Resource Summary Report

Generated by NIF on Aug 1, 2026

PaDEL-Descriptor

RRID:SCR_014272
Type: Tool

Proper Citation

PaDEL-Descriptor (RRID:SCR_014272)

Resource Information

URL: http://www.yapcwsoft.com/dd/padeldescriptor/

Proper Citation: PaDEL-Descriptor (RRID:SCR_014272)

Description: A software to calculate molecular descriptors and fingerprints. The descriptors and fingerprints are calculated using The Chemistry Development Kit with additional descriptors and fingerprints such as atom type electrotopological state descriptors, Crippen's logP and MR, extended topochemical atom (ETA) descriptors, and McGowan volume.

Resource Type: data processing software, data analysis software, software application, software resource

Keywords: data analysis software, calculator, molecular descriptor, fingerprint

Availability: Free, Acknowledgement requested, Source code available

Resource Name: PaDEL-Descriptor

Resource ID: SCR_014272

Record Creation Time: 20220129T080319+0000

Record Last Update: 20260801T190510+0000

Ratings and Alerts

No rating or validation information has been found for PaDEL-Descriptor.

No alerts have been found for PaDEL-Descriptor.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 150 mentions in open access literature.

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

Vaidya H, et al. (2025) Anti-EBV: Artificial intelligence driven predictive modeling for repurposing drugs as potential antivirals against Epstein-Barr virus. Computational and structural biotechnology journal, 27, 1784.

Odugbemi AI, et al. (2025) Machine learning prediction of intestinal ?-glucosidase inhibitors using a diverse set of ligands: a drug repurposing effort with drugBank database screening. In silico pharmacology, 13(2), 95.

Shoombuatong W, et al. (2025) BGATT-GR: accurate identification of glucocorticoid receptor antagonists based on data augmentation combined with BiGRU-attention. Scientific reports, 15(1), 21402.

Alcázar JJ, et al. (2025) A Simple Machine Learning-Based Quantitative Structure-Activity Relationship Model for Predicting pIC50 Inhibition Values of FLT3 Tyrosine Kinase. Pharmaceuticals (Basel, Switzerland), 18(1).

Álvarez-Gómez C, et al. (2025) Design, synthesis, and in vitro evaluation of a carbamazepine derivative with antitumor potential in a model of Acute Lymphoblastic Leukemia. PloS one, 20(4), e0319415.

Ölander M, et al. (2025) A multi-strategy antimicrobial discovery approach reveals new ways to treat Chlamydia. PLoS biology, 23(4), e3003123.

Patil PA, et al. (2025) Structure based drug design and machine learning approaches for identifying natural inhibitors against the human ??III tubulin isotype. Scientific reports, 15(1), 32716.

Malik AA, et al. (2025) DeepEGFR a graph neural network for bioactivity classification of EGFR inhibitors. Scientific reports, 15(1), 38236.

Evangelista M, et al. (2025) New QSAR Models to Predict Human Transthyretin Disruption by Per- and Polyfluoroalkyl Substances (PFAS): Development and Application. Toxics, 13(7).

Sankar J, et al. (2025) ML enhanced bioactivity prediction for angiotensin II receptor: A potential anti-hypertensive drug target. Scientific reports, 15(1), 25367.

Schaduangrat N, et al. (2025) M3S-GRPred: a novel ensemble learning approach for the interpretable prediction of glucocorticoid receptor antagonists using a multi-step stacking strategy. BMC bioinformatics, 26(1), 117.

Aqeel I, et al. (2025) Drug repurposing targeting COVID-19 3CL protease using molecular docking and machine learning regression approaches. Scientific reports, 15(1), 18722.

Nikolopoulos A, et al. (2025) Ionization efficiency prediction of electrospray ionization mass spectrometry analytes based on molecular fingerprints and cumulative neutral losses. Journal of cheminformatics, 17(1), 183.

Illa SE, et al. (2025) Developing a predictive model for blood-brain-barrier permeability to explore relevance of in vitro neurotoxicity data for in vivo risk assessment. Frontiers in toxicology, 7, 1535112.

Le HV, et al. (2025) CaliciBoost: Performance-driven evaluation of molecular representations for caco-2 permeability prediction. Journal of cheminformatics, 17(1), 184.

Hsu KC, et al. (2025) A robust and interpretable graph neural network-based protocol for predicting p-glycoprotein substrates. Briefings in bioinformatics, 26(4).

Maliyakkal N, et al. (2025) Two-dimensional QSAR-driven virtual screening for potential therapeutics against Trypanosoma cruzi. Frontiers in chemistry, 13, 1600945.

Xiao M, et al. (2025) Drug molecular representations for drug response predictions: a comprehensive investigation via machine learning methods. Scientific reports, 15(1), 20.

Paixão VVM, et al. (2025) Novel Antischistosomal Drug Targets: Identification of Alkaloid Inhibitors of SmTGR via Integrated In Silico Methods. Pathogens (Basel, Switzerland), 14(6).

Omoboyede V, et al. (2025) Pharmacological assessment of Coffea arabica compounds as potential therapeutics for cervical cancer. Bioinformatics advances, 5(1), vbaf132.