

Instant JChem as a basis to construct a customized database to store biological activity data

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iTeos Therapeutics in 2012

- A spinoff of the Ludwig Cancer Research, focussed on discovery and development of novel drugs in the immunooncology area
- Completed Round A financing in April 2012
- Raised 3 M EUR in round A plus 6 M non-dilutive grant from Walloon Region
- Start of operations in September 2012
- Five employees at end 2012
- Three initial projects, of which two entailed medicinal chemistry (synthetic chemistry outsourced, biology in-house)
- No Research Informatics team, limited IT support



iTeos Therapeutics Research Informatics needs in 2012

- Focus on using existing capital for projects rather than infrastructure: very low CAPEX...
- ... but at the same time, a drive to ensure high level of quality in data generation and **data handling and reporting**
 - Implementation from day one of an Electronic Notebook for all internal activities
 - **Need for a database to store all compounds produced and all biological data generated (internally and externally)**
- **Need for a fit-for-purpose tool**
- ... which additionally needed to be compatible with Mac computers
- Decision to use Chemaxon Instant JChem as the basis for the database, and to work with Chemaxon to customize the tools for our needs
- Team up with another start-up, Asceneuron SA (Lausanne, CH), which had similar requirements

ASCENEURON
A Neurodegeneration Therapeutics Company



Corporate Database: main deliverables

- A limited customization, with a limited budget
- Fully searchable database
- Capable of handling and associating data to both the molecule as well as batches of the molecule
- Handling different types of data according to predefined rules. E.g. some types of data are aggregated in averages, others not
- Visualization both by individual molecule (with possibility to easily get access to all data for one molecule, batch by batch) or by list (see selected types of data across a list of compounds)
- An easy loading of both structures and biological data
- Easy interface with sd files and with JChem for Excel



Corporate Database I: typical compound view

Instant JChem 15.8.10.0

File Edit View Search Data Lists Chemistry Tools Window Help

Dashboard **Compounds form**

Design Query Browse Code

Batch Code	Salt	Appear	Registrar	Origin	LNB	Supplier Code	Commer	Quantit	Melt Poir	Batch MW	Purity	Project Code
1 EOS100008-01	Parent	Yellow sol	22-jul.-2...	Villapha	SCR000004	PF-05222463-00		30,00	179,	238,27	96%	
2 EOS100008-02	Parent	yellow sol	02-sept.-...	Sundia	SCR000078	PF-05222463-00		340,20	178,	238,26	97	TDO

Avg Enzyme Cell DRC

Batch Code	Assay SOP	Assay Title	Result Avg	Result Type	Ratio Ref Cpd Avg	Amplitude Efficacy Perc	Result Cnt	Result Tot
1 EOS100008-02	1731	TDO THP1 cell	1,96E-07	IC50		98,53	25	25
2 EOS100008-02	1721	hTDO A172 dose response	4,48E-07	IC50	0,97	100,81	286	286
3 EOS100008-02	1711	mTDO P815 dose response	1,05E-07	IC50		96,61	24	24
4 EOS100008-01	1711	mTDO P815 dose response	6,42E-08	IC50	1,00		2	2
5 EOS100008-01	1702	hTDO P815 Dose response IMDM	1,58E-07	IC50		95,07	8	8
6 EOS100008-01	1701	hTDO P815 dose response	1,37E-07	IC50	1,00	100,16	36	36
7 EOS100008-02	1701	hTDO P815 dose response	1,45E-07	IC50		97,57	18	18
8 EOS100008-02	1631	IDO THP1 cell	3,37E-05	IC50		72,67	12	14

