

Resource Summary Report

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PaDEL-Descriptor

RRID:SCR_014272

Type: Tool

Proper Citation

PaDEL-Descriptor (RRID:SCR_014272)

Resource Information

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

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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 analysis software, software resource, software application, data processing software

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: 20260810T040622+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

Usage and Citation Metrics

We found 160 mentions in open access literature.

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

Nilewar SS, et al. (2026) An Integrated QSAR-MD-DCCM Pipeline: A Predictive Computational Platform for the Rational Design and Dynamic Functional Validation of Dual-Target Directed Ligands. *Pharmaceuticals* (Basel, Switzerland), 19(2).

Sharma D, et al. (2026) An integrative machine learning, explainable AI, molecular simulation, and cytotoxicity validation framework for the discovery of selective SIRT1 inhibitors against triple negative breast cancer. *Frontiers in bioinformatics*, 6, 1827014.

Morshed N, et al. (2026) Computational and Experimental Characterization of Mycobacterium marinum γ -Carbonic Anhydrase Inhibitors. *Bioinformatics and biology insights*, 20, 11779322261427120.

Wang NN, et al. (2026) A comprehensive evaluation of advanced methods for identifying structural alerts using extensive toxicity data. *Journal of cheminformatics*, 18(1), 27.

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).

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

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.

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

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.

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

Patil PA, et al. (2025) Structure based drug design and machine learning approaches for identifying natural inhibitors against the human γ -tubulin isotype. *Scientific reports*,

15(1), 32716.

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

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.

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).

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.

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

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.

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).