Development Directions

and

Core Competencies

[Wolf-D. Ihlenfeldt](#)
Xemistry GmbH
Königstein, Germany
wdi@xemistry.com

The Setting

Pharma IT World Evolves:

- Servers/server farms for applications, running Linux or Solaris
- Desktop PCs for researchers, running WIN XP

Tasks and Problems around the Interface:

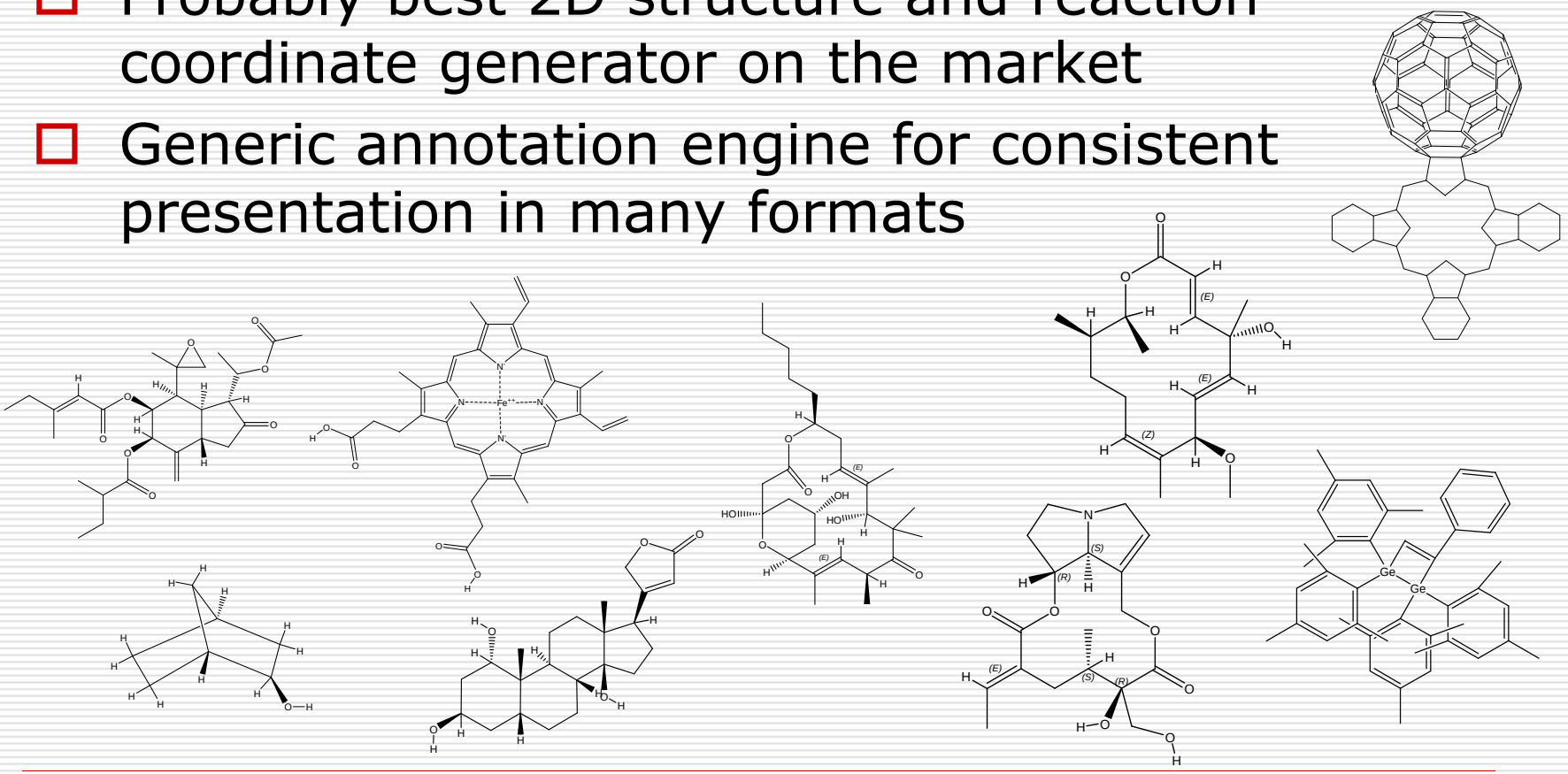
- Submit data – Data conversion technologies
- Display results – Web technologies
- Export results – Cross-platform technologies

