

Resource Summary Report

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BioSolveIT

RRID:SCR_003949

Type: Tool

Proper Citation

BioSolveIT (RRID:SCR_003949)

Resource Information

URL: <http://www.biosolveit.de/>

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Description: Commercial provider of software solutions for drug discovery applications offering tools, services, and research collaborations. The software portfolio ranges from design, over screening, to the visualization of ligand libraries, for hit identification, optimization, and scaffold hopping. With a stellar scientific advisory board and founders from academia who intensely collaborate with pharma, BioSolveIT catalyzes products off of university research successes with proven pharmaceutical industry application. They provide software products within the areas of ligand and structure-based drug design and is the pioneer of computational fragment-based ligand design. BioSolveIT innovate breakthroughs in drug discovery by supplying smooth, user-centered designed tools bringing different researchers together for efficient multidisciplinary drug design.

Abbreviations: BioSolveIT

Synonyms: BioSolveIT GmbH

Resource Type: commercial organization

Keywords: drug discovery, drug, ligand, structure, drug design

Availability: Free for academic use, License required

Resource Name: BioSolveIT

Resource ID: SCR_003949

Alternate IDs: nlx_158346

Record Creation Time: 20220129T080221+0000

Record Last Update: 20260912T195605+0000

Ratings and Alerts

No rating or validation information has been found for BioSolveIT.

No alerts have been found for BioSolveIT.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 126 mentions in open access literature.

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

Ahrens H, et al. (2025) Synthesis and biological profile of substituted hexahydrofuro[3,4-b]furans, a novel class of bicyclic acyl-acyl carrier protein (ACP) thioesterase inhibitors. *Pest management science*, 81(5), 2635.

Abadi MHHE, et al. (2025) Identification of potential COVID-19 Mpro inhibitors through covalent drug docking, molecular dynamics simulation, and MMGBSA calculation. *Scientific reports*, 15(1), 20500.

Afzal M, et al. (2025) Investigation of biometabolites and novel antimicrobial peptides derived from promising source *Cordyceps militaris* and effect of non-small cell lung cancer genes computationally. *PloS one*, 20(1), e0310103.

Fahrenhorst-Jones T, et al. (2025) Scaffold hopping approaches for the exploration of herbicidally active compounds inhibiting Acyl-ACP Thioesterase. *Pest management science*, 81(5), 2617.

Wagner M, et al. (2025) Mapping protein-metabolite interactions in *E. coli* by integrating chromatographic techniques and co-fractionation mass spectrometry. *iScience*, 28(6), 112611.

Hoba SN, et al. (2025) Parallel synthesis of 5'-amino-5'-deoxy-adenosine derivatives for focused chemical space exploration and their application as methyltransferase inhibitors. *RSC medicinal chemistry*.

Bernier D, et al. (2025) Aminoisothiazolamides, a new class of potent inhibitors of lysyl-tRNA synthetase. *Pest management science*, 81(7), 3956.

Lin S, et al. (2025) Drug Screening of Flavonoids as Potential VEGF Inhibitors Through Computational Docking and Cell Models. *Molecules (Basel, Switzerland)*, 30(2).

Kagho MD, et al. (2024) Comprehensive Cell Biological Investigation of Cytochalasin B Derivatives with Distinct Activities on the Actin Network. *Journal of natural products*, 87(10), 2421.

Müller V, et al. (2024) Mapping and Characterization of Target-Site Resistance to Cyclic Ketoenol Insecticides in Cabbage Whiteflies, *Aleyrodes proletella* (Hemiptera: Aleyrodidae). *Insects*, 15(3).

Abbas R, et al. (2024) ARTS and small-molecule ARTS mimetics upregulate p53 levels by promoting the degradation of XIAP. *Apoptosis : an international journal on programmed cell death*, 29(7-8), 1145.

Ciesielska A, et al. (2024) Evaluation of the antidermatophytic activity of potassium salts of N-acylhydrazinecarbodithioates and their aminotriazole-thione derivatives. *Scientific reports*, 14(1), 3521.

Schwalm MP, et al. (2024) Critical assessment of LC3/GABARAP ligands used for degrader development and ligandability of LC3/GABARAP binding pockets. *Nature communications*, 15(1), 10204.

Aftab H, et al. (2024) Design, synthesis, in vitro and in silico studies of novel piperidine derived thiosemicarbazones as inhibitors of dihydrofolate reductase. *Scientific reports*, 14(1), 22645.

Lin S, et al. (2024) Computational Docking as a Tool in Guiding the Drug Design of Rutaecarpine Derivatives as Potential SARS-CoV-2 Inhibitors. *Molecules (Basel, Switzerland)*, 29(11).

Ahmed A, et al. (2024) Acyl pyrazole sulfonamides as new antidiabetic agents: synthesis, glucosidase inhibition studies, and molecular docking analysis. *Frontiers in chemistry*, 12, 1380523.

Rusinko A, et al. (2024) AIDDISON: Empowering Drug Discovery with AI/ML and CADD Tools in a Secure, Web-Based SaaS Platform. *Journal of chemical information and modeling*, 64(1), 3.

Carmona AV, et al. (2024) Discovery of an Aldo-Keto reductase 1C3 (AKR1C3) degrader. *Communications chemistry*, 7(1), 95.

Tran TH, et al. (2024) Inhibition of Pancreatic Lipase by Flavonoid Derivatives: In Vitro and In Silico Investigations. *Advances in pharmacological and pharmaceutical sciences*, 2024, 6655996.

Tettevi EJ, et al. (2024) In Silico Identification of a Potential TNF-Alpha Binder Using a Structural Similarity: A Potential Drug Repurposing Approach to the Management of Alzheimer's Disease. *BioMed research international*, 2024, 9985719.