

# Development Directions

and

# Core Competencies

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# The Setting

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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
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# Data Conversion Technologies

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- ❑ 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
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# 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

The screenshot shows a Windows Internet Explorer browser window displaying the URL <http://www.xemistry.com/molmagic>. The page content is organized into a grid of options and examples:

- Simple display, black on white:** Shows a chemical structure of a substituted benzene ring.
- Colored display on black background:** Shows the same chemical structure with a black background.
- With headers and footers, unusual bond coloring and hidden embedded image data:** Shows the structure with additional styling and a "Confidential" watermark.
- Simple substructure matching and highlighting - and as PNG image, not GIF:** Shows the structure with red highlighting on specific atoms.
- With superatoms, partial superatom expansion, and selected atom highlighting:** Shows the structure with red boxes around specific atoms.
- An inline compressed Molfile with 2D-coordinates as structure source instead of SMILES, a larger coordinate scaling, and a cropped variable-size image with a 2-pixel border:** Shows a smaller version of the structure.
- Note that this file format contains atom plot coordinates - a recomputed drawing would have the nitrogen in the standard position!**
- We can plot reactions from Reaction SMILES or RXN files, too!**: Shows a reaction of Benzene reacting with Heat to form a square.
- And now annotated with a computed CIP stereo descriptor!:** Shows a chiral center with a CIP descriptor.
- Here we have a molecule in a standard computed orientation:** Shows a complex organic molecule.
- We are going to use these templates with preset coordinates to align it. Note that templates cannot just rotate a structure (first example), but also change the overall layout (second example):** Shows two different orientations of the same molecule.
- The same structure, but now aligned according to two different templates:** Shows the molecule aligned to different templates.

# Web Technologies

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

http://www.xemistry.com/pdf3d - Windows Internet Explorer

http://www.xemistry.com/pdf3d

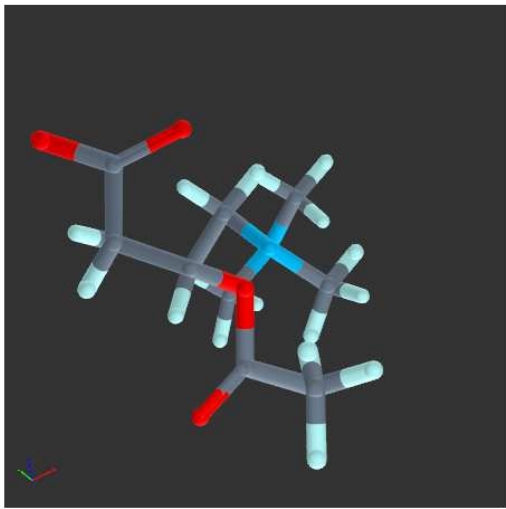
File Edit View Favorites Tools Help

Google Search

Favorites Unicorner Free page-hit - ...

http://www.xemistry.com/pdf3d

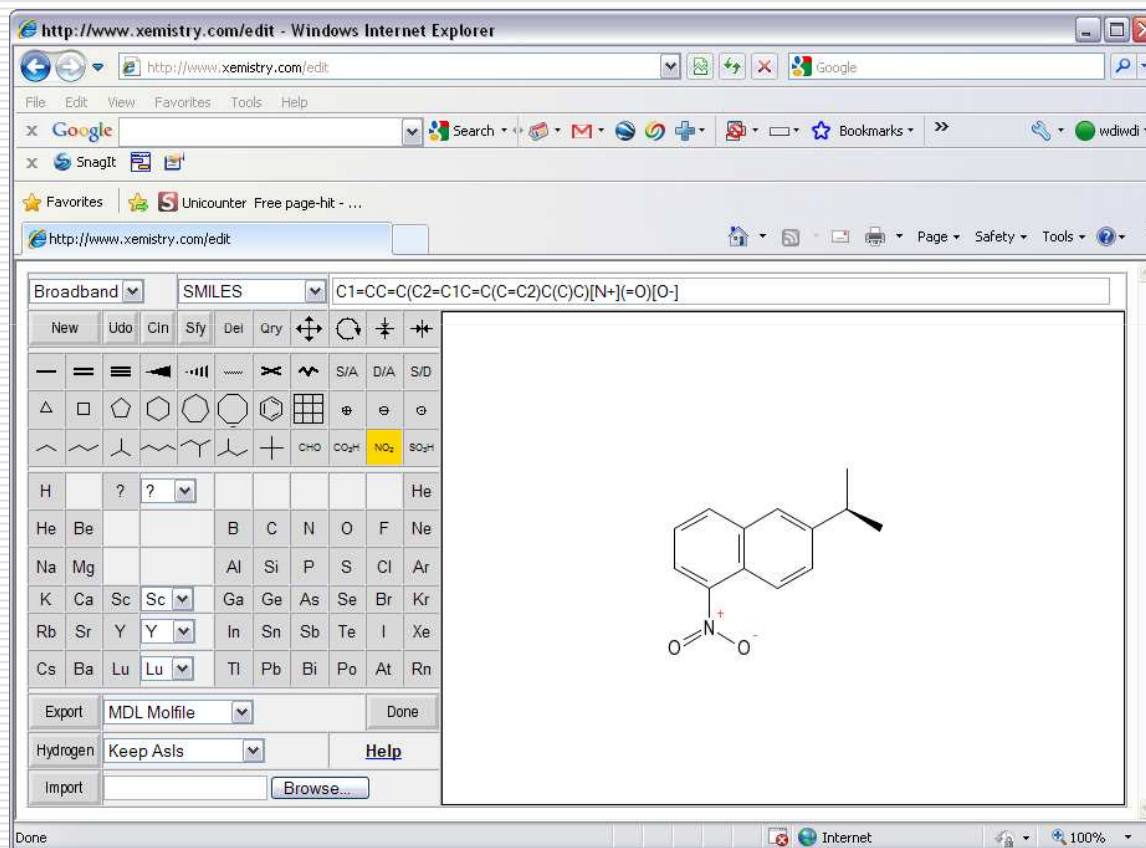
### Embedded PDF Chemical Structure Model Rendering Demonstration