Enzyme Cell DRC

Batch Code	Assay SOP	Assay Title	Result Modif	Result M	Result Type	Result Reado	Amplit. Efficac	Max Conc	Max Conc Result	Min Conc	Min Conc	Slope	Ratio Ref	Invali	Expt ID	LNB	Filename	Commer	PDF	XLS
1 EOS100008-01	1102	hTDO enzyme dose response		3,39E-07	IC50	Kynurei						-1,02			2,871	ADU0000008	ADU0000008 new.xls		file:///file:///	file:///file:///
2 EOS100008-01	1102	hTDO enzyme dose response		3,89E-07	IC50	Kynurei						-0,91			2,871	ADU0000008	ADU0000008 new.xls		file:///file:///	file:///file:///
3 EOS100008-01	1102	hTDO enzyme dose response		3,43E-07	IC50	Kynurei						-0,92			2,871	ADU0000008	ADU0000008 new.xls		file:///file:///	file:///file:///
4 EOS100008-01	1102	hTDO enzyme dose response		6,06E-07	IC50	Kynurei						-1,61	1,00		2,870	ADU0000011	ADU0000011.xls		file:///file:///	file:///file:///
5 EOS100008-01	1102	hTDO enzyme dose response		8,00E-07	IC50	Kynurei						-1,12	1,00		2,870	ADU0000011	ADU0000011.xls		file:///file:///	file:///file:///
6 EOS100008-01	1102	hTDO enzyme dose response		8,13E-07	IC50	Kynurei						-1,98	1,00		2,870	ADU0000011	ADU0000011.xls		file:///file:///	file:///file:///
7 EOS100008-01	1102	hTDO enzyme dose response		6,06E-07	IC50	Kynurei						-1,61	1,00		2,868	ADU0000012	ADU0000012.xls		file:///file:///	file:///file:///
8 EOS100008-01	1102	hTDO enzyme dose response		1,02E-06	IC50	Kynurei						-2,05	1,00		2,868	ADU0000012	ADU0000012.xls		file:///file:///	file:///file:///
9 EOS100008-01	1102	hTDO enzyme dose response		5,36E-07	IC50	Kynurei						-1,54	1,00		2,867	ADU0000013	ADU0000013.xls		file:///file:///	file:///file:///
10 EOS100008-01	1102	hTDO enzyme dose response		1,19E-06	IC50	Kynurei						-1,01	1,00		2,867	ADU0000013	ADU0000013.xls		file:///file:///	file:///file:///
11 EOS100008-01	1102	hTDO enzyme dose response		6,12E-07	IC50	Kynurei						-1,63	1,00		414	ADU0000050	ADU0000050.xls		file:///file:///	file:///file:///
12 EOS100008-01	1102	hTDO enzyme dose response		7,42E-07	IC50	Kynurei						-0,86	1,00		414	ADU0000050	ADU0000050.xls		file:///file:///	file:///file:///
13 EOS100008-01	1102	hTDO enzyme dose response		2,63E-07	IC50	Kynurei						-1,21	1,00		409	ADU0000066	ADU0000066.xls		file:///file:///	file:///file:///

Compounds: 1/5.125. Batches: 2/5.232. Analytical: 0/0. Avg Caco 2: 0/1. Avg Enzyme Cell DRC: 17/2.859. Avg Enzyme Cell One Conc: 0/0. Avg In Vivo PD: 0/0. Avg In Vivo PK: 0/10. Avg Irrev Inhib Params: 0/0. Avg Microsome Stab Clint: 3/330.

Compound view: molecule details

The screenshot displays the Instant JChem 15.8.10.0 interface. The main window is titled 'Compounds form' and shows a sidebar with a tree view containing 'chembioass', 'Compou', 'Gric', 'Cor', 'Batches', 'Gric', 'Vst', 'Stage', 'Sta', 'Assays', 'Experin', 'Enzyme', 'Scripts', and 'Nouveau dk'. The central area is divided into several sections: a 'Cpd Code' field with 'EOS100008', a 'Registration Date' field with '22-jul.-2013 11:25:10', a 'Mol Weight' field with '238,26', and a 'PSA' field with '28,68'. Below these are fields for 'Formula' (C15H11FN2), 'Acidic pKa' (15,91), 'LogP' (3,34), 'Basic pKa' (4,88), 'LogD pH7,4' (3,34), and 'Donors' (1). The 'IUPAC Name' field contains '6-fluoro-3-[(E)-2-(pyridin-3-yl)ethenyl]-1H-indole'. A 'Batches' table is visible on the right, with columns for 'Batch Code', 'Salt Info', 'Appearance', 'Registration Date', 'Origin', 'LNB', 'Supplier Code', 'Commer', 'Quantit', 'Melt Poir', 'Batch MW', 'Purity', and 'Project Code'. The table contains two rows of data.