Data Conversion Technologies

- Extensive library of I/O modules for structures, reactions and tables, support for standard PC formats (ChemDraw CDX/CDXML, IsisDraw SKC/TGF, Marvin Docs, ChemSketch SK2,..)
- Kekulizer, connectivity generation, tautomer normalizer, 2D layouter, wedge assignment, Harworth/Fischer stereo interpretation, etc.
- Scriptable conversion engine
- Data extraction from Windows OLE objects (in RTF, XLS, DOC/X) and from EMF/WMF images written by ChemDraw/IsisDraw

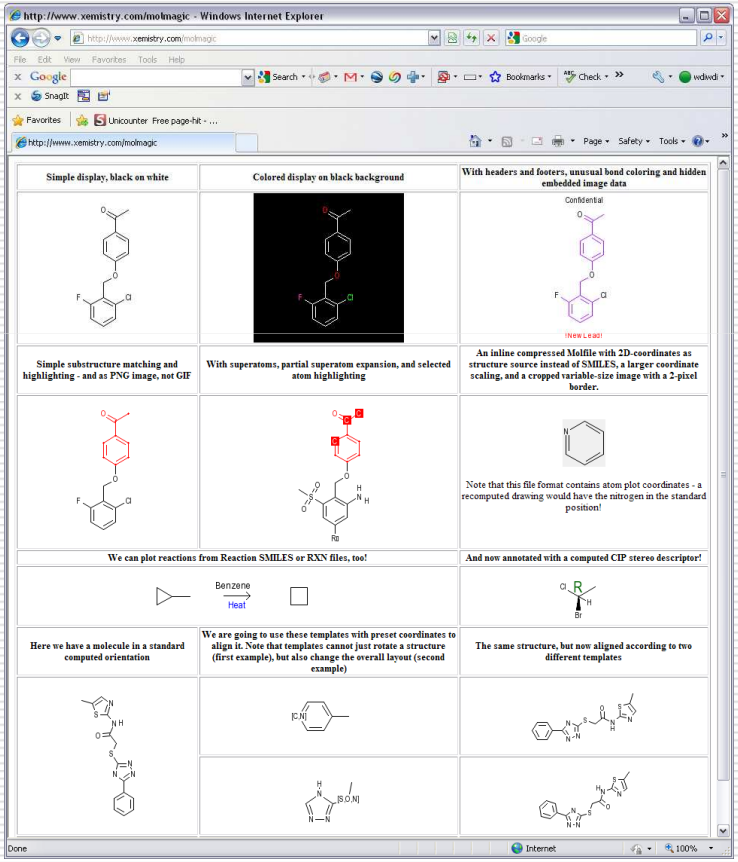
Presentation Technologies

- Probably best 2D structure and reaction coordinate generator on the market
- Generic annotation engine for consistent presentation in many formats



