

Dominik Awad, BSc

Identification of potential ribosome biogenesis inhibitors

MASTER'S THESIS

to achieve the university degree of

Master of Science

Master's degree programme: Molecular Microbiology

submitted to

Graz University of Technology

Supervisor

Ao.Univ.-Prof. Dr. Helmut Bergler

Institute of Molecular Biosciences
University of Graz

Danksagung

Mein größter Dank geht an Helmut, der mir dieses spannende und einzigartige Projekt ermöglichte. Helmut hat mich nicht nur durch sein unglaubliches Wissen unterstützt, sondern stand mir auch bei schwierigen Entscheidungen zur Seite. Seine Betreuung war einzigartig und ging weit über die Aufgaben eines Arbeitsgruppenleiters hinaus. Helmut, ich danke dir vielmals für die lustige und tolle Zeit.

Danke auch an Brigitte, die mir immer mit einem guten Rat zur Seite stand. Selbst in stressigen Zeiten, hat sie sich immer Zeit für mich genommen und mir wertvolle Tipps gegeben. Danke Brigitte für die Unterstützung, die lustigen Momente und das Vertrauen.

Ein Mann, der nicht nur durch seine Kompetenz, sondern auch durch seine Freundlichkeit und Unterstützung auffällt, ist Mathias. Ob zacki, zacki im Labor oder gemütlich bei einem Glas Wein, mit Mathias wird es niemals langweilig.

Ich würde an dieser Stelle gerne auch Gertrude für die schöne Zeit im Labor, die vielen Scherze, aber auch für die tollen Ratschläge danken.

Auch Valentin möchte ich herzlich danken. Viele Kaffeepausen an Wochenenden, Sekt an Weihnachten und Gespräche über Bruce Springsteen haben die teilweise langen Arbeitszeiten zu einem schönen Erlebnis gemacht.

Ebenso danke ich Michi für die endlosen Scherze und Gespräche über die „wichtigen“ Themen der Welt. Ein Danke geht auch an Ingrid und Maria für die lustige Momente im und außerhalb des Labors. Ebenfalls danke ich Nadine, Manu, Chrissi, Julia und Tamysn für ihre Unterstützung.

Ein herzlicher Dank geht auch an Isa. Danke für die vielen lustigen Momente und Kaffeepausen!

Erst am Ende dazu gestoßen, aber unverzichtbar ist Mirjam. Ich danke dir für die Unterstützung im Labor und die tollen Mittagspausen. Anna und Lisa K. möchte ich für die kurze, aber lustige Zeit danken. Des Weiteren danke ich Lisa W. für ihre wunderbaren Abendessen.

Meinem Bruder Luki möchte ich für seine Unterstützung und Ratschläge danken.

Ein großer Dank geht an meine Eltern. Ohne ihre finanzielle Unterstützung und Fürsorge wäre diese Masterarbeit mit Sicherheit nicht zu Stande gekommen.

Am Ende möchte ich auch noch Sadie danken. Mit unglaublicher Geduld und Unterstützung hat sie mich durch die Zeit meines Studiums begleitet.

„It's a long road to wisdom; it's a short one to being ignored”

The Lumineers

Abstract

All living cells depend on the continuous synthesis of proteins in order to grow and adjust to the influence of the environment surrounding them. Therefore, the cell spends a significant amount of its energy on creating and recycling its ribosomes. Ribosomes are nanomachines, located in the cytoplasm and at the endoplasmic reticulum, that translate the genetic code in form of mRNA into proteins. Ribosomes in eukaryotic cells consist of a small (40S) and a large (60S) subunit. The mature 40S subunit contains 33 ribosomal proteins and one 18S rRNA, whereas the mature 60S subunit includes 46 ribosomal proteins and three different rRNAs: 5S, 5.8S and 25S. Ongoing ribosome biogenesis is of special importance for fast growing cells, like tumor cells. Therefore, the ribosome biogenesis is up regulated to keep up the high demand of the proliferating tumor cell.

As a highly conserved cellular process, ribosome biogenesis represents a potential target of cancer drugs. By inhibiting the synthesis of ribosomes directly, uncontrolled proliferation of cancers cells can be suppressed. The pathway of ribosome maturation offers over 200 different non ribosomal proteins and 79 ribosomal proteins as potential targets when screening for inhibitors. New specific inhibitors represent not only potential cancer drugs, but also a powerful tool to study individual steps in ribosome biogenesis. Up to now, only one specific inhibitor for the ribosome biogenesis in yeast is known, the heterocyclic boron containing drug diazaborine. In this work I developed a screening scheme for identifying novel ribosome biogenesis inhibitors. By screening natural and medical compound libraries containing over 1000 compounds, I could identify 130 potential inhibitors for ribosome biogenesis. These inhibitors provide a rich source to study various steps in ribosome biogenesis in detail.

Zusammenfassung

Um sich den stets variablen Umwelteinflüssen anzupassen, benötigt jede Zelle eine ausreichende Proteinsynthese. Daher investieren Zellen einen Großteil ihrer Energie in die Erzeugung von Ribosomen. Diese Nanomaschinen sind im Zytoplasma, sowie am endoplasmatischen Reticulum lokalisiert und übersetzen Abschnitte der Erbinformation in Form von mRNA in Proteine. In Eukaryonten besteht das Ribosom aus einer großen (60S) und kleinen (40S) Untereinheit. Die kleine Untereinheit umfasst eine 18S rRNA und 33 ribosomale Proteine. Im Gegensatz dazu besteht die große Untereinheit aus 46 ribosomalen Proteinen und drei verschiedenen rRNAs (5S, 5.8S und 25S). Eine ungestörte Synthese von Ribosomen ist besonders für schnell proliferierende Zellen von Bedeutung. Deshalb ist in Krebszellen eine erhöhte Ribosomenbiogenese zu beobachten.

Die eukaryontische Ribosomenbiogenese umfasst mehr als 200 non-ribosomale und 79 ribosomale Proteine und ist hoch konserviert. Deshalb bietet dieser Prozess ein ideales Ziel für die Entwicklung von neuen Krebsmedikamenten. Außerdem könnten Inhibitoren zum besseren Verständnis der Ribosomenbiogenese beitragen. Bis jetzt, ist nur ein spezifischer Inhibitor der Ribosomenbiogenese bekannt, die herzyklische Bor-hältige Verbindung Diazaborin. In dieser Arbeit wurde ein neues Screening Protokoll entwickelt und zur Identifizierung von neuen Inhibitoren der Ribosomenbiogenese herangezogen. Dabei wurden über 1000 Substanzen gescreent und 130 potentielle Inhibitoren der Ribosomenbiogenese in *Saccharomyces cerevisiae* identifiziert. Diese Substanzen können nun für weitere Untersuchungen und zur genaueren Analyse der Ribosomenbiogenese herangezogen werden.

Table of content

1. Introduction.....	2
1.1. Ribosome biogenesis in <i>Saccharomyces cerevisiae</i> : A short introduction.....	2
1.2. Cancer and its link to ribosome biogenesis.....	4
1.3. Ribosome biogenesis as target for inhibitors	5
1.4. Aim of this study	6
2. Materials and methods.....	8
2.1. Inhibitors used for this screen	8
2.2. Strains, plasmids and primers.....	9
2.3 Media and growth conditions.....	11
2.4 Strain construction	12
2.4.1. Constructing the cassette for a C-terminal GFP fusion to ribosomal proteins	12
2.4.2. Constructing the cassette for the knockout of <i>BUD20</i>	12
2.4.3. Preparing the amplified DNA for transformation in yeast	13
2.4.4. Yeast transformation	13
2.4.5. Control of the correct integration via colony PCR.....	14
2.4.6. Agarose gel electrophoresis.....	15
2.4.7. Fluorescence Microscopy.....	15
2.5. Strain characterization	16
2.6. The high-through-put screen	18
2.7. The manual screen for ribosome biogenesis inhibitors	18
3. Results and Discussion	20
3.1. Establishing a high-through-put screen measuring whole cell GFP	20
3.1.1 Screening strategy	20
3.1.2. Influence of the Degron-GFP fusion tag on the growth	22
3.1.3. Comparing the GFP Signal using fluorescence microscopy	26
3.1.4. Protein expression levels of the reporter proteins	27
3.1.5. TECAN GENios Pro set up.....	32
3.1.6. Controls of the screen	34
3.2. The manual screen using fluorescence microscopy	36
3.2.1. Strains used while performing the manual screen.....	36
3.2.2. Potential inhibitors identified by the manual screen	41
3.2.3. The manual screen identified 130 potential inhibitors	68
3.2.4. Selected potential inhibitors at a glance.....	69
3.2.5. Additional phenotypes identified by the screen.....	73
4. Outlook.....	74
5. References.....	76
6. Complete list of inhibitors used in this study.....	81

1. Introduction

1.1. Ribosome biogenesis in *Saccharomyces cerevisiae*: A short introduction

All living cells depend on the continuous synthesis of proteins in order to grow and adjust to the influence of the environment surrounding them. Therefore, the cell spends a significant amount of its energy on creating and recycling its ribosomes. Ribosomes are nanomachines, located in the cytoplasm and the endoplasmatic reticulum, that translate the genetic code in form of mRNA into a chain of amino acids. These chains, called polypeptides or proteins, fulfill different tasks throughout the cell (Alberts et al, 2002). First attempts to understand how ribosomes are assembled, included *in vitro* studies in the late 1970s, when bacterial ribosomal proteins were mixed with full-length and partially digested rRNA (Held *et al.*, 1973; Zagorska *et al.*, 1980; Nowotny *et al.*, 1980; Barritault *et al.*, 1979). Since then, genetic interaction studies *in vivo* and protein-protein interaction experiments, especially the powerful method of tandem affinity purification (Rigaut *et al.*, 1999), revealed new insights of this vast, dynamic and highly conserved process. In fast growing yeast cells, the amount of RNA (80% rRNA, 15% tRNA and 5% mRNA) exceeds the amount of DNA by a 50 fold. Thin-section electron micrograph revealed that 30-40% of the cytoplasm is occupied by ribosomes. Thus, roughly 200,000 ribosomes per cell are required to keep up the demands of a growing yeast cell. Close to 60% of the entire cells transcription is devoted to the ribosomal RNA created by PolII and PolIII. Due to the high need of rRNA, the genome of *Saccharomyces cerevisiae* contains a single tandem array of roughly 150 identical repeats as shown in figure 1.1. (reviewed by Warner, 1999). Eukaryotic ribosomes consist of a small (40S) and a large (60S) subunit. The mature 40S subunit contains 33 ribosomal proteins and one 18S rRNA, whereas the mature 60S subunit includes 46 ribosomal proteins and three different rRNAs: 5S, 5.8S and 25S (reviewed by Woolford and Baserga, 2013). The synthesis of ribosomes starts by the transcription of a 35S pre-rRNA by PolII in the nucleolus, a common precursor for both ribosomal subunits (Thiry and Lafontaine 2005, French et al. 2003; Kos and Tollervey 2010). The 35S rRNA is later on processed to become the 5.8S, 25S (large subunit) and 18S (small subunit) as demonstrated in figure 1.1. In contrast, the 5S rRNA is a transcript of RNA Pol III in the opposite direction of the 35S rRNA transcription (Woolford and Baserga, 2013). Not all of the 150 tandem repeats are being actively transcribed, suggesting that the

extra copies are protection against possible mutagenic damage (Toussaint et al. 2005, Ide et al. 2010).

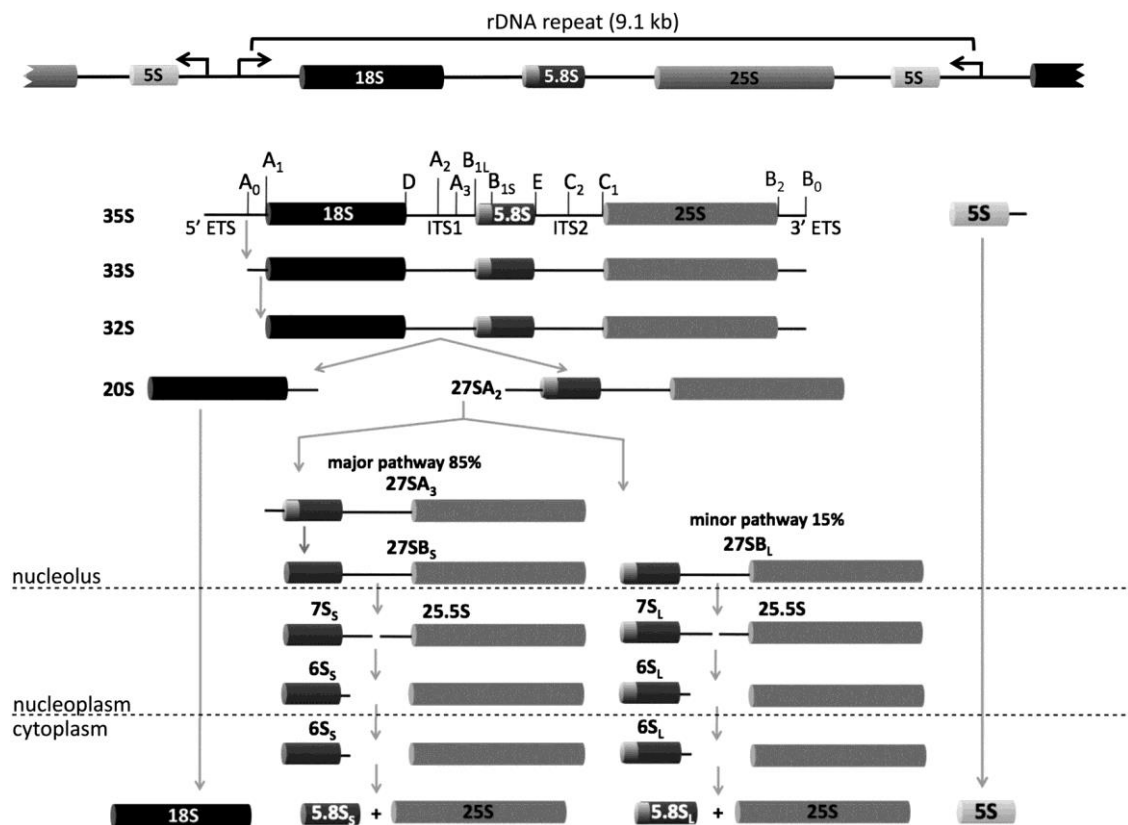


Figure 1.1: Pathway of rRNA processing in yeast. The 35S RNA is a transcript of PolII. In contrast, the 5S RNA is transcribed by the RNA PolIII. External transcribed spacer (ETS), but also internal transcribed spacer (ITS) are featured at the RNA transcript. Different maturation steps include endonucleolytic and exonucleolytic activity and removing the spacers, while the pre-ribosomal particle is being transported to the cytoplasm (taken from Woolford and Baserga, 2013).

The endo- and exonucleolytic processing of the 35S transcript includes removing the external spacer (ETS) and internal spacer (ITS). Additionally about 200 non-ribosomal proteins are involved in processing the ribosomal particles (reviewed by Kressler et al, 2010). Most of this assembly factors have been identified when the tandem affinity purification was introduced (Bassler et al, 2001; Harnpicharnchai et al, 2001, Grandi et al, 2002). The pre-66S particle is associated with almost 90 assembly factors, while the pre 40S particle shows interaction with over 70 non-ribosomal proteins. These proteins include RNA helicases, AAA- ATPases, GTPases, RNA binding proteins, etc. Additionally, there are also proteins with a homology to the ribosomal proteins. Each of these non-ribosomal factors has a particular function when the maturation steps occur and the particles travel from the nucleolus to the cytoplasm (reviewed by Woolford and Baserga, 2013).

1.2. Cancer and its link to ribosome biogenesis

Cancer is a disease that derives from the uncontrolled proliferation of cells within an organism. The growth of tumor cells depends highly on the synthesis of new ribosomes and their translations of proteins to create new cell mass (Dez and Tollervey, 2004). As a consequence, the rate of ribosome biogenesis is upregulated in cancer cells, most likely due to hyper activation of the rDNA transcription (Hein et al, 2013). This effect was already recognized in the 19th century, when cancer cells were found to often demonstrate abnormal and large nucleoli (Pianese, 1896). In recent years the ribosome biogenesis stress checkpoint pathway was described, that causes the activation of p53 via blocking its negative controller MDM2 by ribosomal proteins upon ribosomal impairment (Bursac et al, 2013). Cells that proliferate in an uncontrolled manner feature many times a mutation of the tumor suppressor p53 (Hainaut et al, 1997; Freed-Pastor and Prives 2012; Budanov, 2014). The protein p53 is transcription factor that controls more than 60 genes, including stress response, DNA repair, cell cycle control and apoptosis (reviewed by Smardová et al, 2005). It was shown that the mutations R172H and R270H of the p53 in mouse models resulted in the formation of tumors compared to p53^{-/-} strains (Lang et al, 2004; Olive et al, 2004). These observations suggest that inhibition of ribosome biogenesis could activate p53 and hence represent a promising target for chemotherapy. Indeed, some studies, targeting rRNA transcription, have lead to identification of clinical relevant compounds. For example the inhibition of PolI, using the substances CX-3543 and CX-5461 targeted cancer cells specifically (Bywater et al, 2012; Drygin et al, 2009). However, common cancer treatments include surgery, radiation and chemotherapy. The chemotherapeutic drugs often target essential pathways such as DNA replication or cell division that are needed in all eukaryotic cells (reviewed by American cancer society). As a result, patients suffer from severe side effects. In contrast, advanced treatment options like immunotherapy or the application of hormones is restricted to specific types of cancer (American cancer society). By targeting the ribosome biogenesis directly, the proliferation of the tumor cells can be repressed specifically and could be applied for any type of cancer. Furthermore, ribosomes are stable multi protein complexes and the inhibition of the ribosome biogenesis does not cause an abrupt stop of translation (unpublished data). In other words, the inhibitors could slow down the uncontrolled proliferation and leave all other normally growing cells unharmed, covering their demand of proteins by the existing ribosomes.

1.3. Ribosome biogenesis as target for inhibitors

The hierarchy of the ribosomal proteins joining the rRNA, forming the pre-ribosomal particles, was unraveled by comparing the thermodynamic properties of bacterial complexes of ribosomal proteins associated with rRNA in vitro (Held et al, 1973; Nierhaus and Dohme, 1974). The first information about ribosome biogenesis in vivo was gathered by performing kinetic studies, suggesting that the ribosomal proteins join at a late cytoplasmatic step (Kruiswijk et al, 1978). In contrast, more recent studies predict a joining at an early stage (Babiano and De La Cruz, 2010; Jakovljevic et al, 2012). Thus, only a few ribosomal proteins (S10, S26, L10, L24, L29, L40, L42, P0, P1, P2) join at a very late cytoplasmatic stage (Saveanu et al, 2003; Ferreira-Cerca et al, 2005; Ferreira-Cerca et al, 2007; Lo et al, 2010; Strunk et al, 2011). However, a lot of work has still to be done to fully understand the complex process of ribosome biogenesis in the living cell. Since the process is so dynamic, the use of inhibitors can reveal new information. For example, often times localization studies were conducted by using the substance Leptomycin B. This compound inactivates CRM1/exportin 1 by covalent modification, but requires a single amino acid replacement at Cys-529 with Ser in the *crm1* locus of *Saccharomyces cerevisiae* (Kudo et al, 1999). Adding this mutation to the desired yeast strain, is time consuming and includes the risk of additional mutation due to the DNA transformation. The main advantage of the use of specific inhibitors over mutated or depleted forms of genes for the studying of the ribosome biogenesis is the fast onset of the inhibition. Thus, the use of specific inhibitors could also be helpful to identify novel players in the pathway. For example, the drug diazaborine 2B18, allowed researchers to identify the AAA-ATPase Drg1 as key factor in large subunit formation (Pertschy, 2007; Loibl, 2014). Unfortunately, as of 2015, diazaborine is the only specific inhibitor identified for the ribosome biogenesis in eukaryotic cells. This is astonishing, since the pathway of ribosome maturation offers hundreds of different non-ribosomal proteins and 79 ribosomal proteins as potential targets (see 1.1). Therefore, ribosome biogenesis should represent a promising pathway for the development of novel inhibitors.

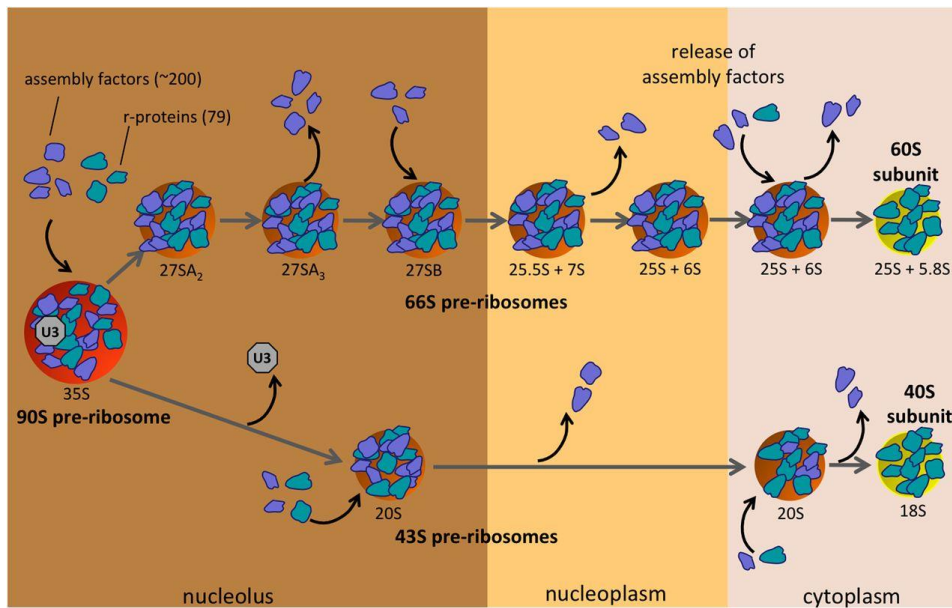


Figure 1.2: Maturation of the 60S and 40S particle in *Saccharomyces cerevisiae*. The majority of ribosomal proteins join in a very early stage of the ribosome biogenesis. The maturation of the pre 90S particle involves processing the rRNA and the export from the nucleolus to the nucleoplasm and later on to the cytoplasm, where the mature ribosomal particles can join to create an active 80S ribosomal complex (taken from Woolford and Baserga, 2013).

1.4. Aim of this study

The aim of this study was to establish a high-throughput screen to identify potential ribosome biogenesis inhibitors, using *Saccharomyces cerevisiae* as a model organism. Such a high-throughput screen could identify additional inhibitors, offering novel chemotherapeutic drugs that inhibit biogenesis downstream of rRNA transcription (Bywater et al, 2012; Drygin et al, 2009).

Such a screen requires an active ribosome biogenesis. Therefore, the fast growing yeast cells offer an ideal model organism, because 100,000 to 200,000 ribosomes are synthesized every 90 minutes (Warner, 1999). Thus, the high ribosome biogenesis rate and the fast proliferation gives *Saccharomyces cerevisiae* the similar characteristics as tumor cells. However, in contrast to mammalian cells, yeast is much more simple to grow in a high throughput system. The screening strategy is based on the observation that most steps of the ribosome biogenesis occur in the nucleus and correct conduction of these maturation steps is required for subsequent export of the pre-ribosome. Furthermore, the inhibition of maturation results in the accumulation of ribosomal reporter proteins in the nucleolus and nucleoplasm (Hurt et al, 1999). This fact allowed identification of many mutants defective in ribosome maturation or export through visual screens (Moy and Silver, 2002). Therefore, the accumulation of ribosomal reporter GFP fusions should be appropriate also to identify inhibitors of ribosome

biogenesis. However, for efficient screening of a larger number of compounds using plate readers would be superior over a visual screen. Therefore, an important step in this work was to set up and evaluate a high throughput compatible screening system using ribosomal reporter constructs. In addition, two low molecular weight compound libraries should be screened to identify novel inhibitors of ribosome biogenesis.

2. Materials and methods

2.1. Inhibitors used for this screen

The inhibitors used for the screen included natural and clinical relevant low molecular weight compound libraries.

a. Natural compound library

The Screen-Well Natural Product Library Version 7.4 from the company Enzo Life Sciences provides 502 small molecular compounds including terpenoids, peptolides, flavones, coumarines, alkaloids, macrolides, isoflavones and synthetic derivatives. The library was supplied in 6x96 Deep-Well plates, each well containing 100µl of the individual purified compounds in DMSO with a final concentration of 2mg/ml (product number: BML-2865-0100). The library was stored at -80°C and thawed at least 60 min before the cell treatment at 32°C while avoiding exposure to any light. For a complete list of all compounds featured in this library see tables of section 6. *Complete list of all inhibitors used in this study.* Additional information on the compounds was provided by the CD supplied with the library or by request from compoundlibraries@enzolifesciences.com.

b. Clinical collection

The National Institutes of Health (NIH) clinical collection included 446 clinical relevant compounds and was supplied in 6x96 well plates. Each well contained 100µl of the compound with a concentration of 10mM dissolved in DMSO. For more information on plate barcodes see table 2.1 and for the entire list of compounds go to tables of section 6. *Complete list of all inhibitors used in this study.*

Table 2.1: List of plates included in the NIH clinical collection

Plate barcode	NCC Plate	Filled wells
NCP003323	NGP-105-01	80
NCP003403	NGP-105-02	80
NCP003483	NGP-105-03	80
NCP003563	NGP-105-04	80
NCP003643	NGP-105-05	80
NCP003723	NGP-105-06	46

2.2. Strains, plasmids and primers

Table 2.2: Strains used for the screen

Strain	Genotype	Source	Info
C303a	<i>MATa leu2 ura3 trp1 his3</i>	I. Podolsky	imb#6580C
C303a FAS1-TEV	<i>MATa leu2 ura3 trp1 his3 FAS1-TEV::natNT2</i>	Mauerhofer	imb#6581C
C303a FAS1-TEV crm1	<i>MATa leu2 ura3 trp1 his3 FAS1-TEV::natNT2 crm1::KanMX</i>	Mauerhofer	<i>crm1</i> T539C
C303a Rps3-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 RPS3-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a Rps3-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 RPS3-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a FAS1-TEV Rps3-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV::natNT2 RPS3-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV Rps3-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 RPS3-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a FAS1-TEV crm1 Rps3-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV::natNT2 crm1::KanMX RPS3-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV crm1 Rps3-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPS3-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a Rpl25-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 RPL25-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a Rpl25-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 RPL25-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a FAS1-TEV Rpl25-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV::natNT2 RPL25-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV Rpl25-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 RPL25-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a FAS1-TEV crm1 Rpl25-Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPL25-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV crm1 Rpl25-Degron(his)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPL25-Degron(his)-GFP:HISMX</i>	This study	Degron (his)
C303a Rpl13a- Degron(asn)- GFP	<i>MATa leu2 ura3 trp1 RPL13A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a Rpl34a- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 RPL34A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a Rpl 38- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 RPL38-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV Rpl 13a- Degron(asn)- GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 RPL13A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV Rpl 34a- Degron(asn)- GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 RPL34A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV Rpl 38- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 RPL38-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn)
C303a FAS1-TEV crm1 Rpl 13a- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPL13A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn), Positive control
C303a FAS1-TEV crm1 Rpl 34a- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPL34A-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn), Positive control
C303a FAS1-TEV crm1 Rpl 38- Degron(asn)-GFP	<i>MATa leu2 ura3 trp1 FAS1-TEV:: natNT2 crm1::KanMX RPL38-Degron(asn)-GFP:HISMX</i>	This study	Degron (asn), Positive control
C303a Δ bud20	<i>MATa leu2 ura3 trp1 his3 Δbud20::hphNT1</i>	This study	Positive control imb#6597B
C303a Rpl7a-GFP K5	<i>MATa leu2 ura3 trp1 RPL7A-GFP::HISMX</i>	This study	60S Screen imb#6598A
C303a Rpl7a-GFP K5 Δ bud20	<i>MATa leu2 ura3 trp1 RPL7A-GFP::HISMX Δbud20::hphNT1</i>	This study	Positive control imb#6594B
C303a Rps9a-GFP K3	<i>MATa leu2 ura3 trp1 RPS9A-GFP::HISMX</i>	M. Loibl	40S Screen imb#6598B

Table 2.3: Primers used for this study

Primer name	Primer sequence
UK_Rps3_Fw	CAAGGACTACAGACCAGCTGAAGAACTGAAGCTCAAGCTGAACCAGTTGAAGCTggtcgacggatccccggg
Rps3_S2	AAGAAATTATTGTACTTATAGTTTATTTATGATTTAATAATTAATCTAatcgaatcgagctcg
UK_Rpl25_Fw	TTGACTGCTGACTACGATGCTTTGGACATTGCTAACAGAATCGGTTACATTGGTCGACGGATCCCCGGG
Rpl25S2	AGAAAAATTTAAAAATAATATTAATTTATTAATTAACCAATTAGATTAATCGATGAATTCGAGCTCG
UK_Rpl13A_fwd	GAAAAGAGAGCTAGAGAAAAGGCTGAAGCTGAAGCTGAAAAGAAGAAAggtcgacggatccccggg
UkRpl13a_S2	TACAAAAATTGTGGATGAAAAATTCCTTGATGAAGTTTTAGATCTAATCGATGAATTCGAGCTCG
UkRpl34a_fwd	GGAACAAACCGAAGCTGCCAAGAAATCTGAAAAGAAGGCTAAGAAAggtcgacggatccccggg
UkRpl34a_S2	AAACAGTTAATTAGGTACATAAGAAAAGTAACATTTTCTTAAAGTTAATCGATGAATTCGAGCTCG
Uk Rpl38_fwd	TAAGAAATTGATCCAATCTTTGCCACCAACTTTGAAGGTTAACAGATTAAggtcgacggatccccggg
UkRpl38_S2	TTCCAGTCTCGTTATGATAACACTCCGATCATTCCTTATTTTCTTAATCGATGAATTCGAGCTCG
RPS3_430-500fw	AGGCTATGAAATTTGCTGACGG
Rpl25_Ctrl_Fw	CCGCTATGAAGAAGGTTGAAG
Rpl13A_tag_ctrl	AGAAATTCAGAGGTATCAGAG
Rpl34A_tag_ctrl	AATTGTCAAGAAGGTTGTCA
Rpl38_tag_ctrl	CAACGATGCTGGTAAGGCTA
Rpl7a-genomfwd	TTTCGGTAACCGTGAAGAATTCATCAACAAATTTGGTTAAGTCCATGAACGGTCGACGGATCCCCGGG
Rpl7a-genomrev	ACAGAACTATATAGGACTTAGATAAAAATAAGTAGTTATATGTAATGATCGATGAATTCGAGCTCG
Rpl7a_Ctrl_Fw	CCGACAATGCTATCATCGAAG
BUD20_fwd_S1	TGAAAGGCAGTTAAACACACAGACAAGTGAAGATAAAAACAATAGCGCATCATGCGTACGCTGCAGGTC GAC
YFPcontrol	TTCCGTATGTTGCATCACC
Bud20 delkontr	TGCTAACTAGTTTCGGAGGGA
KanR5`b	CAAGACTGTCAAGGAGGG

Table 2.4: Plasmids used for this study

Plasmid name	Feature
4020_pFA6a-Degron(asn)-GFP-HISMX	Template for GFP Fusion including Degron
4019_pFA6a-Degron(his)-GFP-HISMX	Template for GFP Fusion including Degron
1510_pFA6a-GFP(S65T)-HIS3	Template for GFP-fusion cassette
3190_pFA6a-hphNT1 (pKS133)	Hygromycin resistance cassette

2.3 Media and growth conditions

Listed in table 2.5 are the media used for culturing *Saccharomyces cerevisiae*. The SD media was supplemented by an amino acid mix (see table 2.6). By separating the ammonium sulfate and yeast nitrogen base from the glucose as well as amino acid mix while sterilizing, the background at the fluorescence microscopy was kept to a minimum. The pH level of the YPD and the SD media was adjusted to 5.5 and afterwards sterilized at 125°C for 20 min. The standard growing condition was 30°C, while at the screen the temperature varied (see 2.7.1).

Table 2.5: Ingredients of culture media

Media type	Component	Concentration (g/l)
YPD	Yeast extract	10.0
	Peptone	20.0
	Glucose	20.0
	Agar (optional)	15.0-20.0
SD	Ammonium sulfate	5.0
	Yeast Nitrogen base	1.4
	Glucose	20.0
	Agar (optional)	15.0-20.0

Table 2.6: Amino acid mix used as supplement for SD media

Amino acid	Concentration (mg/l)
adenine sulfate	20
uracil	20
L-arginine-HCl	20
L-histidine-HCl	20
L-methionine	20
L-tryptophan	20
L-isoleucine	30
L-leucine	30
L-lysine	30
L-phenylalanine	50
L-glutamic acid	100
L-aspartic acid	100
L-valine	150
L-threonine	200
L-serine	400

2.4 Strain construction

2.4.1. Constructing the cassette for a C-terminal GFP fusion to ribosomal proteins

The C-terminal GFP fusion to the ribosomal proteins (Rps3, Rpl25, Rpl13a, Rpl34a, Rpl38, Rpl7a) was introduced via homologous recombination using linear PCR fragments flanked by a 50bp overlay specific to the recombination sites (Petracek and Longtine, 2002). The plasmid, used as template featured a HISMX marker to ensure no interference deriving from an antibiotic resistance while screening for potential inhibitors. See table 2.7 for the PCR reaction, table 2.3 for the primer sequence and table 2.4 for the plasmid used.

Table 2.7: PCR reaction mix for GFP-fusion cassette

Component	Volume (μ l)
Template (~50ng)	1
Q5 High-Fidelity DNA Polymerase (NEB) (2U/ μ l)	0.5
Q5 Puffer (NEB) (5x)	10
dNTPS (2mM stock)	5
Fwd primer (20 μ M stock)	1
Rev primer (20 μ M stock)	1
Aqua bidest. (Fresenius)	31.5
Total	50

Table 2.8: PCR program when using Q5 Polymerase

Step	Temperature ($^{\circ}$ C)	Time	Cycles
Initial Denaturation	98	30''	1
Denaturation	98	10''	
Annealing	55	1'	35
Amplification	72	3'	
Final elongation	72	7'	1
Final	4	∞	

2.4.2. Constructing the cassette for the knockout of *BUD20*

The knockout of *BUD20* was performed via homologous recombination, introducing the cassette amplified with PCR using the setup of table 2.9 and table 2.10. For the sequence of the primers see table 2.3 and for more information on the template see table 2.4.

Table 2.9: PCR reaction mix used for BUD20 knockout cassette

Component	Volume (μl)
3190_pFA6a-hphNT1 (pKS133) (~50ng)	1
Taq Polymerase (NEB) (5U/ μ l)	0.2
Thermo Pol Puffer (NEB) (10x)	5
dNTPS (2mM stock)	5
BUD20_fwd_S1 (20 μ M stock)	1
BUD20_rev_S2 (20 μ M stock)	1
Aqua bidest. (Fresenius)	36.8
Total	50

Table 2.10: PCR program using Taq Polymerase

Step	Temperature ($^{\circ}$C)	Time	Cycles
Initial Denaturation	95	30''	1
Denaturation	95	30''	
Annealing	55	1'30''	35
Amplification	72	3'	
Final elongation	72	7'	1
Final	4	∞	

2.4.3. Preparing the amplified DNA for transformation in yeast

The PCR product was cleaned from polymerase and buffer using the Thermo Scientific Gene Jet Gel Extraction Kit and was afterwards eluted in 30 μ l of water (Fresenius). Then 1-2 μ l of the purified DNA was used for an agarose gel electrophoresis to determine the DNA concentration by comparison with the defined bands of the Lambda DNA standard. The rest of the purified DNA was stored at -20 $^{\circ}$ C until the transformation into yeast cells.

2.4.4. Yeast transformation

To transform the DNA cassettes or plasmid DNA into the desired yeast strain, the standard yeast transformation protocol was performed (Gietz, 2014). Cells were grown in YPD and from this over-night-culture 50ml YPD were inoculated at a starting OD₆₀₀ of 0.2 (Beckman DU 640 Spectrophotometer). After the incubation at 30 $^{\circ}$ C until an OD₆₀₀ of 0.4 to 0.7, the cells were harvested by centrifugation at room temperature for 5 minutes at a speed of 3500rpm. The pellet was washed twice with 10ml of lithium acetate solution (LiAc) and resuspended in 200 to 300 μ l LiAc. The cells were then incubated at 30 $^{\circ}$ C for 30 min and 50 μ l of the cell solution used for the transformation

mix (see table 2.11). The carrier DNA had to be denatured at 95°C prior to use and kept on ice. After mixing the cells, carrier DNA and PEG solution with the PCR product or plasmid DNA (used as control for transformation rate, when using linear DNA), the mix was incubated at 30°C for 30 min. Then a heat shock was applied by switching the incubation temperature to 42°C for 20 min. Immediately after the heat shock, the cells were plated on selective media (SD-his for the GFP fusion) or YPD in case of the knockout of bud20. The bud20 knockout cassette included a Hygromycin resistance marker. Therefore, the cells grown on YPD were transferred the following day onto a YPD plate containing Hygromycin (400µg/ml).

Table 2.11: Transformation mix

Component	Volume (µl)
Cells in LiAc	50
PCR Product/ Plasmid	equal to 50-10µg/1 µg
Carrier DNA (10mg/ml)	5
PEG (40%)	300

2.4.5. Control of the correct integration via colony PCR

By performing colony PCRs, the correct integration of the tag or knockout cassette was confirmed. Transformants from the selective media plates were struck out on YPD and the next day small colonies were suspended in 20µl of water (Fresenius). After incubation at 95°C for 10min, the cell suspension was cooled on ice and later on centrifuged at 13.000 rpm for 10min. Then 7.5 µl of the supernatant was used for the colony PCR mix. Using primers that bind at the DNA region of the insert as well as on chromosomally DNA prior to the insert, a product was only amplified when the tag was integrated at the correct site. See table 2.3 for the primer sequences. The negative control (background strain) was necessary to ensure that the amplified DNA was not due to unspecific binding of the primers. Additionally a positive control was essential.

Table 2.12: Colony PCR mix

Component	Volume (µl)
Supernatant	7.5
Taq Polymerase (NEB) (5U/µl)	0.2
Thermo Pol Puffer (NEB) (10x)	2.5
dNTPS (2mM stock)	2
Primer forward (20µM stock)	1
Primer reverse (20µM stock)	1
Aqua bidest. (Fresenius)	10.8
Total	25

Table 2.13: PCR program using Taq Polymerase

Step	Temperature (°C)	Time	Cycles
Initial Denaturation	95	5′	1
Denaturation	95	1′	
Annealing	55	1′	35
Amplification	72	3′	
Final elongation	72	5′	1
Final	4	∞	

2.4.6. Agarose gel electrophoresis

The PCR products were separated by using an agarose gel containing 1% agarose, TAE puffer (50xTAE: Tris acetate 2M, EDTA pH 8.0 50mM; 1xTAE gel buffer, 0.5xTAE running buffer) and 0.2µg/ml ethidium bromide (Sambrook et al., 1989). 1-2µl of the amplified DNA was mixed with 6xLoading dye (Thermo) and water (Fresenius) to a final concentration of the loading dye 1x. The DNA migrated through the gel with a voltage of 7.5V per centimeter gel length and 0.5x TAE served as a running buffer and the gel was later on put on a UV cabinet with a camera to detect the DNA fragments. Thus, the size of the fragment was determined by comparison of the amplified DNA product to a standard DNA marker (Lamda EcoRI/HindIII or Gene ruler 100bp, Thermo Scientific).

2.4.7. Fluorescence Microscopy

The DIC microscopy for this study was conducted with a Zeiss Axioskop, using a narrow band enhanced GFP (eGFP) filter from Zeiss. Every picture was taken with a 40x objective with 10 fold projective, a secondary magnification of 1.6x and an additional magnification of 10x. The exposure time was 2000ms for the C303a Rpl7a-GFP K5 strain and 800ms for the C303a Rps9a-GFP K3 strain.

2.5. Strain characterization

2.5.1. Rapid cell disruption

To confirm that the GFP-tag was expressed at full size, a rapid cell disruption and protein detection via Western Blot was performed. The cells were cultivated in SD media including all amino acids at 30°C and 170 rpm. From the overnight culture, the cells were diluted in SD media to an OD₆₀₀ of 0.15 and inhibitors were added at an OD₆₀₀ of 0.4. After incubation at 30°C, the cells were harvested at an OD₆₀₀ of 0.8 to compare the proteins levels at logarithmic conditions. The cell pellets were stored at -20°C and later on resuspended in 200µl 1.85 M NaOH including 7.5% β-Mercaptoethanol and incubated 10 min on ice. Afterwards, 200µl of 50% TCA were added to each sample and incubation continued for 10 min on ice. The precipitated proteins were harvested by a 15 min centrifuge step at 14,000 rpm at 4°C. After washing the protein pellet twice with 1ml of water (Fresenius), the proteins were dissolved in 40µl FSB (Final sample buffer, 0.06 M Tris HCl, pH 6.8, 2% (w/v) SDS, 5% (v/v) β –Mercaptoethanol, 8% (v/v) glycerin, 0.04% bromphenolblue). The protein samples were denatured at 95°C for 10 min and centrifuged at 13.000 x g for 10 min before aliquots were separated by SDS-PAGE.

2.5.2. SDS-polyacrylamide gel electrophoresis (SDS-PAGE)

The SDS-PAGE (Ausubel et al., 1995) was conducted by using 12.5% (w/v) polyacrylamide gels and the Mighty Small Minigel Vertical Unit by Hoefer Scientific. The supernatant of the rapid cell disruption (see 2.5.1) was loaded onto the gel and separated by applying 16mA. The Tris-Glycine running buffer (0.25M Tris base, 1.9M glycine, 1%(w/v) SDS) was used to ensure optimal separation of proteins contained in the sample. As molecular weight standard the pre-stained protein Ladder PageRuler by Thermo Scientific was applied.

2.5.3. Western Blot

After the proteins were separated by SDS-PAGE (see 2.5.2), a transfer to a PVDF membrane (Millipore) was performed by using the tank-blot-system (BioRad). The transfer was performed for 1.5 hours, applying 220mA and using CAPS buffer (10mM CAPS, 10% methanol pH 11.0). To block nonspecific binding sites for antibody detection, the membrane was first incubated in 1xTST-Blotto (0.1% Tween20, 0.15 M Sodium chloride, 50 mM Tris HCl pH 7.4, 0.5% milk powder) over night at 4°C. The following day the membrane was incubated with the primary antibody (diluted in 1xTST-blotto with 0.5% milk powder) for one hour and washed with 1xTST three times

for 5 min. Afterwards the secondary antibody was applied (diluted in 1xTST-blotto with 0.5% milk powder) for one hour and washed again three times for 5 minutes with 1xTST. By using the ECL solution of Amersham Bioscience for the detection of Rps3-GFP, Rpl25-GFP, Rpl13a-GFP, Rpl34a-GFP and Rpl38 and BioRad for the detection of Rpl7a-GFP, the chemiluminescence signal was detected via X-ray films (Sterling Diagnostics, USA) or BioRad ChemiDocTouch Imaging system (Rpl7a-GFP and Rps9a-GFP detection). After detection, the membrane was stripped by adding stripping solution (60mM Tris HCl pH 6.8, 2% SDS, 100mM β -Mercaptoethanol) and incubation at 60°C for 20 minutes. After washing the stripped membrane for five times for 5 minutes with 1xTST buffer, the membrane was incubated with the next antibody or dried for storage. See table 2.14 for a list of antibodies used in this study.

Table 2.14: Antibodies used in this study

Antibody	Dilution	Protein size (kDa)	Source	Additional Information
α -GFP	1:1000	27.6	Roche	Diluted antibody stored at 4°C
α -GAPDH	1:40,000	35.75	TuGraz	
α -Rpl25	1:2,000	15.78	Ballesta, Uni. Madrid	Detects also Rpp0 at 33.7 kDa
α -Rps3	1:200,000	26.51	Seedorf ZMBH	
α -FLAG	1:10,000	1.01	Sigma	Conjugated

2.5.4. Spot test

For spot tests, an over night culture of the respective strain was grown at 30°C and 170 rpm. The cell suspension was diluted to an OD₆₀₀ of 0.3. 300 μ l of this dilution were transferred into a 96-Well plate and further diluted three additional times 1:10 using sterile water (Fresenius). Afterwards, the cells were spotted onto YPD plates and/or SD –his plates and incubated at room temperature, 25°C, 28°C, 30°C or 37°C. The SD plates functioned as an additional control for the generated strains and are not presented in this work.

2.5.5. Growth curve

The impact of DMSO on the cells was tested by recording a growth curve for untreated cells and cells treated with different concentrations of DMSO. The cell density was determined by measuring the OD₆₀₀ at different time points (Beckman DU 640 Spectrophotometer). The cells were grown over night until an OD₆₀₀ of 0.4, which was the cell density used for the screen. Then 10ml of the cell suspension were transferred to Erlenmeyer flasks and DMSO in different concentration (from 1% to 8%) was applied. The graph, seen in figure 3.14, only shows the OD₆₀₀ values from one representative result of three independent experiments.

2.6. The high-through-put screen

2.6.1. Set up used for TECANGeniosPro

The measurement of the whole cell GFP signal was performed using the TECAN Genios Pro (Serial number: 507000006; Firmware: V 3.40 01/06 GeniosPRO; XFLUOR4-GENIOSPRO Version: V 4.63). The set up was loosely based on the protocol “*Detection of Green Fluorescent Protein (eGFP) - Tecan Ultra Evolution, Safire and GENios Pro*”, as well as “*Fluorescence Bottom Reading for Cell-Based Assays*” provided by TECAN. Different constructs were tested by using different integration times and gain, searching for the optimal set up of the screen.

2.7. The manual screen for ribosome biogenesis inhibitors

2.7.1. The initial screen set up

The strains C303a Rpl7a-GFP K5 and C303a Rps9a-GFP K3 were grown in synthetic dextrose medium (SD) not including histidine. The culture was diluted with fresh SD-his media and incubated at 30°C until it reached an optical density of 0.4. The optical density was measured at a wavelength of 600nm. This low optical density ensured that the cells were in an early-log-phase and had an active ribosome production, necessary for the screen set up. The half of the culture was then transferred into a 96-Deep-Well plate, the other half in the flask was diluted in SD-his media and grown at 30°C. 56 wells of each deep well plate were filled with 198µl or 196µl (ENZO) or 199µl (NIH) of the cell suspension. To 48 out of 56 wells, potential inhibitors were added (2µl/4µl ENZO, 1µl NIH). In two additional wells diazaborine was added as a positive control for the screen with Rpl7a-GFP or Acivicin for the screen with Rps9a-GFP. The remaining wells with untreated cells were used as a negative control. The 96-deepwell plate was then incubated at 28°C and 320 rpm for three hours. Samples from each well were documented by microscopy, one at a time, leading to final incubation time between 3 to 6 hours, depending on the position of the well. All tested inhibitors were dissolved in DMSO. The impact of DMSO on the cells was tested prior to the screen by incubating the testing strains with different concentrations of DMSO (see strain characterization). By using 1µl of each substance included in the NIH library, the final concentration was 50µM. The Enzo library provided substances with a concentration of 2mg/ml. Since the majority of the compounds had a molecular weight of 400, adding 2µl of the potential inhibitor resulted in a final concentration of about 50µM. When substances exceeded a molecular weight of 800, 4µl were added to the cell suspension.

Table 2.15: Positive controls of the screen

Substance	Reporter	Disolved in	Source	Final Concentration
Diazaborine (2B18)	Rpl7a-GFP	Water (Fresenius)	Novartis	5 µg/ml
Acivicin	Rps9a-GFP	DMSO	Sigma Aldrich	10µg/ml

2.7.2. Confirming hits obtained from initial screen

Cells showing an accumulation of the reporter protein in the nucleolus or nucleoplasm were selected for the second round of microscopy. Depending on the toxicity (forming multiple vacuoles due to the stress for example) and the extent of accumulation seen per picture, the concentration of the inhibitor was adjusted to ensure maximum accumulation and least amount of stress for the yeast cells. A third round of microscopy was performed to confirm the inhibitors effect on the localization of the reporter protein. The duration of inhibitor treatment varied in the second and third round from 3 to 7 hours (see table 3.5 and 3.6).

3. Results and Discussion

3.1. Establishing a high-through-put screen measuring whole cell GFP

The initial step was creating the reporter constructs in the strains *C303a*, *C303a FAS1-TEV* and *C303a FAS1-TEV crm1* (see table 2.2). Afterwards, the whole cell GFP measurements were performed to determine the best possible set up for the TECAN GENios Pro. Many parameters, such as the gain, integration time, etc. had to be tested and optimized.

3.1.1 Screening strategy

The high-through put screening strategy involved the expression of reporter proteins of the large and small subunit (e.g. Rpl25-GFP, Rps3-GFP). A block in ribosome maturation caused by a specific inhibitor is expected to result in accumulation of the reporter construct in the nucleolus. To increase the signal to noise ratio, a cleavage of the GFP tag from the reporter protein after entering the cytoplasm and the subsequent efficient degradation of the GFP moiety were also envisaged. This should be achieved, by introducing a TEV recognition site between the ribosomal protein and the GFP tag and by expressing the TEV protease in the cytoplasm of the reporter strain. By fusing the TEV protease to the Fatty Acid Synthetase (Fas1), the cleavage enzyme was prevented from entering the nucleus due to the high molecular weight of Fas1 (228654.9Da; SGD database). Thus, the GFP marker on the ribosomal protein can only be cleaved off after the pre-ribosomal particle entered the cytoplasm, leading to degradation of the GFP tag via the proteasome. As a result, the fluorescence signal of the cytoplasm should decrease dramatically (see figure 3.1.). The TEV cleavage site, located between the ribosomal protein and the GFP tag, was designed to create a histidine or asparagine located at the N-terminus of the cleaved marker (see linker sequence 1 and 2). According to the N-end rule the half life time of proteins is strongly influenced by the N-terminal residue (reviewed by Finley, 2012).

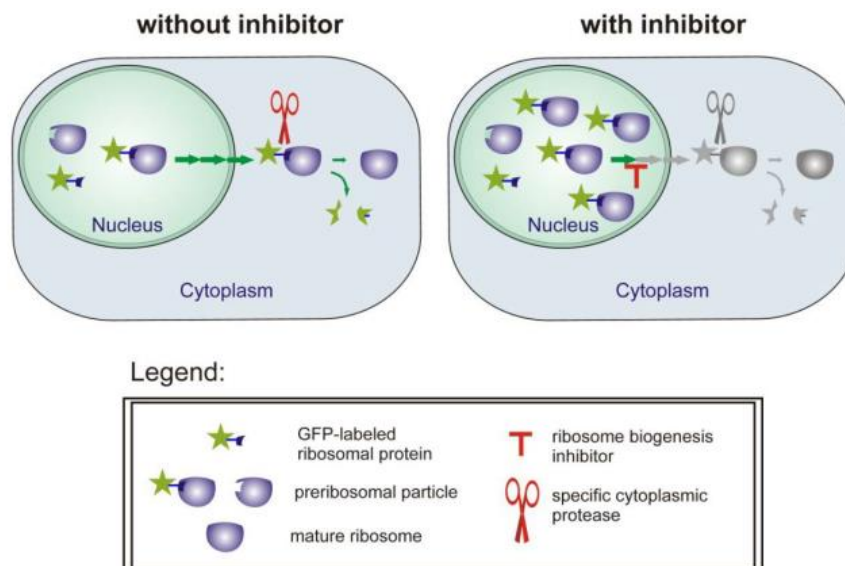


Figure 3.1: Schematic overview of the screening strategy. Taken from “unconventional proposal” by Bergler and Pertschy, 2013.

Linker sequence leading to a N-terminal histidine upon cleavage via TEV protease:

```

      | | | XhoI
      | | |
|| SmaI | |
CCCGGGGTTTCTGGTCTCGAGGCTGGTGGTTCTGGTCCAGGGAAAATTTGTATTTTCAA
P G G S G L E A G G S G P G E N L Y F Q

                                     Sali
                                     ||| BglII
CATCATAAATCTGGTGCTTGAAATTGCCAGTTTCTTTGGTTAAATCTGTCGACAGATCT
H H K S G A W K L P V S L V K S V D R S

GCATCTGGTGGTGGACCTGGTGAGAACTTATACTTCCAGCACCACAAGAGTGGAGCATGG
A S G G G P G E N L Y F Q H H K S G A W

                                     Sali
                                     ||| PacI
                                     ||| BamHI
AAGTTACCTGTCTCATTAGTCAAGTCACTCGACTTAATTAAACGGATCCTCTGGTGCTGGA
K L P V S L V K S V D L I N G S S G A G

GGTCCTGGTGAAAACCTTATATTTCCAACACCACAAAGGAAGTCTTGAAATTACCTTCA
G P G E N L Y F Q H H K G S A W K L P S

      | | | BamHI
      | | |
GTCTTAGTCAAGTCTGGATCC
V L V K S G S

```

Linker sequence leading to a N-terminal asparagine upon cleavage via TEV protease:

```

|   XhoI
|| SmaI   |   ||
CCCGGGGTTCTGGTCTCGAGGCTGGTGGTTCGGTCCAGGGGAAAATTTGTATTTCAA
P G G S G L E A G G S G P G E N L Y F Q

                                     Sali
                                     ||| BglII
AATCATAAATCTGGTGCTTGGAAATTGCCAGTTTCTTTGGTTAAATCTGTCGACAGATCT
N H K S G A W K L P V S L V K S V D R S

GCATCTGGTGGTGGACCTGGTGAGAACTTATACTTCCAGAATCACAAAGAGTGGAGCATGG
A S G G G P G E N L Y F Q N H K S G A W

                                     Sali
                                     |||   ||
                                     ||| BamHI
AAGTTACCTGTCTCATTAGTCAAGTCACTCGACGGATCCTCTGGTGCTGGA
K L P V S L V K S V D G S S G A G

GGTCCTGGTGGAAACTTATATTTCCAAAATCACAAAGGAAGTCTTGGAAATTACCTTCA
G P G E N L Y F Q N H K G S A W K L P S

| |   | | BglIII PacI
GTCTTAGTCAAGTCTAGATCTTTAATTAAC
V L V K S R S L I N

```

3.1.2. Influence of the Degron-GFP fusion tag on the growth

The set up used for the screen required yeast cells with an active ribosome production. Therefore, it was crucial to gather information on cell growth and the influence of the degron-GFP tag itself. The growth of the new strains compared to the wild type was tested by performing a spot test. Interestingly, transformants harboring the same construct showed very different growth, most likely due to different integration of the GFP tag in the pre-ribosomal particle. The first reporter construct (Rps3) showed no growth defect compared to the wild type (see figure 3.2), except the transformant C303a Rps3-Degron(his)-GFP 2-1. This was likely due to the fact that the GFP moiety was cleaved off Rps3 in all other Rps3-Degron strains. This finding suggests that tagged Rps3-GFP is not fully functional, thereby selecting for transformants that are able to cleave the fusion protein. Interestingly, Rps3-Degron(his)-GFP 2-1, which was apparently unable to cleave the fusion protein that was heavily overexpressed, likely to cope with the reduced functionality of the Rps3-fusion protein. Similarly, the C303a FAS1-TEV crm1 Rps3-Degron(asn)-GFP 2-2 strain also showed reduced growth and a failure to form correctly sized Rps3. The transformation of DNA into yeast, using the LiAc method, requires the repair systems to integrate a linear fragment. As a result, additional mutations are highly common and could explain the observed phenotypes. However, when comparing C303a Rps3-Degron(asn)-GFP 2-6 to C303a FAS1-TEV

Rps3-Degron(asn)-GFP 2-5, the size of the single colonies does not differ from each other. This data suggest that the degron-GFP tag of the Rps3 protein does not interfere with the interaction of the pre-ribosomal particle. If the tag would interfere in any way, a growth difference should be seen between the C303a and C303a Fas1-TEV, due to the cleavage of the GFP tag upon entering the cytoplasm when Fas1-TEV is present.

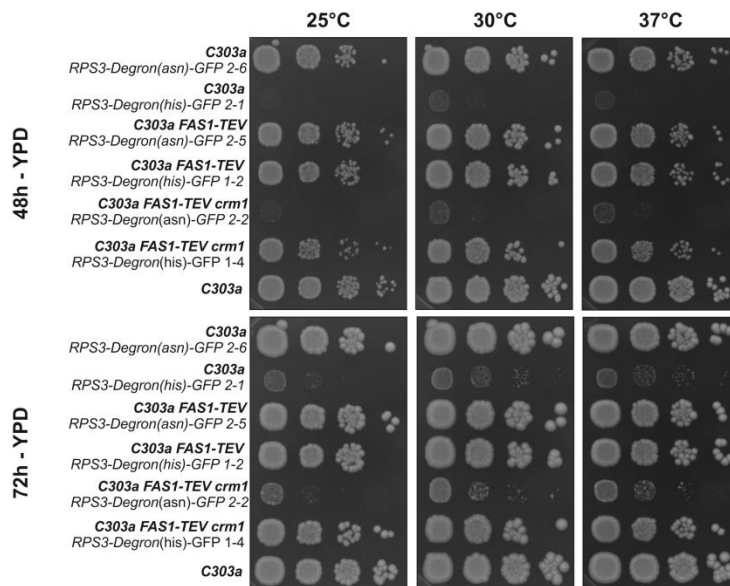


Figure 3.2: Spot test of Rps3-GFP transformants on YPD. Strains were tagged using a fusion tag containing TEV cleavage sites, followed by either one of the two destabilizing residues (his or asn) according to the N-end rule, a degron and a GFP tag. The fusion cassette was present on plasmid 4020_pFA6a-Degron(asn)-GFP-HISMx and 4019_pFA6a-Degron(his)-GFP-HISMx constructed in this study; described in 3.1.1 and in the materials and methods section. The strain Rps3-Degron(asn)-GFP 2-6 shows hardly any growth deficiency compared to C303a FAS1-TEV Rps3-Degron(asn)-GFP 2-5 and the wild type (C303a). This strongly suggests that the degron-GFP tag of the Rps3 protein does not interfere with the interaction of the pre-ribosomal particle. C303a Rps3-Degron(his)-GFP 2-1 and C303a FAS1-TEV crm1 Rps3-Degron(asn)-GFP 2-2 have a strong growth defect, most likely due to the over expression of the GFP tagged protein (see fig 3.7).

When looking at the transformants featuring a Rpl25-GFP construct, the variation within the transformants, strongly suggests that a chromosomal tag of Rpl25 does heavily interfere with growth. It should be mentioned, that Rpl25 localization studies are usually performed by introducing the protein including a GFP tag via plasmid, rather than chromosomal integration (Hurt et al, 1999; Ossareh-Nazari, 2014; Hung and Johnson, 2006;). This leads to the conclusion that the Rpl25-GFP protein needs to be in the cell at higher copy number in order to have a similar growth to the wild type. The differences comparing transformants featuring the same degron-GFP tag lead to the decision that an alternative reporter construct had to be used. Therefore, we created new reporter constructs Rpl13a, Rpl34a and Rpl38, exposing the C-terminus on the outside of the ribosomal particle which should reduce the risk of interference of the GFP tag with incorporation of the protein (Ben-Shem et al, 2011; Jenner et al, 2012). The new

reporter constructs showed no growth deficiency when compared to the wild type, with the exception of Rpl13a-degron-GFP which exhibited a mild phenotype in the *C303a FAS1-TEV* strain. In figure 3.4, representatively one transformants of each construct is shown. The new reporters of the large subunit were only tagged with degron(asn)-GFP. This decision was based on the difference of the GFP signal intensity of the degron(asn)-GFP and degron(his)-GFP (see 3.1.3.), which correlated with the GFP degradation efficiency (see 3.1.4).

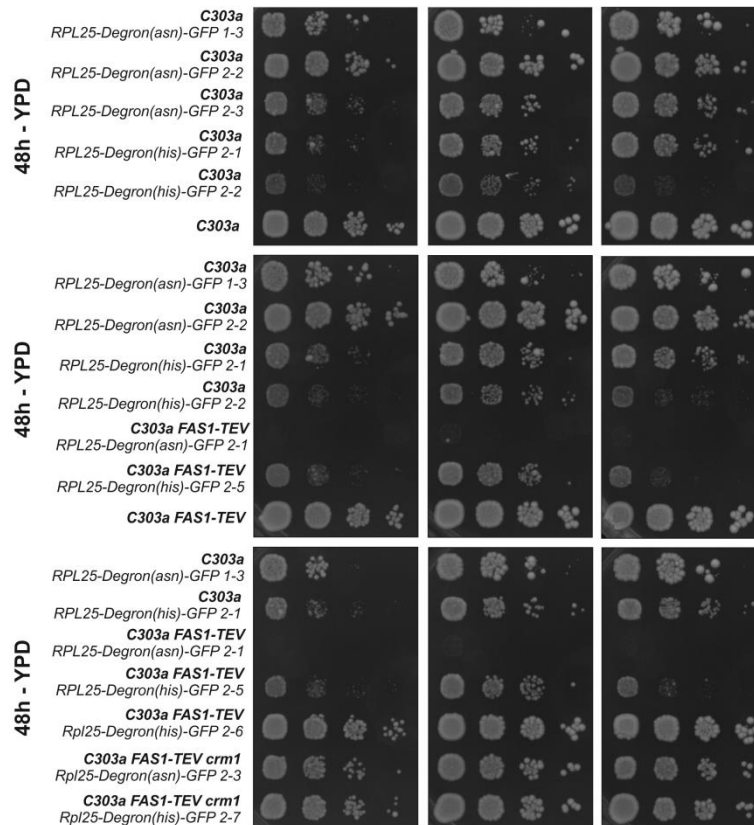


Figure 3.3: Spot test of Rpl25-GFP transformants on YPD. Strains were tagged using a fusion tag containing TEV cleavage sites, followed by either one of the two destabilizing residues (*his* or *asn*) according to the N-end rule, a degron and a GFP tag. The fusion cassette was present on plasmid 4020_pFA6a-Degrone(asn)-GFP-HISMX and 4019_pFA6a-Degrone(his)-GFP-HISMX constructed in this study; described in 3.1.1 and in the materials and methods section. The different transformants of the Rpl25-Degrone-GFP construct show a strong variation. This suggests that the tag of the Rpl25 interferes when the protein interacts with the pre-ribosomal particle or non-ribosomal factors need for the export.

It should be mentioned that the integration of the GFP tag in the *C303a FAS1-TEV crm1* strain lead to a recombination of the HISMX marker (GFP) and the Geneticin marker (*crm1*). This resulted in mainly false positive transformants, able to grow on SD-*his* but not on geneticin containing media. When these strains were tested performing colony PCRs and fluorescence microscopy, the majority of the transformants did not have a GFP signal. Therefore, a recombination of the HISMX and Geneticin marker is a likely explanation.

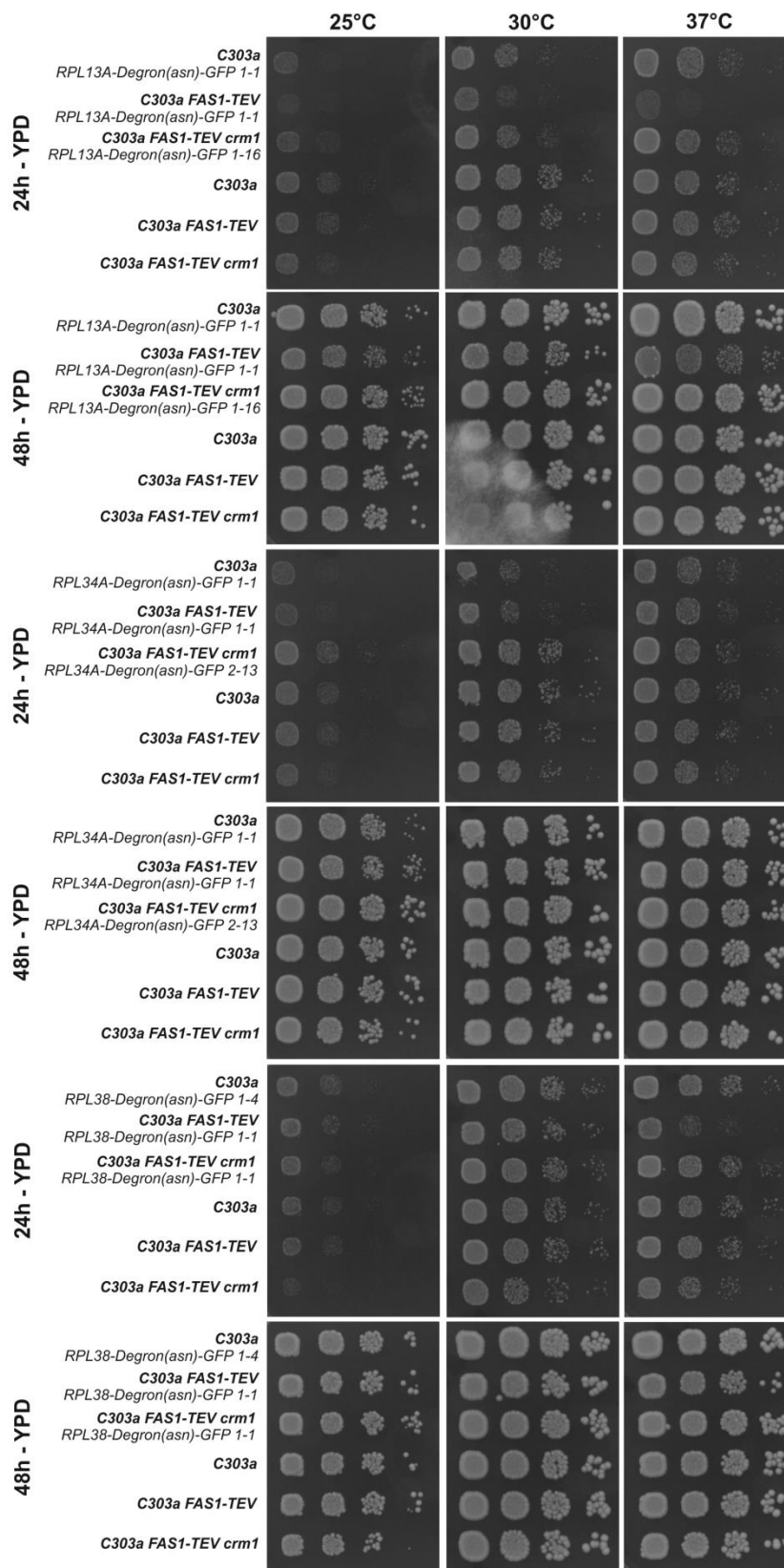


Figure 3.4: Spot test of Rpl13a-GFP, Rpl34a-GFP and Rpl38-GFP transformants on YPD. Strains were tagged using a fusion tag containing TEV cleavage sites, followed by either one of the two destabilizing residues (his or asn) according to the N-end rule, a degron and a GFP tag. The fusion cassette was present on plasmid 4020_pFA6a-Degron(asn)-GFP-HISMX and 4019_pFA6a-Degron(his)-GFP-HISMX constructed in this study; described in 3.1.1 and in the materials and methods section. The new strains, developed to screen for inhibitors of the large subunit, did not exhibit any strong growth deficiency compared to the wild type and therefore present a much better alternative than Rpl25.

