
MedChem Designer™

# FREE! Chemical structure drawing and ADMET property prediction tool

*MedChem Designer™ is a new tool that combines innovative molecule drawing features with a few free fast and accurate ADMET property predictions from our top-ranked ADMET Predictor™.*

*Chemists who design new compounds for pharmaceutical, cosmetic, industrial chemical, herbicide, pesticide, and food applications will enjoy the highly intuitive interface with a number of convenience features and capabilities not available in other molecule drawing software.*

SimulationsPlus
SCIENCE + SOFTWARE = SUCCESS

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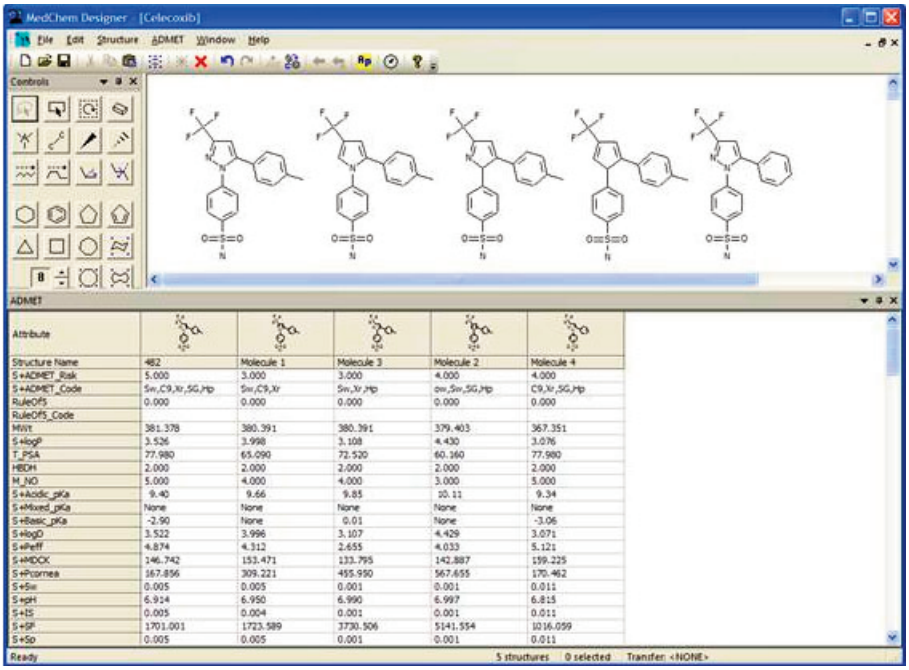
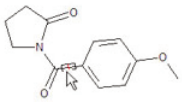
Draw multiple structures on the canvas, manipulate them using innovative drawing capabilities, then instantly generate predicted values of key ADMET properties: S+logP, S+logD(7.4), TPSA, MWt, HBDH, HBA (N+O as M_NO), Rule of 5, and even PEOE sigma charges - for FREE!.

The ability to handle multiple structures means that a structure found to have a desirable property profile can be kept as a reference, so properties of subsequently drawn structures can quickly and easily be compared with the original.

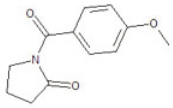



MedChem Designer has a number of innovative sketching features:

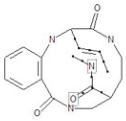
- ability to modify bond and torsional angles of side chains
- alignment tool based on the detection of common scaffolds
- convenient structure-cleanup feature with the option to keep one or more regions of a structure fixed in place
- capture any portion of a structure and save it as a new template
- draw multiple structures on a single canvas view



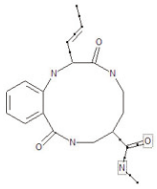
Click on a bond



The torsional angle is "flipped"



