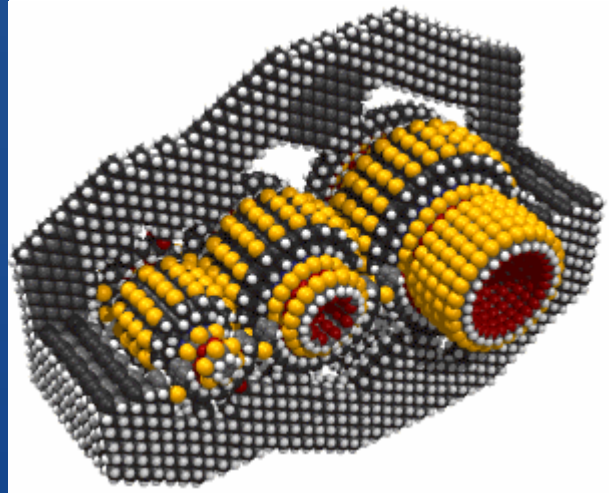

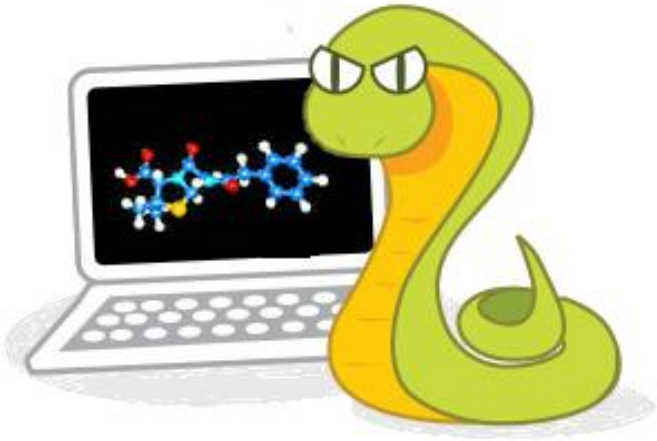

MolGears
cheminformatics tool for bioactive molecules

Adrian Jasiński

Research Scientist

R&D - In Silico Laboratory

Adamed Group

Poland

http://www.adamed.com.pl/en/

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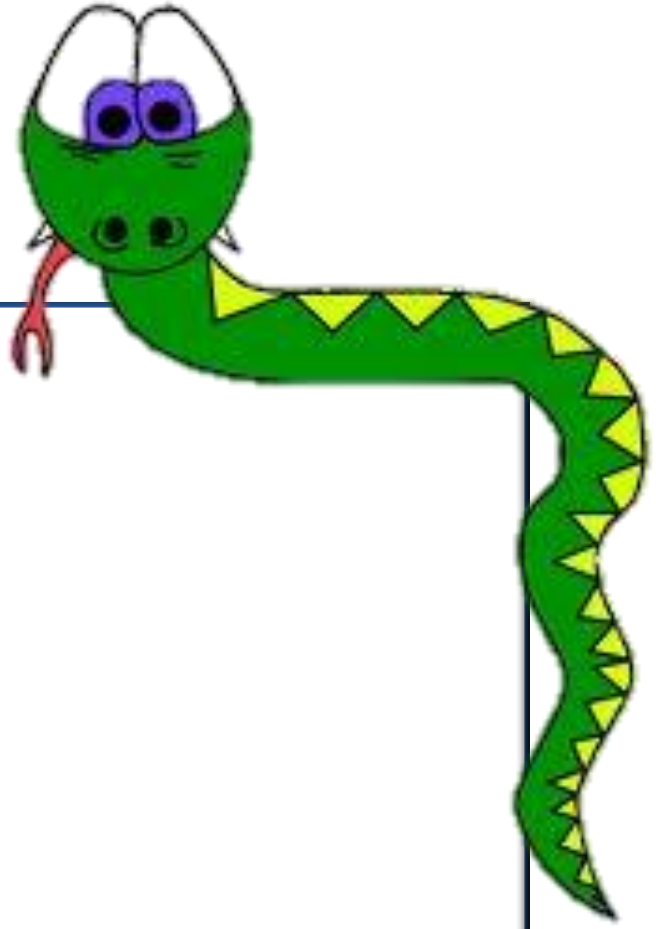
Outline



- Introduction
- Features
- Database model
- Project overview

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Introduction

This is a framework/database programed in Python2.7 language based on a **TurboGears** framework.

It uses:

- RDKiT
- TurboGears
- JSME editor
- Postgresql
- Genshi

And some python based libraries:

- SQLAlchemy
- razi
- Numpy
- Scipy
- Matplotlib
- Xlwt & Xlrd
- xhtml2pdf
- pillow

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Design goal

- Project management tool
- Efficient data storage
- Sorting, analysis, aggregation and reporting of data
- Data visualization
- Improved data access
- Automation of procedures
- Facilitate communication

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Features

- Multi-projects
- Adding molecules by drawing or pasting SMILES code
- Reading molecules from file (csv, smi, sdf, txt, mol)
- Data presenting in sortable columns
- Exporting data to file (file formats: xls, pdf, csv, sdf, txt, png)
- PAINS (Pan Assay Interference Compounds) filtering
- History of changes
- Compound filtering (by similarity, structure, identity, compound name, creator, adding date etc.)
- Stars rating
- IC_{50} determination based on least squares method,
- Automatic data processing
- Graphs generation
- Access managing
- Tags

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Conditions & Source code

Project is free

License: BSD 3-Clause

Source code:
https://github.com/admed/molgears

Forked razi project:
https://github.com/admed/razi

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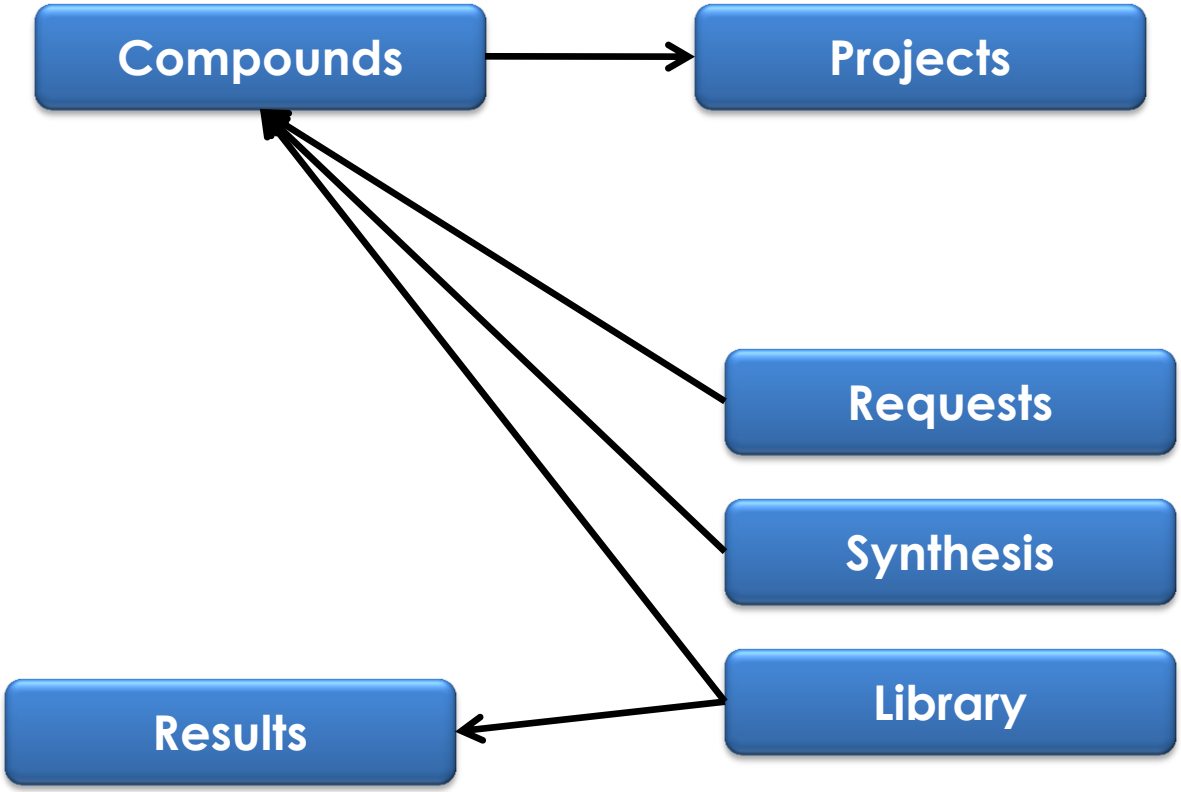
Database Model



