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”

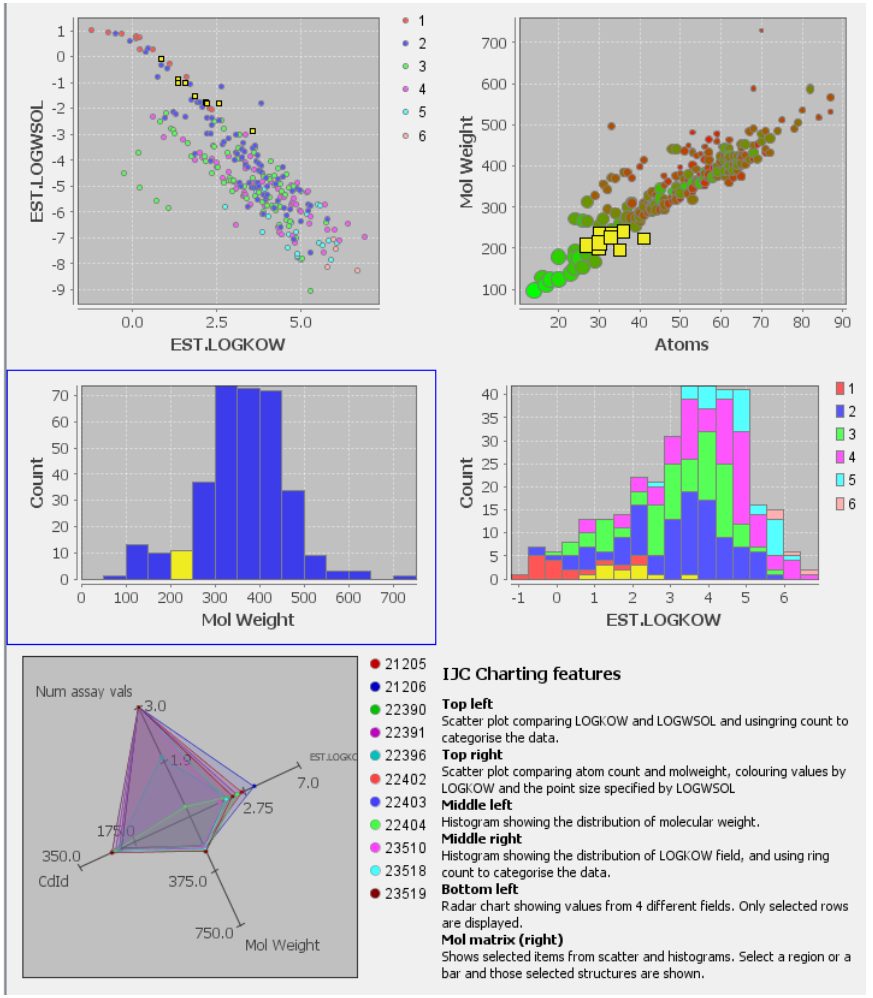
- IJC Visualisation
  - Chart widgets
  - Conditional formatting

