Resource Summary Report

Generated by NIF on Apr 21, 2025

Molecular Discovery

RRID:SCR_004085
Type: Tool

Proper Citation

Molecular Discovery (RRID:SCR_004085)

Resource Information

URL: http://www.moldiscovery.com/

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Description: Commercial organization providing the GRID software to scientists working on the field of drug design. All the products are based on the GRID force field, which is used in connection with experimental design and multivariate analysis tools to transform information into knowledge. The main field of application is drug discovery, property design and prediction by merging molecular modelling techniques and Quantitative structure-activity relationship (QSPR) methods into 3D-QSPR models. The same strategies can also be used in virtual screening, ADME prediction and profile and prediction of human drug metabolism, where selection or prioritization of candidates is required from large collections of compounds to minimize drug failures. Molecular Discovery offers training courses on all MD programs. Workshops and seminars on Drug Design methodologies, DMPK prediction and QSPR are also offered. Consulting agreements are also offered in research areas related with chemometrics and drug discovery. Products * GRID, a program for rational or structure-based design using molecular interaction fields * MetaSite, a program for predicting metabolic hotspots or soft spots and subsequent metabolite formation * Mass-MetaSite, a program for identifying metaoblites based on experimental LC-MSMS data * WebMetaBase, a program for storing, visualising, and data-mining the results from Mass-MetaSite * VolSurf+, a program for modelling pharmacokinetic or ADME properties * SHOP, a program for scaffold replacement * MoKa, a program for modelling pKa and tautomerisation * Pentacle, a program for 3D-QSAR (an update of Almond) * FLAP, a program for virtual screening, pharmacophore modelling, docking, water prediction, and 3D-QSAR

Abbreviations: MD

Synonyms: Molecular Discovery Ltd, Molecular Discovery Ltd.

Resource Type: commercial organization

Keywords: drug discovery, drug design, drug, training service resource, chemometrics, cytochrome p450

Funding:

Resource Name: Molecular Discovery

Resource ID: SCR_004085

Alternate IDs: grid.452579.8, nlx_158543, Wikidata: Q6895943

Alternate URLs: https://ror.org/0576dtf44

Record Creation Time: 20220129T080222+0000

Record Last Update: 20250420T014207+0000

Ratings and Alerts

No rating or validation information has been found for Molecular Discovery.

No alerts have been found for Molecular Discovery.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 30 mentions in open access literature.

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

Goracci L, et al. (2024) MARS: A Multipurpose Software for Untargeted LC-MS-Based Metabolomics and Exposomics. Analytical chemistry, 96(4), 1468.

García Jiménez D, et al. (2022) Designing Soluble PROTACs: Strategies and Preliminary Guidelines. Journal of medicinal chemistry, 65(19), 12639.

Kumar P, et al. (2022) Development of a Novel Pharmacophore Model Guided by the Ensemble of Waters and Small Molecule Fragments Bound to SARS-CoV-2 Main Protease. Molecular informatics, 41(2), e2100178.

Massari S, et al. (2021) Synthesis and characterization of 1,2,4-triazolo[1,5-a]pyrimidine-2-

carboxamide-based compounds targeting the PA-PB1 interface of influenza A virus polymerase. European journal of medicinal chemistry, 209, 112944.

Perrone MG, et al. (2021) An attempt to chemically state the cross-talk between monomers of COX homodimers by double/hybrid inhibitors mofezolac-spacer-mofezolac and mofezolac-spacer-arachidonic acid. European journal of medicinal chemistry, 209, 112919.

Carofiglio F, et al. (2020) Bcr-Abl Allosteric Inhibitors: Where We Are and Where We Are Going to. Molecules (Basel, Switzerland), 25(18).

Lammi C, et al. (2020) Assessment of the Multifunctional Behavior of Lupin Peptide P7 and Its Metabolite Using an Integrated Strategy. Journal of agricultural and food chemistry, 68(46), 13179.

Aichinger G, et al. (2020) Alternaria toxins as casein kinase 2 inhibitors and possible consequences for estrogenicity: a hybrid in silico/in vitro study. Archives of toxicology, 94(6), 2225.

Del Favero G, et al. (2020) Structural Similarity with Cholesterol Reveals Crucial Insights into Mechanisms Sustaining the Immunomodulatory Activity of the Mycotoxin Alternariol. Cells, 9(4).

Dellafiora L, et al. (2020) "Bottom-Up" Strategy for the Identification of Novel Soybean Peptides with Angiotensin-Converting Enzyme Inhibitory Activity. Journal of agricultural and food chemistry, 68(7), 2082.

Dellafiora L, et al. (2020) A Structural Study on the Listeria Monocytogenes Internalin A-Human E-cadherin Interaction: A Molecular Tool to Investigate the Effects of Missense Mutations. Toxins, 12(1).

Dellafiora L, et al. (2020) An In Silico Target Fishing Approach to Identify Novel Ochratoxin A Hydrolyzing Enzyme. Toxins, 12(4).

Ermondi G, et al. (2020) Solubility prediction in the bRo5 chemical space: where are we right now? ADMET & DMPK, 8(3), 207.

Costamagna A, et al. (2019) Modeling ErbB2-p130Cas interaction to design new potential anticancer agents. Scientific reports, 9(1), 3089.

Faisal Z, et al. (2019) Cyclodextrins Can Entrap Zearalenone-14-Glucoside: Interaction of the Masked Mycotoxin with Cyclodextrins and Cyclodextrin Bead Polymer. Biomolecules, 9(8).

Marseglia A, et al. (2019) Simulated Gastrointestinal Digestion of Cocoa: Detection of Resistant Peptides and In Silico/In Vitro Prediction of Their Ace Inhibitory Activity. Nutrients, 11(5).

Dellafiora L, et al. (2018) On the Mechanism of Action of Anti-Inflammatory Activity of Hypericin: An In Silico Study Pointing to the Relevance of Janus Kinases Inhibition.

Molecules (Basel, Switzerland), 23(12).

Del Favero G, et al. (2018) Response of intestinal HT-29 cells to the trichothecene mycotoxin deoxynivalenol and its sulfated conjugates. Toxicology letters, 295, 424.

Desantis J, et al. (2017) Exploring the cycloheptathiophene-3-carboxamide scaffold to disrupt the interactions of the influenza polymerase subunits and obtain potent anti-influenza activity. European journal of medicinal chemistry, 138, 128.

Dellafiora L, et al. (2017) Degradation of Aflatoxins by Means of Laccases from Trametes versicolor: An In Silico Insight. Toxins, 9(1).