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

Topics

- 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”

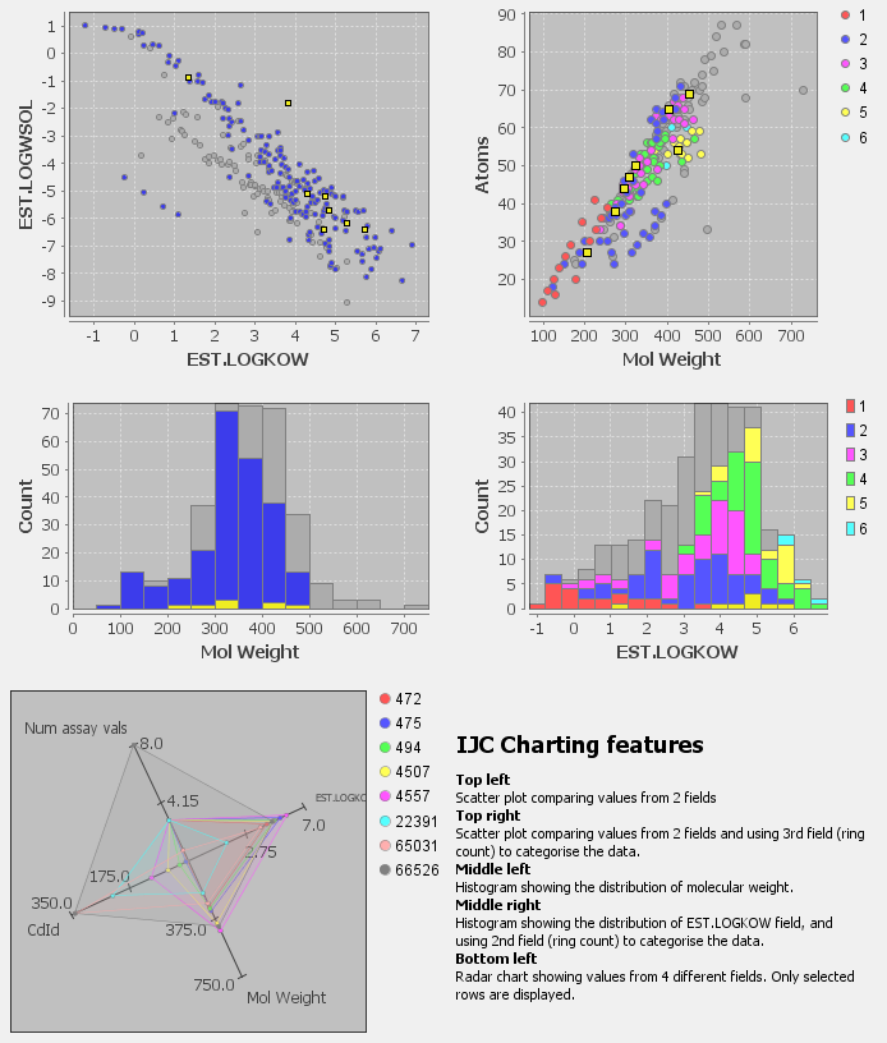
- IJC Visualisation
  - Chart widgets
  - Conditional formatting