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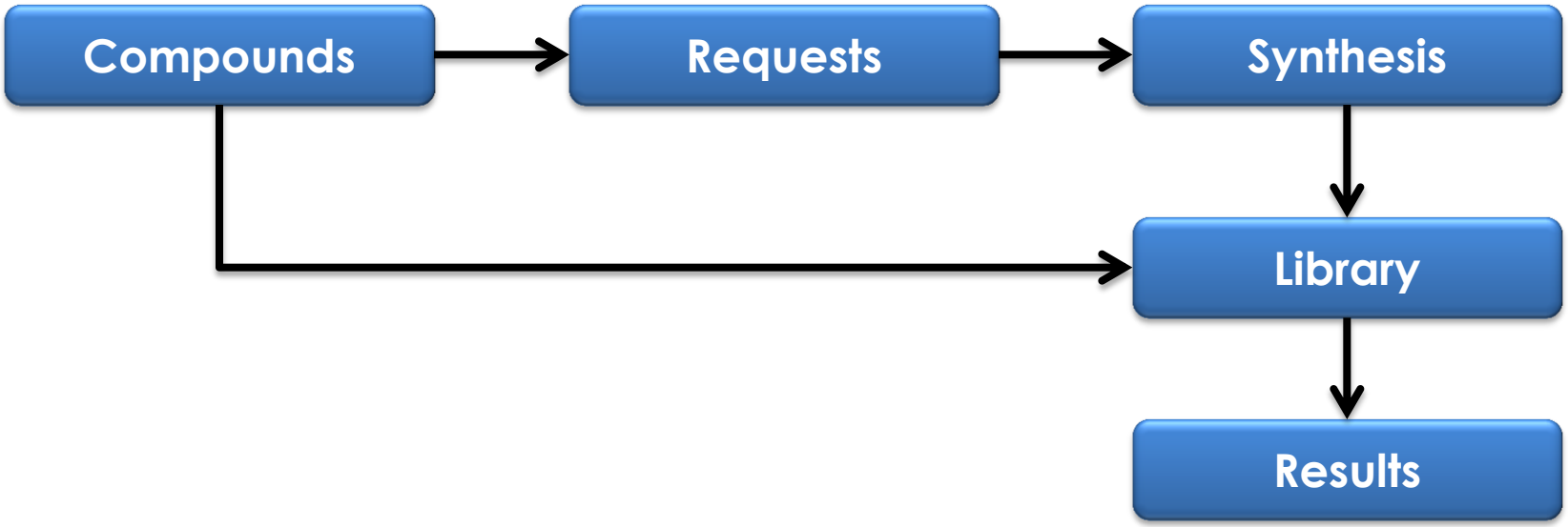
Project Workflow



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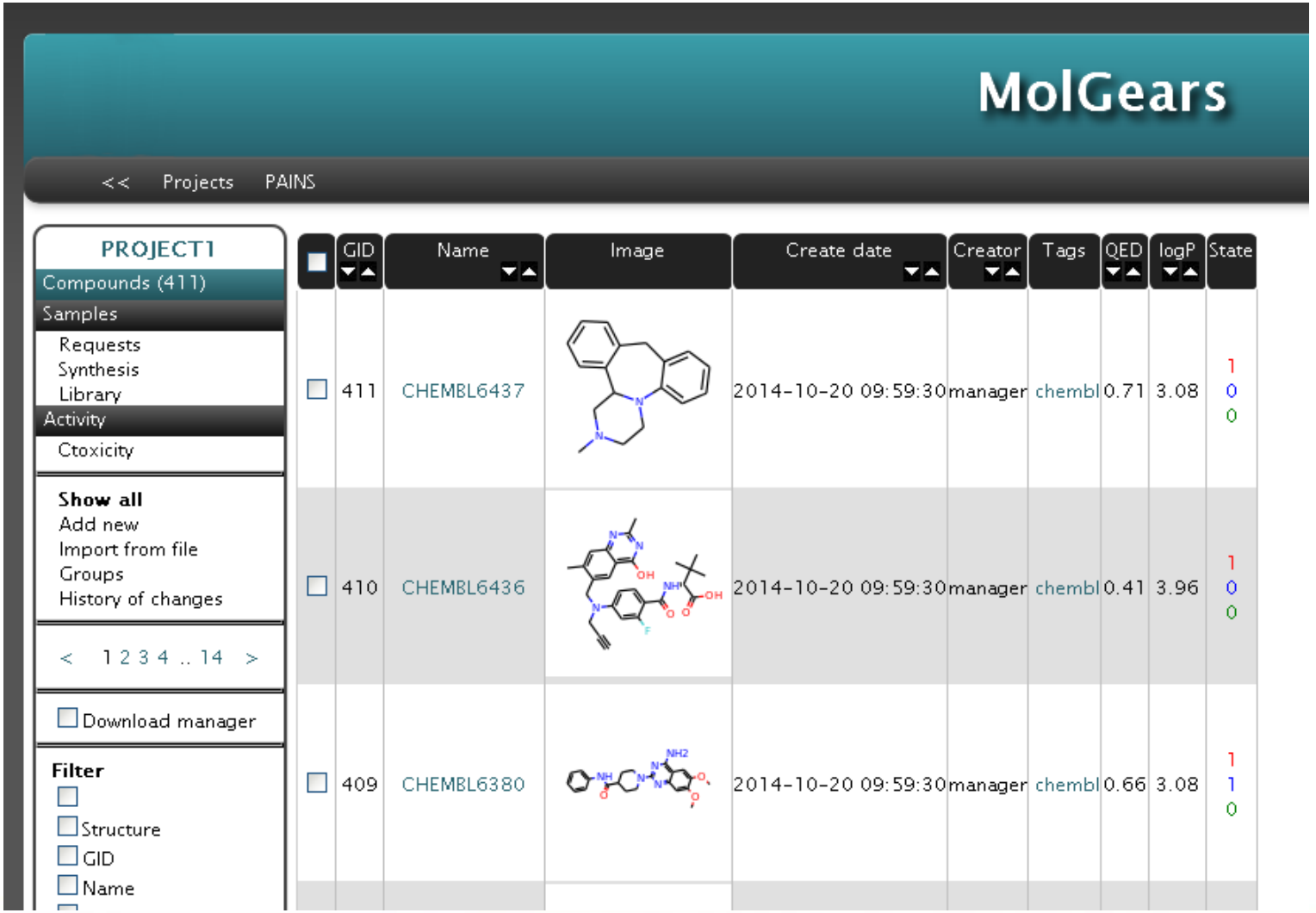
Compounds



