



Instant JChem

More ways to see your data

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Topics

- Licensing changes
- What's new
- What's coming

License changes (5.4)

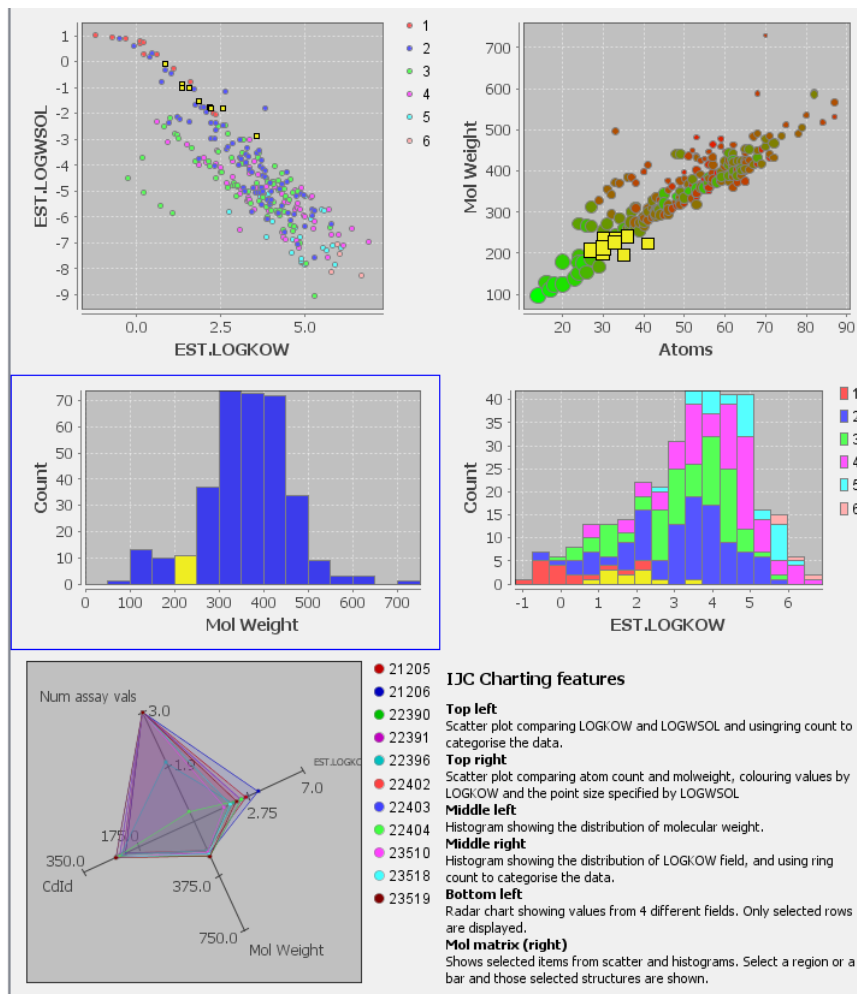
- IJC personal license
 - License now needed for usage with local databases
 - Without license IJC can be used as “free viewer”
- IJC Visualisation
 - Chart widgets
 - Conditional formatting

New in 5.4, 5.5 and 5.6

- Visualisation widgets
- Conditional formatting
- More form widgets
- Form builder improvements
- Cherry picking
- Calculated fields
- Scripting support
- Improved reactor
- Training
- Improved Markush
- R-group decomposition
- Performance improvements
- More options for security

Visualisation widgets (5.4, 5.5, 5.6)

- Chart widgets
 - Histogram
 - Scatter plot
 - Radar chart
- Fully integrated with:
 - Selection
 - Query



Conditional formatting (5.5)

- User defined schemes
- User defined rules
- Templates
- Works for grid and form views