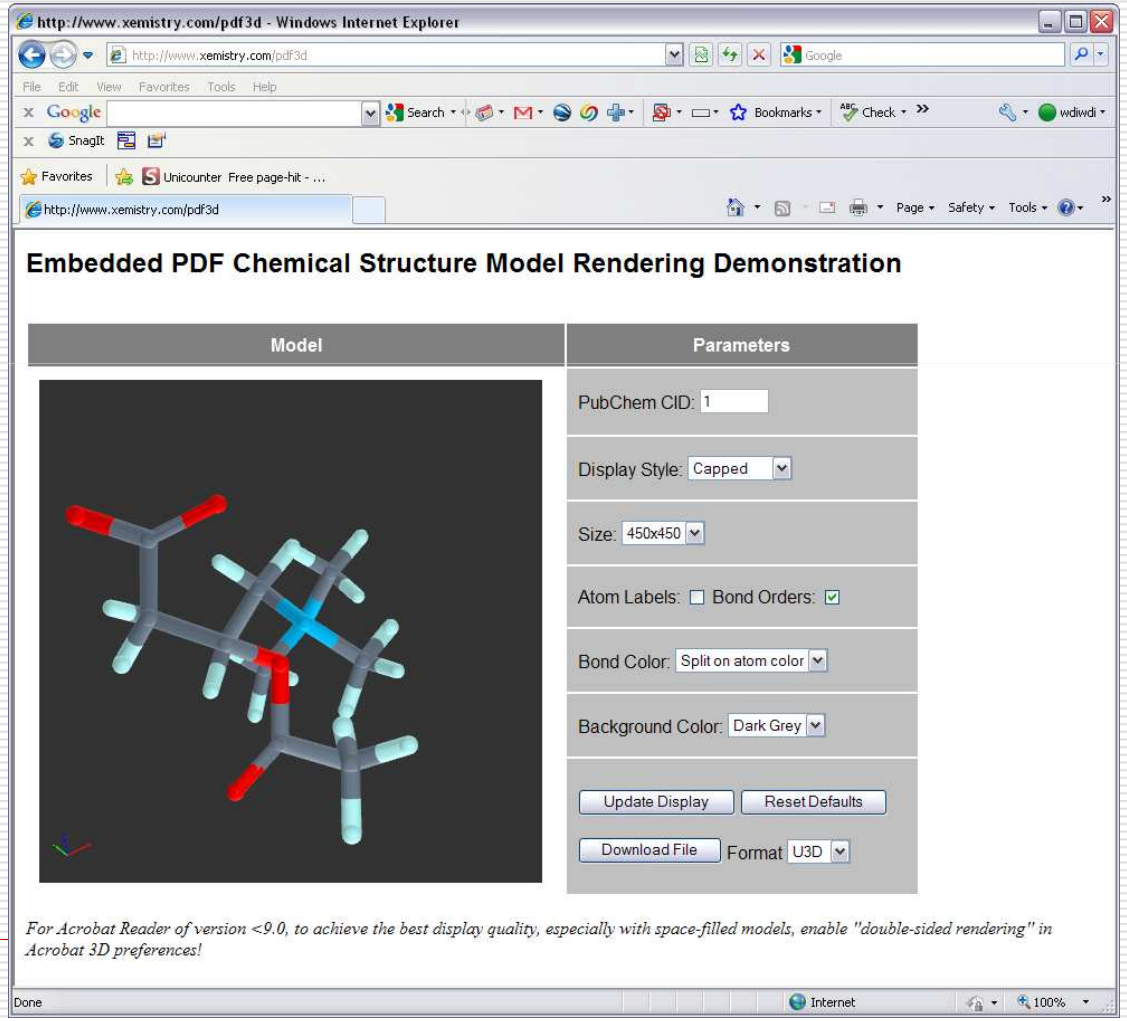
Web Technologies

- GIF/PNG structure image generation as CGI/FCGI Web application designed to link into in-house systems
- PDF and WMF in-place substitution rendering for high-quality Web-page printing
- Animated GIF images, interactive image maps for chemical structures and reactions
- Flash (SWF) and SVG structure drawings