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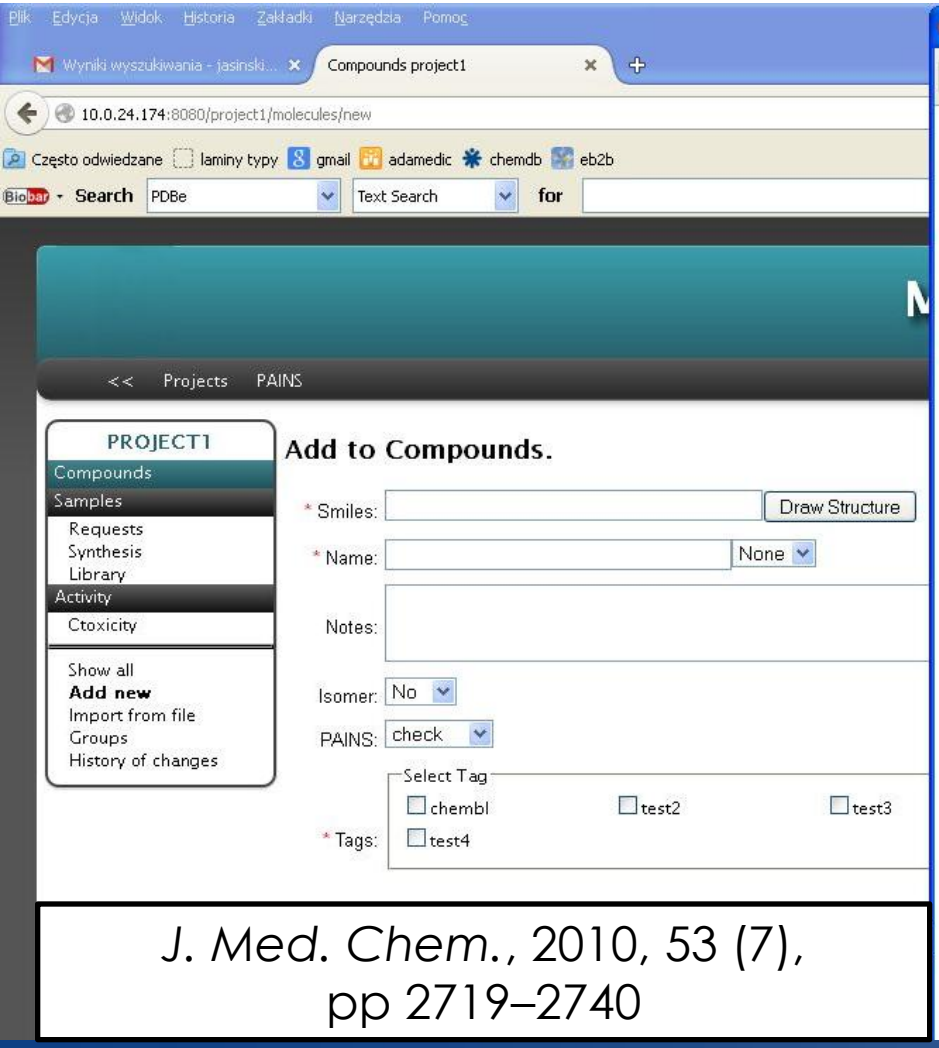
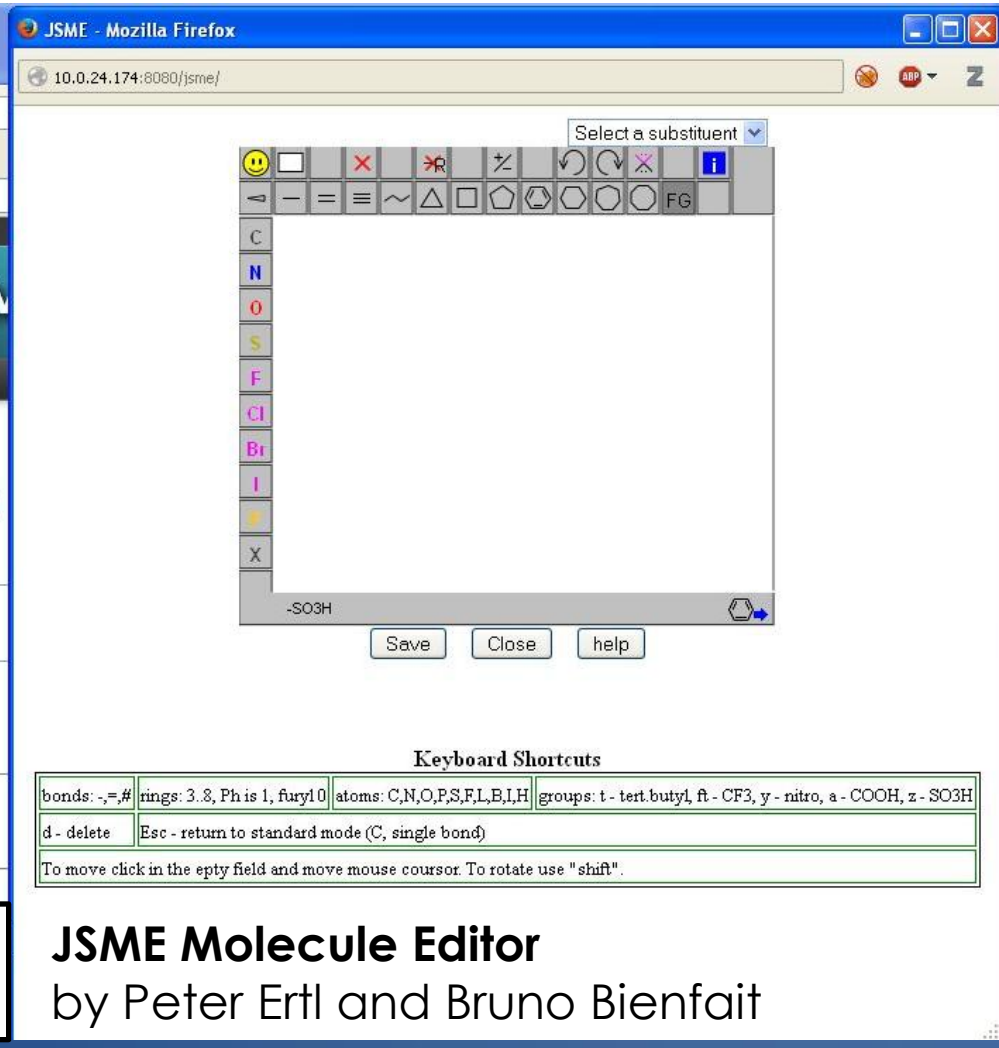
Compounds



J. Med. Chem., 2010, 53 (7), pp 2719–2740



JSME Molecule Editor
by Peter Ertl and Bruno Bienfait

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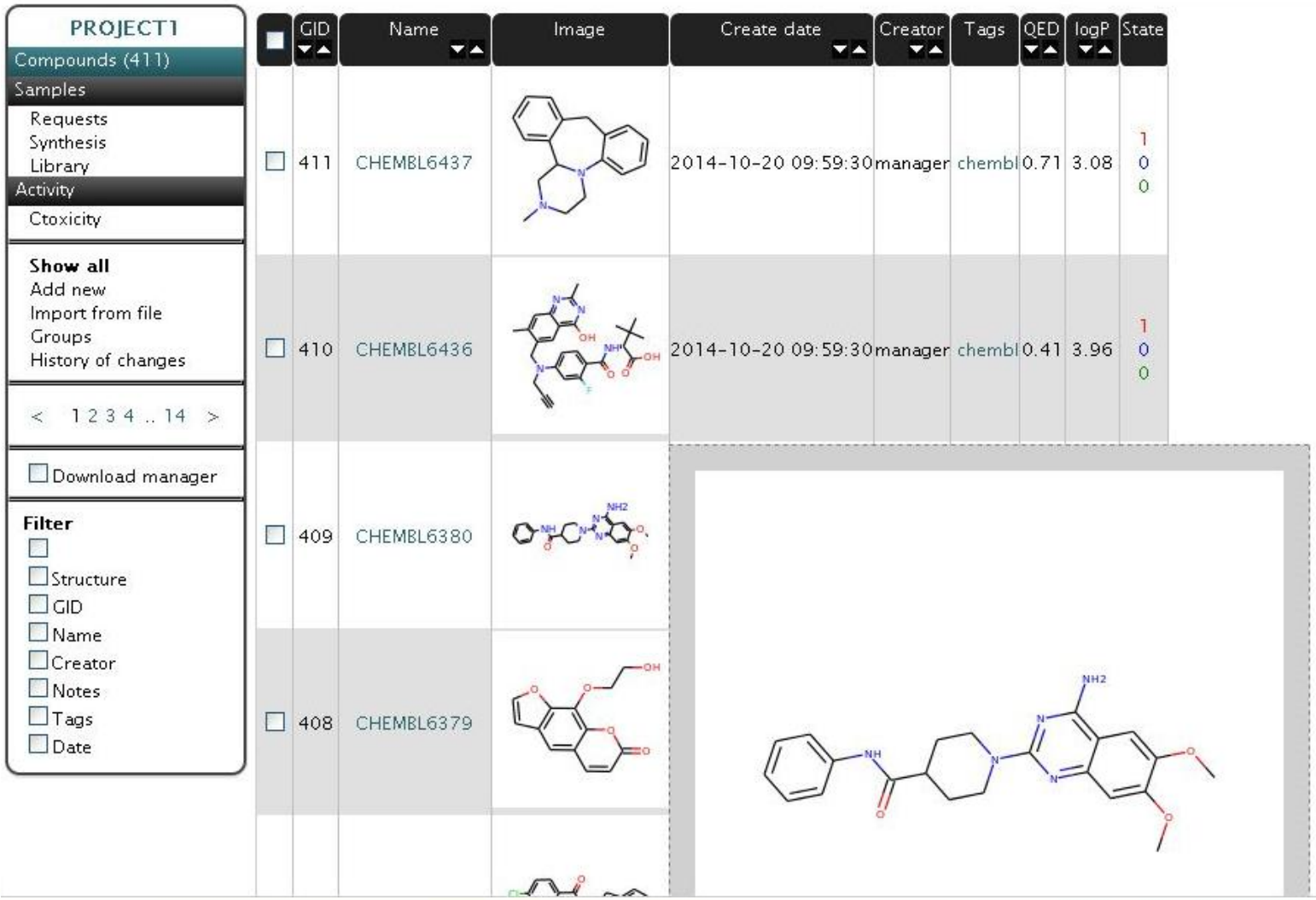
Compounds Table