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

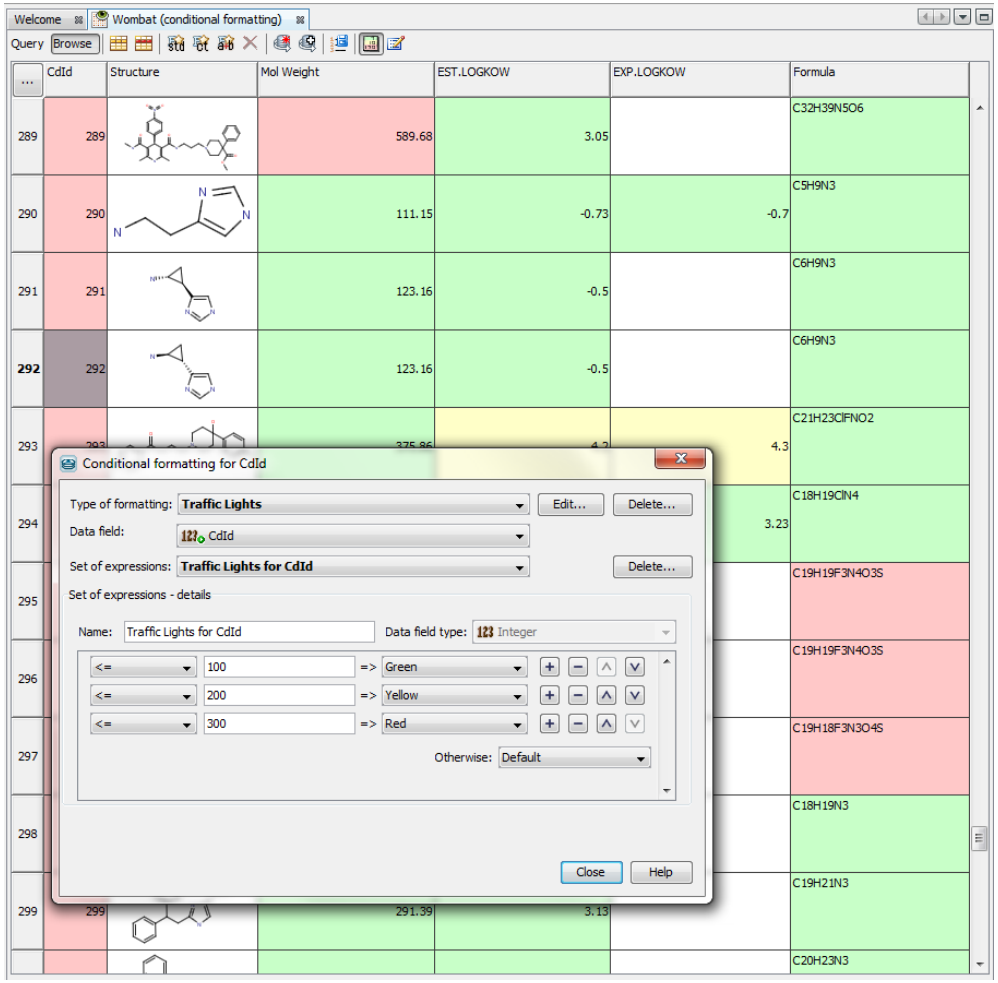
Visualisation widgets (5.4, 5.5, 5.6)

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



Conditional formatting (5.5)

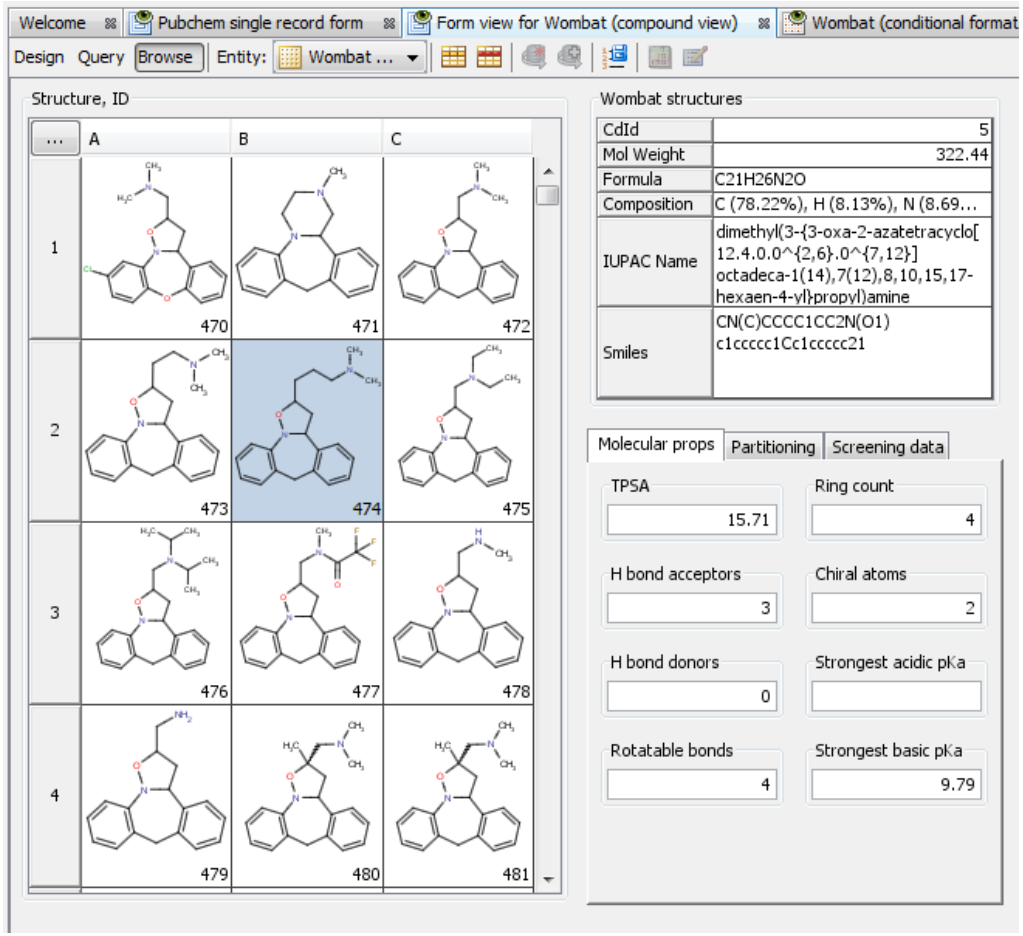
- User defined schemes
- User defined rules
- Templates
- Works for grid and form views



