

Table S1. Softwares utilized for obtain another descriptors, quantities, classifications and used structural representations

Software	Quantities of descriptors	Classifications	Structural representation
ACD/ChemSketch 10.0	9	Sterics, solubility	2D structure
E-Dragon 1.0 ^a	34	Conectivity indices	SMILES
ETState ^a	30	Atom and bond-types E-state indices, and number of determined atoms and bonds	SMILES
Gaussian 03	20	Thermodynamics, electronics	Most stable 3D structure
HyperChem 7.1	4	Sterics	Most stable 3D structure
Marvin 4.1.8 ^b	63	Topologicals, solubility, sterics and constitucionals	Most stable 3D structure / 2D structure
MolSoft ^c	1	Solubility (Log S)	SMILES

^a By the PClient interface - <http://www.vcclab.org/lab/pclient>;

^b Freeware version available in <http://www.chemaxon.com>;

^c www.molsoft.com/mprop.