Daniel Svozil

List of Publications by Year
in descending order

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58	4,906	218381	161609
papers	citations	26 h-index	54 g-index

63	63	63	5752
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	BioPhi: A platform for antibody design, humanization, and humanness evaluation based on natural antibody repertoires and deep learning. MAbs, 2022, 14, 2020203.	2.6	54
2	Novel D2/5-HT receptor modulators related to cariprazine with potential implication to schizophrenia treatment. European Journal of Medicinal Chemistry, 2022, 232, 114193.	2.6	5
3	New psychoactive substances on dark web markets: From deal solicitation to forensic analysis of purchased substances. Drug Testing and Analysis, 2021, 13, 156-168.	1.6	9
4	Pharmacokinetic, pharmacodynamic, and behavioural studies of deschloroketamine (DCK) in Wistar rats. British Journal of Pharmacology, 2021, , .	2.7	3
5	GenUI: interactive and extensible open source software platform for de novo molecular generation and cheminformatics. Journal of Cheminformatics, 2021, 13, 73.	2.8	7
6	Profiling and analysis of chemical compounds using pointwise mutual information. Journal of Cheminformatics, 2021, 13, 3.	2.8	2
7	NERDD: a web portal providing access to in silico tools for drug discovery. Bioinformatics, 2020, 36, 1291-1292.	1.8	46
8	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. Journal of Cheminformatics, 2020, 12, 39.	2.8	26
9	SYBA: Bayesian estimation of synthetic accessibility of organic compounds. Journal of Cheminformatics, 2020, 12, 35.	2.8	52
10	Can X-Ray Powder Diffraction Be a Suitable Forensic Method for Illicit Drug Identification?. Frontiers in Chemistry, 2020, 8, 499.	1.8	5
11	QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction. Journal of Cheminformatics, 2020, 12, 41.	2.8	14
12	An enumeration of natural products from microbial, marine and terrestrial sources. Physical Sciences Reviews, 2020, 5, .	0.8	13
13	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. Journal of Chemical Information and Modeling, 2019, 59, 3400-3412.	2.5	60
14	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. Frontiers in Chemistry, 2019, 7, 402.	1.8	57
15	Comment on â€œThe power metric: a new statistically robust enrichment-type metric for virtual screening applications with early recovery capabilityâ€• Journal of Cheminformatics, 2018, 10, 13.	2.8	2
16	A DNA structural alphabet provides new insight into DNA flexibility. Acta Crystallographica Section D: Structural Biology, 2018, 74, 52-64.	1.1	23
17	Probes & Drugs portal: an interactive, open data resource for chemical biology. Nature Methods, 2017, 14, 759-760.	9.0	59
18	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. Journal of Chemical Information and Modeling, 2017, 57, 1832-1846.	2.5	56

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19	Nonpher: computational method for design of hard-to-synthesize structures. Journal of Cheminformatics, 2017, 9, 20.	2.8	13
20	A DNA Structural Alphabet Distinguishes Structural Features of DNA Bound to Regulatory Proteins and in the Nucleosome Core Particle. Genes, 2017, 8, 278.	1.0	9
21	Activity-driven exploration of chemical space with morphing. , 2015, , .		0
22	Multiple 3D RNA Structure Superposition Using Neighbor Joining. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2015, 12, 520-530.	1.9	8
23	MultiSETTER: web server for multiple RNA structure comparison. BMC Bioinformatics, 2015, 16, 253.	1.2	10
24	InCHlib â€“ interactive cluster heatmap for web applications. Journal of Cheminformatics, 2014, 6, 44.	2.8	50
25	Bioinformatic analysis of the protein/DNA interface. Nucleic Acids Research, 2014, 42, 3381-3394.	6.5	51
26	Molpher: a software framework for systematic chemical space exploration. Journal of Cheminformatics, 2014, 6, 7.	2.8	32
27	Automatic workflow for the classification of local DNA conformations. BMC Bioinformatics, 2013, 14, 205.	1.2	17
28	Developing and Implementing a Combined Chemistry and Informatics Curriculum for Undergraduate and Graduate Students in the Czech Republic. Journal of Chemical Education, 2013, 90, 315-319.	1.1	6
29	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugarâ€“phosphate backbone and their comparison with modern density functional theory. Physical Chemistry Chemical Physics, 2013, 15, 7295.	1.3	33
30	MultiSETTER - Multiple RNA Structure Similarity Algorithm. Lecture Notes in Computer Science, 2013, , 59-70.	1.0	0
31	SETTER: web server for RNA structure comparison. Nucleic Acids Research, 2012, 40, W42-W48.	6.5	27
32	The DNA and RNA sugarâ€“phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. Physical Chemistry Chemical Physics, 2012, 14, 15257.	1.3	76
33	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. Journal of Chemical Theory and Computation, 2012, 8, 2448-2460.	2.3	67
34	Comment on â€œComputational Model for Predicting Experimental RNA and DNA Nearest-Neighbor Free Energy Rankingsâ€• Journal of Physical Chemistry B, 2012, 116, 8331-8332.	1.2	11
35	Efficient RNA pairwise structure comparison by SETTER method. Bioinformatics, 2012, 28, 1858-1864.	1.8	23
36	Understanding the role of base stacking in nucleic acids. MD and QM analysis of tandem GA base pairs in RNA duplexes. Physical Chemistry Chemical Physics, 2012, 14, 12580.	1.3	24