Batch Code	Salt Info	Appearance	Registration Date	Origin	LNB	Supplier Code	Commer	Quantit	Melt Poir	Batch MW	Purity	Project Code
1 EOS100008-01	Parent	Yellow sol	22-jul.-2...	Villapha	SCR000004	PF-05222463-00		30,00	179,4	238,27	96%	
2 EOS100008-02	Parent	yellow sol	02-sept.-...	Sundia	SCR000078	PF-05222463-00		340,20	178,5	238,26	97	TDO

Compound code

Compound structure

Compound calculated properties (InstJChem)

Batch codes

Table can be adapted to have more or less data column visible

Batch data imported from supplier

- All fields searchable (cpd code, structure, batch code, compound or batch properties)
- Editing fields is possible, but requires distinct actions, and cannot really be done by mistake



Compound view: biological data

Tables can be adapted to have more or less data columns visible

6-fluoro-3-[(E)-2-(pyridin-3-yl)ethenyl]-1H-indole 1

Enzyme/Cell DRC | Enzyme/Cell 1 conc | Physchem PPB | Microsomal Stability | Caco-2 | Irrev Inhib Params | In vivo PK | In vivo PD | Analytical

Avg Enzyme Cell DRC

Batch Code	Assay SOP	Assay Title	Result Avg	Result Type	Ratio Ref Cpd Avg	Amplitude Efficacy Perc	Result Cnt	Result Tot
1 EOS100008-02	1731	TDO THP1 cell	1,96E-07	IC50		98,53	25	25
2 EOS100008-02	1721	hTDO A172 dose response	4,48E-07	IC50	0,97	100,81	286	286
3 EOS100008-02	1711	mTDO P815 dose response	1,05E-07	IC50		96,61	24	24
4 EOS100008-01	1711	mTDO P815 dose response	6,42E-08	IC50	1,00		2	2
5 EOS100008-01	1702	hTDO P815 Dose response IMDM	1,58E-07	IC50		95,07	8	8
6 EOS100008-01	1701	hTDO P815 dose response	1,37E-07	IC50	1,00	100,16	36	36
7 EOS100008-02	1701	hTDO P815 dose response	1,45E-07	IC50		97,57	18	18
8 EOS100008-02	1631	hTDO THP1 cell	3,37E-05	IC50		72,67	12	14