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Compounds Table

PROJECT1

Compounds (10)

Samples

- Requests
- Synthesis
- Library

Activity

- Ctoxicity

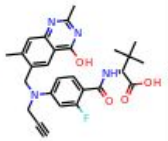
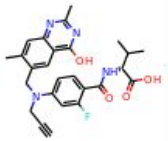
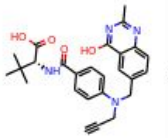
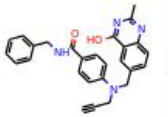
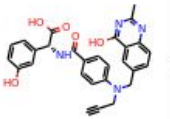
Show all
Add new
Import from file
Groups
History of changes

< 1 >

Download manager

Filter

- Structure
- GID
- Name
- Creator
- Notes
- Tags
- Date

	GID	Name	Image	Create date	Creator	Tags	QED	logP	State	Similarity
☐	410	CHEMBL6436		2014-10-20 09:59:30	manager	chembl	0.41	3.96	1 0 0	100.0
☐	374	CHEMBL6715		2014-10-20 09:59:29	manager	chembl	0.41	3.57	0 0 1	85.29
☐	370	CHEMBL6663		2014-10-20 09:59:29	manager	chembl	0.45	3.51	0 0 1	65.33
☐	328	CHEMBL6829		2014-10-20 09:59:27	manager	chembl	0.41	4.21	0 0 0	50.0
☐	7	CHEMBL6639		2014-10-20 09:59:17	manager	chembl	0.27	3.54	0 0 0	47.67

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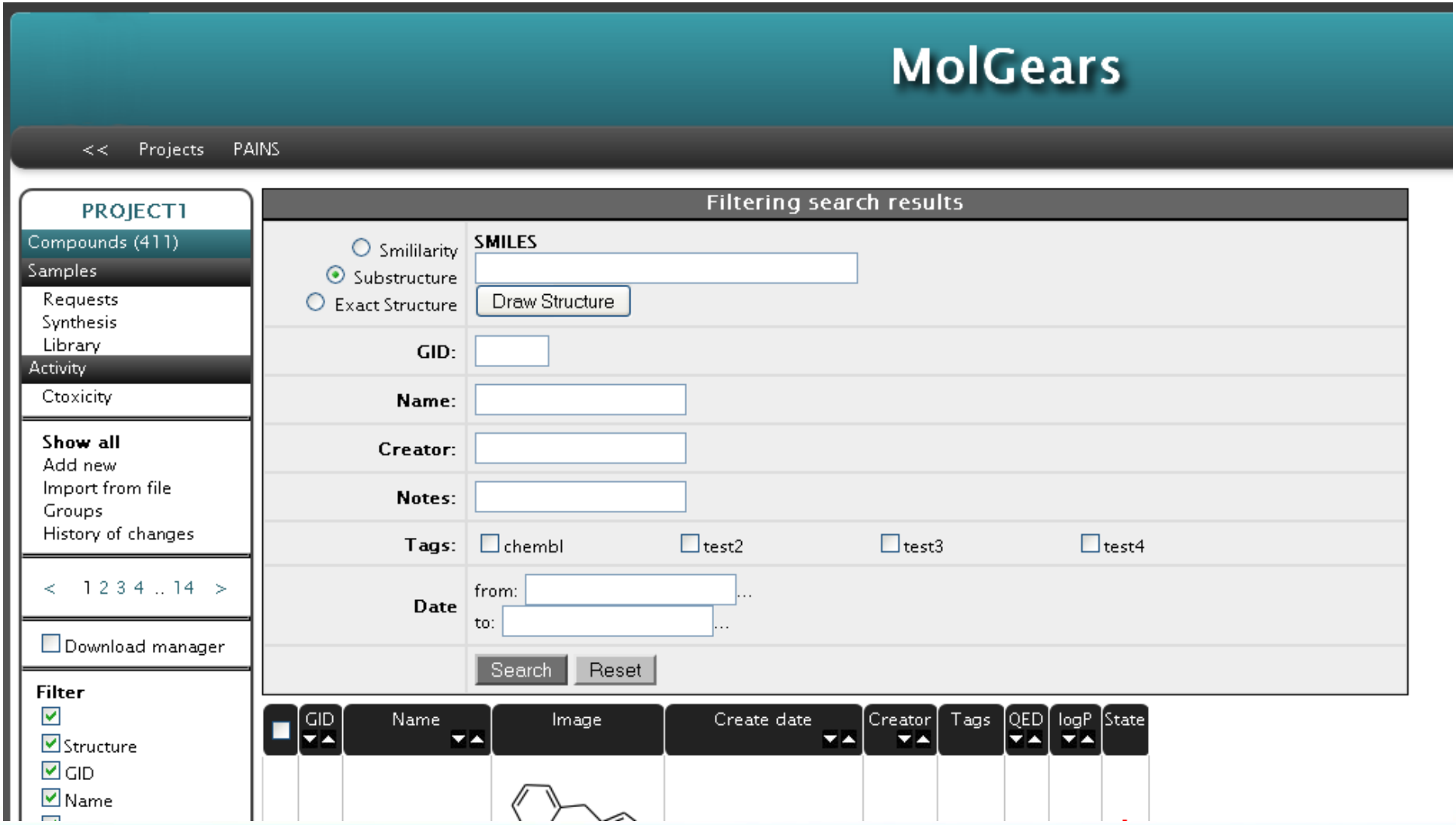
Filtering



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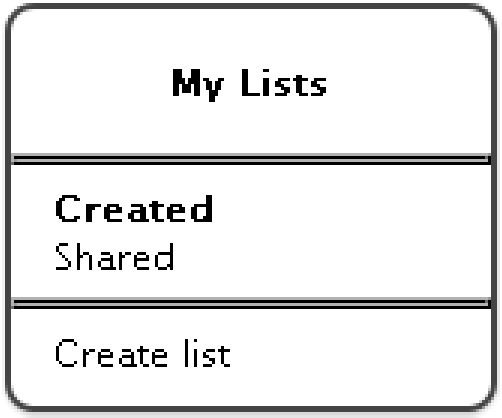
User Lists



	Name	Table	Items num.	Authorized users	Notes
☐	Activity	Activity		• Adrian Jasinski	
☐	test_L	Library	23	• Adrian Jasinski	
☐	test_S	Synthesis	2	• Adrian Jasinski	
☐	test3	Compounds	1		
☐	test22	Compounds	30	• Adrian Jasinski	test