The screenshot displays the Wombat software interface with a table of chemical data. The table has columns for Cdid, Structure, Mol Weight, EST.LOGKOW, EXP.LOGKOW, and Formula. The 'Cdid' column is highlighted in red for values 289, 291, and 292, and in green for values 290, 293, 294, 295, 296, 297, 298, and 299. A dialog box titled 'Conditional formatting for Cdid' is open, showing the following configuration:

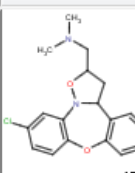
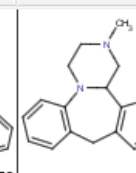
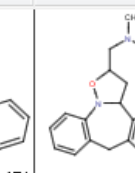
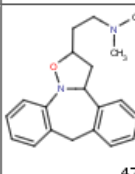
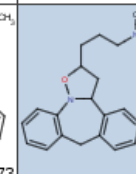
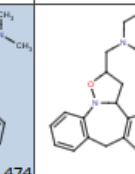
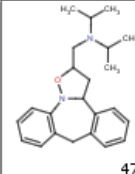
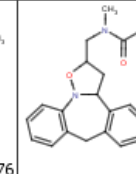
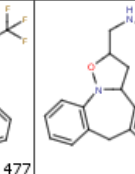
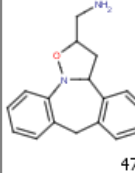
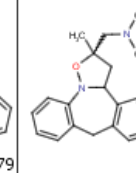
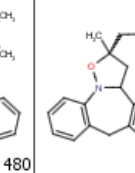
- Type of formatting: Traffic Lights
- Data field: Cdid
- Set of expressions: Traffic Lights for Cdid
- Set of expressions - details:
 - Name: Traffic Lights for Cdid
 - Data field type: Integer
 - Rule 1: <= 100 => Green
 - Rule 2: <= 200 => Yellow
 - Rule 3: <= 300 => Red
 - Otherwise: Default

More form widgets (5.5)

- Structure matrix
- Multi field sheet
- Tabbed pane
- Allow better forms
 - More data rich
 - Less clutter
 - More visual

The screenshot displays a software interface with a structure matrix on the left and a multi-field sheet on the right. The structure matrix is a 4x3 grid of chemical structures, with the central cell (row 2, column B) highlighted in blue. The multi-field sheet contains various data fields and molecular properties.

Structure, ID

	A	B	C
1	 470	 471	 472
2	 473	 474	 475
3	 476	 477	 478
4	 479	 480	 481

Wombat structures

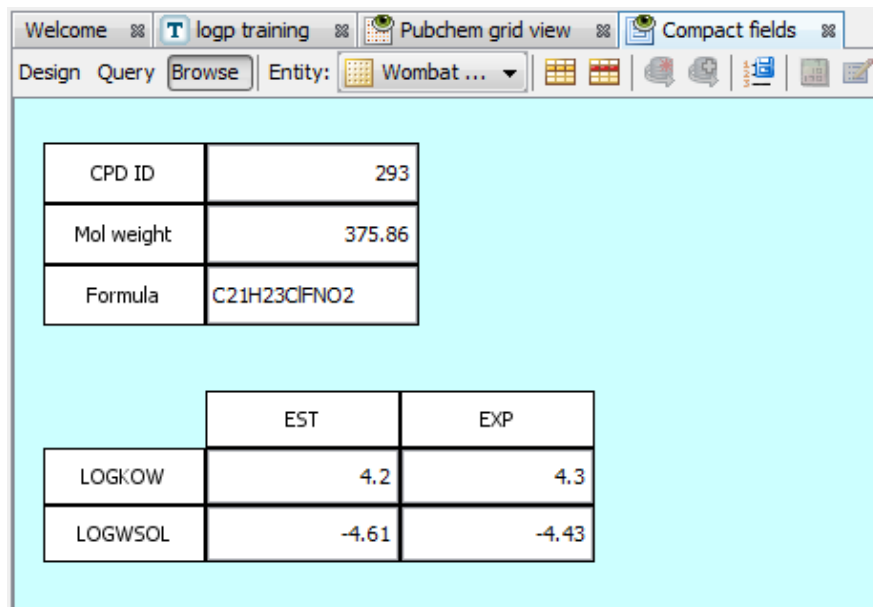
CdId	5
Mol Weight	322.44
Formula	C21H26N2O
Composition	C (78.22%), H (8.13%), N (8.69...)
IUPAC Name	dimethyl(3-{3-oxa-2-azatetracyclo[12.4.0.0 ^{2,6} .0 ^{7,12} }octadeca-1(14),7(12),8,10,15,17-hexaen-4-yl)propyl)amine
Smiles	CN(C)CCCC1CC2N(O1)c1cccc1Cc1cccc21

