

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

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 395 mentions in open access literature.

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

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.

Khan K, et al. (2025) Zapotin mitigates breast cancer progression by targeting PKC γ mediated glycolytic pathway regulation. *BMC cancer*, 25(1), 798.

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.

Doijen J, et al. (2025) A New Fragment-Based Pharmacophore Virtual Screening Workflow Identifies Potent Inhibitors of SARS-CoV-2 NSP13 Helicase. *Journal of computational chemistry*, 46(23), e70201.

Matziol T, et al. (2025) Discovery of Novel Isoxazole-Based Small-Molecule Toll-Like Receptor 8 Antagonists. *Journal of medicinal chemistry*, 68(4), 4888.

Jung HJ, et al. (2025) Design, Synthesis, and Antioxidant and Anti-Tyrosinase Activities of (Z)-5-Benzylidene-2-(naphthalen-1-ylamino)thiazol-4(5H)-one Analogs: In Vitro and In Vivo Insights. *Molecules (Basel, Switzerland)*, 30(2).

Liu S, et al. (2025) Integrated Virtual Screening Approach Identifies New CYP19A1 Inhibitors. *Journal of chemical information and modeling*, 65(7), 3529.

Gündüz MG, et al. (2025) Biginelli dihydropyrimidines and their acetylated derivatives as L-/T-type calcium channel blockers: Synthesis, enantioseparation, and molecular modeling studies. *Archiv der Pharmazie*, 358(3), e2400584.

Ljubić M, et al. (2025) Water-Based Pharmacophore Modeling in Kinase Inhibitor Design: A Case Study on Fyn and Lyn Protein Kinases. *Journal of chemical information and modeling*, 65(18), 9747.

Sarac BE, et al. (2025) A novel 2-oxopyrrolidine derivative (LN-53) efficiently induces Nrf-2 signaling pathway activation in human epidermal keratinocytes. *Pharmacological reports* : PR, 77(5), 1347.

Zahid A, et al. (2025) Characterization of total phenolic and flavonoid content in *Pseudoconyza viscosa* (Mill.) and its in-silico antioxidant evaluation. *Frontiers in plant science*, 16, 1527515.

Saini RS, et al. (2025) In silico exploration of bioactive secondary metabolites with anesthetic effects on sodium channels Nav 1.7, 1.8, and 1.9 in painful human dental pulp. *Molecular pain*, 21, 17448069251327824.

Shen G, et al. (2025) Elevated uric acid induces erectile dysfunction in rats by interacting with MLCK and inhibiting its ubiquitin-mediated degradation. *Communications biology*, 8(1), 1190.

Sauer J, et al. (2025) The sodium/glucose cotransporter 2 inhibitor empagliflozin is a pharmacological chaperone of cardiac Nav1.5 channels. *American journal of physiology. Heart and circulatory physiology*, 329(3), H680.

Moon KM, et al. (2025) Upcycling of Adlay Bran via *Lactobacillus* Fermentation Enhances Anti-Melanogenic and Antioxidant Activities through MITF/Tyrosinase Pathway Modulation. *Journal of microbiology and biotechnology*, 35, e2507049.

Vesnina A, et al. (2025) Antidiabetic Potential of Mangiferin: An In Silico and In Vivo Approach. *Pharmaceutics*, 17(10).

Atlante S, et al. (2025) A Xanthine Derivative With Novel Heat Shock Protein 90-Alpha Inhibitory and Senolytic Properties. *Aging cell*, 24(7), e70047.

Sinsulpsiri S, et al. (2025) Unveiling the antiviral inhibitory activity of ebselen and ebsulfur derivatives on SARS-CoV-2 using machine learning-based QSAR, LB-PaCS-MD, and experimental assay. *Scientific reports*, 15(1), 6956.

Baei B, et al. (2025) Pharmacophore modeling and QSAR analysis of anti-HBV flavonols. *PloS one*, 20(1), e0316765.