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

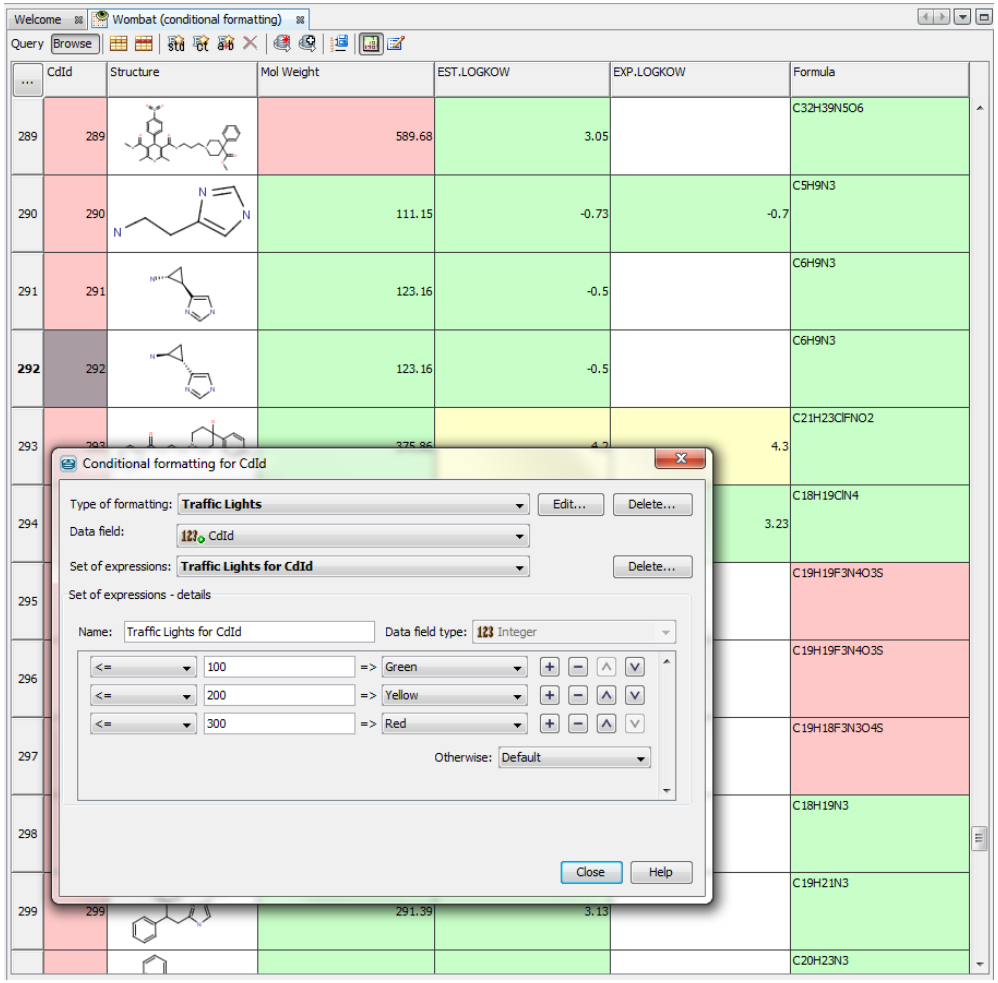
Visualisation widgets

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



Conditional formatting

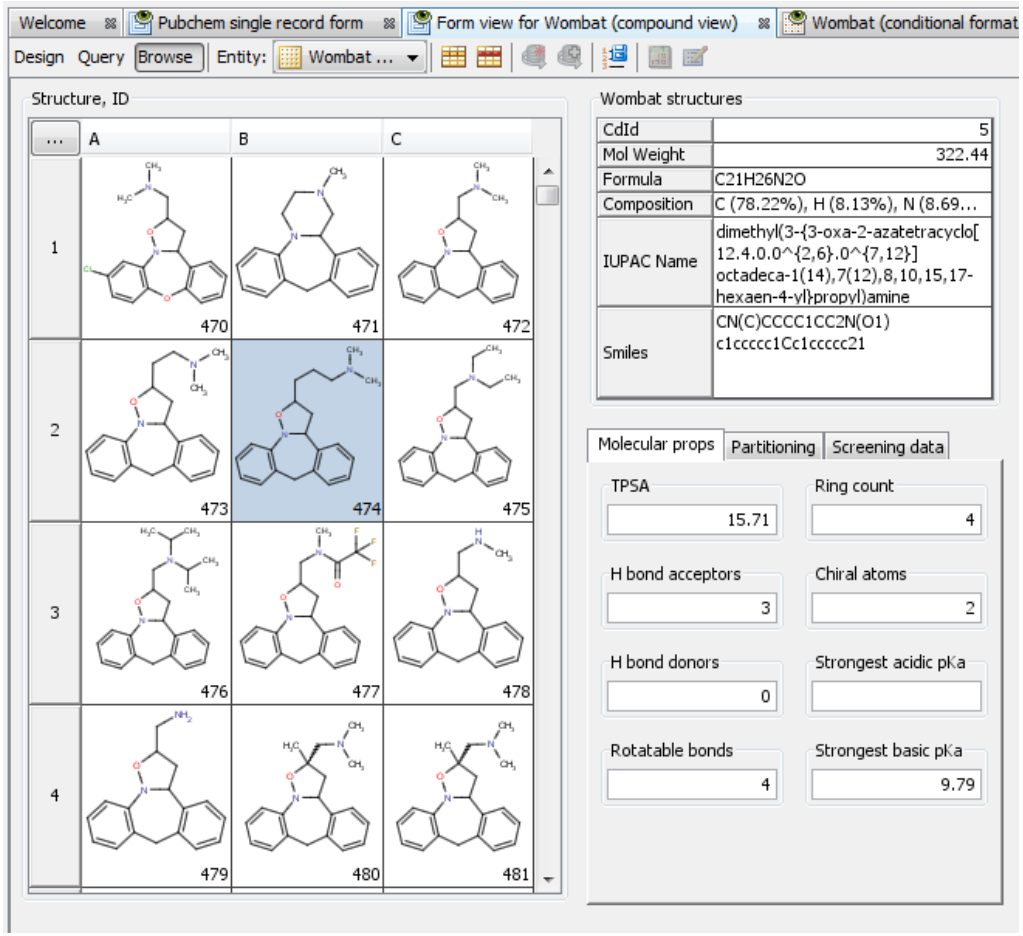
- User define schemes
- User defined rules
- Templates
- Works for grid and form views