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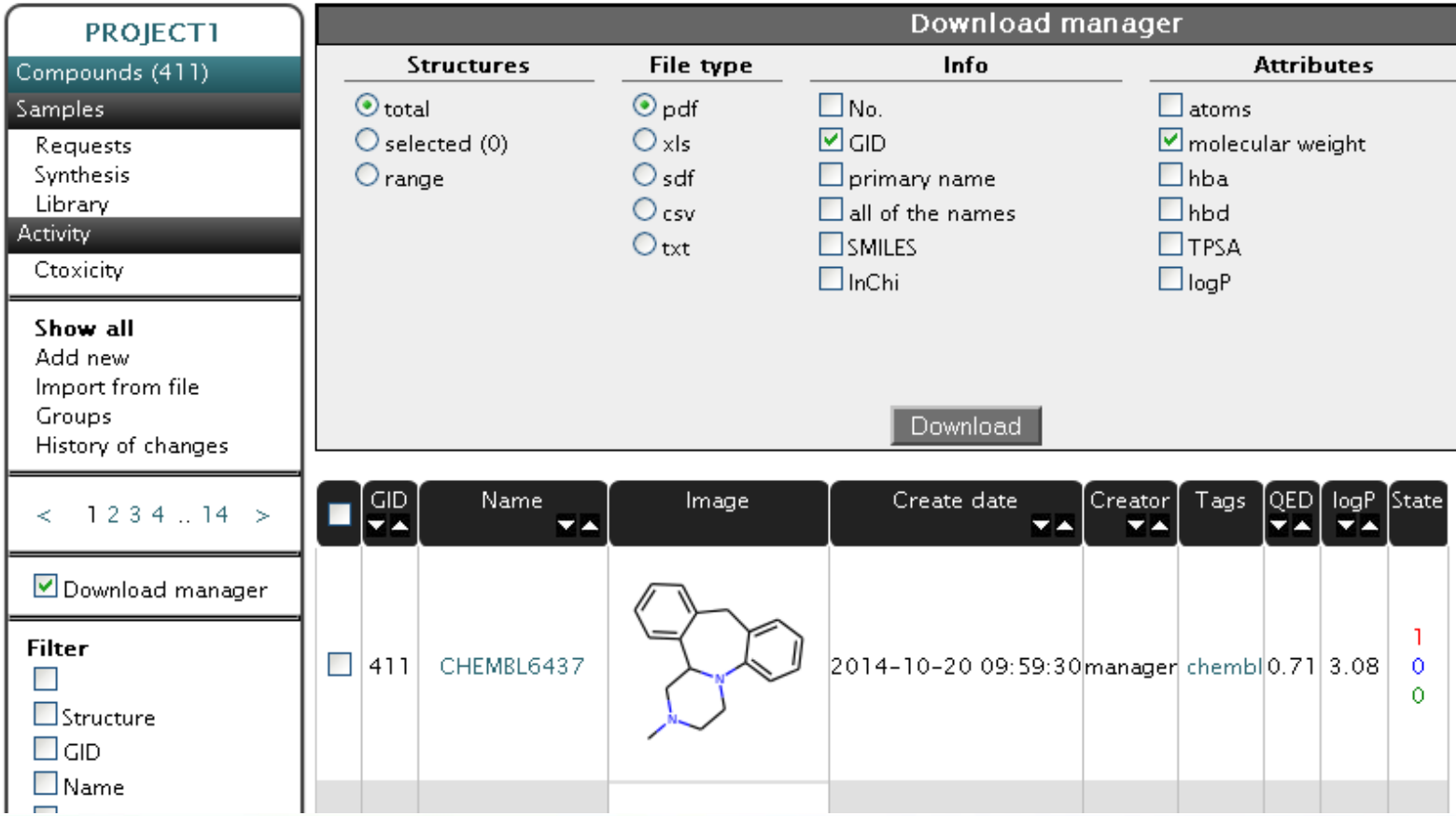
Download



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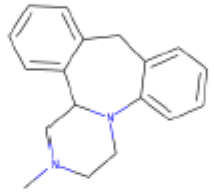
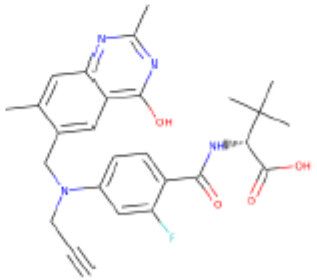
PDF file

Compounds (7)

No.	Name	Image	Molecular weight
1	CHEMBL6437		264
2	CHEMBL6436		493

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Action menu

PROJECT1

Compounds (411)

Samples

- Requests
- Synthesis
- Library

Activity

- Ctoxicity

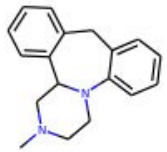
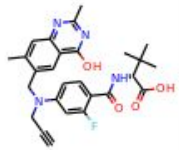
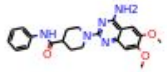
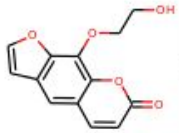
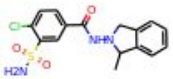
Show all
Add new
Import from file
Groups
History of changes

< 1 2 3 4 .. 14 >

Download manager

Filter

- Structure
- GID
- Name
- Creator
- Notes
- Tags
- Date

	GID	Name	Image	Create date	Creator	Tags	QED	logP	State
☐	411	CHEMBL6437		2014-10-20 09:59:30	manager	chembl	0.71	3.08	1 0 0
☑	410	CHEMBL6436		2014-10-20 09:59:30	manager	chembl	0.41	3.96	1 0 0
☑	409	CHEMBL6380		2014-10-20 09:59:30	manager	chembl	0.66	3.08	1 1 0
☐	408	CHEMBL6379		2014-10-20 09:59:30	manager	chembl	0.72	1.91	1 1 1
☐	407	CHEMBL6378		2014-10-20 09:59:30	manager	chembl	0.87	2.21	1 0 0

Select option:

- Edit
- Create Request
- Add to Library
- Delete
- **Add to List:**
  - + Create new
  - test1

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Compound details

PROJECT1

- Compounds
- Samples
  - Requests
  - Synthesis
  - Library
- Activity
  - Ctoxicity

Show all
Add new
Import from file
Groups
History of changes

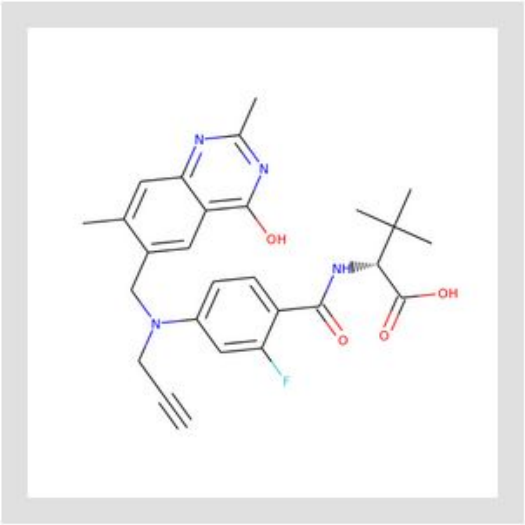
CHEMBL6436 410

atoms	rings	molecular weight	logP	hba	hbd	tpsa	qed
36/65	3	493	3.96	8	3	116	0.41

show

Tags:

chembl



Details | Edit | Create Request | Add to Library | Delete

Requests (1) | Synthesis (0) | Library (0) | Binding (0) | Ctoxicity (0)

Details

GID:	410
Creator:	manager
Author:	
Create date:	2014-10-20 09:59:30
Files from mol. modeling:	

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Compound details

Details

GID:	410
Creator:	manager
Author:	
Create date:	2014-10-20 09:59:30
Files from mol. modeling:	

Similar Compounds (10)

GID	Name	Similarity
410	CHEMBL6436	100.0 %
374	CHEMBL6715	85.29 %
370	CHEMBL6663	65.33 %
328	CHEMBL6829	50.0 %
7	CHEMBL6639	47.67 %
297	CHEMBL6307	47.5 %
149	CHEMBL6357	45.88 %
405	CHEMBL6317	44.71 %
106	CHEMBL6590	43.68 %
380	CHEMBL6775	43.18 %

History of changes

User	Status	Date	Changes
manager	Multi - accept	2014-10-20 10:07:32	Add to requests;
manager	Wczytywanie pliku	2014-10-20 09:59:30	Nazwa:CHEMBL6436; SMILES:Cc1nc(O)c2cc(CN(CC#C)c3ccc(C(=O)N[C@@H](C(=O)O)C(C)(C)C)c(F)c3)c(C)cc2n1; Tags:chembl;