More form widgets (5.5)

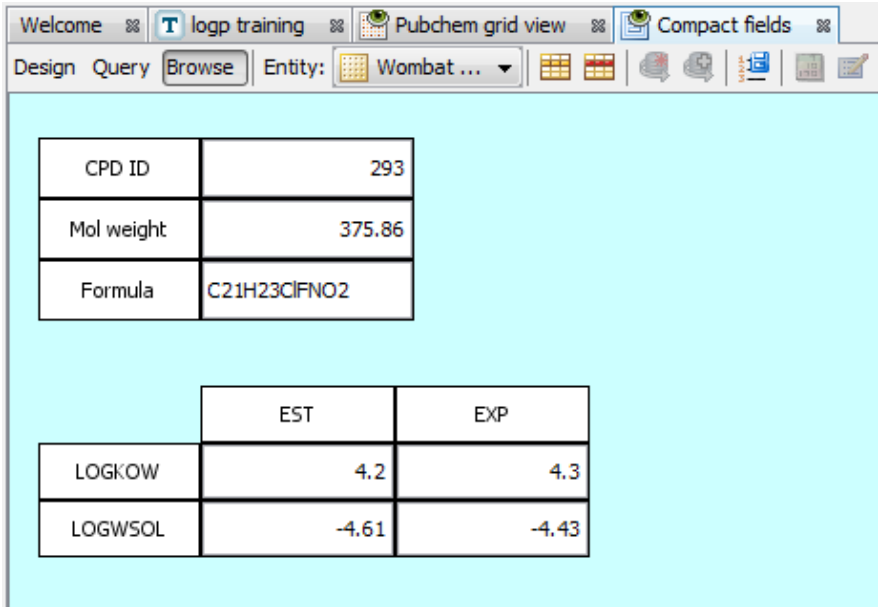
- Structure matrix
- Multi field sheet
- Tabbed pane

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



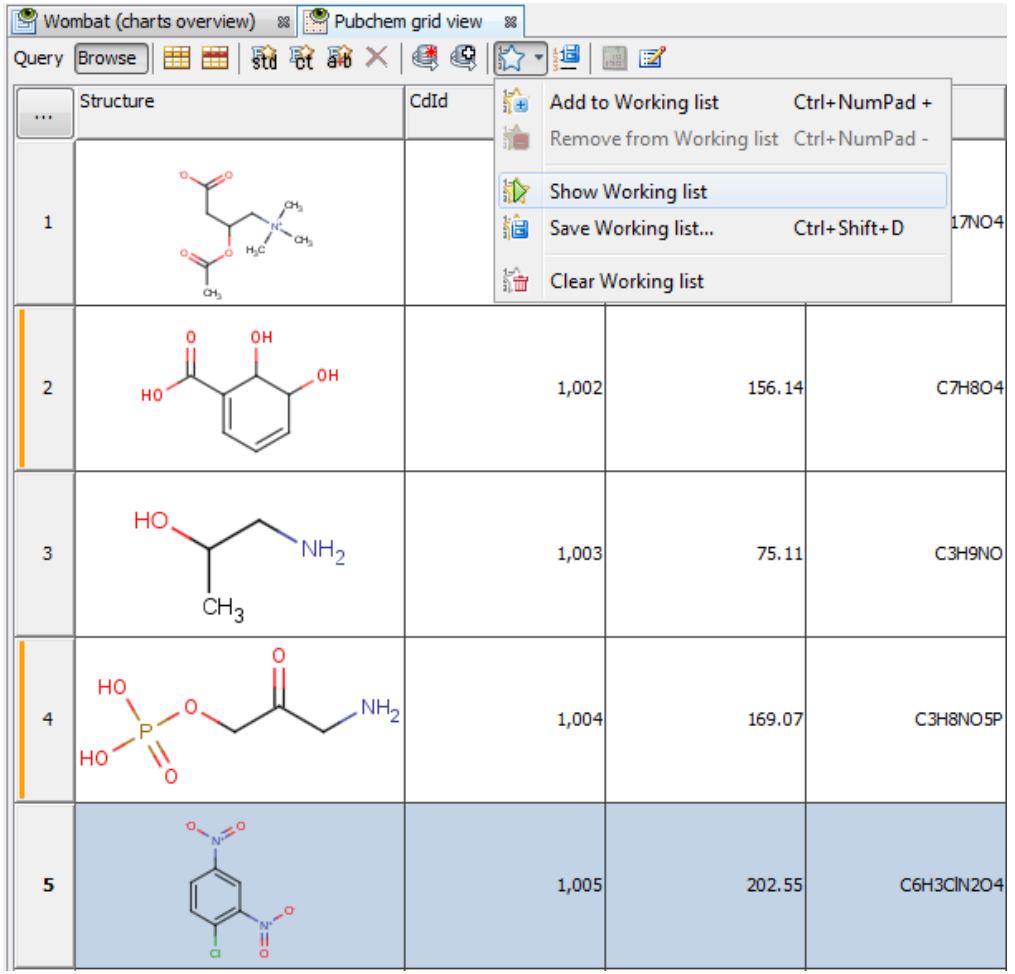
Form builder improvements (5.5)