Enzyme Cell DRC

Batch Code	Assay SOP	Assay Title	Result Modif	Result M	Result Type	Result Reado	Amplitu Efficac	Max Conc	Max Conc Result	Min Conc	Min Conc	Slope	Ratio Ref	Invali	Expt ID	LNB	Filename	Commer	PDF	XLS
1 EOS100008-01	1102	hTDO enzyme dose response		3,39E-07	IC50	Kynurel						-1,02		<input type="checkbox"/>	2,871	ADU000008	ADU000008 new.xls		File:///file:///	File:///file:///
2 EOS100008-01	1102	hTDO enzyme dose response		3,89E-07	IC50	Kynurel						-0,91		<input type="checkbox"/>	2,871	ADU000008	ADU000008 new.xls		File:///file:///	File:///file:///
3 EOS100008-01	1102	hTDO enzyme dose response		3,43E-07	IC50	Kynurel						-0,92		<input type="checkbox"/>	2,871	ADU000008	ADU000008 new.xls		File:///file:///	File:///file:///
4 EOS100008-01	1102	hTDO enzyme dose response		6,06E-07	IC50	Kynurel						-1,61	1,00	<input type="checkbox"/>	2,870	ADU000011	ADU000011.xls		File:///file:///	File:///file:///
5 EOS100008-01	1102	hTDO enzyme dose response		8,00E-07	IC50	Kynurel						-1,12	1,00	<input type="checkbox"/>	2,870	ADU000011	ADU000011.xls		File:///file:///	File:///file:///
6 EOS100008-01	1102	hTDO enzyme dose response		8,13E-07	IC50	Kynurel						-1,98	1,00	<input type="checkbox"/>	2,870	ADU000011	ADU000011.xls		File:///file:///	File:///file:///
7 EOS100008-01	1102	hTDO enzyme dose response		6,06E-07	IC50	Kynurel						-1,61	1,00	<input type="checkbox"/>	2,868	ADU000012	ADU000012.xls		File:///file:///	File:///file:///
8 EOS100008-01	1102	hTDO enzyme dose response		1,02E-06	IC50	Kynurel						-2,05	1,00	<input type="checkbox"/>	2,868	ADU000012	ADU000012.xls		File:///file:///	File:///file:///
9 EOS100008-01	1102	hTDO enzyme dose response		5,36E-07	IC50	Kynurel						-1,54	1,00	<input type="checkbox"/>	2,867	ADU000013	ADU000013.xls		File:///file:///	File:///file:///
10 EOS100008-01	1102	hTDO enzyme dose response		1,19E-06	IC50	Kynurel						-1,01	1,00	<input type="checkbox"/>	2,867	ADU000013	ADU000013.xls		File:///file:///	File:///file:///
11 EOS100008-01	1102	hTDO enzyme dose response		6,12E-07	IC50	Kynurel						-1,63	1,00	<input type="checkbox"/>	414	ADU000050	ADU000050.xls		File:///file:///	File:///file:///
12 EOS100008-01	1102	hTDO enzyme dose response		7,42E-07	IC50	Kynurel						-0,86	1,00	<input type="checkbox"/>	414	ADU000050	ADU000050.xls		File:///file:///	File:///file:///
13 EOS100008-01	1102	hTDO enzyme dose response		2,63E-07	IC50	Kynurel						-1,21	1,00	<input type="checkbox"/>	409	ADU000066	ADU000066.xls		File:///file:///	File:///file:///

Compounds: 1/5.125. Batches: 2/5.232. Analytical: 0/0. Avg Caco 2: 0/1. Avg Enzyme Cell DRC: 17/2.859. Avg Enzyme Cell One Conc: 0/0. Avg In Vivo PD: 0/0. Avg In Vivo PK: 0/10. Avg Irrev Inhib Params: 0/0. Avg Microsome Stab Clint: 3/330.

Aggregated results

Individual results

- Two tables, one for aggregated results and one for individual experimental results
- All fields searchable (both tables)
- Editing fields is not possible, requires reloading of whole experiment by script (safety against data modification)



Compound view: aggregated results

Different tabs have been created for different types of data, which require different data handling (a different « mask ») and different aggregation rules

Mask for Dose-Response experiments

Enzyme/Cell DRC									
Avg Enzyme Cell DRC									
...	Batch Code	Assay SOP ▼ (1)	Assay Title	Result Avg	Result Type	Ratio Ref Cpd Avg	Amplitude Efficacy Perc	Result Cnt	Result Tot
1	EOS100008-02	1731	TDO THP1 cell	1,96E-07	IC50		98,53	25	25
2	EOS100008-02	1721	hTDO A172 dose response	4,48E-07	IC50	0,97	100,81	286	286
3	EOS100008-02	1711	mTDO P815 dose response	1,05E-07	IC50		96,61	24	24
4	EOS100008-01	1711	mTDO P815 dose response	6,42E-08	IC50	1,00		2	2
5	EOS100008-01	1702	hTDO P815 Dose response IMDM	1,58E-07	IC50		95,07	8	8
6	EOS100008-01	1701	hTDO P815 dose response	1,37E-07	IC50	1,00	100,16	36	36
7	EOS100008-02	1701	hTDO P815 dose response	1,45E-07	IC50		97,57	18	18
8	EOS100008-02	1631	IDO THP1 cell	3,37E-05	IC50		72,67	12	14

