



Instant JChem

More ways to see your data

Tim Dudgeon <tdudgeon@chemaxon.com>



IJC team

- **Petr Hamernik** - everything!
- **Petr Zajac** – structure display, reactor, chemistry features
- **Martin Adamek** – IJC server, scripting
- **Max Sauer** - query, database, installers
- **Daniel Butler** – docs, QA
- **Martin Krauskopf** - visualisation
- **Radim Kubacki** – form builder, printing
- **Masoud Kalali** – IJC server, security
- **Vita Stejskel** – Schema editor, deployment
- **Istvan Rabel** – Reactor, Training
- **Ivan Solt** – Application scientist

- Licensing changes
- What's new in 5.4 and 5.5
- What's coming

License changes (5.4)

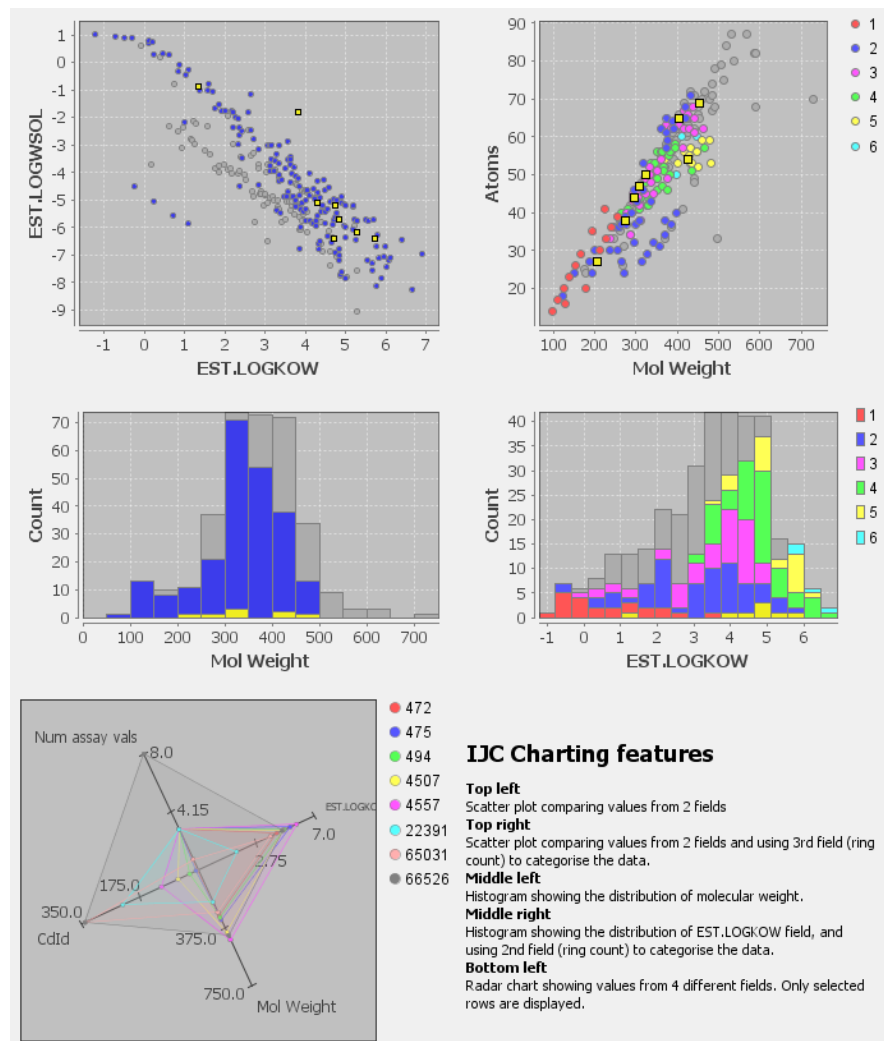
- IJC personal license
 - License now needed for usage with local databases
 - Without license IJC can be used as “free viewer”
- IJC Visualisation
 - Chart widgets
 - Conditional formatting

New in 5.4 and 5.5

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

Visualisation widgets

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



Conditional formatting

- User define 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

- 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 properties panel 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 structures are labeled with IDs 470 through 481. The properties panel on the right is titled 'Wombat structures' and contains a table with the following data:

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

Below the table, there are three tabs: 'Molecular props', 'Partitioning', and 'Screening data'. The 'Molecular props' tab is active and shows the following values:

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

- 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 toolbar with buttons for 'Design', 'Query', and 'Browse'. The 'Entity' dropdown is set to 'Wombat ...'. Below the toolbar, there are two tables. The first table has three rows: 'CPD ID' with value '293', 'Mol weight' with value '375.86', and 'Formula' with value 'C21H23ClFNO2'. The second table has two columns, 'EST' and 'EXP', and two rows: 'LOGKOW' with values '4.2' and '4.3', and 'LOGWSOL' with values '-4.61' and '-4.43'.