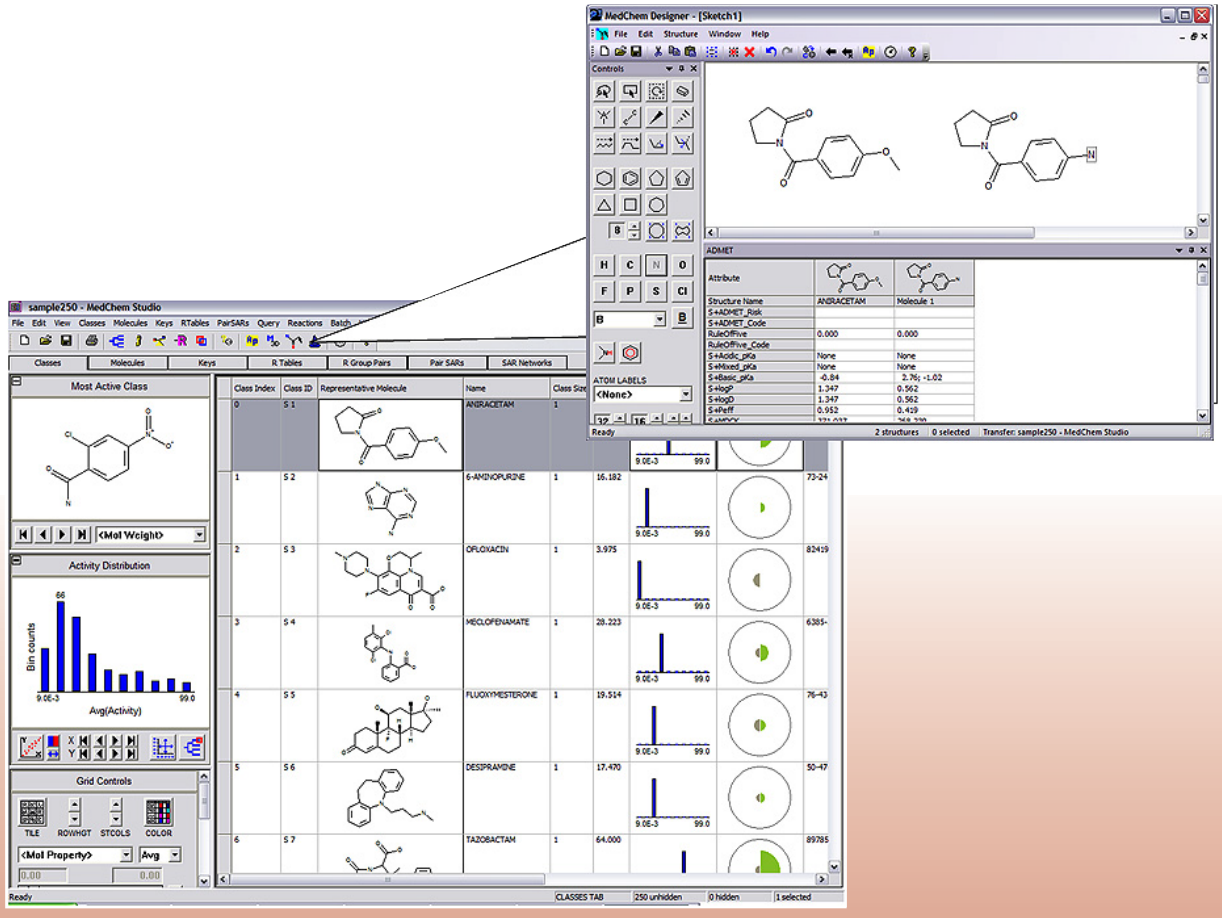
Original structure



Structure after cleanup of selected groups

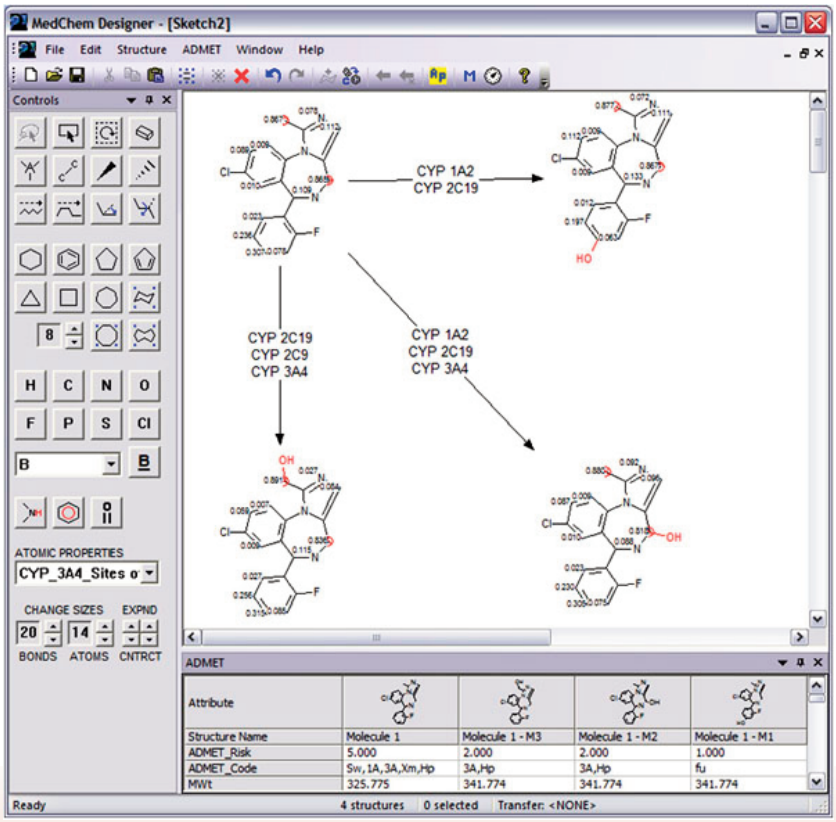
The program also integrates fully with our other software programs (paid licenses required):

- MedChem Studio™: sketch-based input of query structures - define your substructure search without leaving the program!



- ADMET Predictor™: the industry's leading property prediction program!

For full design power, add a paid license to ADMET Predictor™ and get over 120 predicted properties from the industry's leading property prediction program, including pKa(s), logP/logD, solubilities, permeabilities, toxicities, metabolism rates for CYP hydroxylation, CYP inhibitor classification, UGT metabolism classification, and likely sites of metabolic attack for CYP oxidation.




Also with a full ADMET Predictor license, you'll see our unique ADMET Risk™ score based on the World Drug Index that lets you "see" in many dimensions whether your structural modifications produce potential problems with toxicities, metabolism, pharmacokinetic properties, and/or physicochemical properties. Inspired by Lipinski's Rule of 5, but covering a wide range of properties in a single number, you have to experience this to see how molecule design has reached a new level in speed and productivity! Even see numerous rapid estimates of quantum-level atomic properties including partial charges, reactivity indices, and likely sites of CYP oxidation for the five major CYP enzymes. All of this within seconds of drawing your new structures!

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