

Resource Summary Report

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LigandScout

RRID:SCR_014889

Type: Tool

Proper Citation

LigandScout (RRID:SCR_014889)

Resource Information

URL: <http://www.inteligand.com/ligandscout/>

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Description: Software that takes a macromolecular structure containing a bound ligand and identifies the key features on the ligand which are interacting with points on a protein. Its features include: automatic interpretation of PDB ligands using geometry, dictionaries and rule; advanced handling of co-factors, ions, water molecules and covalently bound ligands; pharmacophore export to Catalyst(tm), MOE(tm) and PHASE(tm) for virtual screening; and the ability to treat co-factors and water molecules as part of the ligand or part of the macromolecule.

Resource Type: software application, software resource

Keywords: pharmacophore, macromolecular structure, bound ligand, pdb ligand, virtual screening, ligand based pharmacore design

Availability: Available for purchase

Resource Name: LigandScout

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Alternate URLs: <https://www.chemistryworld.com/ligandscout/1012019.article>

License URLs: <http://www.rsc.org/help-legal/legal/terms-conditions/>

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260904T000431+0000

Ratings and Alerts

No rating or validation information has been found for LigandScout.

No alerts have been found for LigandScout.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 413 mentions in open access literature.

Listed below are recent publications. The full list is available at [NIF](#) .

Saleem A, et al. (2026) Carvacrol from *Moringa oleifera* as a potential antidiabetic agent using integrated in-silico approach inhibiting TCF7L2. *Scientific reports*, 16(1).

Dermawan D, et al. (2026) Integrative molecular simulations reveal NeuroAid II mechanisms in ischemic stroke through network pharmacology, molecular dynamics, and pharmacophore modeling. *Scientific reports*, 16(1), 6161.

Denzler A, et al. (2026) CReM-pharm: de novo 3D pharmacophore-based design with synthetic accessibility awareness. *Journal of cheminformatics*, 18(1).

Kalaba P, et al. (2026) Development and Biological Characterization of Fluorescent Dynorphins for the Visualization of Kappa Opioid Receptors. *Journal of medicinal chemistry*, 69(12), 14098.

Khedraoui M, et al. (2026) Exploring the Biological Potency of Carotenoids Against Alzheimer's Disease: An Integrated Approach of Molecular Docking and Molecular Dynamics. *Current issues in molecular biology*, 48(4).

Sumita M, et al. (2026) Molecular Design with Artificial Intelligence: Progress and Perspectives for Small Molecules. *Chemical reviews*, 126(5), 3007.

Ervina M, et al. (2026) In silico study of *Spatholobus littoralis* Hassk. wood compounds on p38 mitogen-activated protein kinase receptor. *Journal of advanced pharmaceutical technology & research*, 17(2), 87.

Khan MM, et al. (2026) In silico screening and molecular analyses identify apigenin from *Scutellaria barbata* as a potent AKT1 inhibitor in breast cancer. *PloS one*, 21(6), e0338874.

Negishi H, et al. (2026) cGAS-IFN-I responses by extracting nuclear DNA from dying cells via nucleocytosis. *Nature communications*, 17(1), 1658.

Kavaš V, et al. (2026) Structure-Activity Relationship and Crystallographic Study of New Monobactams. *Journal of medicinal chemistry*, 69(4), 3887.

Doering NP, et al. (2026) Mechanistic Insights into G Protein-Biased μ -Opioid Receptor Signaling Using Dual-Charged Naltrexamine Amides. *Journal of medicinal chemistry*, 69(4), 3833.

Lombardo L, et al. (2026) A Multistep Computational Approach to Achieve a Complete Human 5-Lipoxygenase Structure and Provide a Pharmacophore Model for Further Drug Design. *Molecular informatics*, 45(3), e70025.

Desai R, et al. (2026) Deep-Sea Marine Metabolites as Promising Anti-Tubercular Agents: CADD-Guided Targeting of the F420-Dependent Oxidoreductase. *Marine drugs*, 24(2).

Todsaporn D, et al. (2026) Integrating QSAR-Machine Learning, Biochemical Assays, and Molecular Dynamics for the Discovery of JAK2 Inhibitors in Cervical Cancer. *Journal of chemical information and modeling*, 66(10), 6067.

Khazaal Nazal AS, et al. (2026) Structure-based pharmacophore modeling, high-throughput screening, and molecular dynamics identify a novel DrugBank-derived HIV-1 protease inhibitor. *PloS one*, 21(6), e0336765.

Reza R, et al. (2026) Ligand-Based Pharmacophore Mapping and Virtual Screening for the Search of Biguanide-Like Molecules With Antidiabetic Potentials Targeting Liver Kinase B1. *Biochemistry research international*, 2026, 8369459.

Ricci D, et al. (2026) Rescuing TP53 from nonsense: novel triazoles for translational readthrough via optimized drug design. *Scientific reports*, 16(1).

Derwand D, et al. (2025) Effects of the Dietary Supplement 5 β -Hydroxy-Laxogenin in the Orchiectomized Rat Model. *Drug testing and analysis*, 17(9), 1743.

Phetcharawetch J, et al. (2025) Identification of sulfonylated indolo[1,2-a]quinolines as EGFR tyrosine kinase inhibitors. *RSC advances*, 15(5), 3139.

Horgan MJ, et al. (2025) Microtubule inhibition as a proposed mechanism for the anthelmintic effect of phytochemicals isolated from *Cicerbita alpina*. *Scientific reports*, 15(1), 4108.