Averaging of results by batch, not by compound

Averaging of results by assay (same SOP, same title)

Averaging of results by result type (if an assay gives an IC50 and a Ki they will have different lines)

Count of number of experiments



Compound view: individual results (dose response curve tab)

Enzyme Cell DRC

...	Batch Code	Assay SOP	Assay Title	Result Modifier	Result M	Result Type	Result Readout	Amplifi Efficac	Max Conc	Max Conc	Min Conc	Min Conc	Slope	Invalid	Expt ID	LNB ▲ (1)	Filename	Comments	PDF
33	EOS100008-01	1102	hTDO enzyme dose response		4,24E-07	IC50	Kynurenine	104	5,0E-05	97	1,0E-09	-7	-1,00	<input type="checkbox"/>	473	ADU000088	ADU000088.xls		file:///H:/II. Drug Disco
34	EOS100008-01	1102	hTDO enzyme dose response		6,89E-07	IC50	Kynurenine	96	5,0E-05	102	1,0E-09	6	-1,60	<input type="checkbox"/>	473	ADU000088	ADU000088.xls		file:///H:/II. Drug Disco
35	EOS100008-01	1102	hTDO enzyme dose response		8,72E-07	IC50	Kynurenine	94	5,0E-05	93	1,0E-09	-1	-1,05	<input type="checkbox"/>	474	ADU000089	ADU000089.xls		file:///H:/II. Drug Disco
36	EOS100008-01	1102	hTDO enzyme dose response		1,52E-06	IC50	Kynurenine	102	5,0E-05	90	1,0E-09	-12	-0,57	<input type="checkbox"/>	462	ADU000090	ADU000090.xls		file:///H:/II. Drug Disco
37	EOS100008-01	1102	hTDO enzyme dose response		9,79E-07	IC50	Kynurenine	87	5,0E-05	89	1,0E-09	2	-0,69	<input type="checkbox"/>	480	ADU000092	ADU000092.xls		file:///H:/II. Drug Disco
38	EOS100008-01	1102	hTDO enzyme dose response		9,20E-07	IC50	Kynurenine	93	5,0E-05	100	1,0E-09	7	-1,60	<input type="checkbox"/>	480	ADU000092	ADU000092.xls		file:///H:/II. Drug Disco
39	EOS100008-01	1102	hTDO enzyme dose response		4,89E-07	IC50	Kynurenine	97	5,0E-05	96	1,0E-09	-1	-0,83	<input type="checkbox"/>	472	ADU000093	ADU000093.xls		file:///H:/II. Drug Disco
40	EOS100008-01	1102	hTDO enzyme dose response		1,28E-06	IC50	Kynurenine	108	5,0E-05	94	1,0E-09	-13	-1,38	<input type="checkbox"/>	472	ADU000093	ADU000093.xls		file:///H:/II. Drug Disco
41	EOS100008-01	1102	hTDO enzyme dose response		5,71E-07	IC50	Kynurenine	92	5,0E-05	100	1,0E-09	8	-1,59	<input type="checkbox"/>	464	ADU000095	ADU000095.xls		file:///H:/II. Drug Disco
42	EOS100008-01	1102	hTDO enzyme dose response		7,38E-07	IC50	Kynurenine	100	5,0E-05	100	1,0E-09	0	-1,19	<input type="checkbox"/>	464	ADU000095	ADU000095.xls		file:///H:/II. Drug Disco
43	EOS100008-01	1701	hTDO P815 dose response		4,88E-08	IC50	Kynurenine						-0,74	<input type="checkbox"/>	345	ADU000115	ADU000115.xls		file:///H:/II. Drug Disco
44	EOS100008-01	1701	hTDO P815 dose response		8,20E-08	IC50	Kynurenine						-0,93	<input type="checkbox"/>	347	ADU000116	ADU000116.xls		file:///H:/II. Drug Disco

