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	Extended continuous similarity indices: theory and application for QSAR descriptor selection. Journal of Computer-Aided Molecular Design, 2022, 36, 157-173.	2.9	7
2	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
3	Molecular Dynamics Simulations and Diversity Selection by Extended Continuous Similarity Indices. Journal of Chemical Information and Modeling, 2022, 62, 3415-3425.	5.4	9
4	Multicriteria decision making for evergreen problems in food science by sum of ranking differences. Food Chemistry, 2021, 344, 128617.	8.2	16
5	Effect of Dataset Size and Train/Test Split Ratios in QSAR/QSPR Multiclass Classification. Molecules, 2021, 26, 1111.	3.8	106
6	Differential Consistency Analysis: Which Similarity Measures can be Applied in Drug Discovery?. Molecular Informatics, 2021, 40, e2060017.	2.5	12
7	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
8	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
9	Exploring protein hotspots by optimized fragment pharmacophores. Nature Communications, 2021, 12, 3201.	12.8	28
10	Discrimination Ability of Assessors in Check-All-That-Apply Tests: Method and Product Development. Foods, 2021, 10, 1123.	4.3	0
11	Machine learning models for classification tasks related to drug safety. Molecular Diversity, 2021, 25, 1409-1424.	3.9	24
12	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
13	Discovery of a Non-Nucleoside SETD2 Methyltransferase Inhibitor against Acute Myeloid Leukemia. International Journal of Molecular Sciences, 2021, 22, 10055.	4.1	7
14	Extended many-item similarity indices for sets of nucleotide and protein sequences. Computational and Structural Biotechnology Journal, 2021, 19, 3628-3639.	4.1	10
15	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
16	Consensus Virtual Screening Identified [1,2,4]Triazolo[1,5â€•b]isoquinolines As MELK Inhibitor Chemotypes. ChemMedChem, 2021, , .	3.2	3
17	Natural Apocarotenoids and Their Synthetic Glycopeptide Conjugates Inhibit SARS-CoV-2 Replication. Pharmaceuticals, 2021, 14, 1111.	3.8	7
18	Comprehensive chemometric classification of snack products based on their near infrared spectra. LWT - Food Science and Technology, 2020, 133, 110130.	5.2	4

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19	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
20	Discovery of a novel kinase hinge binder fragment by dynamic undocking. RSC Medicinal Chemistry, 2020, 11, 552-558.	3.9	10
21	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
22	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
23	Comparison of Data Fusion Methods as Consensus Scores for Ensemble Docking. Molecules, 2019, 24, 2690.	3.8	14
24	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. Cancers, 2019, 11, 1757.	3.7	45
25	Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR. Molecular Informatics, 2019, 38, e1800154.	2.5	34
26	DUckCov: a Dynamic Undockingâ€Based Virtual Screening Protocol for Covalent Binders. ChemMedChem, 2019, 14, 1011-1021.	3.2	18
27	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
28	Direct Targeting Options for STAT3 and STAT5 in Cancer. Cancers, 2019, 11, 1930.	3.7	65
29	Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics. Molecules, 2019, 24, 2811.	3.8	61
30	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. Leukemia, 2018, 32, 1135-1146.	7.2	112
31	Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition?. RSC Advances, 2018, 8, 10-21.	3.6	30
32	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
33	Binary similarity measures for fingerprint analysis of qualitative metabolomic profiles. Metabolomics, 2018, 14, 29.	3.0	17
34	Life beyond the Tanimoto coefficient: similarity measures for interaction fingerprints. Journal of Cheminformatics, 2018, 10, 48.	6.1	77
35	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
36	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27

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37	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
38	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2235-2259.	2.1	63
39	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
40	Identification of 8â€Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1â€Ðependent Cells. Archiv Der Pharmazie, 2016, 349, 925-933.	4.1	7
41	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 70, 275-283.	2.4	9
42	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
43	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
44	Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations?. Journal of Cheminformatics, 2015, 7, 20.	6.1	775
45	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
46	Property-based characterization of kinase-like ligand space for library design and virtual screening. MedChemComm, 2015, 6, 1898-1904.	3.4	6
47	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
48	Maximizing the integration of virtual and experimental screening in hit discovery. Expert Opinion on Drug Discovery, 0, , 1-12.	5.0	0