Molecular props Partitioning Screening data

TPSA	15.71	Ring count	4
H bond acceptors	3	Chiral atoms	2
H bond donors	0	Strongest acidic pKa	
Rotatable bonds	4	Strongest basic pKa	9.79

Form builder improvements (5.5)

- More configurable
 - Borders
 - Margins
 - Colours
 - Fonts
- Usability improvements
 - Copy and Paste of widgets
 - Move multiple widgets
 - Easier formatting



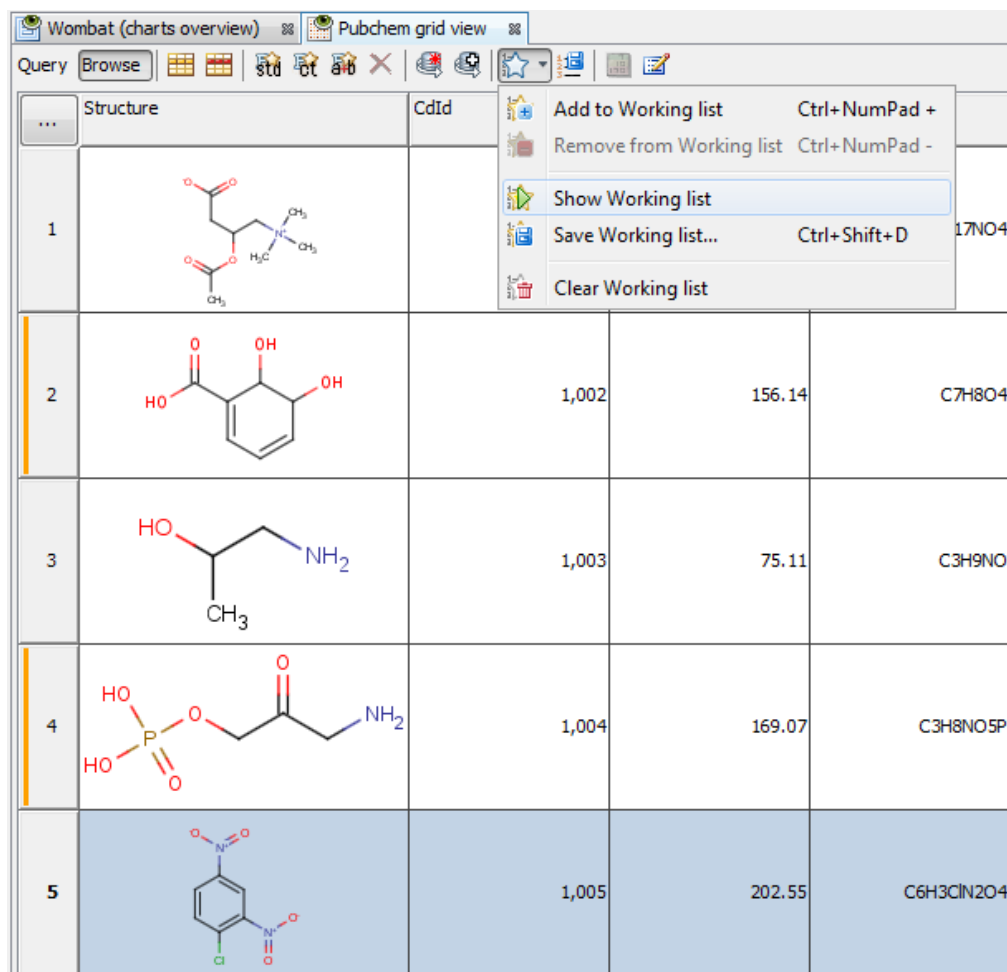
The screenshot shows a software interface with a light blue background. At the top, there is a window title bar with tabs for 'Welcome', 'logp training', 'Pubchem grid view', and 'Compact fields'. Below the title bar is a menu bar with 'Design' and 'Query' options, and a 'Browse' button. To the right of the menu bar is an 'Entity:' dropdown menu currently set to 'Wombat ...'. A toolbar with various icons is located to the right of the dropdown. The main area contains two tables. The first table has three rows and two columns. The second table has three rows and three columns.