cpd batch

Modifier handles <x or >x results

Single conc data captured for high and low conc

Each experiment links to an ELN page, and shows the original upload file

Link to pdf of experiment

each assay is identified by an SOP number and a title for easier reading

All data captured by a number and a result type (IC50, EC50, ...) to leave flexibility



A different mask (microsomal stability)

Microsomal stability requires different (specialized) files, so has a different mask

Enzyme/Cell DRC	Enzyme/Cell 1 conc	Physchem PPB	Microsomal Stability	Caco-2	Irrev Inhib Params	In vivo PK	In vivo PD	Analytical				
Avg Microsome Stab Clint												
...	Batch Code	Assay SOP	Assay Title	Clint Avg	Result Cnt	Result Tot						
1	EOS100008-01	3001	Human Microsome stability	79,20	1	1						
2	EOS100008-02	3021	Rat Microsome stability	50,20	1	1						
3	EOS100008-01	3011	Mouse Microsome stability	109,80	1	1						
Microsome Stab Clint												
...	Batch Code	Assay SOP	Assay Title	Modifier	Clint ug/min/mg Protein	Perc Rem wo NADPH	Expt ID	Invalid	Filename	LNB	Comments	PDF
1	EOS100008-02	3021	Rat Microsome stability		50,20	78,88	1.813	<input type="checkbox"/>	biological assay inp	SCR000188		file:///H:/II. D
2	EOS100008-01	3001	Human Microsome stability		79,20	102,00	320	<input type="checkbox"/>	biological assay inp	SCR000026		file:///H:/II. D
3	EOS100008-01	3011	Mouse Microsome stability		109,80	95,00	321	<input type="checkbox"/>	biological assay inp	SCR000026		file:///H:/II. D

Note: it would be possible to code these results using the same mask as seen before, and giving each type of data (Clint, % remaining without NADPH) a different « result type »
However, since this type of data is used often, we preferred to have a separate worksheet and a different mask to facilitate reading



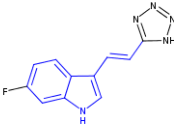
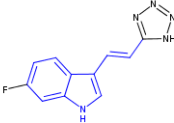
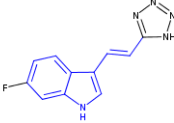
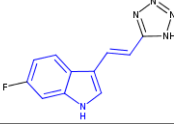
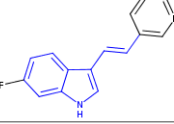
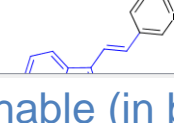
A different mask (in vivo PK)

Enzyme/Cell DRC		Enzyme/Cell 1 conc		Physchem PPB		Microsomal Stability		Caco-2		Irrev Inhib Params		In vivo PK		In vivo PD		Analytical					
...	Batch Code	Assay SOP	Assay Title	AUCz h/ng/ml	Route Of Admin	Bp Ratio	Dose Mpk	Clearance l/kg/h	Clinical Signs	Vz l/kg	Half Life h	AUC Inf	Time h	Brain ng/g	Plasma ng/ml	Vehicle	Csf ng/ml	Dosin ng/ml	Cmax l/kg	Vss l/kg	Fz
1	EOS100006-01	3501	Mouse PK	444	iv		1,00	38.9	no clinical sig		1.44	452				2% DMSO / 20% Kleptose HPB in water		5,00	4617	,607	
2	EOS100006-01	3501	Mouse PK	444	po		5,00		no clinical sig		3.79	682				0.5% HPMC K4M / 0.25% Tween 20 in water		10,00	704		20