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Request

PROJECT1

Compounds

Samples

Requests (30)

Synthesis

Library

Activity

Ctoxicity

< 1 >

Show all

Show requested

History of changes

Download manager

Filter

select all

Structure

GID

ID

Name

Owner

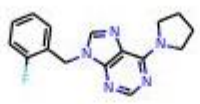
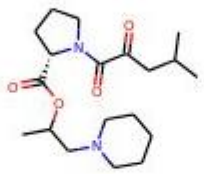
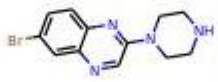
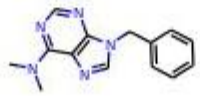
Recipient

Notes

Priority

Tags

Date

	GID	Name	Image	Create date	Creator	Status	Priority	Tags
☐	382	CHEMBL6832		2014-10-20 10:07:33	manager	accepted	★★★★☆	chembl
☐	383	CHEMBL6833		2014-10-20 10:07:33	manager	proposed	★★★☆☆	chembl
☐	384	CHEMBL6837		2014-10-20 10:07:33	manager	rejected	★★☆☆☆	chembl
☐	385	CHEMBL6889		2014-10-20 10:07:33	manager	proposed	★☆☆☆☆	chembl

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Synthesis

PROJECT1

Compounds

Samples

- Requests
- Synthesis (8)
- Library

Activity

- Ctoxicity

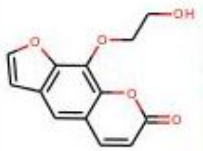
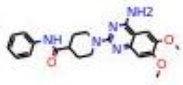
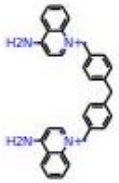
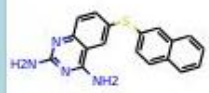
< 1 >

Show all
Show my
Recieve
History of changes

Download manager

Filter

- **select all**
- Structure
- GID
- ID
- Name
- LSO
- Owner
- Recipient
- Notes
- Priority
- Tags
- Date

GID	Name	Image	Create date	Owner	Recipient	Status	Effort	Phase	LSO	Priority	Tags
408	CHEMBL6379		2014-10-20 10:29:44	manager	Example manager	received	1	2/2	TEST3	★★★☆☆	chembl
409	CHEMBL6380		2014-10-20 10:29:30	manager	Example manager	synthesis 0	1	1/2		★★★☆☆	chembl
403	CHEMBL6315		2014-10-20 10:29:15	manager	Example manager	pending	1	-1/2		★★★☆☆	chembl
398	CHEMBL7050		2014-10-20 10:15:11	manager	Example manager	synthesis 0	1	1/3		★★★☆☆	chembl

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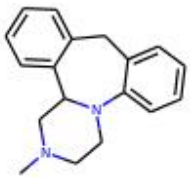
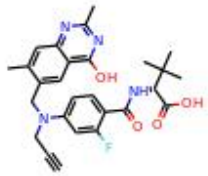
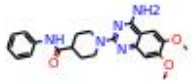
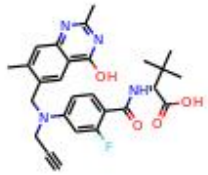
Library

	GID	Name	LCode	Purity [%]	Image	Create date	State [mg]	Entry	Box	LSO	Source	Tags
☐	5365	**8G1**	8G1	k: 100.0 % z: 100.0 %		2014-10-21 09:16:10	9.95	G1	8	3CLA1.133.139.6	LSO: ADAMED	Spirolony
☐	2021	**8F9**	8F9	k: 97.3 % z: 94.4 %		2014-10-14 15:56:43	36.26	F9	8	3CLA1.138.099.05	LSO: ADAMED	Spirolony
☐	5350	**8F8**	8F8	k: 87.6 % z: 81.0 %		2014-10-14 15:56:10	8.2	F8	8	3CLA1.138.088.05	LSO: ADAMED	Spirolony
☐	2019	**8F7**	8F7	k: 98.7 % z: 97.2 %		2014-10-14 15:55:42	10.66	F7	8	3CLA1.138.097.03	LSO: ADAMED	Spirolony

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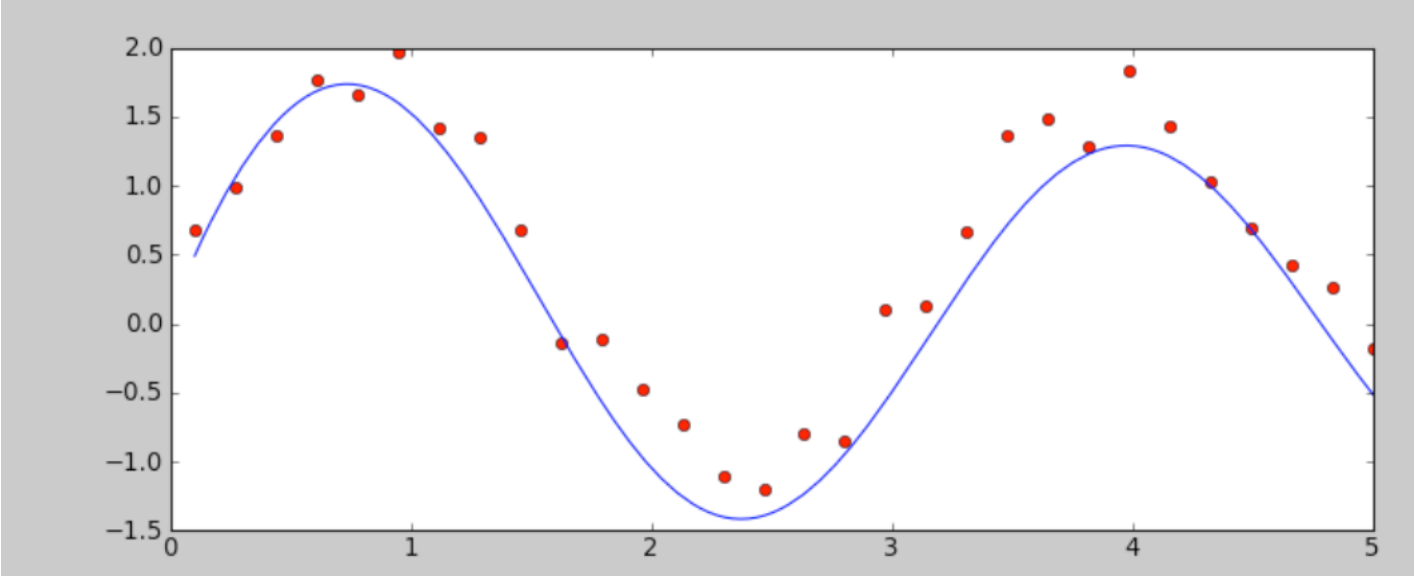
Least-square fitting (leastsq) example



Fit a model to noisy data:

$$y = a/xb \sin(cx)+\varepsilon$$

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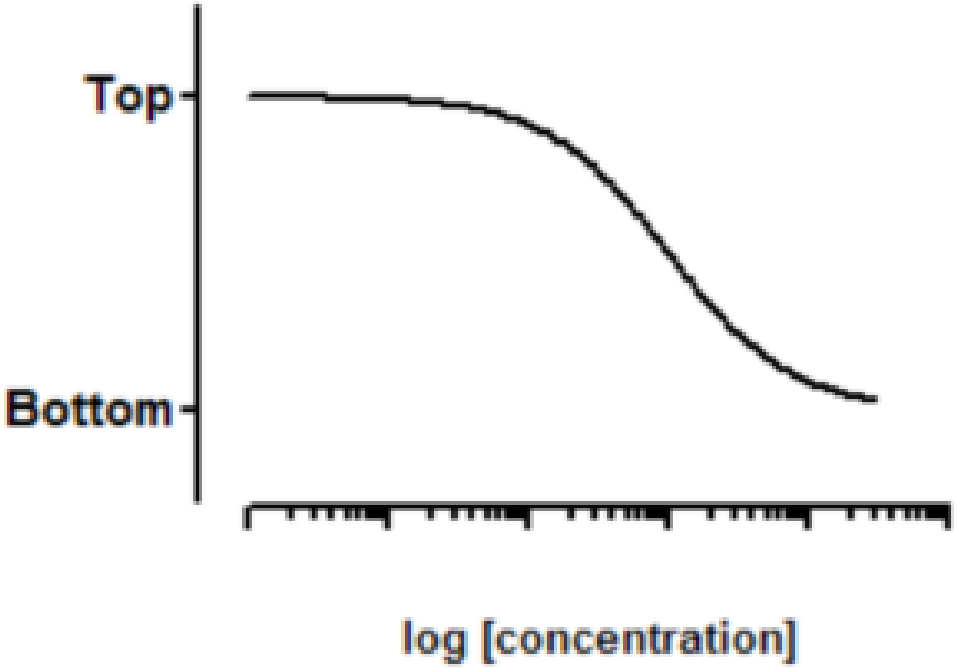
log(inhibitor) vs. response -- Variable slope