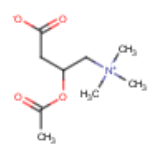
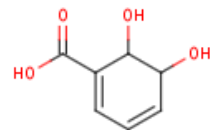
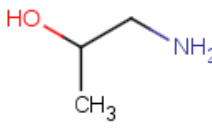
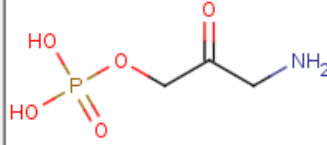
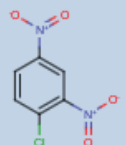
CPD ID	293
Mol weight	375.86
Formula	C ₂₁ H ₂₃ ClFNO ₂

	EST	EXP
LOGKOW	4.2	4.3
LOGWSOL	-4.61	-4.43

Cherry picking (5.6)

- Much easier approach to building up lists



...	Structure	CdId			
1					17NO4
2			1,002	156.14	C7H8O4
3			1,003	75.11	C3H9NO
4			1,004	169.07	C3H8NO5P
5			1,005	202.55	C6H3ClN2O4

Calculated fields (5.4)

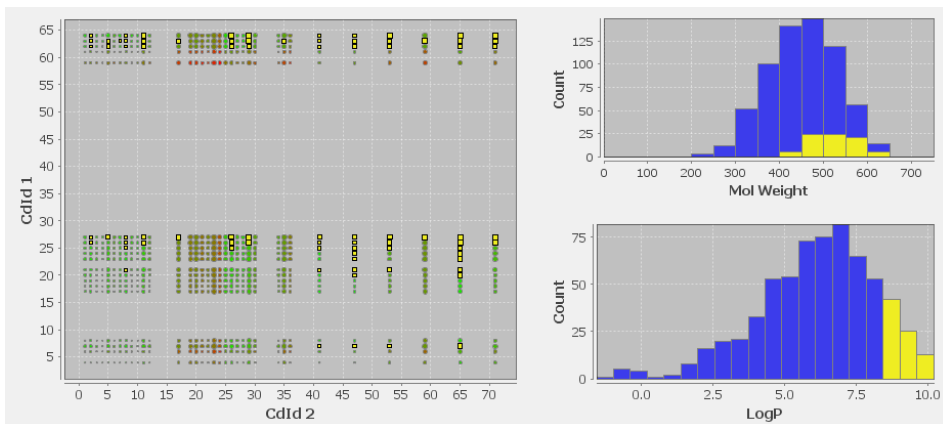
- Calculation is a script
 - Can do something very simple or very complex
 - Field values injected into script for calculation
- Examples
 - Simple “A + B” formulae
 - Aggregate data from related tables
 - Make data from other tables accessible
 - Call out to external services

Scripting support (5.4, 5.6, 5.6)

