# EMPOWER 3 SOFTWARE CHEMICAL STRUCTURES OPTION

## USING CHEMICAL STRUCTURES IN EMPOWER 3 SOFTWARE

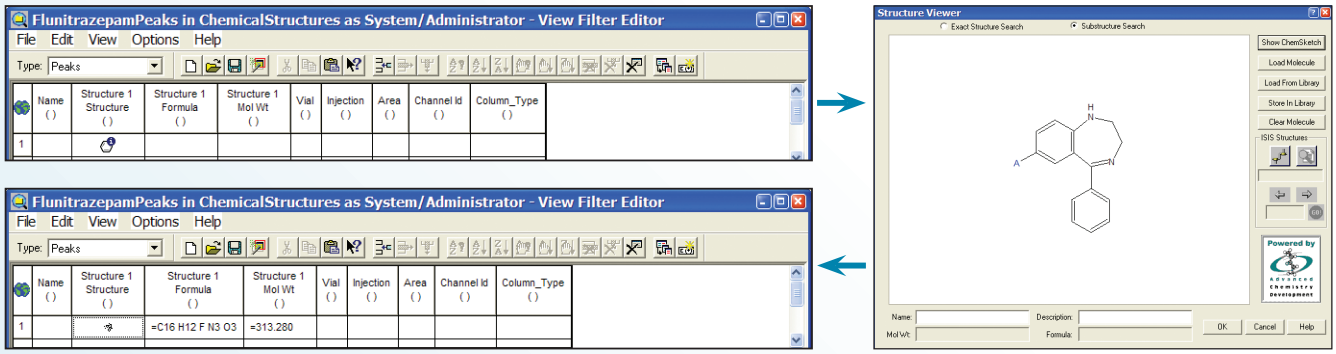
The Chemical Structures Option available with Waters® Empower™ 3 Software allows you to display chemical structures on your chromatograms and spectra as well as print structural information on reports. This option also enables you to effectively search for structural information. Waters is the only chromatography data software (CDS) supplier that provides these capabilities. Through a partnership with ACD Labs, Waters has embedded the ACD Labs ChemSketch structure drawing software directly into Empower 3 Software so that you can create chemical structures without ever having to exit the application.

### Searching by chemical structures

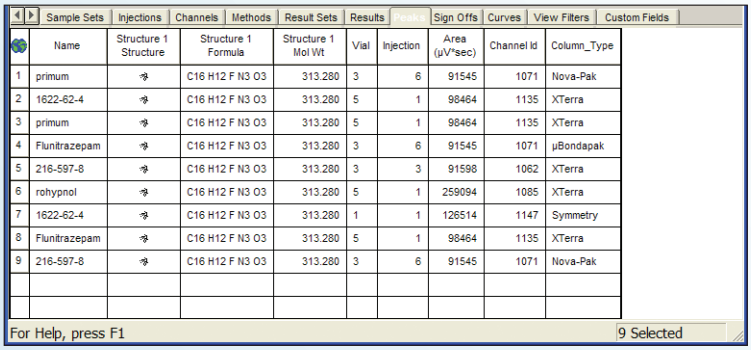
The vast array of naming conventions makes searching for data using a structure much more effective than searching by a compound name. Naming chemical entities can be tricky. Interpreting names of chemical entities can be even trickier. A given chemical entity may have many "correct" names. CAS, IUPAC, EINECS and registry numbers, as well as common names, are frequently used for identification. In some cases, it is difficult to represent a chemical entity with a text string. Take ibuprofen as an example: its CAS number is 15687-27-1 while its EINECS number is 239-784-6. Your lab may refer to a compound differently than another laboratory down the hall, simply based on personal preferences.

Given the wide variety of legitimate names, searching for data using "correct" names may not retrieve any, or all, of the desired data. Searching with structural information gives you assurance that the search results are accurate and complete.