Model:

$$Y = Bottom + \frac{Top - Bottom}{1 + 10^{(logIC50 - X) * Hillslope}}$$



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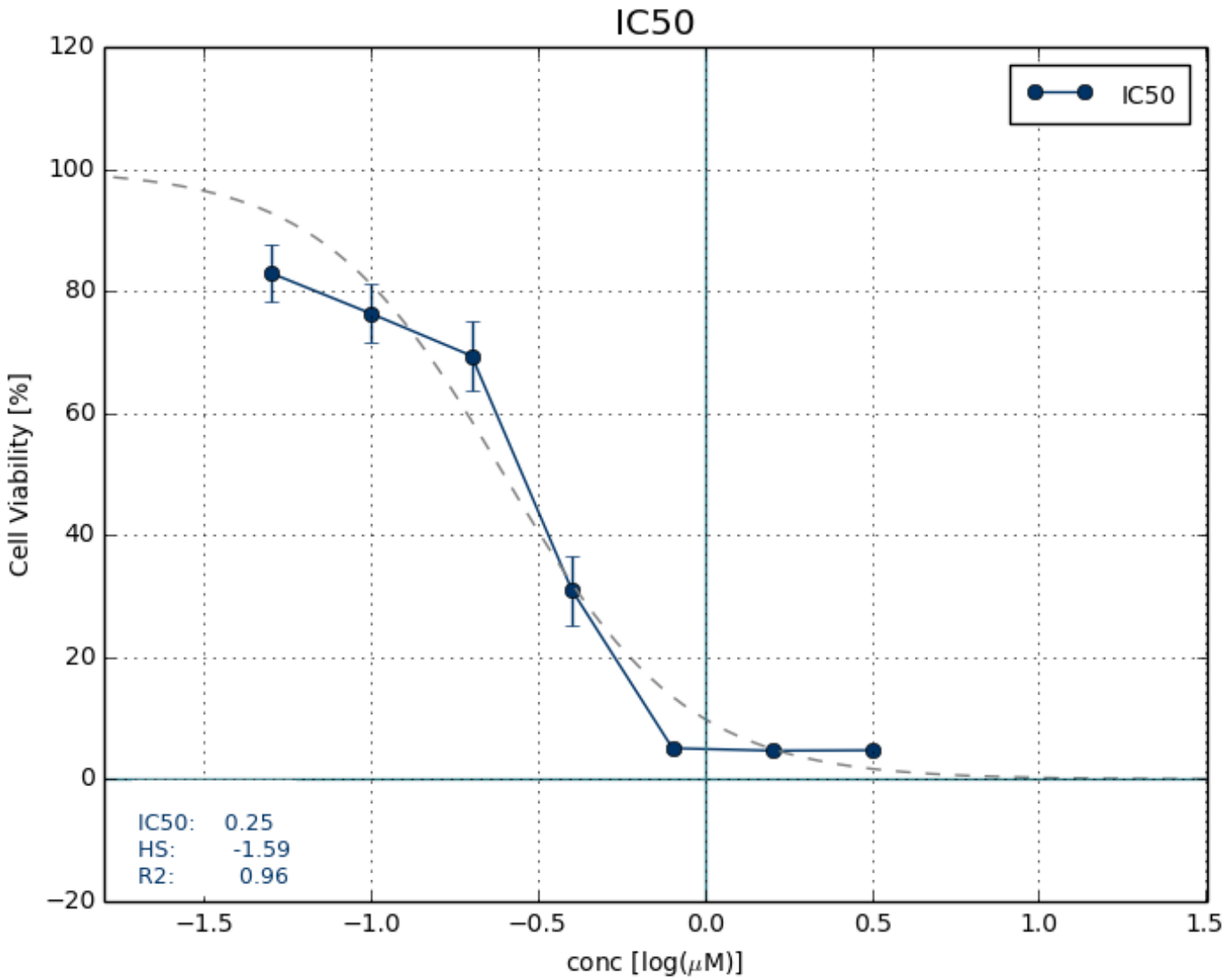

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Results – input data format

Concentration [mM];8D3;8D3;8D3; ← **header**
0,0000;0,916;1,011;1,065; ← **control line**
0,0500;0,844;0,997;1,206;
0,1000;0,964;0,989;1,117;
0,2000;0,849;0,972;1,075;
0,4000;0,843;0,880;1,003; **data**
0,8000;0,715;0,823;0,934;
1,6000;0,501;0,652;0,823;
3,2000;0,251;0,318;0,388;

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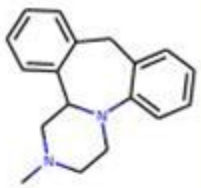
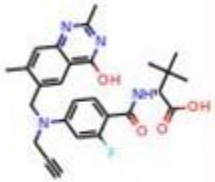
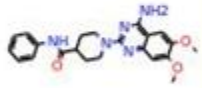
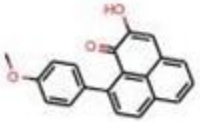
Results

☐	9	1428	**7A3** 7B7	7A3	k: 97.0 % z: 97.0 %		40.6 12.91	15.1 1.31	52.5 4.93	37.1 0.46	39.4 9.57	43.7 5.59	0.0 0	55.9 8.48	27.5 12.05
☐	10	1241	7A2	7A2	k: 97.0 % z: 97.0 %		1.21 0.36	0.080 0.02	11.9 0.16	3.16 1.91	4.43 1.48	0.660 0.16	0.0 0	37.1 31.05	>99.9 447.14
☐	11	328	**6D4** N3aToc	6D4	k: 98.0 % z: 98.0 %		8.55 5.34	1.85 0.43	32.2 5.15	10.5 3.71	19.2 8.96	4.74 1.89	0.0 0	29.6 6.38	31.3 2.99
☐	12	1240	**8D3** 6D3	6D3	k: 98.0 % z: 98.0 %		4.82 2.41	1.44 0.53	15.2 0.59	6.00 1.23	11.5 1.86	4.08 1.52	0.0 0	14.0 2.19	11.6 1.86

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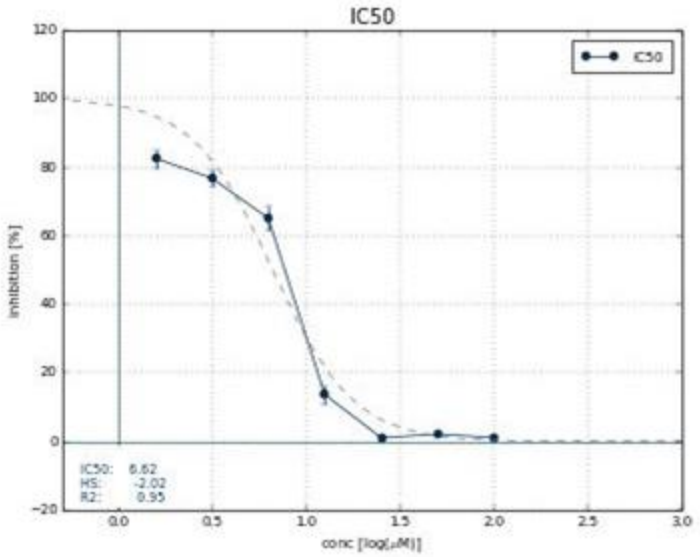
Results

