Resource Summary Report

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Ghemical

RRID:SCR_014899
Type: Tool

Proper Citation

Ghemical (RRID:SCR_014899)

Resource Information

URL: http://bioinformatics.org/ghemical/ghemical/index.html

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Description: Molecular modelling software package with 3D-visualization tools. It supports methods based on both molecular mechanics and quantum mechanics (using MOPAC7, and MPQC for QM). It contains geometry optimization (for MM and QM) and molecular dynamics (for MM) algorithms.

Resource Type: software resource, software toolkit

Keywords: molecular modeling, 3d visualization, molecular mechanics, quantum mechanics, geometry organization, molecular dynamics

Availability: Available for download

Resource Name: Ghemical

Resource ID: SCR_014899

Alternate IDs: OMICS_21304

Alternate URLs: https://sources.debian.org/src/ghemical/

Old URLs: https://www.uku.fi/~thassine/projects/ghemical

Ratings and Alerts

No rating or validation information has been found for Ghemical.

No alerts have been found for Ghemical.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 17 mentions in open access literature.

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

Aghamohammadi M, et al. (2022) Modeling studies on the role of vitamins B1 (thiamin), B3 (nicotinamide), B6 (pyridoxamine), and caffeine as potential leads for the drug design against COVID-19. Journal of molecular modeling, 28(12), 380.

Depommier C, et al. (2021) Beneficial Effects of Akkermansia muciniphila Are Not Associated with Major Changes in the Circulating Endocannabinoidome but Linked to Higher Mono-Palmitoyl-Glycerol Levels as New PPAR? Agonists. Cells, 10(1).

Vitale RM, et al. (2021) Identification and Characterization of Cannabidiol as an OX1R Antagonist by Computational and In Vitro Functional Validation. Biomolecules, 11(8).

Donyapour N, et al. (2021) Predicting partition coefficients for the SAMPL7 physical property challenge using the ClassicalGSG method. Journal of computer-aided molecular design, 35(7), 819.

Iannotti FA, et al. (2020) Identification and Characterization of Cannabimovone, a Cannabinoid from Cannabis sativa, as a Novel PPAR? Agonist via a Combined Computational and Functional Study. Molecules (Basel, Switzerland), 25(5).

Fancellu G, et al. (2020) Novel tacrine-benzofuran hybrids as potential multi-target drug candidates for the treatment of Alzheimer's Disease. Journal of enzyme inhibition and medicinal chemistry, 35(1), 211.

Vitale RM, et al. (2020) Discovery of a Remarkable Methyl Shift Effect in the Vanilloid Activity of Triterpene Amides. Journal of natural products, 83(11), 3476.

Rajeshwari R, et al. (2019) New Multitarget Hybrids Bearing Tacrine and Phenylbenzothiazole Motifs as Potential Drug Candidates for Alzheimer's Disease. Molecules (Basel, Switzerland), 24(3).

D'Aniello E, et al. (2019) Identification and characterization of phytocannabinoids as novel dual PPAR?/? agonists by a computational and in vitro experimental approach. Biochimica et

biophysica acta. General subjects, 1863(3), 586.

D'Aniello E, et al. (2019) In Silico Identification and Experimental Validation of (-)-Muqubilin A, a Marine Norterpene Peroxide, as PPAR?/?-RXR? Agonist and RAR? Positive Allosteric Modulator. Marine drugs, 17(2).

Vitale RM, et al. (2018) Fishing for Targets of Alien Metabolites: A Novel Peroxisome Proliferator-Activated Receptor (PPAR) Agonist from a Marine Pest. Marine drugs, 16(11).

Ruzza P, et al. (2018) Chaperone-like effect of ceftriaxone on HEWL aggregation: A spectroscopic and computational study. Biochimica et biophysica acta. General subjects, 1862(6), 1317.

Ruzza P, et al. (2018) Spectroscopy data of ceftriaxone-lysozyme interaction and computational studies. Data in brief, 18, 1808.

Vitale RM, et al. (2017) Structure-activity relationships of fraxamoside as an unusual xanthine oxidase inhibitor. Journal of enzyme inhibition and medicinal chemistry, 32(1), 345.

Ruzza P, et al. (2016) Interactions of GFAP with ceftriaxone and phenytoin: SRCD and molecular docking and dynamic simulation. Biochimica et biophysica acta, 1860(10), 2239.

Melnikov P, et al. (2014) Structural modeling of djenkolic acid with sulfur replaced by selenium and tellurium. Molecules (Basel, Switzerland), 19(4), 4847.

Marshall TG, et al. (2006) Common angiotensin receptor blockers may directly modulate the immune system via VDR, PPAR and CCR2b. Theoretical biology & medical modelling, 3, 1.