CPD ID	293
Mol weight	375.86
Formula	C21H23ClFNO2

	EST	EXP
LOGKOW	4.2	4.3
LOGWSOL	-4.61	-4.43

Calculated fields

- 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

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

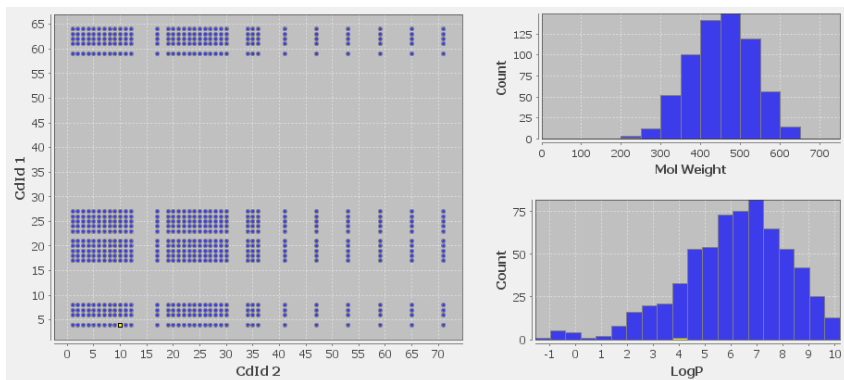
Improved reactor

- 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 'friedel crafts' reactor interface. The main window displays a chemical reaction for Friedel-Crafts acylation. The reactants are benzene (labeled with field (a),1) and acetyl chloride (labeled with fields [C,S],2 and [Cl,Br,I],3). The reaction is catalyzed by AlCl₃. The products are acetophenone (labeled with fields [C,S],2 and (a),1) and HCl (labeled with fields [Cl,Br,I],3 and (a),1). Below the reaction, there are controls for Reactant 1, Reactant 2, Copied Fields, and Output, each with a 'Browse...' button. A 'Copy field' dialog box is open in the foreground, showing a table of fields to be copied from reactants to products.

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, Index 1) and 'Reactant 2 Index' (checked, Index 2). Buttons for 'Add', 'Remove', 'Ok', and 'Cancel' are also present.



Training

- 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

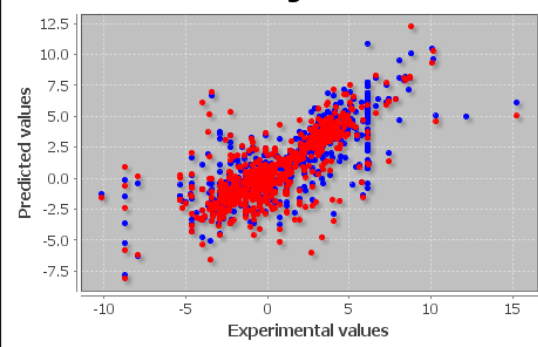
Validation Validate with other set

Validation set <No entity selected>

Experimental values

Statistics

Training Set



Statistics

R²: 0.70

RMS: 1.89

Q²: 0.56

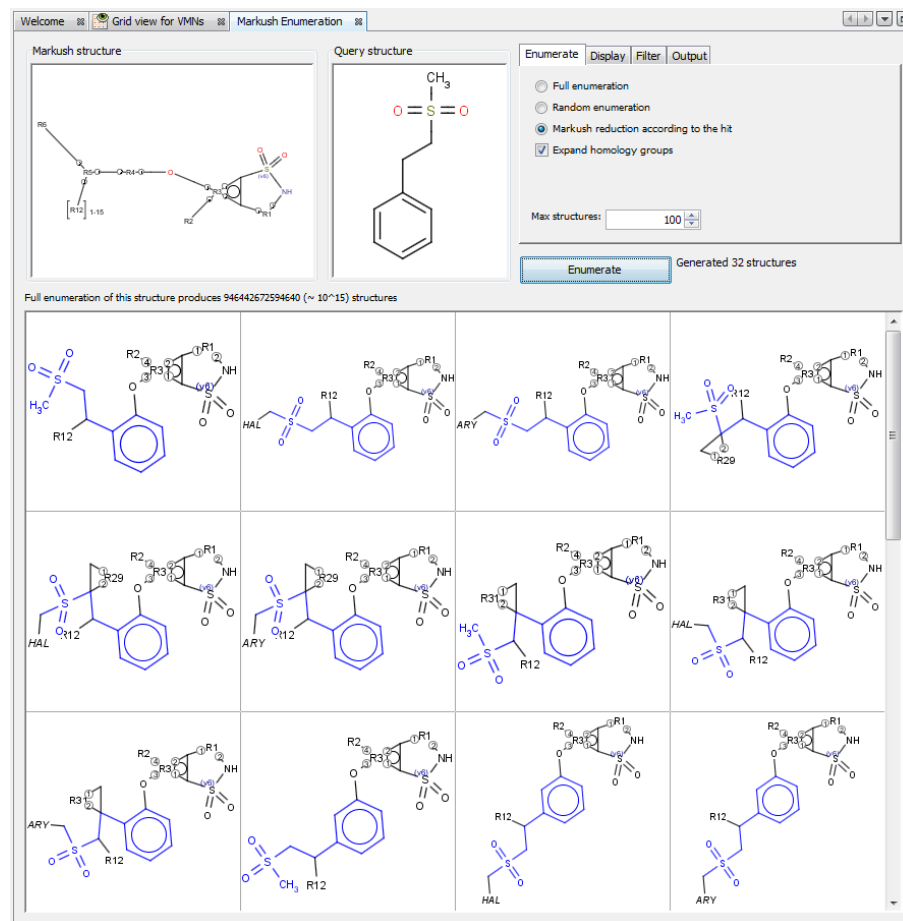
Show Cross-Validation on Chart

No Validation Set Statistics

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

Improved Markush

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



Performance improvements

- Faster startup time, especially on slow networks
 - should be much faster than 5.3 versions
- Less chat with the database
- Lower memory footprint for forms
- Further improvements being investigated

More options for security

- 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 5.5 (core)

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

Beyond 5.5 (chemistry)

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

Thank you

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