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



Cherry picking (5.6)

- Much easier approach to building up lists



Calculated fields (5.4)

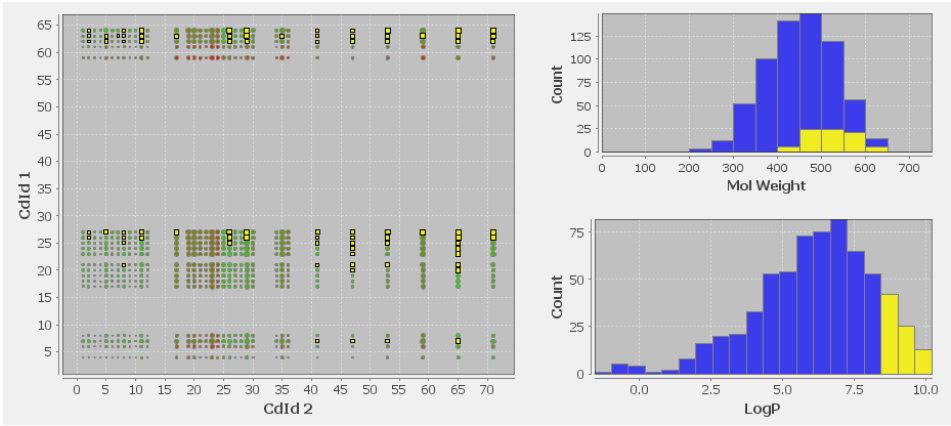
- Calculation is a script
  - Can do something very simple or very complex
  - Field values injected into script for calculation
- Examples
  - Simple “A + B” formulae
  - Aggregate data from related tables
  - Make data from other tables accessible
  - Call out to external services

