



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.

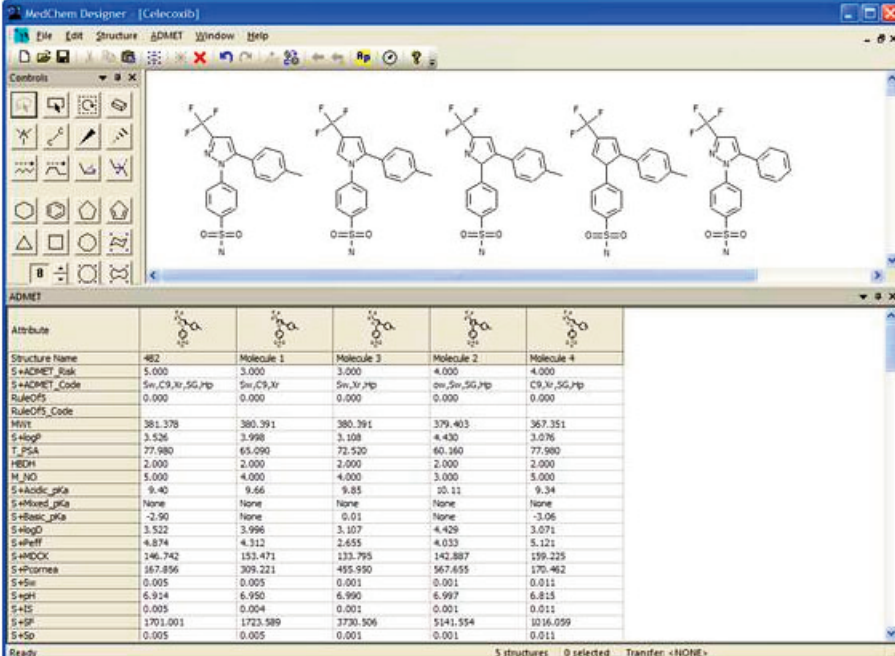


Scan for more information ▶



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.

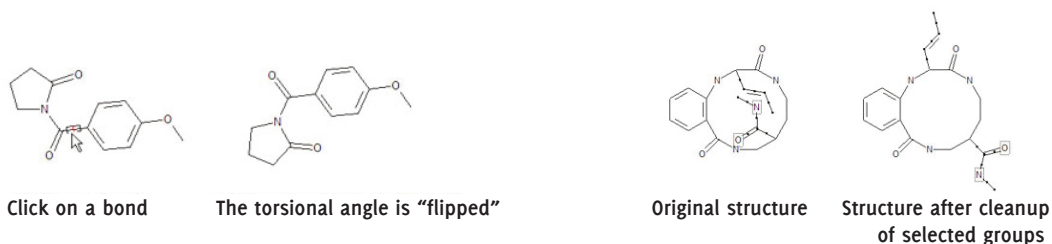


The screenshot displays the MedChem Designer software interface. The top window shows five chemical structures on a canvas. Below the canvas is an ADMET table with the following data:

Attribute	Molecule 1	Molecule 3	Molecule 2	Molecule 4	
Structure Name	482	Molecule 1	Molecule 3	Molecule 2	Molecule 4
S+ADMET_Risk	5.000	3.000	3.000	4.000	4.000
S+ADMET_Code	Sw,C9,Xr,SG,fp	Sw,C9,Xr	Sw,Xr,fp	sw,Sw,SG,fp	C9,Xr,SG,fp
RuleOf5	0.000	0.000	0.000	0.000	0.000
RuleOf5_Code					
MWt	381.378	380.391	380.391	379.403	367.351
S+logP	3.526	3.998	3.108	4.430	3.076
T_PSA	77.980	65.090	72.520	60.160	77.980
HBDH	2.000	2.000	2.000	2.000	2.000
M_NO	5.000	4.000	4.000	3.000	3.000
S+acidic_pKa	9.40	9.66	9.85	10.11	9.34
S+Mixed_pKa	None	None	None	None	None
S+Basic_pKa	-2.90	None	0.01	None	-3.06
S+logD	3.522	3.996	3.107	4.429	3.071
S+eff	4.874	4.312	2.655	4.033	5.121
S+MCK	146.742	153.471	133.795	142.887	159.225
S+Ptoxae	167.656	399.221	455.950	567.655	170.462
S+Si	0.005	0.005	0.001	0.001	0.011
S+piH	6.914	6.950	6.990	6.997	6.815
S+IS	0.005	0.004	0.001	0.001	0.011
S+SF	1701.001	1723.589	1730.506	5141.554	1016.059
S+Sp	0.005	0.005	0.001	0.001	0.011

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



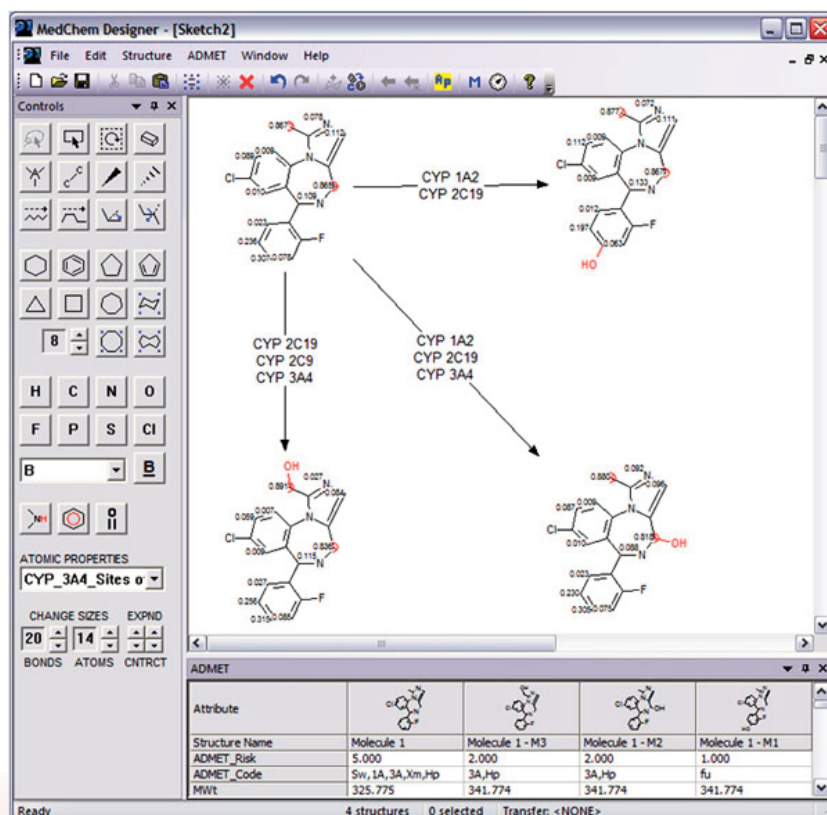
The program also integrates fully with our other software programs (paid licenses required):

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

Attribute	Structure 1	Structure 2
Structure Name	ANRACETAM	Molecule 1
S4ADMET_Brid		
S4ADMET_Code		
RuleOffRate	0.000	0.000
RuleOffRate		
S4Addc_pKa	None	None
S4Mixed_pKa	None	None
S4Basic_pKa	-0.84	2.36/-1.02
S4logP	1.347	0.562
S4eff	0.952	0.453
S4Count	177,113	164,100

- 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!