- Execute scripts on data trees, schemas or forms
- Allows
 - Customised import/export
 - Data migration
 - Custom data processing
 - “Mini-apps”
 - Rapid prototyping
 - Buttons on forms
- Planned improvements
 - Better editor support
 - Allow use of external libraries

Improved reactor (5.5)

- Copy fields from reactants to products
- More reactor runtime options
- May bug fixes and usability improvements
- Chemical terms + charts make powerful analysis tools



The screenshot shows the ChemAxon reactor software interface. The main window displays a reaction scheme for Friedel-Crafts acylation. The reaction is: C1=CC=C(C=C1) + C(=O)Cl >> C1=CC=C(C=C1)C(=O)Cl. The interface includes a 'Reaction' section with a 'Friedel-Crafts acylation' title, a 'Reactant 1' field with 'localdb/2004 Building Blocks Database', a 'Reactant 2' field with 'localdb/2004 Building Blocks Database', a 'Copied Fields' field, and an 'Output' field with 'localdb/friedel crafts Results'. A 'Copy field' dialog box is open, showing a table of fields:

Fields	Reactant Name	Reactant Field Name	Field Name
	1. 2004 Building Bloc...	ID	ID 1
	1. 2004 Building Bloc...	price1g	price1g 1
	2. 2004 Building Bloc...	ID	ID 2
	2. 2004 Building Bloc...	price1g	price1g 2

Below the table, there are checkboxes for 'Reactant 1 Index' (checked) and 'Reactant 2 Index' (checked), with corresponding index values of 'Index 1' and 'Index 2'. The dialog box also has 'Add', 'Remove', 'Ok', and 'Cancel' buttons.

Training (5.4)