3.1.3. Comparing the GFP Signal using fluorescence microscopy

For the screening procedure using a plate reader, it is important that the GFP tag not only is cleaved off by the TEV protease when entering the cytoplasm, but also is degraded efficiently by the proteasome. When designing the degron, the N-end rule gave insights to the protein stability depending on the amino acid present at the N-terminus of the cleaved GFP tag (Finley et al, 2012). By comparing the Rps3-Degron-GFP transformants, the degron including an asparagine at the N-terminus resulted in less cytoplasmic background (fig 3.5.). A comparison between Rpl25-Degron-GFP was not possible because of the problems when tagging Rpl25 chromosomally. Based on the information obtained from the Rps3 constructs, the new large ribosomal reporters, Rpl13a, Rpl34a and Rpl38, only featured a degron with an asparagine at the TEV site. When looking at figure 3.6, a strong decrease in the cytoplasmic background can be seen, when the TEV protease was introduced via Fas1. From the reporter of the large subunit, the Rpl13a-Degron(asn)-GFP showed the most decrease of the cytoplasmic signal.

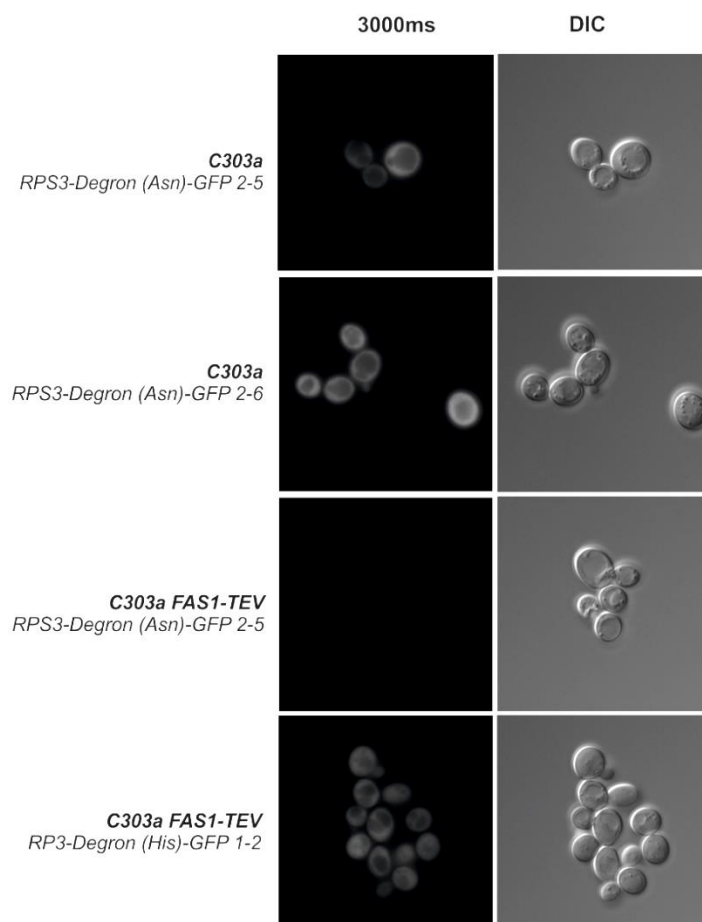


Figure 3.5: Fluorescence microscopy of Rps3-Degron-GFP in C303a and C303a FAS1-TEV. The degron leading to an asparagine at the N-terminus when tag is cleaved by TEV protease, indicated a much better degradation by the proteasome and therefore less background. Because of these results, the new large ribosomal reporter proteins were only featuring the degron version, leading to an asparagine at the N-terminus.

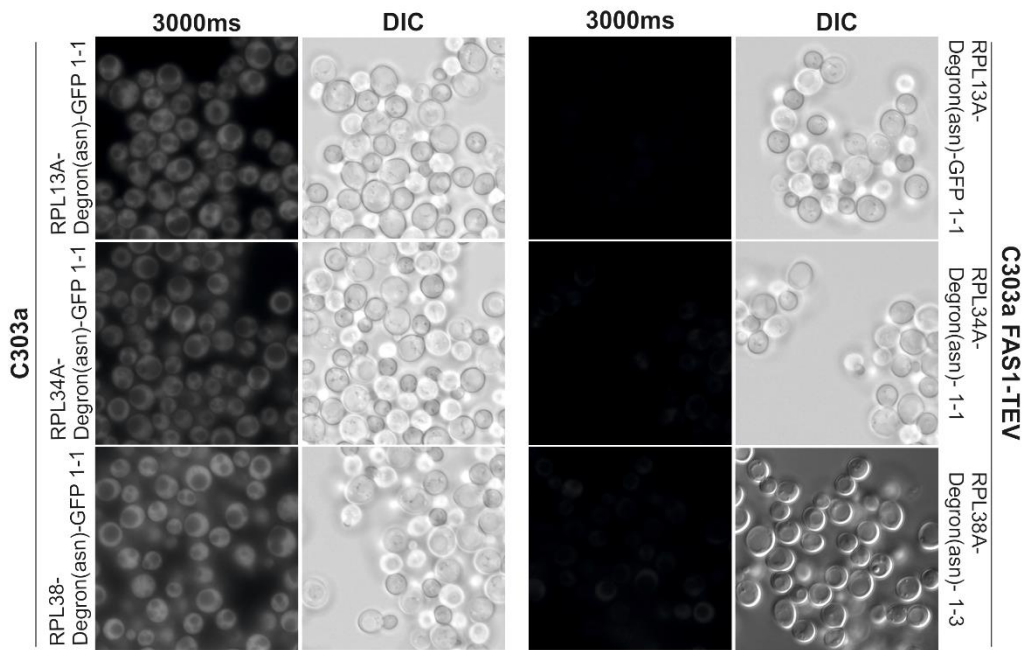


Figure 3.6: Fluorescence microscopy of *Rpl13a-Degron-GFP*, *Rpl34a-Degron-GFP* and *Rpl38-Degron-GFP* in *C303a* and *C303a FAS1-TEV*. All reporter proteins of the large ribosomal subunit showed a dramatic decrease of the cytoplasmic background when the TEV protease was introduced via *Fas1*. The strongest effect was with the reporter *Rpl13A-Degron(asn)-GFP*.

3.1.4. Protein expression levels of the reporter proteins

In order to determine the GFP expression level of the various reporters constructs, the proteins were isolated and detected via Western Blots. When comparing the GFP expression level among the Rps3 strains created in this study (fig 3.7), one can see a strong over expression of Rps3-degrom-GFP (*C303a Rps3-Degron(his)-GFP 2-1* and *C303a FAS1-TEV crm1 Rps3-Degron(asn)-GFP 2-2*). This was most likely due to additional mutations from the transformation process, a common effect since the yeast repair system is used for the recombination (Kawai et al, 2010). The strains also show a very strong growth defect, when analysed at the spot test (fig 3.2). However, the band intensity of Rps3-GFP of the first lane (*C303a Rps3-Degron(his)-GFP 2-1*) is significantly higher compared to the signal in the lane with *C303a FAS1-TEV Rps3-Degron(asn)-GFP 2-5*. The anti-GAPDH detection indicates that the amount of proteins loaded in the first and third lane is nearly the same, but the Rps3-GFP intensity was reduced in the third lane. The TEV protease cuts off the GFP tag when the ribosomal protein enters the cytoplasm, which led to a reduced cytoplasmic signal which was confirmed using fluorescence microscopy (fig 3.5). Another aspect of this protein detection was to determine which N-terminal residue, his or asn, leads to a better degradation by the proteasome. The microscopy in figure 3.5 shows a stronger cytoplasmic signal for the his construct. This suggests that a cut off resulting in a N-

terminal asparagine is degraded by the proteasome more efficiently than with the N-terminal histidine, resulting in less signal detected in the cytoplasm. Indeed, the asn construct showed lower residual levels of GFP in crude extracts as determined by western blotting by comparing the samples C303a FAS1-TEV Rps3-Degron(asn)-GFP 2-5 and C303a FAS1-TEV Rps3-Degron(his)-GFP 1-2 shown in figure 3.7. Nearly the same amount of total protein was loaded as suggested by the band intensity of the GAPDH protein, as well as comparing the intensity of the Rps3 bands using anti-Rps3 antibody. When comparing the GFP signal, which is roughly 27 kDa (Hink et al, 2000), the degron-GFP featuring an asparagine shows a much more efficient degradation resulting in less GFP detected. Therefore, the new large ribosomal proteins only featured an asparagine at the TEV site of the degron. Figure 3.8 shows the different C303a Rpl25-Degron-GFP strains seen in figure 3.3. The Western Blot indicates that all of the transformants have the same Rpl25-Degron-GFP expression, but that the majority of the Rpl25 is untagged in the cell. This effect can be seen by comparing the intensity of the Rpl25 band to the Rpl25-GFP band when detected by the anti-Rpl25 antibody. Since there is no expression of the TEV protease in the C303a strains, there must be an alternative cleavage activity responsible for removal of the tag. To ensure that the cleavage was not due to a mix up, I used an anti-FLAG antibody against the FLAG tag that is featured at the Fas1-TEV protein. In conclusion the Rpl25-Degron-GFP construct does not represent a reliable reporter system when screening for ribosome biogenesis inhibitors. When looking at fig 3.7 and 3.8, different bands above the size of the GFP protein appear. This is most likely due to the ubiquitination, since attachment of multiple ubiquitin chains functions as a signal for degradation by the proteasome (Finley et al, 2012). The same effect can be seen in fig 3.7 at the longer exposure of the GFP antibody. Additionally, degraded GFP can be observed when looking below the GFP band at fig 3.7-3.9. The expression level of the new reporter proteins Rpl13a, Rpl34a and Rpl38 is shown figure 3.9. As already seen in figure 3.7, introducing the TEV protease leads to reduction of the detected reporter protein-degrom-GFP construct, using the anti GFP antibody. The strain harboring the Rpl38-degrom-GFP construct does seem to have a stronger GFP expression compared to Rpl13a and Rpl34a. Minor cleavage of the degrom-GFP tag can be seen when looking at the longer exposed anti-GFP antibody detection at the sample C303a Rpl38-Degrom(asn)-GFP. The anti-FLAG antibody was used as mentioned before as an additional control of the TEV protease expression.

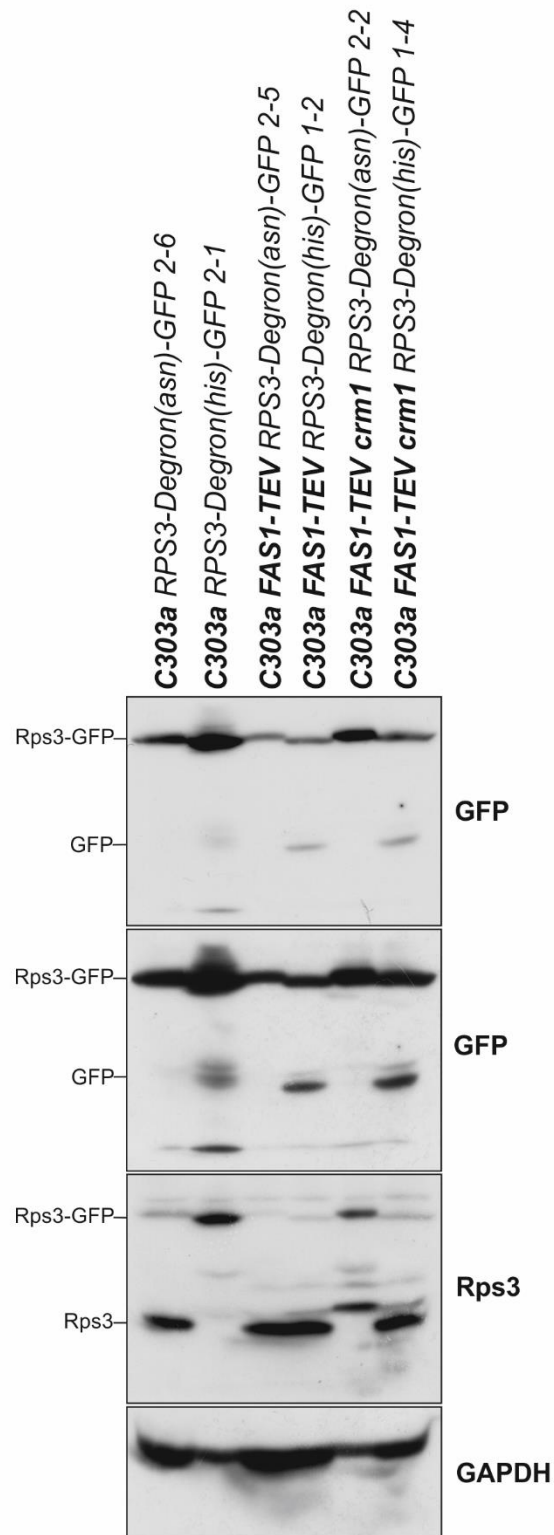


Figure 3.7: Western Blot detection of the Rps3 constructs. Total protein was extracted from the tagged strains and analyzed by western blotting for the presence of the GFP-fusion constructs. C303a Rps3-Degron(his)-GFP 2-1 and C303a FAS1-TEV crm1 Rps3-Degron(asn)-GFP 2-2 show a strong GFP expression. This is coupled with a growth defect (see fig 3.2) and microscopy signal (not presented in this work). Comparing the third and fourth lane (C303a Fas1-TEV strains), it does seem that the asparagine at the N-terminus leads to a better degradation compared to a histidine at the N-terminus.

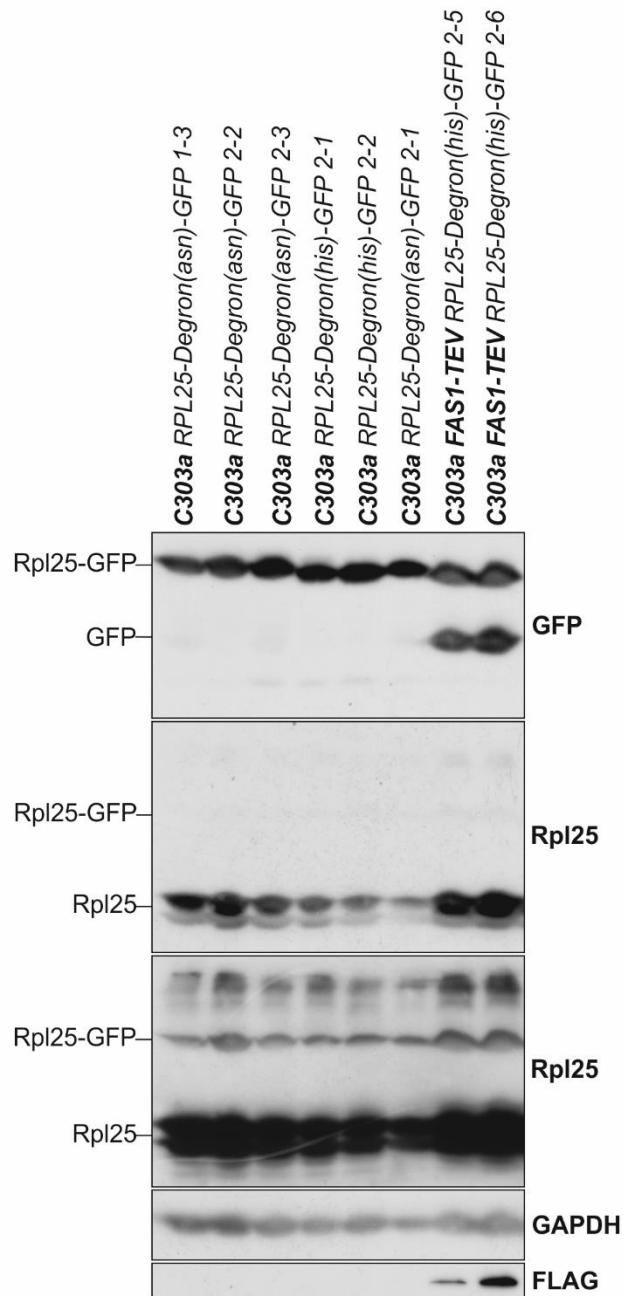


Figure 3.8: Western Blot detection of the Rpl25 constructs. Total protein was extracted from the tagged strains and analyzed by western blotting for the presence of the GFP-fusion constructs. The first six lanes indicate that the C303a strains can efficiently cleave off and degrade the GFP tag and form Rpl25 (see the Rpl25 blot) in the absence of TEV protease. Using the anti-FLAG antibody, the expression of the TEV protease was monitored and is restricted to the strains expressing the TEV-Fas1 fusion protein. The signal above the Rpl25-GFP bands seen in the long exposure blot is likely due to multi ubiquitination.

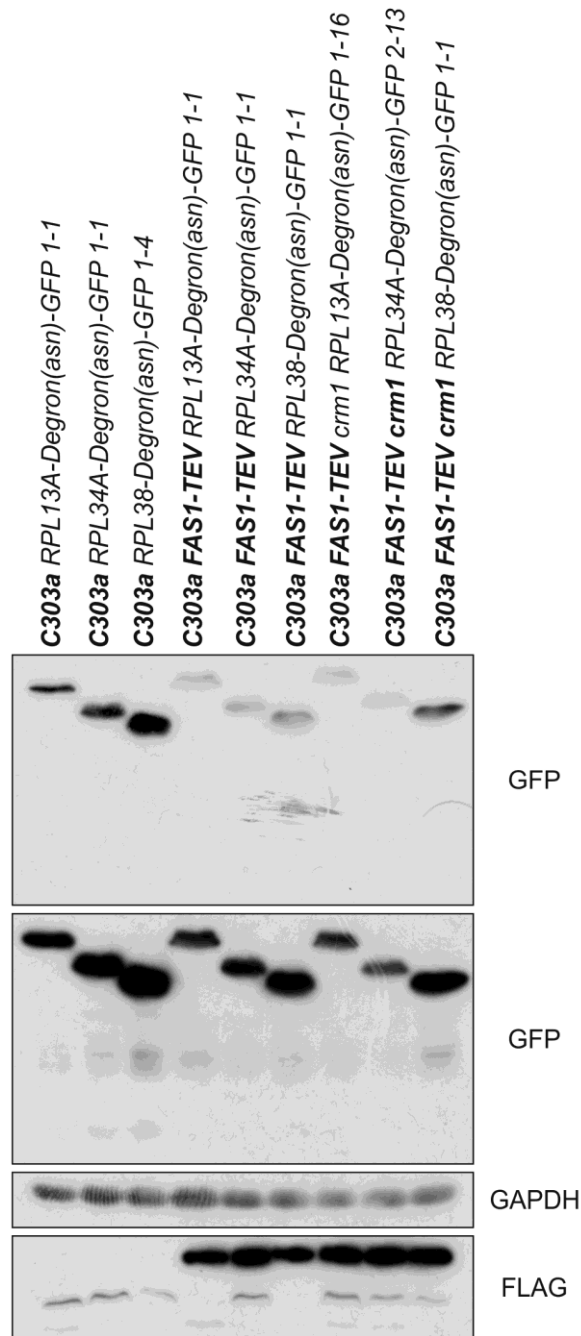


Figure 3.9: Western Blot detection of Rpl13a, Rpl34a and Rpl38. Total protein was extracted from the tagged strains and analyzed by western blotting for the presence of the GFP-fusion construct. The new reporter constructs of the large subunit demonstrate that the introduction of the TEV protease leads to a reduction of the reporter-degdon-GFP detected (compare lane 1-3 to 4-6, counting from the left). The cleaved GFP signal is hardly detectable in the FAS1-TEV expressing strains, even upon longer exposure. The cells featuring a TEV protease are confirmed via the FLAG tag. This strongly suggests that the cleaved GFP is degraded efficiently by the proteasome.

3.1.5. TECAN GENios Pro set up

Different settings for the whole cell GFP measurement using the TECAN GENios Pro were tested while working on this thesis. The technical “*Detection of Green Fluorescent Protein (eGFP), Tecan Ultra Evolution, Safire and GENios Pro*” described a set up for whole cell GFP measurement for cell culture applications and was used to create a modified version for yeast. Many setting variations such as different volumes, gain, integration times, plate types, read modes (bottom/top) and cell densities of the cell suspension were tested. However, table 3.1 only presents the most promising set up for the screen using the constructs described in table 2.2. The minimal media, which did not interfere with the fluorescence microscopy, had strong background when using small volumes or low cell density. By using a volume of 200µl and the cell density of at least 0.5 OD₆₀₀, the background of the media was kept to a minimum.

Table 3.1. Suggested set up for measuring whole cell GFP using the TECAN GENios Pro

Measurement mode:	Fluorescence Bottom
Excitation wavelength:	485nm
Emission wavelength:	535nm
Gain (Optimal):	87
Number of reads:	6
Integration time:	20 µs
Lag time:	0 µs
Mirror selection:	Bottom
Plate definition file:	GRE96fb.pdf
Multiple reads per well (Square):	3x3
Shake duration (Orbital Normal):	6s

The following tables, 3.2 - 3.4, demonstrate the row data of the sample measurements performed with the constructs Rps3-Degron(asn)-GFP and Rpl13a-Degron(asn)-GFP in *C303a* and *C303a FAS1-TEV* using the set up listed in table 3.1. To exclude any mistakes due to the transfer to the 96 well plate, each probe was pipetted four times (see table 3.2). When multiplying the cell density (table 3.3) with the GFP signal measured (table 3.2), the signal was adjusted to the approximately cell number of the well. The mean of the constructs and its standard deviation can be found in table 3.4.

Table 3.2. Whole cell GFP measurements. Each probe was measured four times independently in different wells to exclude any pipetting mistakes or variations due the well position on the plate.

C303a	C303a Rps3-Degron(asn)-GFP 2-5	C303a FasI-TEV Rps3-Degron(asn)-GFP 2-5	C303a Rpl13a-Degron(asn)-GFP 1-1	C303a FasI-TEV Rpl13a-Degron(asn)-GFP 1-1	Media
21119	43072	32334	27556	23112	8351
21061	42713	31534	27371	24213	8278
21116	42383	31832	27656	23009	8297
21081	42338	31655	27389	22927	8142

Table 3.3. Row data of the 600nm absorbance measurements. Using the cell density, the GFP signal could be adjusted to the approximately cell number of the well.

C303a	C303a Rps3-Degron(asn)-GFP 2-5	C303a FasI-TEV Rps3-Degron(asn)-GFP 2-5	C303a Rpl13a-Degron(asn)-GFP 1-1	C303a FasI-TEV Rpl13a-Degron(asn)-GFP 1-1
0,1425	0,1822	0,1549	0,1419	0,1550
0,1427	0,1736	0,1634	0,1449	0,1572
0,1444	0,1797	0,1626	0,1461	0,1599
0,1459	0,1808	0,1609	0,1425	0,1599

Table 3.4. Adjusted whole cell GFP signal. Using table 3.3, the GFP signal was adjusted to the cell number in the well and used to create figure 3.10.

	C303a	C303a Rps3-Degron(asn)-GFP 2-5	C303a FasI-TEV Rps3-Degron(asn)-GFP 2-5	C303a Rpl13a-Degron(asn)-GFP 1-1	C303a FasI-TEV Rpl13a-Degron(asn)-GFP 1-1
Mean	1845.5	6152.99	3781.15	2765.72	2377.26
Std. deviation	20.55	148.39	45.21	48.24	89.58

When looking at table 3.4 and figure 3.10, the GFP signal measured using the Rps3-degrom-GFP construct was easily distinguishable from the cell background. Thus, the cells featuring a TEV-Protease showed a significant reduction of the signal, due to the cleavage of the degrom-GFP tag when entering the cytoplasm and following degradation. The same results were expected when using the Rpl13a-degrom-GFP construct. However, the signal of the cells lacking a TEV-protease was not significantly higher than the cells expressing a TEV-protease. Figure 3.6 suggests that the cells with a TEV protease should have dramatic decrease of the GFP signal and therefore a similar signal to C303a. In contrast, the cells without a cleavage in the cytoplasm should have a much higher signal than the strain background (C303a), as it was suggested from the microscopy pictures (figure 3.6). In conclusion, the screen set up in table 3.1 and reporter constructs with a high GFP signal, such as Rps3, could potentially be used for a high through put screen. Constructs with lower GFP expression, as seen with Rpl13a, should not be used for the screen in the suggested set up. The background of the cell cannot be distinguished from the GFP signal. Assuming that not all cells will show an accumulation when treated with the potential inhibitors, a significant effect will most likely not be detectable when using the plate reader.

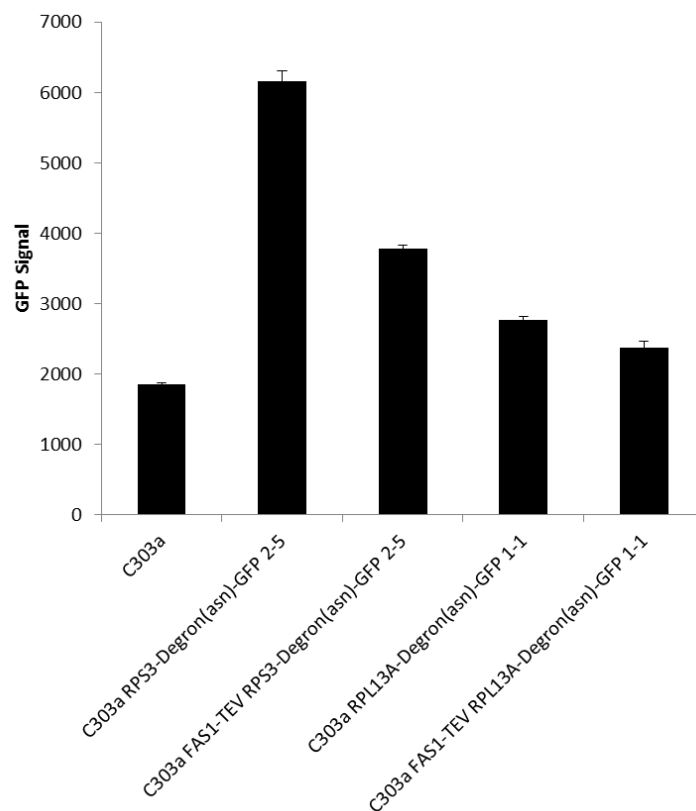


Figure 3.10: Whole cell GFP measurement of the Rps3-Degron(asn)-GFP construct and Rpl13a in C303a and C303a FAS1-TEV. The data suggest that the Rps3 could be used for a screen. However, constructs with lower GFP signals such as Rpl13a, will most likely not show a significant effect when the suggest set up is used.

3.1.6. Controls of the screen

The high trough put screen, based on whole cell GFP measurement did require proper controls. Untreated cells were used as the negative control. However, the positive control had to be a tested substance, leading to an accumulation in the nucleus preferably at all cells. Cells with a *crm1* mutation could have functioned as a positive control, but the strain C303a Fas1-TEV *crm1* used in this work, turned out to do not contain the *crm1*T539C mutation. The strain has been replaced now in the official strain collection, with the C303a Fas1-Tev *crm1* strain, featuring the *crm1* mutation (fig 3.11).

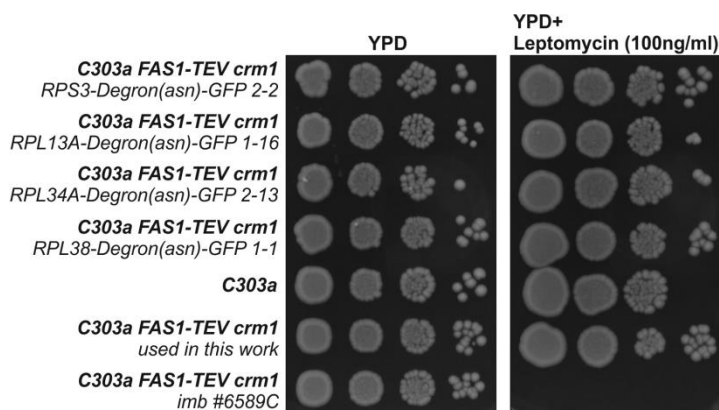


Fig 3.11: The strain C303a FAS1-TEV *crm1* did not feature Leptomycin B sensitivity.

The preferred positive control, over treating different cells, is to treat the same cells that are used for the screen with a known inhibitor of the ribosome biogenesis. The accumulation would only occur when there is an active ribosome production and would serve as control for the cells used for the screen. Diazaborine is a well characterized and up to now the only known specific inhibitor of the ribosome biogenesis (Pertschy et al, 2007; Loibl et al, 2014). However, it does only affect the pre-60S particle and not the pre-40S particle. In addition, cells featuring the large subunit reporter constructs Rpl13a, Rpl34a and Rpl38 did not show any accumulation when they were treated with diazaborine. Strains featuring the reporter Rpl25-GFP did show an accumulation upon treatment with diazaborine but were not suitable for a screen, due to their high variation in growth and amount of untagged Rpl25 protein in the cell. Thus, the accumulation of ribosomal proteins in the nucleus is likely not strong enough to allow discrimination between cells treated with a ribosome biogenesis inhibitor and untreated cells. Finally, it has to be considered, that the compounds in the screen might exhibit different MIC values, resulting in different degrees of accumulation of the reporter protein in the nucleus. In conclusion, set up of a high throughput compatible screen for plate readers is complicated and influenced by many different and partially hard to control parameters. Therefore, for further experiments we used a visual screen to identify novel inhibitors of ribosome biogenesis.

3.2. The manual screen using fluorescence microscopy

3.2.1. Strains used while performing the manual screen

This screen relies on the visual inspection of cells expressing ribosomal protein-GFP reporter fusions by fluorescence microscopy, after growth in microtiter plates and treatment for three to five hours. For experimental details on this manual screen see the materials and methods section (2.7). In brief, at least four to five pictures representing different fields were recorded from each sample and independently evaluated for nuclear accumulation of the reporter proteins by two researchers (Helmut Bergler and me). Compound causing nuclear accumulation of either reporter protein were retested at least two additional times with different drug concentrations (up to three times the concentration of the original screen). Only drug scoring positive in these analyses were classified as possible ribosome biogenesis inhibitors. The constructs of the large subunit (Rpl13a, Rpl34a and Rpl38) created for the high-through-put screen, did not show any effect upon diazaborine treatment upon inspection with the fluorescence microscope. Therefore, an alternative reporter protein had to be used for the manual screen in order to use diazaborine as a positive control. The Rpl7a-GFP fusion is known to accumulate in yeast cells when treated with diazaborine (Morgenstern, 2004, Pertschy et al., 2004). When the plain GFP tag, was fused to Rpl7a in the C303a strain, cells did show a mild growth deficiency compared to the wildtype (fig 3.12). The C303a Rpl7a-GFP K5 strain, which was used for the screen, had a generation time of 180 min in SD media. The wild type strain (C303a) required about 120 min for cells to proliferate. The Western Blot indicated no cleavage of the GFP tag (fig 3.15). This was essential for the screen, because the cleaved GFP could enter the nucleus and create artefacts. Upon diazaborine treatment, Rpl7a-GFP showed a strong accumulation in the cell nucleus. After short time treatment, the signal of Rpl7a-GFP accumulate in the nucleolus, but upon longer incubation, the signal can also be detected in the nucleoplasm (see figure 3.16). Since diazaborine only inhibits the 60S particle when entering the cytoplasm (Loibl et al, 2014), a different positive control for the small subunit was essential. When screening for the inhibitors with Rpl7a-GFP, the potential inhibitor Acivicin was identified (see table 3.5). The reporter Rps3-GFP did not show an effect when treated with Acivicin. For this reason, Mathias Loibl fused a GFP tag to different proteins of the small subunit (Rps13, Rps0, Rps9, etc). When I tested those reporter proteins, Rps9a-GFP showed an accumulation in the nucleolus when the cells were treated with Acivicin (see fig 3.16).

Since all tested inhibitors were dissolved in DMSO, we also tested whether the solvent has an effect on growth of yeast. The growth curve and microscopy, seen in figure 3.14 and 3.13, show the influence of different amounts of DMSO on the yeast cells. This results confirmed that the concentration used for the screen (NIH 1 μ l/200 μ l and ENZO 2 or 4 μ l/200 μ l), leading to a final concentration of 0.5% - 2% of DMSO in the sample, does not lead to an unspecific accumulation in the nucleus due to stress (fig 3.13). The spot test of C303a Rpl7a-GFP and C303a Rps9a-GFP indicates that the GFP fusion to the large subunit protein had a stronger effect on growth than the small subunit reporter (fig 3.12). The strain C303a Rpl7a-GFP K5 Δ bud20, a knockout of one shuttling factor of the pre-60S subunit, demonstrated an already known growth defect (Bassler et al, 2012).

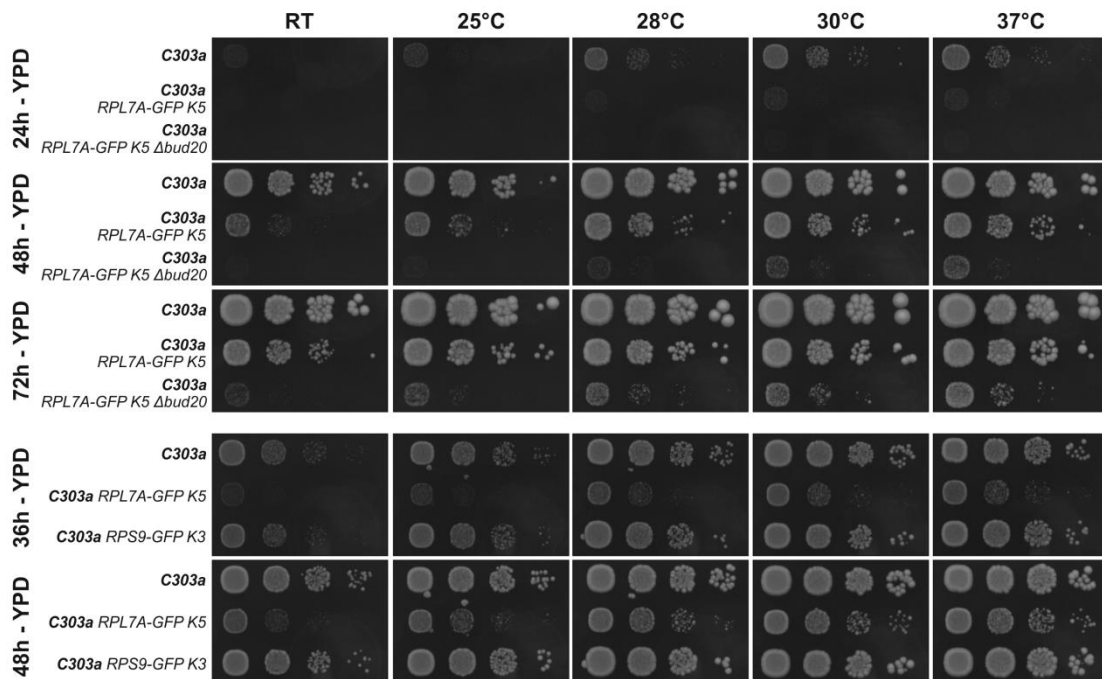


Figure 3.12: Spot test of Rpl7a-GFP and Rps9a-GFP on YPD. The Rpl7a-GFP strain shows a growth deficiency compared to the wild type. In contrast the Rps9a-GFP fusion had hardly any impact on the growth of the cells.

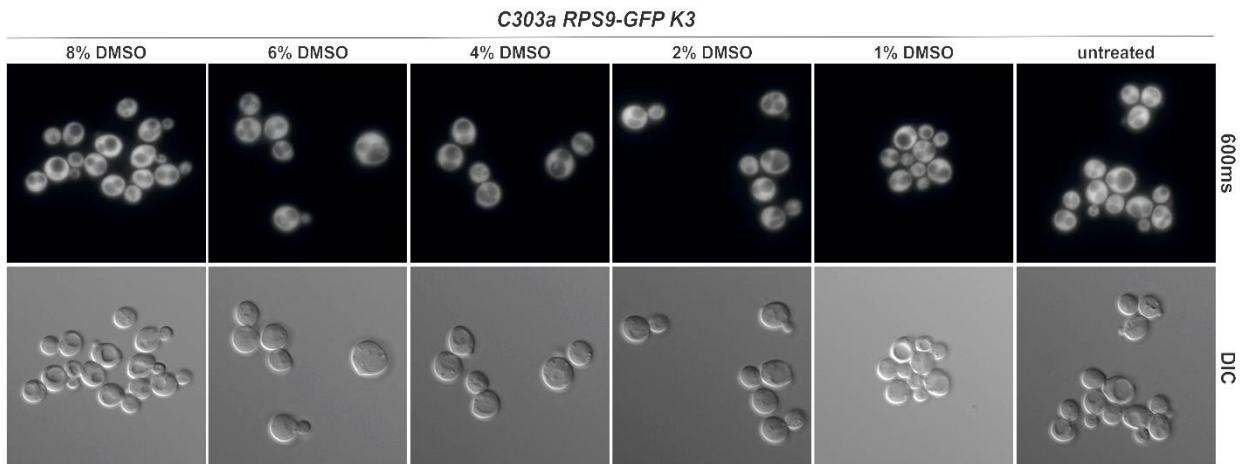


Fig 3.13: C303a Rps9a-GFP K3 treated with DMSO. To determine if DMSO has an impact the cells, they were treated with up to 8% DMSO for 4 hours. Additional vacuoles can be seen, as well as slight changes in the morphology of the cell but there was no accumulation of the reporter protein in the cell nucleus.

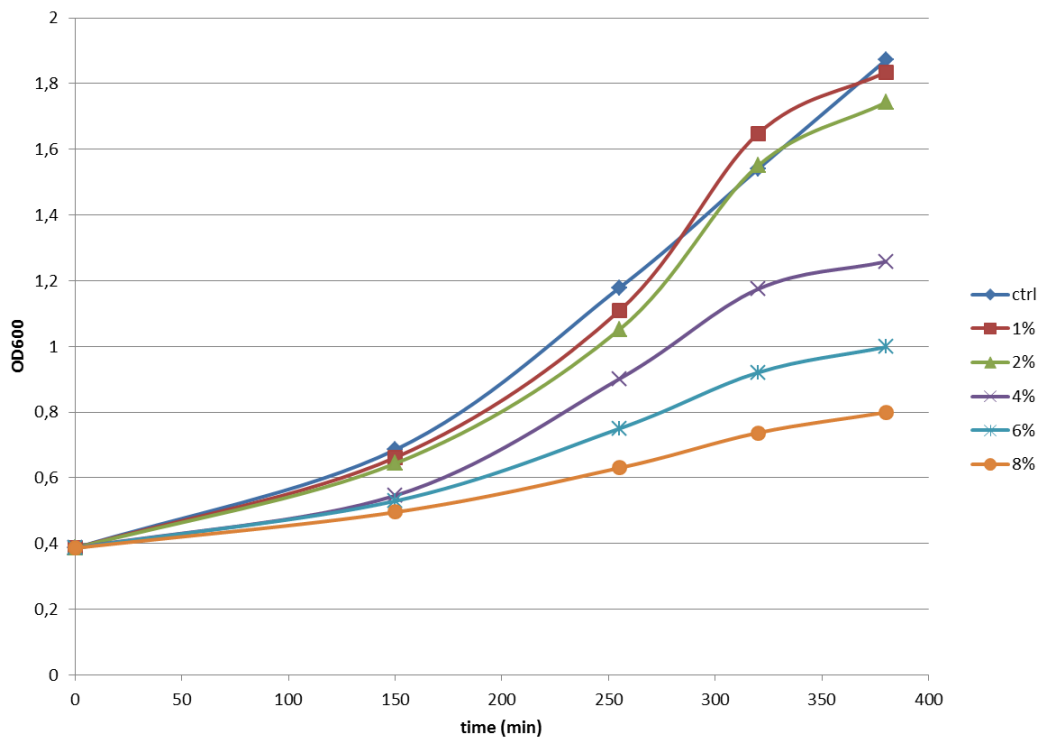


Fig 3.14: Effect of DMSO on the growth of Rpl7a-GFP. Different amounts of DMSO were added to determine the influence of DMSO on the yeast cells. When screening for ribosome biogenesis inhibitors, the final DMSO concentration did not exceed 3%. Therefore, the DMSO should not lead to secondary effects due to the inhibition of the growth of the cells.

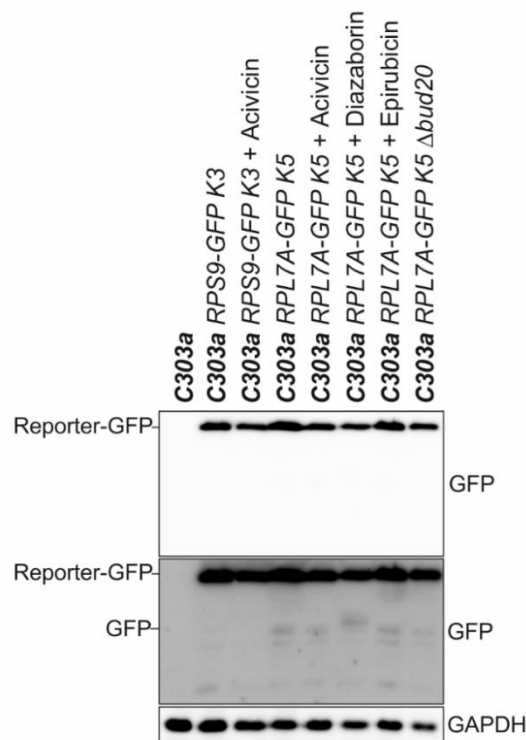


Fig 3.15: Western Blot detection of C303a Rpl7a-GFP and C303a Rps9a-GFP. When the cell lysate was incubated with GFP antibody, almost no degradation products were detected. The reporter proteins Rpl7a (27.6kDa) and Rps9a (22.4 kDa) were detected at the same height, due to its similar size, when the GFP tag (27 kDa) was added. Some degradation can be seen, but the amount is very small compared to the amount of reporter protein-GFP detected. Therefore, the accumulation signal upon inhibitor treatment cannot be caused by the cleaved GFP protein. The cells were treated with 20µg/ml Acivicin, 5µg/ml of diazaborine and 29µg/ml Epirubicin.

To determine the influence of selected compounds on the protein levels of the reporter proteins, I incubated yeast cells at an OD₆₀₀ of 0.4 with the drugs. At a cell density of 0.8 (OD₆₀₀), the cells were harvested and broken using the chemical lysis protocol (materials and methods 2.5.1.) and analyzed by western blotting. The western blot of the reporter constructs is shown in figure 3.15. The blot shows extracts from untreated cells, as well as, of cells treated with Acivicin (20µg/ml, 112µM), diazaborine (5µg/ml, 18.4µM) and Epirubicin (29µg/ml, 50µM). The GFP detection by antibodies, suggests that the amount of reporter-GFP of the treated cells is slightly reduced compared to the reporter-GFP of the untreated cells (see C303a Rpl7a-GFP K5 untreated and treated with Acivicin). When the ribosome biogenesis is inhibited by a substance such as diazaborine, ribosomal proteins accumulate in the nucleus. Since less pre-ribosomal particles are exported or maturation in the nucleus is repressed, the overall amount of ribosomal proteins in the cell decreases. This could be caused by a down regulation of the ribosomal protein synthesis due to the stress, the degradation of the ribosomal proteins not bound to the ribosomal particle or a removal of the GFP tag from the ribosomal proteins incorporated in mature cytoplasmic ribosomes.

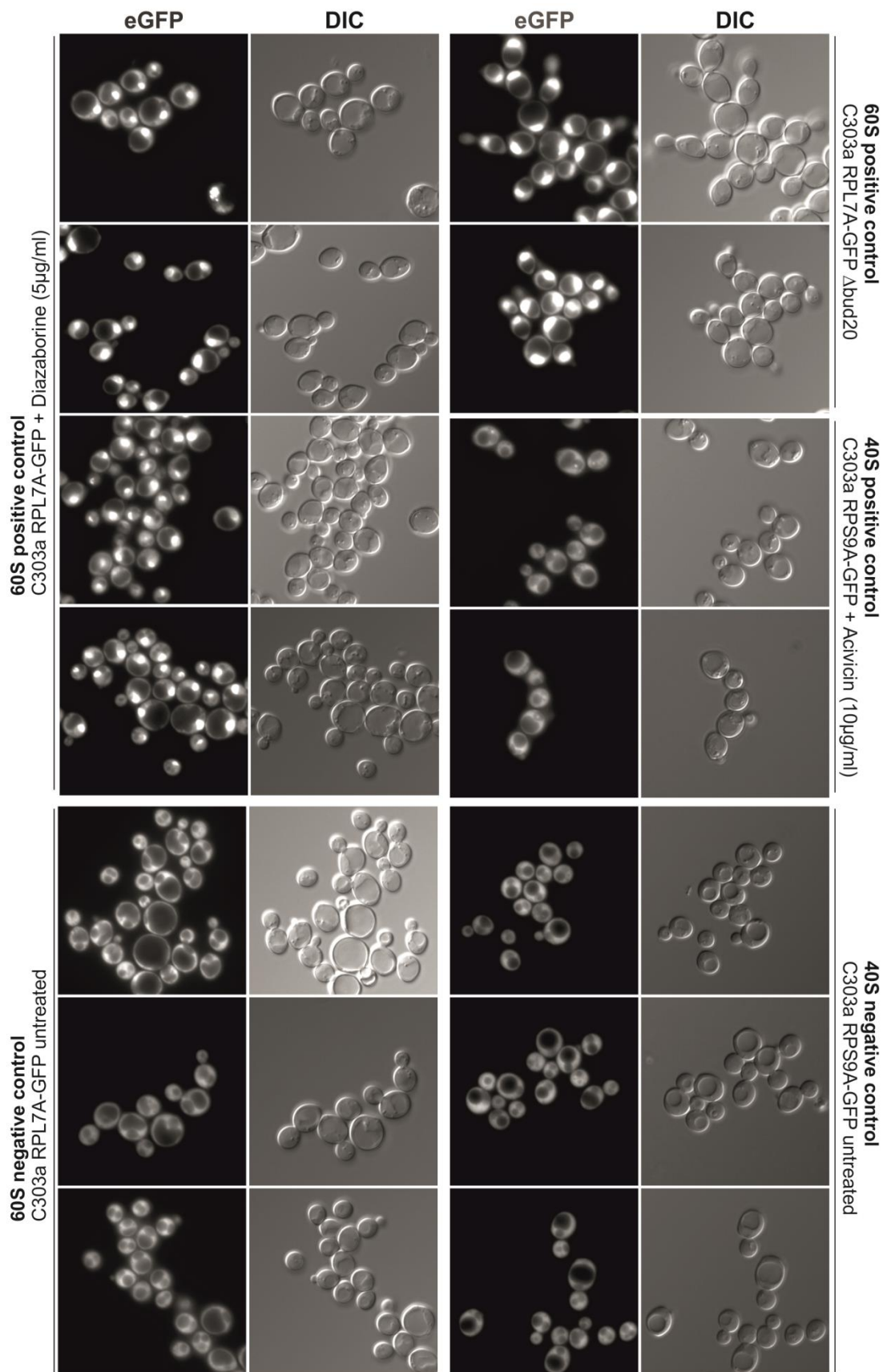


Figure 3.16: Fluorescence microscopy pictures showing the controls of the manual screen

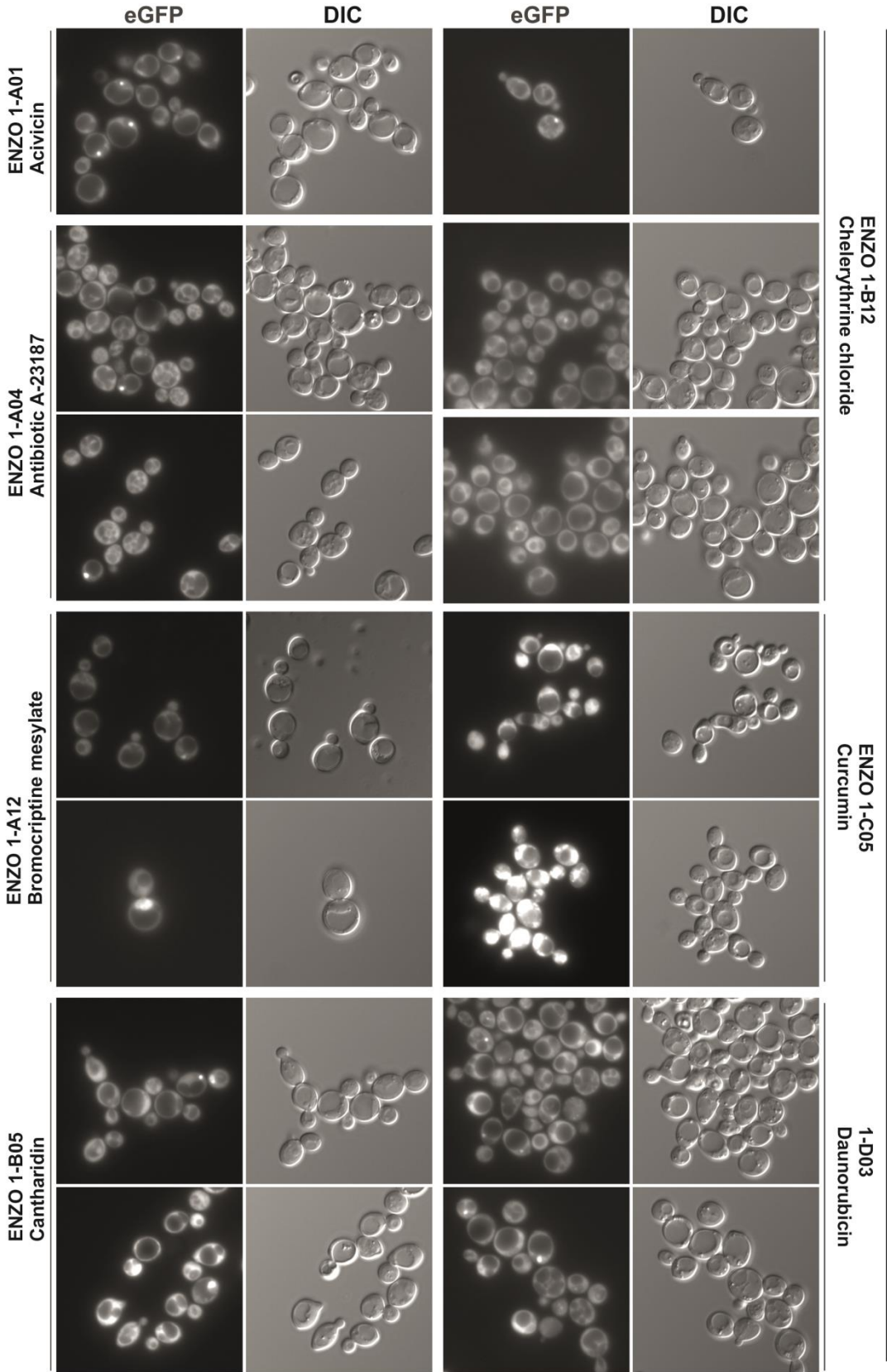
3.2.2. Potential inhibitors identified by the manual screen

Substances that showed an accumulation in the nucleolus and/or the nucleoplasm using the reporter of the large subunit (Rpl7a-GFP) are presented in table 3.5 and figure 3.17. The hits obtained from screening with the small subunit reporter (Rps9a-GFP) are shown in table 3.6 and figure 3.18. Substances that demonstrated an effect in the screen with the large subunit and later on with the small subunit are listed in table 3.7.

Table 3.5: List of all substances that demonstrated an accumulation in the nucleolus and/or nucleoplasm when screening with the Rpl7a-GFP reporter construct. The time of incubation and final concentration only represents the value that gave the most accumulations of the reporter protein in the nucleus when evaluating the pictures from the screen.

Collection	Plate	Well	Substance	Final concentration (µM)	Time of incubation (h)
ENZO	1	1-A1	Acivicin	56	4
ENZO	1	1-A4	Antibiotic A-23187 (Calcimycin)	38	3
ENZO	1	1-A12	Bromocriptine mesylate	53	6
ENZO	1	1-B05	Cantharidin	51	5.5
ENZO	1	1-B12	Chelerythrine chloride	52	4.5
ENZO	1	1-C05	Curcumin	27	4
ENZO	1	1-D03	Daunorubicin . hydrochloride	36	5.75
ENZO	1	1-D10	Doxorubicin HCl	35	4.5
ENZO	1	1-H04	Mycophenolic acid	63	5.75
ENZO	2	2-C05	Tanshinone IIA	68	4.5
ENZO	2	2-F05	Morin	66	5
ENZO	2	2-F09	Nonactin	54	4.5
ENZO	2	2-G02	Quercetin dehydrate	59	5
ENZO	2	2-H09	Kaempferol	70	4
ENZO	3	3-G05	Sinensetine	54	5
ENZO	4	4-A01	Syringetin-3-glucoside	39	4.5
ENZO	4	4-B12	Caryophylline	90	4
ENZO	4	4-E08	Streptonigrin	40	3.5
ENZO	4	4-G05	(+)-Usnic acid	29	3.5
ENZO	5	5-B05	Vulpinic acid	93	5.5
ENZO	5	5-B06	Berberine-HCl	54	3.75
ENZO	5	5-B12	Zerumbone	92	4.5
ENZO	6	6-A04	Senecionine	60	5
ENZO	6	6-B01	Bleomycin sulfate	40	5.5
NIH	NGP-105-01	1-A10	Doxorubicin	50	5
NIH	NGP-105-01	1-E11	Sulfasalazine	50	5
NIH	NGP-105-01	1-H06	Epirubicin Hydrochloride	50	3.5
NIH	NGP-105-02	2-D06	Carmofur	50	5
NIH	NGP-105-02	2-F07	Itraconazole	100	5
NIH	NGP-105-02	2-H08	Idarubicin hydrochloride	20	5
NIH	NGP-105-03	3-A02	Bestatin	100	5
NIH	NGP-105-05	5- A07	Clotrimazole	100	5
NIH	NGP-105-06	6-C07	Parecoxib sodium	50	5
NIH	NGP-105-06	6-F07	Artemether	50	5

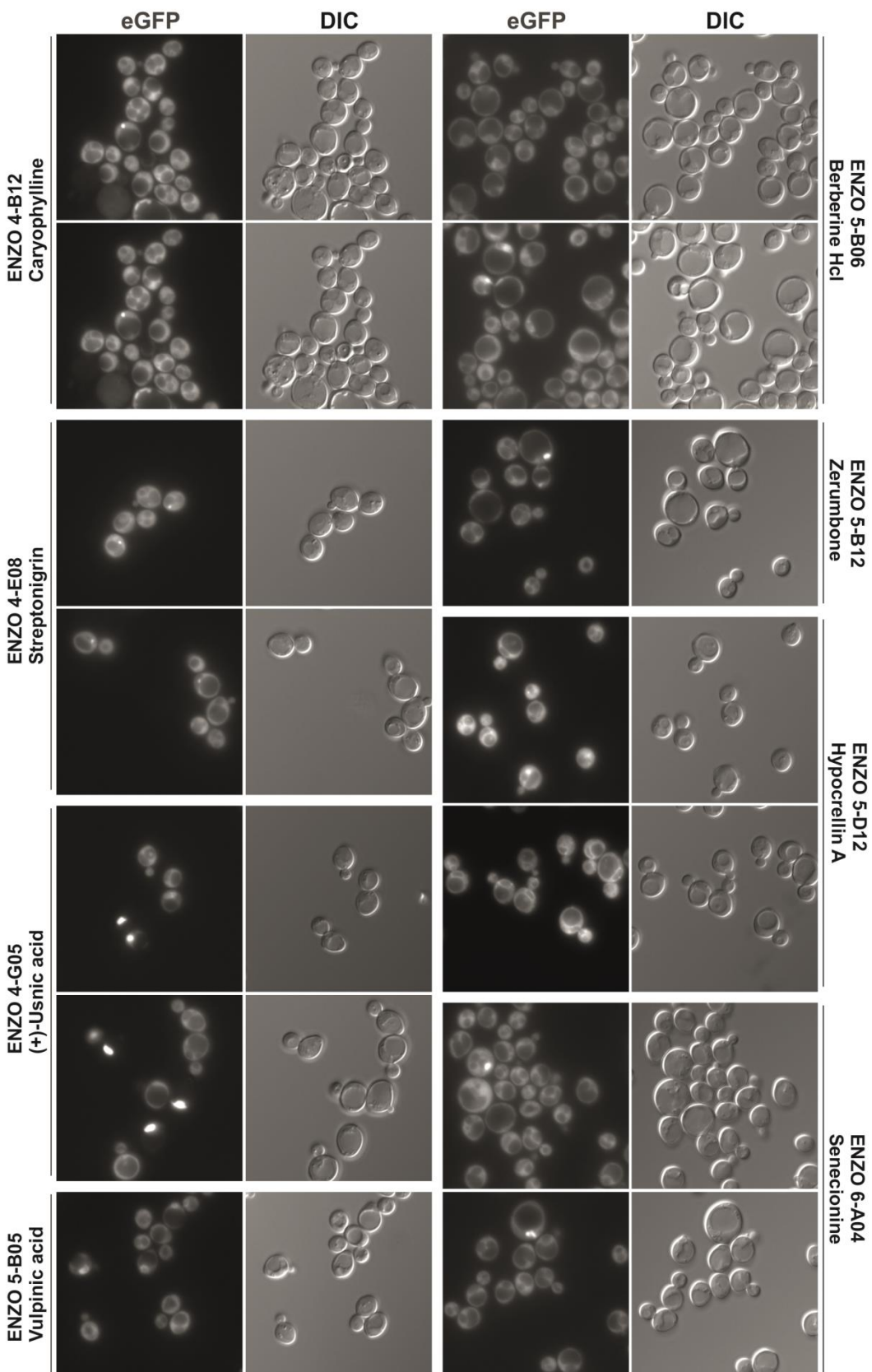
60S Screen Hits (RPL7A-GFP K5)



60S Screen Hits (RPL7A-GFP K5)

ENZO 2-F05 Morin	eGFP	DIC	eGFP	DIC
ENZO 2-F09 Nonactin	eGFP	DIC	eGFP	DIC
ENZO 2-G02 Quercetin dihydrat	eGFP	DIC	eGFP	DIC
ENZO 2-H09 Kaempferol	eGFP	DIC	eGFP	DIC
ENZO 3-G05 Sinensetine	eGFP	DIC	eGFP	DIC
ENZO 4-A01 Syringetine-3-glucoside	eGFP	DIC	eGFP	DIC
ENZO 1-D10 Doxorubicin	eGFP	DIC	eGFP	DIC
ENZO 1-H04 Mycophenolic acid	eGFP	DIC	eGFP	DIC
ENZO 2-C05 Tanshinone IIA	eGFP	DIC	eGFP	DIC

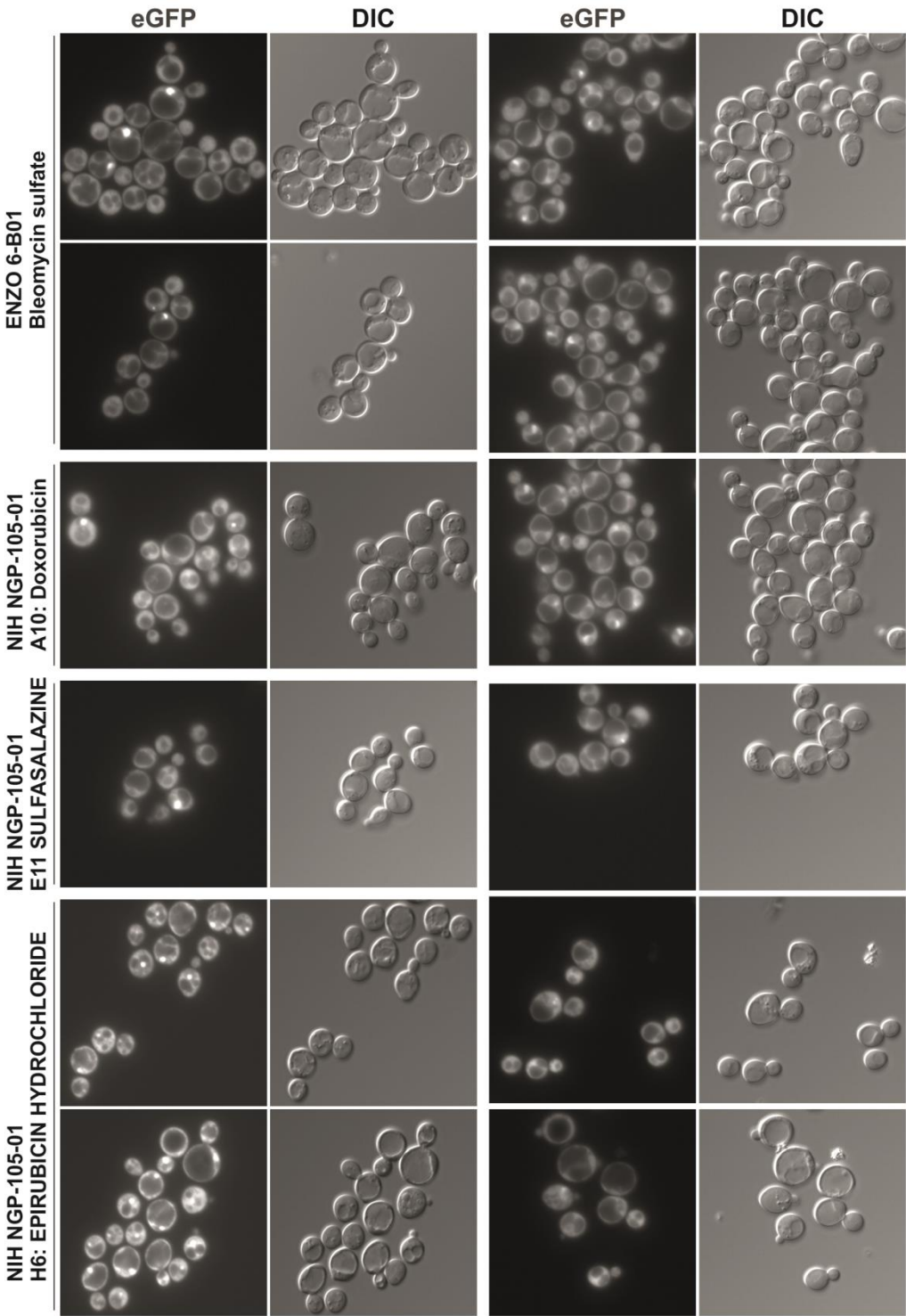
60S Screen Hits (RPL7A-GFP K5)



60S Screen Hits (RPL7A-GFP K5)

NIH NGP-105-02
D6: Carmofur

NIH NGP-105-02
F7: Itraconazole



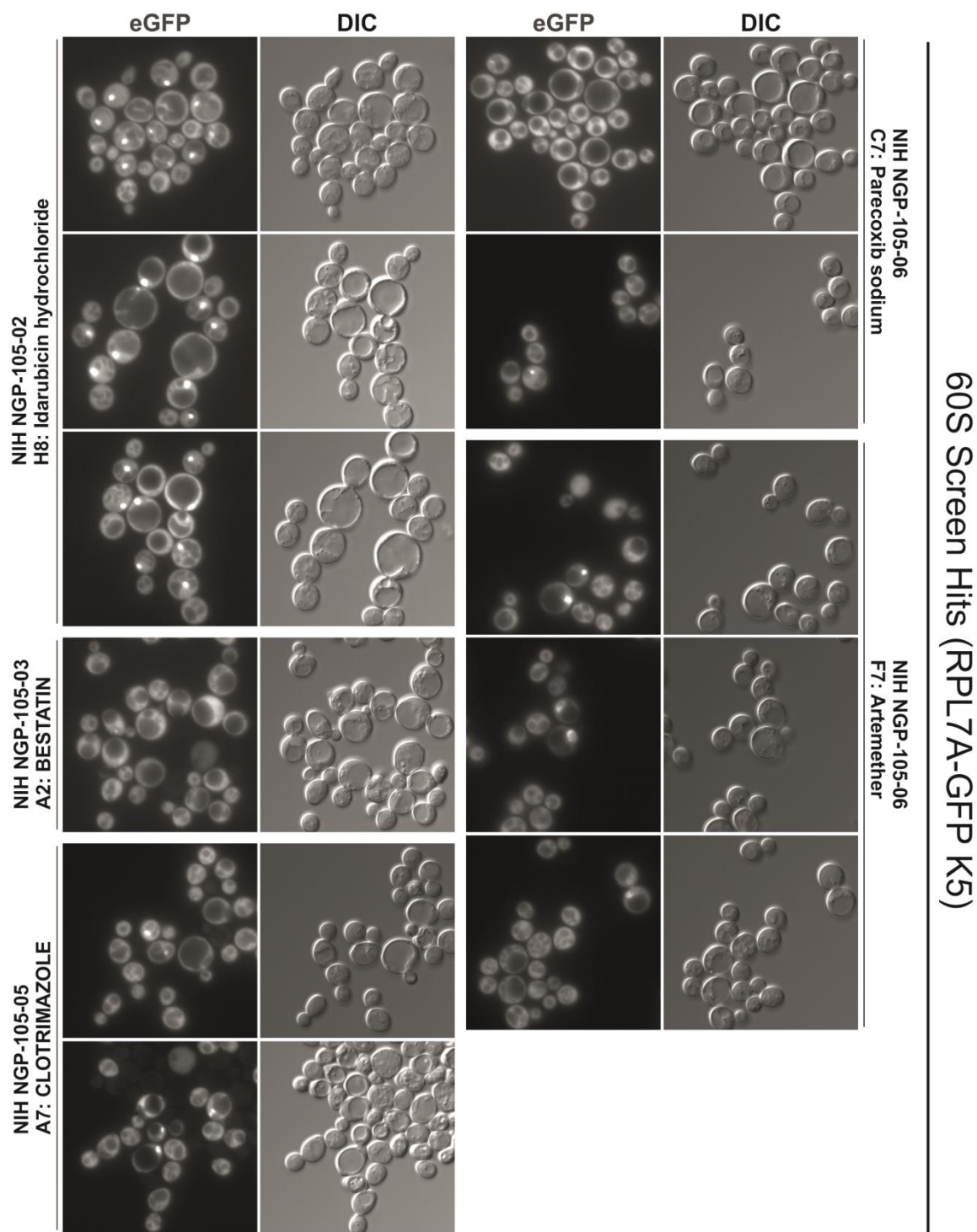


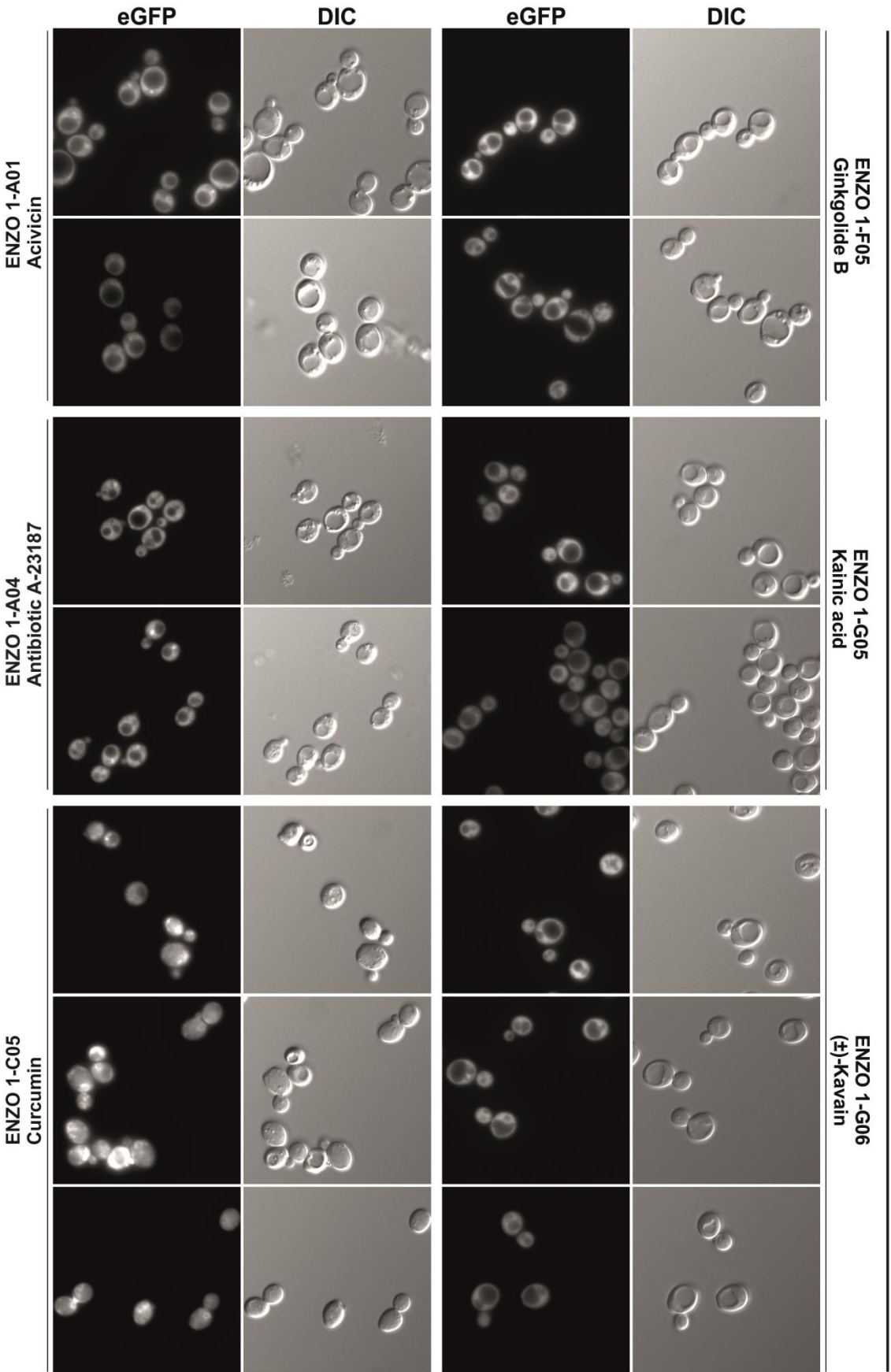
Figure 3.17: Fluorescence microscopy pictures of the hits obtained from the screen, using the Rpl7a-GFP reporter construct.

