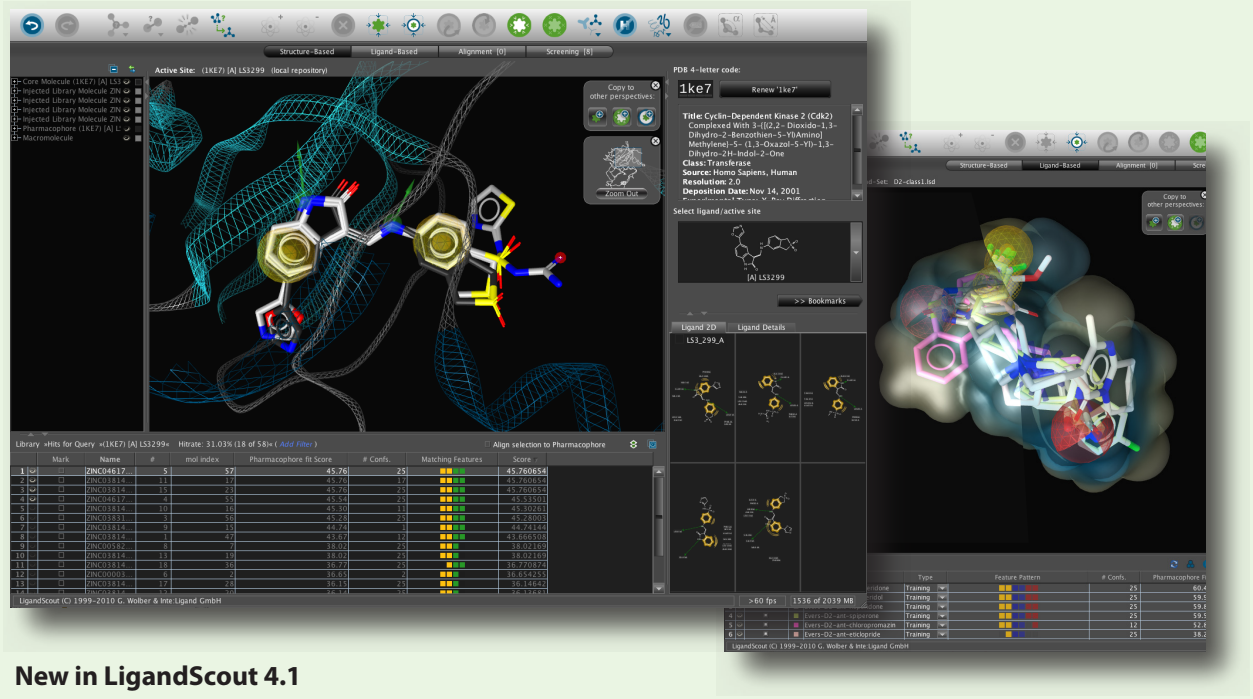
LigandScout 4.1

Advanced Molecular Design

LigandScout 4.1 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.



New in LigandScout 4.1

- Ligand-based pharmacophore modeling, including automatic classification of chemical features, feature weights and generation of exclusion volume spheres
- Analysis of molecular dynamics trajectories with pharmacophore clustering
- Seamless integration of AutoDock program
- Accurate alignment tools for fast and flexible comparison of molecules and pharmacophores with the possibility to interpolate and merge comparable pharmacophores
- Easy 3D compound database generation and management, with parallelization support for efficient use of CPUs in your network
- High performance accurate virtual screening with automated analysis of screening performance using ROC curves and enrichment factor calculations
- Simple workflows for boolean combination of target and anti-target pharmacophore models
- Accurate implementation of the MMFF94 force field for generating high quality geometries
- Extended pharmacophore editing, table export, and multidimensional filtering
- Easy exploration of apo binding sites based on user friendly intuitive modeling workflows, and automated protein pocket finder

inte:ligand

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