**Preamble**

The Chemical Biology Platform at the Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) provides access towards high throughput screening, medicinal chemistry, and cheminformatics support. Further information is provided on the FMP websites, visit <http://www.leibniz-fmp.de/core-facilities/chemical-biology-platform.html>

Your Signature on this form indicates your acceptance of the **AGREEMENT** between you as the Project Leader

|  |  |
| --- | --- |
| Project Leader Title | Klicken Sie hier, um Text einzugeben. |
| Project Leader First name | Klicken Sie hier, um Text einzugeben. |
| Project Leader Last name | Klicken Sie hier, um Text einzugeben. |
| Project Leader Street address | Klicken Sie hier, um Text einzugeben. |
| Project Leader ZIP code | Klicken Sie hier, um Text einzugeben. |
| Project Leader Email | Klicken Sie hier, um Text einzugeben. |
| Project Leader Phone | Klicken Sie hier, um Text einzugeben. |
| Project Leader Fax | Klicken Sie hier, um Text einzugeben. |

and your institution responsible for project finances

|  |  |
| --- | --- |
| Institution Name | Klicken Sie hier, um Text einzugeben. |

(both together in the following named **USER)**, and the “Leibniz-Forschungsinstitut für Molekulare Pharmakologie im Forschungsverbund Berlin e.V. (FMP)” (in the following named **CONTRACTOR)**.

**X** USER accepts to be supported by the FMP on the basis of a **scientific collaboration** and not on the basis of a fee for service interaction.

**X** USER will acknowledge the FMP as contributor as well as “FMP screening collections” as the source of compounds or genomic screening tools in all publications and presentations that make use of the results of this contribution and support. If a **publication** or other public disclosure does result from this collaboration using the screening collections and serving infrastructure, the USER and the served Project Leader agree to inform the CONTRACTOR prior to submission of the manuscript or abstract and name the FMP scientists as co-authors depending on their contribution to the publication. If the USER intends to submit a **patent application** from results originating from this collaboration using the screening collections and serving infrastructure, the USER and the served Project Leader agree to inform the CONTRACTOR prior to submission of the patent. An FMP participation in this patent application depends on the contribution of the FMP scientists and will be discussed between the USER and CONTRACTOR.

**X** USER acknowledges that the project can be stopped at any time if evidence arises that the **assay acceptance criteria** – as described in the scientific part of this document – are not met.

**X** USER authorizes the FMP to store the **generated data** together with this form in a central archive and to include the data in statistical analysis for quality control purposes. Specific information about project aims, target, or experimental protocols will not be visible to others.

**X** USER will declare and give detailed description of all materials falling within **chemical and biological safety regulations** as requested in the organizational part of this document, prior to any initial experiment.

**X** USER will cover the **costs** for assay reagents, consumables and access fee for usage of screening collections as well as invested working time of the staff. A quote for estimated costs will be sent to USER by CONTRACTOR after initial tests have been conducted. Support of the project can start as soon USER has placed a regular order based on the quote prepared by the CONTRACTOR. Initial tests will be provided free-of charge.

**INDEMNITY AND LIABILITY**

1. **Personnel Relationships -** USER shall be responsible for the acts or omissions of all officers, agents and employees participating in the use of the FMP Chemical Biology Platform.

**B.** **Product Liability** - To the extent permitted by German law, if USER utilizes the work derived from this Agreement in the making, using, or selling of a product, process or service, then USER hereby agrees to hold harmless and indemnify CONTRACTOR, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, as a result of or arising out of such utilization of the work by or on behalf of USER, its assignees or licensees.

**C. General** **Indemnity** - To the extent permitted by German law, USER hereby agrees to indemnify and hold harmless CONTRACTOR, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, to the extent such liability, claims, or damages is caused by or contributed to the negligence or intentional misconduct of USER or its employees or representatives during the performance of the work under this Agreement.

###### D. Patent and Copyright Indemnity – To the extent permitted by German law, USER shall fully indemnify the CONTRACTOR and their officers, agents, and employees for infringement of any patent or copyright arising out of any acts required or directed or performed by USER under the Agreement to the extent such acts are not normally performed at the facility.

1. The liability and indemnity provisions in paragraphs B, C and D above shall not apply unless USER shall have been informed as soon as practicable by CONTRACTOR of the suit or action alleging such infringement, and such indemnity shall not apply to a claimed infringement that is settled without the consent of USER unless required by a court of competent jurisdiction.

**F. General Disclaimer -** The CONTRACTOR makes no express or implied warranty as to the conditions of the user facility furnished hereunder. In addition, CONTRACTOR and USER make no express or implied warranty as to the research or any intellectual property, generated information, or product made or developed under this agreement, or the ownership, merchantability, or the fitness for the particular purpose of the research or the resulting product; that the goods, services, materials, products, processes, information, or data to be furnished hereunder will accomplish intended results or are safe for any purpose including the intended purpose; or that any of the above will not interfere with privately owned rights of others. The CONTRACTOR and/or USER shall not be liable for special, consequential, or incidental damages attributed to use of such facilities, research or resulting product, intellectual property, generated information, or product made or delivered under this agreement.