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37	Exploration of Chemical Space by Molecular Morphing. , 2011, , .		3
38	mmView: a web-based viewer of the mmCIF format. BMC Research Notes, 2011, 4, 121.	0.6	0
39	SETTER - RNA SEcondary sTructure-based TERtiary Structure Similarity Algorithm. Lecture Notes in Computer Science, 2011, , 37-48.	1.0	0
40	Conformational Energies of DNA Sugarâ^'Phosphate Backbone: Reference QM Calculations and a Comparison with Density Functional Theory and Molecular Mechanics. Journal of Chemical Theory and Computation, 2010, 6, 3817-3835.	2.3	17
41	Comparison of Intrinsic Stacking Energies of Ten Unique Dinucleotide Steps in A-RNA and B-DNA Duplexes. Can We Determine Correct Order of Stability by Quantum-Chemical Calculations?. Journal of Physical Chemistry B, 2010, 114, 1191-1203.	1.2	97
42	Reference MP2/CBS and CCSD(T) quantum-chemical calculations on stacked adenine dimers. Comparison with DFT-D, MP2.5, SCS(MI)-MP2, M06-2X, CBS(SCS-D) and force field descriptions. Physical Chemistry Chemical Physics, 2010, 12, 3522.	1.3	84
43	Balance of Attraction and Repulsion in Nucleic-Acid Base Stacking: CCSD(T)/Complete-Basis-Set-Limit Calculations on Uracil Dimer and a Comparison with the Force-Field Description. Journal of Chemical Theory and Computation, 2009, 5, 1524-1544.	2.3	51
44	Geometrical and Electronic Structure Variability of the Sugarâ^'phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	1.2	52
45	General Base Catalysis for Cleavage by the Active-Site Cytosine of the Hepatitis Delta Virus Ribozyme: QM/MM Calculations Establish Chemical Feasibility. Journal of Physical Chemistry B, 2008, 112, 11177-11187.	1.2	46
46	DNA conformations and their sequence preferences. Nucleic Acids Research, 2008, 36, 3690-3706.	6.5	177
47	Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of Î±/Î³ Conformers. Biophysical Journal, 2007, 92, 3817-3829.	0.2	2,036
48	The application of piecewise direct standardisation with variable selection to the correction of drift in inductively coupled atomic emission spectrometry. Journal of Analytical Atomic Spectrometry, 2006, 21, 1045.	1.6	17
49	Cluster Model for the Ionic Product of Water:â€‰ Accuracy and Limitations of Common Density Functional Methods. Journal of Physical Chemistry A, 2006, 110, 9194-9199.	1.1	30
50	Valence- and Dipole-Bound Anions of the Thymineâ^'Water Complex:â€‰ Ab Initio Characterization of the Potential Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 2916-2923.	1.1	22
51	Ab initio electronic structure of thymine anions. Physical Chemistry Chemical Physics, 2005, 7, 840.	1.3	35
52	Electron Binding to Nucleic Acid Bases. Experimental and Theoretical Studies. A Review. Collection of Czechoslovak Chemical Communications, 2004, 69, 1395-1428.	1.0	43
53	Variable reduction algorithm for atomic emission spectra: application to multivariate calibration and quantitative analysis of industrial samples. Journal of Analytical Atomic Spectrometry, 2002, 17, 800-812.	1.6	16
54	Comparison of traditional and multivariate calibration techniques applied to complex matrices using inductively coupled plasma atomic emission spectroscopy. Journal of Analytical Atomic Spectrometry, 2000, 15, 967-972.	1.6	26

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55	Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter. Journal of Chemical Information and Computer Sciences, 1997, 37, 338-342.	2.8	27
56	Introduction to multi-layer feed-forward neural networks. Chemometrics and Intelligent Laboratory Systems, 1997, 39, 43-62.	1.8	1,092
57	Electric resistance in a NafionÂ® membrane exposed to air after a step change in the relative humidity. Journal of Electroanalytical Chemistry, 1995, 385, 269-271.	1.9	38
58	Neural Network Prediction of Carbon-13 NMR Chemical Shifts of Alkanes. Journal of Chemical Information and Computer Sciences, 1995, 35, 924-928.	2.8	40