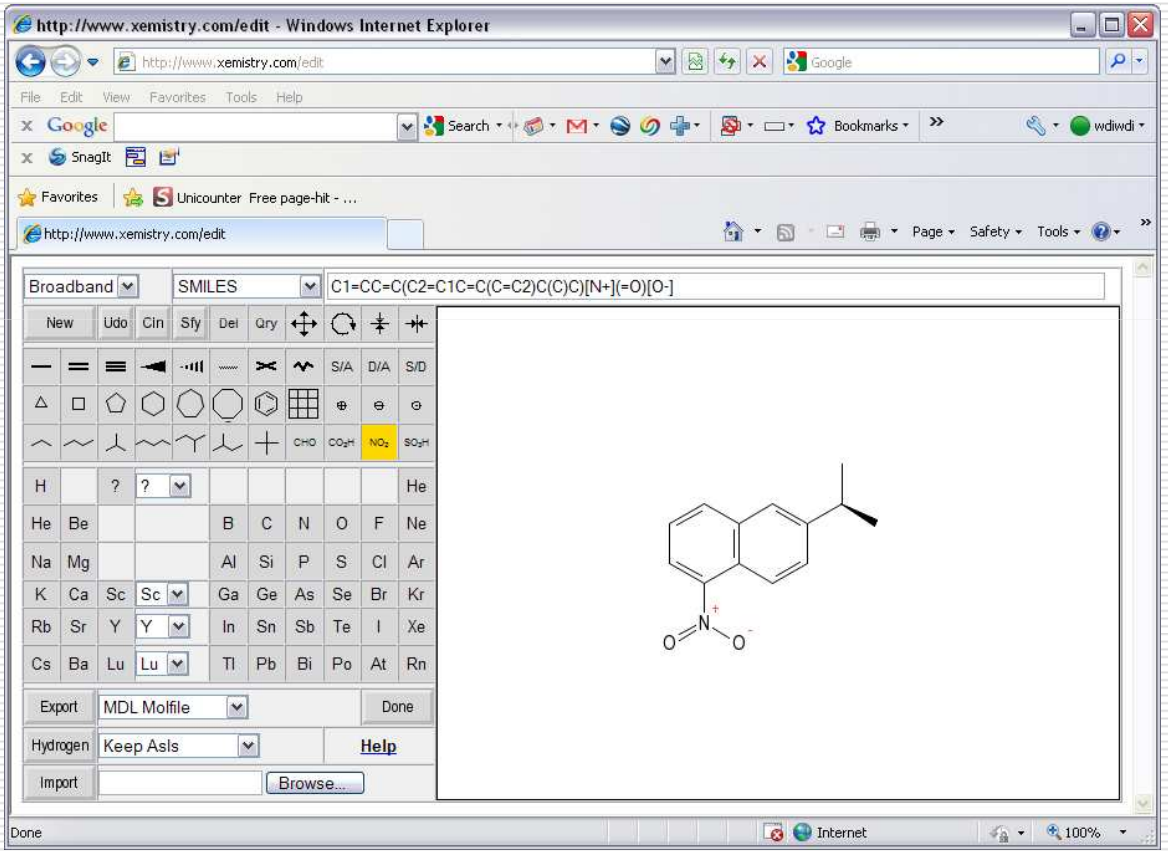
Web Technologies

- 3D portable PDF and VRML rendering for the Web
- 3D PDF rendering for EDocuments



