



Instant JChem

More ways to see your data

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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)

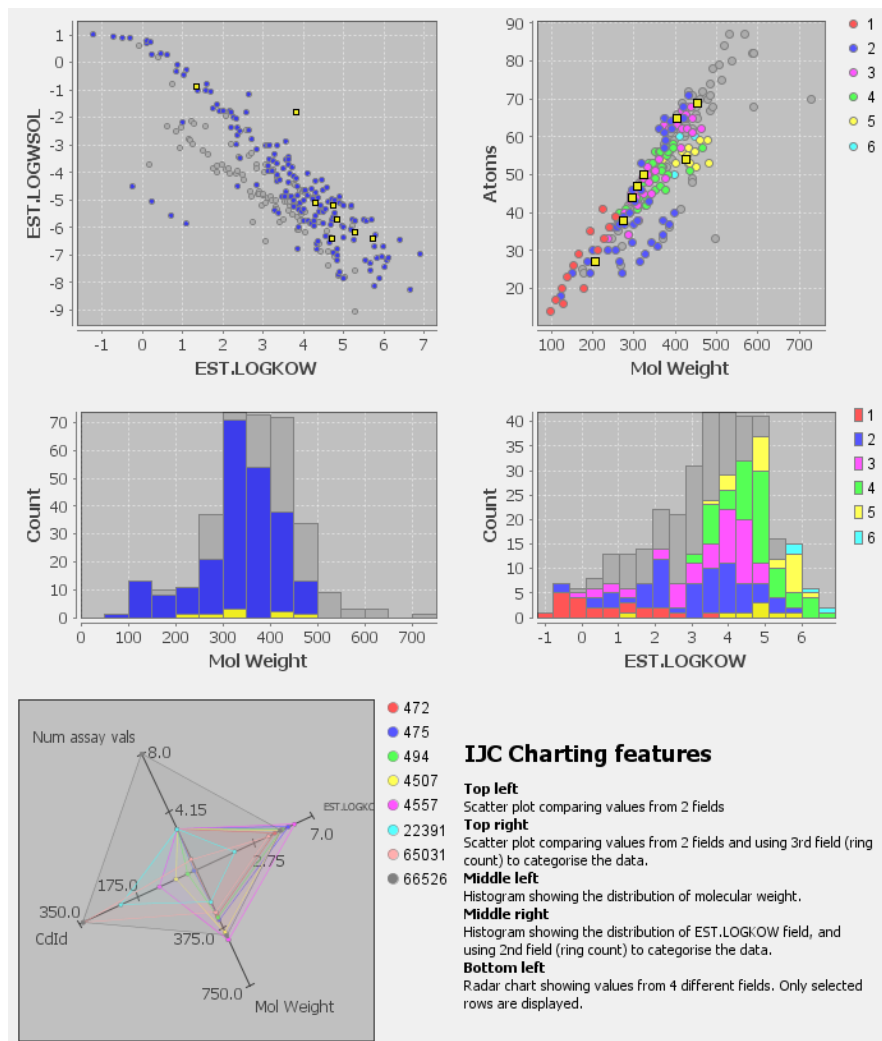
- IJC personal license
 - License now needed for usage with local databases
 - Without license IJC can be used as “free viewer”
- IJC Visualisation
 - Chart widgets
 - Conditional formatting

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 data table and a conditional formatting dialog box. The table has columns for Cdid, Structure, Mol Weight, EST.LOGKOW, EXP.LOGKOW, and Formula. The dialog box shows 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 multi-field sheet on the right.

Structure Matrix: A grid of chemical structures labeled A, B, and C across four rows (1-4). The structures are numbered 470 through 481. Structure 474 is highlighted in blue.

Wombat structures: A multi-field sheet for the selected structure (474).

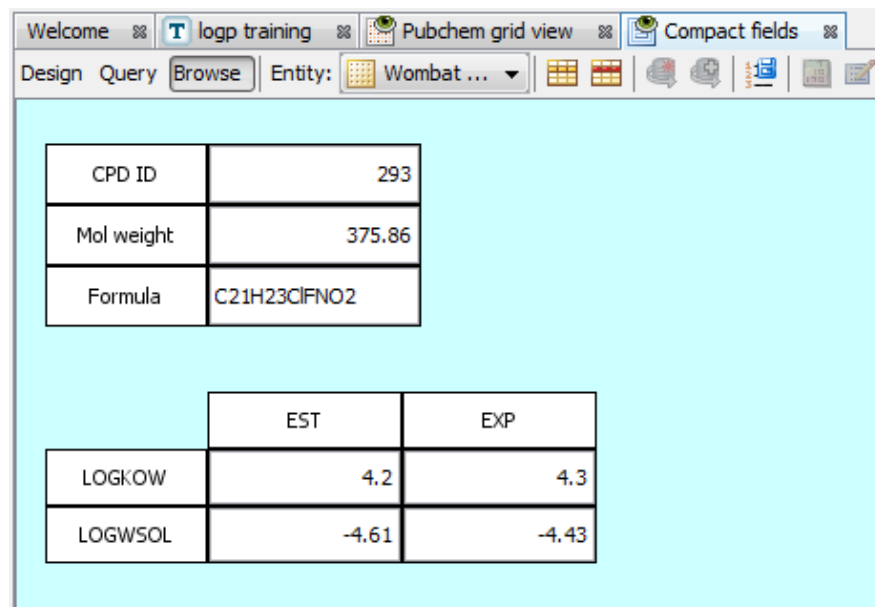
Wombat structures	
CdId	5
Mol Weight	322.44
Formula	C21H26N2O
Composition	C (78.22%), H (8.13%), N (8.69...)
IUPAC Name	dimethyl(3-{3-oxa-2-azatetracyclo[12.4.0.0 ^{2,6} .0 ^{7,12}]}octadeca-1(14),7(12),8,10,15,17-hexaen-4-yl)propyl)amine
Smiles	CN(C)CCCC1CC2N(O1)c1cccc1Cc1cccc21

