

Anita RÄicz

List of Publications by Year in descending order

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Version: 2024-02-01

36
papers

1,610
citations

516710

16
h-index

395702

33
g-index

37
all docs

37
docs citations

37
times ranked

2091
citing authors

#	ARTICLE	IF	CITATIONS
1	Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations?. Journal of Cheminformatics, 2015, 7, 20.	6.1	775
2	Effect of Dataset Size and Train/Test Split Ratios in QSAR/QSPR Multiclass Classification. Molecules, 2021, 26, 1111.	3.8	106
3	Consistency of QSAR models: Correct split of training and test sets, ranking of models and performance parameters. SAR and QSAR in Environmental Research, 2015, 26, 683-700.	2.2	85
4	Life beyond the Tanimoto coefficient: similarity measures for interaction fingerprints. Journal of Cheminformatics, 2018, 10, 48.	6.1	77
5	Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics. Molecules, 2019, 24, 2811.	3.8	61
6	Multivariate assessment of lipophilicity scalesâ€™ computational and reversed phase thin-layer chromatographic indices. Journal of Pharmaceutical and Biomedical Analysis, 2016, 127, 81-93.	2.8	54
7	Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR. Molecular Informatics, 2019, 38, e1800154.	2.5	34
8	Modelling methods and cross-validation variants in QSAR: a multi-level analysis^{\$}. SAR and QSAR in Environmental Research, 2018, 29, 661-674.	2.2	32
9	Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition?. RSC Advances, 2018, 8, 10-21.	3.6	30
10	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27
11	Quantitative determination of coenzyme Q10 from dietary supplements by FT-NIR spectroscopy and statistical analysis. Analytical and Bioanalytical Chemistry, 2015, 407, 2887-2898.	3.7	25
12	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 1: Theory and characteristicsâ€™. Journal of Cheminformatics, 2021, 13, 32.	6.1	25
13	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 2: speed, consistency, diversity selection. Journal of Cheminformatics, 2021, 13, 33.	6.1	24
14	Machine learning models for classification tasks related to drug safety. Molecular Diversity, 2021, 25, 1409-1424.	3.9	24
15	Comparison of antioxidant capacity assays with chemometric methods. Analytical Methods, 2015, 7, 4216-4224.	2.7	23
16	Comparison of Descriptor- and Fingerprint Sets in Machine Learning Models for ADME-Tox Targets. Frontiers in Chemistry, 0, 10, .	3.6	21
17	Quantitative determination and classification of energy drinks using near-infrared spectroscopy. Analytical and Bioanalytical Chemistry, 2016, 408, 6403-6411.	3.7	20
18	Binary similarity measures for fingerprint analysis of qualitative metabolomic profiles. Metabolomics, 2018, 14, 29.	3.0	17

#	ARTICLE	IF	CITATIONS
19	Large-scale evaluation of cytochrome P450 2C9 mediated drug interaction potential with machine learning-based consensus modeling. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 831-839.	2.9	17
20	Multicriteria decision making for evergreen problems in food science by sum of ranking differences. <i>Food Chemistry</i> , 2021, 344, 128617.	8.2	16
21	Comparison of Data Fusion Methods as Consensus Scores for Ensemble Docking. <i>Molecules</i> , 2019, 24, 2690.	3.8	14
22	Comparison of sensory evaluation techniques for Hungarian wines. <i>Journal of Chemometrics</i> , 2020, 34, e3219.	1.3	13
23	Differential Consistency Analysis: Which Similarity Measures can be Applied in Drug Discovery?. <i>Molecular Informatics</i> , 2021, 40, e2060017.	2.5	12
24	Classification of Hungarian medieval silver coins using x-ray fluorescent spectroscopy and multivariate data analysis. <i>Heritage Science</i> , 2013, 1, .	2.3	10
25	Extended many-item similarity indices for sets of nucleotide and protein sequences. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 3628-3639.	4.1	10
26	Molecular Dynamics Simulations and Diversity Selection by Extended Continuous Similarity Indices. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3415-3425.	5.4	9
27	Development and comparison of regression models for the determination of quality parameters in margarine spread samples using NIR spectroscopy. <i>Analytical Methods</i> , 2018, 10, 3089-3099.	2.7	7
28	Extended continuous similarity indices: theory and application for QSAR descriptor selection. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 157-173.	2.9	7
29	Effects of aging in oak barrels on the trans-resveratrol and anthocyanin concentration of red wines from Hungary. <i>Acta Alimentaria</i> , 2019, 48, 349-357.	0.7	6
30	A corneal-PAMPA-based in silico model for predicting corneal permeability. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2021, 203, 114218.	2.8	6
31	Discovery of d-amino acid oxidase inhibitors based on virtual screening against the lid-open enzyme conformation. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018, 28, 1693-1698.	2.2	4
32	Comprehensive chemometric classification of snack products based on their near infrared spectra. <i>LWT - Food Science and Technology</i> , 2020, 133, 110130.	5.2	4
33	Which Performance Parameters Are Best Suited to Assess the Predictive Ability of Models?. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2017, , 89-104.	0.6	4
34	Consensus Virtual Screening Identified [1,2,4]Triazolo[1,5-a]isoquinolines As MELK Inhibitor Chemotypes. <i>ChemMedChem</i> , 2021, , .	3.2	3
35	Synthesis and Biochemical Evaluation of Lid-Open D-Amino Acid Oxidase Inhibitors. <i>Molecules</i> , 2019, 24, 290.	3.8	1
36	Discrimination Ability of Assessors in Check-All-That-Apply Tests: Method and Product Development. <i>Foods</i> , 2021, 10, 1123.	4.3	0