Table 3.6: List of all substances that demonstrated an accumulation in the nucleolus and/or nucleoplasm when screening with the *Rps9a-GFP* reporter construct. The time of incubation and final concentration only represents the value that gave the most accumulations of the reporter protein in the nucleus when evaluating the pictures from the screen.

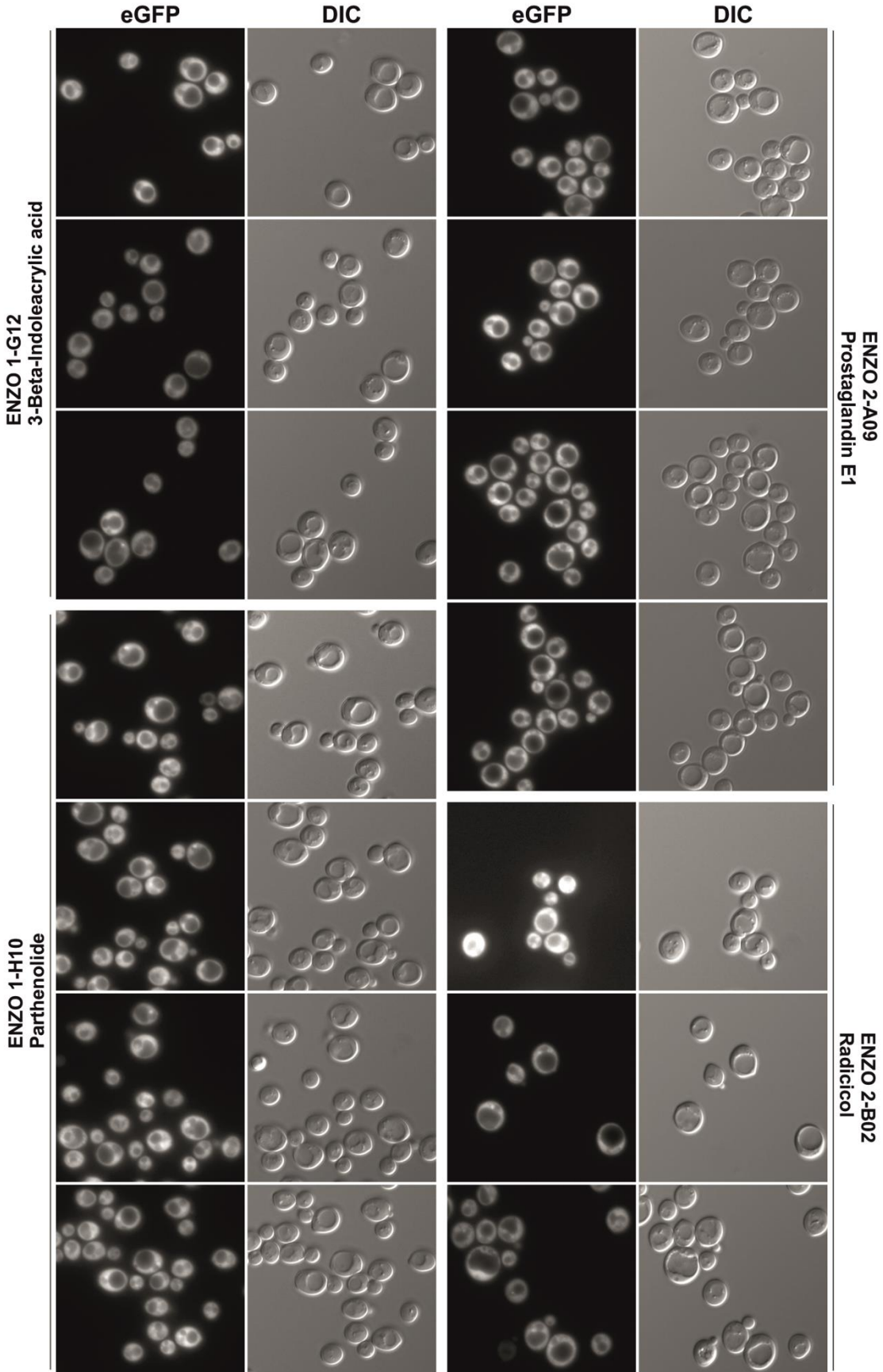
Collection	Plate	Well	Substance	Final concentration (μM)	Time of incubation (h)
ENZO	1	1-A1	Acivicin	28	4
ENZO	1	1-A4	Antibiotic A-23187 (Calcimycin)	38	4.25
ENZO	1	1-C05	Curcumin	27	5.25
ENZO	1	1-F05	Ginkgolide B	47	5.5
ENZO	1	1-G05	Kainic acid	94	6
ENZO	1	1-G06	(±)-Kavain	87	6
ENZO	1	1-G12	3-Beta-Indoleacrylic acid	107	6.75
ENZO	1	1-H10	Parthenolide	40	6.5
ENZO	2	2-A09	Prostaglandin E1	56	5
ENZO	2	2-B02	Radicalol	28	5
ENZO	2	2-B06	All trans retinoic acid	67	5
ENZO	2	2-B10	Rosmarinic acid	83	6
ENZO	2	2-B11	Rotenone	51	6
ENZO	2	2-C08	Thapsigargin	62	6
ENZO	2	2-C10	Troleandomycin	49	6
ENZO	2	2-C11	Tunicamycin B	24	6.5
ENZO	2	2-E05	Catalpol	55	6.5
ENZO	2	2-E08	Veratramine	49	6.5
ENZO	2	2-F02	Ivermectin	46	7.25
ENZO	2	2-F05	Morin	66	6.25
ENZO	2	2-F08	(-)-Nicotine	123	6.5
ENZO	2	2-F09	Nonactin	54	6.5
ENZO	2	2-F10	L-Penicillamine	134	6.5
ENZO	2	2-F11	Picrotoxinin	103	7.5
ENZO	2	2-G02	Quercetin dehydrate	59	6.5
ENZO	2	2-G08	Tryptanthrin	40	6.5-7
ENZO	2	2-G09	Yohimbine-HCl	51	7
ENZO	2	2-G10	(-)-Eburnamonine	102	7.25
ENZO	2	2-H09	Kaempferol	70	6.75
ENZO	2	2-H11	Celastrol	67	7
ENZO	3	3-A06	Condolphine	66	6
ENZO	3	3-E05	Isorhoifolin	52	6.75
ENZO	3	3-F03	Picropodophyllin	72	6.5
ENZO	3	3-F05	Narigenin-7-O-glucoside	70	7
ENZO	3	3-G05	Sinensetine	54	6.75
ENZO	4	4-A01	Syringetine-3-glucoside	39	7
ENZO	4	4-B06	Aloe-emodin	74	5
ENZO	4	4-C04	Trans-4-Cotininecarboxylic acid	91	5.25
ENZO	4	4-C11	Gitoxygenin	51	5.5
ENZO	4	4-C12	Harmaline	110	5.75
ENZO	4	4-D04	Leucomisine	81	6
ENZO	4	4-E08	Streptonigrin	40	4.75
ENZO	4	4-E09	Tetrahydropapaverine-HCl	52	6
ENZO	4	4-E12	Visnagin	87	6.25
ENZO	4	4-F04	Caffeine	103	6.5
ENZO	4	4-F12	Lasalocid A	33	6.5
ENZO	4	4-G05	(+)-Usnic acid	29	5
ENZO	4	4-G10	Cephadrine	58	6.5
ENZO	4	4-G11	Vasicine	53	6.75
ENZO	4	4-H05	Tetrahydrolipistatin	40	6.75
ENZO	4	4-H08	Oleanolic acid	44	7
ENZO	4	4-H10	Phlorizine	92	7.25
ENZO	5	5-B06	Berberine-HCl	54	5.75
ENZO	5	5-C12	Diosmin	66	5.5
ENZO	5	5-E08	Minocycline-HCl	81	5.5
ENZO	5	5-E11	16-Oxocafestol	106	5.5
ENZO	5	5-G11	Yangonin	77	5.5
ENZO	6	6-A04	Senecionine	60	6
ENZO	6	6-A11	Arbutin	73	5
ENZO	6	6-B01	Bleomycin sulfate	40	6
NIH	NGP-105-01	1-A06	Rosiglitazone maleate	50	5
NIH	NGP-105-01	1-C05	Finasteride	50	6
NIH	NGP-105-01	1-D03	Olanzapine	50	6
NIH	NGP-105-01	1-E05	Nevirapine	50	5
NIH	NGP-105-01	1-E07	Icariin	50	5.75
NIH	NGP-105-01	1-E08	Ipriflavone	50	4.75
NIH	NGP-105-01	1-F06	Sertraline hydrochloride	50	5.5
NIH	NGP-105-01	1-F10	Pantoprazole Sodium	50	5

NIH	NGP-105-01	1-G10	Fluticasone Propionate	50	5.75
NIH	NGP-105-02	2-A07	Methyltestosterone	50	4.75
NIH	NGP-105-02	2-A09	Flubendazole	50	6
NIH	NGP-105-02	2-C10	Nifekalant hydrochloride	50	5.85
NIH	NGP-105-02	2-D08	Rofecoxib	50	4.75
NIH	NGP-105-02	2-D11	Famciclovir	50	5.5
NIH	NGP-105-02	2-E10	Megestrol acetate	50	5.15
NIH	NGP-105-02	2-F09	Trimebutine Maleate	50	5
NIH	NGP-105-02	2-G09	Mestanolone	50	5.5
NIH	NGP-105-02	2-G10	Zileuton	50	5.3
NIH	NGP-105-02	2-H08	Idarubicin hydrochloride	50	5.75
NIH	NGP-105-03	3-B03	Fluphenazine dihydrochloride	50	5.15
NIH	NGP-105-03	3-B06	Cefaclor	50	4.75
NIH	NGP-105-03	3-B08	Desoximetasone	50	5.5
NIH	NGP-105-03	3-G11	Nicotinamide	50	5h10
NIH	NGP-105-03	3-H07	Rimcazole	50	5h25
NIH	NGP-105-03	3-H10	Itavastatin Ca	50	5
NIH	NGP-105-03	3-H11	Nialamide	50	5h40
NIH	NGP-105-04	4-E10	Donepezil hydrochloride	50	5h10
NIH	NGP-105-04	4-F03	GR-89696 fumarate	50	5h20
NIH	NGP-105-04	4-F06	Irbesartan	50	5h30
NIH	NGP-105-04	4-F08	Valsartan	50	5h20
NIH	NGP-105-04	4-G07	Levocetirizine	50	5h
NIH	NGP-105-05	5-A05	Pancuronium Bromide	50	6h
NIH	NGP-105-05	5-A08	Cinanserin	50	4h30
NIH	NGP-105-05	5-A10	Hexamethylenebisacetamide (Hmba)	50	4h15
NIH	NGP-105-05	5-B08	Cisapride monohydrate	50	6h10
NIH	NGP-105-05	5-B09	Cidoxepin HCl	50	4h20
NIH	NGP-105-05	5-B11	Tacrine hydrochloride	50	6h
NIH	NGP-105-05	5-C08	Indatraline hydrochloride	50	6h
NIH	NGP-105-05	5-D11	Cytarabine	50	6h10
NIH	NGP-105-05	5-E07	Naltrindole	50	6h10
NIH	NGP-105-05	5-E11	Methotrexate hydrate	50	4h50
NIH	NGP-105-05	5-F08	Urapidil hydrochloride	50	5h
NIH	NGP-105-05	5-F09	Maprotiline hydrochloride	50	4h30
NIH	NGP-105-05	5-F10	SMR000449302	50	5h40
NIH	NGP-105-05	5-G08	Cotinine	50	4h20
NIH	NGP-105-05	5-G09	Pizotifen maleate	50	5h
NIH	NGP-105-05	5-G11	Pramipexole	50	6h30
NIH	NGP-105-05	5-H09	Estradiol	50	4h50
NIH	NGP-105-06	6-A03	Dup 697	50	6h
NIH	NGP-105-06	6-A04	Vindesine sulfate	50	6h
NIH	NGP-105-06	6-A06	Clobenpropit	50	6h20
NIH	NGP-105-06	6-D07	Pergolide Mesylate	50	4h35

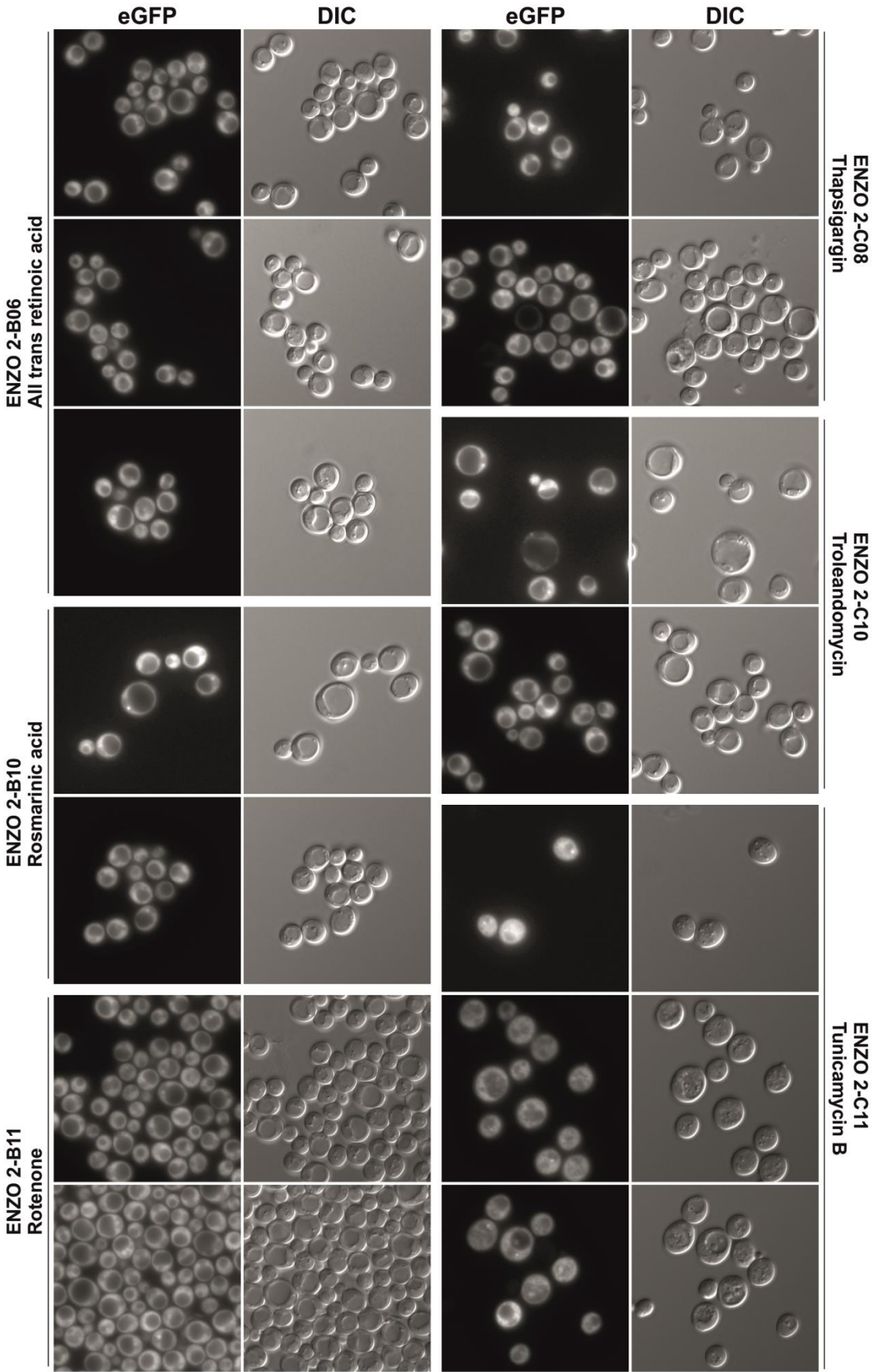
40S Screen Hits (RPS9A-GFP K3)



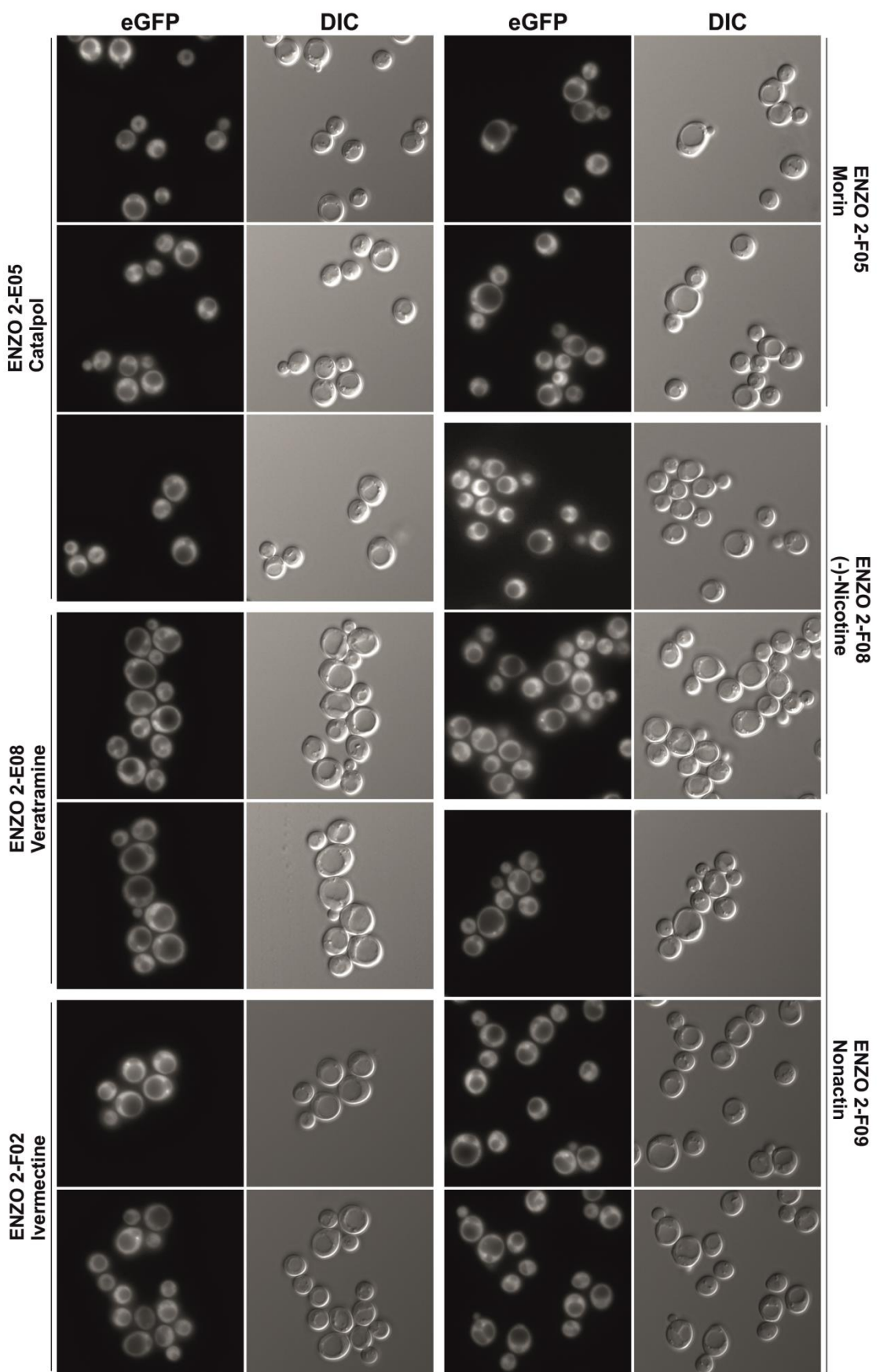
40S Screen Hits (RPS9A-GFP K3)



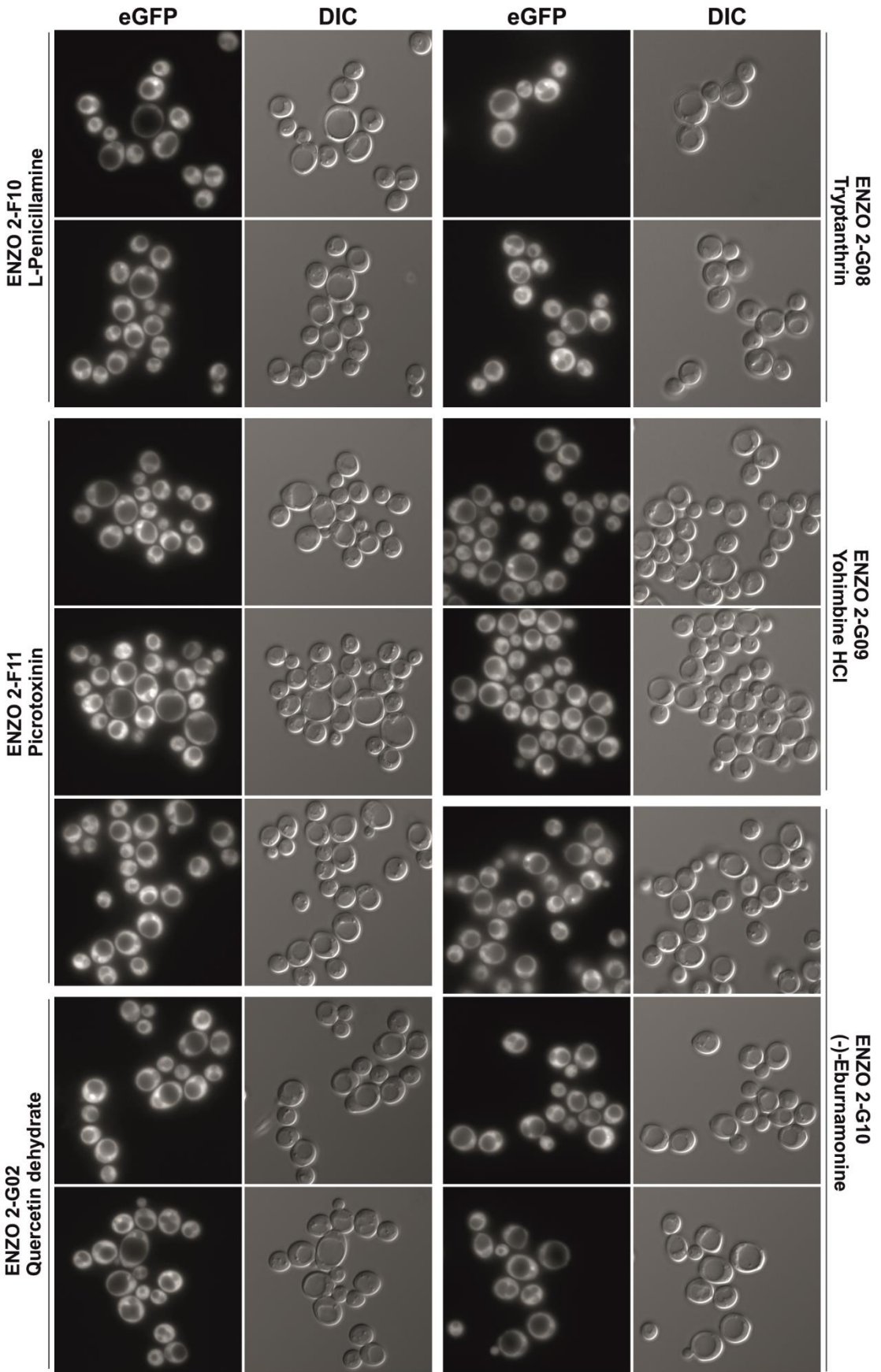
40S Screen Hits (RPS9A-GFP K3)



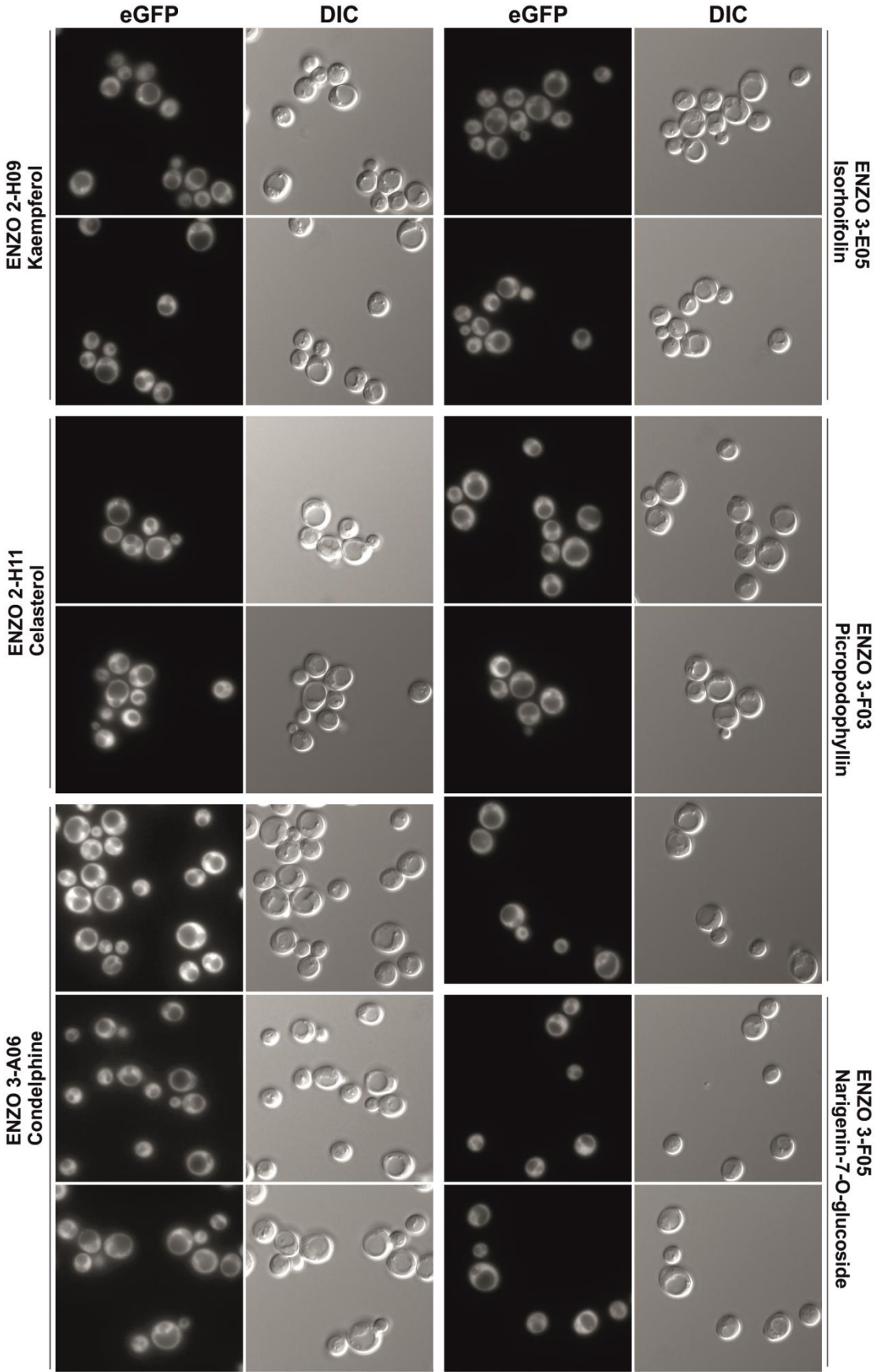
40S Screen Hits (RPS9A-GFP K3)



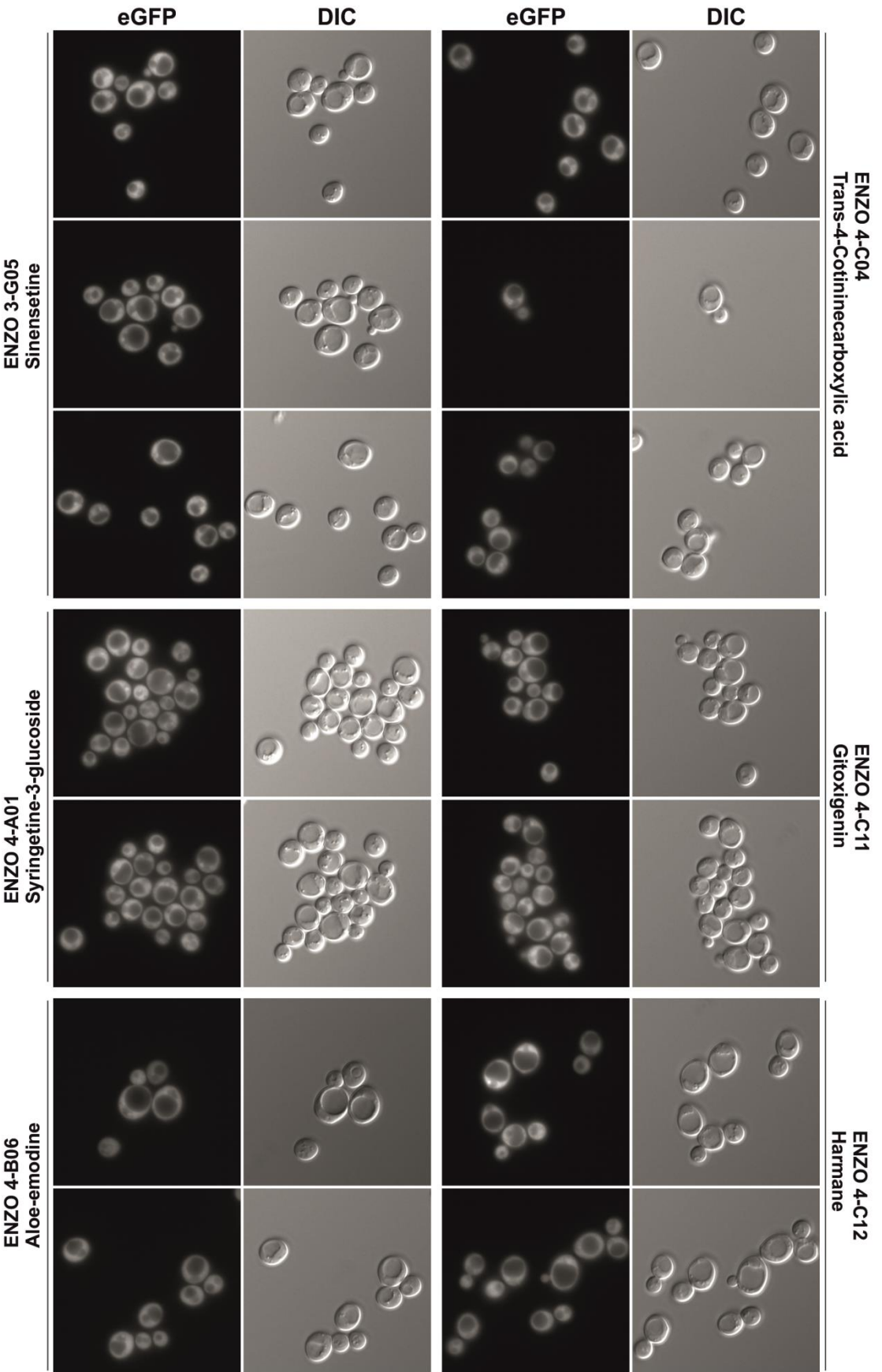
40S Screen Hits (RPS9A-GFP K3)



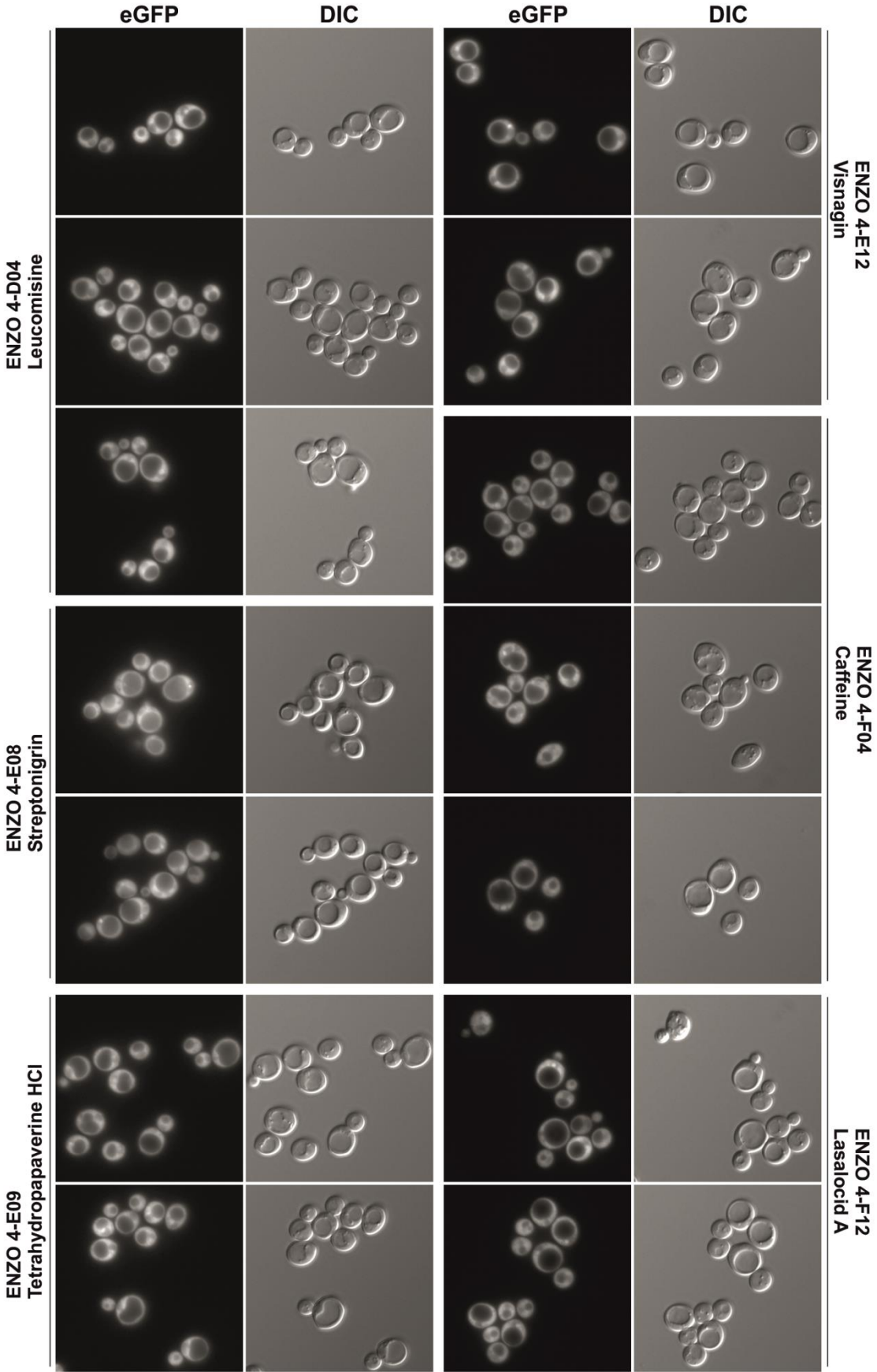
40S Screen Hits (RPS9A-GFP K3)



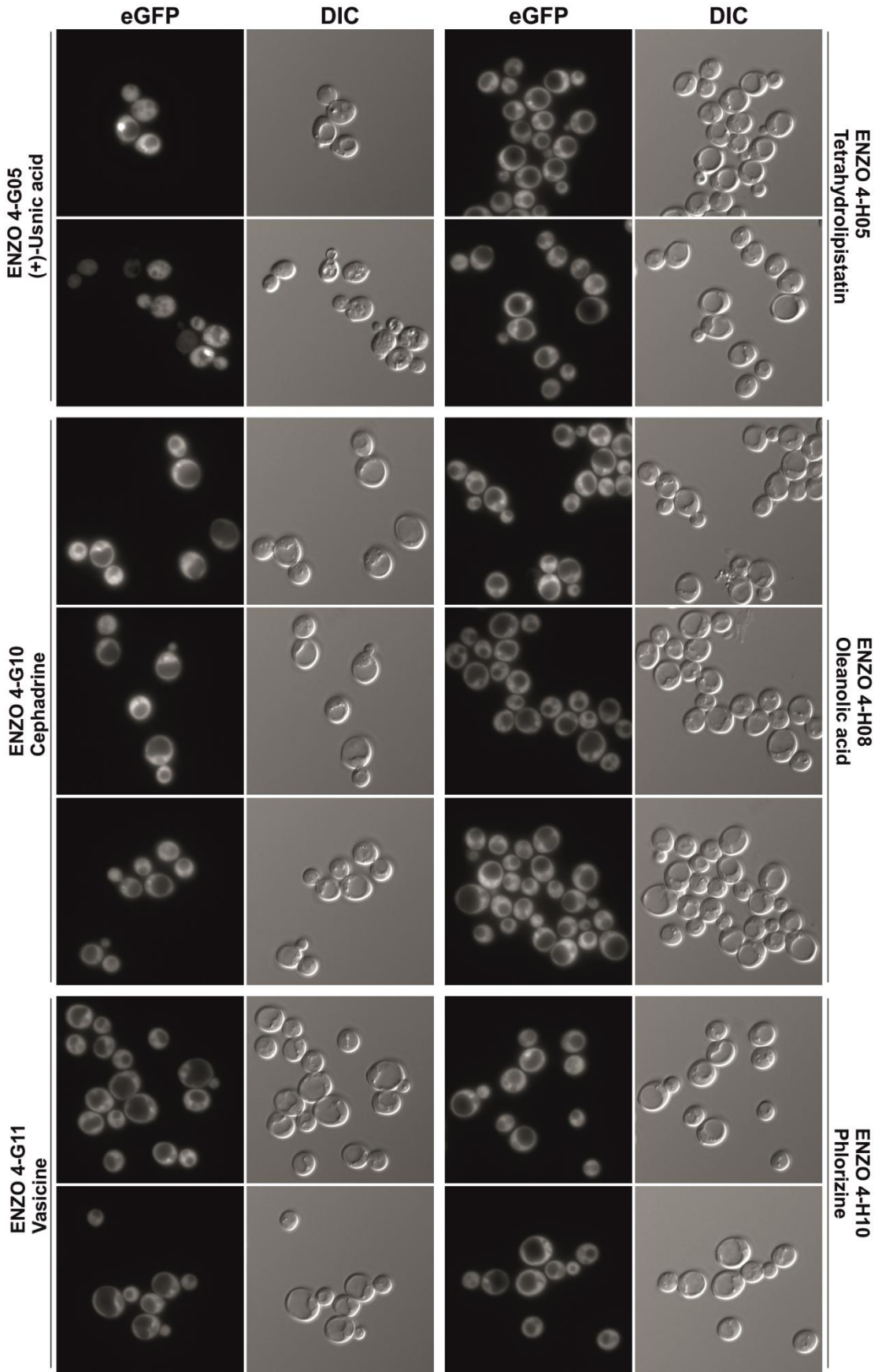
40S Screen Hits (RPS9A-GFP K3)



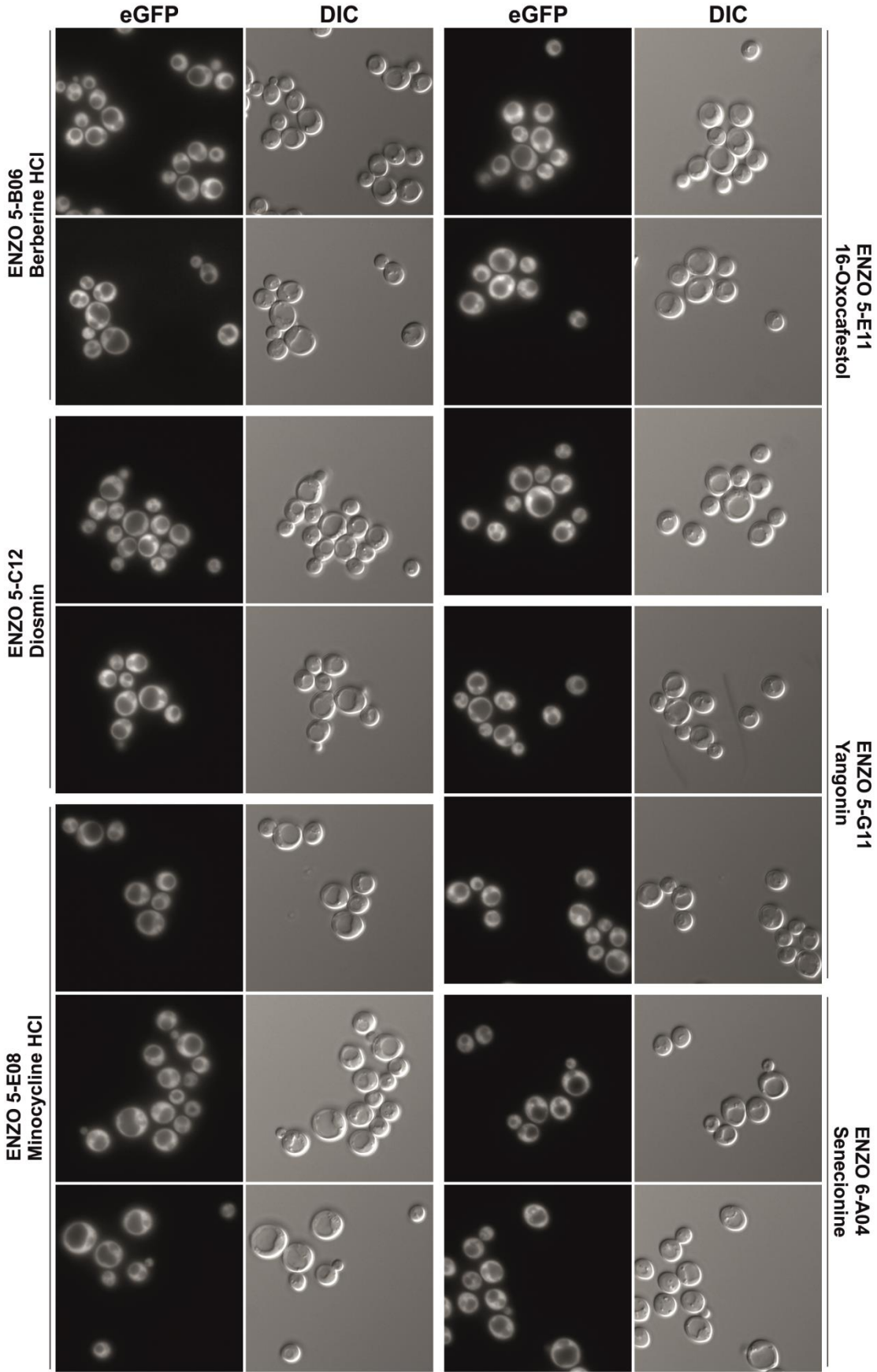
40S Screen Hits (RPS9A-GFP K3)



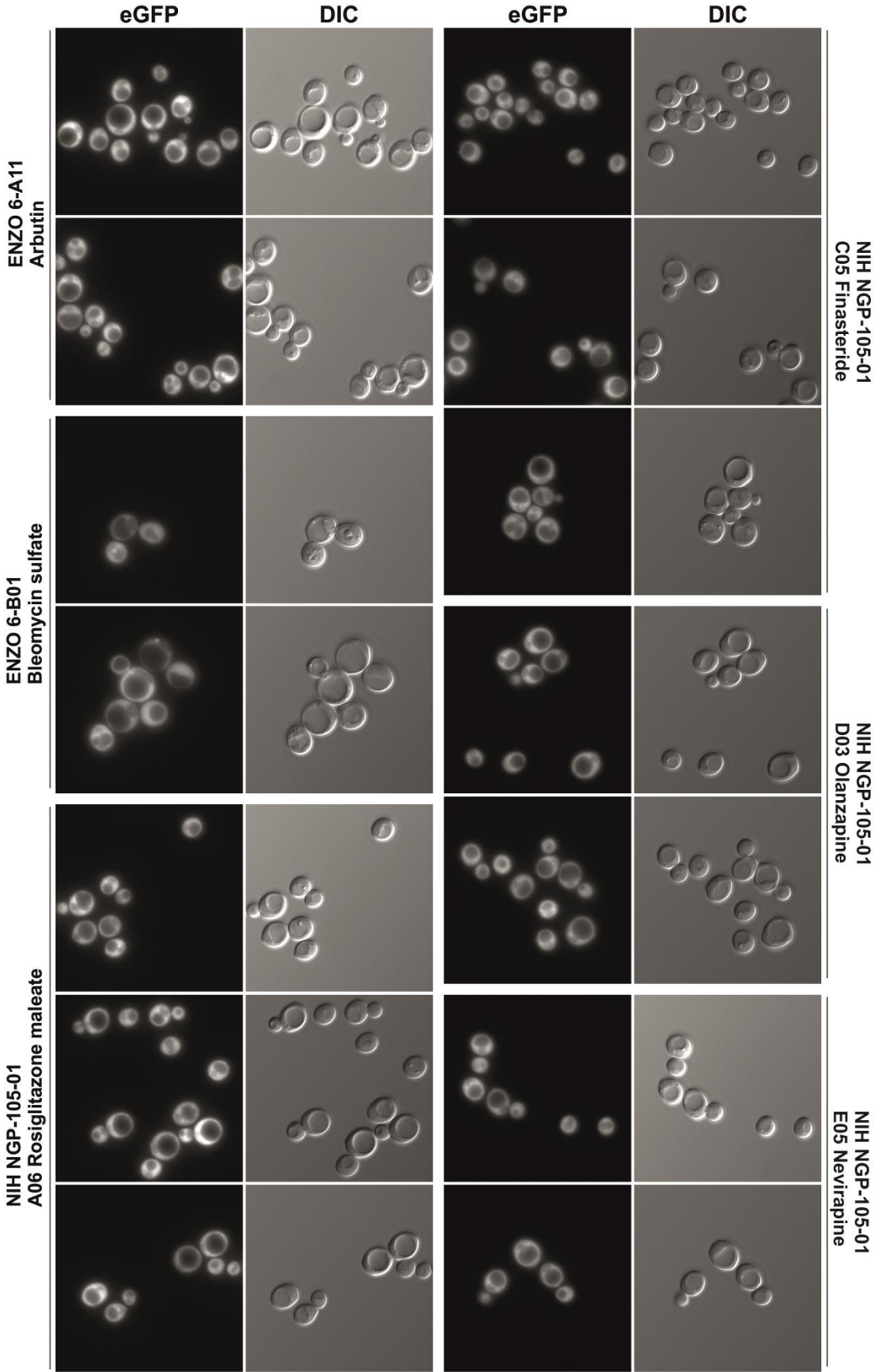
40S Screen Hits (RPS9A-GFP K3)



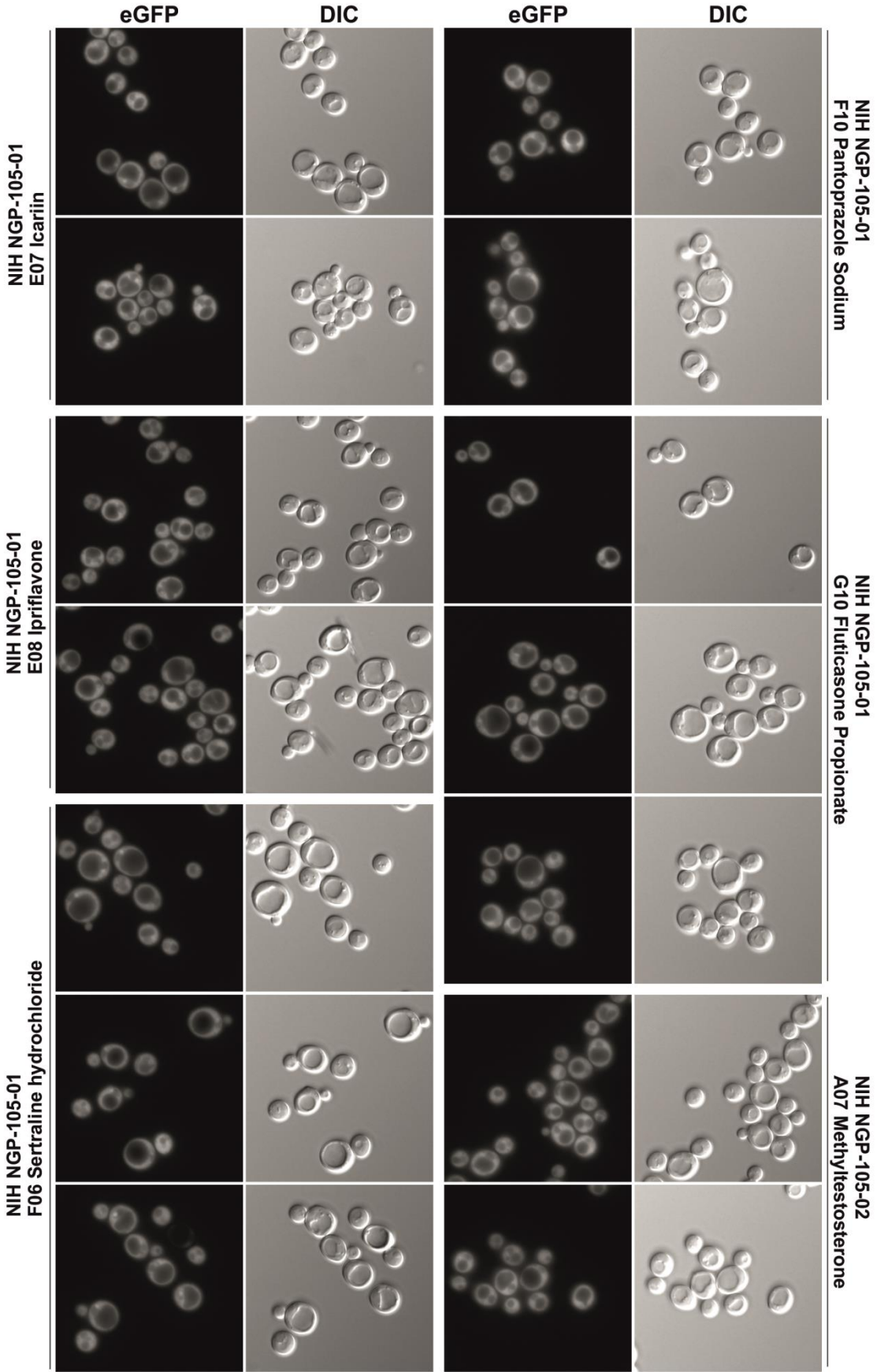
40S Screen Hits (RPS9A-GFP K3)



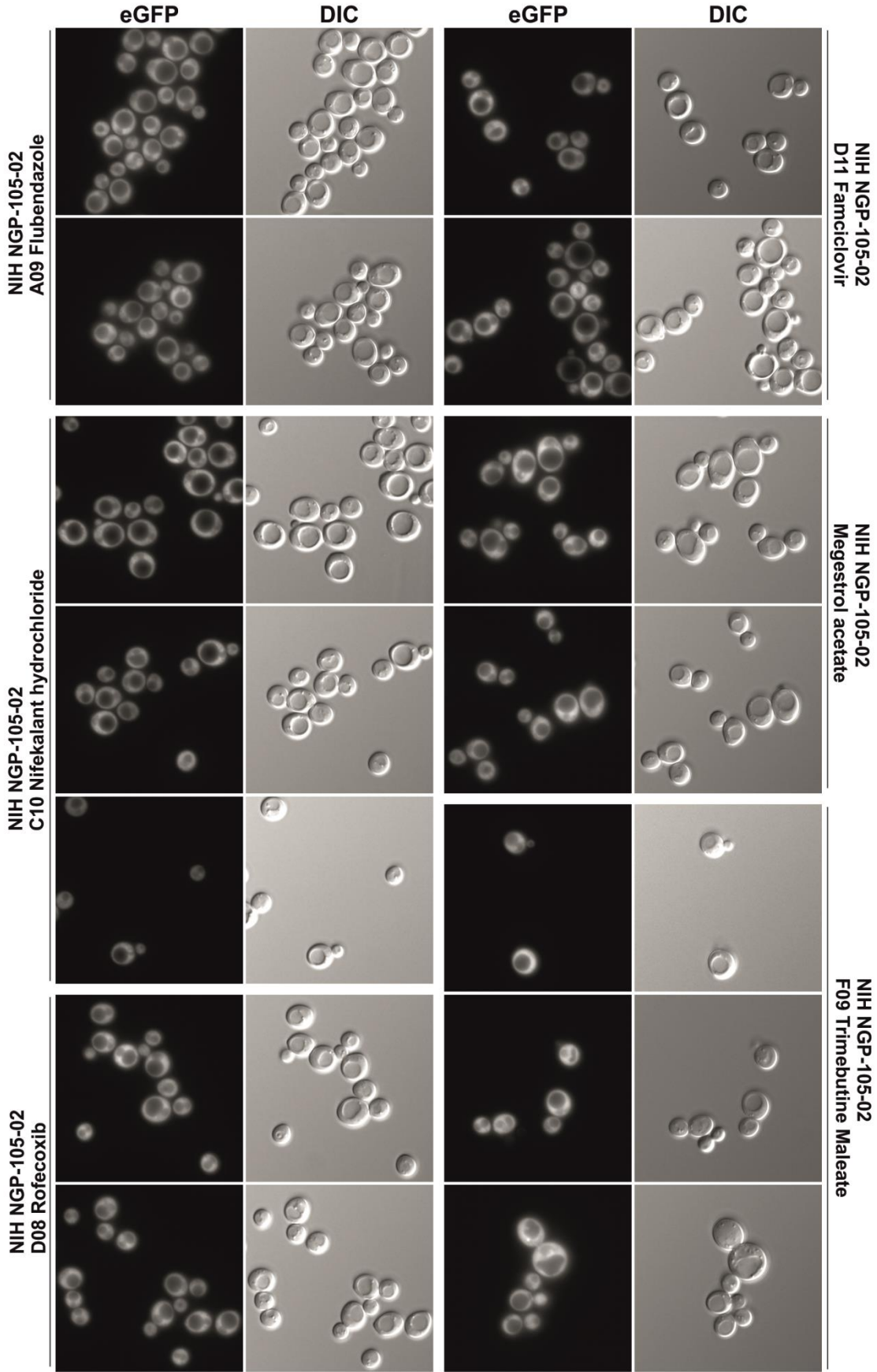
40S Screen Hits (RPS9A-GFP K3)



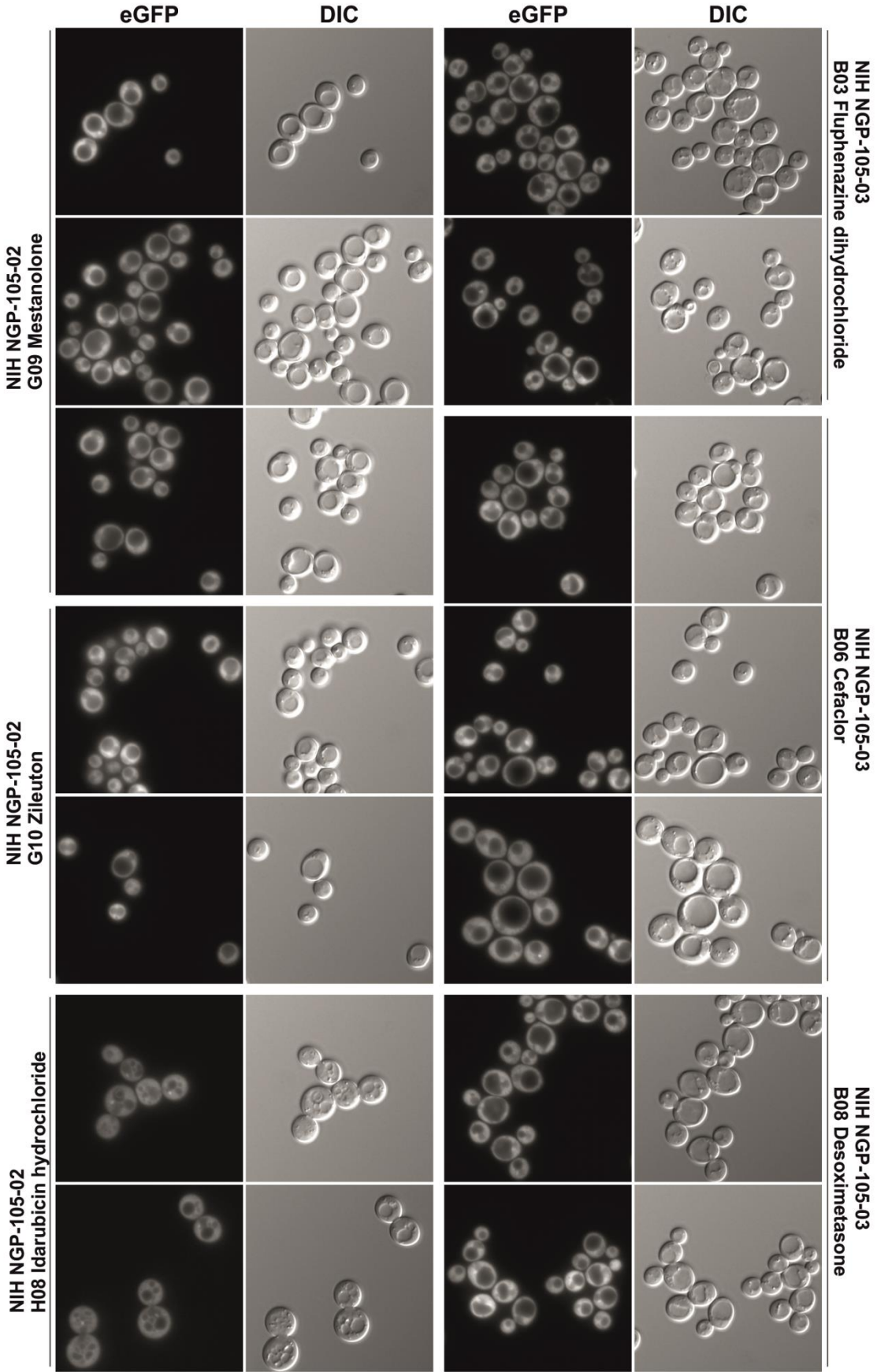
40S Screen Hits (RPS9A-GFP K3)



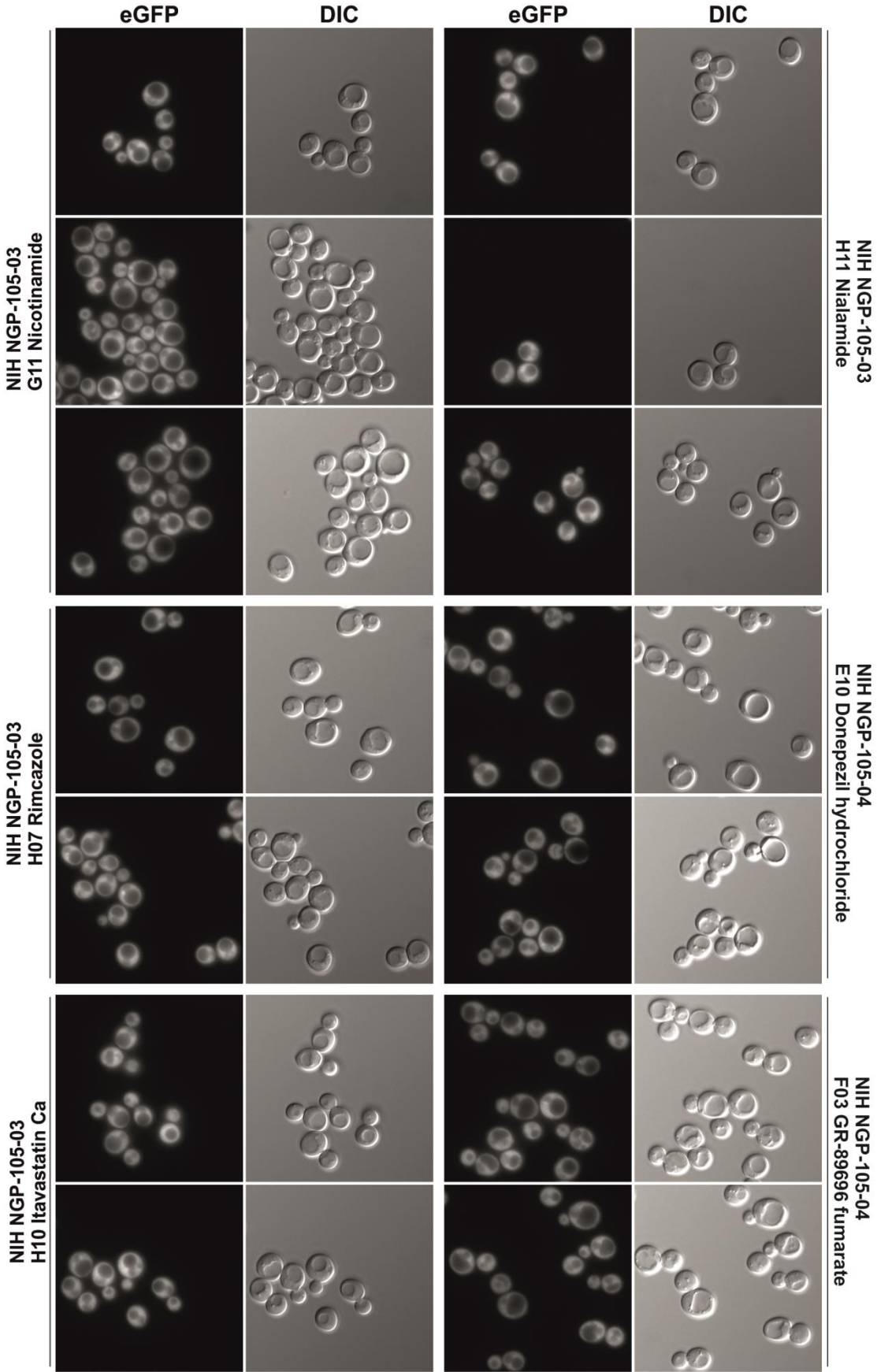
40S Screen Hits (RPS9A-GFP K3)



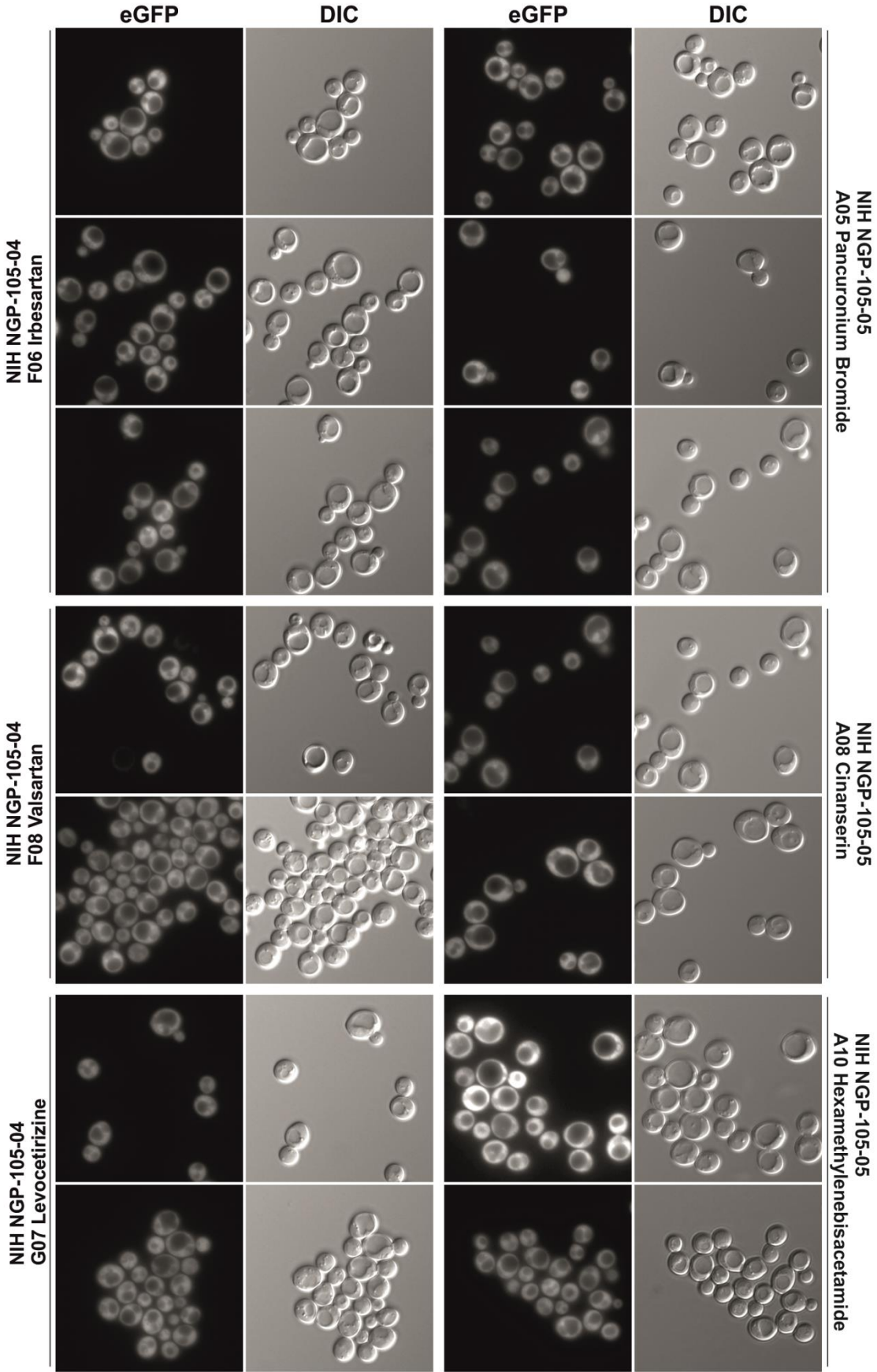
40S Screen Hits (RPS9A-GFP K3)



