# **Resource Summary Report**

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# **ALOGPS**

RRID:SCR\_018786 Type: Tool

**Proper Citation** 

ALOGPS (RRID:SCR\_018786)

#### **Resource Information**

URL: http://www.vcclab.org/lab/alogps/

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**Description:** Software tool to predict lipophilicity and aqueous solubility of molecules. ALOGPS 2.1 can increase its prediction for molecules up to 5 times LIBRARY mode. You can create and use your own LIBRARY.

Synonyms: ALOGPS 2.1

**Resource Type:** data analysis software, software resource, data processing software, service resource, software application

**Keywords:** Molecule lipophilicity prediction, molecule aqueous solubility prediction, molecule, prediction

**Funding:** INTAS ; University of Lausanne

Availability: Free, Freely available

**Resource Name:** ALOGPS

Resource ID: SCR\_018786

**Record Creation Time:** 20220129T080342+0000

Record Last Update: 20250430T060216+0000

**Ratings and Alerts** 

No rating or validation information has been found for ALOGPS.

No alerts have been found for ALOGPS.

## Data and Source Information

Source: SciCrunch Registry

### **Usage and Citation Metrics**

We found 19 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

Zhang K, et al. (2024) Late-stage (radio)fluorination of alkyl phosphonates via electrophilic activation. Nature communications, 15(1), 10338.

Chen Z, et al. (2024) PungentDB: Bridging traditional Chinese medicine of medicine food homology and modern food flavor chemistry. Food chemistry: X, 23, 101742.

Kemas AM, et al. (2024) Compound Absorption in Polymer Devices Impairs the Translatability of Preclinical Safety Assessments. Advanced healthcare materials, 13(11), e2303561.

Ren M, et al. (2022) The structure-activity relationship of aromatic compounds in advanced oxidation processes?a review. Chemosphere, 296, 134071.

Kasthuri T, et al. (2022) Rapid-killing efficacy substantiates the antiseptic property of the synergistic combination of carvacrol and nerol against nosocomial pathogens. Archives of microbiology, 204(9), 590.

Fang J, et al. (2021) Biodegradable self-assembly micelles significantly enhanced the solubility, biological stability and in vivo antitumor efficacy of Hexylselen. RSC chemical biology, 2(6), 1669.

Cassien M, et al. (2021) Improving the Antioxidant Properties of Calophyllum inophyllum Seed Oil from French Polynesia: Development and Biological Applications of Resinous Ethanol-Soluble Extracts. Antioxidants (Basel, Switzerland), 10(2).

Conlon M, et al. (2021) A compendium of kinetic modulatory profiles identifies ferroptosis regulators. Nature chemical biology, 17(6), 665.

Gupta R, et al. (2021) Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Molecular diversity, 25(3), 1315.

Salvador-Mira M, et al. (2021) Immunomodulatory Lectin-like Peptides for Fish Erythrocytes-Targeting as Potential Antiviral Drug Delivery Platforms. International journal of molecular sciences, 22(21).

Sjögren E, et al. (2021) A Physiologically-Based Pharmacokinetic Framework for Prediction of Drug Exposure in Malnourished Children. Pharmaceutics, 13(2).

Bai X, et al. (2021) Network pharmacology integrated molecular docking reveals the bioactive components and potential targets of Morinda officinalis-Lycium barbarum coupled-herbs against oligoasthenozoospermia. Scientific reports, 11(1), 2220.

Bai X, et al. (2021) An Integrated Analysis of Network Pharmacology, Molecular Docking, and Experiment Validation to Explore the New Candidate Active Component and Mechanism of Cuscutae Semen-Mori Fructus Coupled-Herbs in Treating Oligoasthenozoospermia. Drug design, development and therapy, 15, 2059.

Wei MP, et al. (2021) Saponin fraction from Sapindus mukorossi Gaertn as a novel cosmetic additive: Extraction, biological evaluation, analysis of anti-acne mechanism and toxicity prediction. Journal of ethnopharmacology, 268, 113552.

Liu B, et al. (2021) Synthesis, Stability, and Antidiabetic Activity Evaluation of (-)-Epigallocatechin Gallate (EGCG) Palmitate Derived from Natural Tea Polyphenols. Molecules (Basel, Switzerland), 26(2).

, et al. (2020) Risk assessment of aflatoxins in food. EFSA journal. European Food Safety Authority, 18(3), e06040.

Jayakar SS, et al. (2020) Photoaffinity labeling identifies an intersubunit steroid-binding site in heteromeric GABA type A (GABAA) receptors. The Journal of biological chemistry, 295(33), 11495.

Wei Y, et al. (2019) Cubosomes with surface cross-linked chitosan exhibit sustained release and bioavailability enhancement for vinpocetine. RSC advances, 9(11), 6287.

Amoli-Diva M, et al. (2015) Gold nanoparticles grafted modified silica gel as a new stationary phase for separation and determination of steroid hormones by thin layer chromatography. Journal of food and drug analysis, 23(2), 279.