

# Concord<sup>®</sup>

GENERATE ACCURATE 3D COORDINATES


**Tripos<sup>™</sup>**  
 Go. Discover

Concord sets the industry standard for extremely rapid conversion of 2D (or crude 3D) input to accurate, geometry-optimized 3D structures. Although most often used for the conversion of large corporate and commercially distributed databases, Concord is also a productivity tool useful for molecular modeling and QSAR/QSPR research. Concord's proven reliability and versatility have made it a worldwide pharmaceutical and agrochemical research standard.

**Fast, Accurate Structures**

After the extremely rapid, logic-based generation of initial structures, Concord offers the user several options for equally rapid, energy-based geometry optimization. Concord offers a novel, uniquely efficient procedure which emulates molecular dynamic simulated annealing. Concord performs equality assessments on every structure, providing complete control regarding the quality of structures in 3D databases.

**Fast, Complete Conversions**

Indiscriminate conversion of large databases can waste disk space and drastically increase database search-times. Concord allows researchers to specify limits on molecular size, number of rotatable bonds, etc. and exclude compounds from the "conversion domain." Concord typically converts over 99% of the structures in its conversion domain at an average rate of just 0.2 cpu-seconds per compound.

**Multiple Input/Output Formats**

Concord provides many advantageous input/output options. MDL SDfiles, SYBYL<sup>®</sup> mol and mol2 files, and Tripos' SLN formats are supported. The highly compact and easy-to-learn SMILES line-notation is another very popular input format. Additional output formats include MOPAC, MM4, GAUSSIAN, PDB, CSSR, ORTEP, and custom formats. To save time, two or more formats can be output simultaneously.

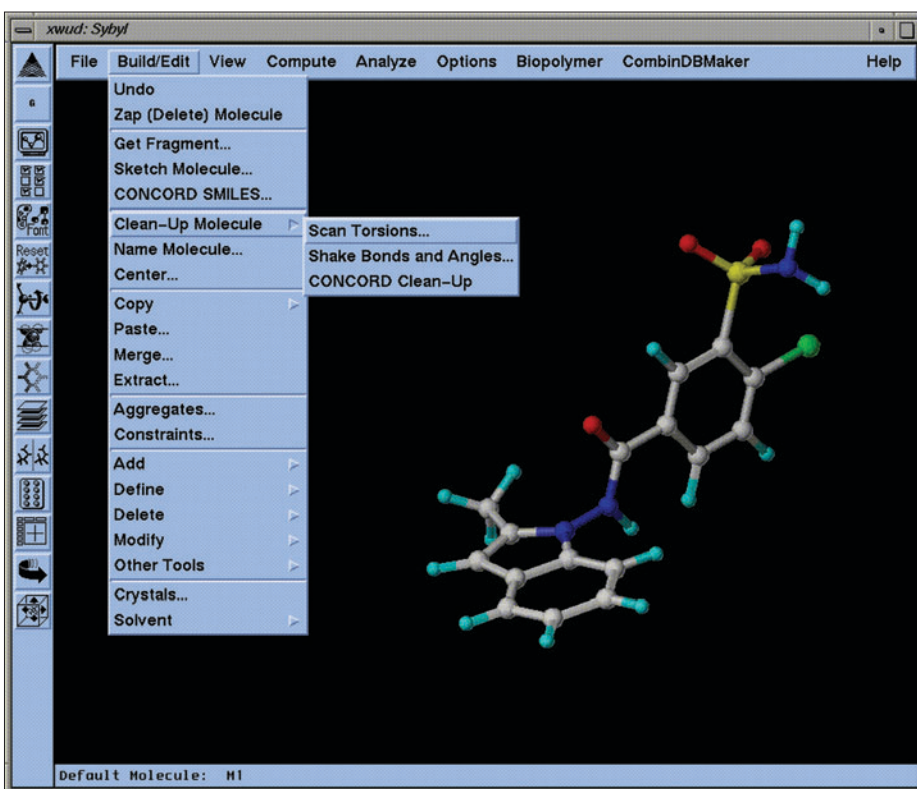
**Interfaced with SYBYL and UNITY**

Concord is a productivity tool which provides substantial added value to the power and versatility of SYBYL and UNITY<sup>®</sup>. The "dbconcord3db" command may be used to automatically convert corporate or custom databases from 2D to 3D, while refining a UNITY 3D-search query.

SYBYL users save time by using SMILES input to Concord rather than sketching. Unlike other clean-up methods, Concord converts even the roughest sketch or 2D structure retrieved from a database into an accurate 3D structure.

**Expand The Stereochemical Diversity of a Database**

Concord generates 3D structures which are 100% consistent with the stereochemical specifications in the 2D input. However, those specifications are frequently incorrect, incomplete, or entirely absent. 3D searches within the resulting 3D database cannot find a stereoisomer which was not in the original 2D database. Subsequently, combinatorial "multiplexing" of all stereocenters is not a practical solution. StereoPlex<sup>®</sup>, coupled with Concord, enables the intelligent stereochemical diversification of a database.



Rapid generation of complex ring systems from SMILES strings.

**Features and Benefits**

- The industry-standard tool for rapid generation of high-quality 3D coordinates from 2D input
- Offers a variety of built-in geometry optimization options
- Handles I/O in all of the common industry-standard formats
- Automatically "strips" salts, waters of hydration, etc.
- Exceptionally attentive to stereochemical and other cheminformatic information
- Provides a variety of input filters (regarding molecular size and flexibility)
- Provides built-in distributed processing on UNIX/Linux machines
- Easily incorporated into other programs, shell scripts, and "pipelined" protocols

**Complementary Products**

- **GASP™** for developing pharmacophore hypotheses using full conformational flexibility.
- **Tuplets™** for pharmacophore-based virtual screening.
- **DISCOtech™** for elucidating pharmacophore models from precalculated conformers.
- **FlexX™** for flexibly docking ligands into a binding site.
- **LeapFrog®** for performing *de novo* ligand design.
- **RACHEL™** for optimizing lead compounds.
- **Legion™/CombiLibMaker™** for generating virtual combinatorial libraries.
- **OptDesign®** for designing and editing combinatorial libraries.
- **StereoPlex®** for expanding the stereochemical diversity of a database.
- **DiverseSolutions®** for designing, comparing, and selecting compound libraries.
- **GeneFold®** for identifying protein function from sequence.
- **MatchMaker™** for building 3D models of proteins from sequence using inverse-folding techniques.
- **UNITY** for locating compounds in databases that match a pharmacophore or fit a receptor site.

**Hardware and Software Requirements**

Concord requires a Concord software license, and is accessible through the SYBYL expert molecular modeling environment or standalone. Concord runs on workstations operating under IRIX® (SGI®) or Linux® (x86).



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