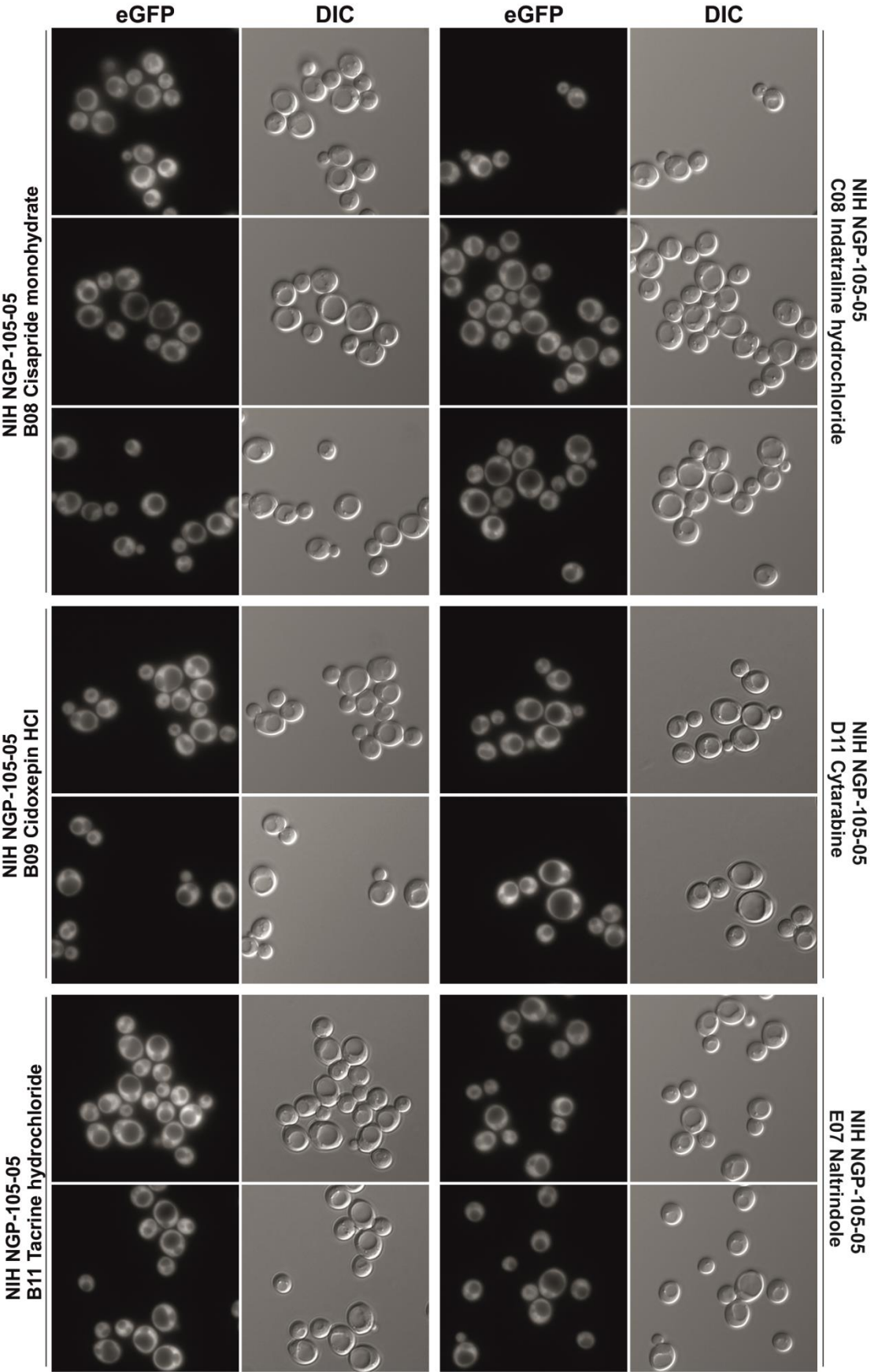
40S Screen Hits (RPS9A-GFP K3)



40S Screen Hits (RPS9A-GFP K3)



40S Screen Hits (RPS9A-GFP K3)

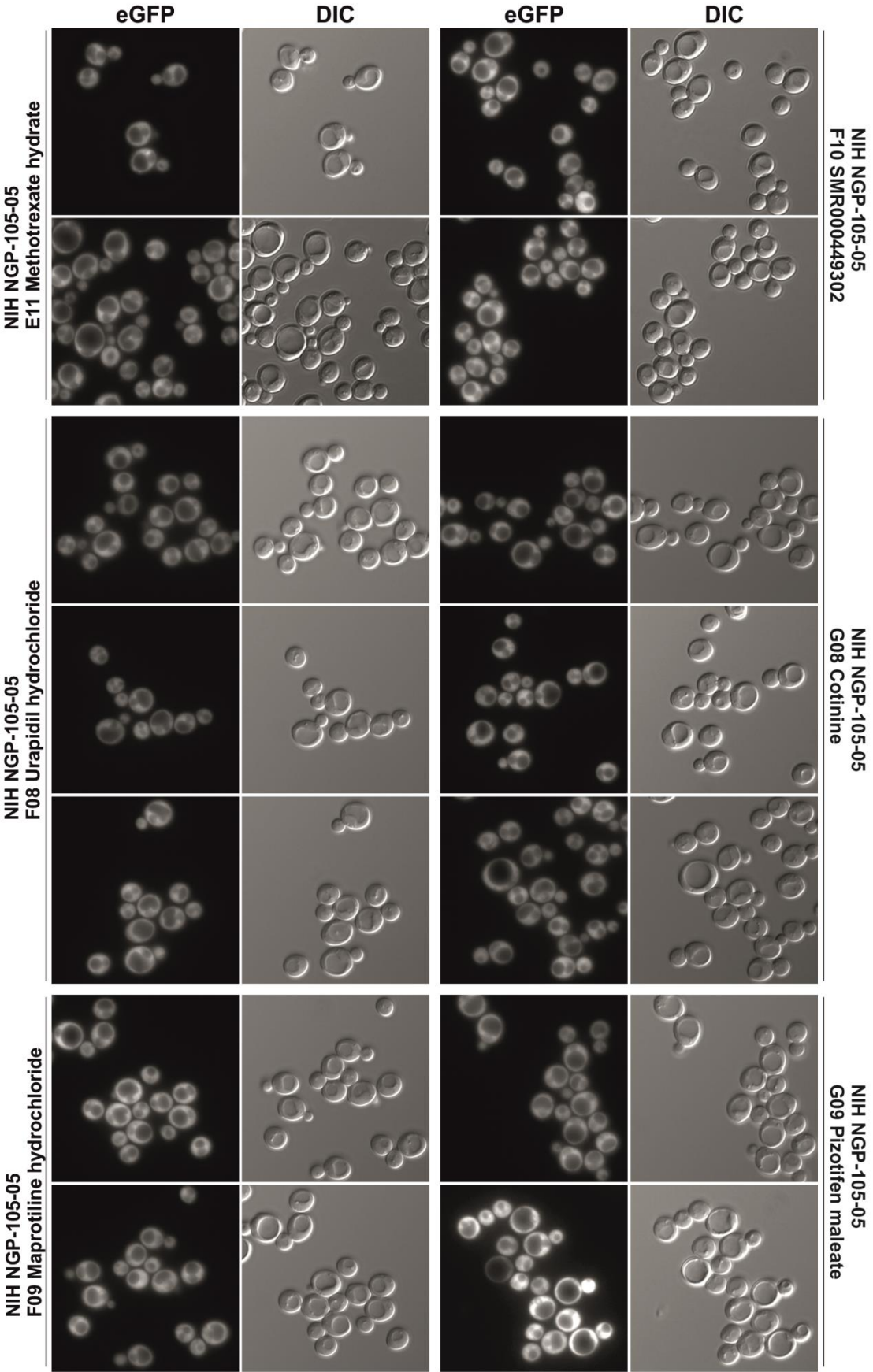


NIH NGP-105-05
C08 Indatraline hydrochloride

NIH NGP-105-05
D11 Cytarabine

NIH NGP-105-05
E07 Naltrindole

40S Screen Hits (RPS9A-GFP K3)



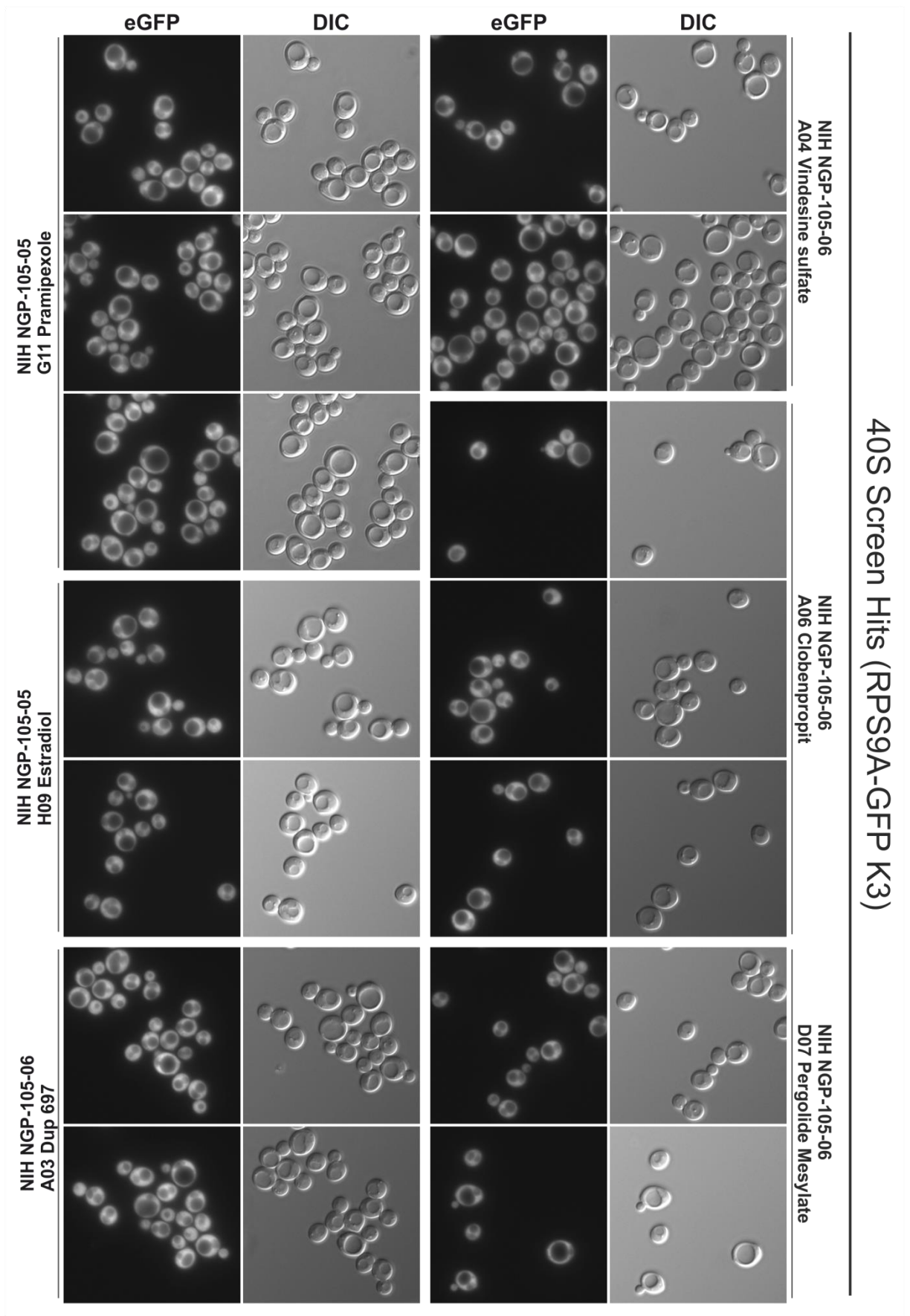


Figure 3.18: Fluorescence microscopy pictures of the hits obtained from the screen using Rps9a-GFP.

Table 3.7: A list of all substances that demonstrated an accumulation in the nucleolus and/or nucleoplasm when screening with the *Rps9a-GFP* and the *Rpl7a-GFP* reporter construct. The time of incubation and final concentration only represents the value that gave the most accumulations of the reporter protein in the nucleus when evaluating the pictures from the screen.

Collection	Plate	Well	Substance
ENZO	1	1-A1	Acivicin
ENZO	1	1-A4	Antibiotic A-23187 (Calcimycin)
ENZO	1	1-C05	Curcumin
ENZO	2	2-C05	Tanshinone IIA
ENZO	2	2-F05	Morin
ENZO	2	2-F09	Nonactin
ENZO	2	2-G02	Quercetin dehydrate
ENZO	2	2-H09	Kaempferol
ENZO	3	3-G05	Sinensetine
ENZO	4	4-A01	Syringetine-3-glucoside
ENZO	4	4-E08	Streptonigrin
ENZO	4	4-G05	(+)-Usnic acid
ENZO	5	5-B06	Berberine-HCl
ENZO	6	6-A04	Senecionine
ENZO	6	6-B01	Bleomycin sulfate
NIH	NGP-105-02	2-H08	Idarubicin hydrochloride

3.2.3. The manual screen identified 130 potential inhibitors

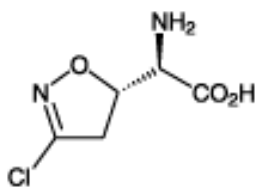
The manual screen using *Rpl7a-GFP* as a reporter identified 34 potential inhibitors targeting the maturation pathway of the large ribosomal subunit (table 3.5). In contrast, the results of the screen for inhibitors interfering with the small subunit revealed 112 potential inhibitors (table 3.6). There was an overlap of 16 substances, mainly from the ENZO natural compound library (table 3.7). These results were obtained from extensive fluorescence microscopy and evaluation of roughly 24,000 microscopy pictures. When deciding on 50 μ M as the final concentration of potential inhibitor, used in the first screening, our intention was to stay close to a concentration that is known from previous work with diazaborine. However, I am aware of the fact that we missed potential inhibitors by deciding on one final concentration for the initial screen, rather than performing an initial screen with multiple concentrations. The decision on the inhibitor concentration involved two fundamental problems. When the concentration is set too low, many inhibitors might not be identified by the screen. If the concentration is set too high, accumulation due to secondary effects will be enhanced. The screen identified 130 potential inhibitors combined. Since the ribosome biogenesis involves 200 non-ribosomal factors in the maturation steps (Henras et al, 2008), the expected amount of potential inhibitors was significantly higher than a screen for one specific target protein, which would have expected to result in 2 to 4 hits as previous high throughput screens with specific proteins resulted in about 1 hit per 250 to 400 compounds. But which inhibitor is specific? The first step was to compare already published data about the obtained hits, in order to exclude substances that do not directly act on the ribosome biogenesis. However, this evaluation should be done with caution, because many

studies have been conducted in vitro or by purely biochemical means and not in living cells.

3.2.4. Selected potential inhibitors at a glance

3.2.4.1. Acivicin

Acivicin, identified as a potential inhibitor in the screen using the large subunit reporter, has been identified as an inhibitor of the gamma-glutamyl transpeptidase (GGT) biochemically (Allen et al, 1980). The enzyme GGT cleaves the gamma-glutamyl bond of glutathione and therefore releases glutamate, cysteine and glycine. By overexpressing GGT in tumor cells, the rate limiting cysteine can be acquired from cleaving oxidized or reduced glutathione and leading to a quick response upon treatment with pro-oxidizing agents (reviewed by Hanigan, 2014). The inhibitor acivicin could target the protein Ecm38, the gamma-glutamyl transpeptidase in yeast. The shortage of cysteine and oxidative stress could lead to a secondary effect that results in an accumulation of Rpl7a



and Rps9a in the nucleus. In 2014, the cytotoxic effect of acivicin was linked to the target ALDH4A1 (delta-1-pyrroline-5-carboxylate dehydrogenase) in cancer cells, which is involved in the glutamate synthesis (Kreuzer et al, 2014).

Figure 3.19: Chemical structure of Acivicin Image taken from <http://www.enzolifesciences.com/BML-E1113/acivicin/> (April 2015)

3.2.4.2. Rubicin derivatives

Doxrubicin, epirubicin, idarubicin and daunorubicin, a group of anthracycline (figure 3.20), are prominent antitumor agents, with a variety of effects on growing cells. The effect in eukaryotic cells include inhibition of topoisomerase II, DNA alkylation, DNA crosslinking, generating free radicals, lipid oxidation resulting in membrane damage, preventing of DNA unwinding and helicase activity (reviewed by Gewirtz, 1999). In addition rubicin derivatives can also form DNA adducts when formaldehyde is present (reviewed by Cutts et al, 2005). Thus, the rubicin derivatives might induce apoptosis (Kotamraju et al, 2000). More recently, the inhibition of the RNA PolII via rubicin was reported (Burger et al, 2010). However, our research revealed a 27SA2 accumulation in yeast upon treatment with different rubicin derivatives, suggesting a target downstream of the transcription (not published data, Loibl M.).

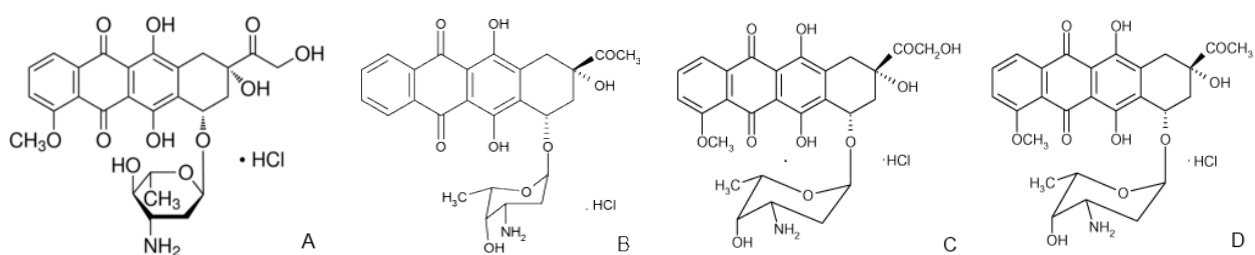


Figure 3.20: Chemical structure of the rubicin derivatives

A) Epirubicin <http://www.sigmaaldrich.com/catalog/product/sigma/e9406> (May, 2015)

B) Idarubicin <http://www.enzolifesciences.com/ALX-380-260/idarubicin-.hydrochloride/> (May, 2015)

C) Doxorubicin <http://www.enzolifesciences.com/BML-GR319/doxorubicin-.hcl/> (May, 2015)

D) Daunorubicin <http://www.enzolifesciences.com/ALX-380-043/daunorubicin-.hydrochloride/> (May, 2015)

3.2.4.3. Flavonoids

Another group sharing a similar chemical structure are the flavonoids kaempferol, sinensetin, quercetin and morin (figure 3.21). The antioxidant effects of the flavonoids have been already reviewed in the mid-1990s (Rice-Evans et al., 1996). Studies on isolated rat liver nuclei suggest that morin and naringenin treatment leads to DNA damage and lipid peroxidation (Sahu and Gray, 1997). More recent studies link morin to cell cycle arrest in human leukemia cells and induction of apoptosis (Kuo et al, 2007; Manna et al, 2007). Furthermore, studies indicate that quercetin can inhibit the mitochondrial ATPase (Lang and Racker, 1974). Effects on the protein kinase C have been reported in vivo and in vitro (Grunicke et al, 1989). When tumor cells were treated with quercetin, nuclear fragmentation, nuclear chromatin condensation occurred and apoptosis in the G1 and S Phase was induced (Wei et al, 1994). Another interesting link has been found between flavonoids and the fatty acid synthase FASN in human, possibly explaining their toxicity and its induction of apoptosis (reviewed by Lupu and Menendez, 2006).

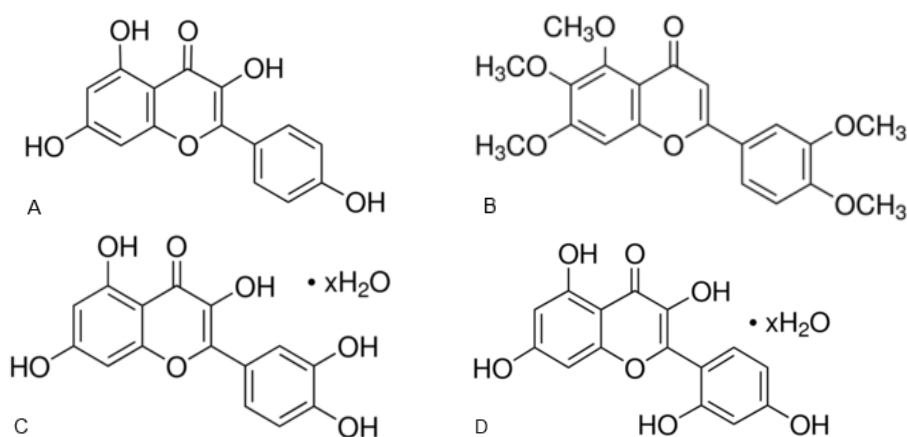


Figure 3.21: Chemical structure of the flavonoids found due to an accumulation of the reporter protein in the nucleus

A) Kaempferol, <http://www.sigmaaldrich.com/catalog/product/sigma/k0133> (May 2015)

B) Sinensetin, <http://www.sigmaaldrich.com/catalog/product/fluka/89392> (May 2015)

C) Quercetin dihydrate, <http://www.sigmaaldrich.com/catalog/product/fluka/phr1488> (May 2015)

D) Morin hydrate, <http://www.sigmaaldrich.com/catalog/product/sigma/m4008> (May 2015)

3.2.4.4. Carmofur and Urapidil hydrochloride

Carmofur (1-Hexylcarbamoyl-5-fluorouracil), a substance included in the NIH library (2-D06), resulted in a strong accumulation of the reporter protein in the nucleolus. Recent publications demonstrated the effect of 5-fluorouracil and its effect on ribosome biogenesis (Burger et al, 2010). Urapidil hydrochloride (NIH 5-F8) was identified by using Rps9a-GFP as a reporter.

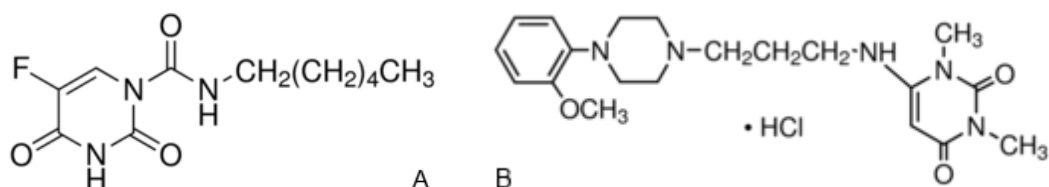


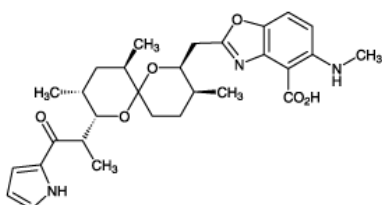
Figure 3.22: Chemical structure of the antibiotic A-23187

A) Carmofur, <http://www.sigmaaldrich.com/catalog/product/sigma/c1494> (May 2015)

B) Urapidil hydrochloride, <http://www.sigmaaldrich.com/catalog/product/sigma/u100> (May 2015)

3.2.4.5. Antibiotic A-23187 (Calcimycin)

Antibiotic A-23187, also known as calcimycin, is a divalent cation ionophor leading to an increase in Ca^{2+} in the cell (Reed and Lardy, 1972).



Thus, the increase of intracellular calcium is within the first five minutes and is accompanied by increased levels of ROS, most likely due to the Ca^{2+} effect on the mitochondria (Przygodzki et al., 2005).

Figure 3.23: Chemical structure of the antibiotic A-23187 Image taken from

<http://www.enzolifesciences.com/BML-CA100/antibiotic-a-23187-calcimycin/> (April 2015)

3.2.4.6. Bromocriptine mesylate

Bromocriptine mesylate is a known ligand of D2 and D3 dopamin receptor (Hubner and Koob, 1990). Taking a closer look at the protein domains of the dopamine receptors using Ensembl, a homology to G-protein coupled receptors can be found. *S. cerevisiae* has a G-protein coupled receptor (GPR1/YDL035C), acting on nutritional signals via PKA and cAMP (Yun et al, 1997; Pan and Heitman 1999; Kraakman et al, 1999; Ansari et al, 1999).

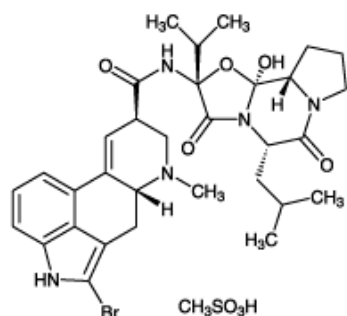
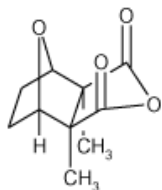


Figure 3.24: Chemical structure of bromocriptine mesylate

Image taken from <http://www.enzolifesciences.com/BML-D102/bromocriptine--mesylate/> (April 2015)

3.2.4.7. Cantharidin

In previous years, cantharidin was identified as a specific inhibitor of the serin/threonine protein phosphatase2A, PP2A (WU et al, 2014; Li and Casida, 1992). Thus, the PP2A

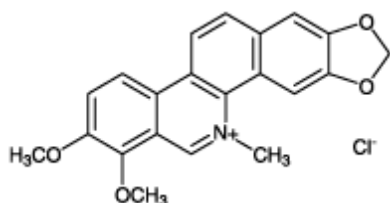


was shown to be a regulator of β -catenin (Bos et al, 2006), which is the homolog of the yeast protein Srp1 (Yano et al, 1994). Srp1, also known as Kap60 is a α -Importin, essential import of many different proteins, including Rps3 (B. Pertschy, unpublished data).

Figure 3.25: Chemical structure of cantharidin <http://www.enzolifesciences.com/ALX-270-063/cantharidin/>

3.2.4.8. Chelerythrine chloride

Chelerythrine chloride, first identified as potential PKC inhibitor (Herbert et al, 1990), seem to have also different biological activities in the cell. Just recently, chelerythrine was used to inhibit the endoplasmic reticulum Ca^{2+} -ATPase, leading to a loss of calcium



homeostasis (Vieira et al, 2015). There are many ATPases involved in the ribosome biogenesis pathway, which could serve as a potential target for chelerythrine (Woolford and Baserga, 2013).

Figure 3.26: Chemical structure of chelerythrine chloride <http://www.enzolifesciences.com/BML-EI225/chelerythrine-chloride/> (April, 2015)

3.2.4.9. Curcumin

Curcumin, a substance used already in ancient indian medicine, has been reported to have several effect on cells of various kinds, including antioxidant and anti-tumor activity (Korutla and Kumar, 1994; Brouet and Okshima, 1995; Commandeur and Vermeulen, 1996; Singh et al, 1996; Kuo et al, 1996). Recently, it also has been associated with *Saccharomyces cerevisiae*'s quinone oxidoreductase Lot6 (Megarity et al, 2014). Other reported effects include the activation of Hog1 in budding yeast (Azad et al, 2014). The screen with the large and small subunit revealed a strong cytotoxic effect of curcumin on yeast cells when exceeding a concentration over 50 μ M for more than one hour.

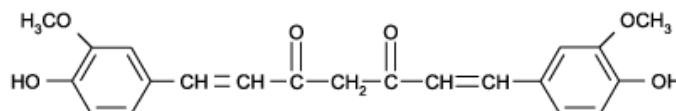
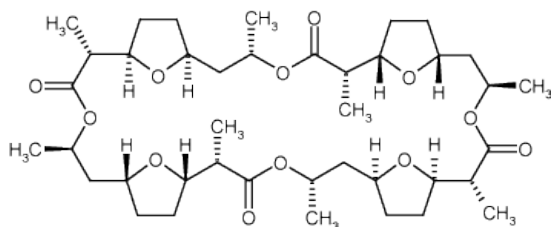


Figure 3.27: Chemical structure of curcumin <http://www.enzolifesciences.com/ALX-350-028/curcumin-high-purity/>

3.2.4.10. Nonactin

Nonactin and its antibacterial effects has been published already decades ago (Köhler et al., 1964). More recent studies revealed that the substance also functions as a p38 MAP kinase inhibitor (Mori et al, 2001). The ribosomal S6 kinase, RSK-B, was published to be under dominant control of p38 MAP kinase (Pierrat et al, 1998). Additionally,



nonactin is an ionophore, high selectivity for potassium (Garcia et al, 2003).

Figure 3.28: Chemical structure of nonactin <http://www.enzolifesciences.com/ALX-450-008/nonactin/> (April 2015)

3.2.5. Additional phenotypes identified by the screen

Hypocrellin A was not identified as a ribosome biogenesis inhibitor, but showed an interesting phenotype. It's photosensitizing activity was discovered during the screen. After stimulation by the light source of the fluorescence microscopy, the cells develop a strong fluorescence signal after one minute. The nuclear membrane, plasma membrane and lipid droplets of the yeast cells had an increased signal (see figure 3.29, far right). Next to its photosensitizing activity, hypocrellin A might have an effect on protein kinase C (Ma G., et al 2004; Dang L. et al, 2004).

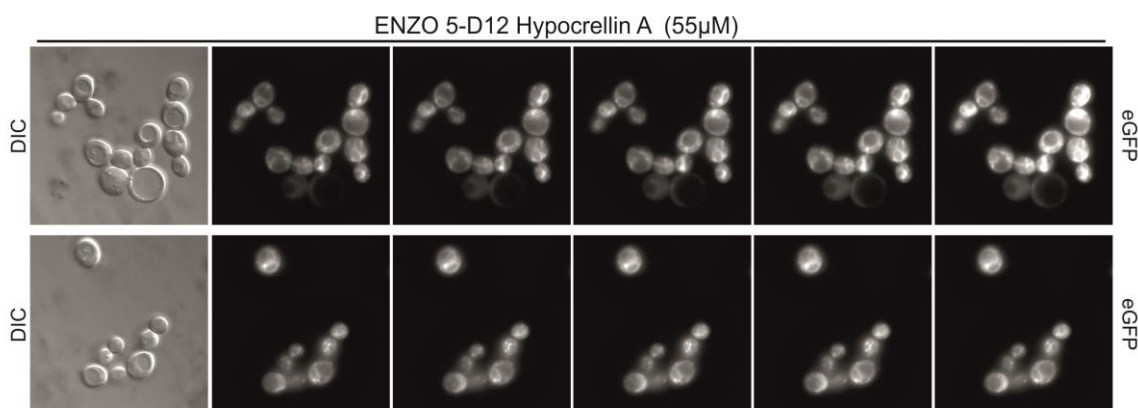


Figure 3.29: Hypocrellin A showed a photosensitizing activity. The pictures were taken within the first minute after exposing the cells to the light source of the microscope. The fluorescence signal detected becomes stronger after the first minute (far right).

Other interesting phenotypes included an abnormal number of vacuoles seen when cells were treated with the substances Enzo 1-C01, Enzo 1-H03, Enzo 1-B06, to name a few. Such a vacuole fragmentation, leading to multiple vacuoles in one cell, has been already observed in yeast cells upon nutrition stress (Zieger and Mayer, 2012).

4. Outlook

The high-throughput screen developed during this thesis, offers a fast way to identify new potential inhibitors. Thus, the set-up suggested in table 3.1, demonstrated that cells with a high expression of the reporter-GFP construct could be used for a high-throughput screen. However, it was not possible to determine if the accumulation of the reporter protein in the nucleus will create a significant signal that can be distinguished from the fluorescence signal of the reporter protein in the cytoplasm of untreated cells. Further testing with different inhibitors is needed to improve the screen set up, especially taking in account that not all cells treated with a certain inhibitor will show an accumulation, thereby reducing the signal to noise ratio.

In contrast, the manual screen identified 130 potential inhibitors. The next step should be an intensive literature study on the inhibitors. My research revealed that multiple inhibitors share the same potential target or share the same chemical structure (see 3.2.4.). Additionally, the wild type (*C303a*) should be treated with the identified inhibitors. This could reveal unspecific fluorescence signals of the inhibitors due to artefacts instead of the actual accumulation of the ribosomal proteins.

The inhibitors identified by using the small subunit reporter protein, should be used to reexamine cells featuring the Rpl7a-GFP reporter. Many of these substances did not show an effect when screening with the large subunit reporter. However, the RNA isolation of the treated wild type (*C303a*) will reveal more specifically the effect of the inhibitors on the ribosome biogenesis. Previous studies included northern blots, of yeast cells treated with diazaborine, and revealed that the processing of the 27S pre-rRNA to the 7S pre-rRNA is blocked (Perstchy et al, 2004). When using diazaborine as a positive control, an accumulation of Rpl7a-GFP in the nucleolus was detected after 60 min of incubation (5µg/ml). However, a clear effect on 27SA2 pre-rRNA can be already seen after 15 min of incubation (Perstchy et al, 2004). This suggests that the RNA detection is highly sensitive and will give more detail about which pre-ribosome maturation step is blocked, and finally results in the accumulation of the reporter protein in the nucleus. Hence, the rRNA of the treated cells will reveal if the inhibitor targets the maturation of the pre-60S, pre-40S or even the pre-90S particle. Additionally, classic genetics will give more detail about the specific target. Although, the rRNA levels will indicate which maturation step is blocked, the target of the inhibitor could be not involved in the

ribosome biogenesis directly (see 3.2.3 and 3.2.4.). The first step would be creating mutants that are resistant to the identified inhibitors. Afterwards the chromosomally DNA can be digested and used to create a gene bank. By later on introducing the gene bank into the wild type (*C303a*), the specific target of the inhibitor, causing the resistance, can be identified. Then, and only then, the identified inhibitors can be differentiated between specific and unspecific ribosome biogenesis inhibitors.

5. References

- Alberts B**, Johnson A, Lewis J, et al. (2002) *Molecular Biology of the Cell*. 4th edition. New York: Garland Science.
- Allen L**, Meck R, Yunis A. (1980) *The inhibition of gamma-glutamyl transpeptidase from human pancreatic carcinoma cells by (alpha S,5S)-alpha-amino-3-chloro-4,5-dihydro-5-isoxazoleacetic acid (AT-125; NSC-163501)* Res. Commun. Chem. Pathol. Pharmacol. 27, 175
- American cancer society** <http://www.cancer.org/treatment/treatmentsandsideeffects/> (May, 2015)
- Ansari K**, Martin S, Farkasovsky M, Ehbrecht IM, Küntzel H. (1999) *Phospholipase C binds to the receptor-like GPR1 protein and controls pseudohyphal differentiation in Saccharomyces cerevisiae*. J Biol Chem 274(42):30052-8
- Ausubel, FM** et al. (1995), eds. *Current Protocols in Molecular Biology*, Wiley-Interscience, New York
- Azad GK**, Singh V, Thakare MJ, Baranwal S, Tomar RS. (2014). *Mitogen-activated protein kinase Hog1 is activated in response to curcumin exposure in the budding yeast Saccharomyces cerevisiae*. BMC Microbiol. Dec 19;14(1):317. doi: 10.1186/s12866-014-0317-0.
- Babiano R** and De La Cruz J. (2010) *Ribosomal protein L35 is required for 27SB prerRNA processing in Saccharomyces cerevisiae*. Nucleic Acids Res. 38: 5177–5192.
- Barritault D**, Guerin MF, Hayes DH. (1979) *Reconstitution of active 30-S ribosomal subunits in vitro using heat-denatured 16-S rRNA* Eur J Biochem. Aug 1;98(2):567-71.
- Bassler J**, Grandi P, Gadal O, Lessmann T, Petfalski E, Tollervey D, Lechner J, Hurt E. (2001). *Identification of a 60S preribosomal particle that is closely linked to nuclear export*. Mol. Cell 8: 517–529
- Baßler J**, Klein I, Schmidt C, Kallas M, Thomson E, Wagner MA,Bergler H. (2012). *The Conserved Bud20 Zinc Finger Protein Is a New Component of the Ribosomal 60S Subunit Export Machinery*. Molecular and Cellular Biology, 32(24), 4898–4912. doi:10.1128/MCB.00910-12
- Ben-Shem A**, Garreau de Loubresse N, Melnikov S, Jenner L, Yusupova G, Yusupov M. (2011) *The structure of the eukaryotic ribosome at 3.0 Å resolution*. Science. 2011 Dec 16;334(6062):1524-9. doi: 10.1126/science.1212642. Epub 2011 Nov 17.
- Bergler and Pertschy** (2013) *Unconventional proposal*.
- Bos CL**, Kodach LL, van den Brink GR, Diks SH, van Santen MM, Richel DJ, Peppelenbosch MP, Hardwick JC. (2006). *Effect of aspirin on the Wnt/beta-catenin pathway is mediated via protein phosphatase 2A*. Oncogene. Oct 19;25(49):6447-56. Epub 2006 Jul 31.
- Brouet I** and Ohshima H. (1995). *Curcumin, an anti-tumour promoter and anti-inflammatory agent, inhibits induction of nitric oxide synthase in activated macrophages*. Biochem Biophys Res Commun. Jan 17;206(2):533-40.
- Budanov AV**. (2014). *The role of tumor suppressor p53 in the antioxidant defense and metabolism*. Sub-Cellular Biochemistry, 85, 337–358. doi:10.1007/978-94-017-9211-0_18
- Burger K**, Mühl B, Harasim T, Rohrmoser M, Malamoussi A, Orban M., ... Eick D. (2010). *Chemotherapeutic Drugs Inhibit Ribosome Biogenesis at Various Levels*. The Journal of Biological Chemistry, 285(16), 12416–12425. doi:10.1074/jbc.M109.074211
- Bursac S**, Brdovcak MC, Donati G, Volarevic S. (2013) *Activation of the tumor suppressor p53 upon impairment of ribosome biogenesis*. Biochim Biophys Acta. 2014 Jun;1842(6):817-30. doi: 10.1016/j.bbadis.2013.08.014. Epub 2013 Oct 26.
- Bywater MJ**, Poortinga G, Sanij E, Hein N, Peck A, Cullinane C, ... Hannan, R. D. (2012). *Inhibition of RNA Polymerase I as a Therapeutic Strategy to Promote Cancer-Specific Activation of p53*. Cancer Cell, 22(1), 51–65. doi:10.1016/j.ccr.2012.05.019

- Cutts SM**, Swift LP, Rephaeli A, Nudelman A, Phillips DR. (2005) *Recent advances in understanding and exploiting the activation of anthracyclines by formaldehyde*. *Curr Med Chem Anticancer Agents*. Sep;5(5):431-47
- Commandeur JN and Vermeulen NP** (1996). *Cytotoxicity and cytoprotective activities of natural compounds. The case of curcumin*. *Xenobiotica*. Jul;26(7):667-80.
- Dang L**, Seale JP, Qu X. (2004) *Reduction of high glucose and phorbol-myristate-acetate-induced endothelial cell permeability by protein kinase C inhibitors LY379196 and hypocrellin A*. *Biochem Pharmacol*. Mar 1;67(5):855-64.
- Dez C and Tollervey D**. (2004) *Ribosome synthesis meets the cell cycle*. *Curr Opin Microbiol*. Dec;7(6):631-7.
- Drygin D**, Siddiqui-Jain A, O'Brien S, Schwaebe M, Lin A, Bliesath J, Ho CB, Proffitt C, Trent K, Whitten JP, Lim JK, Von Hoff D, Anderes K, Rice WG. (2009) *Anticancer activity of CX-3543: a direct inhibitor of rRNA biogenesis*. *Cancer Res*. Oct 1;69(19):7653-61. doi: 10.1158/0008-5472.CAN-09-1304. Epub 2009 Sep 8.
- Ferreira-Cerca S**, Poll G, Gleizes PE, Tschochner H, Milkereit P. (2005) *Roles of eukaryotic ribosomal proteins in maturation and transport of pre-18S rRNA and ribosome function*. *Mol. Cell* 20: 263–275.
- Ferreira-Cerca S**, Pöll G, Kühn H, Neueder A, Jakob S, Tschochner H, Milkereit P. (2007) *Analysis of the in vivo assembly pathway of eukaryotic 40S ribosomal proteins*. *Mol. Cell* 28: 446–457
- Finley D**, Ulrich H D, Sommer T, Kaiser P. (2012). *The Ubiquitin–Proteasome System of Saccharomyces cerevisiae*. *Genetics*, 192(2), 319–360. doi:10.1534/genetics.112.140467
- Freed-Pastor WA and Prives C**. (2012). *Mutant p53: one name, many proteins*. *Genes & Development*, 26(12), 1268–1286. doi:10.1101/gad.190678.112
- French SL**, Osheim YN, Cioci F, Nomura M, Beyer LA. (2003) *In exponentially growing Saccharomyces cerevisiae cells, rRNA synthesis is determined by the summed RNA polymerase I loading rate rather than by the number of active genes*. *Mol. Cell. Biol.* 23: 1558–1568
- Garcia CA**, Júnior LR, Neto Gde O. (2003) *Determination of potassium ions in pharmaceutical samples by FIA using a potentiometric electrode based on ionophore nonactin occluded in EVA membrane*. *J Pharm Biomed Anal*. Feb 5;31(1):11-8.
- Gewirtz DA**. (1999) *A critical evaluation of the mechanisms of action proposed for the antitumor effects of the anthracycline antibiotics adriamycin and daunorubicin*. *Biochem Pharmacol*. Apr 1;57(7):727-41.
- Gietz RD** (2014). *Yeast transformation by the LiAc/SS carrier DNA/PEG method* *Methods Mol Biol.*;1163:33-44. doi: 10.1007/978-1-4939-0799-1_4
- Grandi P**, Rybin V, Bassler J, Petfalski E, Strauss D, Marzioch M, Schäfer T, Kuster B, Tschochner H, Tollervey D, Gavin AC, Hurt E. (2002) *90S pre-ribosomes include the 35S pre-rRNA, the U3 snoRNP, and 40S subunit processing factors but predominantly lack 60S synthesis factors*. *Mol. Cell* 10: 105–115
- Grunicke H, Hofmann J, Maly K, Uberall F, Posch L, Oberhuber H, Fiebig H**. (1989) *The phospholipid- and calcium-dependent protein kinase as a target in tumor chemotherapy*. *Adv Enzyme Regul.*;28:201-16.
- Hainaut P**, Soussi T, Shomer B, Hollstein M, Greenblatt M, Hovig E, Harris CC, Montesano R. (1997) *Database of p53 gene somatic mutations in human tumors and cell lines: updated compilation and future prospects*. *Nucleic Acids Research*, 25(1), 151–157.
- Hanigan MH**. (2014) *Gamma-glutamyl transpeptidase: redox regulation and drug resistance* *Adv Cancer Res.*;122:103-41.
- Harnpicharnchai P**, Jakovljevic J, Horsey E, Miles T, Roman J,Woolford JL Jr. (2001) *Composition and functional characterization of yeast 66S ribosome assembly intermediates*. *Mol. Cell* 8: 505–515
- Henras AK**, Soudet J, Gêrus M, Lebaron S, Caizergues-Ferrer M, Mougïn A, Henry Y. (2008) *The post-transcriptional steps of eukaryotic ribosome biogenesis*. *Cell. Mol. Life Sci.* 65, 2334–59.

- Hink MA**, Griep RA, Borst JW, van Hoek A, Eppink MH, Schots A, Visser AJ. (2000) *Structural dynamics of green fluorescent protein alone and fused with a single chain Fv protein*. J Biol Chem. Jun 9;275(23):17556-60.
- Hein N**, Hannan KM, George AJ, Sanij E, Hannan RD. (2013) *The nucleolus: an emerging target for cancer therapy*. Trends Mol Med. Nov;19(11):643-54. doi: 10.1016/j.molmed.2013.07.005. Epub 2013 Aug 15.
- Held WA**, Mizushima S, Nomura M. (1973) *Reconstitution of Escherichia coli 30 S ribosomal subunits from purified molecular components*. J. Biol. Chem. 248: 5720–5730
- Herbert JM**, Augereau JM, Gleye J, Maffrand JP. (1990) *Chelerythrine is a potent and specific inhibitor of protein kinase C*. Biochem Biophys Res Commun. Nov 15;172(3):993-9.
- Hubner CB** and Koob GF. (1990) *Bromocriptine produces decreases in cocaine self-administration in the rat*. Neuropsychopharmacology. Apr;3(2):101-8
- Hung NJ** and Johnson AW. (2006) *Nuclear recycling of the pre-60S ribosomal subunit-associated factor Arx1 depends on Rei1 in Saccharomyces cerevisiae*. Mol Cell Biol. May;26(10):3718-27.
- Hurt E**, Hannus S, Schmelzl B, Lau D, Tollervey D and Simos G. (1999). *A Novel In Vivo Assay Reveals Inhibition of Ribosomal Nuclear Export in Ran-Cycle and Nucleoporin Mutants*. The Journal of Cell Biology, 144(3), 389–401.
- Ide S**, Miyazaki T, Maki H, Kobayashi T. (2010) *Abundance of ribosomal RNA gene copies maintains genome integrity*. Science 327: 693–696
- Jakovljevic J**, Gamalinda M, Talkish J, Alexander L, Linnemann J, Milkereit P, Woolford JL Jr. (2012) *Ribosomal proteins L7 and L8 function in concert with six A3 assembly factors to propagate assembly of domain I of 25S rRNA in yeast 60S ribosomal subunits*. RNA 18: 1805–1822.
- Jenner L**, Melnikov S, Garreau de Loubresse N, Ben-Shem A, Iskakova M, Urzhumtsev A, Meskauskas A, Dinman J, Yusupova G, Yusupov M. (2012) *Crystal structure of the 80S yeast ribosome*. Curr Opin Struct Biol. Dec;22(6):759-67. doi: 10.1016/j.sbi.2012.07.013. Epub 2012 Aug 8
- Kawai S**, Hashimoto W and Murata, K. (2010) *Transformation of Saccharomyces cerevisiae and other fungi: Methods and possible underlying mechanism*. Bioengineered Bugs, 1(6), 395–403. doi:10.4161/bug.1.6.13257
- Koch B**, Mitterer V, Niederhauser J, Stanborough T, Murat G, Rechberger G, Bergler H, Kressler D, Pertschy B. (2012) *Yar1 protects the ribosomal protein Rps3 from aggregation*. J. Biol. Chem. 287, 21806–21815 10.1074/jbc.M112.365791
- Köhler W**, Thrum H, Schlegel R. (1964) *Antibacterial spectrum of nonactin with special consideration of Corynebacteriaceae*. Zentralbl Bakteriolog Orig. 1964 Dec;194(4):457-61
- Korutla L and Kumar R**. (1994) *Inhibitory effect of curcumin on epidermal growth factor receptor kinase activity in A431 cells*. Biochim Biophys Acta. Dec 30;1224(3):597-600.
- Kos M and Tollervey D**. (2010) *Yeast pre-rRNA processing and modification occur cotranscriptionally*. Mol. Cell 37: 809–820
- Kotamraju S**, Konorev EA, Joseph J, Kalyanaraman B. (2000) *Doxorubicin-induced apoptosis in endothelial cells and cardiomyocytes is ameliorated by nitron spin traps and ebselen. Role of reactive oxygen and nitrogen species*. J Biol Chem. Oct 27;275(43):33585-92.
- Kraakman L**, Lemaire K, Ma P, Teunissen AW, Donaton MC, Van Dijk P, Winderickx J, de Winde JH, Thevelein JM. (1999) *A Saccharomyces cerevisiae G-protein coupled receptor, Gpr1, is specifically required for glucose activation of the cAMP pathway during the transition to growth on glucose*. Mol Microbiol 32(5):1002-12 PMID: 10361302
- Kressler D**, Hurt E, Bassler J. (2010) *Driving ribosome assembly*. Biochim Biophys Acta. Jun;1803(6):673-83. doi: 10.1016/j.bbamcr.2009.10.009. Epub 2009 Oct 30.

- Kreuzer J**, Bach NC, Forler D, Sieber SA. (2014) *Target discovery of acivicin in cancer cells elucidates its mechanism of growth inhibition†Electronic supplementary information (ESI) available: Synthesis, cloning, protein expression, purification and biochemical assays.* Chem Sci. 2014 Dec 1;6(1):237-245. Epub Sep 26.
- Krogan NJ**, Peng WT, Cagney G, Robinson MD, HawR, Zhong G, Guo X, Zhang X, ...Greenblatt JF. (2004) *High-definition macromolecular composition of yeast RNA-processing complexes* Mol. Cell 13 225–239.
- Kruiswijk T**, Planta RJ, Krop JM. (1978) *The course of the assembly of ribosomal subunits in yeast.* Biochim. Biophys. Acta 517: 378–389.
- Kudo N**, Matsumori N, Taoka H, Fujiwara D, Schreiner EP, Wolff B, Yoshida M, Horinouchi S. (1999) *Leptomycin B inactivates CRM1/exportin 1 by covalent modification at a cysteine residue in the central conserved region.* Proceedings of the National Academy of Sciences of the United States of America. 1999;96(16):9112–9117. doi: 10.1073/pnas.96.16.9112.
- Kuo HM**, Chang LS, Lin YL, Lu HF, Yang JS, Lee JH, Chung JG. (2007) *Morin inhibits the growth of human leukemia HL-60 cells via cell cycle arrest and induction of apoptosis through mitochondria dependent pathway.* Anticancer Res. 27, 395
- Kuo ML**, Huang TS, Lin JK. (1996) *Curcumin, an antioxidant and anti-tumor promoter, induces apoptosis in human leukemia cells.* Biochim Biophys Acta. Nov 15;1317(2):95-100.
- Lang GA**, Iwakuma T, Suh YA, Liu G, Rao VA, Parant JM, Valentin-Vega YA, Terzian T, Caldwell LC, Strong LC, et al. (2004) *Gain of function of a p53 hot spot mutation in a mouse model of Li-Fraumeni syndrome.* Cell.;119:861–872.
- Lang DR and Racker E.** (1974) *Effects of quercetin and F1 inhibitor on mitochondrial ATPase and energy-linked reactions in submitochondrial particles.* Biochim Biophys Acta. Feb 22;333(2):180-6.
- Li YM and Casida JE.** (1992) *Cantharidin-binding protein: identification as protein phosphatase 2A.* Proceedings of the National Academy of Sciences of the United States of America, 89(24), 11867–11870.
- Lo KY**, Li Z, Bussiere C, Bresson S, Marcotte EM, Johnson AW. (2010) *Defining the pathway of cytoplasmic maturation of the 60S ribosomal subunit.* Mol. Cell 39: 196–208.
- Loibl M**, Klein I, Prattes M, Schmidt C, Kappel L, Zisser G, Gungl A, Krieger E, Pertschy B, Bergler H. (2014) *The drug histidine blocks ribosome biogenesis by inhibiting the AAA-ATPase Drg1.* J Biol Chem. Feb 14;289(7):3913-22. doi: 10.1074/jbc.M113.536110. Epub 2013 Dec 26.
- Lupu R and Menendez JA.** (2006) *Pharmacological inhibitors of Fatty Acid Synthase (FASN)--catalyzed endogenous fatty acid biogenesis: a new family of anti-cancer agents?* Curr Pharm Biotechnol. Dec;7(6):483-93.
- Ma G**, Khan SI, Jacob MR, Tekwani BL, Li Z, Pasco DS, ..., Khan IA. (2004) *Antimicrobial and Antileishmanial Activities of Hypocrellins A and B.* Antimicrobial Agents and Chemotherapy, 48(11), 4450–4452. doi:10.1128/AAC.48.11.4450-4452.2004
- Manna SK**, Aggarwal RS, Sethi G, Aggarwal BB, Ramesh GT. (2007) *Morin (3,5,7,2',4'-Pentahydroxyflavone) Abolishes Nuclear Factor- κ B Activation Induced by Various Carcinogens and Inflammatory Stimuli, Leading to Suppression of Nuclear Factor- κ B-Regulated Gene Expression and Up-regulation of Apoptosis.* Clinical Cancer Research : An Official Journal of the American Association for Cancer Research, 13(7), 2290–2297. doi:10.1158/1078-0432.CCR-06-2394
- Megarity CF**, Looi HK, Timson DJ. (2014) *The Saccharomyces cerevisiae quinone oxidoreductase Lot6p: stability, inhibition and cooperativity.* FEMS Yeast Res. 2014 Aug;14(5):797-807. doi: 10.1111/1567-1364.12167. Epub Jun 19.
- Morgenstern C.** (2004) *Identifizierung von möglichen Interaktionspartnern des Drg1 Proteins in Saccharomyces cerevisiae.* Master thesis
- Mori A**, Okudaira H, Kobayashi N, Akiyama K. (2001) *Selective regulation of T cell IL-5 synthesis by OM-01, JTE-711 and p38 MAP kinase inhibitor: independent control of Th2 cytokines, IL-4 and IL-5.* Int Arch Allergy Immunol. Jan-Mar;124(1-3):172-5.

- Moy T and Silver P.** (2002) *Requirements for the nuclear export of the small ribosomal subunit.* J Cell Sci. 2002 Jul 15;115(Pt 14):2985-95.
- Nierhaus KH and Dohme F.** (1974) *Total reconstitution of functionally active 50S ribosomal subunits from Escherichia coli.* Proc. Natl. Acad. Sci. USA 71: 4713–4717
- Nissan TA,** Bassler J, Petfalski E, Tollervey D, Hurt E. (2002) *60S pre-ribosome formation viewed from assembly in the nucleolus until export to the cytoplasm.* EMBO J. 21: 5539–5547
- Nowotny V,** Rheinberger HJ, Nierhaus K, Tesche B, Amils R. (1980) *Preparation procedures of proteins and RNA influence the total reconstitution of 50S subunits from E. coli ribosomes.* Nucleic Acids Res. Mar 11;8(5):989-98.
- Olive KP,** Tuveson DA, Ruhe ZC, Yin B, Willis NA, Bronson RT, Crowley D, Jacks T. (2004) *Mutant p53 gain of function in two mouse models of Li-Fraumeni syndrome.* Cell.;119:847–860.
- Ossareh-Nazari B,** Niño CA, Bengtson MH, Lee JW, Joazeiro CA, Dargemont C. (2014) *Ubiquitylation by the Ltn1 E3 ligase protects 60S ribosomes from starvation-induced selective autophagy.* J Cell Biol. 2014 Mar 17;204(6):909-17. doi: 10.1083/jcb.201308139. Epub Mar 10.
- Sambrook J,** Fritsch EF, Maniatis T. (1989) *Molecular Cloning: A Laboratory Manual. 2nd ed.* Plainview, N.Y.: Cold Spring Harbor Laboratory Press.
- Vieira SM,** de Oliveira VH, Valente Rdo C, Moreira Oda C, Fontes CF, Mignaco JA. (2015) *Chelerythrine inhibits the sarco/endoplasmic reticulum Ca(2+)-ATPase and results in cell Ca(2+) imbalance.* Arch Biochem Biophys. 2015 Mar 15;570:58-65. doi: 10.1016/j.abb.2015.02.019. Epub Feb 23.
- Pan X and Heitman J.** (1999) *Cyclic AMP-dependent protein kinase regulates pseudohyphal differentiation in Saccharomyces cerevisiae.* Mol Cell Biol 19(7):4874-87
- Perez-Fernandez J,** Roman A, De Las Rivas J, Bustelo XR, Dosil M. (2007) *The 90S preribosome is a multimodular structure that is assembled through a hierarchical mechanism.* Mol. Cell. Biol. 27 5414–5429.
- Pertschy B,** Zisser G, Schein H, Köffel R, Rauch G, Grillitsch K, Morgenstern C, Durchschlag M, Högenauer G, Bergler H. (2004) *Diazaborine treatment of yeast cells inhibits maturation of the 60S ribosomal subunit.* Mol Cell Biol 24(14):6476-87
- Pertschy B,** Saveanu C, Zisser G, Lebreton A, Tengg M, Jacquier A, Liebming E, Nobis B, Kappel L, van der Klei I. (2007) *Cytoplasmic recycling of 60S preribosomal factors depends on the AAA protein Drg1.* Mol Cell Biol.;27:6581–6592.
- Petracek ME and Longtine MS.** (2002) *PCR-based engineering of yeast genome.* Methods Enzymol. 2002;350:445-69.
- Pianese G.** (1896) Beitrag zur Histologie und Aetiologie der Carcinoma. Histologische und experimentelle Untersuchungen Beitr Pathol Anat Allg Pathol., 142:1–193.
- Pierrat B,** Correia JS, Mary JL, Tomas-Zuber M, Lesslauer W. (1998) *RSK-B, a novel ribosomal S6 kinase family member, is a CREB kinase under dominant control of p38alpha mitogen-activated protein kinase (p38alphaMAPK).* J Biol Chem; 273:29661–71.
- Planta RJ and Mager WH.** (1998) *The list of cytoplasmic ribosomal proteins of Saccharomyces cerevisiae.* Yeast. Mar 30;14(5):471-7.
- Przygodzki T,** Sokal A, Bryszewska M. (2005) *Calcium ionophore A23187 action on cardiac myocytes is accompanied by enhanced production of reactive oxygen species.* Biochim Biophys Acta. 2005 Jun 10;1740(3):481-8. Epub Apr 9
- Reed PW,** Lardy HA. (1972) *A23187: a divalent cation ionophore.* J Biol Chem. Nov 10; 247(21):6970-7
- Rice-Evans CA,** Miller NJ, Paganga G. (1996) *Structure-antioxidant activity relationships of flavonoids and phenolic acids.* Free Radic Biol Med.;20(7):933-56.