- In vivo PK is another type of mask which require many datafields associated to the same experiment. It would not be practical to use the data/datatype system for each of them
- In addition, several fileds require text rather then numerical data
- For this worksheet, there is no data aggregation, since we do not do averaging for in vivo experiments



Table (SAR) view

Structure	Batch Code	Batch MW	HTDO P815 IC50	HTDO A172 IC50
	EOS100007-01	229,22	3,0E-05	2,4E-05
	EOS100007-02	229,22		
	EOS100007-03	229,22		
	EOS100007-04	229,21		
	EOS100008-01	238,27	1,4E-07	
	EOS100008-02	238,26	1,5E-07	4,5E-07

- Fully searchable (in blue, the search structure), including all datafields
- Can select the fields to display from all SOPs/result types
- Gives the aggregated value (if selected for this readout) or a concatenation of the individual results (if no aggregation selected for this datatype)
- Table can be exported as sd file (with independent selection of fields to be exported)
- Further Instant JChem functions are available (conditional formatting, list management etc)



Assays and experiments view

Mask and averaging determined by choice at this level

Assays								
ID	Title	SOP	Target	Species	Tissue Gene	Result Table	Comments	
1	1 CYP1A2	1501				BA_ENZ_CELL_DRC		
2	2 CYP2C9	1511				BA_ENZ_CELL_DRC		
3	3 CYP2C19	1521				BA_ENZ_CELL_DRC		
4	4 CYP2D6	1531				BA_ENZ_CELL_DRC		
5	5 CYP3A4	1541				BA_ENZ_CELL_DRC		
6	6 Kv11.1_PATCH_CLAMP_ONE_CONC	1551				BA_ENZ_CELL_ONE_C		
7	7 Kv11.1_PATCH_CLAMP_DRC	1552				BA_ENZ_CELL_DRC		
8	8 Human Microsome stability	3001				BA_MICROSOME_STAB		
9	9 Mouse Microsome stability	3011				BA_MICROSOME_STAB		
10	10 Rat Microsome stability	3021				BA_MICROSOME_STAB		
11	11 Caco2 pH7.4 no inhibitor	3101				BA_CACO_2		

Experiments								
ID	Assay ID	LNB	Expt Date	Registratio Date	Comments	PDF expt file	PDF 2	
1	318	8 SCR000022	18-sept.-2012	22-juil.-2...	Testosterone 81/433;	smb://10.0file:///iteos		
2	320	8 SCR000026	28-déc.-2012	22-juil.-2...	Testosterone 103/499	smb://10.0file:///iteos		
3	322	8 SCR000038	02-avr.-2013	22-juil.-2...	Testosterone 108/467	smb://10.0file:///iteos		
4	323	8 SCR000045	06-mai-2013	22-juil.-2...	Testosterone 95/520;	smb://10.0file:///iteos		
5	324	8 SCR000054	13-juin-2013	22-juil.-2...	Testosterone 82/448;	smb://10.0file:///iteos		
6	325	8 SCR000055	10-juil.-2013	22-juil.-2...	Testosterone 84/476;	smb://10.0file:///iteos		
7	326	8 SCR000056	10-juil.-2013	22-juil.-2...	Testosterone 98/518;	smb://10.0file:///iteos		
8	327	8 SCR000057	12-juil.-2013	22-juil.-2...	Testosterone 107/444	smb://10.0file:///iteos		
9	334	8 SCR000063	19-juil.-2013	22-juil.-2...	Testosterone 89/539;	smb://10.0file:///iteos		
10	424	8 SCR000083	01-août-2013	16-sept.-...		smb://10.0file:///iteos		
11	426	8 SCR000089	10-sept.-2013	16-sept.-...		smb://10.0file:///iteos		

A LabNoteBook number and a date together identify unambiguously an experiment

Loading new experimental results and creating new SOPs or new masks

- Loading data for new experiments is easy. Data are organized in an Excel sheet, with precise column headers which are automatically recognized by the program
- To modify existing data, one has to modify the original Excel file and load it again. Data cannot be changed directly in the system, to avoid mistakes