*In the View Filter Editor, clicking on the structure icon opens the Structure Viewer.*




*The Structure Viewer allows you to select the structure on which to search.*




*The search results are displayed in the Project Window. Although the names of the structures vary, all data matching the specified structure is retrieved. Specifying your structural search criteria in a View Filter allows you to search the Empower Database for structural information and retrieve the desired data regardless of which naming convention was used.*

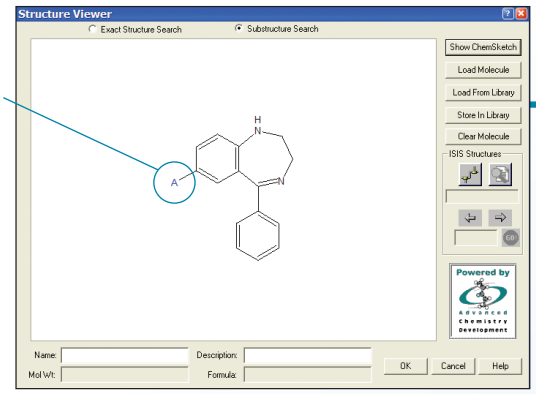
# [PRODUCT SOLUTION]

The ability to integrate structural information with chromatograms into a database offers exciting benefits to the chromatographer. A database of successful separations linked to chemical structures is a valuable tool for choosing columns, separation conditions and even types of chromatography. It is an ideal solution where a chromatographer needs to quickly determine appropriate conditions for the separation of specific chemical structure classes. Substructure searches allow you to retrieve related compounds. You can then view acquisition conditions and use these parameters as a starting point in your own method development.

- Selecting conditions based on previously studied compounds reduces method development time.
- Past projects can become a part of the method development process.
- Legacy data is available as an experimental design tool, both in Empower 3 Software and by using links to method development software.
- Structures and retention times can be utilized by chromatographic prediction tools such as ACD/LC Simulator.
- Expected retention times for new compounds can be predicted by using physicochemical properties such as pKa, LogP and LogD.

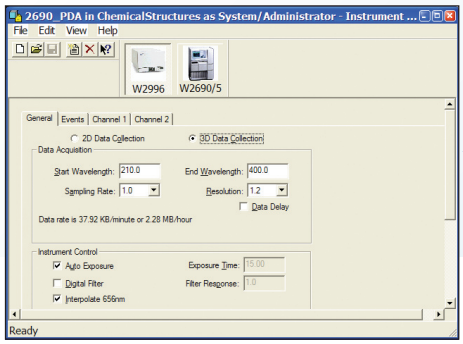
**Substructure searching allows you to retrieve information on related compounds for use in method development**

*Wildcards such as 'A' (any functional group) allow retrieval of related compounds.*




*Substructure searching allows you to retrieve related compounds.*

| | Name | Structure 1 Structure | Structure 1 Formula | Structure 1 Mol Wt | Vial | Injection | Area (µV*sec) | Channel Id | Column_Type |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Alprazolam | | C17 H13 Cl N4 | 308.760 | 3 | 6 | 9552 | 1071 | Nova-Pak |
| 2 | primum | | C16 H12 F N3 O3 | 313.280 | 3 | 6 | 91545 | 1071 | Nova-Pak |
| 3 | 1622-62-4 | | C16 H12 F N3 O3 | 313.280 | 5 | 1 | 98464 | 1135 | XTerra |
| 4 | primum | | C16 H12 F N3 O3 | 313.280 | 5 | 1 | 98464 | 1135 | XTerra |
| 5 | Alprazolam | | C17 H13 Cl N4 | 308.760 | 3 | 6 | 9552 | 1071 | µBondapak |
| 6 | Flunitrazepam | | C16 H12 F N3 O3 | 313.280 | 3 | 6 | 91545 | 1071 | µBondapak |
| 7 | Alprazolam | | C17 H13 Cl N4 | 308.760 | 3 | 3 | 9476 | 1062 | XTerra |
| 8 | 216-597-8 | | C16 H12 F N3 O3 | 313.280 | 3 | 3 | 91598 | 1062 | XTerra |
| 9 | rohypnol | | C16 H12 F N3 O3 | 313.280 | 5 | 1 | 259094 | 1085 | XTerra |
| 10 | 1622-62-4 | | C16 H12 F N3 O3 | 313.280 | 1 | 1 | 126514 | 1147 | Symmetry |
| 11 | Flunitrazepam | | C16 H12 F N3 O3 | 313.280 | 5 | 1 | 98464 | 1135 | XTerra |
| 12 | Alprazolam | | C17 H13 Cl N4 | 308.760 | 3 | 6 | 9552 | 1071 | Nova-Pak |
| 13 | 216-597-8 | | C16 H12 F N3 O3 | 313.280 | 3 | 6 | 91545 | 1071 | Nova-Pak |




*Column information and separation conditions for related compounds can then be used in method development.*

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™




**Waters Corporation**
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com