- Sahu SC and Gray GC.** (1997) *Lipid peroxidation and DNA damage induced by morin and naringenin in isolated rat liver nuclei.* Food Chem. Toxicol. 35, 443
- Saveanu C, Namane A, Gleizes PE, Lebreton A, Rousselle JC, Noaillac-Depeyre J, Gas N, Jacquier A, Fromont-Racine M.** (2003) *Sequential protein association with nascent 60S ribosomal particles.* Mol. Cell. Biol. 23: 4449–4460.
- Schafer T, Strauss D, Petfalski E, Tollervey D, Hurt E.** (2003) *The path from nucleolar 90S to cytoplasmic 40S pre-ribosomes.* EMBO J. 22: 1370–1380
- SGD database,** Fas1 information; <http://www.yeastgenome.org/locus/S000001665/overview> (May, 2015)
- Singh AK, Sidhu GS, Deepa T, Maheshwari RK.** (1996) *Curcumin inhibits the proliferation and cell cycle progression of human umbilical vein endothelial cell.* Cancer Lett. Oct 1;107(1):109-15
- Smardová J, Smarda J, Koptíková J.** (2005) *Functional analysis of p53 tumor suppressor in yeast.* Differentiation. Jul;73(6):261-77.
- Strunk BS, Loucks CR, Su M, Vashisth H, Cheng S, Schilling J, Brooks CL 3rd, Karbstein K, Skiniotis G.** (2011) *Ribosome assembly factors prevent premature translation initiation by 40S assembly intermediates.* Science 333: 1449–1453.
- TECAN technical note:** *Detection of Green Fluorescent Protein (eGFP), Tecan Ultra Evolution, Safire and GENios Pro*
- Thiry M and Lafontaine DL.** (2005) *Birth of a nucleolus: the evolution of nucleolar compartments.* Trends Cell Biol. 15: 194–199
- Toussaint M, Levasseur G, Tremblay M, Paquette M, Conconi A.** (2005) *Psoralen photocrosslinking, a tool to study the chromatin structure of RNA polymerase I-transcribed ribosomal genes.* Biochem. Cell Biol. 83: 449–459
- Wei YQ, Zhao X, Kariya Y, Fukata H, Teshigawara K, Uchida A.** (1994) *Induction of apoptosis by quercetin: involvement of heat shock protein.* Cancer Res. Sep 15;54(18):4952-7
- Woolford J L and Baserga SJ.** (2013) *Ribosome biogenesis in the yeast Saccharomyces cerevisiae.* Genetics 195, 643–81
- Wu M-Y, Xie X, Xu, ZK, Xie L, Chen Z, Shou L-M, ... Tao M.** (2014) *PP2A inhibitors suppress migration and growth of PANC-1 pancreatic cancer cells through inhibition on the Wnt/ β -catenin pathway by phosphorylation and degradation of β -catenin.* Oncology Reports, 32(2), 513–522. doi:10.3892/or.2014.3266
- Yano R, Oakes ML, Tabb MM, Nomura M.** (1994) *Yeast Srp1p has homology to armadillo/plakoglobin/ β -catenin and participates in apparently multiple nuclear functions including the maintenance of the nucleolar structure.* Proc Natl Acad Sci U S A. Jul 19;91(15):6880-4.
- Yun CW, Tamaki H, Nakayama R, Yamamoto K, Kumagai H.** (1997) *G-protein coupled receptor from yeast Saccharomyces cerevisiae.* Biochem Biophys Res Commun. Nov 17;240(2):287-92.
- Zagórska L, Szkopińska A, Klita S, Szafranski P.** (1980) *Effect of removal of 160 nucleotides from the 3' end of Escherichia coli 16s rRNA on the reconstitution and activity of 30S ribosomes.* Biochem Biophys Res Commun. Aug 14;95(3):1152-9.
- Zieger M and Mayer A.** (2012). *Yeast vacuoles fragment in an asymmetrical two-phase process with distinct protein requirements.* Molecular Biology of the Cell, 23(17), 3438–3449. doi:10.1091/mbc.E12-05-0347

6. Complete list of inhibitors used in this study

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-01	NCP003323	A02	CPD000058423	SAM001246723	46386703	CPD000058423	BUPROPION HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B02	CPD000471621	SAM001246718	46386698	CPD000471621	IRSOGLADINE MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C02	CPD000466376	SAM001246733	46386746	CPD000466376	ACARBOSE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D02	CPD000469294	SAM001246739	46386752	CPD000469294	BENPROPERINE PHOSPHATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E02	CPD000466378	SAM001246740	46386753	CPD000466378		18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F02	CPD000058926	SAM001246743	46386756	CPD000058926		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G02	CPD000449280	SAM001246736	46386749	CPD000449280	Carvedilol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H02	CPD000466379	SAM001246741	46386754	CPD000466379	LOMIFYLLINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A03	CPD000466380	SAM001246742	46386755	CPD000466380	PAZUFLOXACIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B03	CPD000466381	SAM001246745	46386758	CPD000466381	MIGLITOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C03	CPD000058373	SAM001246737	46386750	CPD000058373		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D03	CPD000466345	SAM001246652	46386668	CPD000466345	OLANZAPINE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E03	CPD000449297	SAM001246653	46386669	CPD000449297	Nefazodone	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F03	CPD000469185	SAM001246654	46386670	CPD000469185	Moxifloxacin hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G03	CPD000469186	SAM001246655	46386712	CPD000469186	NELFINAVIR MESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H03	CPD000469187	SAM001246656	46386713	CPD000469187	PRAVASTATIN Sodium	18.Jun.13	9,5	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A04	CPD000466344	SAM001246651	46386667	CPD000466344	Topotecan Hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B04	CPD000466303	SAM001246539	46386557	CPD000466303	LEVETIRACETAM	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C04	CPD000469142	SAM001246540	46386558	CPD000469142	PRAMIPEXOLE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D04	CPD000466323	SAM001246595	46386613	CPD000466323	RISPERIDONE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E04	CPD000469167	SAM001246600	46386618	CPD000469167	pioglitazone hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F04	CPD000469147	SAM001246552	46386570	CPD000469147	Cilastatin sodium	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G04	CPD000466348	SAM001246661	46386718	CPD000466348	ARGATROBAN	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H04	CPD000466327	SAM001246603	46386621	CPD000466327	VALDECOXIB	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A05	CPD000466346	SAM001246658	46386715	CPD000466346	NAFTOPIDIL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B05	CPD000156231	SAM001246662	46386719	CPD000156231	Nobiletin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C05	CPD000466304	SAM001246541	46386559	CPD000466304	FINASTERIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D05	CPD000469145	SAM001246549	46386567	CPD000469145	ZOLPIDEM TARTRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E05	CPD000048458	SAM001246551	46386569	CPD000048458	Viramune	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F05	CPD000466325	SAM001246601	46386619	CPD000466325	TOPIRAMATE	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-01	NCP003323	G05	CPD000466350	SAM001246664	46386721	CPD000466350	VORICONAZOLE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H05	CPD000469190	SAM001246665	46386722	CPD000469190	FENOLDOPAM MESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A06	CPD000471612	SAM001246610	46386628	CPD000471612	ROSIGLITAZONE MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B06	CPD000469191	SAM001246668	46386725	CPD000469191	ESCITALOPRAM OXALATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C06	CPD000058866	SAM001246609	46386627	CPD000058866		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D06	CPD000466354	SAM001246671	46386728	CPD000466354	LATANOPROST	18.Jun.13	10,3	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E06	CPD000058576	SAM001246673	46386730	CPD000058576		18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F06	CPD000466298	SAM001246666	46386723	CPD000466298	Sertraline	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G06	CPD000466353	SAM001246670	46386727	CPD000466353	CALCIOTRIOL	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H06	CPD000466308	SAM001246559	46386577	CPD000466308	EPIRUBICIN HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A07	CPD000466329	SAM001246612	46386630	CPD000466329	BICALUTAMIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B07	CPD000469192	SAM001246672	46386729	CPD000469192	BENIDIPINE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C07	CPD000466352	SAM001246669	46386726	CPD000466352	AMLEXANOX	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D07	CPD000469148	SAM001246554	46386572	CPD000469148	CERIVASTATIN SODIUM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E07	CPD000466309	SAM001246560	46386578	CPD000466309	ICARIIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F07	CPD000466310	SAM001246562	46386580	CPD000466310	METHYLANDROS TENEDIOL	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G07	CPD000466307	SAM001246553	46386571	CPD000466307	TRIPITOLIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H07	CPD000469170	SAM001246608	46386626	CPD000469170	ROSIGLITAZONE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A08	CPD000059106	SAM001246561	46386579	CPD000059106		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B08	CPD000466392	SAM001246769	46386782	CPD000466392	OLIGOMYCIN C	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C08	CPD000469199	SAM001246712	46386692	CPD000469199	BENAZEPRIL HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D08	CPD000058877	SAM001246765	46386778	CPD000058877		18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E08	CPD000059060	SAM001246714	46386694	CPD000059060	35212-22-7	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F08	CPD000058286	SAM001246770	46386783	CPD000058286	OXAPROZIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G08	CPD000058510	SAM001246766	46386779	CPD000058510		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H08	CPD000469200	SAM001246713	46386693	CPD000469200	MOSAPRIDE CITRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A09	CPD000466391	SAM001246767	46386780	CPD000466391	Isoquercitrin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B09	CPD000058450	SAM001246763	46386776	CPD000058450		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C09	CPD000469164	SAM001246593	46386611	CPD000469164		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D09	CPD000466394	SAM001246776	46386811	CPD000466394	HYPEROSIDE	18.Jun.13	8,8	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E09	CPD000466322	SAM001246589	46386607	CPD000466322	RIFABUTIN	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-01	NCP003323	F09	CPD000469141	SAM001246533	46386551	CPD000469141	ESMOLOL HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G09	CPD000466321	SAM001246586	46386604	CPD000466321	TADALAFIL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H09	CPD000058957	SAM001246587	46386605	CPD000058957		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A10	CPD000058570	SAM001246768	46386781	CPD000058570	DOXORUBICIN HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B10	CPD000469209	SAM001246764	46386777	CPD000469209	MOXONIDINE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C10	CPD000058302	SAM001246711	46386691	CPD000058302		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D10	CPD000387024	SAM001246571	46386589	CPD000387024	PEFLOXACIN MESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E10	CPD000469154	SAM001246572	46386590	CPD000469154	Venlafaxine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F10	CPD000469592	SAM001246591	46386609	CPD000469592	Pantoprazole Sodium	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G10	CPD000469159	SAM001246583	46386601	CPD000469159	FLUTICASON PROPIONATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H10	CPD000469161	SAM001246588	46386606	CPD000469161	Indinavir Sulfate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	A11	CPD000469160	SAM001246585	46386603	CPD000469160	Midazolam Hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	B11	CPD000466319	SAM001246582	46386600	CPD000466319	LAMIVUDINE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	C11	CPD000469151	SAM001246564	46386582	CPD000469151	366-70-1	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	D11	CPD000469280	SAM001246538	46386556	CPD000469280	ESOMEPRAZOLE Mg	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	E11	CPD000059146	SAM001246530	46386548	CPD000059146	SULFASALAZINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	F11	CPD000466313	SAM001246567	46386585	CPD000466313	TORASEMIDE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	G11	CPD000469156	SAM001246576	46386594	CPD000469156	tropisetron- γ hyd rochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-01	NCP003323	H11	CPD000326795	SAM001246534	46386552	CPD000326795	Ranolazine dihydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A02	CPD000338536	SAM001246761	46386774	CPD000338536		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B02	CPD000466390	SAM001246762	46386775	CPD000466390	PIDOTIMOD	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C02	CPD000466386	SAM001246757	46386770	CPD000466386	RAMIPRIL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D02	CPD000469284	SAM001246642	46386658	CPD000469284	FENPIVERINIUM BROMIDE	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E02	CPD000058610	SAM001246751	46386764	CPD000058610	19- Nortestosterone	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F02	CPD000466384	SAM001246752	46386765	CPD000466384		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G02	CPD000059047	SAM001246753	46386766	CPD000059047		18.Jun.13	10,5	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H02	CPD000048684	SAM001246754	46386767	CPD000048684		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A03	CPD000466385	SAM001246756	46386769	CPD000466385	TROXIPIDE	18.Jun.13	10,1	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-02	NCP003403	B03	CPD000466341	SAM001246647	46386663	CPD000466341	ACTARIT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C03	CPD000469183	SAM001246645	46386661	CPD000469183	azelastine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D03	CPD000466388	SAM001246759	46386772	CPD000466388	TOCAINIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E03	CPD000499525	SAM001246760	46386773	CPD000499525	TAXIFOLIN-(+/-)	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F03	CPD000466387	SAM001246758	46386771	CPD000466387	LEVOFLOXACIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G03	CPD000469182	SAM001246643	46386659	CPD000469182	CEFATRIZINE PROPYLENE GLYCOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H03	CPD000466364	SAM001246700	46386682	CPD000466364	IDEBENONE	18.Jun.13	10,2	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A04	CPD000466366	SAM001246703	46386685	CPD000466366	LEVOSULPIRIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B04	CPD000238142	SAM001246706	46386687	CPD000238142		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C04	CPD000466343	SAM001246649	46386665	CPD000466343	LETROZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D04	CPD000469184	SAM001246650	46386666	CPD000469184	MEROPENEM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E04	CPD000466339	SAM001246637	46386654	CPD000466339	ORLISTAT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F04	CPD000469179	SAM001246631	46386648	CPD000469179		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G04	CPD000059117	SAM001246694	46386677	CPD000059117		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H04	CPD000469197	SAM001246695	46386678	CPD000469197	CETRAXATE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A05	CPD000149316	SAM001246696	46386679	CPD000149316		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B05	CPD000058464	SAM001246697	46386680	CPD000058464		18.Jun.13	10,3	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C05	CPD000059145	SAM001246702	46386684	CPD000059145	N-Ethyl-o-crotonoluidide	18.Jun.13	10,3	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D05	CPD000472526	SAM001246699	46386681	CPD000472526	Amfebutamone	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E05	CPD000466340	SAM001246638	46386655	CPD000466340	ALFUZOSIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F05	CPD000449309	SAM001246639	46386656	CPD000449309	Amisulpride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G05	CPD000469292	SAM001246632	46386649	CPD000469292	LOFEPRAMINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H05	CPD000466362	SAM001246688	46386671	CPD000466362	PEROSPIRONE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A06	CPD000059010	SAM001246689	46386672	CPD000059010	DOCETAXEL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B06	CPD000387107	SAM001246690	46386673	CPD000387107	HONOKIOL	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C06	CPD000469196	SAM001246691	46386674	CPD000469196	TOLTERODINE TARTRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D06	CPD000466363	SAM001246692	46386675	CPD000466363	CARMOFUR	18.Jun.13	10,3	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E06	CPD000469181	SAM001246633	46386650	CPD000469181	PAROXETINE	18.Jun.13	9,7	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F06	CPD000466337	SAM001246634	46386651	CPD000466337	OLMESARTAN MEDOXOMIL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G06	CPD000469593	SAM001246635	46386652	CPD000469593	LOSARTAN Potassium	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H06	CPD000466338	SAM001246636	46386653	CPD000466338	TEMOZOLOMIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A07	CPD000058528	SAM001246682	46386739	CPD000058528		18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-02	NCP003403	B07	CPD000469195	SAM001246686	46386743	CPD000469195	tosufloxacin tosilate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C07	CPD000466361	SAM001246687	46386744	CPD000466361	MECILLINAM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D07	CPD000469177	SAM001246626	46386643	CPD000469177	Atomoxetine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E07	CPD000466336	SAM001246628	46386645	CPD000466336	ARTESUNATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F07	CPD000058959	SAM001246679	46386736	CPD000058959		18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G07	CPD000469193	SAM001246674	46386731	CPD000469193	CEFPODOXIME PROXETIL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H07	CPD000058803	SAM001246680	46386737	CPD000058803	Buflomedil HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A08	CPD000012114	SAM001246614	46386631	CPD000012114	4-Chloro-N-(2-morpholin-4-yl-ethyl)-benzamide	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B08	CPD000466330	SAM001246616	46386633	CPD000466330	HALOMETASONE MONOHYDRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C08	CPD000466357	SAM001246681	46386738	CPD000466357	TRICLABENDAZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D08	CPD000466331	SAM001246617	46386634	CPD000466331	ROFECOXIB	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E08	CPD000471619	SAM001246618	46386635	CPD000471619	BISOPROLOL FUMARATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F08	CPD000466334	SAM001246623	46386640	CPD000466334	EZETIMIBE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G08	CPD000469176	SAM001246625	46386642	CPD000469176	TIAGABINE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H08	CPD000466355	SAM001246676	46386733	CPD000466355	idarubicin hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A09	CPD000466360	SAM001246685	46386742	CPD000466360	FLUBENDAZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B09	CPD000466356	SAM001246677	46386734	CPD000466356	TACROLIMUS	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C09	CPD000469208	SAM001246749	46386762	CPD000469208	VALACICLOVIR HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D09	CPD000466382	SAM001246748	46386761	CPD000466382	CLARITHROMYCIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E09	CPD000466383	SAM001246750	46386763	CPD000466383	ARIPIRAZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F09	CPD000471622	SAM001246747	46386760	CPD000471622	TRIMEBUTINE MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G09	CPD000238198	SAM001246746	46386759	CPD000238198		18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H09	CPD000466370	SAM001246719	46386699	CPD000466370	NISOLDIPINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A10	CPD000466371	SAM001246720	46386700	CPD000466371	PICEID	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B10	CPD000149359	SAM001246716	46386696	CPD000149359	1-(2-Methyl-5-nitroimidazol-1-yl)-propan-2-ol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C10	CPD000466369	SAM001246717	46386697	CPD000466369	Nifekalant hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D10	CPD000466372	SAM001246721	46386701	CPD000466372	NATEGLINIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	E10	CPD000058691	SAM001246722	46386702	CPD000058691		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F10	CPD000466374	SAM001246728	46386708	CPD000466374	ORMETOPRIM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G10	CPD000466377	SAM001246738	46386751	CPD000466377	ZILEUTON	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H10	CPD000058350	SAM001246729	46386709	CPD000058350		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	A11	CPD000058918	SAM001246730	46386710	CPD000058918		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	B11	CPD000469293	SAM001246724	46386704	CPD000469293	OXICONAZOLE NITRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	C11	CPD000469235	SAM001246731	46386711	CPD000469235	KITASAMYCIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	D11	CPD000466375	SAM001246732	46386745	CPD000466375	FAMCICLOVIR	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-02	NCP003403	E11	CPD000326828	SAM001246725	46386705	CPD000326828		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	F11	CPD000466373	SAM001246726	46386706	CPD000466373	rufloxacin monohydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	G11	CPD000466389	SAM001246778	46386813	CPD000466389	TAXIFOLIN-(+)	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-02	NCP003403	H11	CPD000469211	SAM001246782	46386816	CPD000469211	alosetron monohydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A02	CPD000059165	SAM001246806	46386830	CPD000059165	BESTATIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B02	CPD000469213	SAM001246774	46386786	CPD000469213	TOREMIFENE CITRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C02	CPD000469214	SAM001246784	46386818	CPD000469214	GOSERELIN ACETATE	18.Jun.13	9,7	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D02	CPD000469212	SAM001246678	46386735	CPD000469212	SECOISOLARICINESINOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E02	CPD000469217	SAM001246796	46386823	CPD000469217	RALTITREXED	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F02	CPD000469229	SAM001246792	46386821	CPD000469229	DOXAPRAM HYDROCHLORIDE	18.Jun.13	10,4	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G02	CPD000466294	SAM001247095	46387004	CPD000466294	RU 24969	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H02	CPD000112281	SAM001246865	46386939	CPD000112281	Brucine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A03	CPD000059115	SAM001246862	46386936	CPD000059115	16502-01-5	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B03	CPD000058411	SAM001246863	46386937	CPD000058411		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D03	CPD000058746	SAM001246874	46386948	CPD000058746	NAPROXEN SODIUM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E03	CPD000058904	SAM001246875	46386949	CPD000058904		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F03	CPD000058310	SAM001246877	46386951	CPD000058310	3-[3,5-DIBROMO-4-HYDROXYBENZOYL]-2-ETHYLBENZOFURAN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G03	CPD000058300	SAM001246890	46386964	CPD000058300		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H03	CPD000058701	SAM001246892	46386966	CPD000058701		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A04	CPD000058715	SAM001246891	46386965	CPD000058715		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B04	CPD000058273	SAM001246876	46386950	CPD000058273		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C04	CPD000466922	SAM001246889	46386963	CPD000466922	Reichsteins substance S	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D04	CPD000059086	SAM001246894	46386968	CPD000059086	3-PYRIDINEMETHANOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E04	CPD000449283	SAM001246979	46386806	CPD000449283	Haloperidol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F04	CPD000449279	SAM001247042	46386912	CPD000449279	Stiripentol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G04	CPD000449303	SAM001247034	46386904	CPD000449303	Fluperlapine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H04	CPD000058660	SAM001246887	46386961	CPD000058660		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A05	CPD000112358	SAM001246869	46386943	CPD000112358	Homoveratrylamine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B05	CPD000058194	SAM001246913	46387025	CPD000058194		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C05	CPD000058741	SAM001246912	46387024	CPD000058741	XANTHINOL NICOTINATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D05	CPD000059111	SAM001246896	46386970	CPD000059111	SYNEPHRINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E05	CPD000058206	SAM001246888	46386962	CPD000058206	501-36-0	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F05	CPD000059093	SAM001246871	46386945	CPD000059093	118-71-8	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G05	CPD000059077	SAM001246854	46386887	CPD000059077		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H05	CPD000059011	SAM001246856	46386889	CPD000059011	ENROFLOXACIN	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-03	NCP003483	A06	CPD000058603	SAM001246857	46386890	CPD000058603		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B06	CPD000058250	SAM001246884	46386958	CPD000058250		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C06	CPD000059044	SAM001246858	46386891	CPD000059044		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D06	CPD000469136	SAM001246523	46386541	CPD000469136	duloxetine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E06	CPD000469155	SAM001246573	46386591	CPD000469155	VARDENAFIL CITRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F06	CPD000469137	SAM001246524	46386542	CPD000469137	Ropivacaine hydrochloride	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G06	CPD000466301	SAM001246525	46386543	CPD000466301	ANASTROZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H06	CPD000058462	SAM001246984	46386834	CPD000058462	KETOTIFEN FUMARATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A07	CPD000058769	SAM001246906	46387018	CPD000058769		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B07	CPD000466919	SAM001246907	46387019	CPD000466919	Pinacidil monohydrate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C07	CPD000058266	SAM001246908	46387020	CPD000058266		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D07	CPD000112269	SAM001246909	46387021	CPD000112269		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E07	CPD000059045	SAM001246855	46386888	CPD000059045	92-84-2	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F07	CPD000058553	SAM001246526	46386544	CPD000058553		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G07	CPD000469138	SAM001246527	46386545	CPD000469138	Granisetron Hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H07	CPD000466293	SAM001247094	46387003	CPD000466293	Rimcazole	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A08	CPD000466292	SAM001247092	46387001	CPD000466292	Nafadotride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B08	CPD000058856	SAM001246885	46386959	CPD000058856		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C08	CPD000471617	SAM001246557	46386575	CPD000471617	DEXCHLORPHENIRAMINE MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D08	CPD000466288	SAM001247088	46386997	CPD000466288	Guanidine	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E08	CPD000466290	SAM001247090	46386999	CPD000466290	L-694,247	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F08	CPD000466284	SAM001247081	46386990	CPD000466284	AM-251	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G08	CPD000466289	SAM001247089	46386998	CPD000466289	HTMT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H08	CPD000466286	SAM001247083	46386992	CPD000466286	Benzo[a]phenanthridine-10,11-diol, 5,6,6a,7,8,12b-hexahydro-, trans- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A09	CPD000466291	SAM001247091	46387000	CPD000466291	Methanesulfonamide, N-[4-[[1-[2-(6-methyl-2-pyridinyl)ethyl]-4-piperidinyl]carbonyl]phenyl]-, dihydrochloride [CAS]	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B09	CPD000466279	SAM001247076	46386985	CPD000466279	2H-Indol-2-one, 1,3-dihydro-1-phenyl-3,3-bis(4-pyridinylmethyl)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-03	NCP003483	C09	CPD000466920	SAM001246898	46386972	CPD000466920	Beclomethasone	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D09	CPD000058847	SAM001246900	46386973	CPD000058847	73590-58-6	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E09	CPD000469228	SAM001246842	46386881	CPD000469228	DOLASETRON MESYLATE	18.Jun.13	10,4	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F09	CPD000449310	SAM001246841	46386880	CPD000449310	Zolmitriptan	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G09	CPD000469223	SAM001246852	46386886	CPD000469223	TREMULACIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H09	CPD000469227	SAM001246846	46386883	CPD000469227	DACTINOMYCIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A10	CPD000449308	SAM001246847	46386884	CPD000449308	Tramadol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B10	CPD000469226	SAM001246815	46386831	CPD000469226	CHLORDIAZEPOXIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C10	CPD000469225	SAM001246816	46386832	CPD000469225	CEFIXIME TRIHYDRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D10	CPD000469224	SAM001246818	46386833	CPD000469224		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E10	CPD000469232	SAM001246820	46386875	CPD000469232	Lofexidine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F10	CPD000469221	SAM001246804	46386828	CPD000469221	BALSALAZIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G10	CPD000469220	SAM001246802	46386826	CPD000469220	OLOPATADINE HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H10	CPD000469287	SAM001246803	46386827	CPD000469287	ITAVASTATIN Ca	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	A11	CPD000058334	SAM001246882	46386956	CPD000058334		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	B11	CPD000058431	SAM001246883	46386957	CPD000058431		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	C11	CPD000469230	SAM001246822	46386877	CPD000469230	HOMOHARRINGTONINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	D11	CPD000058318	SAM001246879	46386953	CPD000058318	50-22-6	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	E11	CPD000471625	SAM001246821	46386876	CPD000471625	VECURONIUM BROMIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	F11	CPD000469219	SAM001246801	46386825	CPD000469219	TIBOLONE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	G11	CPD000058212	SAM001246860	46386893	CPD000058212	98-92-0	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-03	NCP003483	H11	CPD000059131	SAM001246861	46386894	CPD000059131		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A02	CPD000058612	SAM001246886	46386960	CPD000058612		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B02	CPD000058726	SAM001246873	46386947	CPD000058726		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C02	CPD000058572	SAM001246914	46387026	CPD000058572	1,1-DIMETHYL-4-PHENYLPYPERAZINIUM IODIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D02	CPD000058507	SAM001246893	46386967	CPD000058507		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E02	CPD000059128	SAM001246866	46386940	CPD000059128	72-33-3	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F02	CPD000059142	SAM001246868	46386942	CPD000059142	BENACTYZINE HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G02	CPD000059100	SAM001246867	46386941	CPD000059100		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H02	CPD000059158	SAM001246870	46386944	CPD000059158	79-43-6	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A03	CPD000466283	SAM001247080	46386989	CPD000466283	Altanserin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B03	CPD000466281	SAM001247078	46386987	CPD000466281	Acetamide, 2-amino-N-(1-methyl-1,2-diphenylethyl)-, (+/-)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-04	NCP003563	C03	CPD000058420	SAM001247084	46386993	CPD000058420		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D03	CPD000466311	SAM001246563	46386581	CPD000466311		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E03	CPD000466285	SAM001247082	46386991	CPD000466285	Azasetron	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F03	CPD000466287	SAM001247087	46386996	CPD000466287	GR 89696	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G03	CPD000058773	SAM001246897	46386971	CPD000058773	DELTA1-HYDROCORTISONE 21-HEMISUCCINATE SODIUM SALT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H03	CPD000058392	SAM001246872	46386946	CPD000058392		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A04	CPD000058366	SAM001246531	46386549	CPD000058366		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B04	CPD000469290	SAM001246578	46386596	CPD000469290	SAQUINAVIR MESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C04	CPD000058970	SAM001246775	46386787	CPD000058970	60628-96-8	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D04	CPD000469158	SAM001246579	46386597	CPD000469158	SUMATRIPTAN SUCCINATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E04	CPD000466314	SAM001246574	46386592	CPD000466314	EXEMESTANE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F04	CPD000466367	SAM001246708	46386689	CPD000466367	NITAZOXANIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G04	CPD000058398	SAM001246536	46386554	CPD000058398		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H04	CPD000471623	SAM001246777	46386812	CPD000471623	QUETIAPINE HEMIFUMARATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A05	CPD000112560	SAM001246528	46386546	CPD000112560	RUTIN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B05	CPD000466317	SAM001246580	46386598	CPD000466317	PENCICLOVIR	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C05	CPD000466393	SAM001246772	46386784	CPD000466393	CALCITRIOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D05	CPD000469140	SAM001246532	46386550	CPD000469140	DIPHENOXYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E05	CPD000449307	SAM001247005	46386855	CPD000449307	Felbamate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F05	CPD000058855	SAM001247013	46386863	CPD000058855		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G05	CPD000035998	SAM001247011	46386861	CPD000035998		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H05	CPD000466277	SAM001247074	46386983	CPD000466277	1H-Imidazole-5-carboxylic acid, 1-(1-phenylethyl)-, ethyl ester, (R)- [CAS]	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A06	CPD000466395	SAM001246783	46386817	CPD000466395	RITONAVIR	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B06	CPD000469210	SAM001246780	46386815	CPD000469210	vinorelbine tartrate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C06	CPD000466335	SAM001246624	46386641	CPD000466335	LINEZOLID	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D06	CPD000469203	SAM001246727	46386707	CPD000469203	LOMERIZINE DIHCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E06	CPD000466351	SAM001246667	46386724	CPD000466351	EFAVIRENZ	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F06	CPD000466306	SAM001246548	46386566	CPD000466306	IRBESARTAN	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G06	CPD000466305	SAM001246546	46386564	CPD000466305		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H06	CPD000238204	SAM001246555	46386573	CPD000238204		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A07	CPD000440694	SAM001246605	46386623	CPD000440694		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B07	CPD000469144	SAM001246547	46386565	CPD000469144	roxatidine acetate hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-04	NCP003563	C07	CPD000471616	SAM001246556	46386574	CPD000471616	DEXBROMPHENIRAMINE MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D07	CPD000469168	SAM001246604	46386622	CPD000469168	anagrelide hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E07	CPD000471618	SAM001246606	46386624	CPD000471618	TEGASEROD MALEATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F07	CPD000058475	SAM001246611	46386629	CPD000058475	MILRINONE	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G07	CPD000466315	SAM001246575	46386593	CPD000466315	LEVOCETIRIZINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H07	CPD000326936	SAM001246599	46386617	CPD000326936	Citalopram	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A08	CPD000048468	SAM001246558	46386576	CPD000048468	Ticlopidine Hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B08	CPD000469165	SAM001246594	46386612	CPD000469165	sodium-áloxoprofen	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C08	CPD000466316	SAM001246577	46386595	CPD000466316	ZAFIRLUKAST	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D08	CPD000469152	SAM001246565	46386583	CPD000469152	Terbinafine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E08	CPD000466320	SAM001246584	46386602	CPD000466320	ISRADIPINE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F08	CPD000466318	SAM001246581	46386599	CPD000466318	VALSARTAN	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G08	CPD000449291	SAM001247048	46386918	CPD000449291	Piroxicam	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H08	CPD000469282	SAM001246629	46386646	CPD000469282		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A09	CPD000449286	SAM001246992	46386842	CPD000449286	Physostigmine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B09	CPD000466278	SAM001247075	46386984	CPD000466278	1H-Indole-2-propanoic acid, 1-[(4-chlorophenyl)methyl]-3-[[1,1-dimethylethyl]thio]-Alpha,Alpha-dimethyl-5-(1-methylethyl)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C09	CPD000058436	SAM001247030	46386900	CPD000058436	562-10-7	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D09	CPD000449266	SAM001247035	46386905	CPD000449266	Milnacipran	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E09	CPD000449315	SAM001247017	46386867	CPD000449315	5-fluoro-2-pyrimidone	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F09	CPD000466271	SAM001247022	46386872	CPD000466271	Chlorpheniramine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G09	CPD000466333	SAM001246621	46386638	CPD000466333	DOFETILIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H09	CPD000471620	SAM001246675	46386732	CPD000471620	FORMOTEROL FUMARATE DIHYDRATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A10	CPD000525252	SAM001246615	46386632	CPD000525252	RIZATRIPTAN BENZOATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B10	CPD000466332	SAM001246620	46386637	CPD000466332	RIFAPENTINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	C10	CPD000469178	SAM001246630	46386647	CPD000469178	LOTEPREDNOL ETABONATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D10	CPD000466359	SAM001246684	46386741	CPD000466359	ENALAPRILAT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E10	CPD000449292	SAM001246627	46386644	CPD000449292	Donepezil	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F10	CPD000238177	SAM001246755	46386768	CPD000238177		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G10	CPD000466365	SAM001246701	46386683	CPD000466365		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H10	CPD000466326	SAM001246602	46386620	CPD000466326		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	A11	CPD000469143	SAM001246542	46386560	CPD000469143	ITOPRIDE HCl	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	B11	CPD000466324	SAM001246597	46386615	CPD000466324	RIFAXIMIN	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-04	NCP003563	C11	CPD000469188	SAM001246657	46386714	CPD000469188	MONTELUKAST SODIUM	18.Jun.13	9,6	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	D11	CPD000058253	SAM001246779	46386814	CPD000058253	2',3'-DIDEOXYCYTIDINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	E11	CPD000466276	SAM001247073	46386982	CPD000466276	1H-Imidazol-2-amine, N-(2,6-dichlorophenyl)-4,5-dihydro- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	F11	CPD000466280	SAM001247077	46386986	CPD000466280	6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 11-[[2-[(diethylamino)methyl]-1-piperidinyl]acetyl]-5,11-dihydro- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	G11	CPD000449316	SAM001246964	46386791	CPD000449316	3'-deoxyadenosine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-04	NCP003563	H11	CPD000449296	SAM001246980	46386807	CPD000449296	Ifenprodil	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A02	CPD000145728	SAM001247020	46386870	CPD000145728	5-Amino-2-hydroxy-benzoic acid	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	B02	CPD000466269	SAM001246991	46386841	CPD000466269	Paroxetine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C02	CPD000058465	SAM001247050	46386920	CPD000058465	LOBELINE HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D02	CPD000449329	SAM001247049	46386919	CPD000449329	L-Ornithine, N5-[imino(methylamino)methyl]-[CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E02	CPD000058461	SAM001246596	46386614	CPD000058461		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F02	CPD000449321	SAM001247025	46386895	CPD000449321	Oxiranecarboxylic acid, 2-[6-(4-chlorophenoxy)hexyl]-, ethyl ester- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G02	CPD000449288	SAM001247031	46386901	CPD000449288	Epigallocatechin gallate	18.Jun.13	10,3	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H02	CPD000449275	SAM001247072	46386981	CPD000449275	Raclopride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A03	CPD000449271	SAM001247069	46386978	CPD000449271	Zacopride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	B03	CPD000449276	SAM001247068	46386977	CPD000449276	SKF 83566	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C03	CPD000449274	SAM001246965	46386792	CPD000449274	AM 404	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D03	CPD000449281	SAM001247063	46386933	CPD000449281	Nalbuphine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E03	CPD000059053	SAM001246962	46386789	CPD000059053	PILOCARPINE HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F03	CPD000058291	SAM001246963	46386790	CPD000058291		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G03	CPD000042823	SAM001246961	46386788	CPD000042823	Flurbiprofen	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H03	CPD000059136	SAM001247015	46386865	CPD000059136	3-HYDROXY-1,2-DIMETHYL-4(1H)-PYRIDONE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A04	CPD000058470	SAM001247061	46386931	CPD000058470	Loxapine	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-05	NCP003643	B04	CPD000326694	SAM001247062	46386932	CPD000326694	d-3-Methoxy-N-methylmorphinan hydrobromide	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C04	CPD000449282	SAM001247059	46386929	CPD000449282	Duloxetine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D04	CPD000449320	SAM001247060	46386930	CPD000449320	Glycine, N-[2-[(acetylthio)methyl]-1-oxo-3-phenylpropyl]-, phenylmethyl ester [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E04	CPD000449318	SAM001247057	46386927	CPD000449318	Benzeneacetic acid, 2-[(2,6-dichlorophenyl)amino]-, monosodium salt [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F04	CPD000058345	SAM001247039	46386909	CPD000058345		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G04	CPD000058961	SAM001247033	46386903	CPD000058961	FAMOTIDINE	18.Jun.13	10,2	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H04	CPD000449299	SAM001246999	46386849	CPD000449299	SR 57227A	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A05	CPD000466270	SAM001247003	46386853	CPD000466270	Pancuronium	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	B05	CPD000058175	SAM001247010	46386860	CPD000058175	443-48-1	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C05	CPD000449327	SAM001246967	46386794	CPD000449327	Benzeneacetic acid, Alpha-(hydroxymethyl)-, 9-methyl-3-oxa-9-azatricyclo[3.3.1.0 ^{2,4}]non-7-yl ester, [7(S)-(1Alpha,2,4,5Alpha,7)]- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D05	CPD000449323	SAM001246968	46386795	CPD000449323	Benzeneacetonitrile, Alpha-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy-Alpha-(1-methylethyl)-, (R)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E05	CPD000449328	SAM001246969	46386796	CPD000449328		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F05	CPD000449294	SAM001246970	46386797	CPD000449294	zucapsaicin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G05	CPD000058513	SAM001246971	46386798	CPD000058513	SALBUTAMOL SULFATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H05	CPD000057879	SAM001246972	46386799	CPD000057879	(+/-)-Vesamicol hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A06	CPD000469289	SAM001246993	46386843	CPD000469289	Picrotin - Picrotoxinin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	B06	CPD000449268	SAM001247000	46386850	CPD000449268	Terazosin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C06	CPD000449319	SAM001247027	46386897	CPD000449319	diphenylcyclopropenone	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D06	CPD000449326	SAM001247016	46386866	CPD000449326	4-Thiazolidinecarboxylic acid, 2-oxo-, (R)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E06	CPD000466274	SAM001247051	46386921	CPD000466274	Mesoridazine	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC	PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-05		NCP003643	F06	CPD000449313	SAM001247053	46386923	CPD000449313	3(2H)-Pyridazinone, 6-[4-(difluoromethoxy)-3-methoxyphenyl]- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	G06	CPD000466275	SAM001247054	46386924	CPD000466275	10H-Phenothiazine, 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	H06	CPD000449322	SAM001247055	46386925	CPD000449322	1H-Cyclopenta[b]quinolin-9-amine, 2,3,5,6,7,8-hexahydro-, monohydrochloride- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	A07	CPD000058306	SAM001247056	46386926	CPD000058306	CLOTRIMAZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	B07	CPD000058255	SAM001246987	46386837	CPD000058255	79794-75-5	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	C07	CPD000058500	SAM001247037	46386907	CPD000058500	Phenelzine sulfate	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	D07	CPD000449311	SAM001246997	46386847	CPD000449311	Riluzole	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	E07	CPD000449312	SAM001247004	46386854	CPD000449312	Naltrindole	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	F07	CPD000449277	SAM001247026	46386896	CPD000449277	Nornicotine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	G07	CPD000449269	SAM001247052	46386922	CPD000449269	Bifemelane	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	H07	CPD000449284	SAM001246973	46386800	CPD000449284	CGS 15943	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	A08	CPD000449287	SAM001246974	46386801	CPD000449287	Cinanserin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	B08	CPD000449272	SAM001246975	46386802	CPD000449272	Cisapride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	C08	CPD000449273	SAM001246981	46386808	CPD000449273	Indatraline	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	D08	CPD000058520	SAM001247045	46386915	CPD000058520	25332-39-2	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	E08	CPD000449301	SAM001246995	46386845	CPD000449301	Prazosin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	F08	CPD000058525	SAM001247001	46386851	CPD000058525	URAPIDIL HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	G08	CPD000449278	SAM001247007	46386857	CPD000449278	(-)-Cotinine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	H08	CPD000058313	SAM001247014	46386864	CPD000058313	D-CYCLOSERINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	A09	CPD000466268	SAM001246977	46386804	CPD000466268	Fluvoxamine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	B09	CPD000449270	SAM001246976	46386803	CPD000449270	Doxepin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	C09	CPD000059133	SAM001247046	46386916	CPD000059133		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	D09	CPD000058908	SAM001247023	46386873	CPD000058908	(+)-3-HYDROXY-N-METHYLMORPHINAN D-TARTRATE	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	E09	CPD000058555	SAM001246988	46386838	CPD000058555	LY 171883	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	F09	CPD000148117	SAM001246989	46386839	CPD000148117	Maprotiline hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	G09	CPD000466272	SAM001247038	46386908	CPD000466272	Pizotyline	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	H09	CPD000059126	SAM001247032	46386902	CPD000059126	BETA-ESTRADIOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	A10	CPD000059046	SAM001247019	46386869	CPD000059046	N,N'-DIACETYL-1,6-DIAMINOHEXANE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	B10	CPD000058353	SAM001247024	46386874	CPD000058353	147-24-0	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05		NCP003643	C10	CPD000449267	SAM001246978	46386805	CPD000449267	Galanthamine	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-05	NCP003643	D10	CPD000449290	SAM001246982	46386809	CPD000449290	Indomethacin	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E10	CPD000059171	SAM001247028	46386898	CPD000059171	TETRAETHYLTHIURAM DISULFIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F10	CPD000449302	SAM001246994	46386844	CPD000449302	Piribedil	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G10	CPD000058460	SAM001246983	46386810	CPD000058460		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H10	CPD000058623	SAM001247047	46386917	CPD000058623		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	A11	CPD000449325	SAM001246996	46386846	CPD000449325	Pyrazinecarboxamide, 3,5-diamino-N-(aminoiminomethyl)-6-chloro- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	B11	CPD000059105	SAM001247002	46386852	CPD000059105	9-AMINO-1,2,3,4-TETRAHYDROACRIDINE HYDROCHLORIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	C11	CPD000058319	SAM001247008	46386858	CPD000058319	ETHYNYLESTRADIOL	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	D11	CPD000449317	SAM001247012	46386862	CPD000449317	2(1H)-Pyrimidinone, 4-amino-1-γ-D-arabinofuranosyl- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	E11	CPD000449324	SAM001246985	46386835	CPD000449324	L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	F11	CPD000449305	SAM001247043	46386913	CPD000449305	TFMPP	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	G11	CPD000449298	SAM001247006	46386856	CPD000449298	Pramipexole	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-05	NCP003643	H11	CPD000058189	SAM001247018	46386868	CPD000058189		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A02	CPD000466297	SAM001247099	46387008	CPD000466297	SDM25N	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B02	CPD000466300	SAM001247103	46387012	CPD000466300	5-Nonyloxytryptamine	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C02	CPD000466296	SAM001247097	46387006	CPD000466296	SB 205607	18.Jun.13	9,8	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D02	CPD000058344	SAM001246921	46501387	CPD000058344		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	E02	CPD000238180	SAM001246641	46386657	CPD000238180		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F02	CPD000468734	SAM001247067	46386976	CPD000468734	PD 81723	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	G02	CPD000469222	SAM001246805	46386829	CPD000469222		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	H02	CPD000058445	SAM001247071	46386980	CPD000058445		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A03	CPD000466299	SAM001247101	46387010	CPD000466299	Thiophene, 5-bromo-2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B03	CPD000466295	SAM001247096	46387005	CPD000466295	Salmeterol	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C03	CPD000326935	SAM001247098	46387007	CPD000326935	R(+)-SCH-23390 hydrochloride	18.Jun.13	9,9	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D03	CPD000059075	SAM001246922	46387028	CPD000059075	DEHYDROEPIANDROSTERONE	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-06	NCP003723	E03	CPD000112594	SAM001246840	46386879	CPD000112594	Prostaglandin E1	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F03	CPD000058878	SAM001246590	46386608	CPD000058878		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	G03	CPD000468732	SAM001247065	46386935	CPD000468732	CCPA	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	H03	CPD000468733	SAM001247066	46386975	CPD000468733	CGS 12066B	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A04	CPD000469153	SAM001246568	46386586	CPD000469153	VINDESINE SULFATE	18.Jun.13	9,7	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B04	CPD000058540	SAM001246570	46386588	CPD000058540	VINCRISTINE SULFATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C04	CPD000466342	SAM001246648	46386664	CPD000466342	LACIDIPINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D04	CPD000466347	SAM001246659	46386716	CPD000466347		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	E04	CPD000469285	SAM001246707	46386688	CPD000469285	AMPIROXICAM	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F04	CPD000466368	SAM001246710	46386690	CPD000466368	GLIMEPIRIDE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	G04	CPD000469198	SAM001246705	46386686	CPD000469198	Amlodipine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	H04	CPD000469174	SAM001246619	46386636	CPD000469174	RABEPRAZOLE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A05	CPD000058704	SAM001246878	46386952	CPD000058704	CLOFAZIMINE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B05	CPD000469166	SAM001246598	46386616	CPD000469166	Irinotecan hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C05	CPD000058469	SAM001246544	46386562	CPD000058469	103577-45-3	18.Jun.13	10,1	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D05	CPD000149358	SAM001246545	46386563	CPD000149358	8-Chloro-11-piperidin-4-ylidene-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	E05	CPD000058772	SAM001246904	46386974	CPD000058772	1,3,5(10)-ESTRATRIEN-3-OL-17-ONE SULPHATE, SODIUM SALT	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F05	CPD000058481	SAM001246881	46386955	CPD000058481		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	G05	CPD000112002	SAM001246880	46386954	CPD000112002		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	H05	CPD000238156	SAM001247105	46387014	CPD000238156	Sibutramine	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A06	CPD000469632	SAM001247107	46387016	CPD000469632		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B06	CPD000469231	SAM001246851	46386885	CPD000469231		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C06	CPD000472527	SAM001246592	46386610	CPD000472527	Sibutramine hydrochloride	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D06	CPD000058410	SAM001246833	46386878	CPD000058410		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	E06	CPD000469633	SAM001247108	46387017	CPD000469633	8-Azaspiro[4.5]decane-7,9-dione, 8-[2-[[[2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]ethyl]-, monomethanesulfonate [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F06	CPD000469631	SAM001247106	46387015	CPD000469631	Adenosine, N-(2-hydroxycyclopentyl)-, (1S-trans)- [CAS]	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	G06	CPD000058296	SAM001246646	46386662	CPD000058296	19774-82-4	18.Jun.13	9,5	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	H06	CPD000336944	SAM001246644	46386660	CPD000336944		18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	A07	CPD000469175	SAM001246622	46386639	CPD000469175	IMATINIB MESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	B07	CPD000468736	SAM001247102	46387011	CPD000468736	Metylperon	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	C07	CPD000469594	SAM001246773	46386785	CPD000469594	Parecoxib sodium	18.Jun.13	9,8	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	D07	CPD000058504	SAM001247070	46386979	CPD000058504		18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE ID	SAMPLE ID	PUBCHEM SID	STRUCTURE SYNONYMS [1]	STRUCTURE SYNONYMS [2]	DATE	CONC	CONC UNIT	VOLUME	VOLUME UNIT	SOLVENT
NGP-105-06	NCP003723	E07	CPD000471626	SAM001246793	46386822	CPD000471626	ATRACURIUM BESYLATE	18.Jun.13	10.0	mM	50.0	uL	DMSO
NGP-105-06	NCP003723	F07	CPD000469218	SAM001246799	46386824	CPD000469218	ARTEMETHER	18.Jun.13	10.0	mM	50.0	uL	DMSO

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-01	NCP003323	A02	C13H18ClNO.HCl	2.762.070	2.397.461	2.391.076	Sequoia Research Products Ltd.	SRP03446b	1	2
NGP-105-01	NCP003323	B02	C9H7Cl2N5.C4H4O4	3.721.665	2.560.945	2.550.078	Sequoia Research Products Ltd.	SRP01510i	4	5
NGP-105-01	NCP003323	C02	C25H43NO18	6.456.149	6.456.149	6.452.480	Sequoia Research Products Ltd.	SRP00375a	14	19
NGP-105-01	NCP003323	D02	C21H27NO.H3PO4	4.074.485	3.094.531	3.092.092	Sequoia Research Products Ltd.	SRP01065b	0	2
NGP-105-01	NCP003323	E02	C10H13NO2	1.792.195	1.792.195	1.790.946	Sequoia Research Products Ltd.	SRP014251p	2	3
NGP-105-01	NCP003323	F02	C12H21N.HCl	2.157.676	1.793.067	1.791.673	Sequoia Research Products Ltd.	SRP02040m	2	1
NGP-105-01	NCP003323	G02	C24H26N2O4	4.064.830	4.064.830	4.061.892	Sequoia Research Products Ltd.	SRP01625c	3	6
NGP-105-01	NCP003323	H02	C13H18N4O3	2.783.120	2.783.120	2.781.378	Sequoia Research Products Ltd.	SRP01571l	0	7
NGP-105-01	NCP003323	A03	C16H15FN2O4	3.183.054	3.183.054	3.181.015	Sequoia Research Products Ltd.	SRP010775p	3	6
NGP-105-01	NCP003323	B03	C8H17NO5	2.072.277	2.072.277	2.071.106	Sequoia Research Products Ltd.	SRP06560m	5	6
NGP-105-01	NCP003323	C03	C18H17NO5	3.273.377	3.273.377	3.271.106	Sequoia Research Products Ltd.	SRP02572t	2	6
NGP-105-01	NCP003323	D03	C17H20N4S	3.124.338	3.124.338	3.121.408	Sequoia Research Products Ltd.	SRP01035o	1	4
NGP-105-01	NCP003323	E03	C25H32ClN5O2.HCl	5.064.772	4.700.163	4.692.244	Sequoia Research Products Ltd.	SRP03327n	0	7
NGP-105-01	NCP003323	F03	C21H24FN3O4.HCl	4.379.000	4.014.391	4.011.750	Sequoia Research Products Ltd.	SRP06644m	2	7
NGP-105-01	NCP003323	G03	C32H45N3O4S.CH4O3S	6.638.954	5.677.897	5.673.130	Sequoia Research Products Ltd.	SRP03330n	4	7
NGP-105-01	NCP003323	H03	C23H35O7.Na+	4.465.186	4.235.288	4.232.382	Sequoia Research Products Ltd.	SRP02590p	3	7
NGP-105-01	NCP003323	A04	C23H23N3O5.HCl	4.579.150	4.214.541	4.211.637	Sequoia Research Products Ltd.	SRP02510t	2	8
NGP-105-01	NCP003323	B04	C8H14N2O2	1.702.122	1.702.122	1.701.055	Sequoia Research Products Ltd.	SRP01381l	2	4
NGP-105-01	NCP003323	C04	C10H17N3S.HCl	2.477.870	2.113.261	2.111.143	Sequoia Research Products Ltd.	SRP02587p	3	3
NGP-105-01	NCP003323	D04	C23H27FN4O2	4.104.930	4.104.930	4.102.118	Sequoia Research Products Ltd.	SRP01295r	0	6
NGP-105-01	NCP003323	E04	C19H20N2O3S.HCl	3.929.015	3.564.406	3.561.194	Sequoia Research Products Ltd.	SRP02425p	1	5
NGP-105-01	NCP003323	F04	C16H25N2O5S.Na+	3.804.362	3.574.464	3.571.484	Sequoia Research Products Ltd.	SRP035055c	4	7
NGP-105-01	NCP003323	G04	C23H36N6O5S	5.086.382	5.086.382	5.082.467	Sequoia Research Products Ltd.	SRP07170a	7	11
NGP-105-01	NCP003323	H04	C16H14N2O3S	3.143.596	3.143.596	3.140.725	Sequoia Research Products Ltd.	SRP00825v	2	5
NGP-105-01	NCP003323	A05	C24H28N2O3	3.924.996	3.924.996	3.922.099	Sequoia Research Products Ltd.	SRP00825n	1	5
NGP-105-01	NCP003323	B05	C21H22O8	4.024.022	4.024.022	4.021.314	Sequoia Research Products Ltd.	SRP05400n	0	8
NGP-105-01	NCP003323	C05	C23H36N2O2	3.725.532	3.725.532	3.722.776	Sequoia Research Products Ltd.	SRP00500f	2	4
NGP-105-01	NCP003323	D05	C19H21N3O.0.5C4H6O6	3.824.407	3.073.965	3.071.684	Sequoia Research Products Ltd.	SRP01500z	0	4
NGP-105-01	NCP003323	E05	C15H14N4O	2.663.032	2.663.032	2.661.167	Sequoia Research Products Ltd.	SRP03408n	1	5
NGP-105-01	NCP003323	F05	C12H21NO8S	3.393.619	3.393.619	3.390.987	Sequoia Research Products Ltd.	SRP02505t	2	9
NGP-105-01	NCP003323	G05	C16H14F3N5O	3.493.162	3.493.162	3.491.150	Sequoia Research Products Ltd.	SRP01070v	1	6
NGP-105-01	NCP003323	H05	C16H16ClNO3.CH4O3S	4.018.676	3.057.619	3.050.818	Sequoia Research Products Ltd.	SRP00426r	4	4
NGP-105-01	NCP003323	A06	C18H19N3O3S.C4H4O4	4.735.003	3.574.283	3.571.147	Sequoia Research Products Ltd.	SRP01315r	1	6
NGP-105-01	NCP003323	B06	C20H21FN2O.C2H2O4	4.144.341	3.243.992	3.241.637	Sequoia Research Products Ltd.	SRP01460e	0	3
NGP-105-01	NCP003323	C06	C18H26O5	3.224.030	3.224.030	3.221.780	Sequoia Research Products Ltd.	SRP00600z	3	5
NGP-105-01	NCP003323	D06	C26H40O5	4.326.030	4.326.030	4.322.875	Sequoia Research Products Ltd.	SRP01328l	3	5
NGP-105-01	NCP003323	E06	C10H12N4O3	2.362.310	2.362.310	2.360.909	Sequoia Research Products Ltd.	SRP02715d	2	7
NGP-105-01	NCP003323	F06	C17H17Cl2N.HCl	3.426.966	3.062.357	3.050.738	Sequoia Research Products Ltd.	SRP01325s	1	1
NGP-105-01	NCP003323	G06	C27H40O3	4.126.152	4.126.152	4.122.977	Sequoia Research Products Ltd.	SRP01060c	3	3

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-01	NCP003323	H06	C27H29NO11.HCl	5.799.900	5.435.291	5.431.740	Sequoia Research Products Ltd.	SRP01310e	7	12
NGP-105-01	NCP003323	A07	C18H14F4N2O4S	4.303.748	4.303.748	4.300.610	Sequoia Research Products Ltd.	SRP02002b	2	6
NGP-105-01	NCP003323	B07	C28H31N3O6.HCl	5.420.334	5.055.725	5.052.212	Sequoia Research Products Ltd.	SRP010651b	1	9
NGP-105-01	NCP003323	C07	C16H14N2O4	2.982.990	2.982.990	2.980.953	Sequoia Research Products Ltd.	SRP05620a	3	6
NGP-105-01	NCP003323	D07	C26H33FNO5.Na+	4.815.419	4.585.521	4.582.342	Sequoia Research Products Ltd.	SRP02030c	2	6
NGP-105-01	NCP003323	E07	C33H40O15	6.766.740	6.766.740	6.762.367	Sequoia Research Products Ltd.	SRP00325i	8	15
NGP-105-01	NCP003323	F07	C20H32O2	3.044.748	3.044.748	3.042.402	Sequoia Research Products Ltd.	SRP02900m	2	2
NGP-105-01	NCP003323	G07	C20H24O6	3.604.084	3.604.084	3.601.572	Sequoia Research Products Ltd.	SRP02915t	1	6
NGP-105-01	NCP003323	H07	C18H19N3O3S.HCl	3.938.892	3.574.283	3.571.147	Sequoia Research Products Ltd.	SRP01314r	1	6
NGP-105-01	NCP003323	A08	C8H9FN2O3	2.001.700	2.001.700	2.000.597	Sequoia Research Products Ltd.	SRP01185t	1	5
NGP-105-01	NCP003323	B08	C45H74O10	7.750.810	7.750.810	7.745.281	Sequoia Research Products Ltd.	SRP01150o	4	10
NGP-105-01	NCP003323	C08	C24H28N2O5.HCl	4.609.593	4.244.984	4.241.998	Sequoia Research Products Ltd.	SRP01060b	2	7
NGP-105-01	NCP003323	D08	C21H32O3	3.324.852	3.324.852	3.322.351	Sequoia Research Products Ltd.	SRP01300o	2	3
NGP-105-01	NCP003323	E08	C18H16O3	2.803.242	2.803.242	2.801.099	Sequoia Research Products Ltd.	SRP01425i	0	3
NGP-105-01	NCP003323	F08	C18H15NO3	2.933.229	2.933.229	2.931.051	Sequoia Research Products Ltd.	SRP012475o	1	4
NGP-105-01	NCP003323	G08	C16H21NO3	2.753.489	2.753.489	2.751.521	Sequoia Research Products Ltd.	SRP013047r	1	4
NGP-105-01	NCP003323	H08	C21H25ClFN3O3.C6H8O7	6.140.247	4.219.007	4.211.568	Sequoia Research Products Ltd.	SRP066435m	3	6
NGP-105-01	NCP003323	A09	C21H20O12	4.643.838	4.643.838	4.640.954	Sequoia Research Products Ltd.	SRP01950i	8	12
NGP-105-01	NCP003323	B09	C15H14FN3O3	3.032.937	3.032.937	3.031.019	Sequoia Research Products Ltd.	SRP01035f	0	6
NGP-105-01	NCP003323	C09	C13H12N2O2.HCl	2.647.121	2.282.512	2.280.898	Sequoia Research Products Ltd.	SRP01500o	1	4
NGP-105-01	NCP003323	D09	C21H20O12	4.643.838	4.643.838	4.640.954	Sequoia Research Products Ltd.	SRP03990h	8	12
NGP-105-01	NCP003323	E09	C46H62N4O11	8.470.222	8.470.222	8.464.415	Sequoia Research Products Ltd.	SRP01275r	5	15
NGP-105-01	NCP003323	F09	C16H25NO4.HCl	3.318.412	2.953.803	2.951.783	Sequoia Research Products Ltd.	SRP01475e	2	5
NGP-105-01	NCP003323	G09	C22H19N3O4	3.894.117	3.894.117	3.891.375	Sequoia Research Products Ltd.	SRP000800t	1	7
NGP-105-01	NCP003323	H09	C15H15NO2S	2.733.505	2.733.505	2.730.823	Sequoia Research Products Ltd.	SRP06607m	2	3
NGP-105-01	NCP003323	A10	C27H29NO11.HCl	5.799.900	5.435.291	5.431.740	Sequoia Research Products Ltd.	SRP04600d	7	12
NGP-105-01	NCP003323	B10	C9H12ClN5O.HCl	2.781.418	2.416.809	2.410.730	Sequoia Research Products Ltd.	SRP06645m	2	6
NGP-105-01	NCP003323	C10	C15H11N3O3	2.812.713	2.812.713	2.810.800	Sequoia Research Products Ltd.	SRP03417n	1	6
NGP-105-01	NCP003323	D10	C17H20FN3O3.CH4O3S	4.294.694	3.333.637	3.331.488	Sequoia Research Products Ltd.	SRP01078p	1	6
NGP-105-01	NCP003323	E10	C17H27NO2.HCl	3.138.694	2.774.085	2.772.041	Sequoia Research Products Ltd.	SRP01015v	1	3
NGP-105-01	NCP003323	F10	C16H14F2N3O4S.Na+	4.053.524	3.823.626	3.820.673	Sequoia Research Products Ltd.	SRP01075p	0	7
NGP-105-01	NCP003323	G10	C25H31F3O5S	5.005.753	5.005.753	5.001.844	Sequoia Research Products Ltd.	SRP01977f	1	5
NGP-105-01	NCP003323	H10	C36H47N5O4.H2O4S	7.118.816	6.138.031	6.133.628	Sequoia Research Products Ltd.	SRP00675i	4	9
NGP-105-01	NCP003323	A11	C18H13ClFN3.HCl	3.622.344	3.257.735	3.250.782	Sequoia Research Products Ltd.	SRP065525m	0	3
NGP-105-01	NCP003323	B11	C8H11N3O3S	2.292.543	2.292.543	2.290.521	Sequoia Research Products Ltd.	SRP01125l	3	6
NGP-105-01	NCP003323	C11	C12H19N3O.HCl	2.577.644	2.213.035	2.211.528	Sequoia Research Products Ltd.	SRP03580p	3	4
NGP-105-01	NCP003323	D11	C34H36MgNO6S2	7.131.236	7.131.236	7.125.187	Sequoia Research Products Ltd.	SRP01485e	0	12
NGP-105-01	NCP003323	E11	C18H14N4O5S	3.983.938	3.983.938	3.980.684	Sequoia Research Products Ltd.	SRP01700s	3	9
NGP-105-01	NCP003323	F11	C16H20N4O3S	3.484.210	3.484.210	3.481.256	Sequoia Research Products Ltd.	SRP02525t	3	7
NGP-105-01	NCP003323	G11	C17H20N2O2.HCl	3.208.201	2.843.592	2.841.524	Sequoia Research Products Ltd.	SRP02985t	1	4

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-01	NCP003323	H11	C24H33N3O4.2HCI	5.004.675	4.275.457	4.272.471	Sequoia Research Products Ltd.	SRP010131r	2	7
NGP-105-02	NCP003403	A02	C16H17N3O4S	3.473.897	3.473.897	3.470.939	Sequoia Research Products Ltd.	SRP01880c	4	7
NGP-105-02	NCP003403	B02	C9H12N2O4S	2.442.660	2.442.660	2.440.517	Sequoia Research Products Ltd.	SRP02360p	2	6
NGP-105-02	NCP003403	C02	C23H32N2O5	4.165.194	4.165.194	4.162.311	Sequoia Research Products Ltd.	SRP0101151r	2	7
NGP-105-02	NCP003403	D02	C22H29N2O.Br-	4.173.908	3.374.868	3.372.279	Sequoia Research Products Ltd.	SRP00470f	2	3
NGP-105-02	NCP003403	E02	C18H26O2	2.744.048	2.744.048	2.741.932	Sequoia Research Products Ltd.	SRP00900n	1	2
NGP-105-02	NCP003403	F02	C12H21N5O2S2	3.314.523	3.314.523	3.311.136	Sequoia Research Products Ltd.	SRP05385n	2	7
NGP-105-02	NCP003403	G02	C4H4FN3O	1.290.939	1.290.939	1.290.338	Sequoia Research Products Ltd.	SRP01027f	3	4
NGP-105-02	NCP003403	H02	C15H12N2O2	2.522.732	2.522.732	2.520.898	Sequoia Research Products Ltd.	SRP012480o	2	4
NGP-105-02	NCP003403	A03	C15H22N2O4	2.943.520	2.943.520	2.941.579	Sequoia Research Products Ltd.	SRP02990t	2	6
NGP-105-02	NCP003403	B03	C10H11NO3	1.932.029	1.932.029	1.930.738	Sequoia Research Products Ltd.	SRP02538a	2	4
NGP-105-02	NCP003403	C03	C22H24ClN3O.HCl	4.183.674	3.819.065	3.811.607	Sequoia Research Products Ltd.	SRP07805a	0	4
NGP-105-02	NCP003403	D03	C11H16N2O	1.922.618	1.922.618	1.921.262	Sequoia Research Products Ltd.	SRP02375t	3	3
NGP-105-02	NCP003403	E03	C15H12O7	3.042.568	3.042.568	3.040.583	Sequoia Research Products Ltd.	SRP01176t	5	7
NGP-105-02	NCP003403	F03	C18H20FN3O4	3.613.741	3.613.741	3.611.437	Sequoia Research Products Ltd.	SRP01385l	1	7
NGP-105-02	NCP003403	G03	C18H18N6O5S2.C3H8O2	5.385.936	4.624.992	4.620.780	Sequoia Research Products Ltd.	SRP01886c	6	11
NGP-105-02	NCP003403	H03	C19H30O5	3.384.460	3.384.460	3.382.093	Sequoia Research Products Ltd.	SRP00400i	1	5
NGP-105-02	NCP003403	A04	C15H23N3O4S	3.414.267	3.414.267	3.411.409	Sequoia Research Products Ltd.	SRP01395l	3	7
NGP-105-02	NCP003403	B04	C9H8N2O2	1.761.752	1.761.752	1.760.585	Sequoia Research Products Ltd.	SRP01090p	2	4
NGP-105-02	NCP003403	C04	C17H11N5	2.853.085	2.853.085	2.851.014	Sequoia Research Products Ltd.	SRP01285l	0	5
NGP-105-02	NCP003403	D04	C17H25N3O5S	3.834.641	3.834.641	3.831.514	Sequoia Research Products Ltd.	SRP02110m	3	8
NGP-105-02	NCP003403	E04	C29H53NO5	4.957.467	4.957.467	4.953.923	Sequoia Research Products Ltd.	SRP01240o	1	6
NGP-105-02	NCP003403	F04	C18H19N3O.HCl	3.298.304	2.933.695	2.931.528	Sequoia Research Products Ltd.	SRP01235o	0	4
NGP-105-02	NCP003403	G04	C21H28O2	3.124.538	3.124.538	3.122.089	Sequoia Research Products Ltd.	SRP01390l	1	2
NGP-105-02	NCP003403	H04	C17H23NO4.HCl	3.418.362	3.053.753	3.051.627	Sequoia Research Products Ltd.	SRP02040c	3	5
NGP-105-02	NCP003403	A05	C17H13ClN4	3.087.708	3.087.708	3.080.828	Sequoia Research Products Ltd.	SRP04905a	0	4
NGP-105-02	NCP003403	B05	C9H7Cl2N5	2.560.945	2.560.945	2.550.078	Sequoia Research Products Ltd.	SRP01130l	4	5
NGP-105-02	NCP003403	C05	C13H17NO	2.032.851	2.032.851	2.031.310	Sequoia Research Products Ltd.	SRP04515c	0	2
NGP-105-02	NCP003403	D05	C13H18ClNO	2.397.461	2.397.461	2.391.076	Sequoia Research Products Ltd.	SRP03725a	1	2
NGP-105-02	NCP003403	E05	C19H27N5O4	3.894.561	3.894.561	3.892.063	Sequoia Research Products Ltd.	SRP04165a	3	9
NGP-105-02	NCP003403	F05	C17H27N3O4S	3.694.807	3.694.807	3.691.722	Sequoia Research Products Ltd.	SRP05612a	3	7
NGP-105-02	NCP003403	G05	C26H27ClN2O.HCl	4.554.287	4.189.678	4.181.811	Sequoia Research Products Ltd.	SRP015615l	0	3
NGP-105-02	NCP003403	H05	C23H30N4O2S.HCl	4.630.395	4.265.786	4.262.089	Sequoia Research Products Ltd.	SRP01320P	0	6
NGP-105-02	NCP003403	A06	C43H53NO14	8.078.953	8.078.953	8.073.466	Sequoia Research Products Ltd.	SRP04571d	5	15
NGP-105-02	NCP003403	B06	C18H18O2	2.663.408	2.663.408	2.661.306	Sequoia Research Products Ltd.	SRP02135h	2	2
NGP-105-02	NCP003403	C06	C22H31NO.C4H6O6	4.755.845	3.254.961	3.252.405	Sequoia Research Products Ltd.	SRP02390t	1	2
NGP-105-02	NCP003403	D06	C11H16FN3O3	2.572.657	2.572.657	2.571.175	Sequoia Research Products Ltd.	SRP01460c	2	6
NGP-105-02	NCP003403	E06	C20H22FNO3	3.433.993	3.433.993	3.431.583	Sequoia Research Products Ltd.	SRP04325m	0	4
NGP-105-02	NCP003403	F06	C24H26N6O3	4.465.104	4.465.104	4.462.066	Sequoia Research Products Ltd.	SRP01205o	3	9

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-02	NCP003403	G06	C22H22CIN6O.K+	4.610.089	4.219.106	4.211.543	Sequoia Research Products Ltd.	SRP01580l	1	7
NGP-105-02	NCP003403	H06	C6H6N6O2	1.941.530	1.941.530	1.940.552	Sequoia Research Products Ltd.	SRP011925t	2	8
NGP-105-02	NCP003403	A07	C20H30O2	3.024.588	3.024.588	3.022.245	Sequoia Research Products Ltd.	SRP04150m	1	2
NGP-105-02	NCP003403	B07	C19H15F3N4O3.C7H8O3S	5.765.485	4.043.493	4.041.096	Sequoia Research Products Ltd.	SRP02535t	3	7
NGP-105-02	NCP003403	C07	C15H23N3O3S	3.254.273	3.254.273	3.251.460	Sequoia Research Products Ltd.	SRP01690m	1	6
NGP-105-02	NCP003403	D07	C17H21NO.HCl	2.918.220	2.553.611	2.551.623	Sequoia Research Products Ltd.	SRP07328a	1	2
NGP-105-02	NCP003403	E07	C19H28O8	3.844.282	3.844.282	3.841.784	Sequoia Research Products Ltd.	SRP073035a	1	8
NGP-105-02	NCP003403	F07	C35H38Cl2N8O4	7.056.462	7.056.462	7.042.393	Sequoia Research Products Ltd.	SRP02500i	0	12
NGP-105-02	NCP003403	G07	C21H27N5O9S2	5.575.951	5.575.951	5.571.250	Sequoia Research Products Ltd.	SRP018875c	3	14
NGP-105-02	NCP003403	H07	C17H25NO4.HCl	3.438.522	3.073.913	3.071.783	Sequoia Research Products Ltd.	SRP03422b	0	5
NGP-105-02	NCP003403	A08	C13H17CIN2O2	2.687.442	2.687.442	2.680.978	Sequoia Research Products Ltd.	SRP06605m	1	4
NGP-105-02	NCP003403	B08	C22H27ClF2O5	4.449.049	4.449.049	4.441.515	Sequoia Research Products Ltd.	SRP01205h	3	5
NGP-105-02	NCP003403	C08	C14H9Cl3N2OS	3.596.578	3.596.578	3.579.501	Sequoia Research Products Ltd.	SRP02865t	1	3
NGP-105-02	NCP003403	D08	C17H14O4S	3.143.566	3.143.566	3.140.612	Sequoia Research Products Ltd.	SRP013045r	0	4
NGP-105-02	NCP003403	E08	C18H31NO4.0.5C4H4O4	3.834.863	3.254.503	3.252.253	Sequoia Research Products Ltd.	SRP020366b	2	5
NGP-105-02	NCP003403	F08	C24H21F2NO3	4.094.338	4.094.338	4.091.489	Sequoia Research Products Ltd.	SRP04000e	2	4
NGP-105-02	NCP003403	G08	C20H25NO2S2.HCl	4.120.064	3.755.455	3.751.326	Sequoia Research Products Ltd.	SRP023505t	1	3
NGP-105-02	NCP003403	H08	C26H27NO9.HCl	5.339.642	4.975.033	4.971.685	Sequoia Research Products Ltd.	SRP000350i	6	10
NGP-105-02	NCP003403	A09	C16H12FN3O3	3.132.887	3.132.887	3.130.862	Sequoia Research Products Ltd.	SRP01021f	2	6
NGP-105-02	NCP003403	B09	C44H69NO12	8.040.355	8.040.355	8.034.819	Sequoia Research Products Ltd.	SRP00750t	3	13
NGP-105-02	NCP003403	C09	C13H20N6O4.HCl	3.608.017	3.243.408	3.241.546	Sequoia Research Products Ltd.	SRP00800v	5	10
NGP-105-02	NCP003403	D09	C38H69NO13	7.479.689	7.479.689	7.474.768	Sequoia Research Products Ltd.	SRP03660c	4	14
NGP-105-02	NCP003403	E09	C23H27Cl2N3O2	4.483.939	4.483.939	4.471.480	Sequoia Research Products Ltd.	SRP06795a	1	5
NGP-105-02	NCP003403	F09	C22H29NO5.C4H4O4	5.035.497	3.874.777	3.872.045	Sequoia Research Products Ltd.	SRP02875t	0	6
NGP-105-02	NCP003403	G09	C20H32O2	3.044.748	3.044.748	3.042.402	Sequoia Research Products Ltd.	SRP02260m	1	2
NGP-105-02	NCP003403	H09	C20H24N2O6	3.884.218	3.884.218	3.881.634	Sequoia Research Products Ltd.	SRP03410n	1	8
NGP-105-02	NCP003403	A10	C20H22O8	3.903.912	3.903.912	3.901.314	Sequoia Research Products Ltd.	SRP02318p	6	8
NGP-105-02	NCP003403	B10	C7H11N3O3	1.851.833	1.851.833	1.850.800	Sequoia Research Products Ltd.	SRP010965s	1	6
NGP-105-02	NCP003403	C10	C19H27N5O5.HCl	4.419.164	4.054.555	4.052.012	Sequoia Research Products Ltd.	SRP034084n	2	10
NGP-105-02	NCP003403	D10	C19H27NO3	3.174.299	3.174.299	3.171.990	Sequoia Research Products Ltd.	SRP03325n	2	4
NGP-105-02	NCP003403	E10	C24H32O4	3.845.176	3.845.176	3.842.300	Sequoia Research Products Ltd.	SRP01730m	0	4
NGP-105-02	NCP003403	F10	C14H18N4O2	2.743.236	2.743.236	2.741.429	Sequoia Research Products Ltd.	SRP01245o	4	6
NGP-105-02	NCP003403	G10	C11H12N2O2S	2.362.892	2.362.892	2.360.619	Sequoia Research Products Ltd.	SRP01100z	3	4
NGP-105-02	NCP003403	H10	C10H12N2O4	2.242.170	2.242.170	2.240.797	Sequoia Research Products Ltd.	SRP1625s	2	6
NGP-105-02	NCP003403	A11	C16H23N3O4.CH4O3S	4.174.834	3.213.777	3.211.688	Sequoia Research Products Ltd.	SRP00500g	4	7
NGP-105-02	NCP003403	B11	C18H13Cl4N3O.HNO3	4.921.463	4.291.335	4.269.812	Sequoia Research Products Ltd.	SRP012492o	0	4
NGP-105-02	NCP003403	C11	C42H69NO15	8.280.117	8.280.117	8.274.667	Sequoia Research Products Ltd.	SRP01340k	3	16
NGP-105-02	NCP003403	D11	C14H19N5O4	3.213.371	3.213.371	3.211.437	Sequoia Research Products Ltd.	SRP00400f	2	9
NGP-105-02	NCP003403	E11	C12H20N2O3S.HCl	3.088.245	2.723.636	2.721.194	Sequoia Research Products Ltd.	SRP01610s	3	5
NGP-105-02	NCP003403	F11	C17H18FN3O3S	3.634.077	3.634.077	3.631.052	Sequoia Research Products Ltd.	SRP01330r	1	6