- logP
- General

Welcome Pubchem grid view logp training

Training type LogP

Training input Training set localdb/Pubchem demo

Experimental values XLogP

Add ChemAxon's data

Cross-validate training set

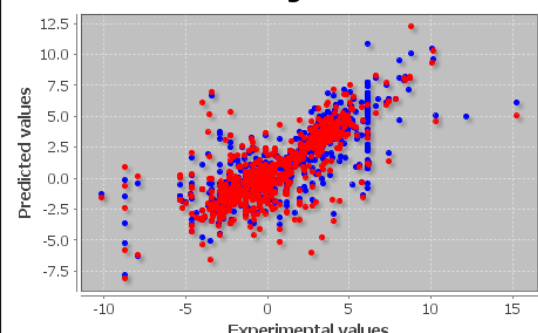
Validation Validate with other set

Validation set <No entity selected>

Experimental values

Statistics

Training Set



Predicted values

Experimental values

R²: 0.70

RMS: 1.89

Q²: 0.56

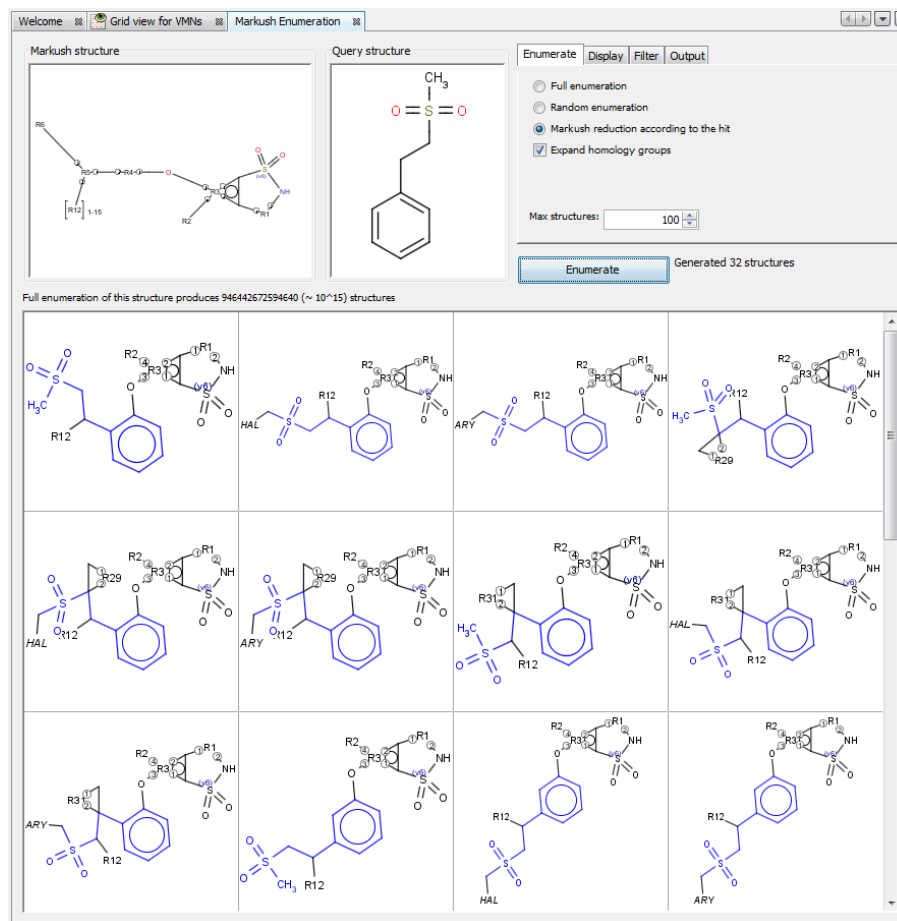
Show Cross-Validation on Chart

No Validation Set Statistics

Tip: To exclude structures from training set, mark them by left click, and re-run training.

Improved Markush (5.5, 5.6)

- Faster Markush search
- Markush enumeration
- Filtering using chemical terms expressions
- Homology group expansion
- Homology group search options



R-group decomposition (5.6)

- View R-group definitions
- Search options for R-group queries
- Generate Markush structure from R-group search results
- R-group tables planned

...	Structure				Cdid	Mol Weight	Formula
	S	R1	R2	R3			
1					1,005	202.55	C6H3ClN2O4
2					1,009	473.44	C20H23N7O7
3					1,011	181.45	C6H3Cl3
4					1,046	625.02	C45H68O
5					1,054	163.00	C6H4Cl2O
6					1,060	154.12	C7H6O4

Performance improvements

- Faster startup time, especially when database is on WAN, internet or VPN
- Less chat with the database
- Lower memory footprint for forms
- Further improvements being investigated

More options for security (5.4, 5.5)

- Ability to use database accounts for IJC user
- Oracle schema can be specified
- More flexible use of LDAP and Active Directory
 - Groups in directory can be mapped to IJC roles
- Filter out IJC schema items based on roles

