Resource Summary Report

Generated by T1D on Sep 19, 2026

LeadIT

RRID:SCR_014881
Type: Tool

Proper Citation

LeadIT (RRID:SCR_014881)

Resource Information

URL: http://www.biosolveit.de/LeadIT/

Proper Citation: LeadIT (RRID:SCR_014881)

Description: Drug discovery platform for medicinal and computational researchers. Users can assess the binding affinity and contributions to binding of a complex, find new scaffolds, grow molecules towards pharmacophore points, link fragments, and investigate possible dock binding conformations.

Resource Type: software resource

Keywords: drug discovery, platform, binding, docking, complex, small molecule, software package, drug design

Availability: License must be purchased, Older versions are available

Resource Name: LeadIT

Resource ID: SCR_014881

License: Full licenses are issued for a fixed term on a contract or leasing basis.

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260912T195822+0000

Ratings and Alerts

No rating or validation information has been found for LeadIT.

No alerts have been found for LeadIT.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 151 mentions in open access literature.

Listed below are recent publications. The full list is available at T1D .

Almena Rodriguez L, et al. (2026) Comparative Evaluation of Explicit Solvent Models for RNA-Ligand Docking. Journal of chemical information and modeling, 66(11), 6719.

Lyu Y, et al. (2026) Development and application of an instrument for microstructure matrix inclusion distribution analysis in oversized metallic materials. iScience, 29(2), 114620.

Zareen W, et al. (2026) Synthesis and biological evaluation of 6-hydroxychromone based thiosemicarbazones as potential antidiabetic and antioxidant agents. Scientific reports, 16(1).

Saeed R, et al. (2025) Design, synthesis, and multi-target evaluation of 4-phenyl quinoline-8-sulfonate thiosemicarbazones as potential anti-Alzheimer agents. Scientific reports, 15(1), 44212.

Sharma A, et al. (2025) CADD based designing and biological evaluation of novel triazole based thiazolidinedione coumarin hybrids as antidiabetic agent. Scientific reports, 15(1), 4302.

Slimani A, et al. (2025) Phytochemical Characterization and Assessment of Antioxidant and Anti-Alzheimer Effects of Algerian Seseli Tortuosum. Chemistry & biodiversity, 22(1), e202400482.

Chen LC, et al. (2025) Exploring diarylheptanoid derivatives to target LIMK1 as potential agents against colorectal cancer. Journal of enzyme inhibition and medicinal chemistry, 40(1), 2583826.

Bordoni C, et al. (2025) New Anticancer 4-Aryldihydropyrimidinone-5-Carboxylates Targeting Hsp90. Chemical biology & drug design, 106(6), e70221.

Rani M, et al. (2025) Molecular Dynamics (MD) Simulation of GPR87-LPA Binding: Therapeutic Implications for Targeted Cancer Treatment. Anti-cancer agents in medicinal chemistry, 25(17), 1342.

Naseer I, et al. (2025) Synthesis, in vitro, and in silico studies of 4-chlorophenyl-sulfonyl Indole based thiosemicarbazones as competitive ?-glucosidase inhibitors. Scientific reports, 15(1), 38832.

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.

Bekaddour N, et al. (2024) The histamine analogue clobenpropit modulates IRF7 phosphorylation and interferon production by targeting CXCR4 in systemic lupus erythematosus models. Frontiers in immunology, 15, 1490593.

Djehiche C, et al. (2024) Exploring the Therapeutic Potential of Ammodaucus leucotrichus Seed Extracts: A Multi-Faceted Analysis of Phytochemical Composition, Anti-Inflammatory Efficacy, Predictive Anti-Arthritic Properties, and Molecular Docking Insights. Pharmaceuticals (Basel, Switzerland), 17(3).

Soni S, et al. (2024) Highly efficient synthesis of isoxazolones and pyrazolones using g-C3N4·OH nanocomposite with their in silico molecular docking, pharmacokinetics and simulation studies. Scientific reports, 14(1), 19123.

Ngernsombat C, et al. (2024) Repurposing FDA-approved drugs targeting FZD10 in nasopharyngeal carcinoma: insights from molecular dynamics simulations and experimental validation. Scientific reports, 14(1), 31461.

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.

Luo L, et al. (2024) Development of broad-spectrum immunoassay with monoclonal antibody to detect five eugenols and study of their molecular recognition mechanism. Food chemistry: X, 22, 101255.

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.

Munir R, et al. (2024) Exploration of morpholine-thiophene hybrid thiosemicarbazones for the treatment of ureolytic bacterial infections via targeting urease enzyme: Synthesis, biochemical screening and computational analysis. Frontiers in chemistry, 12, 1403127.

Chin HK, et al. (2023) Exploration of anti-leukemic effect of soft coral-derived 13-acetoxysarcocrassolide: Induction of apoptosis via oxidative stress as a potent inhibitor of heat shock protein 90 and topoisomerase II. The Kaohsiung journal of medical sciences, 39(7), 718.