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-02	NCP003403	G11	C15H12O7	3.042.568	3.042.568	3.040.583	Sequoia Research Products Ltd.	SRP01175t	5	7
NGP-105-02	NCP003403	H11	C17H18N4O.HCl	3.308.181	2.943.572	2.941.480	Sequoia Research Products Ltd.	SRP04894a	1	5
NGP-105-03	NCP003483	A02	C16H24N2O4	3.083.790	3.083.790	3.081.736	Sequoia Research Products Ltd.	SRP00500u	5	6
NGP-105-03	NCP003483	B02	C26H28ClNO.C6H8O7	5.980.931	4.059.691	4.051.859	Sequoia Research Products Ltd.	SRP02530t	0	2
NGP-105-03	NCP003483	C02	C59H84N18O14.C2H4O2	13.294.852	12.694.332	12.686.414	Sequoia Research Products Ltd.	SRP02570g	20	32
NGP-105-03	NCP003483	D02	C20H26O6	3.624.244	3.624.244	3.621.729	Sequoia Research Products Ltd.	SRP01097s	4	6
NGP-105-03	NCP003483	E02	C21H22N4O6S	4.584.902	4.584.902	4.581.260	Sequoia Research Products Ltd.	SRP010115r	4	10
NGP-105-03	NCP003483	F02	C24H30N2O2.HCl	4.149.771	3.785.162	3.782.307	Sequoia Research Products Ltd.	SRP04574d	0	4
NGP-105-03	NCP003483	G02	C14H16N2O.0.5C4H6O4	2.873.388	2.282.948	2.281.262	Tocris Bioscience	912	2	3
NGP-105-03	NCP003483	H02	C23H26N2O4	3.944.720	3.944.720	3.941.892	Sigma Chemical Company	399027	0	6
NGP-105-03	NCP003483	A03	C11H12N2	1.722.304	1.722.304	1.721.000	Sigma Chemical Company	300764	2	2
NGP-105-03	NCP003483	B03	C22H26F3N3OS.2HCl	5.104.466	4.375.248	4.371.748	Sigma Chemical Company	F4765	1	4
NGP-105-03	NCP003483	C03	C19H24N2O.HCl	3.328.747	2.964.138	2.961.888	Sequoia Research Products Ltd.	SRP02460p	0	3
NGP-105-03	NCP003483	D03	C14H13O3.Na+	2.522.460	2.292.562	2.290.864	Sigma Chemical Company	M1275	0	3
NGP-105-03	NCP003483	E03	C15H22N2O.HCl	2.828.147	2.463.538	2.461.732	Sigma Chemical Company	M3189	1	3
NGP-105-03	NCP003483	F03	C17H12Br2O3	4.240.892	4.240.892	4.219.153	Sigma Chemical Company	B5774	1	3
NGP-105-03	NCP003483	G03	C21H26N2O7	4.184.482	4.184.482	4.181.740	Sigma Chemical Company	N149	1	9
NGP-105-03	NCP003483	H03	C27H33N3O8	5.275.763	5.275.763	5.272.267	Sigma Chemical Company	R2253	6	11
NGP-105-03	NCP003483	A04	C11H14N4O2	2.342.586	2.342.586	2.341.116	Sigma Chemical Company	M9017	0	6
NGP-105-03	NCP003483	B04	C8H11N3O6	2.451.925	2.451.925	2.450.647	Sigma Chemical Company	A1882	4	9
NGP-105-03	NCP003483	C04	C21H30O4	3.464.686	3.464.686	3.462.144	Sigma Chemical Company	R0500	2	4
NGP-105-03	NCP003483	D04	C6H7NO	1.091.281	1.091.281	1.090.527	Sigma Chemical Company	P66807	1	2
NGP-105-03	NCP003483	E04	C21H23ClFNO2.HCl	4.123.328	3.758.719	3.751.401	Tocris Bioscience	100330	1	3
NGP-105-03	NCP003483	F04	C14H18O3	2.342.962	2.342.962	2.341.255	Tocris Bioscience	100267	1	3
NGP-105-03	NCP003483	G04	C19H20FN3	3.093.875	3.093.875	3.091.641	Tocris Bioscience	100737	0	3
NGP-105-03	NCP003483	H04	C21H34NO3.Br-	4.284.119	3.485.079	3.482.538	Sigma Chemical Company	O5501	1	4
NGP-105-03	NCP003483	A05	C10H15NO2	1.812.355	1.812.355	1.811.102	Sigma Chemical Company	D136204	2	3
NGP-105-03	NCP003483	B05	C8H13N3O4S	2.472.697	2.472.697	2.470.626	Sigma Chemical Company	T3021	0	7
NGP-105-03	NCP003483	C05	C13H21N5O4.C6H5NO2	4.344.511	3.113.421	3.111.593	Sigma Chemical Company	X6750	2	9
NGP-105-03	NCP003483	D05	C9H13NO2	1.672.085	1.672.085	1.670.946	Sigma Chemical Company	s0752	3	3
NGP-105-03	NCP003483	E05	C14H12O3	2.282.482	2.282.482	2.280.786	Sigma Chemical Company	R5010	3	3
NGP-105-03	NCP003483	F05	C6H6O3	1.261.122	1.261.122	1.260.316	Sigma Chemical Company	H43407	1	3
NGP-105-03	NCP003483	G05	C7H7N3	1.331.531	1.331.531	1.330.639	Sigma Chemical Company	A59565	3	3
NGP-105-03	NCP003483	H05	C19H22FN3O3	3.594.017	3.594.017	3.591.645	Sigma Chemical Company	17849	1	6
NGP-105-03	NCP003483	A06	C24H34O5	4.025.330	4.025.330	4.022.406	Sigma Chemical Company	30830	1	5
NGP-105-03	NCP003483	B06	C15H14ClN3O4S	3.678.077	3.678.077	3.670.393	Sigma Chemical Company	C6895	4	7
NGP-105-03	NCP003483	C06	C10H10N2	1.582.034	1.582.034	1.580.843	Sigma Chemical Company	116416	0	2
NGP-105-03	NCP003483	D06	C18H19NOS.HCl	3.338.770	2.974.161	2.971.187	Sequoia Research Products Ltd.	SRP05005d	1	2
NGP-105-03	NCP003483	E06	C23H32N6O4S.C6H8O7	6.807.308	4.886.068	4.882.205	Sequoia Research Products Ltd.	SRP01005v	1	10

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-03	NCP003483	F06	C17H26N2O.HCl	3.108.687	2.744.078	2.742.045	Sequoia Research Products Ltd.	SRP01307r	1	3
NGP-105-03	NCP003483	G06	C17H19N5	2.933.725	2.933.725	2.931.640	Sequoia Research Products Ltd.	SRP05647a	0	5
NGP-105-03	NCP003483	H06	C19H19NOS.C4H4O4	4.254.991	3.094.271	3.091.187	Tocris Bioscience	100029	0	2
NGP-105-03	NCP003483	A07	C22H32O3	3.444.962	3.444.962	3.442.351	Sigma Chemical Company	M6013	1	3
NGP-105-03	NCP003483	B07	C13H19N5.H2O	2.633.438	2.453.285	2.451.640	Sigma Chemical Company	P154	2	5
NGP-105-03	NCP003483	C07	C7H5N3O2	1.631.359	1.631.359	1.630.381	Sigma Chemical Company	N7778	1	5
NGP-105-03	NCP003483	D07	C11H14N2O	1.902.458	1.902.458	1.901.106	Sigma Chemical Company	286583	3	3
NGP-105-03	NCP003483	E07	C12H9NS	1.992.707	1.992.707	1.990.455	Sigma Chemical Company	P14831	1	1
NGP-105-03	NCP003483	F07	C10H12ClN5O3	2.856.907	2.856.907	2.850.628	Sequoia Research Products Ltd.	SRP03655c	4	8
NGP-105-03	NCP003483	G07	C18H24N4O.HCl	3.488.771	3.124.162	3.121.950	Sequoia Research Products Ltd.	SRP02575g	1	5
NGP-105-03	NCP003483	H07	C21H27N3.0.5H2O.2HCl	4.033.966	3.214.671	3.212.204	Tocris Bioscience	1497	1	3
NGP-105-03	NCP003483	A08	C22H27N3O2	3.654.769	3.654.769	3.652.103	Tocris Bioscience	1347	1	5
NGP-105-03	NCP003483	B08	C22H29FO4	3.764.700	3.764.700	3.762.049	Sigma Chemical Company	D6038	2	4
NGP-105-03	NCP003483	C08	C16H19ClN2.C4H4O4	3.908.664	2.747.944	2.741.236	Sequoia Research Products Ltd.	SRP02129d	0	2
NGP-105-03	NCP003483	D08	C12H17N5	2.313.015	2.313.015	2.311.483	Tocris Bioscience	1355	2	5
NGP-105-03	NCP003483	E08	C20H21N5O3S.2H2O	4.475.103	4.114.797	4.111.365	Tocris Bioscience	781	4	8
NGP-105-03	NCP003483	F08	C22H21Cl2IN4O	5.552.467	5.552.467	5.540.137	Tocris Bioscience	1117	1	5
NGP-105-03	NCP003483	G08	C19H25F3N4O.2C4H4O4	6.145.745	3.824.305	3.821.980	Tocris Bioscience	646	3	5
NGP-105-03	NCP003483	H08	C17H17NO2.1H2O.HCl	3.353.162	2.673.285	2.671.259	Tocris Bioscience	884	3	3
NGP-105-03	NCP003483	A09	C21H27N3O3S.2HCl	4.744.471	4.015.253	4.011.773	Tocris Bioscience	1808	1	6
NGP-105-03	NCP003483	B09	C26H21N3O.0.25H2O.2HC l	4.688.991	3.914.735	3.911.684	Tocris Bioscience	1999	0	4
NGP-105-03	NCP003483	C09	C22H29ClO5	4.089.240	4.089.240	4.081.703	Sigma Chemical Company	B0385	3	5
NGP-105-03	NCP003483	D09	C17H19N3O3S	3.454.173	3.454.173	3.451.147	Sigma Chemical Company	O104	1	6
NGP-105-03	NCP003483	E09	C19H20N2O3.CH4O3S	4.204.863	3.243.806	3.241.473	Sequoia Research Products Ltd.	SRP045724d	1	5
NGP-105-03	NCP003483	F09	C16H21N3O2	2.873.629	2.873.629	2.871.633	Sequoia Research Products Ltd.	SRP01300z	2	5
NGP-105-03	NCP003483	G09	C27H28O11	5.285.144	5.285.144	5.281.631	Sequoia Research Products Ltd.	SRP02720t	4	11
NGP-105-03	NCP003483	H09	C62H86N12O16	12.554.408	12.554.408	12.546.284	Sequoia Research Products Ltd.	SRP00450d	6	28
NGP-105-03	NCP003483	A10	C16H25NO2.HCl	2.998.424	2.633.815	2.631.885	Sequoia Research Products Ltd.	SRP02565t	1	3
NGP-105-03	NCP003483	B10	C16H14ClN3O	2.997.605	2.997.605	2.990.825	Sequoia Research Products Ltd.	SRP02170c	1	4
NGP-105-03	NCP003483	C10	C16H15N5O7S2.3H2O	5.074.912	4.534.453	4.530.412	Sequoia Research Products Ltd.	SRP018865c	5	12
NGP-105-03	NCP003483	D10	C14H13N5O5S2	3.954.085	3.954.085	3.950.358	Sequoia Research Products Ltd.	SRP018855c	5	10
NGP-105-03	NCP003483	E10	C11H12Cl2N2O.HCl	2.955.967	2.591.358	2.580.326	Sequoia Research Products Ltd.	SRP01565l	1	3
NGP-105-03	NCP003483	F10	C17H15N3O6	3.573.235	3.573.235	3.570.960	Sequoia Research Products Ltd.	SRP00900b	4	9
NGP-105-03	NCP003483	G10	C21H23NO3.HCl	3.738.808	3.374.199	3.371.677	Sequoia Research Products Ltd.	SRP01210o	1	4
NGP-105-03	NCP003483	H10	C50H46CaF2N2O8	8.810.035	8.810.035	8.804.022	Sequoia Research Products Ltd.	SRP02390i	4	10
NGP-105-03	NCP003483	A11	C21H28O5	3.604.520	3.604.520	3.601.936	Sigma Chemical Company	C2755	2	5
NGP-105-03	NCP003483	B11	C21H21N.HCl	3.238.666	2.874.057	2.871.673	Sigma Chemical Company	C6022	0	1
NGP-105-03	NCP003483	C11	C29H39NO9	5.456.323	5.456.323	5.452.624	Sequoia Research Products Ltd.	SRP02125h	3	10
NGP-105-03	NCP003483	D11	C21H30O4	3.464.686	3.464.686	3.462.144	Sigma Chemical Company	C2505	2	4

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-03	NCP003483	E11	C34H57N2O4.Br-	6.377.450	5.578.410	5.574.318	Sequoia Research Products Ltd.	SRP01010v	0	6
NGP-105-03	NCP003483	F11	C21H28O2	3.124.538	3.124.538	3.122.089	Sequoia Research Products Ltd.	SRP02352t	1	2
NGP-105-03	NCP003483	G11	C6H6N2O	1.221.268	1.221.268	1.220.480	Sigma Chemical Company	240206	2	3
NGP-105-03	NCP003483	H11	C16H18N4O2	2.983.456	2.983.456	2.981.429	Sigma Chemical Company	252999	3	6
NGP-105-04	NCP003563	A02	C10H12CIN5O4	3.016.901	3.016.901	3.010.577	Sigma Chemical Company	C5134	5	9
NGP-105-04	NCP003563	B02	C7H10CIN3O3	2.196.283	2.196.283	2.190.410	Sigma Chemical Company	O5879	1	6
NGP-105-04	NCP003563	C02	C12H19N2.I-	3.182.014	1.912.974	1.911.548	Sigma Chemical Company	D5891	0	2
NGP-105-04	NCP003563	D02	C23H24FN3O2	3.934.623	3.934.623	3.931.852	Sigma Chemical Company	P126	0	5
NGP-105-04	NCP003563	E02	C21H26O2	3.104.378	3.104.378	3.101.932	Sigma Chemical Company	855871	1	2
NGP-105-04	NCP003563	F02	C20H25NO3.HCl	3.638.858	3.274.249	3.271.834	Sigma Chemical Company	B704	1	4
NGP-105-04	NCP003563	G02	C7H10N2	1.221.704	1.221.704	1.220.843	Sigma Chemical Company	A55306	2	2
NGP-105-04	NCP003563	H02	C2H2Cl2O2	1.289.428	1.289.428	1.279.431	Sigma Chemical Company	D54702	1	2
NGP-105-04	NCP003563	A03	C22H22FN3O2S.1H2O.HCl	4.749.792	4.114.953	4.111.416	Tocris Bioscience	1809	1	5
NGP-105-04	NCP003563	B03	C17H20N2O.HCl	3.048.207	2.683.598	2.681.575	Tocris Bioscience	1622	3	3
NGP-105-04	NCP003563	C03	C18H29NO3.HCl	3.438.958	3.074.349	3.072.147	Tocris Bioscience	906	2	4
NGP-105-04	NCP003563	D03	C16H10N2O2	2.622.682	2.622.682	2.620.742	Sequoia Research Products Ltd.	SRP00750i	2	4
NGP-105-04	NCP003563	E03	C17H20CIN3O3.HCl	3.862.792	3.498.183	3.491.193	Tocris Bioscience	380	1	6
NGP-105-04	NCP003563	F03	C19H25Cl2N3O3.C4H4O4	5.304.053	4.143.333	4.131.272	Tocris Bioscience	1483	0	6
NGP-105-04	NCP003563	G03	C25H31O8.Na+	4.825.080	4.595.182	4.592.018	Sigma Chemical Company	P4153	2	8
NGP-105-04	NCP003563	H03	C8H7CIN2O2S	2.306.692	2.306.692	2.299.916	Sigma Chemical Company	D9035	1	4
NGP-105-04	NCP003563	A04	C18H20N2O6	3.603.678	3.603.678	3.601.321	Sequoia Research Products Ltd.	SRP00418n	1	8
NGP-105-04	NCP003563	B04	C38H50N6O5.CH4O3S	7.669.609	6.708.552	6.703.842	Sequoia Research Products Ltd.	SRP01070s	6	11
NGP-105-04	NCP003563	C04	C22H18N2	3.103.994	3.103.994	3.101.469	Sequoia Research Products Ltd.	SRP02006b	0	2
NGP-105-04	NCP003563	D04	C14H21N3O2S.C4H6O4	4.134.889	2.954.009	2.951.354	Sequoia Research Products Ltd.	SRP01780s	2	5
NGP-105-04	NCP003563	E04	C20H24O2	2.964.108	2.964.108	2.961.776	Sequoia Research Products Ltd.	SRP03000e	0	2
NGP-105-04	NCP003563	F04	C12H9N3O5S	3.072.811	3.072.811	3.070.262	Sequoia Research Products Ltd.	SRP03412n	1	8
NGP-105-04	NCP003563	G04	C16H13CIN2O	2.847.458	2.847.458	2.840.716	Sequoia Research Products Ltd.	SRP02375d	0	3
NGP-105-04	NCP003563	H04	C21H25N3O2S.C4H4O4	4.995.819	3.835.099	3.831.667	Sequoia Research Products Ltd.	SRP01075q	1	5
NGP-105-04	NCP003563	A05	C27H30O16	6.105.274	6.105.274	6.101.533	Sequoia Research Products Ltd.	SRP01350r	10	16
NGP-105-04	NCP003563	B05	C10H15N5O3	2.532.617	2.532.617	2.531.174	Sequoia Research Products Ltd.	SRP01095p	5	8
NGP-105-04	NCP003563	C05	C27H44O3	4.166.472	4.166.472	4.163.290	Sequoia Research Products Ltd.	SRP01075c	3	3
NGP-105-04	NCP003563	D05	C30H32N2O2.HCl	4.890.591	4.525.982	4.522.463	Sequoia Research Products Ltd.	SRP04225d	0	4
NGP-105-04	NCP003563	E05	C11H14N2O4.0.33H2O	2.441.890	2.382.440	2.380.953	Tocris Bioscience	100813	4	6
NGP-105-04	NCP003563	F05	C22H22FN3O2	3.794.353	3.794.353	3.791.696	Tocris Bioscience	101276	1	5
NGP-105-04	NCP003563	G05	C13H18N4O3	2.783.120	2.783.120	2.781.378	Tocris Bioscience	101755	0	7
NGP-105-04	NCP003563	H05	C14H16N2O2	2.442.942	2.442.942	2.441.211	Tocris Bioscience	1471	0	4
NGP-105-04	NCP003563	A06	C37H48N6O5S2	7.209.482	7.209.482	7.203.127	Sequoia Research Products Ltd.	SRP01303r	4	11
NGP-105-04	NCP003563	B06	C45H54N4O8.2C4H6O6	10.791.258	7.789.490	7.783.941	Sequoia Research Products Ltd.	SRP01040v	2	12
NGP-105-04	NCP003563	C06	C16H20FN3O4	3.373.521	3.373.521	3.371.437	Sequoia Research Products Ltd.	SRP01440l	1	7

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-04	NCP003563	D06	C27H30F2N2O3.2HCl	5.414.673	4.685.455	4.682.224	Sequoia Research Products Ltd.	SRP01568l	0	5
NGP-105-04	NCP003563	E06	C14H9ClF3NO2	3.156.798	3.156.798	3.150.273	Sequoia Research Products Ltd.	SRP01025e	1	3
NGP-105-04	NCP003563	F06	C25H28N6O	4.285.386	4.285.386	4.282.324	Sequoia Research Products Ltd.	SRP01502i	1	7
NGP-105-04	NCP003563	G06	C27H36N2O4	4.525.960	4.525.960	4.522.675	Sequoia Research Products Ltd.	SRP01040r	2	6
NGP-105-04	NCP003563	H06	C20H32O	2.884.754	2.884.754	2.882.453	Sequoia Research Products Ltd.	SRP02030e	1	1
NGP-105-04	NCP003563	A07	C16H16O3	2.563.022	2.563.022	2.561.099	Sequoia Research Products Ltd.	SRP03680p	1	3
NGP-105-04	NCP003563	B07	C19H28N2O4.HCl	3.849.049	3.484.440	3.482.049	Sequoia Research Products Ltd.	SRP01326r	1	6
NGP-105-04	NCP003563	C07	C16H19BrN2.C4H4O4	4.353.174	3.192.454	3.180.731	Sequoia Research Products Ltd.	SRP02128d	0	2
NGP-105-04	NCP003563	D07	C10H7Cl2N3O.HCl	2.925.524	2.560.915	2.549.966	Sequoia Research Products Ltd.	SRP05646a	1	4
NGP-105-04	NCP003563	E07	C16H23N5O.C4H4O4	4.174.649	3.013.929	3.011.902	Sequoia Research Products Ltd.	SRP01187t	4	6
NGP-105-04	NCP003563	F07	C12H9N3O	2.112.235	2.112.235	2.110.745	Sequoia Research Products Ltd.	SRP06575m	1	4
NGP-105-04	NCP003563	G07	C21H25ClN2O3	3.888.956	3.888.956	3.881.553	Sequoia Research Products Ltd.	SRP01384l	1	5
NGP-105-04	NCP003563	H07	C20H21FN2O.HBr	4.053.111	3.243.992	3.241.637	Sequoia Research Products Ltd.	SRP03585c	0	3
NGP-105-04	NCP003563	A08	C14H14ClNS.HCl	3.002.466	2.637.857	2.630.535	Sequoia Research Products Ltd.	SRP02355t	0	1
NGP-105-04	NCP003563	B08	C15H17O3.Na+	2.682.890	2.452.992	2.451.177	Sequoia Research Products Ltd.	SRP01595l	0	3
NGP-105-04	NCP003563	C08	C31H33N3O6S	5.756.815	5.756.815	5.752.090	Sequoia Research Products Ltd.	SRP00200z	2	9
NGP-105-04	NCP003563	D08	C21H25N.HCl	3.278.986	2.914.377	2.911.986	Sequoia Research Products Ltd.	SRP01197t	0	1
NGP-105-04	NCP003563	E08	C19H21N3O5	3.713.941	3.713.941	3.711.481	Sequoia Research Products Ltd.	SRP01970i	1	8
NGP-105-04	NCP003563	F08	C24H29N5O3	4.355.277	4.355.277	4.352.270	Sequoia Research Products Ltd.	SRP00900v	2	8
NGP-105-04	NCP003563	G08	C15H13N3O4S.0.25H2O	3.358.505	3.313.467	3.310.626	Tocris Bioscience	100486	2	7
NGP-105-04	NCP003563	H08	C19H28NO3.Br-	3.983.419	3.184.379	3.182.069	Sequoia Research Products Ltd.	SRP02450g	1	4
NGP-105-04	NCP003563	A09	C15H21N3O2.0.5H2O4S	3.243.912	2.753.519	2.751.633	Tocris Bioscience	100352	1	5
NGP-105-04	NCP003563	B09	C27H34ClNO2S	4.720.875	4.720.875	4.711.998	Tocris Bioscience	1311	1	3
NGP-105-04	NCP003563	C09	C17H22N2O.C4H6O4	3.884.638	2.703.758	2.701.732	Tocris Bioscience	100918	0	3
NGP-105-04	NCP003563	D09	C15H22N2O.HCl	2.828.147	2.463.538	2.461.732	Tocris Bioscience	100047	2	3
NGP-105-04	NCP003563	E09	C4H3FN2O	1.140.792	1.140.792	1.140.229	Tocris Bioscience	101322	1	3
NGP-105-04	NCP003563	F09	C16H19ClN2.C4H4O4	3.908.664	2.747.944	2.741.236	Tocris Bioscience	100728	0	2
NGP-105-04	NCP003563	G09	C19H27N3O5S2	4.415.621	4.415.621	4.411.392	Sequoia Research Products Ltd.	SRP045723d	2	8
NGP-105-04	NCP003563	H09	C19H24N2O4.2H2O.C4H4O4	4.965.146	3.444.120	3.441.736	Sequoia Research Products Ltd.	SRP02131f	4	6
NGP-105-04	NCP003563	A10	C15H19N5.C7H6O2	3.914.715	2.693.505	2.691.640	Sequoia Research Products Ltd.	SRP013035r	1	5
NGP-105-04	NCP003563	B10	C47H64N4O12	8.770.486	8.770.486	8.764.520	Sequoia Research Products Ltd.	SRP01280r	6	16
NGP-105-04	NCP003563	C10	C24H31ClO7	4.669.608	4.669.608	4.661.758	Sequoia Research Products Ltd.	SRP01583l	1	7
NGP-105-04	NCP003563	D10	C18H24N2O5	3.484.004	3.484.004	3.481.685	Sequoia Research Products Ltd.	SRP010855e	3	7
NGP-105-04	NCP003563	E10	C24H29NO3.HCl	4.159.618	3.795.009	3.792.147	Sequoia Research Products Ltd.	SRP04573d	0	4
NGP-105-04	NCP003563	F10	C16H13N3O3	2.952.983	2.952.983	2.950.956	Sequoia Research Products Ltd.	SRP034095n	0	6
NGP-105-04	NCP003563	G10	C8H9N3O4	2.111.777	2.111.777	2.110.593	Sequoia Research Products Ltd.	SRP034079n	1	7
NGP-105-04	NCP003563	H10	C33H30N4O2	5.146.286	5.146.286	5.142.368	Sequoia Research Products Ltd.	SRP01192t	1	6
NGP-105-04	NCP003563	A11	C20H26N2O4.HCl	3.948.999	3.584.390	3.581.892	Sequoia Research Products Ltd.	SRP02400i	1	6
NGP-105-04	NCP003563	B11	C43H51N3O11	7.858.945	7.858.945	7.853.523	Sequoia Research Products Ltd.	SRP01281r	5	14

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-04	NCP003563	C11	C35H35ClNO3S.Na+	6.081.727	5.851.829	5.842.026	Sequoia Research Products Ltd.	SRP06641m	1	4
NGP-105-04	NCP003563	D11	C9H13N3O3	2.112.213	2.112.213	2.110.956	Sequoia Research Products Ltd.	SRP00250z	3	6
NGP-105-04	NCP003563	E11	C9H9Cl2N3.HCl	2.665.580	2.300.971	2.290.173	Tocris Bioscience	690	2	3
NGP-105-04	NCP003563	F11	C24H31N5O2	4.215.443	4.215.443	4.212.477	Tocris Bioscience	1105	1	7
NGP-105-04	NCP003563	G11	C10H13N5O3.0.25H2O	2.557.495	2.512.457	2.511.018	Tocris Bioscience	101399	4	8
NGP-105-04	NCP003563	H11	C21H27NO2.0.5H2O.0.5C4H6O6	4.095.044	3.254.525	3.252.041	Tocris Bioscience	100657	2	3
NGP-105-05	NCP003643	A02	C7H7NO3	1.531.379	1.531.379	1.530.425	Tocris Bioscience	101661	4	4
NGP-105-05	NCP003643	B02	C19H20FNO3.C4H4O4	4.454.443	3.293.723	3.291.427	Tocris Bioscience	100038	1	4
NGP-105-05	NCP003643	C02	C22H27NO2.HCl	3.739.244	3.374.635	3.372.041	Tocris Bioscience	100344	1	3
NGP-105-05	NCP003643	D02	C7H16N4O2.C2H4O2	2.482.826	1.882.306	1.881.273	Tocris Bioscience	101931	6	6
NGP-105-05	NCP003643	E02	C15H13NO3.C4H11NO3	3.764.089	2.552.739	2.550.895	Sequoia Research Products Ltd.	SRP01182k	1	4
NGP-105-05	NCP003643	F02	C17H23ClO4	3.268.216	3.268.216	3.261.284	Tocris Bioscience	101478	0	4
NGP-105-05	NCP003643	G02	C22H18O11	4.583.794	4.583.794	4.580.849	Tocris Bioscience	100468	8	11
NGP-105-05	NCP003643	H02	C15H20Cl2N2O3	3.472.426	3.472.426	3.460.850	Tocris Bioscience	100155	2	5
NGP-105-05	NCP003643	A03	C15H20ClN3O2.H2O.HCl	3.642.731	3.097.969	3.091.244	Tocris Bioscience	100111	3	5
NGP-105-05	NCP003643	B03	C17H18BrNO.HBr	4.131.530	3.322.411	3.310.571	Tocris Bioscience	100174	1	2
NGP-105-05	NCP003643	C03	C26H37NO2	3.955.875	3.955.875	3.952.824	Tocris Bioscience	100122	2	3
NGP-105-05	NCP003643	D03	C21H27NO4.HCl	3.939.122	3.574.513	3.571.940	Tocris Bioscience	100313	3	5
NGP-105-05	NCP003643	E03	C11H16N2O2.HCl	2.447.221	2.082.612	2.081.211	Tocris Bioscience	101761	0	4
NGP-105-05	NCP003643	F03	C17H18N2O6	3.463.408	3.463.408	3.461.164	Tocris Bioscience	101709	1	8
NGP-105-05	NCP003643	G03	C15H13FO2	2.442.662	2.442.662	2.440.899	Tocris Bioscience	101507	1	2
NGP-105-05	NCP003643	H03	C7H9NO2	1.391.545	1.391.545	1.390.633	Tocris Bioscience	101427	1	3
NGP-105-05	NCP003643	A04	C18H18ClN3O.C4H6O4	4.459.025	3.278.145	3.271.138	Tocris Bioscience	100738	0	4
NGP-105-05	NCP003643	B04	C18H25NO.H2O.HBr	3.703.313	2.714.041	2.711.936	Tocris Bioscience	101433	0	2
NGP-105-05	NCP003643	C04	C18H19NOS	2.974.161	2.974.161	2.971.187	Tocris Bioscience	100318	1	2
NGP-105-05	NCP003643	D04	C21H23NO4S	3.854.793	3.854.793	3.851.347	Tocris Bioscience	101458	1	5
NGP-105-05	NCP003643	E04	C14H10Cl2N2NaO2	3.181.352	3.181.352	3.169.986	Tocris Bioscience	101435	1	3
NGP-105-05	NCP003643	F04	C21H30O2	3.144.698	3.144.698	3.142.245	Tocris Bioscience	101771	0	2
NGP-105-05	NCP003643	G04	C8H15N7O2S3	3.374.337	3.374.337	3.370.449	Tocris Bioscience	101156	8	9
NGP-105-05	NCP003643	H04	C10H14ClN3.HCl	2.481.560	2.116.951	2.110.876	Tocris Bioscience	100714	2	3
NGP-105-05	NCP003643	A05	C35H60N2O4.2Br-	7.326.840	5.728.760	5.724.553	Tocris Bioscience	100349	0	6
NGP-105-05	NCP003643	B05	C6H9N3O3	1.711.563	1.711.563	1.710.643	Tocris Bioscience	101667	1	6
NGP-105-05	NCP003643	C05	C17H21NO4.3H2O.HBr	4.383.171	3.033.593	3.031.470	Tocris Bioscience	101890	1	5
NGP-105-05	NCP003643	D05	C27H38N2O4.0.5H2O.HCl	5.000.806	4.546.120	4.542.831	Tocris Bioscience	101617	0	6
NGP-105-05	NCP003643	E05	C13H17N.HCl	2.237.466	1.872.857	1.871.360	Tocris Bioscience	101891	0	1
NGP-105-05	NCP003643	F05	C18H27NO3	3.054.189	3.054.189	3.051.990	Tocris Bioscience	100605	2	4
NGP-105-05	NCP003643	G05	C13H21NO3.0.5H2O4S	2.883.552	2.393.159	2.391.521	Tocris Bioscience	101881	4	4
NGP-105-05	NCP003643	H05	C17H25NO.HCl	2.958.540	2.593.931	2.591.936	Tocris Bioscience	100353	1	2

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-05	NCP003643	A06	C15H18O7.C15H16O6	6.025.887	3.103.048	3.101.052	Tocris Bioscience	100596	2	7
NGP-105-05	NCP003643	B06	C19H25N5O4.2H2O.HCl	4.599.316	3.874.401	3.871.906	Tocris Bioscience	100080	2	9
NGP-105-05	NCP003643	C06	C15H10O	2.062.444	2.062.444	2.060.731	Tocris Bioscience	101438	0	1
NGP-105-05	NCP003643	D06	C4H5NO3S	1.471.489	1.471.489	1.469.990	Tocris Bioscience	101743	2	4
NGP-105-05	NCP003643	E06	C21H26N2O52.C6H6O3S	5.447.440	3.865.718	3.861.486	Tocris Bioscience	100739	0	3
NGP-105-05	NCP003643	F06	C12H10F2N2O3	2.682.205	2.682.205	2.680.659	Tocris Bioscience	101260	1	5
NGP-105-05	NCP003643	G06	C20H24ClN3S.2C4H4O4	6.060.891	3.739.451	3.731.379	Tocris Bioscience	101287	0	3
NGP-105-05	NCP003643	H06	C12H16N2	1.882.734	1.882.734	1.881.313	Tocris Bioscience	101561	2	2
NGP-105-05	NCP003643	A07	C22H17ClN2	3.448.444	3.448.444	3.441.080	Tocris Bioscience	101397	0	2
NGP-105-05	NCP003643	B07	C22H23ClN2O2	3.828.912	3.828.912	3.821.448	Tocris Bioscience	100099	0	4
NGP-105-05	NCP003643	C07	C8H12N2.H2O4S	2.342.759	1.361.974	1.361.000	Tocris Bioscience	100790	3	2
NGP-105-05	NCP003643	D07	C8H5F3N2O5.HCl	2.706.570	2.341.961	2.340.074	Tocris Bioscience	100955	2	3
NGP-105-05	NCP003643	E07	C26H26N2O3.1H2O.HCl	4.779.894	4.145.056	4.141.943	Tocris Bioscience	101181	3	5
NGP-105-05	NCP003643	F07	C9H12N2	1.482.084	1.482.084	1.481.000	Tocris Bioscience	100188	1	2
NGP-105-05	NCP003643	G07	C18H23NO.HCl	3.058.490	2.693.881	2.691.779	Tocris Bioscience	100103	1	2
NGP-105-05	NCP003643	H07	C13H8ClN5O	2.856.929	2.856.929	2.850.417	Tocris Bioscience	100341	2	6
NGP-105-05	NCP003643	A08	C20H24N2O5.0.25H2O.HCl	3.814.495	3.404.848	3.401.609	Tocris Bioscience	100354	1	3
NGP-105-05	NCP003643	B08	C23H29ClFN3O4.H2O	4.839.694	4.659.541	4.651.830	Tocris Bioscience	100112	3	7
NGP-105-05	NCP003643	C08	C16H15Cl2N.HCl	3.286.696	2.922.087	2.910.581	Tocris Bioscience	100118	1	1
NGP-105-05	NCP003643	D08	C19H22ClN5O.HCl	4.083.318	3.718.709	3.711.512	Tocris Bioscience	100843	0	6
NGP-105-05	NCP003643	E08	C19H21N5O4.0.75H2O.HCl	4.333.805	3.834.081	3.831.593	Tocris Bioscience	100730	2	9
NGP-105-05	NCP003643	F08	C20H29N5O3.HCl	4.239.446	3.874.837	3.872.270	Tocris Bioscience	100121	1	8
NGP-105-05	NCP003643	G08	C10H12N2O	1.762.188	1.762.188	1.760.949	Tocris Bioscience	100252	0	3
NGP-105-05	NCP003643	H08	C3H6N2O2	1.020.932	1.020.932	1.020.429	Tocris Bioscience	101840	3	4
NGP-105-05	NCP003643	A09	C15H21F3N2O2.C4H4O4	4.344.125	3.183.405	3.181.555	Tocris Bioscience	100328	2	4
NGP-105-05	NCP003643	B09	C19H21NO.HCl	3.158.440	2.793.831	2.791.623	Tocris Bioscience	100107	0	2
NGP-105-05	NCP003643	C09	C21H24F3N3S.2HCl	4.804.202	4.074.984	4.071.643	Tocris Bioscience	100741	0	3
NGP-105-05	NCP003643	D09	C17H23NO.C4H6O6	4.074.655	2.573.771	2.571.779	Tocris Bioscience	100721	1	2
NGP-105-05	NCP003643	E09	C16H22N4O3	3.183.770	3.183.770	3.181.691	Tocris Bioscience	100601	2	7
NGP-105-05	NCP003643	F09	C20H23N.HCl	3.138.716	2.774.107	2.771.830	Tocris Bioscience	100747	1	1
NGP-105-05	NCP003643	G09	C19H21NS.C4H4O4	4.115.157	2.954.437	2.951.394	Tocris Bioscience	100752	0	1
NGP-105-05	NCP003643	H09	C18H24O2	2.723.888	2.723.888	2.721.776	Tocris Bioscience	101474	2	2
NGP-105-05	NCP003643	A10	C10H20N2O2	2.002.822	2.002.822	2.001.524	Tocris Bioscience	101533	2	4
NGP-105-05	NCP003643	B10	C17H21NO.HCl	2.918.220	2.553.611	2.551.623	Tocris Bioscience	100917	0	2
NGP-105-05	NCP003643	C10	C17H21NO3.HBr	3.682.718	2.873.599	2.871.521	Tocris Bioscience	100060	1	4
NGP-105-05	NCP003643	D10	C19H16ClNO4.0.25H2O	3.622.981	3.577.943	3.570.767	Tocris Bioscience	100475	1	5
NGP-105-05	NCP003643	E10	C10H20N2S4	2.965.234	2.965.234	2.960.509	Tocris Bioscience	100320	0	2
NGP-105-05	NCP003643	F10	C16H18N4O2.0.5H2O.HCl	3.438.142	2.983.456	2.981.429	Tocris Bioscience	100731	0	6
NGP-105-05	NCP003643	G10	C26H28Cl2N4O4	5.314.404	5.314.404	5.301.487	Tocris Bioscience	100180	0	8

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-05	NCP003643	H10	C16H21N3.HCl	2.918.250	2.553.641	2.551.735	Tocris Bioscience	100727	0	3
NGP-105-05	NCP003643	A11	C6H8ClN7O.2H2O.HCl	3.021.208	2.296.293	2.290.478	Tocris Bioscience	101735	8	8
NGP-105-05	NCP003643	B11	C13H14N2.HCl	2.347.293	1.982.684	1.981.156	Tocris Bioscience	101925	2	2
NGP-105-05	NCP003643	C11	C20H24O2	2.964.108	2.964.108	2.961.776	Tocris Bioscience	101476	2	2
NGP-105-05	NCP003643	D11	C9H13N3O5	2.432.201	2.432.201	2.430.855	Tocris Bioscience	101401	5	8
NGP-105-05	NCP003643	E11	C20H22N8O5.3H2O	5.084.925	4.544.466	4.541.713	Tocris Bioscience	101662	7	13
NGP-105-05	NCP003643	F11	C11H13F3N2.HCl	2.666.946	2.302.337	2.301.030	Tocris Bioscience	100743	1	2
NGP-105-05	NCP003643	G11	C10H17N3S	2.113.261	2.113.261	2.111.143	Tocris Bioscience	100677	3	3
NGP-105-05	NCP003643	H11	C14H22N2O	2.343.428	2.343.428	2.341.732	Tocris Bioscience	101620	1	3
NGP-105-06	NCP003723	A02	C26H26N2O3.H2O.HCl	4.689.818	4.145.056	4.141.943	Tocris Bioscience	1410	3	5
NGP-105-06	NCP003723	B02	C19H30N2O.HCl	3.389.227	3.024.618	3.022.358	Tocris Bioscience	100337	3	3
NGP-105-06	NCP003723	C02	C23H24N2O.H2O.2HBr	5.242.969	3.444.578	3.441.888	Tocris Bioscience	921	1	3
NGP-105-06	NCP003723	D02	C19H28O2	2.884.318	2.884.318	2.882.089	Tocris Bioscience	101473	1	2
NGP-105-06	NCP003723	E02	C17H15N5O	3.053.399	3.053.399	3.051.276	Sequoia Research Products Ltd.	SRP00300z	0	6
NGP-105-06	NCP003723	F02	C14H12F3NOS	2.993.114	2.993.114	2.990.591	Tocris Bioscience	100115	2	2
NGP-105-06	NCP003723	G02	C43H65N5O10	8.120.205	8.120.205	8.114.731	Sequoia Research Products Ltd.	SRP01191t	1	15
NGP-105-06	NCP003723	H02	C13H9NOSe	2.741.811	2.741.811	2.749.849	Tocris Bioscience	101457	0	2
NGP-105-06	NCP003723	A03	C17H12BrFO2S2	4.113.042	4.113.042	4.099.446	Tocris Bioscience	101416	0	2
NGP-105-06	NCP003723	B03	C25H37NO4	4.155.753	4.155.753	4.152.722	Tocris Bioscience	1660	4	5
NGP-105-06	NCP003723	C03	C17H18ClNO.HCl	3.242.510	2.877.901	2.871.076	Tocris Bioscience	925	1	2
NGP-105-06	NCP003723	D03	C19H28O2	2.884.318	2.884.318	2.882.089	Tocris Bioscience	101406	1	2
NGP-105-06	NCP003723	E03	C20H34O5	3.544.890	3.544.890	3.542.406	Sequoia Research Products Ltd.	SRP04907a	3	5
NGP-105-06	NCP003723	F03	C21H32N2O	3.284.998	3.284.998	3.282.514	Sequoia Research Products Ltd.	SRP01623s	2	3
NGP-105-06	NCP003723	G03	C15H20ClN5O4.H2O	3.878.244	3.698.091	3.691.203	Tocris Bioscience	100086	4	9
NGP-105-06	NCP003723	H03	C17H17F3N4.2C4H4O4	5.664.891	3.343.451	3.341.405	Tocris Bioscience	100333	0	4
NGP-105-06	NCP003723	A04	C43H55N5O7.H2O4S	8.520.208	7.539.423	7.534.101	Sequoia Research Products Ltd.	SRP01038v	6	12
NGP-105-06	NCP003723	B04	C46H56N4O10.H2O4S	9.230.533	8.249.748	8.243.996	Sequoia Research Products Ltd.	SRP01037v	3	14
NGP-105-06	NCP003723	C04	C26H33NO6	4.555.531	4.555.531	4.552.307	Sequoia Research Products Ltd.	SRP00900l	1	7
NGP-105-06	NCP003723	D04	C17H19N3	2.653.591	2.653.591	2.651.578	Sequoia Research Products Ltd.	SRP06582m	0	3
NGP-105-06	NCP003723	E04	C20H21N3O7S	4.474.639	4.474.639	4.471.100	Sequoia Research Products Ltd.	SRP05637a	1	10
NGP-105-06	NCP003723	F04	C24H34N4O5S	4.906.198	4.906.198	4.902.249	Sequoia Research Products Ltd.	SRP01525g	3	9
NGP-105-06	NCP003723	G04	C20H25ClN2O5	4.088.834	4.088.834	4.081.451	Sequoia Research Products Ltd.	SRP05624a	3	7
NGP-105-06	NCP003723	H04	C18H21N3O3S	3.594.443	3.594.443	3.591.303	Sequoia Research Products Ltd.	SRP00950r	1	6
NGP-105-06	NCP003723	A05	C27H22Cl2N4	4.734.058	4.734.058	4.721.221	Sigma Chemical Company	C8895	1	4
NGP-105-06	NCP003723	B05	C33H38N4O6.3H2O.HCl	6.771.970	5.866.902	5.862.791	Sequoia Research Products Ltd.	SRP01505i	1	10
NGP-105-06	NCP003723	C05	C16H14F3N3O2S	3.693.622	3.693.622	3.690.758	Sequoia Research Products Ltd.	SRP01175l	1	5
NGP-105-06	NCP003723	D05	C19H19ClN2	3.108.274	3.108.274	3.101.236	Sequoia Research Products Ltd.	SRP02090d	1	2
NGP-105-06	NCP003723	E05	C18H21O5S.Na+	3.724.128	3.494.230	3.491.109	Sigma Chemical Company	E0251	0	5
NGP-105-06	NCP003723	F05	C29H35NO2	4.296.045	4.296.045	4.292.667	Sigma Chemical Company	M8046	1	3
NGP-105-06	NCP003723	G05	C29H32O13	5.885.672	5.885.672	5.881.842	Sigma Chemical Company	E1383	3	13

NCC PLATE	PLATE BARCODE	WELL ID	STRUCTURE REAL MF	STRUCTURE REAL AMW	PARENT AMW	PARENT EMW	SAMPLE SUPPLIER	SUPPLIER STRUCTURE ID	NUM H DONORS	NUM H ACCEPTORS
NGP-105-06	NCP003723	H05	C17H26CIN	2.798.547	2.798.547	2.791.753	Tocris Bioscience	2290	0	1
NGP-105-06	NCP003723	A06	C14H17CIN4S	3.088.298	3.088.298	3.080.862	Tocris Bioscience	752	3	4
NGP-105-06	NCP003723	B06	C15H18N2O	2.423.218	2.423.218	2.421.419	Sequoia Research Products Ltd.	SRP02175h	3	3
NGP-105-06	NCP003723	C06	C17H26CIN.H2O.HCl	3.343.309	2.798.547	2.791.753	Sequoia Research Products Ltd.	SRP01355s	0	1
NGP-105-06	NCP003723	D06	C15H10Cl2N2O2	3.211.632	3.211.632	3.200.119	Sequoia Research Products Ltd.	SRP01577l	2	4
NGP-105-06	NCP003723	E06	C20H26N2O4.2HBr	5.202.628	3.584.390	3.581.892	Tocris Bioscience	411	1	6
NGP-105-06	NCP003723	F06	C15H21N5O5.H2O.HCl	4.058.397	3.513.635	3.511.542	Tocris Bioscience	1957	5	10
NGP-105-06	NCP003723	G06	C25H29I2NO3.HCl	6.817.818	6.453.209	6.450.237	Sequoia Research Products Ltd.	SRP05610a	0	4
NGP-105-06	NCP003723	H06	C23H34O5	3.905.220	3.905.220	3.902.406	Sequoia Research Products Ltd.	SRP06551m	1	5
NGP-105-06	NCP003723	A07	C29H31N7O.CH4O3S	5.897.190	4.936.133	4.932.590	Sequoia Research Products Ltd.	SRP000530i	2	8
NGP-105-06	NCP003723	B07	C16H22FNO.HCl	2.998.174	2.633.565	2.631.685	Tocris Bioscience	100740	0	2
NGP-105-06	NCP003723	C07	C19H17N2O4S.Na+	3.924.058	3.694.160	3.690.909	Sequoia Research Products Ltd.	SRP010755P	0	6
NGP-105-06	NCP003723	D07	C19H26N2S.CH4O3S	4.105.961	3.144.904	3.141.816	Tocris Bioscience	101757	1	2
NGP-105-06	NCP003723	E07	C53H72N2O12.2C6H5O3S	12.434.936	9.291.652	9.285.085	Sequoia Research Products Ltd.	SRP07340a	0	14
NGP-105-06	NCP003723	F07	C16H26O5	2.983.810	2.983.810	2.981.780	Sequoia Research Products Ltd.	SRP07301a	0	5