Model	Parameters	
	PubChem CID: <input type="text" value="1"/>	
	Display Style: <input type="text" value="Capped"/>	
	Size: <input type="text" value="450x450"/>	
	Atom Labels: <input type="checkbox"/> Bond Orders: <input checked="" type="checkbox"/>	
	Bond Color: <input type="text" value="Split on atom color"/>	
	Background Color: <input type="text" value="Dark Grey"/>	
	<input type="button" value="Update Display"/> <input type="button" value="Reset Defaults"/>	
	<input type="button" value="Download File"/> <input type="text" value="Format U3D"/>	
	<p><i>For Acrobat Reader of version &lt;9.0, to achieve the best display quality, especially with space-filled models, enable "double-sided rendering" in Acrobat 3D preferences!</i></p>	
	Done	

# Web Technologies

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



# Cross-Platform Technologies

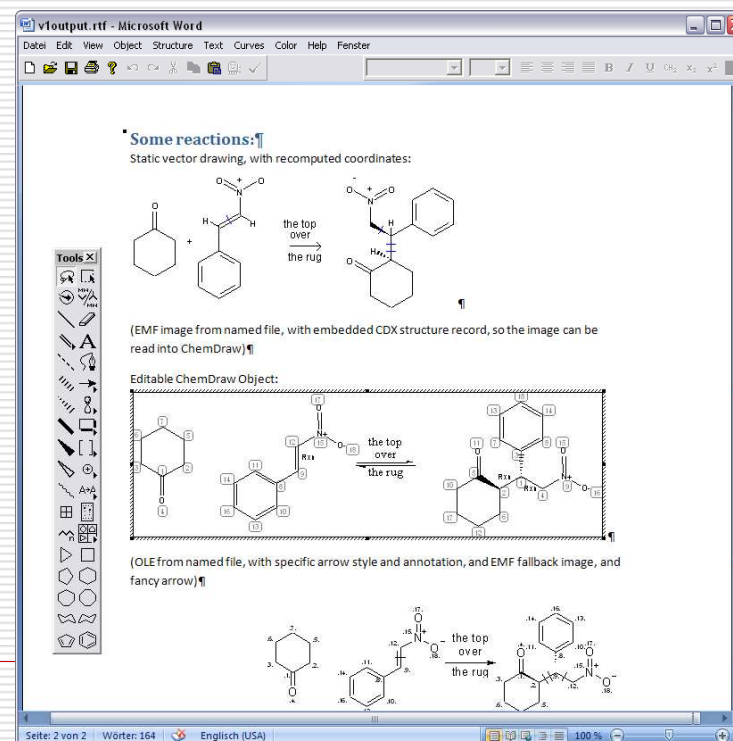
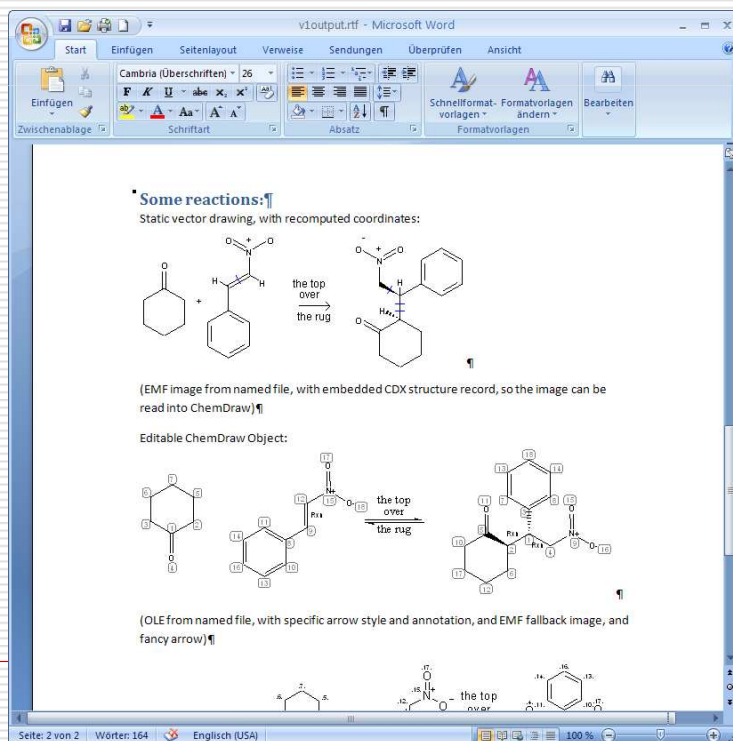
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- WMF/EMF/PCT structure and reaction drawings for import/paste into Word/Powerpoint
  - Optionally with embedded structure data for re-editing with ISIS/Draw and ChemDraw
  