More form widgets

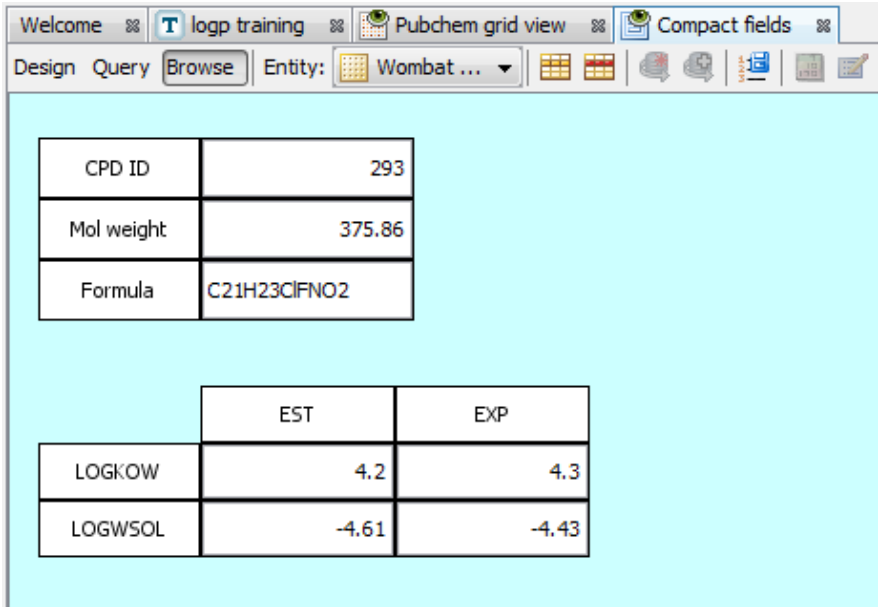
- Structure matrix
- Multi field sheet
- Tabbed pane

- Allow better forms
  - More data rich
  - Less clutter
  - More visual



Form builder improvements

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



Calculated fields

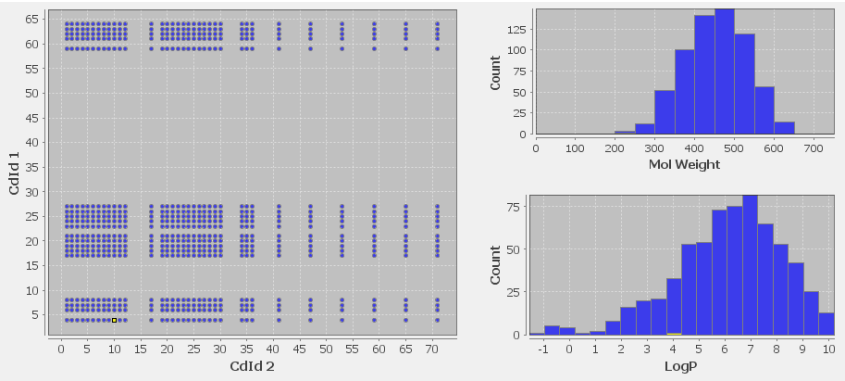
- Calculation is a script
  - Can do something very simple or very complex
  - Field values injected into script for calculation
- Examples
  - Simple “A + B” formulae
  - Aggregate data from related tables
  - Make data from other tables accessible
  - Call out to external services