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

- 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

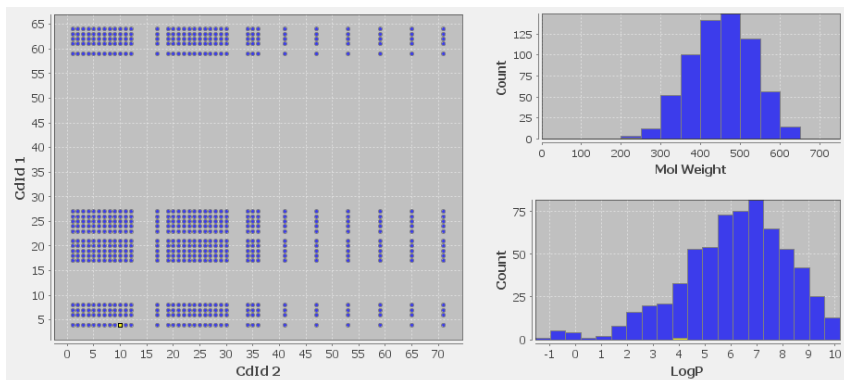
Improved reactor

- 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:

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). The dialog also has 'Add', 'Remove', 'Ok', and 'Cancel' buttons.



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

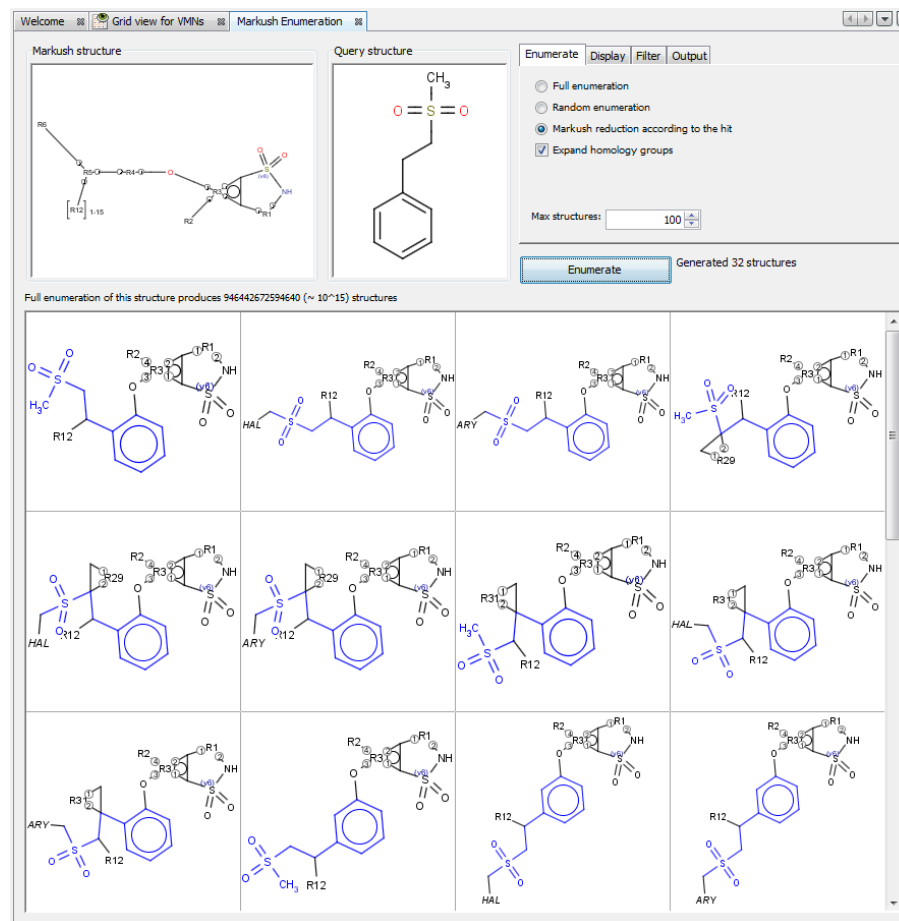
Show Cross-Validation on Chart

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>