Web Technologies

- Ultra-portable (no Java or Plug-Ins) Web structure sketcher



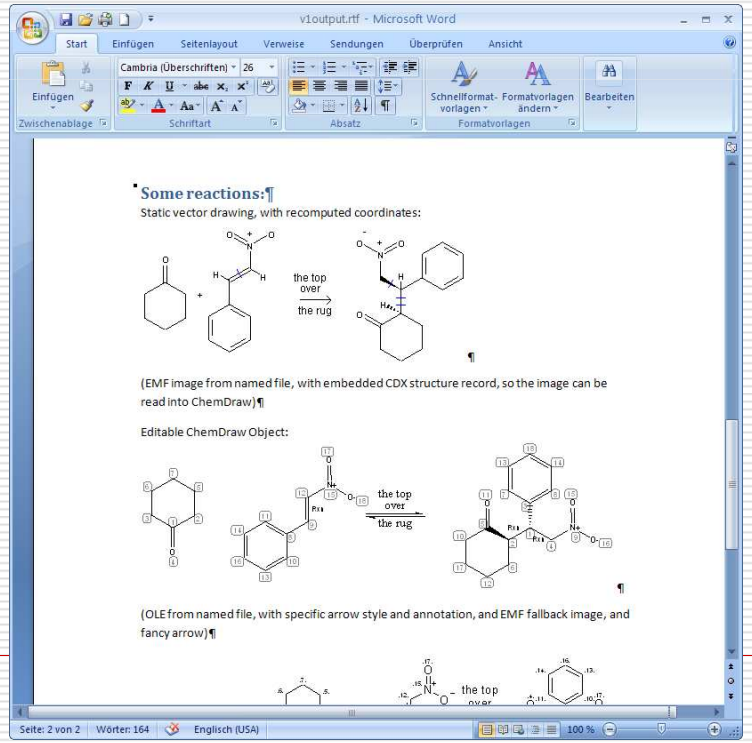
Cross-Platform Technologies

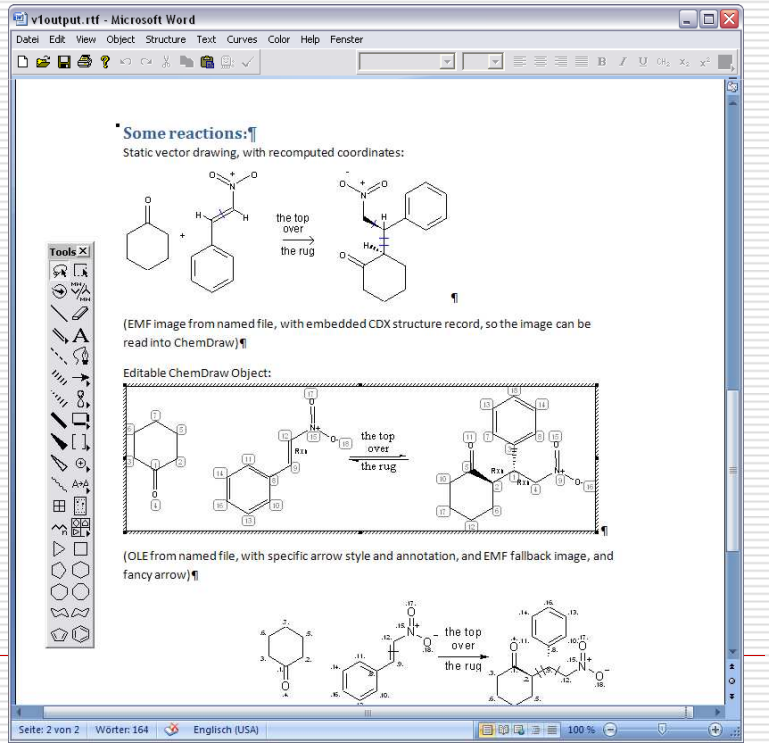
- WMF/EMF/PCT structure and reaction drawings for import/paste into Word/Powerpoint
- Optionally with embedded structure data for re-editing with ISIS/Draw and ChemDraw

- RTF template expansion engine
  - Enter formatted structure and reaction data, links and drawing into template pages…

Cross-Platform Technologies

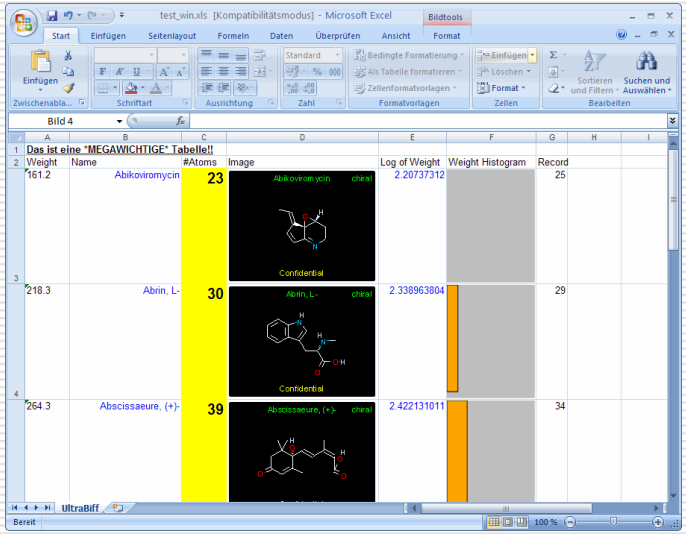
- Expanded structures and reactions can be simple images – or *editable* OLE objects for ISIS/Draw or ChemDraw

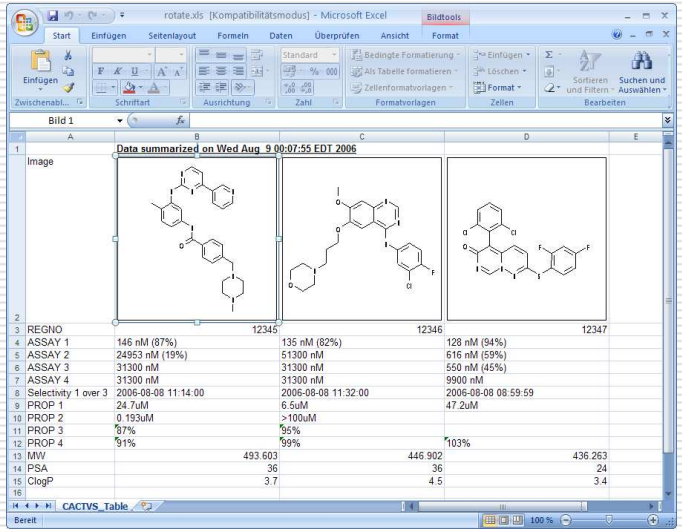




Cross-Platform Technologies

- MS Excel (Windows & Mac versions) table data exporter, with typed cells, embedded structure renderings, programmable layout, data-dependent cell attributes





Universal Chemistry Tables

- Assemble, extract, merge, filter, format tabular data from chemistry and table data files
- Direct access to PubChem assay data
  - Native ASN.1 interface – zero information loss
  - Complete information content, including descriptions, column types
  - Automatic association/download of deposited and standardized PubChem structures

Universal Chemistry Tables

- Native table file I/O of MS Excel (BIFF & XML), Sybyl, SPSS, SAS, Stata, Matlab, WEKA, R – with proper support for data types, NULLs, etc.

