

# Resource Summary Report

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## Molecular Discovery

RRID:SCR\_004085

Type: Tool

### Proper Citation

Molecular Discovery (RRID:SCR\_004085)

### Resource Information

**URL:** <http://www.moldiscovery.com/>

**Proper Citation:** Molecular Discovery (RRID:SCR\_004085)

**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 metabolites 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

**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:** 20260815T182246+0000

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## Ratings and Alerts

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

No alerts have been found for Molecular Discovery.

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## Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We found 36 mentions in open access literature.

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

Di Cristofano S, et al. (2025) Selection of short Gadd45 $\gamma$ -binding peptides through a synergistic computational and biophysical approach. Protein science : a publication of the Protein Society, 34(12), e70380.

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

Sipala F, et al. (2023) Different In Silico Approaches Using Heterocyclic Derivatives against the Binding between Different Lineages of SARS-CoV-2 and ACE2. Molecules (Basel, Switzerland), 28(9).

Rossi Sebastiano M, et al. (2022) Personalized Treatment for Infantile Ascending Hereditary Spastic Paralysis Based on In Silico Strategies. Molecules (Basel, Switzerland), 27(20).

Mercorelli B, et al. (2022) Discovery of novel SARS-CoV-2 inhibitors targeting the main protease Mpro by virtual screenings and hit optimization. Antiviral research, 204, 105350.

Mar $\gamma$  MA, et al. (2022) Pharmaceutical and Safety Profile Evaluation of Novel Selenocompounds with Noteworthy Anticancer Activity. Pharmaceutics, 14(2).

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.

Smirnova M, et al. (2022) Pharmacophore-Based Discovery of Substrates of a Novel Drug/Proton-Antiporter in the Human Brain Endothelial hCMEC/D3 Cell Line. *Pharmaceutics*, 14(2).

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.

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.

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.

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.

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

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).

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

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).

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.

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).