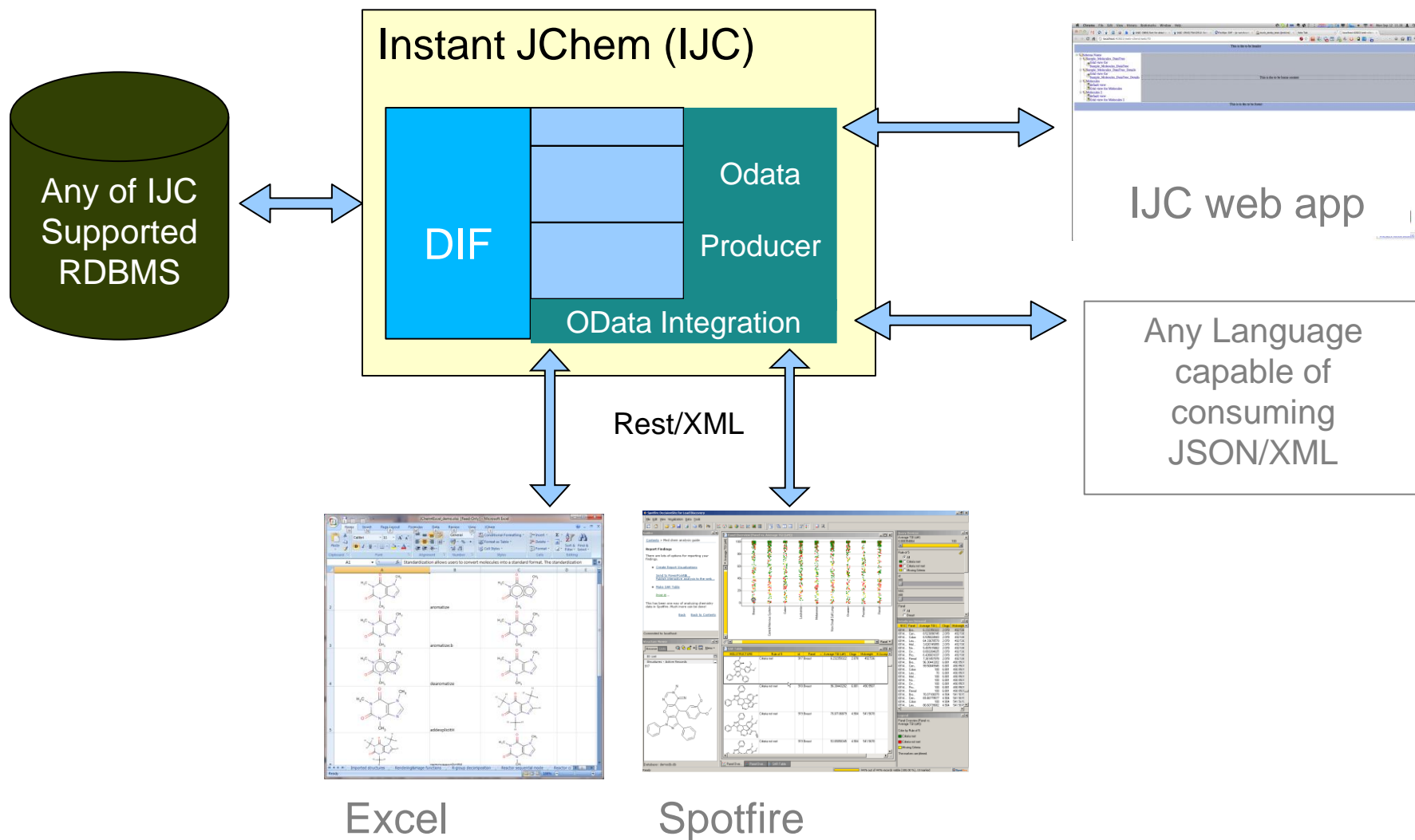
Beyond 5.6 (core)

- Performance
- More and improved visualisation widgets
 - parallel coordinate plot, X-Y plot, curve fits, stats
- Improved scripting
- Improved manipulation of data from DB
 - pivoting, aggregation, joining
- Improved display of data in forms
 - grouping, matrix display, filtering

Beyond 5.6 (chemistry)

- Clustering/grouping
 - MCS, hierarchical, scaffold
- R-group tables
- Markush enumeration browser
- Chemical space analysis
- Library design

Beyond 5.6 (integration)



What is OData?

A Web protocol for querying and updating data that provides a way to unlock your data and free it from silos that exist in applications today. OData does this by applying and building upon Web technologies such as HTTP, Atom Publishing protocol and JSON to provide access to information from a variety of applications, services, and stores

- Led by Microsoft
 - Supported in Excel 2010, Sharepoint
- Libraries for .NET, Java, Objective C, PHP, Javascript, Ruby (and more)
- Pushed by Pistoia as interoperability standard
- <http://www.odata.org/>

Thank you

- IJC product page
 - <http://www.chemaxon.com/products/instant-jchem/>
- Forum
 - <https://www.chemaxon.com/forum/forum62.html>