☐	10	1241	7A2	7				**4.43** 4.21 2.45 4.43 6.62	0.660 0.16	0.0 0	37.1 31.05	>99.9 447.14
☐	11	328	**6D4**	6				19.2 8.96	4.74 1.89	0.0 0	29.6 6.38	31.3 2.99
☐	12	1240	**8D3** 6D3	6				11.5 1.86	4.08 1.52	0.0 0	14.0 2.19	11.6 1.86
☐	13	328	6D4					19.2	10.0	1.84	35.6	38.6

HCT-116++ (MTT) 2014-02-18

IC50:	6.618
Hillslope:	-2.016
R²:	0.952
Notes:	



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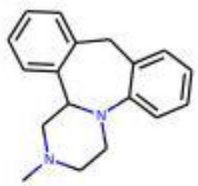
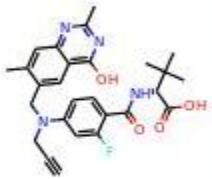
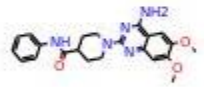
Results

7A3	k: 97.0 % z: 97.0 %		40.6 12.91	15.1 1.31	52.5 4.93	37.1 0.46	39.4 9.57	43.7 5.59	0.0 0	55.9 8.48	27.5 12.05	35.6 0.0	35.2 1.33	55.5 2.23
7A2	k: 97.0 % z: 97.0 %		1.21 0.36	0.080 0.02	11.9 0.16	3.16 1.91	4.43 1.48	0.660 0.16	0.0 0	37.1 31.05	>99.9 447.14	24.6 15.71	3.76 1.34	5.58 1.15
6D4	k: 98.0 % z: 98.0 %		**8.55** 25.2 6.16 8.18 5.97 5.34 9.27 3.24 9.84 8.31 8.88 6.49 5.71	**1.85** 2.15 1.46 1.42 1.22 2.35 1.26 1.79 1.43 2.34 2.15 1.90 2.29 2.34	**32.2** 32.0 32.5 36.0 22.9 39.5 30.1	**10.5** 6.22 8.26 8.52 16.5 12.8	**19.2** 20.9 28.5 36.8 19.2 14.9 7.07 7.59 12.9 17.4 26.9	**4.74** 3.86 2.48 7.62 5.01	0.0 0	**29.6** 35.9 28.6 34.1 20.2 36.3 22.5	**31.3** 33.9 25.3 30.1 32.7 28.9 35.6 31.5 32.3	**22.3** 25.2 27.8 25.7 24.9 22.4 11.6 24.0 15.5 23.4	**10.6** 10.4 6.20 1.00 27.1 10.8 8.37	**28.7** 33.6 16.8 28.8 35.8

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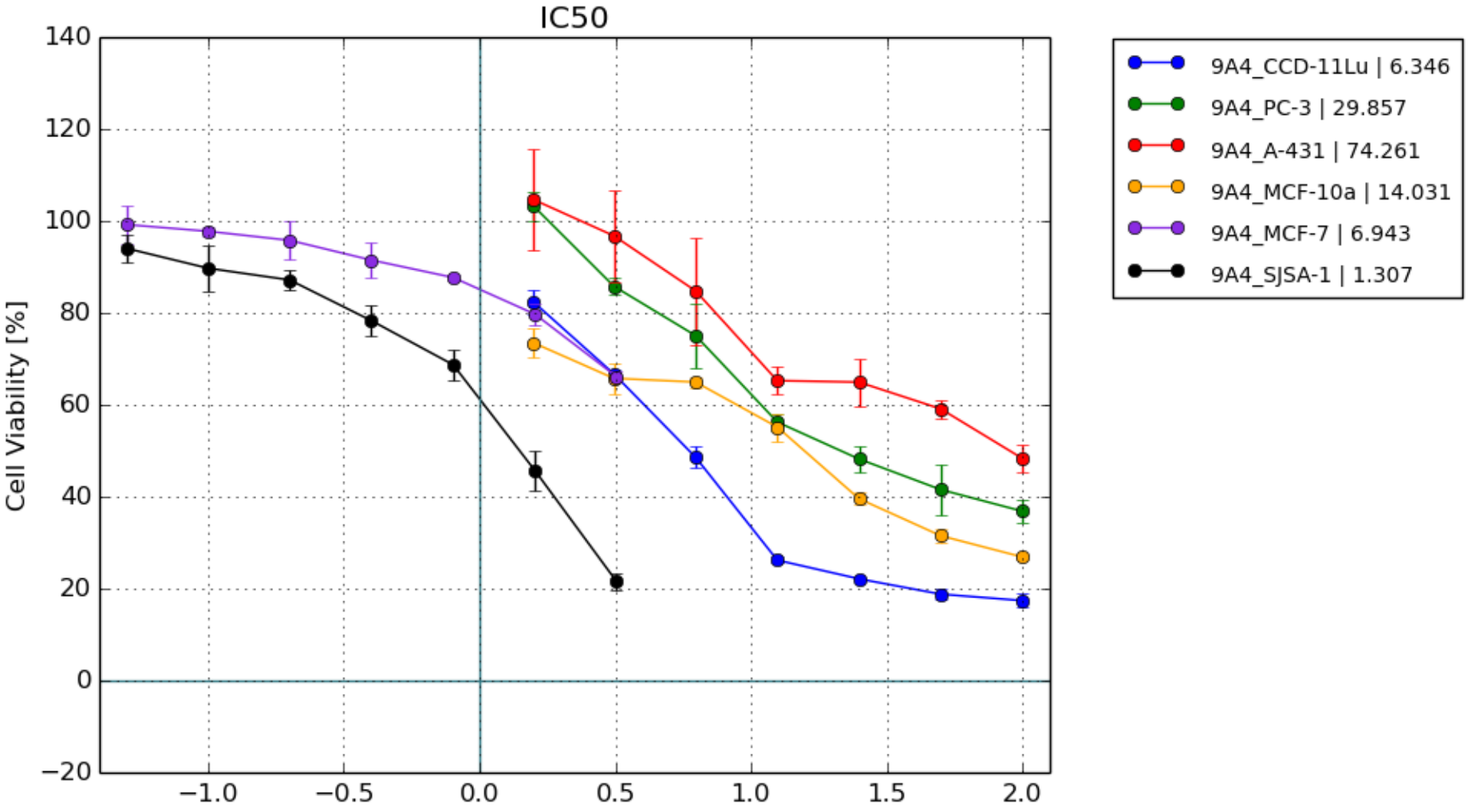

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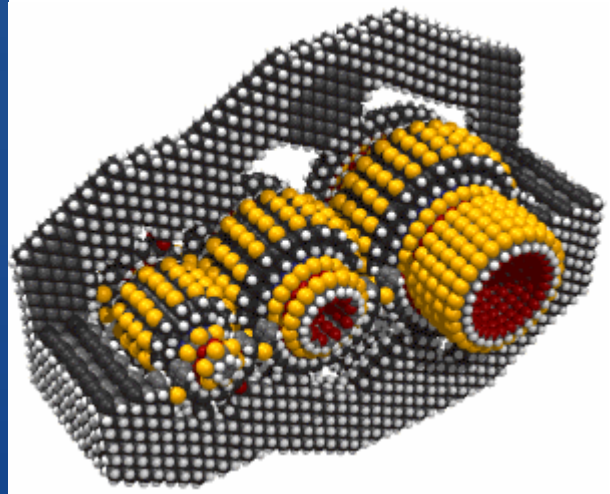

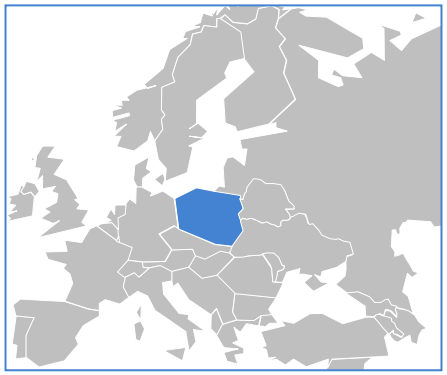

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THANK YOU FOR YOUR TIME

Questions?

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