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-A01	Acivicin	(2R)-2-amino-2-[(5S)-3-chloro-4,5-dihydro-1,2-oxazol-5-yl]acetic acid	178,6	42228-92-2	EI-113	2mg/ml	DMSO	2865	Natural Products Library
1	1-A02	Actinomycin D	2-amino-4,6-dimethyl-3-oxo-1-N,9-N-bis[7,11,14-trimethyl-2,5,9,12,15-pentaoxo-3,10-di(propan-2-yl)-8-oxa-1,4,11,14-tetraabicyclo[14.3.0]nonadecan-6-yl]phenoxazine-1,9-dicarboxamide	1255,5	50-76-0	GR-300	2mg/ml	DMSO	2865	Natural Products Library
1	1-A03	Anisomycin	(2R,3S,4S)-4-hydroxy-2-[(3-methoxyphenyl)methyl]pyrrolidin-3-yl acetate	265,3	22862-76-6	ST-102	2mg/ml	DMSO	2865	Natural Products Library
1	1-A04	Antibiotic A-23187	5-(methylamino)-2-[[[2S,3S,8S,9R,11R]-3,9,11-trimethyl-8-[1-oxo-1-(1H-pyrrol-2-yl)propan-2-yl]-1,7-dioxaspiro[5.5]undecan-2-yl]methyl]-1,3-benzoxazole-4-carboxylic acid	523,6	52665-69-7	CA-100	2mg/ml	DMSO	2865	Natural Products Library
1	1-A05	Aristolochic acid A	6-methoxy-9-nitro-14,16-dioxatetracyclo[8.7.0.0 ^{2,7} .0 ^{13,17}]heptadeca-1(10),2(7),3,5,8,11,13(17)-heptaene-11-carboxylic acid	341,3	313-67-7	EI-175	2mg/ml	DMSO	2865	Natural Products Library
1	1-A06	Artesunate	4-oxo-4-[(1S,4S,5R,8S,9R,10S,12R,13R)-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0 ^{4,13} .0 ^{8,13}]hexadecan-10-yl]oxybutanoic acid	384,4	88495-63-0	PR-117	2mg/ml	DMSO	2865	Natural Products Library
1	1-A07	Australine-HCl	(1R,2R,3R,7S,7aR)-3-(hydroxymethyl)-hexahydro-1H-pyrrolizine-1,2,7-triol hydrochloride	225,7	118396-02-4	S-105	2mg/ml	DMSO	2865	Natural Products Library
1	1-A08	Baicalein	5,6,7-trihydroxy-2-phenyl-4H-chromen-4-one	270,2	491-67-8	EI-106	2mg/ml	DMSO	2865	Natural Products Library
1	1-A09	Betulinic acid	(1R,2R,5S,8R,9R,10R,13R,14R,17S,19R)-17-hydroxy-1,2,14,18,18-pentamethyl-8-(prop-1-en-2-yl)pentacyclo[11.8.0.0 ^{2,10} .0 ^{5,9} .0 ^{14,19}]henicosane-5-carboxylic acid	456,7	472-15-1	AP-301	2mg/ml	DMSO	2865	Natural Products Library
1	1-A10	Bilobalide	(1S,4R,7R,8S,9R,11S)-9-tert-butyl-7,9-dihydroxy-3,5,12-trioxatetracyclo[6.6.0.0 ^{1,11} .0 ^{4,8}]tetradecane-2,6,13-trione	326,3	33570-04-6	N-140	2mg/ml	DMSO	2865	Natural Products Library
1	1-A11	Brefeldin A	(1R,6S,11aS,13S,14aR)-1,13-dihydroxy-6-methyl-1H,4H,6H,7H,8H,9H,11aH,12H,13H,14H,14aH-cyclopenta[f]oxacyclotridecan-4-one	280,4	20350-15-6	G-405	2mg/ml	DMSO	2865	Natural Products Library
1	1-A12	Bromocriptine mesylate	(4R,7R)-10-bromo-N-[(1S,2S,4R,7S)-2-hydroxy-7-(2-methylpropyl)-5,8-dioxo-4-(propan-2-yl)-3-oxa-6,9-diazatricyclo[7.3.0.0 ^{2,6}]dodecan-4-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.0 ^{2,7} .0 ^{12,16}]hexadeca-1(15),2,9,12(16),13-pentaene-4-carboxamide methanesulfonate	749,7	22260-51-1	D-102	2mg/ml	DMSO	2865	Natural Products Library
1	1-B01	C2 Phytoceramide	N-[(2S,3S,4R)-1,3,4-trihydroxyoctadecan-2-yl]acetamide	359,5		SL-151	2mg/ml	DMSO	2865	Natural Products Library
1	1-B02	C6 Ceramide	N-[(2S,3R,4E)-1,3-dihydroxyoctadec-4-en-2-yl]hexanamide	397,6	124753-97-5	SL-110	2mg/ml	DMSO	2865	Natural Products Library
1	1-B03	Caffeic acid	(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid	180,2	331-39-5	EI-124	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-B04	Camptothecin	(16S)-16-ethyl-16-hydroxy-18-oxa-1,10-diazapentacyclo[11.8.0.0.0 ² ; ¹¹ .0 ⁴ , ⁹ .0 ¹⁵ , ²⁰]henicosa-2,4,6,8,10,13,15(20)-heptaene-17,21-dione	348,4	7689-03-4	GR-301	2mg/ml	DMSO	2865	Natural Products Library
1	1-B05	Cantharidin	2,6-dimethyl-4,10-dioxatricyclo[5.2.1.0 ² , ⁶]decane-3,5-dione	196,2	56-25-7	PR-105	2mg/ml	DMSO	2865	Natural Products Library
1	1-B06	CAPE	2-phenylethyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	284,3	104594-70-9	FR-102	2mg/ml	DMSO	2865	Natural Products Library
1	1-B07	Capsaicin	(6E)-N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methylnon-6-enamide	305,4	404-86-4	EI-125	2mg/ml	DMSO	2865	Natural Products Library
1	1-B08	Castanospermine	(1S,6S,7R,8R,8aR)-octahydroindolizine-1,6,7,8-tetrol	189,2	79831-76-8	S-107	2mg/ml	DMSO	2865	Natural Products Library
1	1-B09	Cerulenin	(2R,3S)-3-[(4E,7E)-nona-4,7-dienyl]oxirane-2-carboxamide	223,3	17397-89-6	G-237	2mg/ml	DMSO	2865	Natural Products Library
1	1-B10	Cevadine	(1R,2S,6S,9S,10R,11S,12S,14R,15S,18S,19S,22S,23S,25R)-1,10,11,12,14,23-hexahydroxy-6,10,19-trimethyl-24-oxa-4-azaheptacyclo[12.12.0.0.0 ² ; ¹¹ .0 ⁴ , ⁹ .0 ¹⁵ , ²⁵ .0 ¹⁸ , ²³ .0 ¹⁹ , ²⁵]hexacosan-22-yl (2E)-2-methylbut-2-enoate	591,7	62-59-9	NA-104	2mg/ml	DMSO	2865	Natural Products Library
1	1-B11	Chaetomelic acid A	disodium (2Z)-2-methyl-3-tetradecylbut-2-enedioate	370,4	148796-51-4	G-229	2mg/ml	DMSO	2865	Natural Products Library
1	1-B12	Chelerythrine	17,18-dimethoxy-21-methyl-5,7-dioxo-21-azapentacyclo[11.8.0.0.0 ² ; ¹⁰ .0 ⁴ , ⁸ .0 ¹⁴ , ¹⁹]henicosa-1(13),2(10),3,8,11,14,16,18,20-nonaen-21-ium chloride	383,8	3895-92-9	EI-225	2mg/ml	DMSO	2865	Natural Products Library
1	1-C01	Chromomycin A3	6-[[[(6S,7S)-6-[(4-[[[5-(acetyloxy)-4-hydroxy-4,6-dimethyloxan-2-yl]oxy]-5-hydroxy-6-methyloxan-2-yl]oxy]-5-hydroxy-6-methyloxan-2-yl]oxy]-7-[[[1S,3S,4R)-3,4-dihydroxy-1-methoxy-2-oxopentyl]-4,10-dihydroxy-3-methyl-5-oxo-5,6,7,8-tetrahydroanthracen-2-yl]oxy]-4-[(4-hydroxy-5-methoxy-6-methyloxan-2-yl]oxy]-2-methyloxan-3-yl]acetate	1183,2	7059-24-7	GR-302	2mg/ml	DMSO	2865	Natural Products Library
1	1-C02	Citrinin	(3R,4S)-8-hydroxy-3,4,5-trimethyl-6-oxo-4,6-dihydro-3H-2-benzopyran-7-carboxylic acid	250,2	518-75-2	CM-116	2mg/ml	DMSO	2865	Natural Products Library
1	1-C03	Colchicine	N-[(10S)-3,4,5,14-tetramethoxy-13-oxotricyclo[9.5.0.0.0 ² , ⁷]hexadeca-1(16),2(7),3,5,11,14-hexaen-10-yl]acetamide	399,4	64-86-8	T-118	2mg/ml	DMSO	2865	Natural Products Library
1	1-C04	Coumermycin A1	(3S,4R,5S)-5-hydroxy-6-[(4-hydroxy-3-{5-[(4-hydroxy-7-[[[3R,4S,5R)-3-hydroxy-5-methoxy-6,6-dimethyl-4-(5-methyl-1H-pyrrole-2-carbonyloxy)oxan-2-yl]oxy]-8-methyl-2-oxo-2H-chromen-3-yl]carbonyl]-4-methyl-1H-pyrrole-3-amido)-8-methyl-2-oxo-2H-chromen-7-yl]oxy]-3-methoxy-2,2-dimethyloxan-4-yl 5-methyl-1H-pyrrole-2-carboxylate	1110,1	4434-05-3	GR-317	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-C05	Curcumin	1-(3-hydroxy-2-methoxyphenyl)-7-(3-hydroxy-4-methoxyphenyl)hepta-1,6-diene-3,5-dione	368,4	458-37-7	EI-135	2mg/ml	DMSO	2865	Natural Products Library
1	1-C06	Cycloheximide	4-[(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl]piperidine-2,6-dione	281,3	66-81-9	GR-310	2mg/ml	DMSO	2865	Natural Products Library
1	1-C07	Cyclopamine	(3S,3'R,3'aS,6'S,6aS,6bS,7'aR,9R,11aS,11bR)-3',6',10,11b-tetramethyl-1,2,3,3'a,4,4',5',6,6',6a,6b,7,7',7'a,8,11,11a,11b-octadecahydro-3'H-spiro[cyclohexa[a]fluorene-9,2'-furo[3,2-b]pyridine]-3-ol	411,6	4449-51-8	GR-334	2mg/ml	DMSO	2865	Natural Products Library
1	1-C08	Cyclopiazonic acid	(2R,3S,5Z,9R)-5-(1-hydroxyethylidene)-8,8-dimethyl-7,16-diazapentacyclo[9.6.1.0 ^{2,9} .0 ^{3,7} .0 ^{15,18}]octadeca-1(17),11,13,15(18)-tetraene-4,6-dione	336,4	18172-33-3	CA-415	2mg/ml	DMSO	2865	Natural Products Library
1	1-C09	L-Cycloserine	(4R)-4-amino-1,2-oxazolidin-3-one	102,1	339-72-0	SL-200	2mg/ml	DMSO	2865	Natural Products Library
1	1-C10	Cyclosporin A	(3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-30-ethyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-1,4,7,10,12,15,19,25,28-nonamethyl-6,9,18,24-tetrakis(2-methylpropyl)-3,21-bis(propan-2-yl)-1,4,7,10,13,16,19,22,25,28,31-undecaazacyclotritriacontan-2,5,8,11,14,17,20,23,26,29,32-undecone	1202,6	59865-13-3	A-195	2mg/ml	DMSO	2865	Natural Products Library
1	1-C11	Cytochalasin B	(5R,9R,13S,15S,15aS,16S,18aS,18bS)-16-benzyl-5,13-dihydroxy-9,15-dimethyl-14-methylidene-2H,5H,6H,7H,8H,9H,10H,13H,14H,15H,15aH,16H,17H,18H,18bH-oxacyclotetradeca[3,2-e]isoindole-2,18-dione	479,6	14930-96-2	T-108	2mg/ml	DMSO	2865	Natural Products Library
1	1-C12	Cytochalasin D	(3S,4S,6S,6aR,10S,12S,15R,15aR,15bR)-3-benzyl-6,12-dihydroxy-4,10,12-trimethyl-5-methylidene-1,11-dioxo-1H,2H,3H,4H,5H,6H,6aH,9H,10H,11H,12H,15H,15bH-cycloundeca[e]isoindol-15-yl acetate	507,6	22144-77-0	T-109	2mg/ml	DMSO	2865	Natural Products Library
1	1-D01	Cytochalasin E	(1S,5E,7S,9S,11E,13S,14S,16R,17S,18S,19S)-19-benzyl-7-hydroxy-7,9,16,17-tetramethyl-2,4,15-trioxa-20-azatetracyclo[11.8.0.0 ^{1,18} .0 ^{4,16}]henicosa-5,11-diene-3,8,21-trione	495,6	36011-19-5	CT-120	2mg/ml	DMSO	2865	Natural Products Library
1	1-D02	Daidzein	7-hydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one	254,2	486-66-8	ST-110	2mg/ml	DMSO	2865	Natural Products Library
1	1-D03	Daunorubicin	(8S,10S)-8-acetyl-10-[(4-amino-5-hydroxy-6-methylloxan-2-yl)oxy]-6,8,11-trihydroxy-1-methoxy-5,7,8,9,10,12-hexahydrotetracene-5,12-dione hydrochloride	564,0	23541-50-6	GR-318	2mg/ml	DMSO	2865	Natural Products Library
1	1-D04	Decoyinine	(2R,3R,4S)-2-(6-amino-9H-purin-9-yl)-2-(hydroxymethyl)-5-methylideneoxolane-3,4-diol	279,3	2004-04-8	A-230	2mg/ml	DMSO	2865	Natural Products Library
1	1-D05	Degeulin	(1S,14S)-17,18-dimethoxy-7,7-dimethyl-2,8,21-trioxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{15,20}]docosa-3(12),4(9),5,10,15(20),16,18-heptaen-13-one	394,4	522-17-8	EI-329	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-D06	13-O-Acetylphorbol	(1R,2S,6R,10S,11R,13S,15R)-1,6-dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxotetracyclo[8.5.0.0.0 ² ,6.0 ¹¹ ,13]pentadeca-3,8-dien-13-yl acetate	390,5	60857-08-1	PE-187	2mg/ml	DMSO	2865	Natural Products Library
1	1-D07	12-Deoxyphorbol 13-phenylacetate 20-acetate	[(1R,2S,6R,10S,11R,13S,15R)-1,6-dihydroxy-4,12,12,15-tetramethyl-5-oxo-13-[(2-phenylacetyl)oxy]tetracyclo[8.5.0.0.0 ² ,6.0 ¹¹ ,13]pentadeca-3,8-dien-8-yl)methyl acetate	508,6	54662-30-5	PE-182	2mg/ml	DMSO	2865	Natural Products Library
1	1-D08	Dihydroergocristine mesylate	(2R,4R,7R)-N-[(1S,2S,4R,7S)-7-benzyl-2-hydroxy-5,8-dioxo-4-(propan-2-yl)-3-oxa-6,9-diazatricyclo[7.3.0.0.0 ² ,6]dodecan-4-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.0.0 ² ,7.0 ¹² ,16]hexadeca-1(15),9,12(16),13-tetraene-4-carboxamide; methanesulfonic acid	707,8	24730-10-7	NS-108	2mg/ml	DMSO	2865	Natural Products Library
1	1-D09	Domoic acid	(2S,3S,4S)-4-[(2Z,4E,6R)-6-carboxy-6-methylhexa-2,4-dien-2-yl]-3-(carboxymethyl)pyrrolidine-2-carboxylic acid	311,3	14277-97-5	EA-117	2mg/ml	DMSO	2865	Natural Products Library
1	1-D10	Doxorubicin	(8S,10S)-10-[(4-amino-5-hydroxy-6-methyloxan-2-yl)oxy]-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-5,7,8,9,10,12-hexahydrotetracene-5,12-dione hydrochloride	580,0	25316-40-9	GR-319	2mg/ml	DMSO	2865	Natural Products Library
1	1-D11	E6 Berbamine	(1S,14R)-20,21,25-trimethoxy-15,30-dimethyl-7,23-dioxo-15,30-diazaheptacyclo[22.6.2.2.0 ³ ,6.1 ⁸ ,12.1 ¹⁴ ,18.0 ²⁷ ,31.0 ²² ,33]hexatriaconta-3,5,8(34),9,11,18(33),19,21,24,26,31,35-dodecaen-9-yl 4-nitrobenzoate	757,8	73885-53-7	CA-302	2mg/ml	DMSO	2865	Natural Products Library
1	1-D12	E-64	(2S,3S)-3-[[[(1S)-1-[(4-carbamimidamidobutyl)carbamoyl]-3-methylbutyl]carbamoyl]oxirane-2-carboxylic acid	357,4	66701-25-5	PI-105	2mg/ml	DMSO	2865	Natural Products Library
1	1-E01	E-64-C	(2S,3S)-3-[[[(1S)-3-methyl-1-[(3-methylbutyl)carbamoyl]butyl]carbamoyl]oxirane-2-carboxylic acid	314,4	76684-89-4	PI-106	2mg/ml	DMSO	2865	Natural Products Library
1	1-E02	E-64-D	ethyl (2S)-3-[[[(1S)-3-methyl-1-[(3-methylbutyl)carbamoyl]butyl]carbamoyl]oxirane-2-carboxylate	342,4	88321-09-9	PI-107	2mg/ml	DMSO	2865	Natural Products Library
1	1-E03	Ebelactone B	(3S,4S)-3-ethyl-4-[(2S,4E,6R,8S,9R,10R)-9-hydroxy-4,6,8,10-tetramethyl-7-oxododec-4-en-2-yl]oxetan-2-one	352,5	76808-15-6	G-223	2mg/ml	DMSO	2865	Natural Products Library
1	1-E04	Ellipticine	5,11-dimethyl-6H-pyrido[4,3-b]carbazole	246,3	519-23-3	GR-315	2mg/ml	DMSO	2865	Natural Products Library
1	1-E05	Embelin	2,5-dihydroxy-3-undecylcyclohexa-2,5-diene-1,4-dione	294,4	550-24-3	CM-125	2mg/ml	DMSO	2865	Natural Products Library
1	1-E06	(±)-Epibatadine	2-(6-chloropyridin-3-yl)-7-azabicyclo[2.2.1]heptane	208,7	140111-52-0	C-114	2mg/ml	DMSO	2865	Natural Products Library
1	1-E07	Epigallocatechin	(2R,3R)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3-yl 3,4,5-trihydroxybenzoate	458,4	989-51-5	FR-109	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-E08	Etoposide	(10R,11R,15R,16S)-16-({7,8-dihydroxy-2-methyl-hexahydro-2H-pyrano[3,2-d][1,3]dioxin-6-yl}oxy)-10-(4-hydroxy-3,5-dimethoxyphenyl)-4,6,13-trioxatetracyclo[7.7.0.0 ^{3,7} .0 ^{11,15}]hexadeca-1,3(7),8-trien-12-one	588,6	33419-42-0	GR-307	2mg/ml	DMSO	2865	Natural Products Library
1	1-E09	Forskolin	(3R,4aR,5S,6S,6aS,10R,10aR,10bS)-3-ethenyl-6,10,10b-trihydroxy-3,4a,7,7,10a-pentamethyl-1-oxo-dodecahydro-1H-naphtho[2,1-b]pyran-5-yl acetate	410,5	66575-29-9	CN-100	2mg/ml	DMSO	2865	Natural Products Library
1	1-E10	Fumagillin	(2Z,4E,6E,8E)-10-(((3R,4S,5S)-5-methoxy-4-((2R,3R)-2-methyl-3-(3-methylbut-2-en-1-yl)oxiran-2-yl)-1-oxaspiro[2.5]octan-6-yl)oxy)-10-oxodeca-2,4,6,8-tetraenoic acid	458,5	23110-15-8	CT-100	2mg/ml	DMSO	2865	Natural Products Library
1	1-E11	Fumonisin B2	(2R)-2-(2-(((5R,6R,7S,9S,16R,18S,19S)-19-amino-6-(((3R)-3,4-dicarboxybutanoyl)oxy)-16,18-dihydroxy-5,9-dimethylicosan-7-yl)oxy)-2-oxoethyl)butanedioic acid	705,8	116355-84-1	SL-219	2mg/ml	DMSO	2865	Natural Products Library
1	1-E12	Galanthamine-HBr	(1S,12S,14R)-9-methoxy-4-methyl-11-oxa-4-azatetracyclo[8.6.1.0 ^{1,12} .0 ^{6,17}]heptadeca-6,8,10(17),15-tetraen-14-ol hydrobromide	368,3	1953-04-4	C-115	2mg/ml	DMSO	2865	Natural Products Library
1	1-F01	Gambogic acid	(2Z)-4-(((1R,2S,8R,19R)-12-hydroxy-8,21,21-trimethyl-5-(3-methylbut-2-en-1-yl)-8-(4-methylpent-3-en-1-yl)-14,18-dioxo-3,7,20-trioxahexacyclo[15.4.1.0 ^{2,15} .0 ^{2,19} .0 ^{4,13} .0 ^{6,11}]docosa-4,6(11),9,12,15-pentaen-19-yl)-2-methylbut-2-enoic acid	628,8	2752-65-0	AP-305	2mg/ml	DMSO	2865	Natural Products Library
1	1-F02	Genistein	5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one	270,2	446-72-0	ALX-350-006	2mg/ml	DMSO	2865	Natural Products Library
1	1-F03	Streptozocin	3-methyl-3-nitroso-1-((2S,5S)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-yl)urea	265,2	18883-66-4	ALX-380-010	2mg/ml	DMSO	2865	Natural Products Library
1	1-F04	Gingerol	(5S)-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)decan-3-one	294,4	23513-14-6	CA-422	2mg/ml	DMSO	2865	Natural Products Library
1	1-F05	Ginkgolide B	(3S,6R,7S,8S,11R,12R,13S,16S,17R)-8-tert-butyl-6,12,17-trihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.0 ^{1,11} .0 ^{3,7} .0 ^{7,11} .0 ^{13,17}]nonadecane-5,15,18-trione	424,4	15291-77-7	L-135	2mg/ml	DMSO	2865	Natural Products Library
1	1-F06	Gliotoxin	(1R,7S,8S,11R)-7-hydroxy-11-(hydroxymethyl)-15-methyl-12,13-dithia-9,15-diazatetracyclo[9.2.2.0 ^{1,9} .0 ^{3,8}]pentadeca-3,5-diene-10,14-dione	326,4	67-99-2	PI-129	2mg/ml	DMSO	2865	Natural Products Library
1	1-F07	Gossypol	7-[8-formyl-1,6,7-trihydroxy-3-methyl-5-(propan-2-yl)naphthalen-2-yl]-2,3,8-trihydroxy-6-methyl-4-(propan-2-yl)naphthalene-1-carbaldehyde	518,6	303-45-7	EI-130	2mg/ml	DMSO	2865	Natural Products Library
1	1-F08	Grayanotoxin III	(1S,3R,4R,6S,8S,9R,10R,16R)-5,5,9,14-tetramethyltetracyclo[11.2.1.0 ^{1,10} .0 ^{4,8}]hexadecane-3,4,6,9,14,16-hexol; acetaldehyde	414,5	4678-45-9	NA-135	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-F09	Himbacine	(3S,3aR,4R,4aS,8aR,9aS)-4-[(E)-2-[(2R,6S)-1,6-dimethylpiperidin-2-yl]ethenyl]-3-methyl-dodecahydronaphtho[2,3-c]furan-1-one	345,5	6879-74-9	C-116	2mg/ml	DMSO	2865	Natural Products Library
1	1-F10	(-)-Huperazine	(1R,13E)-1-amino-13-ethylidene-11-methyl-6-azatricyclo[7.3.1.0 ^{2,7}]trideca-2(7),3,10-trien-5-one	242,3	102518-79-6	C-117	2mg/ml	DMSO	2865	Natural Products Library
1	1-F11	10-Hydroxycamptothecin	(19S)-19-ethyl-8,19-dihydroxy-17-oxa-3,13-diazapentacyclo[11.8.0.0 ^{2,11} .0 ^{4,9} .0 ^{15,20}]henicosa-1(21),2,4,6,8,10,15(20)-heptaene-14,18-dione	364,4	64439-81-2	GR-316	2mg/ml	DMSO	2865	Natural Products Library
1	1-F12	Hypericin	5,7,11,18,22,24-hexahydroxy-13,16-dimethyloctacyclo[13.11.1.1 ^{2,10} .0 ^{3,8} .0 ^{4,25} .0 ^{19,27} .0 ^{21,26} .0 ^{14,28}]octacosa-1,3,5,7,10(28),11,13,15,17,19(27),21(26),22,24-tridecaene-9,20-dione	504,4	548-04-9	EI-226	2mg/ml	DMSO	2865	Natural Products Library
1	1-G01	Indirubin	2-(2-oxo-2,3-dihydro-1H-indol-3-ylidene)-2,3-dihydro-1H-indol-3-one	262,3	479-41-4	CC-206	2mg/ml	DMSO	2865	Natural Products Library
1	1-G02	Ingenol 3,20-dibenzoate	[(1S,4R,5S,6R,9S,10R,12R,14R)-3-(benzoyloxy)-4,5,6-trihydroxy-11,11,14-trimethyl-15-oxotetracyclo[7.5.1.0 ^{1,5} .0 ^{10,12}]pentadeca-2,7-dien-7-yl]methyl benzoate	558,6	59086-90-7	PE-186	2mg/ml	DMSO	2865	Natural Products Library
1	1-G03	Isotetrandrine	(1S,14R)-9,20,21,25-tetramethoxy-15,30-dimethyl-7,23-dioxa-15,30-diazaheptacyclo[22.6.2.2 ^{3,6} .1 ^{8,12} .1 ^{14,18} .0 ^{27,31} .0 ^{22,33}]hexatriaconta-3,5,8(34),9,11,18(33),19,21,24(32),25,27(31),35-dodecaene	622,7	477-57-6	G-520	2mg/ml	DMSO	2865	Natural Products Library
1	1-G04	Jervine	(2'R,3S,3'R,3'aS,6'S, 6aS,6bS,7'aR,11aS,11bR)-2,3,3'a,4,4',5',6,6',6a, 6b,7,7',7'a,8,11a,11b-Hexadecahydro-3-hydroxy-3',6',10,11b-tetramethyl-spiro [9H-benzo [a] fluorene-9,2'(3'H)-furo [3,2-b]pyridin]-11(1H)-one	425,6	469-59-0	GR-337	2mg/ml	DMSO	2865	Natural Products Library
1	1-G05	Kainic acid	(2S,3S,4S)-3-(carboxymethyl)-4-(prop-1-en-2-yl)pyrrolidine-2-carboxylic acid	213,2	487-79-6	EA-123	2mg/ml	DMSO	2865	Natural Products Library
1	1-G06	(±)-Kavain	4-methoxy-6-[(E)-2-phenylethenyl]-5,6-dihydro-2H-pyran-2-one	230,3	500-64-1	NA-136	2mg/ml	DMSO	2865	Natural Products Library
1	1-G07	Kenpaulone	14-bromo-8,18-diazatetracyclo[9.7.0.0 ^{2,7} .0 ^{12,17}]octadeca-1(11),2(7),3,5,12(17),13,15-heptaen-9-one	327,2	142273-20-9	EI-310	2mg/ml	DMSO	2865	Natural Products Library
1	1-G08	β-Lapachone	2,2-dimethyl-2H,3H,4H,5H,6H-naphtho[1,2-b]pyran-5,6-dione	242,3	4707-32-8	GR-308	2mg/ml	DMSO	2865	Natural Products Library
1	1-G09	Lincomycin	(2S,4R)-N-[(1R,2R)-2-hydroxy-1-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(methylsulfanyl)oxan-2-yl]propyl]-1-methyl-4-propylpyrrolidine-2-carboxamide	406,5	154-21-2	A-240	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-G10	Lycorine	(1S,17S,18S,19S)-5,7-dioxo-12-azapentacyclo[10.6.1.0 ² , ¹⁰ .0 ⁴ , ⁸ .0 ¹⁵ , ¹⁹]nonadeca-2,4(8),9,15-tetraene-17,18-diol	287,3	476-28-8	GR-313	2mg/ml	DMSO	2865	Natural Products Library
1	1-G11	Mevastatin	(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate	390,5	73573-88-3	G-233	2mg/ml	DMSO	2865	Natural Products Library
1	1-G12	3-Beta-Indoleacrylic acid	(2E)-3-(1H-indol-3-yl)prop-2-enoic acid	187,2	1204-06-4	NP-565	2mg/ml	DMSO	2865	Natural Products Library
1	1-H01	L-Mimosine	(2S)-2-amino-3-(3-hydroxy-4-oxo-1,4-dihydropyridin-1-yl)propanoic acid	198,2	500-44-7	CC-102	2mg/ml	DMSO	2865	Natural Products Library
1	1-H02	Mithramycin A	(2S,3S)-3-[(1S,3S,4R)-3,4-dihydroxy-1-methoxy-2-oxopentyl]-2-[[4-[(4,5-dihydroxy-4,6-dimethyloxan-2-yl)oxy]-5-hydroxy-6-methyloxan-2-yl]oxy]-5-hydroxy-6-methyloxan-2-yl]oxy]-6-[[4-[(4,5-dihydroxy-6-methyloxan-2-yl)oxy]-5-hydroxy-6-methyloxan-2-yl]oxy]-8,9-dihydroxy-7-methyl-1,2,3,4-tetrahydroanthracen-1-one	1085,1	18378-89-7	GR-305	2mg/ml	DMSO	2865	Natural Products Library
1	1-H03	Monensin	sodium (3R,4S)-4-[(2S,5R,7S,8R,9S)-2-[(2R,5S)-5-ethyl-5-[(2R,3S,5R)-5-[(2S,3S,5R,6R)-6-hydroxy-6-(hydroxymethyl)-3,5-dimethyloxan-2-yl]-3-methyloxolan-2-yl]oxolan-2-yl]-9-hydroxy-2,8-dimethyl-1,6-dioxaspiro[4.5]decan-7-yl]-3-methoxy-2-methylpentanoate	692,9	22373-78-0	A-248	2mg/ml	DMSO	2865	Natural Products Library
1	1-H04	Mycophenolic acid	(4E)-6-(4-hydroxy-6-methoxy-7-methyl-3-oxo-1,3-dihydro-2-benzofuran-5-yl)-4-methylhex-4-enoic acid	320,3	24280-93-1	A-249	2mg/ml	DMSO	2865	Natural Products Library
1	1-H05	Myriocin	(2S,3R,4R,6E)-2-amino-3,4-dihydroxy-2-(hydroxymethyl)-14-oxoicos-6-enoic acid	401,5	35891-70-4	SL-226	2mg/ml	DMSO	2865	Natural Products Library
1	1-H06	Neomycin	(2R,3S,4R,5R,6R)-5-amino-2-(aminomethyl)-6-[[[(1R,2R,3S,4R,6S)-4,6-diamino-2-[[[(2S,3R,4S,5R)-4-[[[(3R,4R,5S,6S)-3-amino-6-(aminomethyl)-4,5-dihydroxyoxan-2-yl]oxy]-3-hydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy]-3-hydroxycyclohexyl]oxy]oxane-3,4-diol	614,6	1405-10-3	EI-180	2mg/ml	DMSO	2865	Natural Products Library
1	1-H07	Nigericin-Na	sodium (2R)-2-[(2R,3S,6R)-6-[[[(2S,4R,5R,7R,9R,10R)-2-[[[(2R,5S)-5-[(2R,3S,5R)-5-[(2S,3S,5R,6R)-6-hydroxy-6-(hydroxymethyl)-3,5-dimethyloxan-2-yl]-3-methyloxolan-2-yl]-5-methyloxolan-2-yl]-9-methoxy-2,4,10-trimethyl-1,6-dioxaspiro[4.5]decan-7-yl]methyl]-3-methyloxan-2-yl]propanoate	746,9	28380-24-7	CA-421	2mg/ml	DMSO	2865	Natural Products Library
1	1-H08	Oligomycin A	(1S,4E,5'R,6R,6'R,7S,8R,10S,11S,12R,14S,15R,16S,18E,20E,22S,25R,27S,28R,29S)-22-ethyl-7,11,14,15-tetrahydroxy-6'-[(2S)-2-hydroxypropyl]-5',6,8,10,12,14,16,28,29-nonamethyl-2,26-dioxaspiro[bicyclo[23.3.1]nonacosane-27,2'-oxane]-4,18,20-triene-3,9,13-trione	791,1	579-13-5	CM-111	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
1	1-H09	(-)-Ouabain	4-[[[1S,2R,3R,5S,7S,10R,11S,14R,15R,17R]-3,7,11,17-tetrahydroxy-2-(hydroxymethyl)-15-methyl-5-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]tetracyclo[8.7.0.0.0 ^{2,7} .0 ^{11,15}]heptadecan-14-yl]-2,5-dihydrofuran-2-one	584,7	11018-89-6	CM-109	2mg/ml	DMSO	2865	Natural Products Library
1	1-H10	Parthenolide	(1S,2R,4R,7E,11S)-4,8-dimethyl-12-methylidene-3,14-dioxatricyclo[9.3.0.0.0 ^{2,4}]tetradec-7-en-13-one	248,3	20554-84-1	T-113	2mg/ml	DMSO	2865	Natural Products Library
1	1-H11	Perillic acid	(4S)-4-(prop-1-en-2-yl)cyclohex-1-ene-1-carboxylic acid	166,2	7694-45-3	G-210	2mg/ml	DMSO	2865	Natural Products Library
1	1-H12	Phloretin	3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)propan-1-one	274,3	60-82-2	EI-154	2mg/ml	DMSO	2865	Natural Products Library
2	2-A01	Phorbol 12,13-dibutyrate	(1S,2S,6R,10S,11R,13S,14R,15R)-14-(butanoyloxy)-1,6-dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxotetracyclo[8.5.0.0.0 ^{2,6} .0 ^{11,13}]pentadeca-3,8-dien-13-yl butanoate	504,6	37558-16-0	PE-135	2mg/ml	DMSO	2865	Natural Products Library
2	2-A02	(-)-Guaiol	2-[[[3S,5R,8S)-3,8-dimethyl-1,2,3,4,5,6,7,8-octahydroazulen-5-yl]propan-2-ol	222,4	489-86-1	NP-531	2mg/ml	DMSO	2865	Natural Products Library
2	2-A03	Phorbol 12-myristate 13-acetate	(1S,2S,6R,10S,11R,13S,14R,15R)-13-(acetyloxy)-1,6-dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxotetracyclo[8.5.0.0.0 ^{2,6} .0 ^{11,13}]pentadeca-3,8-dien-14-yl tetradecanoate	616,8	16561-29-8	PE-160	2mg/ml	DMSO	2865	Natural Products Library
2	2-A04	4 α -Phorbol 12-myristate 13-acetate	(1S,2S,6S,10S,11R,13S,14R,15R)-13-(acetyloxy)-1,6-dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxotetracyclo[8.5.0.0.0 ^{2,6} .0 ^{11,13}]pentadeca-3,8-dien-14-yl tetradecanoate	616,8	63597-44-4	PE-162	2mg/ml	DMSO	2865	Natural Products Library
2	2-A05	Phytosphingosine	(2S,3S,4R)-2-aminooctadecane-1,3,4-triol	317,5	554-62-1	SL-150	2mg/ml	DMSO	2865	Natural Products Library
2	2-A06	Piceatannol	5-[(E)-2-(3,4-dihydroxyphenyl)ethenyl]benzene-1,3-diol	244,2	10083-24-6	EI-271	2mg/ml	DMSO	2865	Natural Products Library
2	2-A07	Prostaglandin A ₁	7-[[[1R,2S)-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-3-en-1-yl]heptanoic acid	336,5	14152-28-4	PG-001	2mg/ml	DMSO	2865	Natural Products Library
2	2-A08	Prostaglandin B ₁	7-{2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	336,5	13345-51-2	PG-003	2mg/ml	DMSO	2865	Natural Products Library
2	2-A09	Prostaglandin E ₁	7-[[[1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoic acid	354,5	745-65-3	PG-006	2mg/ml	DMSO	2865	Natural Products Library
2	2-A10	Prostaglandin E ₂	(5Z)-7-[[[1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoic acid	352,5	363-24-6	PG-007	2mg/ml	DMSO	2865	Natural Products Library
2	2-A11	Prostaglandin F _{2α}	(5Z)-7-[[[1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoic acid	354,5	38562-01-5	PG-008	2mg/ml	DMSO	2865	Natural Products Library
2	2-A12	Kahweol Acetate	[[[1S,4S,12S,13R,16R,17R)-17-hydroxy-12-methyl-8-oxapentacyclo[14.2.1.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadeca-5(9),6,10-trien-17-yl]methyl acetate	356,5	81760-47-6	NP-577	2mg/ml	DMSO	2865	Natural Products Library
2	2-B01	Quisqualic acid	(2S)-2-amino-3-(3,5-dioxo-1,2,4-oxadiazolidin-2-yl)propanoic acid	189,1	52809-07-1	EA-132	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-B02	Radicicol	(4R,6R,8R,9Z,11E)-16-chloro-17,19-dihydroxy-4-methyl-3,7-dioxatricyclo[13.4.0.0 ^{6,8}]nonadeca-1(15),9,11,16,18-pentaene-2,13-dione	364,8	12772-57-5	EI-285	2mg/ml	DMSO	2865	Natural Products Library
2	2-B03	Rapamycin	(1R,9S,15R,16E,18R,19R,21R,23S,24E,26E,28E,30S,32S,35R)-1,18-dihydroxy-12-[(2R)-1-[(1R,3S,4S)-4-hydroxy-3-methoxycyclohexyl]propan-2-yl]-19,30-dimethoxy-15,17,21,23,29,35-hexamethyl-11,36-dioxo-4-azatricyclo[30.3.1.0 ^{4,9}]hexatriaconta-16,24,26,28-tetraene-2,3,10,14,20-pentone	914,2	53123-88-9	A-275	2mg/ml	DMSO	2865	Natural Products Library
2	2-B04	Rauwolscine	methyl (1S,15S,18S,19S,20S)-18-hydroxy-3,13-diazapentacyclo[11.8.0.0 ^{2,10} .0 ^{4,9} .0 ^{15,20}]henicosa-2(10),4(9),5,7-tetraene-19-carboxylate hydrochloride	390,9	6211-32-1	AR-106	2mg/ml	DMSO	2865	Natural Products Library
2	2-B05	Resveratrol	5-[(E)-2-(4-hydroxyphenyl)ethenyl]benzene-1,3-diol	228,2	501-36-0	FR-104	2mg/ml	DMSO	2865	Natural Products Library
2	2-B06	All trans retinoic acid	(2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenoic acid	300,4	302-79-4	GR-100	2mg/ml	DMSO	2865	Natural Products Library
2	2-B07	13-cis-Retinoic acid	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenoic acid	300,4	4759-48-2	GR-102	2mg/ml	DMSO	2865	Natural Products Library
2	2-B08	9-cis-Retinoic acid	(2E,4E,6Z,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenoic acid	300,4	5300-03-8	GR-101	2mg/ml	DMSO	2865	Natural Products Library
2	2-B09	Rifampicin	(7S,9E,11S,12R,13S,14R,15R,16R,17S,18S,19E,21Z)-2,15,17,27,29-pentahydroxy-11-methoxy-3,7,12,14,16,18,22-heptamethyl-26-[(E)-N-(4-methylpiperazin-1-yl)carboximidoyl]-6,23-dioxo-8,30-dioxo-24-azatetracyclo[23.3.1.1 ^{4,7} .0 ^{5,28}]triaconta-1,3,5(28),9,19,21,25(29),26-octaen-13-yl acetate	822,9	13292-46-1	GR-306	2mg/ml	DMSO	2865	Natural Products Library
2	2-B10	Rosmarinic acid	(2R)-3-(3,4-dihydroxyphenyl)-2-([(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy)propanoic acid	360,3	20283-92-5	EI-291	2mg/ml	DMSO	2865	Natural Products Library
2	2-B11	Rotenone	(1S,6R,13S)-16,17-dimethoxy-6-(prop-1-en-2-yl)-2,7,20-trioxapentacyclo[11.8.0.0 ^{3,11} .0 ^{4,8} .0 ^{14,19}]henicosa-3(11),4(8),9,14(19),15,17-hexaen-12-one	394,4	83-79-4	ALX-350-360	2mg/ml	DMSO	2865	Natural Products Library
2	2-B12	Rottlerin	(2E)-1-[6-[(3-acetyl-2,4,6-trihydroxy-5-methylphenyl)methyl]-5,7-dihydroxy-2,2-dimethyl-2H-chromen-8-yl]-3-phenylprop-2-en-1-one	516,5	82-08-6	ALX-350-075	2mg/ml	DMSO	2865	Natural Products Library
2	2-C01	Ryanodine	(1R,2R,3S,6S,7S,9S,10R,11R,12R,13S,14R)-2,6,9,11,13,14-hexahydroxy-3,7,10-trimethyl-11-(propan-2-yl)-15-oxapentacyclo[7.5.1.0 ^{1,6} .0 ^{7,13} .0 ^{10,14}]pentadecan-12-yl 1H-pyrrole-2-carboxylate	493,5	15662-33-6	CA-450	2mg/ml	DMSO	2865	Natural Products Library
2	2-C02	Shikonin	5,8-dihydroxy-2-[(1R)-1-hydroxy-4-methylpent-3-en-1-yl]-1,4-dihydronaphthalene-1,4-dione	288,3	517-89-5	CT-115	2mg/ml	DMSO	2865	Natural Products Library
2	2-C03	Spectinomycin	(1R,3S,5R,8R,10R,11S,12S,13R,14S)-8,12,14-trihydroxy-5-methyl-11,13-bis(methylamino)-2,4,9-trioxatricyclo[8.4.0.0 ^{3,8}]tetradecan-7-one	332,3	1695-77-8	A-281	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-C04	Swainsonine	(1S,2R,8R,8aR)-octahydroindolizine-1,2,8-triol	173,2	72741-87-8	S-112	2mg/ml	DMSO	2865	Natural Products Library
2	2-C05	Tanshinone IIA	6,6,14-trimethyl-12-oxatetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadeca-1(10),2(7),8,11(15),13-pentaene-16,17-dione	294,3	568-73-0	GR-336	2mg/ml	DMSO	2865	Natural Products Library
2	2-C06	Taxol	(1S,2S,4S,7R,9S,10S,12R,15S)-4,12-bis(acetyloxy)-1,9-dihydroxy-15-(((2R,3S)-2-hydroxy-3-phenyl-3-(phenylformamido)propanoyl]oxy)-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.0 ^{3,10} .0 ^{4,7}]heptadec-13-en-2-yl benzoate	853,9	33069-62-6	T-104	2mg/ml	DMSO	2865	Natural Products Library
2	2-C07	Tetrandrine	(1S,14S)-9,20,21,25-tetramethoxy-15,30-dimethyl-7,23-dioxo-15,30-diazaheptacyclo[22.6.2.2 ^{3,6} .1 ^{8,12} .1 ^{14,18} .0 ^{27,31} .0 ^{22,33}]hexatriaconta-3,5,8(34),9,11,18(33),19,21,24(32),25,27(31),35-dodecaene	622,7	518-34-3	CA-260	2mg/ml	DMSO	2865	Natural Products Library
2	2-C08	Thapsigargin	(3S,3aR,4S,6S,6aR,7S,8S,9bS)-6-(acetyloxy)-4-(butanoyloxy)-3,3a-dihydroxy-3,6,9-trimethyl-8-(((2Z)-2-methylbut-2-enoyl]oxy)-2-oxo-2H,3H,3aH,4H,5H,6H,6aH,7H,8H,9bH-azuleno[4,5-b]furan-7-yl octanoate	650,8	67526-95-8	PE-180	2mg/ml	DMSO	2865	Natural Products Library
2	2-C09	Tomatidine	(1R,2S,4S,5'S,6S,7S,8R,9S,12S,13S,16S,18S)-5',7,9,13-tetramethyl-5-oxaspiro[pentacyclo[10.8.0.0 ^{2,9} .0 ^{4,8} .0 ^{13,18}]icosane-6,2'-piperidine]-16-ol	415,7	77-59-8	GR-335	2mg/ml	DMSO	2865	Natural Products Library
2	2-C10	Troleandomycin	(3S,5R,6S,7S,8R,11S,12S,13R,14S,15S)-14-[[3-(acetyloxy)-4-(dimethylamino)-6-methyloxan-2-yl]oxy]-12-[[5-(acetyloxy)-4-methoxy-6-methyloxan-2-yl]oxy]-5,7,8,11,13,15-hexamethyl-4,10-dioxo-1,9-dioxaspiro[2.13]hexadecan-6-yl acetate	814,0	2751-09-9	EI-249	2mg/ml	DMSO	2865	Natural Products Library
2	2-C11	Tunicamycin B	(2Z)-N-(6-{2-[5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]-2-hydroxyethyl}-2-[[3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-4,5-dihydroxyoxan-3-yl)-13-methyltetradec-2-enamide	830,9	11089-65-9	CC-104	2mg/ml	DMSO	2865	Natural Products Library
2	2-C12	Ursolic acid	(1S,2R,4aS,6aS,6bR,8aR,10S,12aR,12bR,14bS)-10-hydroxy-1,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	456,7	77-52-1	CT-105	2mg/ml	DMSO	2865	Natural Products Library
2	2-D01	Valinomycin	(3S,6S,9R,12R,15S,18S,21R,24R,27S,30S,33R,36R)-6,18,30-trimethyl-3,9,12,15,21,24,27,33,36-nonakis(propan-2-yl)-1,7,13,19,25,31-hexaoxa-4,10,16,22,28,34-hexaazacyclohexatriacontane-2,5,8,11,14,17,20,23,26,29,32,35-dodecane	1111,3	2001-95-8	KC-140	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-D02	Aconitine	(1S,2R,3R,4R,5R,6S,7S,8R,10R,13R,14R,16S,17S,18R)-8-(acetyloxy)-11-ethyl-5,7,14-trihydroxy-6,16,18-trimethoxy-13-(methoxymethyl)-11-azahexacyclo[7.7.2.1 ² . ⁵ .0 ¹ .0 ³ . ⁸ .0 ¹³ . ¹⁷]nonadecan-4-yl benzoate	645,7	302-27-2	AC-126	2mg/ml	DMSO	2865	Natural Products Library
2	2-D03	Veratridine	(1R,2S,6S,9S,10R,11S,12S,14R,15S,18S,19S,22S,23S,25R)-1,10,11,12,14,23-hexahydroxy-6,10,19-trimethyl-24-oxa-4-azaheptacyclo[12.12.0.0 ² . ¹¹ .0 ⁴ . ⁹ .0 ¹⁵ . ²⁵ .0 ¹⁸ . ²³ .0 ¹⁹ . ²⁵]hexacosan-22-yl 3,4-dimethoxybenzoate	673,8	71-62-5	NA-125	2mg/ml	DMSO	2865	Natural Products Library
2	2-D04	Vinblastine sulfate	sulfuric acid methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(1S,14S,15R)-17-ethyl-17-hydroxy-13-(methoxycarbonyl)-1,11-diazatetracyclo[13.3.1.0 ⁴ . ¹² .0 ⁵ . ¹⁰]nonadeca-4(12),5(10),6,8-tetraen-14-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0 ¹ . ⁹ .0 ² . ⁷ .0 ¹⁶ . ¹⁹]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	909,1	143-67-9	T-116	2mg/ml	DMSO	2865	Natural Products Library
2	2-D05	Vincristine sulfate	sulfuric acid methyl (1R,9R,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(1S,13R,14S,15R)-17-ethyl-17-hydroxy-13-(methoxycarbonyl)-1,11-diazatetracyclo[13.3.1.0 ⁴ . ¹² .0 ⁵ . ¹⁰]nonadeca-4(12),5(10),6,8-tetraen-14-yl]-8-formyl-10-hydroxy-5-methoxy-8,16-diazapentacyclo[10.6.1.0 ¹ . ⁹ .0 ² . ⁷ .0 ¹⁶ . ¹⁹]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	923,0	2068-78-2	T-117	2mg/ml	DMSO	2865	Natural Products Library
2	2-D06	Vinpocetin	ethyl (15S,19S)-15-ethyl-1,11-diazapentacyclo[9.6.2.0 ² . ⁷ .0 ⁸ . ¹⁸ .0 ¹⁵ . ¹⁹]nonadeca-2(7),3,5,8(18),16-pentaene-17-carboxylate	350,5	42971-09-5	PD-185	2mg/ml	DMSO	2865	Natural Products Library
2	2-D07	Wedelolactone	3,13,14-trihydroxy-5-methoxy-8,17-dioxatetracyclo[8.7.0.0 ² . ⁷ .0 ¹¹ . ¹⁶]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-9-one	314,2	524-12-9	EI-316	2mg/ml	DMSO	2865	Natural Products Library
2	2-D08	Wortmannin	(1R,3R,5S,9R,18S)-18-(methoxymethyl)-1,5-dimethyl-6,11,16-trioxo-13,17-dioxapentacyclo[10.6.1.0 ² . ¹⁰ .0 ⁵ . ⁹ .0 ¹⁵ . ¹⁹]nonadeca-2(10),12(19),14-trien-3-yl acetate	428,4	19545-26-7	ST-415	2mg/ml	DMSO	2865	Natural Products Library
2	2-D09	Apigenin	5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one	270,2	520-36-5	EI-345	2mg/ml	DMSO	2865	Natural Products Library
2	2-D10	Arecoline-HBr	methyl 1-methyl-1,2,5,6-tetrahydropyridine-3-carboxylate hydrobromide	236,1	300-08-3	AC-784	2mg/ml	DMSO	2865	Natural Products Library
2	2-D11	Atropine sulfate	sulfuric acid bis(8-methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropanoate) hydrate	694,8	55-48-1	AC-735	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-D12	Berberamine-2HCl	(1S,14R)-20,21,25-trimethoxy-15,30-dimethyl-7,23-dioxo-15,30-diazaheptacyclo[22.6.2.2 ^{3,6} .1 ^{8,12} .1 ^{14,18} .0 ^{27,31} .0 ^{22,33}]hexatriaconta-3,5,8(34),9,11,18(33),19,21,24(32),25,27(31),35-dodecaen-9-ol dihydrochloride	681,6	6078-17-7	NP-403	2mg/ml	DMSO	2865	Natural Products Library
2	2-E01	(+)-Bicuculline	(10R)-10-[(5S)-6-methyl-2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinolin-5-yl]-3,5,11-trioxatricyclo[7.3.0.0 ^{2,6}]dodeca-1(9),2(6),7-trien-12-one	367,4	485-49-4	NP-031	2mg/ml	DMSO	2865	Natural Products Library
2	2-E02	Bufalin	5-[(1S,2S,5S,7R,10R,11R,14R,15R)-5,11-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecan-14-yl]-2H-pyran-2-one	386,5	465-21-4	AP-303	2mg/ml	DMSO	2865	Natural Products Library
2	2-E03	Brucine-N-oxide	(1R,11S,18S,20R,21R,22S)-4,5-dimethoxy-12-oxa-8,17-diazaheptacyclo[15.5.2.0 ^{1,18} .0 ^{2,7} .0 ^{8,22} .0 ^{11,21} .0 ^{15,20}]tetracosan-2(7),3,5,14-tetraen-9-one	394,5	357-57-3	NP-038	2mg/ml	DMSO	2865	Natural Products Library
2	2-E04	Butein	(2E)-1-(2,4-dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)prop-2-en-1-one	272,3	487-52-5	NP-040	2mg/ml	DMSO	2865	Natural Products Library
2	2-E05	Catalpol	(2S,3R,4S,5S,6R)-2-([(1S,2S,4S,5S,6R,10S)-5-hydroxy-2-(hydroxymethyl)-3,9-dioxatricyclo[4.4.0.0 ^{2,4}]dec-7-en-10-yl]oxy)-6-(hydroxymethyl)oxane-3,4,5-triol	362,3	2415-24-9	NP-046	2mg/ml	DMSO	2865	Natural Products Library
2	2-E06	Chrysine	5,7-dihydroxy-2-phenyl-4H-chromen-4-one	254,2	480-40-0	NP-051	2mg/ml	DMSO	2865	Natural Products Library
2	2-E07	Desoxypeganine	1H,2H,3H,9H-pyrrolo[2,1-b]quinazoline dihydrate hydrochloride	244,7	61939-05-7	NP-073	2mg/ml	DMSO	2865	Natural Products Library
2	2-E08	Veratramine	(3R,5S)-2-([(1R)-1-[(3S,6aR,11aR,11bR)-3-hydroxy-10,11b-dimethyl-1H,2H,3H,4H,6H,6aH,11H,11aH,11bH-cyclohexa[a]fluoren-9-yl]ethyl]-5-methylpiperidin-3-ol	409,6	60-70-8	CA-214	2mg/ml	DMSO	2865	Natural Products Library
2	2-E09	Emodin	1,3,8-trihydroxy-6-methyl-9,10-dihydroanthracene-9,10-dione	270,2	518-82-1	NP-094	2mg/ml	DMSO	2865	Natural Products Library
2	2-E10	Gramine	(1H-indol-3-ylmethyl)dimethylamine	174,2	87-52-5	AC-913	2mg/ml	DMSO	2865	Natural Products Library
2	2-E11	Harmaline	7-methoxy-1-methyl-3H,4H,9H-pyrido[3,4-b]indole	214,3	304-21-2	AC-1051	2mg/ml	DMSO	2865	Natural Products Library
2	2-E12	Harmine	7-methoxy-1-methyl-9H-pyrido[3,4-b]indole	212,2	442-51-3	AC-1053	2mg/ml	DMSO	2865	Natural Products Library
2	2-F01	Hyoscyamine	8-methyl-8-azabicyclo[3.2.1]octan-3-yl (2S)-3-hydroxy-2-phenylpropanoate	289,4	101-31-5	AC-922	2mg/ml	DMSO	2865	Natural Products Library
2	2-F02	Ivermectin	(1'R,2R,4'S,5S,6R,8'R,10'E,13'S,14'E,16'E,20'R,21'R,24'S)-6-(butan-2-yl)-21',24'-dihydroxy-12'-([(2R,4S,6S)-5-([(2S,4S,5S,6S)-5-hydroxy-4-methoxy-6-methyloxan-2-yl]oxy)-4-methoxy-6-methyloxan-2-yl]oxy)-5,11',13',22'-tetramethyl-3',7',19'-trioxaspiro[oxane-2,6'-tetracyclo[15.6.1.1 ^{4,8} .0 ^{20,24}]pentacosane]-10',14',16',22'-tetraen-2'-one	875,1	70288-86-7	AC-238	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-F03	Luteolin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one	286,2	491-70-3	NP-176	2mg/ml	DMSO	2865	Natural Products Library
2	2-F04	Melatonin	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]acetamide	232,3	73-31-4	NS-520	2mg/ml	DMSO	2865	Natural Products Library
2	2-F05	Morine	2-(2,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one	302,2	480-16-0	NP-193	2mg/ml	DMSO	2865	Natural Products Library
2	2-F06	Myricetin	3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one	318,2	529-44-2	NP-195	2mg/ml	DMSO	2865	Natural Products Library
2	2-F07	Naringenin	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	272,3	480-41-1	NP-200	2mg/ml	DMSO	2865	Natural Products Library
2	2-F08	(-)-Nicotine	3-[(2S)-1-methylpyrrolidin-2-yl]pyridine	162,2	54-11-5	AC-782	2mg/ml	DMSO	2865	Natural Products Library
2	2-F09	Nonactin	(1R,2R,5R,7R,10S,11S,14S,16S,19R,20R,23R,25R,28S,29S,32S,34S)-2,5,11,14,20,23,29,32-octamethyl-4,13,22,31,37,38,39,40-octaoxapentacyclo[32.2.1.1 ^{7,10} .1 ¹⁶ ,1 ⁹ .1 ²⁵ ,2 ⁸]tetracontane-3,12,21,30-tetrone	736,9	6833-84-7	NP-207	2mg/ml	DMSO	2865	Natural Products Library
2	2-F10	L-Penicillamine	(2R)-2-amino-3-methyl-3-sulfanylbutanoic acid	149,2	1113-41-3	NP-226	2mg/ml	DMSO	2865	Natural Products Library
2	2-F11	Picrotoxinin	(1R,3R,5S,8S,9R,12S,13R,14R)-1-hydroxy-13-methyl-14-(prop-1-en-2-yl)-4,7,10-trioxapentacyclo[6.4.1.1 ⁹ ,1 ² .0 ³ ,5 ⁰ ,1 ³]tetradecane-6,11-dione	292,3	17617-45-7	NP-401	2mg/ml	DMSO	2865	Natural Products Library
2	2-F12	Pilocarpine	(3S,4R)-3-ethyl-4-[(1-methyl-1H-imidazol-5-yl)methyl]oxolan-2-one hydrochloride	244,7	54-71-7	AC-214	2mg/ml	DMSO	2865	Natural Products Library
2	2-G01	Quassin	(1S,2S,6S,7S,9R,13R,17S)-4,15-dimethoxy-2,6,14,17-tetramethyl-10-oxatetracyclo[7.7.1.0 ² ,7 ⁰ ,1 ³ ,1 ⁷]heptadeca-4,14-diene-3,11,16-trione	388,5	76-78-8	NP-245	2mg/ml	DMSO	2865	Natural Products Library
2	2-G02	Quercetin·2H ₂ O	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one dihydrate	338,3	6151-25-3	AC-1142	2mg/ml	DMSO	2865	Natural Products Library
2	2-G03	Quinidine·HCl·H ₂ O	(S)-[(2R,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](6-methoxyquinolin-4-yl)methanol hydrate hydrochloride	378,9	6151-40-2	AC-129	2mg/ml	DMSO	2865	Natural Products Library
2	2-G04	Quinine·HCl·2H ₂ O	(S)-[(1R,2S)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](6-methoxyquinolin-4-yl)methanol dihydrate hydrochloride	396,9	6119-47-7	AC-122	2mg/ml	DMSO	2865	Natural Products Library
2	2-G05	Robinetine	3,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one	302,2	490-31-3	NP-261	2mg/ml	DMSO	2865	Natural Products Library
2	2-G06	Menadione	2-methyl-1,4-dihydronaphthalene-1,4-dione	172,2	58-27-5	NP-528	2mg/ml	DMSO	2865	Natural Products Library
2	2-G07	Strychnine·HCl	(1R,11S,18S,20R,21R,22S)-12-oxa-8,17-diazahaptacyclo[15.5.2.0 ¹ ,1 ⁸ .0 ² ,7 ⁰ .0 ⁸ ,2 ² .0 ¹¹ ,2 ¹ .0 ¹⁵ ,2 ⁰]tetracosan-2(7),3,5,14-tetraen-9-one hydrochloride	370,9	1421-86-9	AC-745	2mg/ml	DMSO	2865	Natural Products Library
2	2-G08	Tryptanthrin	6H,12H-indolo[2,1-b]quinazoline-6,12-dione	248,2	13220-57-0	NP-467	2mg/ml	DMSO	2865	Natural Products Library
2	2-G09	Yohimbine·HCl	methyl (1S,15R,18S,19R,20S)-18-hydroxy-3,13-diazapentacyclo[11.8.0.0 ² ,1 ⁰ .0 ⁴ ,9 ⁰ .0 ¹⁵ ,2 ⁰]hencosane-2(10),4(9),5,7-tetraene-19-carboxylate hydrochloride	390,9	65-19-0	AC-161	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
2	2-G10	(-)-Eburnamonine	(15S,19S)-15-ethyl-1,11-diazapentacyclo[9.6.2.0 ² .7.0 ⁸ .18.0 ¹⁵ .19]nonadeca-2,4,6,8(18)-tetraen-17-one	294,4	4880-88-0	NP-088	2mg/ml	DMSO	2865	Natural Products Library
2	2-G11	Lysergol	[(4S,7S)-6-methyl-6,11-diazatetracyclo[7.6.1.0 ² .7.0 ¹² .16]hexadeca-1(16),2,9,12,14-pentaen-4-yl]methanol	254,3	602-85-7	NP-180	2mg/ml	DMSO	2865	Natural Products Library
2	2-G12	Monocrotaline	(1R,4R,5R,6R,16R)-5,6-dihydroxy-4,5,6-trimethyl-2,8-dioxa-13-azatricyclo[8.5.1.0 ¹³ .16]hexadec-10-ene-3,7-dione	325,4	315-22-0	NP-192	2mg/ml	DMSO	2865	Natural Products Library
2	2-H01	α -Apo-Oxytetracycline	(4R,5S)-4-{4,5-dihydroxy-9-methyl-3-oxo-1H,3H-naphtho[2,3-c]furan-1-yl}-3-(dimethylamino)-2,5-dihydroxy-6-oxocyclohex-1-ene-1-carboxamide	442,4	18695-01-7	NP-219	2mg/ml	DMSO	2865	Natural Products Library
2	2-H02	Pseudopelletierine-HCl	9-methyl-9-azabicyclo[3.3.1]nonan-3-one hydrochloride	189,7	6164-62-1	NP-244	2mg/ml	DMSO	2865	Natural Products Library
2	2-H03	Salsoninol-HBr	(1S)-1-methyl-1,2,3,4-tetrahydroisoquinoline-6,7-diol hydrobromide	260,1	38221-21-5	NP-268	2mg/ml	DMSO	2865	Natural Products Library
2	2-H04	β -Sitosterol	(1S,2R,5S,10S,11S,14R,15R)-14-[(2R,5R)-5-ethyl-6-methylheptan-2-yl]-2,15-dimethyltetracyclo[8.7.0.0 ² .7.0 ¹¹ .15]heptadec-7-en-5-ol	414,7	83-46-5	NP-294	2mg/ml	DMSO	2865	Natural Products Library
2	2-H05	Sterigmatocystin	(7R)-15-hydroxy-11-methoxy-6,8,20-trioxapentacyclo[10.8.0.0 ² .9.0 ³ .7.0 ¹⁴ .19]jicosa-1(12),2(9),4,10,14(19),15,17-heptaen-13-one	324,3	10048-13-2	NP-304	2mg/ml	DMSO	2865	Natural Products Library
2	2-H06	4,5',8-Trimethylpsoralen	2,5,9-trimethyl-7H-furo[3,2-g]chromen-7-one	228,2	3902-71-4	NP-323	2mg/ml	DMSO	2865	Natural Products Library
2	2-H07	Cinobufagin	(1R,2S,4R,5R,6S,7R,10S,11S,14S,16R)-14-hydroxy-7,11-dimethyl-6-(2-oxo-2H-pyran-5-yl)-3-oxapentacyclo[8.8.0.0 ² .4.0 ² .7.0 ¹¹ .16]octadecan-5-yl acetate	442,5	470-37-1	NP-055	2mg/ml	DMSO	2865	Natural Products Library
2	2-H08	Emetine·2HCl	(1R)-1-[[[(2S,3R,11bS)-3-ethyl-9,10-dimethoxy-1H,2H,3H,4H,6H,7H,11bH-pyrido[2,1-a]isoquinolin-2-yl]methyl]-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline dihydrochloride	553,6	316-42-7	NP-093	2mg/ml	DMSO	2865	Natural Products Library
2	2-H09	Kaempferol	3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one	286,2	520-18-3	NP-156	2mg/ml	DMSO	2865	Natural Products Library
2	2-H10	Kanamycin sulfate	(3S,4R,6R)-2-(aminomethyl)-6-[[[(1R,4R,6R)-4,6-diamino-3-[[[(2S,4R,5S)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-2-hydroxycyclohexyl]oxy]oxane-3,4,5-triol; sulfuric acid	582,6	25389-94-0	NP-160	2mg/ml	DMSO	2865	Natural Products Library
2	2-H11	Celastrol	(2R,4aS,6aS,12bR,14aS,14bR)-10-hydroxy-2,4a,6a,9,12b,14a-hexamethyl-11-oxo-1,2,3,4,4a,5,6,6a,11,12b,13,14,14a,14b-tetradecahydricene-2-carboxylic acid	450,6	34157-83-0	NP-568	2mg/ml	DMSO	2865	Natural Products Library
2	2-H12	(+)-Taxifolin	(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	304,3	480-18-2	NP-313	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-A01	Theobromine	3,7-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	180,2	83-67-0	NP-317	2mg/ml	DMSO	2865	Natural Products Library
3	3-A02	Baccatin III	(1S,2S,3R,4S,7R,9S,10S,12R,15S)-4,12-bis(acetyloxy)-1,9,15-trihydroxy-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.0 ^{3,10} .0 ^{4,7}]heptadec-13-en-2-yl benzoate	586,6	27548-93-2	NP-402	2mg/ml	DMSO	2865	Natural Products Library
3	3-A03	Carminic acid	3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxo-7-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-9,10-dihydroanthracene-2-carboxylic acid	492,4	1260-17-9	NP-043	2mg/ml	DMSO	2865	Natural Products Library
3	3-A04	(-)-Cotinine	(5S)-1-methyl-5-(pyridin-3-yl)pyrrolidin-2-one	176,2	486-56-6	NP-064	2mg/ml	DMSO	2865	Natural Products Library
3	3-A05	Austricin	(3S,3aR,4S,9bR)-4-hydroxy-3,6,9-trimethyl-2H,3H,3aH,4H,5H,7H,9aH,9bH-azuleno[4,5-b]furan-2,7-dione	262,3	10180-88-8	NP-024	2mg/ml	DMSO	2865	Natural Products Library
3	3-A06	Condorphine	(4S,5R,8S,9S,10R,16S)-11-ethyl-8,16-dihydroxy-6-methoxy-13-(methoxymethyl)-11-azahexacyclo[7.7.2.1 ^{2,5} .0 ^{1,10} .0 ^{3,8} .0 ^{13,17}]nonadecan-4-yl acetate	449,6	7633-69-4	NP-057	2mg/ml	DMSO	2865	Natural Products Library
3	3-A07	Delcorine	(1S,4S,5R,6S,8R,16S,19S,21S)-14-ethyl-4,6,19-trimethoxy-16-(methoxymethyl)-9,11-dioxo-14-azaheptacyclo[10.7.2.1 ^{2,5} .0 ^{1,13} .0 ^{3,8} .0 ^{8,12} .0 ^{16,20}]docosan-21-ol	479,6	52358-55-1	AC-918	2mg/ml	DMSO	2865	Natural Products Library
3	3-A08	Deltaline	(1R,2S,4S,5R,8R,12S,16R,19S,21S)-14-ethyl-2-hydroxy-4,6,19-trimethoxy-16-methyl-9,11-dioxo-14-azaheptacyclo[10.7.2.1 ^{2,5} .0 ^{1,13} .0 ^{3,8} .0 ^{8,12} .0 ^{16,20}]docosan-21-yl acetate	507,6	6836-11-9	NP-071	2mg/ml	DMSO	2865	Natural Products Library
3	3-A09	Diacetylkorseveriline	(1S,2R,6R,9S,10R,11S,14R,15R,17R,18S,20R,23R,24S)-20-(acetyloxy)-14-hydroxy-6,10,23-trimethyl-4-azahexacyclo[12.11.0.0 ^{2,11} .0 ^{4,9} .0 ^{15,24} .0 ^{18,23}]pentacosan-17-yl acetate	515,7	21851-07-0	NP-074	2mg/ml	DMSO	2865	Natural Products Library
3	3-A10	Dubinidine	2-[4-methoxy-2H,3H-furo[2,3-b]quinolin-2-yl]propane-1,2-diol	275,3	22964-77-8	NP-087	2mg/ml	DMSO	2865	Natural Products Library
3	3-A11	Eudesmine	(1S,4S)-1,4-bis(3,4-dimethoxyphenyl)-hexahydrofuro[3,4-c]furan	386,4	526-06-7	NP-100	2mg/ml	DMSO	2865	Natural Products Library
3	3-A12	Feroline	(7E,9R,10R)-9-hydroxy-3,7-dimethyl-10-(propan-2-yl)cyclodeca-3,7-dien-1-yl 4-hydroxybenzoate	358,5	39380-12-6	NP-102	2mg/ml	DMSO	2865	Natural Products Library
3	3-B01	Fillalbin	8-methyl-8-azabicyclo[3.2.1]octan-3-yl 4-hydroxy-3-methoxybenzoate	291,3	4540-25-4	NP-103	2mg/ml	DMSO	2865	Natural Products Library
3	3-B02	Graveoline	2-(2H-1,3-benzodioxol-5-yl)-1-methyl-1,4-dihydroquinolin-4-one	279,3	485-61-0	NP-118	2mg/ml	DMSO	2865	Natural Products Library
3	3-B03	Heliotrine	[(1S,7aR)-1-hydroxy-2,3,5,7a-tetrahydro-1H-pyrrolizin-7-yl]methyl 2-hydroxy-3-methoxy-2-(propan-2-yl)butanoate	313,4	303-33-3	NP-125	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-B04	Hernandezine	(1S,14S)-9,19,20,21,25-pentamethoxy-15,30-dimethyl-7,23-dioxa-15,30-diazaheptacyclo[22.6.2.2 ^{3,6} .1 ^{8,12} .1 ^{14,18} .0 ^{27,31} .0 ^{22,33}]hexatriaconta-3,5,8,10,12(34),18(33),19,21,24(32),25,27(31),35-dodecaene	652,8	6681-13-6	NP-126	2mg/ml	DMSO	2865	Natural Products Library
3	3-B05	Heteratisine	(1S,6S,9S,10R,11R,14R)-12-ethyl-9,19-dihydroxy-17-methoxy-14-methyl-5-oxa-12-azahexacyclo[8.7.2.1 ^{2,6} .0 ^{1,11} .0 ^{3,9} .0 ^{14,18}]icosan-4-one	391,5	3328-84-5	NP-129	2mg/ml	DMSO	2865	Natural Products Library
3	3-B06	Imperialine	(1R,2S,6S,9S,10S,11S,14S,15S,18S,20S,23R,24S)-10,20-dihydroxy-6,10,23-trimethyl-4-azahexacyclo[12.11.0.0 ^{2,11} .0 ^{4,9} .0 ^{15,24} .0 ^{18,23}]pentacosan-17-one	429,6	18059-10-4	AC-916	2mg/ml	DMSO	2865	Natural Products Library
3	3-B07	Karakoline	(1S,4S,5S,6S,8S,9S,10R,13R,16S)-11-ethyl-6-methoxy-13-methyl-11-azahexacyclo[7.7.2.1 ^{2,5} .0 ^{1,10} .0 ^{3,8} .0 ^{13,17}]nonadecane-4,8,16-triol	377,5	39089-30-0	AC-920	2mg/ml	DMSO	2865	Natural Products Library
3	3-B08	Lapidin	(3R,3aS,4S,8aS)-3-hydroxy-6,8a-dimethyl-8-oxo-3-(propan-2-yl)-1,2,3,3a,4,5,8,8a-octahydroazulen-4-yl (2Z)-2-methylbut-2-enoate	334,4	79863-24-4	NP-164	2mg/ml	DMSO	2865	Natural Products Library
3	3-B09	Lapiferine	(1aS,2S,5R,5aS,6S,7aR)-2-(acetyloxy)-5-hydroxy-2a,7a-dimethyl-5-(propan-2-yl)-decahydroazuleno[5,6-b]oxiren-6-yl (2Z)-2-methylbut-2-enoate	394,5	86992-41-8	NP-165	2mg/ml	DMSO	2865	Natural Products Library
3	3-B10	Nitrarine-2HCl	4,14,20-triazaheptacyclo[13.6.2.0 ^{2,14} .0 ^{3,11} .0 ^{5,10} .0 ^{16,21}]tricosan-3(11),5(10),6,8-tetraene dihydrochloride	380,4	20069-05-0	NP-206	2mg/ml	DMSO	2865	Natural Products Library
3	3-B11	Norfluorourarine	(1R,11S,12E,17S)-12-ethylidene-8,14-diazapentacyclo[9.5.2.0 ^{1,9} .0 ^{2,7} .0 ^{14,17}]octadeca-2(7),3,5,9-tetraene-10-carbaldehyde	292,4	6880-54-2	NP-209	2mg/ml	DMSO	2865	Natural Products Library
3	3-B12	Peganole	1H,2H,3H,9H-pyrrolo[2,1-b]quinazolin-9-ol	188,2	36101-54-9	NP-224	2mg/ml	DMSO	2865	Natural Products Library
3	3-C01	Pinoembrin	(2S)-5,7-dihydroxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one	256,3	480-39-7	NP-233	2mg/ml	DMSO	2865	Natural Products Library
3	3-C02	Protopine	15-methyl-7,9,19,21-tetraoxa-15-azapentacyclo[15.7.0.0 ^{4,12} .0 ^{6,10} .0 ^{18,22}]tetracosan-1(17),4(12),5,10,18(22),23-hexaen-3-one	353,4	130-86-9	NP-242	2mg/ml	DMSO	2865	Natural Products Library
3	3-C03	Remerine-HCl	(12R)-11-methyl-3,5-dioxa-11-azapentacyclo[10.7.1.0 ^{2,6} .0 ^{8,20} .0 ^{14,19}]jicosa-1,6,8(20),14,16,18-hexaene hydrochloride	315,8	17669-16-8	NP-252	2mg/ml	DMSO	2865	Natural Products Library
3	3-C04	Sevedindione	(1S,2R,6R,9S,10R,11S,14R,15R,18S,23R,24S)-14-hydroxy-6,10,23-trimethyl-4-azahexacyclo[12.11.0.0 ^{2,11} .0 ^{4,9} .0 ^{15,24} .0 ^{18,23}]pentacosane-17,20-dione	427,6		NP-289	2mg/ml	DMSO	2865	Natural Products Library
3	3-C05	Skimmianine	4,7,8-trimethoxyfuro[2,3-b]quinoline	259,3	83-95-4	NP-295	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-C06	Songorine	(1R,7R,8R,9R,10R,13R,16S)-11-ethyl-7,16-dihydroxy-13-methyl-6-methylidene-11-azahehexacyclo[7.7.2.1 ⁵ , ⁸ .0 ¹ , ¹⁰ .0 ² , ⁸ .0 ¹³ , ¹⁷]nonadecan-4-one	357,5	509-24-0	NP-300	2mg/ml	DMSO	2865	Natural Products Library
3	3-C07	Trichodesmine	(1R,4R,5R,6R,16R)-5,6-dihydroxy-5,6-dimethyl-4-(propan-2-yl)-2,8-dioxa-13-azatricyclo[8.5.1.0 ³ , ⁶]hexadec-10-ene-3,7-dione	353,4	548-90-3	NP-321	2mg/ml	DMSO	2865	Natural Products Library
3	3-C08	Tschimganidin	(1S,7E,9R,10R)-9-hydroxy-3,7-dimethyl-10-(propan-2-yl)cyclodeca-3,7-dien-1-yl 4-hydroxy-3-methoxybenzoate	388,5	39380-16-0	NP-325	2mg/ml	DMSO	2865	Natural Products Library
3	3-C09	Tschimganine	(1R,2R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 4-hydroxy-3-methoxybenzoate	304,4	38970-49-9	NP-326	2mg/ml	DMSO	2865	Natural Products Library
3	3-C10	Ungerine nitrate	(3R,9R,10S)-9-methoxy-4-methyl-11,16,18-trioxa-4-azapentacyclo[11.7.0.0 ² , ¹⁰ .0 ³ , ⁷ .0 ¹⁵ , ¹⁹]icosa-1(13),7,14,19-tetraen-12-one; nitric acid	392,4		NP-329	2mg/ml	DMSO	2865	Natural Products Library
3	3-C11	Genistin	5-hydroxy-3-(4-hydroxyphenyl)-7-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-4H-chromen-4-one	432,4	529-59-9	NP-111	2mg/ml	DMSO	2865	Natural Products Library
3	3-C12	Laudanosine methiodide	1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium iodide	499,4	24770-59-0	NP-566	2mg/ml	DMSO	2865	Natural Products Library
3	3-D01	Apigenin-7-glucoside	5-hydroxy-2-(4-hydroxyphenyl)-7-(((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-4H-chromen-4-one	432,4	578-74-5	NP-013	2mg/ml	DMSO	2865	Natural Products Library
3	3-D02	Bavachinin A	(2S)-2-(4-hydroxyphenyl)-7-methoxy-6-(3-methylbut-2-en-1-yl)-3,4-dihydro-2H-1-benzopyran-4-one	338,4	19879-30-2	NP-025	2mg/ml	DMSO	2865	Natural Products Library
3	3-D03	Decylubiquinone	2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione	322,4	55486-00-5	CM-115	2mg/ml	DMSO	2865	Natural Products Library
3	3-D04	Convolvamine	8-methyl-8-azabicyclo[3.2.1]octan-3-yl 3,4-dimethoxybenzoate	305,4	500-56-1	NP-058	2mg/ml	DMSO	2865	Natural Products Library
3	3-D05	Daidzin	3-(4-hydroxyphenyl)-7-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-4H-chromen-4-one	416,4	552-66-9	NP-067	2mg/ml	DMSO	2865	Natural Products Library
3	3-D06	Daticetin	3,5,7-trihydroxy-2-(2-hydroxyphenyl)-4H-chromen-4-one	286,2	480-15-9	NP-068	2mg/ml	DMSO	2865	Natural Products Library
3	3-D07	N-Formyl-Deacetylcolchicine	N-[(10S)-3,4,5,14-tetramethoxy-13-oxotricyclo[9.5.0.0 ² , ⁷]hexadeca-1(16),2(7),3,5,11,14-hexaen-10-yl]formamide	385,4	7411-12-3	NP-069	2mg/ml	DMSO	2865	Natural Products Library
3	3-D08	Oridonin	(1S,2S,5S,8R,9S,10S,11R,15S,18R)-9,10,15,18-tetrahydroxy-12,12-dimethyl-6-methylidene-17-oxapentacyclo[7.6.2.1 ⁵ , ⁸ .0 ¹ , ¹¹ .0 ² , ⁸]octadecan-7-one	364,4	16964-56-0	NP-567	2mg/ml	DMSO	2865	Natural Products Library
3	3-D09	Eriocitrin	(2S)-2-(3,4-dihydroxyphenyl)-5-hydroxy-7-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(((2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methylloxan-2-yl)oxy)methyl)oxan-2-yl)oxy)-3,4-dihydro-2H-1-benzopyran-4-one	596,5	13463-28-0	NP-096	2mg/ml	DMSO	2865	Natural Products Library
3	3-D10	Eriodictyol	(3S)-3-(3,4-dihydroxyphenyl)-6,8-dihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	288,3	4049-38-1	NP-097	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-D11	Eriodictyol-7-O-glucoside	(2S)-2-(3,4-dihydroxyphenyl)-5-hydroxy-7- {[(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]oxy}-3,4-dihydro-2H-1- benzopyran-4-one	450,4	38965-51-4	NP-098	2mg/ml	DMSO	2865	Natural Products Library
3	3-D12	Homobutein	(2E)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxy-3- methoxyphenyl)prop-2-en-1-one	286,3	34000-39-0	NP-132	2mg/ml	DMSO	2865	Natural Products Library
3	3-E01	Homoeriodictyol	(2S)-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,4- dihydro-2H-1-benzopyran-4-one	302,3	446-71-9	NP-133	2mg/ml	DMSO	2865	Natural Products Library
3	3-E02	Homoorientin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6- [(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	448,4	4261-42-1	NP-134	2mg/ml	DMSO	2865	Natural Products Library
3	3-E03	7-Hydroxyflavone	7-hydroxy-2-phenyl-4H-chromen-4-one	238,2	6665-86-7	NP-138	2mg/ml	DMSO	2865	Natural Products Library
3	3-E04	Isorhamnetine-3-glucoside	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3- {[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one	478,4	5041-82-7	NP-149	2mg/ml	DMSO	2865	Natural Products Library
3	3-E05	Isorhoifolin	5-hydroxy-2-(4-hydroxyphenyl)-7- {[(2S,3S,4R,5S)-3,4,5-trihydroxy-6- {[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6- methyloxan-2-yl]oxy}oxan-2-yl]methoxy}-4H-chromen-4- one	578,5	552-57-8	NP-151	2mg/ml	DMSO	2865	Natural Products Library
3	3-E06	Isosakuranetin	(2S)-5,7-dihydroxy-2-(4-methoxyphenyl)-3,4-dihydro-2H- 1-benzopyran-4-one	286,3	480-43-3	NP-152	2mg/ml	DMSO	2865	Natural Products Library
3	3-E07	Isovitexin	5,7-dihydroxy-2-(4-hydroxyphenyl)-6- {[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]-4H- chromen-4-one	432,4	29702-25-8	NP-154	2mg/ml	DMSO	2865	Natural Products Library
3	3-E08	Dihydromethysticin	(6S)-6-[2-(2H-1,3-benzodioxol-5-yl)ethyl]-4-methoxy-5,6- dihydro-2H-pyran-2-one	276,3	19902-91-1	NP-537	2mg/ml	DMSO	2865	Natural Products Library
3	3-E09	(β,β-Dimethylacryl) Shikonin	(1R)-1-(5,8-dihydroxy-1,4-dioxo-1,4-dihydronaphthalen- 2-yl)-4-methylpent-3-en-1-yl 3-methylbut-2-enoate	370,4	24502-79-2	NP-572	2mg/ml	DMSO	2865	Natural Products Library
3	3-E10	Kaempferol-7-neohesperidoside	7- {[(3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3- {[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2- yl]oxy}oxan-2-yl]oxy}-3,5-dihydroxy-2-(4-hydroxyphenyl)- 4H-chromen-4-one	594,5	17353-03-6	NP-159	2mg/ml	DMSO	2865	Natural Products Library
3	3-E11	Luteolin-3',7-diglucoside	2-(3,4-dihydroxy-5- {[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]phenyl}-5-hydroxy-7- {[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one	610,5	52187-80-1	NP-177	2mg/ml	DMSO	2865	Natural Products Library
3	3-E12	Flavokawain B	(2E)-1-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenylprop-2- en-1-one	284,3	1775-97-9	NP-539	2mg/ml	DMSO	2865	Natural Products Library
3	3-F01	Marein	(2E)-1-(2,3-dihydroxy-4- {[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]oxy}phenyl)-3- (3,4-dihydroxyphenyl)prop-2-en-1-one	450,4	535-96-6	NP-182	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-F02	Maritimein	(2E)-2-[(3,4-dihydroxyphenyl)methylidene]-7-hydroxy-6-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-2,3-dihydro-1-benzofuran-3-one	448,4	490-54-0	NP-183	2mg/ml	DMSO	2865	Natural Products Library
3	3-F03	Picropodophyllin	(10R,11S,15R,16R)-16-hydroxy-10-(3,4,5-trimethoxyphenyl)-4,6,13-trioxatetracyclo[7.7.0.0 ^{3,7} .0 ^{11,15}]hexadeca-1,3(7),8-trien-12-one	414,4	447-47-4	EI-372	2mg/ml	DMSO	2865	Natural Products Library
3	3-F04	Myricitrin	5,7-dihydroxy-3-[[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one	464,4	17912-87-7	NP-196	2mg/ml	DMSO	2865	Natural Products Library
3	3-F05	Narigenin-7-O-glucoside	(2S)-5-hydroxy-2-(4-hydroxyphenyl)-7-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-3,4-dihydro-2H-1-benzopyran-4-one	434,4	529-55-5	NP-201	2mg/ml	DMSO	2865	Natural Products Library
3	3-F06	Narirutin	5-hydroxy-2-(4-hydroxyphenyl)-7-[[[(3,4,5-trihydroxy-6-[[[(3,4,5-trihydroxy-6-methyloxan-2-yl]oxy)methyl]oxan-2-yl]oxy]-3,4-dihydro-2H-1-benzopyran-4-one	580,5	14259-46-2	NP-203	2mg/ml	DMSO	2865	Natural Products Library
3	3-F07	Picrotonin	(1R,3R,5S,8S,9R,12S,13R,14S)-1-hydroxy-14-(2-hydroxypropan-2-yl)-13-methyl-4,7,10-trioxapentacyclo[6.4.1.1 ^{9,12} .0 ^{3,5} .0 ^{5,13}]tetradecane-6,11-dione	310,3	21416-53-5	NP-400	2mg/ml	DMSO	2865	Natural Products Library
3	3-F08	Plumbagin	5-hydroxy-2-methyl-1,4-dihydronaphthalene-1,4-dione	188,2	481-42-5	NP-236	2mg/ml	DMSO	2865	Natural Products Library
3	3-F09	Ketopinic acid	(1S,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptane-1-carboxylic acid	182,2	40724-67-2	NP-543	2mg/ml	DMSO	2865	Natural Products Library
3	3-F10	Scopolamine N-butylbromide	(1R,2R,4S,5S,7R)-9-butyl-7-[[[(2S)-3-hydroxy-2-phenylpropanoyl]oxy]-9-methyl-3-oxa-9-azatricyclo[3.3.1.0 ^{2,4}]nonan-9-ium bromide	440,4	149-64-4	NP-527	2mg/ml	DMSO	2865	Natural Products Library
3	3-F11	Rhamnetine	2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-7-methoxy-4H-chromen-4-one	316,3	90-19-7	NP-257	2mg/ml	DMSO	2865	Natural Products Library
3	3-F12	Rhoifolin	7-[[[(2S,3R,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]oxan-2-yl]oxy]-5-hydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one	578,5	17306-46-6	NP-259	2mg/ml	DMSO	2865	Natural Products Library
3	3-G01	Sanguinarine	24-methyl-5,7,18,20-tetraoxa-24-azahexacyclo[11.11.0.0 ^{2,10} .0 ^{4,8} .0 ^{14,22} .0 ^{17,21}]tetracosan-1(13),2(10),3,8,11,14(22),15,17(21),23-nonaen-24-ium	332,3	5578-73-4	NP-269	2mg/ml	DMSO	2865	Natural Products Library
3	3-G02	Saponarin	5-hydroxy-2-(4-hydroxyphenyl)-6-[[[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-7-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-4H-chromen-4-one	594,5	20310-89-8	NP-271	2mg/ml	DMSO	2865	Natural Products Library
3	3-G03	Manool	(3R)-5-[[[(1S,4aS,8aS)-5,5,8a-trimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpent-1-en-3-ol	290,5	596-85-0	NP-545	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-G04	Citreoviridin	6-[(1E,3E,5E,7E)-8-(3,4-dihydroxy-2,4,5-trimethyloxolan-2-yl)-7-methylocta-1,3,5,7-tetraen-1-yl]-4-methoxy-5-methyl-2H-pyran-2-one	402,5	25425-12-1	NP-541	2mg/ml	DMSO	2865	Natural Products Library
3	3-G05	Sinensetine	2-(3,4-dimethoxyphenyl)-5,6,7-trimethoxy-4H-chromen-4-one	372,4	2306-27-6	NP-292	2mg/ml	DMSO	2865	Natural Products Library
3	3-G06	Sulfuretine	(2E)-2-[(3,4-dihydroxyphenyl)methylidene]-6-hydroxy-2,3-dihydro-1-benzofuran-3-one	270,2	120-05-8	NP-308	2mg/ml	DMSO	2865	Natural Products Library
3	3-G07	Atropine-N-oxide-HCl	(1R,3S,5S)-3-[(3-hydroxy-2-phenylpropanoyl)oxy]-8-methyl-8-azabicyclo[3.2.1]octan-8-ium-8-olate hydrochloride	341,8	4574-60-1	NP-544	2mg/ml	DMSO	2865	Natural Products Library
3	3-G08	Tamarixetine	3,5,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one	316,3	603-61-2	NP-311	2mg/ml	DMSO	2865	Natural Products Library
3	3-G09	Tetrahydroalstonine	methyl (1S,15S,16S,20S)-16-methyl-17-oxa-3,13-diazapentacyclo[11.8.0.0 ^{2,10} .0 ^{4,9} .0 ^{15,20}]henicosa-2(10),4,6,8,18-pentaene-19-carboxylate	352,4	6474-90-4	NP-314	2mg/ml	DMSO	2865	Natural Products Library
3	3-G10	Diacetoxyscirpenol	(1'S,2R,2'R,7'R,9'R,10'R,11'S)-11'-{(acetyloxy)-10'-hydroxy-1',5'-dimethyl-8'-oxaspiro[oxirane-2,12'-tricyclo[7.2.1.0 ^{2,7}]dodecan]-5'-en-2'-ylmethyl acetate	366,4	2270-40-8	NP-563	2mg/ml	DMSO	2865	Natural Products Library
3	3-G11	Vitexin-2''-O-rhamnoside	5,7-dihydroxy-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-2-(2-[(3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy)phenyl)-4H-chromen-4-one	578,5	64820-99-1	NP-336	2mg/ml	DMSO	2865	Natural Products Library
3	3-G12	Laudanosoline-HBr·3H ₂ O	1-[(3,4-dihydroxyphenyl)methyl]-2-methyl-1,2,3,4-tetrahydroisoquinoline-6,7-diol trihydrate hydrobromide	436,3	485-33-6	NP-169	2mg/ml	DMSO	2865	Natural Products Library
3	3-H01	(±)-6'-Bromolaudanosine	1-[(2-bromo-4,5-dimethoxyphenyl)methyl]-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline	436,3	53392-66-8	NP-037	2mg/ml	DMSO	2865	Natural Products Library
3	3-H02	Andrographolide	(3E,4S)-3-{2-[(1R,4aS,5R,6R,8aS)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]ethylidene}-4-hydroxyoxolan-2-one	350,4	5508-58-7	NP-008	2mg/ml	DMSO	2865	Natural Products Library
3	3-H03	Ajmaline	(1R,9R,10S,12R,13S,14R,16S,17S,18R)-13-ethyl-8-methyl-8,15-diazahexacyclo[14.2.1.0 ^{1,9} .0 ^{2,7} .0 ^{10,15} .0 ^{12,17}]nonadeca-2,4,6-triene-14,18-diol	326,4	4360-12-7	NP-004	2mg/ml	DMSO	2865	Natural Products Library
3	3-H04	(+)-Chelidoniumine	(1S,12S,13R)-24-methyl-5,7,18,20-tetraoxa-24-azahexacyclo[11.11.0.0 ^{2,10} .0 ^{4,8} .0 ^{14,22} .0 ^{17,21}]tetracosaa-2(10),3,8,14(22),15,17(21)-hexaen-12-ol	353,4	476-32-4	NP-050	2mg/ml	DMSO	2865	Natural Products Library
3	3-H05	6,7-Dihydroxyflavone	6,7-dihydroxy-2-phenyl-4H-chromen-4-one	254,2	38183-04-9	NP-081	2mg/ml	DMSO	2865	Natural Products Library
3	3-H06	Fisetin	2-(3,4-dihydroxyphenyl)-3,7-dihydroxy-4H-chromen-4-one	286,2	528-48-3	NP-104	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
3	3-H07	Harmalol-HCl-2H ₂ O	1-methyl-3H,4H,9H-pyrido[3,4-b]indol-7-ol dihydrate hydrochloride	272,7	6028-00-8	NP-121	2mg/ml	DMSO	2865	Natural Products Library
3	3-H08	Harmol-HCl-2H ₂ O	1-methyl-9H-pyrido[3,4-b]indol-7-ol dihydrate hydrochloride	270,7	40580-83-4	NP-124	2mg/ml	DMSO	2865	Natural Products Library
3	3-H09	Isorhamnetine-3-rutinoside	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-(((2S,3S,4R,5S)-3,4,5-trihydroxy-6-(((2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl)oxy)oxan-2-yl)methoxy)-4H-chromen-4-one	624,5	604-80-8	NP-150	2mg/ml	DMSO	2865	Natural Products Library
3	3-H10	Isoscooletine	6-hydroxy-7-methoxy-2H-chromen-2-one	192,2	776-86-3	NP-153	2mg/ml	DMSO	2865	Natural Products Library
3	3-H11	5-Methoxyflavone	5-methoxy-2-phenyl-4H-chromen-4-one	252,3	42079-78-7	NP-186	2mg/ml	DMSO	2865	Natural Products Library
3	3-H12	Pratol	7-hydroxy-2-(4-methoxyphenyl)-4H-chromen-4-one	268,3	487-24-1	NP-241	2mg/ml	DMSO	2865	Natural Products Library
4	4-A01	Syringetine-3-glucoside	5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-3-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-4H-chromen-4-one	508,4	40039-49-4	NP-309	2mg/ml	DMSO	2865	Natural Products Library
4	4-A02	Conessine	(1R,5S,6S,9R,13R,16S)-N,N,6,7,13-pentamethyl-7-azapentacyclo[10.8.0.0.0 ^{2,9} .0 ^{5,9} .0 ^{13,18}]icos-18-en-16-amine	356,6	546-06-5	NP-495	2mg/ml	DMSO	2865	Natural Products Library
4	4-A03	Sarsasapogenin	(1'R,2R,2'S,4'S,5S,7'S,8'R,9'S,12'S,13'S,16'S,18'R)-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0.0 ^{2,9} .0 ^{4,8} .0 ^{13,18}]icosane]-16'-ol	416,6	126-19-2	NP-272	2mg/ml	DMSO	2865	Natural Products Library
4	4-A04	Strophantidin	(2S,5S,7S,11S,15R)-5,7,11-trihydroxy-15-methyl-14-(5-oxo-2,5-dihydrofuran-3-yl)tetracyclo[8.7.0.0.0 ^{2,7} .0 ^{11,15}]heptadecane-2-carbaldehyde	404,5	66-28-4	NP-306	2mg/ml	DMSO	2865	Natural Products Library
4	4-A05	Hordenine sulfate	bis(4-[2-(dimethylamino)ethyl]phenol); sulfuric acid	428,5	622-64-0	NP-494	2mg/ml	DMSO	2865	Natural Products Library
4	4-A06	Ferutinin	(3R,3aR,4S,8aR)-3-hydroxy-6,8a-dimethyl-3-(propan-2-yl)-1,2,3,3a,4,5,8a-octahydroazulen-4-yl 4-hydroxybenzoate	358,5		NP-534	2mg/ml	DMSO	2865	Natural Products Library
4	4-A07	Piperine	(2E,4E)-5-(2H-1,3-benzodioxol-5-yl)-1-(piperidin-1-yl)penta-2,4-dien-1-one	285,3	94-62-2	NP-235	2mg/ml	DMSO	2865	Natural Products Library
4	4-A08	Quercitrin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(((2S,3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl)oxy)-4H-chromen-4-one	448,4	522-12-3	NP-246	2mg/ml	DMSO	2865	Natural Products Library
4	4-A09	(-)-Scopolamine N-oxide	(1S,2R,4S,5S,7R)-7-[(3-hydroxy-2-phenylpropanoyl)oxy]-9-methyl-3-oxa-9-azatricyclo[3.3.1.0.0 ^{2,4}]nonan-9-ium-9-olate	319,4	6106-81-6	NP-278	2mg/ml	DMSO	2865	Natural Products Library
4	4-A10	Shikimic acid	(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid	174,2	138-59-0	NP-290	2mg/ml	DMSO	2865	Natural Products Library
4	4-A11	Stachydrine-HCl	(2S)-1,1-dimethylpyrrolidin-1-ium-2-carboxylate hydrochloride	179,6	4136-37-2	NP-303	2mg/ml	DMSO	2865	Natural Products Library
4	4-A12	Ochratoxin A	(2S)-2-(((3R)-5-chloro-8-hydroxy-3-methyl-1-oxo-3,4-dihydro-1H-2-benzopyran-7-yl]formamido)-3-phenylpropanoic acid	403,8	303-47-9	NP-212	2mg/ml	DMSO	2865	Natural Products Library
4	4-B01	Patulin	4-hydroxy-2H,4H,6H-furo[3,2-c]pyran-2-one	154,1	149-29-1	NP-223	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-B02	Zearalenone	(3S)-13,15-dihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecine-1,7-dione	318,4	17924-92-4	NP-341	2mg/ml	DMSO	2865	Natural Products Library
4	4-B03	Isorhamnetine	3,5,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one	316,3	418-19-3	NP-148	2mg/ml	DMSO	2865	Natural Products Library
4	4-B04	(±)-Abscisic acid	(2Z,4E)-5-(1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl)-3-methylpenta-2,4-dienoic acid	264,3	14375-45-2	NP-001	2mg/ml	DMSO	2865	Natural Products Library
4	4-B05	Rifamycin-Na	sodium (7S,9E,11R,12R,13R,14R,15R,16R,17R,18R,19E,21Z)-2,15,17,29-tetrahydroxy-11-methoxy-13-(methoxycarbonyl)-3,7,12,14,16,18,22-heptamethyl-6,23-dioxo-8,30-dioxo-24-azatetracyclo[23.3.1.1 ^{4,7} .0 ^{5,28}]triaconta-1(28),2,4,9,19,21,25(29),26-octaen-27-olate	719,8	14897-39-3	NP-526	2mg/ml	DMSO	2865	Natural Products Library
4	4-B06	Aloe-emodin	1,8-dihydroxy-3-(hydroxymethyl)-9,10-dihydroanthracene-9,10-dione	270,2	481-72-1	NP-005	2mg/ml	DMSO	2865	Natural Products Library
4	4-B07	Antimycin A1	(2R,3S,6S,7R,8R)-3-(3-formamido-2-hydroxybenzamido)-8-hexyl-2,6-dimethyl-4,9-dioxo-1,5-dioxonan-7-yl 3-methylbutanoate	548,6	642-15-9	NP-009	2mg/ml	DMSO	2865	Natural Products Library
4	4-B08	(-)-Asarinin	5-[(3aR,6aR)-4-(2H-1,3-benzodioxol-5-yl)-hexahydrofuro[3,4-c]furan-1-yl]-2H-1,3-benzodioxole	354,4	133-05-1	NP-017	2mg/ml	DMSO	2865	Natural Products Library
4	4-B09	Aucubin	(3R,4S,5S,6R)-2-[[[(1S,4aR,5S,7aS)-5-hydroxy-7-(hydroxymethyl)-1H,4aH,5H,7aH-cyclopenta[c]pyran-1-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	346,3	479-98-1	NP-021	2mg/ml	DMSO	2865	Natural Products Library
4	4-B10	Deoxyshikonin	5,8-dihydroxy-2-(4-methylpent-3-en-1-yl)-1,4-dihydronaphthalene-1,4-dione	272,3	43043-74-9	NP-022	2mg/ml	DMSO	2865	Natural Products Library
4	4-B11	Boldine	(9S)-4,16-dimethoxy-10-methyl-10-azatetracyclo[7.7.1.0 ^{2,7} .0 ^{13,17}]heptadeca-1(16),2(7),3,5,13(17),14-hexaene-5,15-diol	327,4	476-70-0	NP-036	2mg/ml	DMSO	2865	Natural Products Library
4	4-B12	Caryophylline	(1R,4R,6R,10S)-4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.0 ^{4,6}]dodecane	220,4	1139-30-6	NP-045	2mg/ml	DMSO	2865	Natural Products Library
4	4-C01	(+)-Catechine	(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol	290,3	225937-10-0	NP-047	2mg/ml	DMSO	2865	Natural Products Library
4	4-C02	(-)-Cinchonidine	(R)-[(2S,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](quinolin-4-yl)methanol	294,4	485-71-2	NP-053	2mg/ml	DMSO	2865	Natural Products Library
4	4-C03	(+)-Cinchonine	[(1R,2R,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](quinolin-4-yl)methanol	294,4	118-10-5	NP-054	2mg/ml	DMSO	2865	Natural Products Library
4	4-C04	Trans-4-Cotinicarboxylic acid	(3S)-1-methyl-5-oxo-2-(pyridin-3-yl)pyrrolidine-3-carboxylic acid	220,2	33224-01-0	NP-065	2mg/ml	DMSO	2865	Natural Products Library
4	4-C05	Demissidine	(1S,2R,5S,7S,10S,11S,14S,15R,16S,17R,20S,23S)-10,14,16,20-tetramethyl-22-azahexacyclo[12.10.0.0 ^{2,11} .0 ^{5,10} .0 ^{15,23} .0 ^{17,22}]tetracosan-7-ol	399,7	474-08-8	NP-072	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-C06	Dipterocarpol	(1R,2R,7R,10R,11R,14S,15R)-14-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-2,6,6,10,11-pentamethyltetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecan-5-one	442,7	471-69-2	NP-085	2mg/ml	DMSO	2865	Natural Products Library
4	4-C07	Dehydrocostus lactone	(3aS,6aR,9aR,9bS)-3,6,9-trimethylidene-dodecahydroazuleno[4,5-b]furan-2-one	230,3	477-43-0	NP-542	2mg/ml	DMSO	2865	Natural Products Library
4	4-C08	Friedelin	(4R,4aS,6aS,6bR,8aR,12aR,12bS,14aS,14bS)-4,4a,6b,8a,11,11,12b,14a-octamethyl-docosahydropicen-3-one	426,7	559-74-0	NP-107	2mg/ml	DMSO	2865	Natural Products Library
4	4-C09	Indole-3-butyric acid	4-(1H-indol-3-yl)butanoic acid	203,2	133-32-4	NP-532	2mg/ml	DMSO	2865	Natural Products Library
4	4-C10	(+)-Gibberellic acid	(1R,2R,5S,8S,9S,10R,11S,12S)-5,12-dihydroxy-11-methyl-6-methylidene-16-oxo-15-oxapentacyclo[9.3.2.1 ^{5,8} .0 ^{1,10} .0 ^{2,8}]heptadec-13-ene-9-carboxylic acid	346,4	77-06-5	NP-113	2mg/ml	DMSO	2865	Natural Products Library
4	4-C11	Gitoxigenin	4-[(1S,2S,5S,7R,10R,11S,13S,14R,15R)-5,11,13-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecan-14-yl]-2,5-dihydrofuran-2-one	390,5	545-26-6	NP-114	2mg/ml	DMSO	2865	Natural Products Library
4	4-C12	Harmane	1-methyl-9H-pyrido[3,4-b]indole	182,2	486-84-0	AC-1050	2mg/ml	DMSO	2865	Natural Products Library
4	4-D01	6-Hydroxytropinone	6-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-one	155,2	5932-53-6	NP-139	2mg/ml	DMSO	2865	Natural Products Library
4	4-D02	(+)-Isocorydine hydrochloride	(9S)-4,15,16-trimethoxy-10-methyl-10-azatetracyclo[7.7.1.0 ^{2,7} .0 ^{13,17}]heptadeca-1(17),2(7),3,5,13,15-hexaen-3-ol hydrochloride	377,9	13552-72-2	NP-144	2mg/ml	DMSO	2865	Natural Products Library
4	4-D03	(-)-Isoreserpine	methyl (1S,15S,17R,18R,19S,20S)-6,18-dimethoxy-17-(3,4,5-trimethoxybenzoyloxy)-3,13-diazapentacyclo[11.8.0.0 ^{2,7} .0 ^{4,9} .0 ^{15,20}]henicosa-2(10),4(9),5,7-tetraene-19-carboxylate	608,7	482-85-9	NP-147	2mg/ml	DMSO	2865	Natural Products Library
4	4-D04	Leucomisine	(3S,3aS,9aS,9bS)-3,6,9-trimethyl-2H,3H,3aH,4H,5H,7H,9aH,9bH-azuleno[4,5-b]furan-2,7-dione	246,3	17946-87-1	NP-170	2mg/ml	DMSO	2865	Natural Products Library
4	4-D05	Methylergonovine maleate	(2Z)-but-2-enedioic acid; (4R,7R)-N-[(2S)-1-hydroxybutan-2-yl]-6-methyl-6,11-diazatetracyclo[7.6.1.0 ^{2,7} .0 ^{12,16}]hexadeca-1(15),2,9,12(16),13-pentaene-4-carboxamide	455,5	57432-61-8	NP-189	2mg/ml	DMSO	2865	Natural Products Library
4	4-D06	Corydaline	(12bR,13S)-3,4,10,11-tetramethoxy-13-methyl-7,8,12b,13-tetrahydro-5H-6-azatetraphene	369,5	518-69-4	NP-061	2mg/ml	DMSO	2865	Natural Products Library
4	4-D07	(+)-Muscarine chloride	{[(2S,4R,5S)-4-hydroxy-5-methyloxolan-2-yl]methyl}trimethylazanium chloride	209,7	2303-35-7	AC-742	2mg/ml	DMSO	2865	Natural Products Library
4	4-D08	Nalidixic acid	1-ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid	232,2	389-08-2	NP-197	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-D09	Narasin	(2R)-2-[(3S,5S,6R)-6-[(2S,3S,4S,6R)-6-[(2S,5S,7R,9S,10S,12R,15R)-2-[(2R,5R,6S)-5-ethyl-5-hydroxy-6-methyloxan-2-yl]-15-hydroxy-2,10,12-trimethyl-1,6,8-trioxadispiro[4.1.5 ⁷ .3 ⁵]pentadec-13-en-9-yl]-3-hydroxy-4-methyl-5-oxooctan-2-yl]-3,5-dimethyloxan-2-yl]butanoic acid	765,0	55134-13-9	NP-198	2mg/ml	DMSO	2865	Natural Products Library
4	4-D10	Noreleagnine	1H,2H,3H,4H,9H-pyrido[3,4-b]indole	172,2	16502-01-5	NP-208	2mg/ml	DMSO	2865	Natural Products Library
4	4-D11	Norharmine	9H-pyrido[3,4-b]indole	168,2	244-63-3	NP-210	2mg/ml	DMSO	2865	Natural Products Library
4	4-D12	Palmatine chloride	3,4,10,11-tetramethoxy-7,8-dihydro-6λ ⁵ -azatetraphen-6-ylum chloride	387,9	171869-95-7	NP-220	2mg/ml	DMSO	2865	Natural Products Library
4	4-E01	Peruvoside	(1S,2R,5S,7R,10R,11S,14R,15R)-5-[[[(2R,4S,5S)-3,5-dihydroxy-4-methoxy-6-methyloxan-2-yl]oxy]-11-hydroxy-15-methyl-14-(5-oxo-2,5-dihydrofuran-3-yl)tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecane-2-carbaldehyde	548,7	1182-87-2	NP-227	2mg/ml	DMSO	2865	Natural Products Library
4	4-E02	Physostigmine	(3aS,8aR)-1,3a,8-trimethyl-1H,2H,3H,3aH,8H,8aH-pyrrolo[2,3-b]indol-5-yl N-methylcarbamate	275,3	57-47-6	AC-241	2mg/ml	DMSO	2865	Natural Products Library
4	4-E03	6-Acetamido-6-deoxy-castanospermine	N-[(1S,6S,7R,8R,8aR)-1,7,8-trihydroxy-octahydroindolizin-6-yl]acetamide	230,3	134100-29-1	NP-573	2mg/ml	DMSO	2865	Natural Products Library
4	4-E04	Podocarpic acid	(1S,4aS,10aR)-6-hydroxy-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylic acid	274,4	5947-49-9	NP-237	2mg/ml	DMSO	2865	Natural Products Library
4	4-E05	Retrorsine	(1R,4Z,6R,7S,17R)-4-ethylidene-7-hydroxy-7-(hydroxymethyl)-6-methyl-2,9-dioxo-14-azatricyclo[9.5.1.0 ^{14,17}]heptadec-11-ene-3,8-dione	351,4	480-54-6	NP-255	2mg/ml	DMSO	2865	Natural Products Library
4	4-E06	Rhapontin	(2S,3R,4S,5S,6R)-2-{3-hydroxy-5-[(E)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]phenoxy}-6-(hydroxymethyl)oxane-3,4,5-triol	420,4	155-58-8	NP-258	2mg/ml	DMSO	2865	Natural Products Library
4	4-E07	(3aR)-(+)-Sclaerolide	(3aR,5aS,9aS,9bR)-3a,6,6,9a-tetramethyl-dodecahydronaphtho[2,1-b]furan-2-one	250,4	564-20-5	NP-275	2mg/ml	DMSO	2865	Natural Products Library
4	4-E08	Streptonigrin	5-amino-6-(7-amino-6-methoxy-5,8-dioxo-5,8-dihydroquinolin-2-yl)-4-(2-hydroxy-3,4-dimethoxyphenyl)-3-methylpyridine-2-carboxylic acid	506,5	3930-19-6	NP-305	2mg/ml	DMSO	2865	Natural Products Library
4	4-E09	Tetrahydropapa-verine-HCl	1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride	379,9	6429-04-5	NP-315	2mg/ml	DMSO	2865	Natural Products Library
4	4-E10	Ingenol	(4S,5R,6R,10R,12R,14R)-4,5,6-trihydroxy-7-(hydroxymethyl)-3,11,11,14-tetramethyltetracyclo[7.5.1.0 ^{1,5} .0 ^{10,12}]pentadeca-2,7-dien-15-one	348,4	30220-46-3	NP-525	2mg/ml	DMSO	2865	Natural Products Library
4	4-E11	Syrosingopine	methyl (1R,15S,17R,18R,19S,20S)-17-{4-[(ethoxycarbonyl)oxy]-3,5-dimethoxybenzoyloxy}-6,18-dimethoxy-3,13-diazapentacyclo[11.8.0.0 ^{2,9} .0 ^{4,9} .0 ^{15,20}]hencosa-2(10),4,6,8-tetraene-19-carboxylate	666,7	84-36-6	NP-574	2mg/ml	DMSO	2865	Natural Products Library
4	4-E12	Visnagin	4-methoxy-7-methyl-5H-furo[3,2-g]chromen-5-one	230,2	82-57-5	NP-334	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-F01	Wogonin	5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one	284,3	632-85-9	NP-337	2mg/ml	DMSO	2865	Natural Products Library
4	4-F02	β -Zearalanol	(3S,7S)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10,11,12-decahydro-1H-2-benzoxacyclotetradecin-1-one	322,4	42422-68-4	NP-340	2mg/ml	DMSO	2865	Natural Products Library
4	4-F03	4-Methylumbelliferone	7-hydroxy-4-methyl-2H-chromen-2-one	176,2	90-33-5	NP-547	2mg/ml	DMSO	2865	Natural Products Library
4	4-F04	Caffeine	1,3,7-trimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione	194,2	58-08-2	ALX-550-322	2mg/ml	DMSO	2865	Natural Products Library
4	4-F05	Ellagic acid	6,7,13,14-tetrahydroxy-2,9-dioxatetracyclo[6.6.2.0 ⁴ , ¹⁶ .0 ¹¹ , ¹⁵]hexadeca-1(15),4,6,8(16),11,13-hexaene-3,10-dione	302,2	476-66-4	NP-091	2mg/ml	DMSO	2865	Natural Products Library
4	4-F06	(-)-Epicatechin	(2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol	290,3	490-46-0	NP-095	2mg/ml	DMSO	2865	Natural Products Library
4	4-F07	Puromycin	(2S)-2-amino-N-[(2S,3S,4R,5R)-5-[6-(dimethylamino)-9H-purin-9-yl]-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]-3-(4-methoxyphenyl)propanamide	471,5	58-58-2	GR-312	2mg/ml	DMSO	2865	Natural Products Library
4	4-F08	18- β -Glycyrrhetic acid	(2S,4aS,6aS,6bR,8aR,10S,12aS,12bR,14bR)-10-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydricene-2-carboxylic acid	470,7	471-53-4	NP-116	2mg/ml	DMSO	2865	Natural Products Library
4	4-F09	(+)-Griseofulvin	(2S,6'R)-7-chloro-2',4,6-trimethoxy-6'-methyl-3H-spiro[1-benzofuran-2,1'-cyclohexan]-2'-ene-3,4'-dione	352,8	126-07-8	NP-119	2mg/ml	DMSO	2865	Natural Products Library
4	4-F10	Isoquercitrine	3-[[[(2S,3R,4R)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one	464,4	21637-25-2	NP-146	2mg/ml	DMSO	2865	Natural Products Library
4	4-F11	Kinetin	N-(furan-2-ylmethyl)-7H-purin-6-amine	215,2	525-79-1	NP-163	2mg/ml	DMSO	2865	Natural Products Library
4	4-F12	Lasalocid A	sodium 6-[(3R,4S,5S,7R)-7-[(3S,5S)-5-ethyl-5-[(5R,6S)-5-ethyl-5-hydroxy-6-methyloxan-2-yl]-3-methyloxolan-2-yl]-4-hydroxy-3,5-dimethyl-6-oxononyl]-2-hydroxy-3-methylbenzoate	612,8	25999-20-6	NP-167	2mg/ml	DMSO	2865	Natural Products Library
4	4-G01	Vannilylacetone	4-(4-hydroxy-3-methoxyphenyl)butan-2-one	194,2	122-48-5	NP-560	2mg/ml	DMSO	2865	Natural Products Library
4	4-G02	Sclareol	(1R,2R,4aS,8aS)-1-[(3S)-3-hydroxy-3-methylpent-4-en-1-yl]-2,5,5,8a-tetramethyl-decahydronaphthalen-2-ol	308,5	515-03-7	NP-274	2mg/ml	DMSO	2865	Natural Products Library
4	4-G03	Trigonelline-HCl	3-carboxy-1-methylpyridin-1-ium hydrochloride	174,6	6138-41-6	NP-322	2mg/ml	DMSO	2865	Natural Products Library
4	4-G04	Tuberlicidin	(2R,4R,5R)-2-[4-amino-7H-pyrrolo[2,3-d]pyrimidin-7-yl]-5-(hydroxymethyl)oxolane-3,4-diol	266,3	69-33-0	NP-327	2mg/ml	DMSO	2865	Natural Products Library
4	4-G05	(+)-Usnic acid	(2R)-4,10-diacetyl-3,11,13-trihydroxy-2,12-dimethyl-8-oxatricyclo[7.4.0.0 ^{2,7}]trideca-1(9),3,6,10,12-pentaen-5-one	344,3	7562-61-0	NP-330	2mg/ml	DMSO	2865	Natural Products Library
4	4-G06	Vitexin	5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[[[2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	432,4	3681-93-4	NP-335	2mg/ml	DMSO	2865	Natural Products Library
4	4-G07	Acacetine	5,7-dihydroxy-2-(4-methoxyphenyl)-4H-chromen-4-one	284,3	480-44-4	NP-002	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-G08	Capreomycin	3,6-diamino-N-[[[8Z]-15-amino-8-[[[carbamoylamino)methylidene]-11-(2-imino-1,3-diazinan-4-yl)-2-methyl-3,6,9,12,16-pentaaxo-1,4,7,10,13-pentaazacyclohexadecan-5-yl]methyl]hexanamide	652,7	1405-37-4	NP-042	2mg/ml	DMSO	2865	Natural Products Library
4	4-G09	(±)-Carnitine	3-hydroxy-4-(trimethylazaniumyl)butanoate hydrochloride	197,7	461-05-2	NP-044	2mg/ml	DMSO	2865	Natural Products Library
4	4-G10	Cephadrine	(6R,7R)-7-[[2R]-2-amino-2-(cyclohexa-1,4-dien-1-yl)acetamido]-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	349,4	38821-53-3	NP-048	2mg/ml	DMSO	2865	Natural Products Library
4	4-G11	Vasicine	1H,2H,3H,9H-pyrrolo[2,1-b]quinazolin-3-ol	188,2	50591-64-5	NP-450	2mg/ml	DMSO	2865	Natural Products Library
4	4-G12	Homatropine-H Br	8-methyl-8-azabicyclo[3.2.1]octan-3-yl 2-hydroxy-2-phenylacetate hydrobromide	356,3	51-56-9	NP-131	2mg/ml	DMSO	2865	Natural Products Library
4	4-H01	D-β-Hydrastine	(3S)-6,7-dimethoxy-3-[(5R)-6-methyl-2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinolin-5-yl]-1,3-dihydro-2-benzofuran-1-one	383,4	118-08-1	NP-136	2mg/ml	DMSO	2865	Natural Products Library
4	4-H02	Khellin	4,9-dimethoxy-7-methyl-5H-furo[3,2-g]chromen-5-one	260,2	82-02-0	NP-162	2mg/ml	DMSO	2865	Natural Products Library
4	4-H03	Lobeline-HCl	2-[(2R,6S)-6-[(2S)-2-hydroxy-2-phenylethyl]-1-methylpiperidin-2-yl]-1-phenylethan-1-one hydrochloride	373,9	134-63-4	AC-227	2mg/ml	DMSO	2865	Natural Products Library
4	4-H04	Osthole	7-methoxy-8-(3-methylbut-2-en-1-yl)-2H-chromen-2-one	244,3	484-12-8	NP-522	2mg/ml	DMSO	2865	Natural Products Library
4	4-H05	Tetrahydrolipist atin	(2S)-1-[(2S,3S)-3-hexyl-4-oxooxetan-2-yl]tridecan-2-yl (2S)-2-formamido-4-methylpentanoate	495,7	96829-58-2	NP-521	2mg/ml	DMSO	2865	Natural Products Library
4	4-H06	Neohesperidin	(2S)-7-[[[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[[[3R,4R,5R,6S]-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]oxan-2-yl]oxy]-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	610,6	13241-33-3	NP-205	2mg/ml	DMSO	2865	Natural Products Library
4	4-H07	(±)-Noscapine	(3S)-6,7-dimethoxy-3-[(5R)-4-methoxy-6-methyl-2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinolin-5-yl]-1,3-dihydro-2-benzofuran-1-one	413,4	128-62-1	NP-211	2mg/ml	DMSO	2865	Natural Products Library
4	4-H08	Oleanolic acid	(4aS,6aS,6bR,8aR,10S,12aR,12bR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	456,7	508-02-1	NP-213	2mg/ml	DMSO	2865	Natural Products Library
4	4-H09	Papaverine-HCl	1-[[3,4-dimethoxyphenyl)methyl]-6,7-dimethoxyisoquinoline hydrochloride	375,8	61-25-6	NP-221	2mg/ml	DMSO	2865	Natural Products Library
4	4-H10	Phlorizine	1-(2,4-dihydroxy-6-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]phenyl]-3-(4-hydroxyphenyl)propan-1-one	436,4	60-81-1	NP-229	2mg/ml	DMSO	2865	Natural Products Library
4	4-H11	Protoveratrine B	(1S,2S,6S,9S,10S,11R,12R,13S,14S,15S,16S,17R,18R,19S,22S,23R,25R)-16,17-bis(acetyloxy)-10,12,14,23-tetrahydroxy-6,10,19-trimethyl-13-[[[(2R)-2-methylbutanoyl]oxy]-24-oxa-4-azaheptacyclo[12.12.0.0 ^{2,11} .0 ^{4,9} .0 ^{15,25} .0 ^{18,23} .0 ^{19,25}]hexacosan-22-yl 2,3-dihydroxy-2-methylbutanoate	809,9	124-97-0	NP-243	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
4	4-H12	Reserpine	methyl (1R,15S,17R,18R,19S,20S)-6,18-dimethoxy-17-(3,4,5-trimethoxybenzoyloxy)-3,13-diazapentacyclo[11.8.0.0.2 ⁹ .0.0 ¹⁰ .0 ¹⁵ .2 ²⁰]henicosa-2(10),4,6,8-tetraene-19-carboxylate	608,7	50-55-5	NP-254	2mg/ml	DMSO	2865	Natural Products Library
5	5-A01	Salinomycin	(2R)-2-[(2R,5S,6R)-6-[(2S,3S,4S,6R)-6-[(2S,5S,7R,9S,10S,12R,15R)-2-[(2R,5R,6S)-5-ethyl-5-hydroxy-6-methyloxan-2-yl]-15-hydroxy-2,10,12-trimethyl-1,6,8-trioxadispiro[4.1.5 ⁷ .3 ⁵]pentadec-13-en-9-yl]-3-hydroxy-4-methyl-5-oxooctan-2-yl]-5-methyloxan-2-yl]butanoic acid	751,0	53003-10-4	NP-267	2mg/ml	DMSO	2865	Natural Products Library
5	5-A02	Xanthotoxin	9-methoxy-7H-furo[3,2-g]chromen-7-one	216,2	298-81-7	NP-554	2mg/ml	DMSO	2865	Natural Products Library
5	5-A03	Scopoletin	7-hydroxy-6-methoxy-2H-chromen-2-one	192,2	92-61-5	NP-282	2mg/ml	DMSO	2865	Natural Products Library
5	5-A04	Digitoxin	4-[(1S,2S,5S,7R,10R,11S,14R,15R)-5-[(2R,4S,5S,6R)-5-[(2S,4S,5S,6R)-5-[(2S,4S,5S,6R)-4,5-dihydroxy-6-methyloxan-2-yl]oxy)-4-hydroxy-6-methyloxan-2-yl]oxy)-4-hydroxy-6-methyloxan-2-yl]oxy)-11-hydroxy-2,15-dimethyltetracyclo[8.7.0.0.2 ⁷ .0 ¹¹ .1 ⁵]heptadecan-14-yl]-2,5-dihydrofuran-2-one	764,9	71-63-6	NP-548	2mg/ml	DMSO	2865	Natural Products Library
5	5-A05	α -Solanine	(2R,3R,4R,5R,6S)-2-[(2R,3R,4S,5S,6R)-5-hydroxy-6-(hydroxymethyl)-2-[[[(1S,2S,7S,10R,11S,14S,15R,16S,17R,20S,23S)-10,14,16,20-tetramethyl-22-azahexacyclo[12.10.0.0.0 ² .1 ¹ .0 ⁵ .1 ⁰ .0 ¹⁵ .2 ³ .0 ¹⁷ .2 ²²]tetracos-4-en-7-yl]oxy)-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]oxan-3-yl]oxy)-6-methyloxane-3,4,5-triol	868,1	20562-02-1	NP-298	2mg/ml	DMSO	2865	Natural Products Library
5	5-A06	Solasodine	(1S,2S,4S,5'R,7R,8R,9S,12S,13R,16S)-5',7,9,13-tetramethyl-5-oxaspiro[pentacyclo[10.8.0.0.0 ² .9.0 ⁴ .8.0 ¹³ .1 ⁸]icosane-6,2'-piperidin]-18-en-16-ol	413,6	80-78-4	NP-299	2mg/ml	DMSO	2865	Natural Products Library
5	5-A07	Tropine	8-methyl-8-azabicyclo[3.2.1]octan-3-ol	141,2	120-29-6	NP-324	2mg/ml	DMSO	2865	Natural Products Library
5	5-A08	(+)-Tubocurarine chloride	(1S,16R)-9,21-dihydroxy-10,25-dimethoxy-15,15,30-trimethyl-7,23-dioxa-15,30-diazaheptacyclo[22.6.2.2 ³ .6.1 ⁸ .1 ² .1 ¹⁸ .2 ² .0 ²⁷ .3 ¹ .0 ¹⁶ .3 ⁴]hexatriaconta-3,5,8,10,12(34),18,20,22(33),24(32),25,27(31),35-dodecaene-15,30-diium chloride hydrochloride	682,7	57-94-3	AC-746	2mg/ml	DMSO	2865	Natural Products Library
5	5-A09	Myristicin	4-methoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxole	192,2	607-91-0	NP-520	2mg/ml	DMSO	2865	Natural Products Library
5	5-A10	Vincamine	methyl (15S,17S,19S)-15-ethyl-17-hydroxy-1,11-diazapentacyclo[9.6.2.0.2 ⁷ .0 ⁸ .1 ⁸ .0 ¹⁵ .1 ⁹]nonadeca-2(7),3,5,8(18)-tetraene-17-carboxylate	354,4	1617-90-9	NP-332	2mg/ml	DMSO	2865	Natural Products Library
5	5-A11	(\pm)-Anabasine	3-(piperidin-2-yl)pyridine	162,2	15251-47-5	NP-007	2mg/ml	DMSO	2865	Natural Products Library
5	5-A12	Cephaeline-HBr	(1R)-1-[(2S,3R,11bS)-3-ethyl-9,10-dimethoxy-1H,2H,3H,4H,6H,7H,11bH-pyrido[2,1-a]isoquinolin-2-yl]methyl-7-methoxy-1,2,3,4-tetrahydroisoquinolin-6-ol hydrobromide	547,5	483-17-0	NP-569	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-B01	Dicoumarol	4-hydroxy-3-[(4-hydroxy-2-oxo-2H-chromen-3-yl)methyl]-2H-chromen-2-one	336,3	66-76-2	NP-535	2mg/ml	DMSO	2865	Natural Products Library
5	5-B02	Artemesinin	(1S,4S,5R,8S,9R,12S,13R)-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0 ⁴ , ¹³ .0 ⁸ , ¹³]hexadecan-10-one	282,3	63968-64-9	NP-016	2mg/ml	DMSO	2865	Natural Products Library
5	5-B03	Asiatic acid	(1S,2R,4aS,6aS,6bR,8aR,9R,10R,11R,12aR,12bR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydronicene-4a-carboxylic acid	488,7	464-92-6	NP-412	2mg/ml	DMSO	2865	Natural Products Library
5	5-B04	Auraptene	7-[[[(2E)-3,7-dimethylocta-2,6-dien-1-yl]oxy]-2H-chromen-2-one	298,4	495-02-3	NP-413	2mg/ml	DMSO	2865	Natural Products Library
5	5-B05	Vulpinic acid	methyl 2-[(2E)-3-hydroxy-5-oxo-4-phenyl-2,5-dihydrofuran-2-ylidene]-2-phenylacetate	322,3	521-52-8	NP-553	2mg/ml	DMSO	2865	Natural Products Library
5	5-B06	Berberine-HCl	16,17-dimethoxy-5,7-dioxo-13λ ⁵ -azapentacyclo[11.8.0.0 ² , ¹⁰ .0 ⁴ , ⁸ .0 ¹⁵ , ²⁰]henicosa-1(21),2,4(8),9,13,15(20),16,18-octaen-13-ylum hydrochloride	372,8	633-65-8	NP-027	2mg/ml	DMSO	2865	Natural Products Library
5	5-B07	Bergenin	(2S,4R,5S,6S,7R)-5,6,12,14-tetrahydroxy-4-(hydroxymethyl)-13-methoxy-3,8-dioxatricyclo[8.4.0.0 ² , ⁷]tetradeca-1(14),10,12-trien-9-one	328,3	477-90-7	NP-414	2mg/ml	DMSO	2865	Natural Products Library
5	5-B08	Biochanin A	5,7-dihydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one	284,3	491-80-5	NP-034	2mg/ml	DMSO	2865	Natural Products Library
5	5-B09	Bulleyaconotine A	(4R,5S,8R,9R,10S,18R)-8-(acetyloxy)-11-ethyl-5-hydroxy-6,16,18-trimethoxy-13-(methoxymethyl)-11-azahehexacyclo[7.7.2.1 ² , ⁵ .0 ¹ , ¹⁰ .0 ³ , ⁸ .0 ¹³ , ¹⁷]nonadecan-4-yl 4-methoxybenzoate	643,8	107668-79-1	NP-416	2mg/ml	DMSO	2865	Natural Products Library
5	5-B10	Cafestol	(1S,4S,12S,13R,16R,17R)-17-(hydroxymethyl)-12-methyl-8-oxapentacyclo[14.2.1.0 ¹ , ¹³ .0 ⁴ , ¹² .0 ⁵ , ⁹]nonadeca-5(9),6-dien-17-ol	316,4	469-83-0	NP-418	2mg/ml	DMSO	2865	Natural Products Library
5	5-B11	Cafestol acetate	[(4S,12S,13R,16R,17R)-17-hydroxy-12-methyl-8-oxapentacyclo[14.2.1.0 ¹ , ¹³ .0 ⁴ , ¹² .0 ⁵ , ⁹]nonadeca-5(9),6-dien-17-yl]methyl acetate	358,5	81760-48-7	NP-419	2mg/ml	DMSO	2865	Natural Products Library
5	5-B12	Zerumbone	(2E,6E,10E)-2,6,9,9-tetramethylcycloundeca-2,6,10-trien-1-one	218,3	471-05-6	NP-570	2mg/ml	DMSO	2865	Natural Products Library
5	5-C01	Catharanthine	methyl (1R)-17-ethyl-3,13-diazapentacyclo[13.3.1.0 ² , ¹⁰ .0 ⁴ , ⁹ .0 ¹³ , ¹⁸]nonadeca-2(10),4(9),5,7,16-pentaene-1-carboxylate	336,4	2468-21-5	NP-421	2mg/ml	DMSO	2865	Natural Products Library
5	5-C02	Cepharanthine	(14S,27R)-22,33-dimethoxy-13,28-dimethyl-2,5,7,20-tetraoxa-13,28-diazaoctacyclo[25.6.2.2 ¹⁶ , ¹⁹ .1 ³ , ¹⁰ .1 ²¹ , ²⁵ .0 ⁴ , ⁸ .0 ³¹ , ³⁵ .0 ¹⁴ , ³⁹]nonatriaconta-1(34),3,8,10(39),16,18,21,23,25(36),31(35),32,37-dodecaene	606,7	481-49-2	NP-404	2mg/ml	DMSO	2865	Natural Products Library
5	5-C03	Cryptotanshinone	(14R)-6,6,14-trimethyl-12-oxatetracyclo[8.7.0.0 ² , ⁷ .0 ¹¹ , ¹⁵]heptadeca-1,7,9,11(15)-tetraene-16,17-dione	296,4	35825-57-1	NP-422	2mg/ml	DMSO	2865	Natural Products Library
5	5-C04	5,6-Dehydrokawain	4-methoxy-6-[(E)-2-phenylethenyl]-2H-pyran-2-one	228,2	15345-89-8	NP-423	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-C05	4'-Demethylpipodophyllotoxin	(10R,11R,15R,16S)-16-hydroxy-10-(4-hydroxy-3,5-dimethoxyphenyl)-4,6,13-trioxatetracyclo[7.7.0.0 ^{3,7} .0 ^{11,15}]hexadeca-1,3(7),8-trien-12-one	400,4	6559-91-7	NP-424	2mg/ml	DMSO	2865	Natural Products Library
5	5-C06	Mitomycin C	[(4S,6S,7R,8S)-11-amino-7-methoxy-12-methyl-10,13-dioxo-2,5-diazatetracyclo[7.4.0.0 ^{2,7} .0 ^{4,6}]trideca-1(9),11-dien-8-yl]methyl carbamate	334,3	50-07-7	GR-311	2mg/ml	DMSO	2865	Natural Products Library
5	5-C07	Methysticin	(6S)-6-[(E)-2-(2H-1,3-benzodioxol-5-yl)ethenyl]-4-methoxy-5,6-dihydro-2H-pyran-2-one	274,3	495-85-2	NP-518	2mg/ml	DMSO	2865	Natural Products Library
5	5-C08	Thymoquinone	2-methyl-5-(propan-2-yl)cyclohexa-2,5-diene-1,4-dione	164,2	490-91-5	NP-536	2mg/ml	DMSO	2865	Natural Products Library
5	5-C09	Dihydrotanshinone	(14R)-6,14-dimethyl-12-oxatetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadeca-1(10),2(7),3,5,8,11(15)-hexaene-16,17-dione	278,3	20958-18-3	NP-428	2mg/ml	DMSO	2865	Natural Products Library
5	5-C10	Azomycin	2-nitro-1H-imidazole	113,1	527-73-1	NP-533	2mg/ml	DMSO	2865	Natural Products Library
5	5-C11	Diosmetine	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-chromen-4-one	300,3	520-34-3	NP-082	2mg/ml	DMSO	2865	Natural Products Library
5	5-C12	Diosmin	5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(((2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methylloxan-2-yl)oxy)methyl)oxan-2-yl)oxy)-4H-chromen-4-one	608,5	520-27-4	NP-084	2mg/ml	DMSO	2865	Natural Products Library
5	5-D01	Ecdysone	(1R,2R,4S,5R,7R,11S,14R,15R)-14-[(2S,3R)-3,6-dihydroxy-6-methylheptan-2-yl]-4,5,11-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadec-9-en-8-one	464,6	3604-87-3	NP-089	2mg/ml	DMSO	2865	Natural Products Library
5	5-D02	β-Ecdysone	(1R,2R,4S,5R,7R,11S,14S,15R)-4,5,11-trihydroxy-2,15-dimethyl-14-[(2S,3R)-2,3,6-trihydroxy-6-methylheptan-2-yl]tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadec-9-en-8-one	480,6	5289-74-7	NP-430	2mg/ml	DMSO	2865	Natural Products Library
5	5-D03	Euphorbiasteroid	(1'R,2R,3'E,5'R,7'S,11'S,12'R,13'S,14'S)-1',11'-bis(acetyloxy)-3',6',6',14'-tetramethyl-2'-oxospiro[oxirane-2,10'-tricyclo[10.3.0.0 ^{5,7}]pentadecan]-3'-en-13'-yl 2-phenylacetate	552,7	28649-59-4	NP-431	2mg/ml	DMSO	2865	Natural Products Library
5	5-D04	Flavokawain A	(2E)-1-(4-hydroxy-2,6-dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one	314,3	3420-72-2	NP-432	2mg/ml	DMSO	2865	Natural Products Library
5	5-D05	Lupinine	(1R,9aR)-octahydro-1H-quinolizin-1-ylmethanol	169,3	545-47-1	NP-516	2mg/ml	DMSO	2865	Natural Products Library
5	5-D06	Formononetin	7-hydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one	268,3	485-72-3	NP-106	2mg/ml	DMSO	2865	Natural Products Library
5	5-D07	Ginkgolide A	(3S,6R,7S,8S,11S,13S,16S,17R)-8-tert-butyl-6,17-dihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.0 ^{1,11} .0 ^{3,7} .0 ^{7,11} .0 ^{13,17}]nonadecane-5,15,18-trione	408,4	15291-75-5	NP-342	2mg/ml	DMSO	2865	Natural Products Library
5	5-D08	Harringtonine	(2R,3S,6R)-4-methoxy-16,18-dioxo-10-azapentacyclo[11.7.0.0 ^{2,6} .0 ^{6,10} .0 ^{15,19}]icosa-1(13),4,14,19-tetraen-3-yl 1-methyl (3S)-3-hydroxy-3-(3-hydroxy-3-methylbutyl)butanedioate	531,6	26833-85-2	NP-435	2mg/ml	DMSO	2865	Natural Products Library
5	5-D09	Hesperitine	(2S)-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	302,3	520-33-2	NP-127	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-D10	Hesperidine	(2S)-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7- {[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6- {[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy)methyl}oxan-2-yl]oxy}-3,4-dihydro-2H-1-benzopyran-4-one	610,6	520-26-3	NP-128	2mg/ml	DMSO	2865	Natural Products Library
5	5-D11	Honokiol	2-[4-hydroxy-3-(prop-2-en-1-yl)phenyl]-4-(prop-2-en-1-yl)phenol	266,3	35354-74-6	NP-135	2mg/ml	DMSO	2865	Natural Products Library
5	5-D12	Hypocrellin A	(12S,13R)-12-acetyl-9,13,19-trihydroxy-5,10,16,21-tetramethoxy-13-methylhexacyclo[13.8.0.0 ² . ¹¹ .0 ³ . ⁸ .0 ⁴ . ²² .0 ¹⁸ . ²³]tricosan-1,3,5,8,10,15,18(23),19,21-nonaene-7,17-dione	546,5	77029-83-5	NP-437	2mg/ml	DMSO	2865	Natural Products Library
5	5-E01	Hypocrellin B	7-acetyl-14,21-dihydroxy-6,12,17,19-tetramethoxy-9-methylhexacyclo[13.8.0.0 ² . ¹¹ .0 ³ . ⁸ .0 ⁴ . ²² .0 ¹⁸ . ²³]tricosan-1(23),2,4(22),6,8,11,14,16,18,20-decaene-5,13-dione	528,5	123940-54-5	NP-438	2mg/ml	DMSO	2865	Natural Products Library
5	5-E02	Lagochiline	(1S,2R,5R,6S,8aS)-5'-(2-hydroxyethyl)-5,5'-bis(hydroxymethyl)-2,5,8a-trimethyl-octahydro-2H-spiro[naphthalene-1,2'-oxolane]-6-ol	356,5	23554-81-6	NP-439	2mg/ml	DMSO	2865	Natural Products Library
5	5-E03	Lappaconitine	(1S,4S,5R,8S,9S,10R,13S)-11-ethyl-3,8-dihydroxy-4,6,16-trimethoxy-11-azahehexacyclo[7.7.2.1 ² . ⁵ .0 ¹ . ¹⁰ .0 ³ . ⁸ .0 ¹³ . ¹⁷]nonadecan-13-yl 2-acetamidobenzoate	584,7	32854-75-4	NP-166	2mg/ml	DMSO	2865	Natural Products Library
5	5-E04	Limonin	(1R,2R,7S,10R,13R,14R,19R,20S)-19-(furan-3-yl)-9,9,13,20-tetramethyl-4,8,15,18-tetraoxahexacyclo[11.9.0.0 ² . ⁷ .0 ² . ¹⁰ .0 ¹⁴ . ¹⁶ .0 ¹⁴ . ²⁰]docosane-5,12,17-trione	470,5	1180-71-8	NP-440	2mg/ml	DMSO	2865	Natural Products Library
5	5-E05	Madecassic acid	(1S,2R,4aS,6aS,6bR,8R,8aR,9R,10R,11R,12aR,12bR,14bS)-8,10,11-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	504,7	18449-41-7	NP-442	2mg/ml	DMSO	2865	Natural Products Library
5	5-E06	Magnolol	2-[2-hydroxy-5-(prop-2-en-1-yl)phenyl]-4-(prop-2-en-1-yl)phenol	266,3	528-43-8	NP-181	2mg/ml	DMSO	2865	Natural Products Library
5	5-E07	Matrine	(1R,2R,9S,17S)-7,13-diazatetracyclo[7.7.1.0 ² . ⁷ .0 ¹³ . ¹⁷]heptadecan-6-one	248,4	519-02-8	NP-443	2mg/ml	DMSO	2865	Natural Products Library
5	5-E08	Minocycline-HCl	(4S,4aS,5aR,12aS)-4,7-bis(dimethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide hydrochloride	493,9	13614-98-7	NP-191	2mg/ml	DMSO	2865	Natural Products Library
5	5-E09	Naringin	(2S)-7- {[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3- {[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}oxan-2-yl]oxy}-5-hydroxy-2-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	580,5	10236-47-2	NP-202	2mg/ml	DMSO	2865	Natural Products Library
5	5-E10	Indole-3-acetic acid	2-(1H-indol-3-yl)acetic acid	175,2	87-51-4	NP-546	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-E11	16-Oxocafestol	(1S,4S,12S,13R)-12-methyl-8-oxapentacyclo[14.2.1.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadeca-5(9),6-dien-17-one	284,4	108664-98-8	NP-446	2mg/ml	DMSO	2865	Natural Products Library
5	5-E12	16-Oxokahweol	(1S,4S,12S,13R)-12-methyl-8-oxapentacyclo[14.2.1.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadeca-5(9),6,10-trien-17-one	282,4	108664-99-9	NP-447	2mg/ml	DMSO	2865	Natural Products Library
5	5-F01	Panaxadiol	(1R,2R,5S,7R,10R,11R,14S,15R,16R)-2,6,6,10,11-pentamethyl-14-[(2S)-2,6,6-trimethyloxan-2-yl]tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecane-5,16-diol	460,7	19666-76-3	NP-448	2mg/ml	DMSO	2865	Natural Products Library
5	5-F02	Panaxatriol	(1R,2R,5S,7R,8S,10R,11R,14S,15R,16R)-2,6,6,10,11-pentamethyl-14-[(2S)-2,6,6-trimethyloxan-2-yl]tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadecane-5,8,16-triol	476,7	32791-84-7	NP-449	2mg/ml	DMSO	2865	Natural Products Library
5	5-F03	GERI-BP002-A	2-tert-butyl-6-[(3-tert-butyl-2-hydroxy-5-methylphenyl)methyl]-4-methylphenol	340,5	119-47-1	EI-363	2mg/ml	DMSO	2865	Natural Products Library
5	5-F04	Pimaricin	(1S,3R,5S,7S,8E,12R,14E,16E,18E,20E,24R,25S,26R)-22-[[[(2R,3R,5S)-4-amino-3,5-dihydroxy-6-methyloxan-2-yl]oxy]-1,3,26-trihydroxy-12-methyl-10-oxo-6,11,28-trioxatricyclo[22.3.1.0 ^{5,7}]octacosane-8,14,16,18,20-pentaene-25-carboxylic acid	665,7	7681-93-8	NP-232	2mg/ml	DMSO	2865	Natural Products Library
5	5-F05	Podophyllotoxin	(10R,11R,16R)-16-hydroxy-10-(3,4,5-trimethoxyphenyl)-4,6,13-trioxatetracyclo[7.7.0.0 ^{3,7} .0 ^{11,15}]hexadeca-1(9),2,7-trien-12-one	414,4	518-28-5	NP-238	2mg/ml	DMSO	2865	Natural Products Library
5	5-F06	Rubescensin A	(1S,2S,5S,8R,9R,10R,11R,15S,18R)-9,10,15,18-tetrahydroxy-12,12-dimethyl-6-methylidene-17-oxapentacyclo[7.6.2.1 ^{5,8} .0 ^{1,11} .0 ^{2,8}]octadecan-7-one	364,4	28957-04-2	NP-451	2mg/ml	DMSO	2865	Natural Products Library
5	5-F07	Rutaecarpine	3,13,21-triazapentacyclo[11.8.0.0 ^{2,10} .0 ^{4,9} .0 ^{15,20}]henicosane-1(21),2(10),4(9),5,7,15,17,19-octaen-14-one	287,3	84-26-4	NP-452	2mg/ml	DMSO	2865	Natural Products Library
5	5-F08	Rutin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(((2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy)methyl)oxan-2-yl]oxy)-4H-chromen-4-one	610,5	153-18-4	NP-266	2mg/ml	DMSO	2865	Natural Products Library
5	5-F09	Salsolodine	(1R)-6,7-dimethoxy-1-methyl-1,2,3,4-tetrahydroisoquinoline	207,3	493-48-1	NP-453	2mg/ml	DMSO	2865	Natural Products Library
5	5-F10	Salsoline	(1R)-7-methoxy-1-methyl-1,2,3,4-tetrahydroisoquinolin-6-ol	193,2	101467-40-7	NP-454	2mg/ml	DMSO	2865	Natural Products Library
5	5-F11	Santonin	(3S,3aS,5aS,9bS)-3,5a,9-trimethyl-2H,3H,3aH,4H,5H,5aH,8H,9bH-naphtho[1,2-b]furan-2,8-dione	246,3	481-06-1	NP-270	2mg/ml	DMSO	2865	Natural Products Library
5	5-F12	R(+)-Schisandrin A	3,4,5,14,15,16-hexamethoxy-9,10-dimethyltricyclo[10.4.0.0 ^{2,7}]hexadeca-1(12),2(7),3,5,13,15-hexaene	416,5	61281-38-7	NP-455	2mg/ml	DMSO	2865	Natural Products Library
5	5-G01	S(-)-Schisandrin A	3,4,5,19-tetramethoxy-9,10-dimethyl-15,17-dioxatetracyclo[10.7.0.0 ^{2,7} .0 ^{14,18}]nonadeca-1(12),2(7),3,5,13,18-hexaene	400,5	61281-37-6	NP-456	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-G02	Schisantherin A	9-hydroxy-3,4,5,19-tetramethoxy-9,10-dimethyl-15,17-dioxatetracyclo[10.7.0.0 ² ,7.0 ¹⁴ ,18]nonadeca-1(12),2(7),3,5,13,18-hexaen-8-yl benzoate	536,6	58546-56-8	NP-457	2mg/ml	DMSO	2865	Natural Products Library
5	5-G03	Securinine	(1S,2R,8S)-14-oxa-7-azatetracyclo[6.6.1.0 ¹ ,11.0 ² ,7]pentadeca-9,11-dien-13-one	217,3	5610-40-2	NP-285	2mg/ml	DMSO	2865	Natural Products Library
5	5-G04	Sedanolid	3-(2-methylpropyl)-1,3,3a,4,5,6-hexahydro-2-benzofuran-1-one	194,3	6415-59-4	NP-458	2mg/ml	DMSO	2865	Natural Products Library
5	5-G05	Silybine	(2R,3R)-3,5,7-trihydroxy-2-[(2R,3R)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-3,4-dihydro-2H-1-benzopyran-4-one	482,4	22888-70-6	NP-291	2mg/ml	DMSO	2865	Natural Products Library
5	5-G06	Silymarin	(2S,3R)-3,5,7-trihydroxy-2-[(2R,3R)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-3,4-dihydro-2H-1-benzopyran-4-one	482,4	65666-07-1	NP-459	2mg/ml	DMSO	2865	Natural Products Library
5	5-G07	Sinomenine	(1R,9S,10S)-3-hydroxy-4,12-dimethoxy-17-methyl-17-azatetracyclo[7.5.3.0 ¹ ,10.0 ² ,7]heptadeca-2(7),3,5,11-tetraen-13-one	329,4	115-53-7	NP-293	2mg/ml	DMSO	2865	Natural Products Library
5	5-G08	Solanesol	(2E,6E,10E,14E,18E,22E,26E,30E)-3,7,11,15,19,23,27,31,35-nonamethylhexatriaconta-2,6,10,14,18,22,26,30,34-nonaen-1-ol	631,1	13190-97-1	NP-296	2mg/ml	DMSO	2865	Natural Products Library
5	5-G09	Vindoline	methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0 ¹ ,9.0 ² ,7.0 ¹⁶ ,19]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	456,5	2182-14-1	NP-460	2mg/ml	DMSO	2865	Natural Products Library
5	5-G10	Vinorelbine	methyl (1R,9R,10S,11R,12R,19R)-11-(acetyloxy)-12-ethyl-4-[(1R,12S,14R)-16-ethyl-12-(methoxycarbonyl)-1,10-diazatetracyclo[12.3.1.0 ³ ,11.0 ⁴ ,9]octadeca-3(11),4(9),5,7,15-pentaen-12-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.0 ¹ ,9.0 ² ,7.0 ¹⁶ ,19]nonadeca-2(7),3,5,13-tetraene-10-carboxylate	778,9	71486-22-1	NP-461	2mg/ml	DMSO	2865	Natural Products Library
5	5-G11	Yangonin	4-methoxy-6-[(E)-2-(4-methoxyphenyl)ethenyl]-2H-pyran-2-one	258,3	500-62-9	NP-462	2mg/ml	DMSO	2865	Natural Products Library
5	5-G12	Bergapten	4-methoxy-7H-furo[3,2-g]chromen-7-one	216,2	484-20-8	NP-028	2mg/ml	DMSO	2865	Natural Products Library
5	5-H01	Betulin	(1R,2R,5S,8R,9R,10R,13R,14R,17S,19R)-5-(hydroxymethyl)-1,2,14,18,18-pentamethyl-8-(prop-1-en-2-yl)pentacyclo[11.8.0.0 ² ,10.0 ⁵ ,9.0 ¹⁴ ,19]heneicosan-17-ol	442,7	473-98-3	NP-030	2mg/ml	DMSO	2865	Natural Products Library
5	5-H02	Corynanthine	methyl (1S,15R,18S,19S,20S)-18-hydroxy-3,13-diazapentacyclo[11.8.0.0 ² ,10.0 ⁴ ,9.0 ¹⁵ ,20]heneicosa-2(10),4,6,8-tetraene-19-carboxylate	354,4	483-10-3	NP-062	2mg/ml	DMSO	2865	Natural Products Library
5	5-H03	(-)-Cytisine	(1R,9S)-7,11-diazatricyclo[7.3.1.0 ² ,7]trideca-2,4-dien-6-one	190,2	485-35-8	NP-066	2mg/ml	DMSO	2865	Natural Products Library
5	5-H04	Sparteine sulfate·5H ₂ O	(1S,2R,9S,10S)-7,15-diazatetracyclo[7.7.1.0 ² ,7.0 ¹⁰ ,15]heptadecane sulfuric acid pentahydrate	422,5	6160-12-9	NP-301	2mg/ml	DMSO	2865	Natural Products Library
5	5-H05	Brassinin	N-(1H-indol-3-ylmethyl)(methylsulfanyl)carbothioamide	236,4	105748-59-2	NP-415	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
5	5-H06	Dihydrorobinetine	(2R,3R)-3,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	304,3	4382-33-6	NP-079	2mg/ml	DMSO	2865	Natural Products Library
5	5-H07	Flavanomarein	(2S)-2-(3,4-dihydroxyphenyl)-8-hydroxy-7-[[2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-3,4-dihydro-2H-1-benzopyran-4-one	450,4	577-38-8	NP-105	2mg/ml	DMSO	2865	Natural Products Library
5	5-H08	Lavendustin B	5-{bis[(2-hydroxyphenyl)methyl]amino}-2-hydroxybenzoic acid	365,4	125697-91-8	EI-254	2mg/ml	DMSO	2865	Natural Products Library
5	5-H09	Evodiamine	21-methyl-3,13,21-triazapentacyclo[11.8.0.0.0 ^{2,10} .0 ^{4,9} .0 ^{15,20}]henicosa-2(10),4(9),5,7,15(20),16,18-heptaen-14-one	303,4	518-17-2	NP-101	2mg/ml	DMSO	2865	Natural Products Library
5	5-H10	Oxyacanthine sulfate	(1R,14S)-20,26-dimethoxy-15,31-dimethyl-8,24-dioxa-15,31-diazaheptacyclo[23.6.2.2 ^{9,12} .1 ^{3,7} .1 ^{14,18} .0 ^{28,32} .0 ^{22,34}]heptatriacont a-3,5,7(37),9,11,18,20,22(34),25(33),26,28(32),35-dodecaene-6,21-diol; sulfuric acid	706,8	548-40-3	NP-217	2mg/ml	DMSO	2865	Natural Products Library
5	5-H11	Galangine	3,5,7-trihydroxy-2-phenyl-4H-chromen-4-one	270,2	548-83-4	NP-109	2mg/ml	DMSO	2865	Natural Products Library
5	5-H12	Lavendustin A	5-[[2,5-dihydroxyphenyl)methyl]amino]-2-hydroxybenzoic acid	381,4	125697-92-9	EI-185	2mg/ml	DMSO	2865	Natural Products Library
6	6-A01	Verruculogen	(9S,14S,17S,23R,24S)-23,24-dihydroxy-5-methoxy-12,12-dimethyl-9-(2-methylprop-1-en-1-yl)-10,11-dioxa-8,15,21-triazahexacyclo[12.10.1.0 ^{2,7} .0 ^{8,25} .0 ^{15,23} .0 ^{17,21}]pentacos a-2(7),3,5-triene-16,22-dione	513,6	12771-72-1	NP-575	2mg/ml	DMSO	2865	Natural Products Library
6	6-A02	Gelsemine-HCl	(2'S,3S,6'S)-2'-ethenyl-4'-methyl-1,2-dihydro-9'-oxa-4'-azaspiro[indole-3,7'-tetracyclo[6.3.1.0 ^{2,6} .0 ^{5,11}]dodecane]-2-one hydrochloride	358,9	35306-33-3	NP-110	2mg/ml	DMSO	2865	Natural Products Library
6	6-A03	Hydrocotarnine HBr	4-methoxy-6-methyl-2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinoline hydrobromide	302,2	550-10-7	NP-137	2mg/ml	DMSO	2865	Natural Products Library
6	6-A04	Senecionine	(1R,4Z,6R,7R,17R)-4-ethylidene-7-hydroxy-6,7-dimethyl-2,9-dioxa-14-azatricyclo[9.5.1.0 ^{14,17}]heptadec-11-ene-3,8-dione	335,4	130-01-8	NP-286	2mg/ml	DMSO	2865	Natural Products Library
6	6-A05	Bis demethoxycurcumin	(1E,6E)-1,7-bis(4-hydroxyphenyl)hepta-1,6-diene-3,5-dione	308,3	24939-16-0	NP-576	2mg/ml	DMSO	2865	Natural Products Library
6	6-A06	9,10-Dihydrolysergol	[(4R,7R)-6-methyl-6,11-diazatetracyclo[7.6.1.0 ^{2,7} .0 ^{12,16}]hexadeca-1(16),9,12,14-tetraen-4-yl]methanol	256,3	18051-16-6	NP-077	2mg/ml	DMSO	2865	Natural Products Library
6	6-A07	Amphotericin B	(1R,3R,5S,6S,9S,11S,15S,16R,17R,18S,19E,21E,23E,25E,27E,29E,31E,33R,35S,36R,37S)-33-[[2R,3S,4S,5S,6R)-4-amino-3,5-dihydroxy-6-methyloxan-2-yl]oxy]-1,3,5,6,9,11,17,37-octahydroxy-15,16,18-trimethyl-13-oxo-14,39-dioxabicyclo[33.3.1]nonatriaconta-19,21,23,25,27,29,31-heptaene-36-carboxylic acid	924,1	1397-89-3	NP-500	2mg/ml	DMSO	2865	Natural Products Library