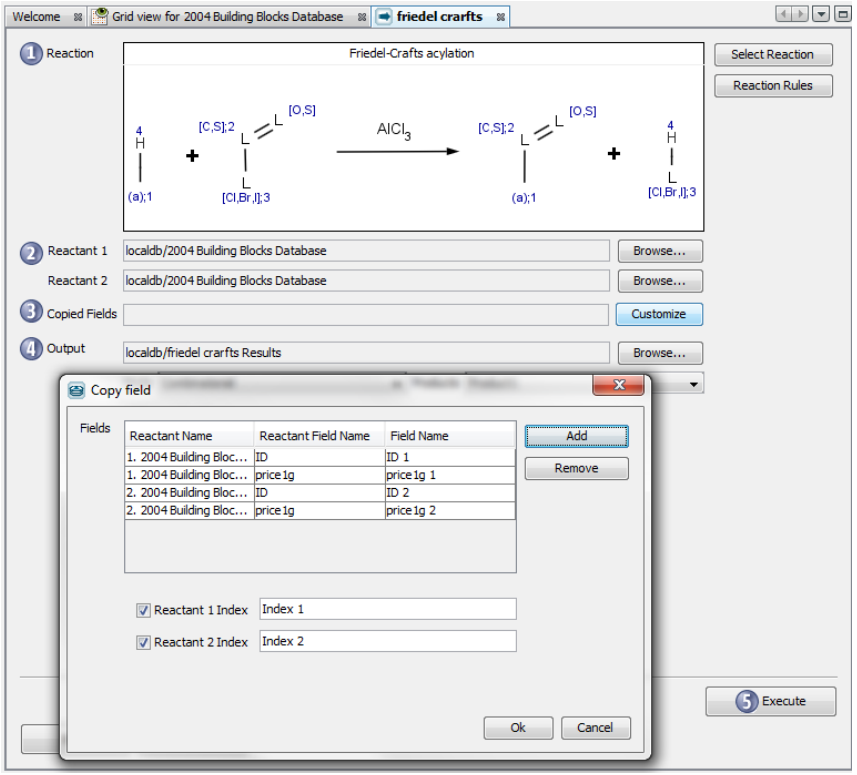
Scripting support

- 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



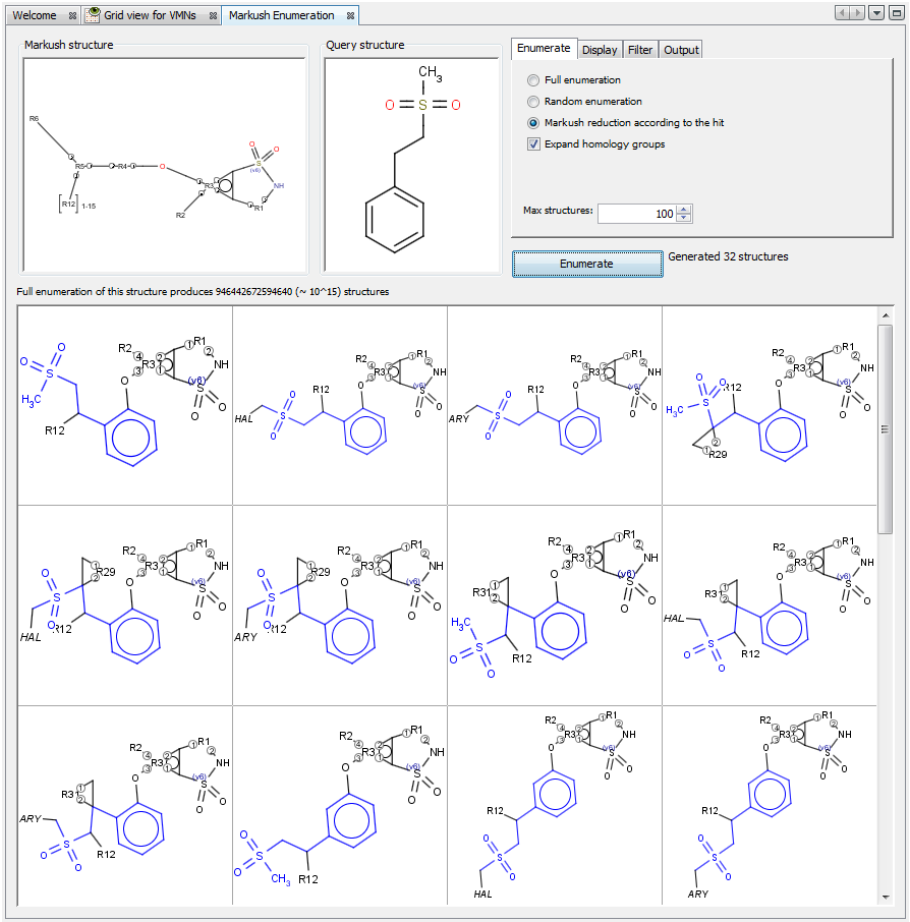


Training

- logP
- General

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