**Date/ Signature (USER/ Project Leader):**

**Date/ Signature (USER/ Institution):**

Before signing you are requested to discuss all matters related to this agreement with the head of the ‘Screening Unit’, Dr. Jens Peter von Kries, who can be contacted by phone: +49 (0) 30-9406-2982, fax: -2922 or e-mail: kries@fmp-berlin.de.

**ORGANIZATIONAL PART**

**Desired screening target shortcut name** (consecutive short word, like “hsp70”, letters & numbers only, 4 to 8 chars):

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| Klicken Sie hier, um Text einzugeben. |

Will be used for naming the data archive

**Collaboration partners** (please indicate the contact information of all people that are allowed to receive results or that are involved in setting up the assay):

|  |  |  |
| --- | --- | --- |
| Name | email | phone |
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| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |
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**Biosafety**

Please declare if biosafety regulations apply to the biological materials provided.

|  |  |
| --- | --- |
| No | |
| Yes | The project leader declares that the provided cell lines:  Klicken Sie hier, um Text einzugeben.  are safe to be handled at biosafety level 1 (S1).  For laboratories located in Germany only:  Gentechnik-Anlagennummer: Klicken Sie hier, um Text einzugeben.  Bundesland der genehmigenden Behörde: Hessen |
|  | The project leader declares that the provided cell material is free of mycoplasma or other infectious agents and contaminants. |

**In case of cell lines**

Please enter recommended handling guidelines for the provided cell lines.

**In case of genetically modified cell lines**

Please provide detailed description including construct drawings and selection conditions.

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| Klicken Sie hier, um Text einzugeben. |

\*Copy and paste vector map picture here\*

**In case of iPSC–derived or primary cells**

Please enter the source (institution, vendor) and contact.

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| Klicken Sie hier, um Text einzugeben. |

**Transfer of materials**

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| Carrier | Your customer number |
| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |

With the carrier customer number we can send you proteins and compounds on dry ice

**SCIENTIFIC PART – SMALL MOLECULE SCREENING**

**Project aims**

Please indicate whether you search either for activators or inhibitors or for both. Inform also whether the identified molecules shall be used as tool compounds or build a starting point for a drug discovery project, and what type of experiment is planned after screening for hit validation.

Klicken Sie hier, um Text einzugeben.

**Literature describing the screening target**

|  |  |
| --- | --- |
| Reference | PubMed Abstract ID |
| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |

**Known molecules**

If there are any molecules known in the literature that are active against this target, please indicate a few of those that might be useful for validating the assay.

|  |  |
| --- | --- |
| CAS-Number | PubMed Abstract ID |
| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |
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| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |

The CAS-Number can be derived from a structural search on [www.chemspider.com](http://www.chemspider.com), known biological activities can be derived from a target name search on <https://www.ebi.ac.uk/chembl/>

**Plate preparation protocol:**

Please describe in detail how assay reagents should be prepared and used for creating the assay plates. Indicate volumes to be pipetted or dispensed and all final component concentrations as well as incubation times. Describe handling of components in regard to their stability (proteins, fluorescent dyes).

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| Klicken Sie hier, um Text einzugeben. |

**Signal detection protocol:**

**Literature describing signal detection method**

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| Reference or URL | PubMed Abstract ID |
| Klicken Sie hier, um Text einzugeben. | Klicken Sie hier, um Text einzugeben. |

**Sketch proteins/elements involved in signal detection**

Include a schematic drawing or picture how the biological activity generates the assay readout (also indicate excitation and emission wavelength and bandwidth). Please also indicate how positive and negative control signals are generated (usage of small molecules, omitting assay components like substrate or enzyme, genetic constructs)

\*Copy and paste picture here\*

**Compound libraries to be screened**

|  |  |  |  |
| --- | --- | --- | --- |
| Compound Collection | | Library Plate ID´s | # 384 plates |
|  | CBB\_1 (16544 cpds, Diversity Set) | 2001-2047 | 47 |
|  | CBB\_2 (7744 cpds, Diversity Set) | 1001-1032 | 32 |
|  | CBB\_3 (4576 cpds, Fragments) | 3001-3013 | 13 |
|  | ChEMBL reference set (part of CBB\_2) | 1030-1031 | 2 |
|  | CBB\_4 (4224 cpds, Diversity Set ArtChem) | 4001-4012 | 12 |
|  | LOPAC 1280 cpds (**L**ibrary **o**f **p**harmacologically **a**ctive **C**pds) | 4013-4016 | 4 |
|  | Selleck Library 1760 cpds (FDA approved drugs) | 4017-4021 | 5 |
|  | CBB\_5 (4928 cpds donated by academic chemists) | 5001-5028 | 28 |
|  | CBB\_7 (20064 cpds AnalytiCon) | 7001-7085 | 85 |