Plate number	Plate Location	Name	IUPAC	MW	CAS	Catalog number	Conc	Solvent	Plate part number	Plate description
6	6-A08	Amygdalin	2-phenyl-2-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)methyl)oxan-2-yl)oxy)acetoneitrile	457,4	29883-15-6	NP-501	2mg/ml	DMSO	2865	Natural Products Library
6	6-A09	Anisodamine	6-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropanoate hydrobromide	386,3	55869-99-3	NP-502	2mg/ml	DMSO	2865	Natural Products Library
6	6-A10	Aphidicolin	(1S,2S,5R,6R,7R,10S,12R,13R)-6,13-bis(hydroxymethyl)-2,6-dimethyltetracyclo[10.3.1.0 ^{1,6} .0 ^{2,7}]hexadecane-5,13-diol	338,5	38966-21-1	CC-101	2mg/ml	DMSO	2865	Natural Products Library
6	6-A11	Arbutin	(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-(4-hydroxyphenoxy)oxane-3,4,5-triol	272,3	497-76-7	NP-504	2mg/ml	DMSO	2865	Natural Products Library
6	6-A12	Sclerotiorin	(7S)-5-chloro-3-[(1E,3E,5S)-3,5-dimethylhepta-1,3-dien-1-yl]-7-methyl-6,8-dioxo-7,8-dihydro-6H-isochromen-7-yl acetate	390,9	549-23-5	NP-276	2mg/ml	DMSO	2865	Natural Products Library
6	6-B01	Bleomycin sulfate	(3-[[2-(2-[[2-(2R,3R)-2-[[2S,3S,4R)-4-[[2R,3R)-2-[[6-amino-2-[[1S)-1-[[[(2S)-2-amino-2-carbamoylethyl]amino]-2-carbamoylethyl]-5-methylpyrimidin-4-yl]formamido]-3-[[[(2R,3S,4S,5S,6S)-3-[[[(2S,3S,4R,5R,6R)-4-(carbamoyloxy)-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-3-(1H-imidazol-4-yl)propanamido]-3-hydroxy-2-methylpentanamido]-3-hydroxybutanamido]ethyl]-1,3-thiazol-4-yl)-1,3-thiazol-5-yl]formamido]propyl]dimethylsulfanium sulfate	1511,6	9041-93-4	AP-302	2mg/ml	DMSO	2865	Natural Products Library
6	6-B02	Chartreusin	3-[[[(2S,3R,4S,5R,6R)-3-[[[(2R,3R,4S,5S,6R)-3,5-dihydroxy-4-methoxy-6-methyloxan-2-yl]oxy]-4,5-dihydroxy-6-methyloxan-2-yl]oxy]-8-hydroxy-15-methyl-11,18-dioxapentacyclo[10.6.2.0 ^{2,7} .0 ^{9,19} .0 ^{16,20}]icosane-1(19),2(7),3,5,8,12(20),13,15-octaene-10,17-dione	640,6	6377-18-0	NP-506	2mg/ml	DMSO	2865	Natural Products Library
6	6-B03	Chlorogenic acid	(1S,3R,4R,5R)-3-[[[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy]-1,4,5-trihydroxycyclohexane-1-carboxylic acid	354,3	327-97-9	NP-507	2mg/ml	DMSO	2865	Natural Products Library
6	6-B04	Geraldol	3,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one	300,3	21511-25-1	NP-112	2mg/ml	DMSO	2865	Natural Products Library
6	6-B05	Coumestrol	5,14-dihydroxy-8,17-dioxatetracyclo[8.7.0.0 ^{2,7} .0 ^{11,16}]heptadecane-1(10),2(7),3,5,11,13,15-heptaen-9-one	268,2	479-13-0	S-180	2mg/ml	DMSO	2865	Natural Products Library
6	6-B06	Diindolylmethane	3-(1H-indol-3-ylmethyl)-1H-indole	246,3	01968-05-4	GR-207	2mg/ml	DMSO	2865	Natural Products Library
6	6-B07	Ferulic acid	(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	194,2	1135-24-6	NP-510	2mg/ml	DMSO	2865	Natural Products Library
6	6-B08	Bakuchiol	4-[(1E,3S)-3-ethenyl-3,7-dimethylocta-1,6-dien-1-yl]phenol	256,4	10309-37-2	NP-571	2mg/ml	DMSO	2865	Natural Products Library
6	6-B09	L-Theanine	(2R)-2-amino-4-(ethylcarbamoyl)butanoic acid	174,2	3081-61-6	AC-1565	2mg/ml	DMSO	2865	Natural Products Library
6	6-B10	Indole-3-carbinol	1H-indol-3-ylmethanol	147,2	700-06-1	NP-512	2mg/ml	DMSO	2865	Natural Products Library

