

LigandScout 3.0

Fully integrated pharmacophore modeling and virtual screening

LigandScout 3.0 is a fully integrated platform for accurate virtual screening based on 3D chemical feature pharmacophore models. It offers seamless workflows, starting both from ligand- and structure based-pharmacophore modeling, and includes novel high performance alignment algorithms for excellent prediction quality with unprecedented screening speed. Additionally, we have included user-friendly screening analysis tools, including the automated generation of ROC curves for performance assessments. All functions are accessible through a well elaborated graphic user interface that reflects our years of experience in creation of the most user-friendly pharmacophore modeling tools. The algorithms are scientifically validated and based on our well-established knowledge in pharmacophore research, while the application corresponds to state-of-the-art information technology.

Mark	Name	#	mol index	Pharmacophore fit score	# Confs.	Matching Features	Score
1	ZINC048137	5	17	45.761	25	100%	1.457260036
2	ZINC018114	11	12	45.476	12	100%	45.2600034
3	ZINC018114	13	25	45.476	25	100%	45.7200034
4	ZINC018114	4	25	45.476	25	100%	45.7300034
5	ZINC018114	10	12	45.101	11	100%	45.1020034
6	ZINC018114	9	12	45.101	12	100%	45.1020034
7	ZINC018114	7	12	44.724	7	100%	44.7240034
8	ZINC018114	1	12	43.801	11	100%	43.8050034
9	ZINC00552	8	7	18.302	25	100%	18.3010034
10	ZINC018114	13	12	18.022	25	100%	18.0210034
11	ZINC018114	11	12	18.022	25	100%	18.0200034
12	ZINC00500	9	2	16.653	2	100%	16.6520034
13	ZINC018114	12	12	16.453	25	100%	16.4440034
14	ZINC00500	7	2	16.271	2	100%	16.2720034

New in LigandScout 3.0:

- o Ligand-based pharmacophore modeling, including automatic classification of chemical features, feature weights and generation of exclusion volume spheres
- o Automated training set selection by pharmacophore-based cluster analysis
- o Smart enumeration of tautomers
- o Accurate alignment tools for fast and flexible comparison of molecules and pharmacophores with the possibility to interpolate and merge comparable pharmacophores
- o Easy 3D compound database generation and management, with parallelization support for efficient use of CPUs in your network
- o High performance accurate virtual screening with automated analysis of screening performance using ROC curves and enrichment factor calculations
- o Simple workflows for boolean combination of target and anti-target pharmacophore models
- o Accurate implementation of the MMFF94 force field for generating high quality geometries
- o Excellent graphics capabilities for generating exciting figures for your reports
- o Seamless integration of structure- and ligand-based modeling workflows allowing the use of structure-based information to improve ligand-based modeling

inte:ligand

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