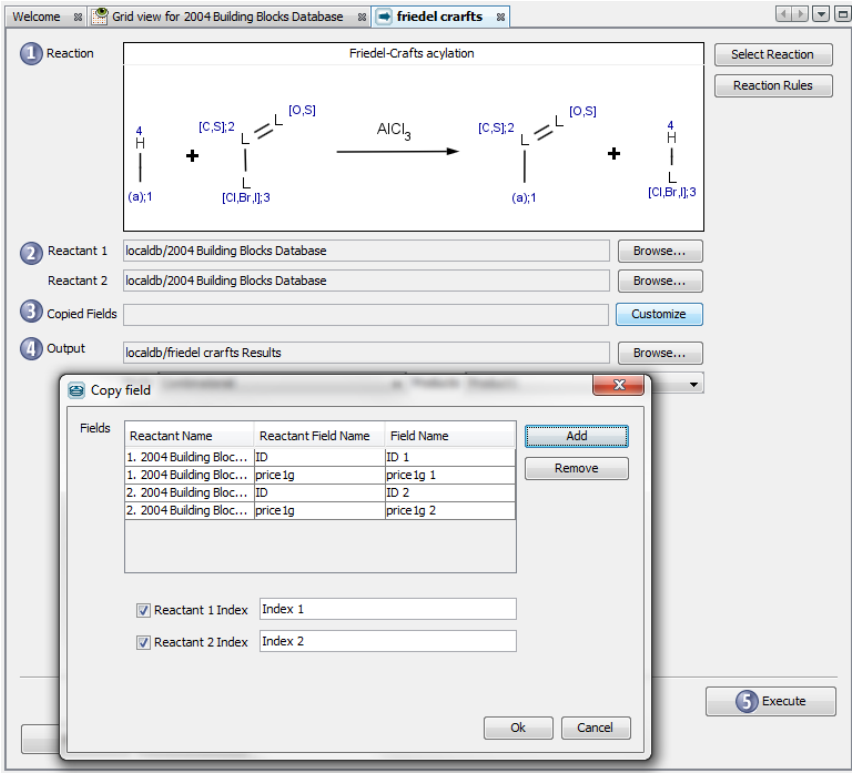
Scripting support (5.4, 5.6, 5.6)

- 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



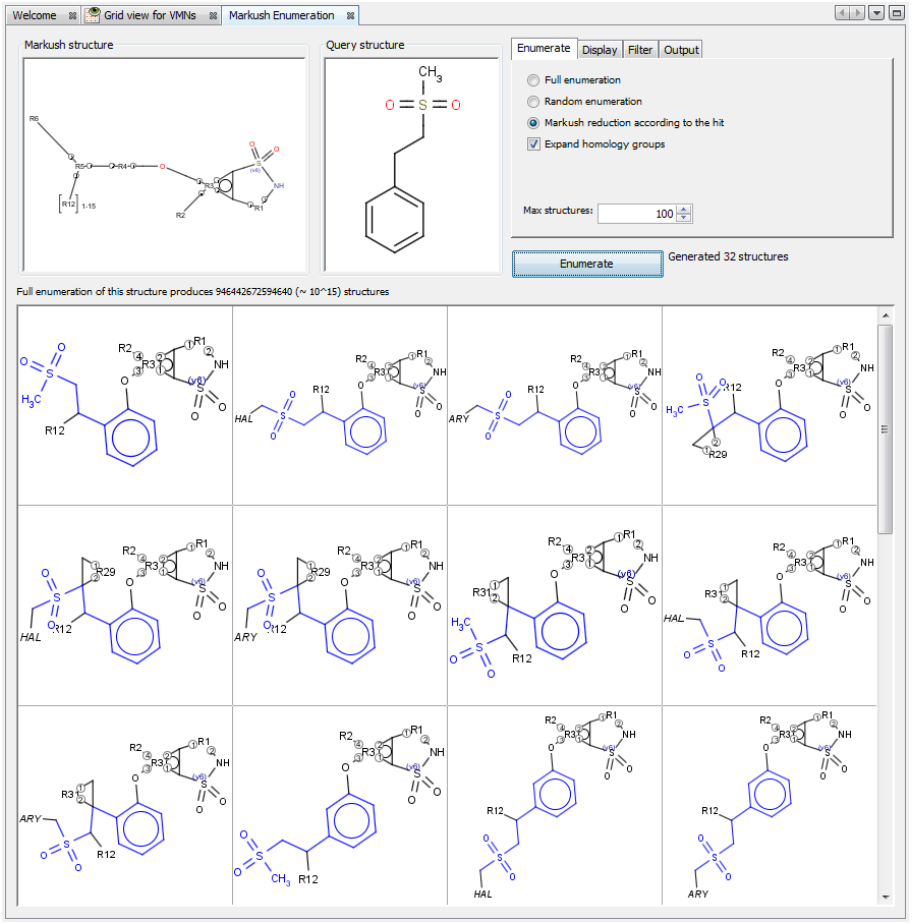


Training (5.4)