Collections CBB\_1 - CBB\_4 consist of compounds which were bought by commercial vendors and the user has got the freedom to operate with the hits identified in these libraries. ChEMBL is an annotated set of commercially available compounds that are described in the scientific literature and are active against a defined protein complex or single protein target with an activity < 5 M. CBB\_5 contains compounds which were donated by different academic research groups. If you wish to screen compounds donated by academic chemists or the AnalytiCon library and hits are found after the validation screen both partners are contacted by the Screening Unit and the contact details will be exchanged. Upon agreement between both partners, the target and the molecular structures of the hits are revealed in the same report which will be simultaneously sent to both partners via E-mail. The donators of compounds are listed below:

* [Prof. Dr. Laufer (Pharmaceutical Chemistry, University of Tübingen)](http://www.uni-tuebingen.de/en/faculties/mathematisch-naturwissenschaftliche-fakultaet/fachbereiche/pharmazie-und-biochemie/pharmazie/pharmazeutische-chemie/prof-dr-stefan-laufer.html)
* [Prof. Dr. Klebe (Pharmaceutical Chemistry, University of Marburg)](http://www.agklebe.de/)
* [Prof. Dr. Link (Pharmaceutical Chemistry, University of Greifswald)](http://pharm1.pharmazie.uni-greifswald.de/pmc/index.html)
* [Prof. Dr. Schmalz (Organic Chemistry, University of Cologne)](http://www.schmalz.uni-koeln.de/)
* [Dr. Frank (Chemical Biology, Leibniz Institute of Molecular Pharmacology)](http://www.fmp-berlin.info/research/chemical-biology/res-groups-chembio/frank/research.html)
* [Prof. Dr. Rault (Organic Chemistry, University of Caen)](http://www.cermn.unicaen.fr/)
* [Prof. Dr. Kirschning (Organic Chemistry, University of Hanover)](http://www.akoci.uni-hannover.de/AK_Kirschning/index.htm)
* [Prof. Dr. Kaufmann (Organic Chemistry, Technical University of Clausthal)](http://www.ioc.tu-clausthal.de/abteilungen/abteilung-prof-kaufmann/)
* [Prof. Dr. Schlitzer (Pharmaceutical Chemistry, University of Marburg)](http://www.ak-schlitzer.de/)
* [Prof. Dr. Geyer (Organic Chemistry, University of Marburg)](http://www.uni-marburg.de/fb15/ag-geyer?language_sync=1)
* [Prof. Dr. Speicher (Organic Chemistry, University of Saarbrücken)](http://www.uni-saarland.de/fak8/speicher/)
* [Prof. Dr. Tsogoeva (Organic Chemistry, University of Erlangen)](http://www.chemie.uni-erlangen.de/dcp/forschung/arbeitskreise/welcome-to-the-tsogoeva-laboratory-science-is-our-passion-s/)
* [Prof. Dr. Bracher (Pharmaceutical Chemistry, University of Munich)](http://www.cup.uni-muenchen.de/dept/ph/pharmachemie/bracher.php)

**Assay acceptance criteria and workflow:**

**DMSO-Tolerance:**

The assay system should tolerate DMSO-concentrations up to 1% (for cell-based screens 0.1%).

**Z´-factor determination:**

A 384 well plate containing 192 positive controls and 192 negative controls is measured. The Z´-factor must be > 0.5. You can use the Z´-factor calculation tool on our website (<http://www.screeningunit-fmp.net/tools/z-prime.php>).

For further information about the Z´-factor see:

Zhang JH, Chung TD, Oldenburg KR, *A simple statistical parameter for use in evaluation and validation of high throughput screening assays.* J Biomol Screen. 1999;4(2):67-73

**Failure rate:**

After initial quality control, no more than 20% of the measured plates shall have to be re-measured. An initially failed plate can be repeated, but to a maximum of 3 repetitions.

**Ingredient stability:**

For biochemical assays, the ingredients (e.g. proteins, buffers) shall be stable at room temperature for at least 2 hours, with less than 30% activity loss.

**Pilot screen hit rate:**

Up to 10 plates are measured in the pilot screen at 10 M compound concentration. In the absence of any z-score based primary hit the screening campaign is stopped (assay sensitivity too low). In the case of high hit rates above 5 %, the compound concentration is reduced (assay specificity too low). The pilot screen serves to establish the assay protocol, data evaluation and the test for robustness of the assay against compound-induced measurement artifacts (as frequently caused by cytotoxicity, auto-fluorescence or aggregation).

**Scheduling:**

This form should arrive at least 3 month before the first experimental steps are planned.