DÃ¡vid Bajusz

List of Publications by Year
in descending order

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48	2,139	430874	243625
papers	citations	18 h-index	44 g-index

51	51	51	3134
all docs	docs citations	times ranked	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	One- Versus Two-Electron Oxidation with Peroxomonosulfate Ion: Reactions with Iron(II), Vanadium(IV), Halide Ions, and Photoreaction with Cerium(III). Inorganic Chemistry, 2009, 48, 1763-1773.	4.0	194
3	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. Leukemia, 2018, 32, 1135-1146.	7.2	112
4	Effect of Dataset Size and Train/Test Split Ratios in QSAR/QSPR Multiclass Classification. Molecules, 2021, 26, 1111.	3.8	106
5	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
6	Life beyond the Tanimoto coefficient: similarity measures for interaction fingerprints. Journal of Cheminformatics, 2018, 10, 48.	6.1	77
7	Direct Targeting Options for STAT3 and STAT5 in Cancer. Cancers, 2019, 11, 1930.	3.7	65
8	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2235-2259.	2.1	63
9	Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics. Molecules, 2019, 24, 2811.	3.8	61
10	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
11	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. Cancers, 2019, 11, 1757.	3.7	45
12	Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR. Molecular Informatics, 2019, 38, e1800154.	2.5	34
13	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
14	Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition?. RSC Advances, 2018, 8, 10-21.	3.6	30
15	An electrophilic warhead library for mapping the reactivity and accessibility of tractable cysteines in protein kinases. European Journal of Medicinal Chemistry, 2020, 207, 112836.	5.5	28
16	Exploring protein hotspots by optimized fragment pharmacophores. Nature Communications, 2021, 12, 3201.	12.8	28
17	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27
18	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

#	ARTICLE	IF	CITATIONS
19	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
20	Machine learning models for classification tasks related to drug safety. Molecular Diversity, 2021, 25, 1409-1424.	3.9	24
21	Discovery of Subtype Selective Janus Kinase (JAK) Inhibitors by Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 234-247.	5.4	23
22	DUckCov: a Dynamic Undockingâ€Based Virtual Screening Protocol for Covalent Binders. ChemMedChem, 2019, 14, 1011-1021.	3.2	18
23	Binary similarity measures for fingerprint analysis of qualitative metabolomic profiles. Metabolomics, 2018, 14, 29.	3.0	17
24	Multicriteria decision making for evergreen problems in food science by sum of ranking differences. Food Chemistry, 2021, 344, 128617.	8.2	16
25	Comparison of Data Fusion Methods as Consensus Scores for Ensemble Docking. Molecules, 2019, 24, 2690.	3.8	14
26	Differential Consistency Analysis: Which Similarity Measures can be Applied in Drug Discovery?. Molecular Informatics, 2021, 40, e2060017.	2.5	12
27	Comparison of classification methods with â€œn-classâ€•receiver operating characteristic curves: A case study of energy drinks. Chemometrics and Intelligent Laboratory Systems, 2016, 151, 34-43.	3.5	11
28	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
29	Human Serum Albumin Binding in a Vial: A Novel UV-pH Titration Method To Assist Drug Design. Journal of Medicinal Chemistry, 2020, 63, 1763-1774.	6.4	11
30	Discovery of a novel kinase hinge binder fragment by dynamic undocking. RSC Medicinal Chemistry, 2020, 11, 552-558.	3.9	10
31	Extended many-item similarity indices for sets of nucleotide and protein sequences. Computational and Structural Biotechnology Journal, 2021, 19, 3628-3639.	4.1	10
32	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 70, 275-283.	2.4	9
33	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
34	Molecular Dynamics Simulations and Diversity Selection by Extended Continuous Similarity Indices. Journal of Chemical Information and Modeling, 2022, 62, 3415-3425.	5.4	9
35	Identification of 8â€Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1â€Dependent Cells. Archiv Der Pharmazie, 2016, 349, 925-933.	4.1	7
36	Validation of tautomeric and protomeric binding modes by free energy calculations. A case study for the structure based optimization of d-amino acid oxidase inhibitors. Journal of Computer-Aided Molecular Design, 2018, 32, 331-345.	2.9	7

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37	Discovery of a Non-Nucleoside SETD2 Methyltransferase Inhibitor against Acute Myeloid Leukemia. International Journal of Molecular Sciences, 2021, 22, 10055.	4.1	7
38	Natural Apocarotenoids and Their Synthetic Glycopeptide Conjugates Inhibit SARS-CoV-2 Replication. Pharmaceuticals, 2021, 14, 1111.	3.8	7
39	Extended continuous similarity indices: theory and application for QSAR descriptor selection. Journal of Computer-Aided Molecular Design, 2022, 36, 157-173.	2.9	7
40	Property-based characterization of kinase-like ligand space for library design and virtual screening. MedChemComm, 2015, 6, 1898-1904.	3.4	6
41	The impact of binding site waters on the activity/selectivity trade-off of Janus kinase 2 (JAK2) inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 1497-1508.	3.0	5
42	Comprehensive chemometric classification of snack products based on their near infrared spectra. LWT - Food Science and Technology, 2020, 133, 110130.	5.2	4
43	Which Performance Parameters Are Best Suited to Assess the Predictive Ability of Models?. Challenges and Advances in Computational Chemistry and Physics, 2017, , 89-104.	0.6	4
44	Effect of An 84-bp Deletion of the Receptor-Binding Domain on the ACE2 Binding Affinity of the SARS-CoV-2 Spike Protein: An In Silico Analysis. Genes, 2021, 12, 194.	2.4	3
45	Consensus Virtual Screening Identified [1,2,4]Triazolo[1,5â€•b]isoquinolines As MELK Inhibitor Chemotypes. ChemMedChem, 2021, , .	3.2	3
46	Designed Peptide Inhibitors of STEP Phosphataseâ€“GluA2 AMPA Receptor Interaction Enhance the Cognitive Performance in Rats. Journal of Medicinal Chemistry, 2022, 65, 217-233.	6.4	3
47	Discrimination Ability of Assessors in Check-All-That-Apply Tests: Method and Product Development. Foods, 2021, 10, 1123.	4.3	0
48	Maximizing the integration of virtual and experimental screening in hit discovery. Expert Opinion on Drug Discovery, 0, , 1-12.	5.0	0