Resource Summary Report

Generated by RRID on Aug 4, 2026

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 resource, software application

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 395 mentions in open access literature.

Listed below are recent publications. The full list is available at RRID .

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

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.

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? mediated glycolytic pathway regulation. BMC cancer, 25(1), 798.

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.

Ljubi? 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.

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.

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.

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.

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.

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.

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

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.

Asrar B, et al. (2025) In silico investigation of ketamine and methylphenidate drug-drug conjugate for MDD and ADHD treatment using MD simulations and MMGBSA. Scientific reports, 15(1), 24565.

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

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.