  - RTF template expansion engine
    - Enter formatted structure and reaction data, links and drawing into template pages...
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# Cross-Platform Technologies

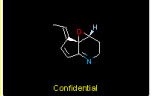

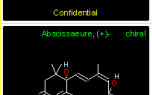
- Expanded structures and reactions can be simple images – or *editable* OLE objects for ISIS/Draw or ChemDraw



# Cross-Platform Technologies

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

Das ist eine "MEGAWICHTIGE" Tabelle!!

Weight	Name	#Atoms	Image	Log of Weight	Weight Histogram	Record
161.2	Abikovromycin	23		2.20737312		25
218.3	Abim, L.	30		2.338963804		29
264.3	Abcissaure, (+)	39		2.422131011		34

Data summarized on Wed Aug 9 00:07:55 EDT 2006

REGNO	12345	12346	12347
ASSAY 1	146 nM (87%)	135 nM (82%)	128 nM (94%)
ASSAY 2	24953 nM (19%)	51300 nM	616 nM (59%)
ASSAY 3	31300 nM	31300 nM	550 nM (45%)
ASSAY 4	31300 nM	31300 nM	9900 nM
Selectivity 1 over 3	2006-08-08 11:14:00	2006-08-08 11:32:00	2006-08-08 08:59:59
PROP 1	24.7uM	6.5uM	47.2uM
PROP 2	0.193uM	>100uM	
PROP 3	97%	96%	
PROP 4	91%	99%	103%
MW	493.603	446.902	436.263
PSA	36	36	24
ClogP	3.7	4.5	3.4

# Universal Chemistry Tables

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- ❑ 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
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# Universal Chemistry Tables

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- ❑ 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
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# Universal Chemistry Tables

- Direct platform-independent PDF reporting

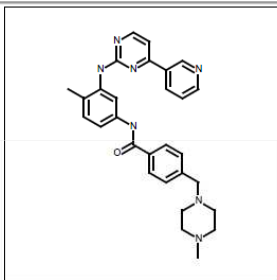
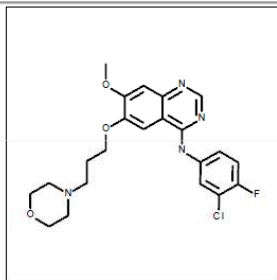
merged.pdf - Adobe Reader

File Edit View Document Tools Window Help

1 / 2 100% Find

Debugger

Data summarized on Tue Sep 29 11:44:09 EDT 2009

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	24.7uM	6.5uM
PROP 2	0.193uM	>100uM
PROP 3	87%	95%
PROP 4	91%	99%
MW	493.603	446.902
PSA	36	36
ClogP	3.7	4.5

210 x 297 mm

# Final Slide

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

[www.xemistry.com](http://www.xemistry.com)  
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