

# MDL<sup>®</sup> ISIS for Excel

*MDL ISIS for Excel is a spreadsheet-based application that enables scientists to visualize and analyze chemical structures, properties, and associated biological data, search local and remote databases, import data from other applications, and create reports.*

The screenshot displays the MDL ISIS for Excel application within a Microsoft Excel spreadsheet. The spreadsheet has columns for ID, Structure, R1, R2, R3, mol weight, Structure, Compound name, and E950. Rows 1 through 9 contain chemical structures and their corresponding data. A search dialog box is open, showing search criteria for 'Chem-3' and 'Tosparyl'. The dialog box includes fields for 'Field name', 'Field type', 'Condition', and 'Structure', and a preview window showing a chemical structure.

ID	Structure	R1	R2	R3	mol weight	Structure	Compound name	E950
000101					214.10215		1,4-Dimethyl-2-[[carbamoyloxy(methyl)-5-nitroimidazole	1
000102					235.21865		1,4-Dimethyl-2-(4-Bucophenyl)-5-nitroimidazole	10
000103								21.0
000104								
000105								
000106								
000107								
000108								

*MDL ISIS for Excel presents searching options and can store queries. Users can then select which of the available fields to retrieve and display in the spreadsheet.*

*An example of this is shown for Rgroup substituents for a core structure, which is shown color-highlighted in the "structure" field.*

## Enhanced performance and features

MDL ISIS for Excel offers a number of powerful features to assist the discovery workflow. You can quickly import and retrieve structures and data and manipulate them in the spreadsheet. Expanded capacity makes it easy to work with large libraries and data files. You can share spreadsheets with colleagues who have Microsoft® Excel but do not have the MDL ISIS for Excel add-in and present your results in other Microsoft Office tools by simply pasting structures and data.

## Outstanding flexibility

Functional components within MDL ISIS for Excel allow easy customization to suit your organization's unique workflow. Companies can even assemble new applications by accessing core functionality, including dialog objects like search and retrieve, through Visual Basic for Applications (VBA). For instance, a company can tailor a reporting tool to run repetitive tasks, store queries, and filter structures by criteria such as molecular weight.



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Powering  
the Process  
of Invention™

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#### About MDL

Over 1,000 life science companies supercharge their discovery engines with MDL software solutions to generate fresh ideas and make breakthrough discoveries. By synchronizing and streamlining the sharing and management of vital information and knowledge, we enable scientists to work more efficiently and invent drugs faster. This saves time, money, and lives. In support of our customers and the momentous challenges they face, everything we do must be reliable, resourceful, innovative, and insightful.

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COMPOUND ID	MOLSTRUCTURE	empiric formula	empiric molweight	rotatable bonds	XLogP	HTS PKCA VALUE	HTS EGFR VALUE	HTS CBRA VALUE	IC50 PKCA VALUE
5815 OTSM496-05874	<chem>C1=CC=C(C=C1)C(=O)N</chem>	C14H18N2O2	248.31	6	3.1	125	110.04	76.95	
5812 OTSM496-05875	<chem>C1=CC=C(C=C1)N</chem>	C10H14N2O	206.3	6	3.09	90.22	104.75	67.39	
5818 OTSM496-05876	<chem>C1=CC=C(C=C1)C(=O)N</chem>		313.42	1					
5813 OTSM496-05877	<chem>C1=CC=C(C=C1)C(=O)N</chem>		167.18	7					
5820 OTSM496-05878	<chem>C1=CC=C(C=C1)C(=O)N</chem>	C23H26N4O4		6	3.31	93.36	100.31	70.86	

MDL ISIS for Excel uses standard Microsoft Excel features for arranging and organizing data. A pop-up calculator lets you determine molecular values (such as molecular weight) for individual structures, and the spreadsheet makes it easy to visualize, analyze, and report SAR (structure-activity relationship) trends. The spreadsheet in this illustration contains more than 5,000 structures.

#### Familiar features

MDL ISIS for Excel enables scientists to easily visualize chemical structures and associated biological data. With MDL ISIS for Excel, scientists can:

- Import structures and data from various sources
- Search local and remote MDL<sup>®</sup> ISIS and Oracle<sup>®</sup> databases
- Pivot data and manipulate lists
- Perform MDL ISIS structure-based searches
- Explore structure-activity relationships
- Conduct Rgroup analyses
- Communicate and share results in a variety of formats

#### Part of an integrated solution

MDL ISIS for Excel offers off-the-shelf compatibility and interoperability advantages not available in competing Microsoft Excel-based applications. By integrating with widely used MDL software, scientists can expedite information access while ensuring data integrity. MDL ISIS for Excel is part of a complete experiment management solution from MDL that spans activities from synthesis planning to biological testing. Throughout the discovery process, MDL ISIS for Excel provides scientists with intuitive means to visualize, analyze, and report on experimental data.