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, ligad based pharmacore design

Availability: Available for purchase

Resource Name: LigandScout

Resource ID: SCR_014889

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

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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 ASWG .

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 ?-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?-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.