

Chemical Biology Platform

Applicant(s)

Name main Applicant *	<input type="text"/>
Position *	<input type="text"/>
Affiliation *	<input type="text"/>
Department *	<input type="text"/>
Email address *	<input type="text"/>

Co-Applicant(s)	<input type="checkbox"/>
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Project name

Title of project (max 150 characters) *
<input type="text"/>
(0 characters)

Acronym (max 30 characters)
<input type="text"/>
(0 characters)

Status Biology

Describe relevant aspects of the biology (e.g., human genetics, in vivo expression studies; human epidemiology; cellular models vs animal models)	<input type="text"/>
Target validation by at least two independent technologies? (antibody, SiRNA, knock-outs, chemical interference)	<input type="checkbox"/>
Uniprot sequence information available? *	<input type="checkbox"/>
Xray structures available?	<input type="checkbox"/>
Xray structure of homologous protein available?	<input type="checkbox"/>
Expression system available? * ?	<input type="checkbox"/> Yes <input type="checkbox"/> No
Purified target protein available? * ?	<input type="checkbox"/> Yes <input type="checkbox"/> No

Status Screening

Are the following screening assays available for screening compounds?

Available test systems: (multiple answers represent screening cascade)	<input type="checkbox"/> binding assay <input type="checkbox"/> cell assay <input type="checkbox"/> functional assay <input type="checkbox"/> in vivo assay
Has any of these assays been validated by measuring the activity or affinity of one or more small molecule reference compounds? * ?	<input type="radio"/> Yes <input type="radio"/> No

Potential screening formats

Radioligand displacement assay	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Bulk fluorescence	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Fluorescence polarisation	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Fluorescence lifetime	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
TR-FRET	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
FRET	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Luminescence	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Absorbance	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature
Calcium mobilization (FLIPR)	<input type="checkbox"/> Available in lab <input type="checkbox"/> Commercially available <input type="checkbox"/> Described in literature

ELISA	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
ALPHAscreen	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Cellular imaging	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Fluorescent Microscopy	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Enzyme fragment complementation assay	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Enzyme Assays	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Reporter Assays	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Viability Assays	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Protein Translocation	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
NMR ligand screening	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
SPR ligand screening	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
ITC ligand screening	<input type="checkbox"/> Available in lab	<input type="checkbox"/> Commercially available	<input type="checkbox"/> Described in literature
Other means of ligand screening: ?	<input type="text"/>		

Target Biology Tractability

Please provide brief details on the following (max ½ page per question)

Description of the target ?
<div style="background-color: #e0f0ff; height: 40px;"></div>
<input type="checkbox"/> Unknown <input type="checkbox"/> Novel target (no known function) <input type="checkbox"/> Novel target (amenable to small molecule intervention) <input type="checkbox"/> Target inferred from phenotypic data <input type="checkbox"/> Known drug target / family <input type="checkbox"/> Other

Validation that the therapeutic approach or target is relevant to human disease?
<div style="background-color: #e0f0ff; height: 40px;"></div>
<input type="checkbox"/> Hypothetical <input type="checkbox"/> Genetic or proteomic <input type="checkbox"/> In vitro studies <input type="checkbox"/> In vivo animal model <input type="checkbox"/> Exploratory clinical studies <input type="checkbox"/> biomarker available

Status Chemistry

Known small molecule ligands published or identified?	<input type="checkbox"/>
Any PK/ADME data available?	<input type="checkbox"/>
Measured aqueous solubility?	<input type="checkbox"/>
In vitro metabolism data known?	<input type="checkbox"/>
hERG and/or CYP450 inhibition measured?	<input type="checkbox"/>
Any activity in an in vivo model of disease known?	<input type="checkbox"/>

Are there off-target activities or other properties that need to be monitored?	<div style="background-color: #e0f0ff; height: 40px;"></div>
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Chemistry Tractability

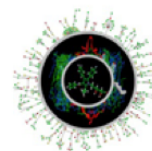
Please describe known reference compounds	
<input type="checkbox"/> Endogenous ligand <input type="checkbox"/> Drug-like compound reported in the patent literature <input type="checkbox"/> Proprietary compound previously identified	<input type="checkbox"/> Commercially available ligand <input type="checkbox"/> A drug-like compound reported in peer reviewed literature <input type="checkbox"/> Existing licensed drug <input type="checkbox"/> Virtual screen based on X-ray / crystal structure
Proprietary ligand structures can be uploaded here (pdf, doc, chemdraw)	<input type="button" value="Browse..."/> No file selected.
How has it been validated that these compounds bind to the desired target? Indicate the techniques used and outline the results.	<div style="background-color: #e0f0ff; height: 40px;"></div>

Computer-Aided Drug Design Tractability

Is there a homology protein model available?	<input type="checkbox"/> Yes (proprietary made by applicant) <input type="checkbox"/> No (AIMMS input requested) <input type="checkbox"/> Not relevant
Pharmacophore model available?	<input type="checkbox"/> Yes (proprietary made by applicant) <input type="checkbox"/> No (AIMMS input requested) <input type="checkbox"/> Not relevant
Virtual screening results available?	<input type="checkbox"/> Yes (virtual screening hits selected by applicant) <input type="checkbox"/> No (AIMMS input requested) <input type="checkbox"/> Not relevant
Ligand-protein models derived by docking studies? ?	<input type="checkbox"/> Yes (models and protocols developed by applicant) <input type="checkbox"/> No (AIMMS input requested) <input type="checkbox"/> Not relevant

Funding and allocation of resources

Do you have funding available for hit finding & hit exploration? *	<input type="checkbox"/> Yes <input type="checkbox"/> No
Issues that hamper freedom to operate ?	



Contact:
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