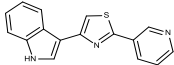
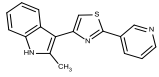
SOP_NUMBER	LNB	BATCH_CODE	RESULT_TYPE	RESULT_MODIFIER	RESULT_M	RESULT_READOUT	AMPLITUDE_EFFICACY_%	MAX_CONC_TESTED_M	MAX_CONC_RESULT_%	MIN_CONC_TESTED_M	MIN_CONC_RESULT_%	SLOPE	COMMENTS
1721	MMA000110	EOS300525-01	IC50		6.7E-08	Kynurenine	102	1.00E-05	101	1.00E-10	-1	-0.88	
1721	MMA000110	EOS300550-01	IC50		8.3E-08	Kynurenine	98	1.00E-05	101	1.00E-10	3	-1.05	
1721	MMA000110	EOS300532-01	IC50		3.2E-08	Kynurenine	103	1.00E-05	100	1.00E-10	-3	-1.67	
1721	MMA000110	EOS300533-01	IC50		3.0E-08	Kynurenine	98	1.00E-05	99	1.00E-10	1	-0.87	
1721	MMA000110	EOS300588-01	IC50		3.5E-08	Kynurenine	96	1.00E-05	99	1.00E-10	4	-0.8	
1721	MMA000110	EOS300589-01	IC50		8.0E-08	Kynurenine	94	1.00E-05	99	1.00E-10	5	-0.77	
1721	MMA000110	EOS300587-01	IC50		2.4E-07	Kynurenine	96	1.00E-05	98	1.00E-10	2	-0.89	
1721	MMA000110	EOS100008-02	IC50		7.5E-07	Kynurenine	107	1.00E-05	98	1.00E-10	-10	-1.04	

- New SOPs can be easily added. It just requires to create a new SOP number, to associate it with the correct mask (is it a SOP that generate an IC50 type of data? A single concentration result? A PK?) and to do a minor modification to the script that generates the tables. It can be easily done at the final client (even without RI or IT resources)
- Creating a new mask (ie a new type of data which requires different datafields and different averaging rules) can only be done by Chemaxon's team


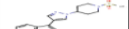


Loading compounds

- Similarly to loading biological data, loading compounds is done via an sd file

Product	Molecular weight (g/mol)	Amount weighted (mg)	External supplier	External Cat number	ID iTeos
	277.3	1	VitasM	STK723928	EOS500004
	291.4	1	VitasM	STK723931	EOS500005

- Molecules are imported from the sd file into the « stage » part of Instant JChem
- Columns of data from the sd file can be matched to the existing fields in the database, for added flexibility
- The system will check against previously registered compounds to see if a structure is already registered. If compound codes match, the batch number is increased by one, if the codes do not match an error is reported
- Structures can be modified at stage level of a mistake happened (for example, different reporting of chiral structures)

Stage	ID	Structure	Cpd Code	Status	Entered Date	Errors	Registration Date	Cpd ID	Batch ID	LNB	Origin	Supplier Code	Appearance	Commer	Salt	Qu mc	HPH Pul	Batc MW
1	5.882		EOS20024	REGISTERED	20-sept.-2...			4...	4...	SCR000093	Sundia	S36620.001	white solid		Parer3...	0,9%	4...	
2	5.883		EOS20024	REGISTERED	20-sept.-2...			4...	4...	SCR000093	Sundia	S36940.001	white solid		Parer4...	0,9%	3...	

After checking for consistency, initiate registration

Reports errors in registration



Conclusion

- Instant JChem can be used as a basis to create a simple, versatile system to handle biological data
- Can be easily adapted to different needs, as it can accommodate different types of data with different rules
- Easy to maintain for customers, including extension to additional projects/SOPs etc
- Next step for iTeos: extend the system beyond small molecules to biologicals, using Chemaxon's Biomolecule Toolkit



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