- logP
- General

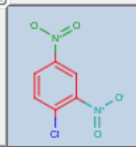
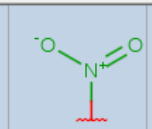
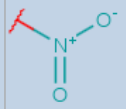
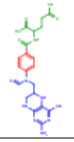
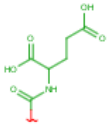
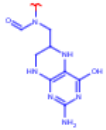
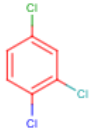
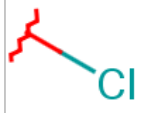
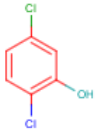
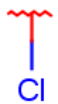
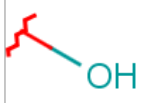
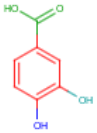
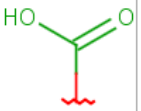
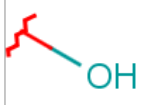
Improved Markush (5.5, 5.6)

- 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

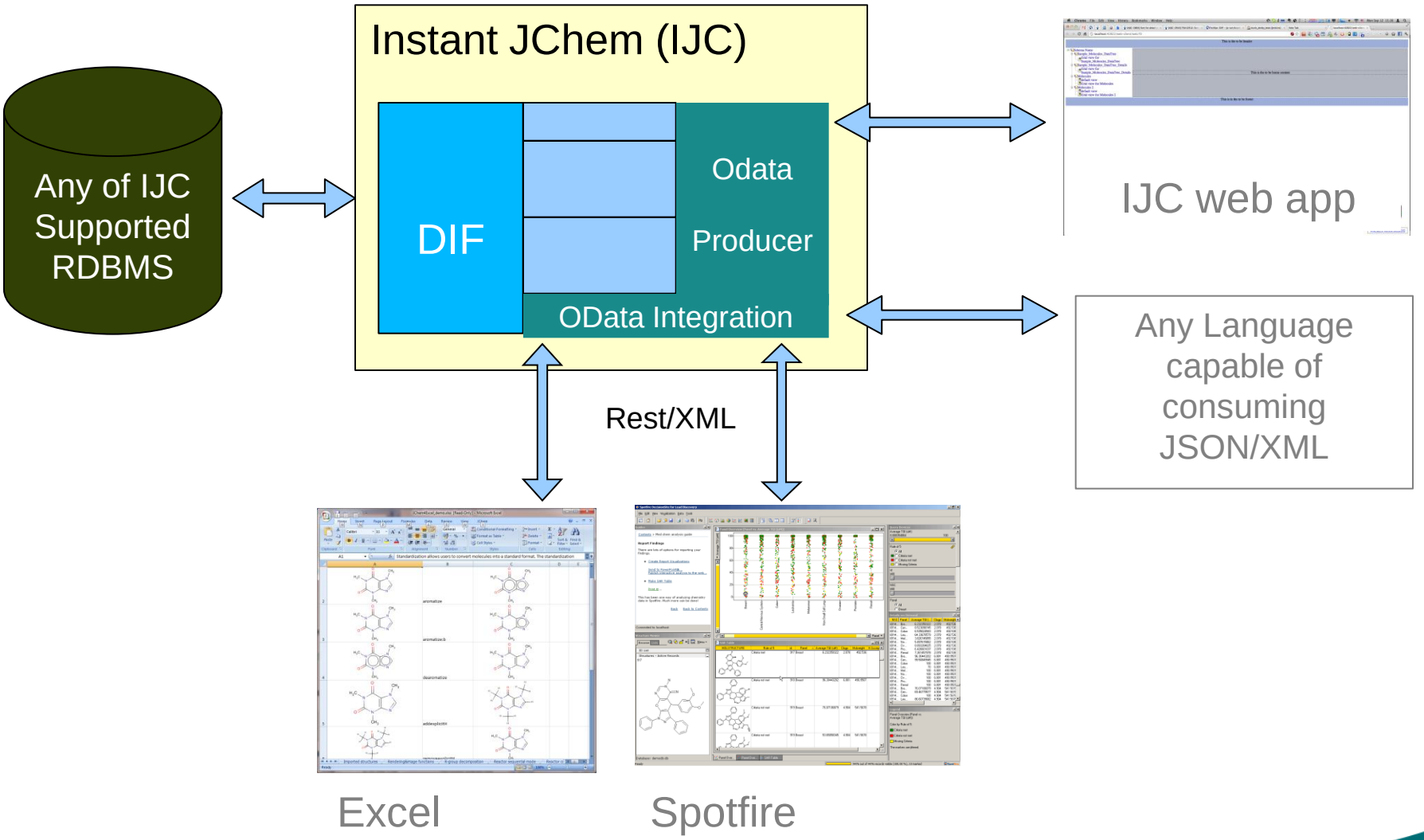
Beyond 5.6 (core)

- 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