- Generic container files - FITS, HDF5, SQLITE
- Legacy data in DIF, SYLK, DBASE3
- Presentation formatting as HTML, PDF
- Internet data exchange as XML, JSON
- SQL database table loader

Universal Chemistry Tables

- Direct platform-independent PDF reporting

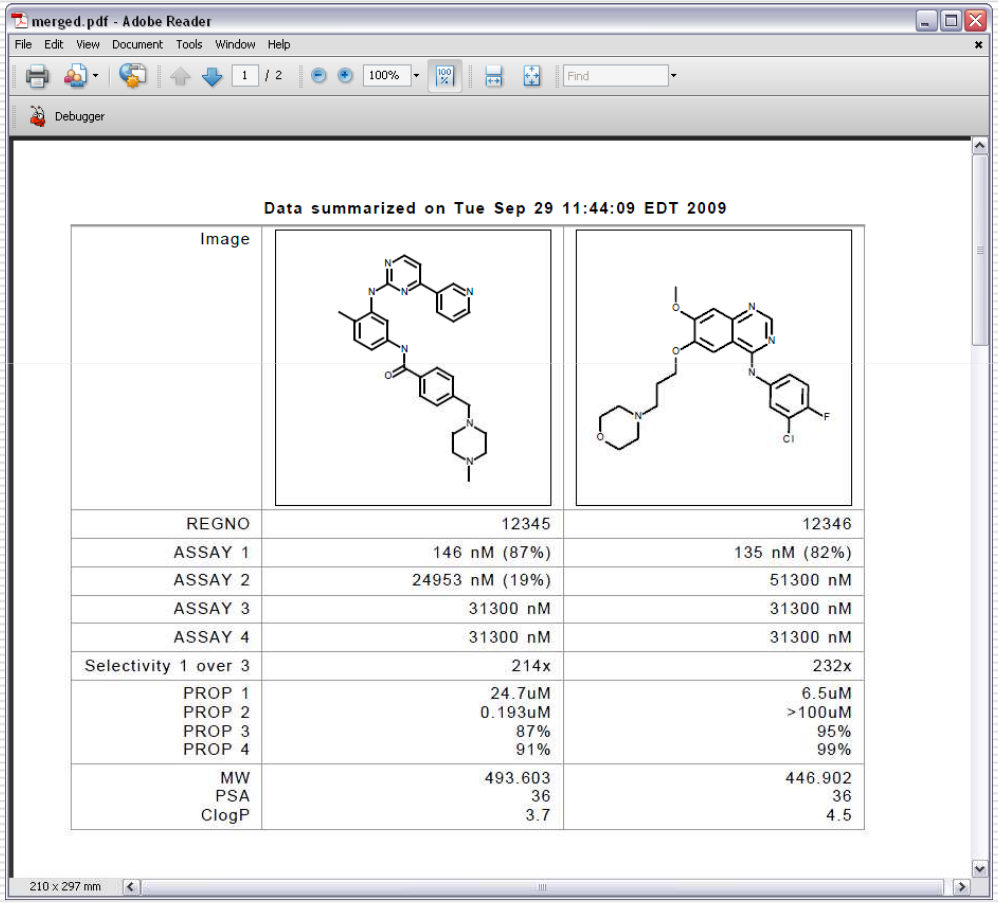


Image		
REGNO	12345	12346
ASSAY 1	146 nM (87%)	135 nM (82%)
ASSAY 2	24953 nM (19%)	51300 nM
ASSAY 3	31300 nM	31300 nM
ASSAY 4	31300 nM	31300 nM
Selectivity 1 over 3	214x	232x
PROP 1 PROP 2 PROP 3 PROP 4	24.7uM 0.193uM 87% 91%	6.5uM >100uM 95% 99%
MW PSA ClogP	493.603 36 3.7	446.902 36 4.5

Final Slide

Xemistry chemoinformatics

- Turnkey applications and scriptable tools
- Custom development
- Component licensing (in-house & software vendors)
- Consulting
- Visit our booth!
- Talk to us!

www.xemistry.com
info@xemistry.com