Sunghwan Kim

List of Publications by Year
in descending order

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59 papers	11,546 citations	279798 23 h-index	138484 58 g-index
59 all docs	59 docs citations	59 times ranked	15928 citing authors

#	Article	IF	Citations
1	PubChem Substance and Compound databases. Nucleic Acids Research, 2016, 44, D1202-D1213.	14.5	3,471
2	PubChem 2019 update: improved access to chemical data. Nucleic Acids Research, 2019, 47, D1102-D1109.	14.5	2,217
3	PubChem in 2021: new data content and improved web interfaces. Nucleic Acids Research, 2021, 49, D1388-D1395.	14.5	2,146
4	Database resources of the national center for biotechnology information. Nucleic Acids Research, 2022, 50, D20-D26.	14.5	887
5	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2021, 49, D10-D17.	14.5	545
6	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2019, 47, D23-D28.	14.5	502
7	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2020, 48, D9-D16.	14.5	381
8	PubChem3D: a new resource for scientists. Journal of Cheminformatics, 2011, 3, 32.	6.1	121
9	Getting the most out of PubChem for virtual screening. Expert Opinion on Drug Discovery, 2016, 11, 843-855.	5.0	98
10	PubChem3D: conformer ensemble accuracy. Journal of Cheminformatics, 2013, 5, 1.	6.1	96
11	Molecular structures of (trifluoromethyl)iodine dihalides CF3IX2 (X=F, Cl): ab initio and DFT calculations. Computational and Theoretical Chemistry, 2002, 587, 1-8.	1.5	88
12	PubChem chemical structure standardization. Journal of Cheminformatics, 2018, 10, 36.	6.1	83
13	PUG-SOAP and PUG-REST: web services for programmatic access to chemical information in PubChem. Nucleic Acids Research, 2015, 43, W605-W611.	14.5	80
14	An update on PUG-REST: RESTful interface for programmatic access to PubChem. Nucleic Acids Research, 2018, 46, W563-W570.	14.5	69
15	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	3.0	58
16	Literature information in PubChem: associations between PubChem records and scientific articles. Journal of Cheminformatics, 2016, 8, 32.	6.1	58
17	Microhydration of cytosine and its radical anion: Cytosineâˆ™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2007, 126, 064301.	3.0	52
18	Exploring Chemical Information in PubChem. Current Protocols, 2021, 1, e217.	2.9	42

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19	Effects of microsolvation on uracil and its radical anion: Uracilâˆ™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2006, 125, 144305.	3.0	41
20	PubChem3D: Conformer generation. Journal of Cheminformatics, 2011, 3, 4.	6.1	37
21	Effects of Microsolvation on the Adenineâ€'Uracil Base Pair and Its Radical Anion:Â Adenineâ€'Uracil Mono- and Dihydratesâ€. Journal of Physical Chemistry A, 2007, 111, 10381-10389.	2.5	29
22	PubChem3D: Similar conformers. Journal of Cheminformatics, 2011, 3, 13.	6.1	28
23	PubChem Protein, Gene, Pathway, and Taxonomy Data Collections: Bridging Biology and Chemistry through Target-Centric Views of PubChem Data. Journal of Molecular Biology, 2022, 434, 167514.	4.2	26
24	Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861.	2.8	23
25	PUG-View: programmatic access to chemical annotations integrated in PubChem. Journal of Cheminformatics, 2019, 11, 56.	6.1	23
26	A theoretical investigation into the conformational changes of dibenzo-p-dioxin, thianthrene, and selenanthrene. Journal of Molecular Structure, 2003, 655, 451-458.	3.6	19
27	PubChem3D: Biologically relevant 3-D similarity. Journal of Cheminformatics, 2011, 3, 26.	6.1	19
28	Effects of multiple conformers per compound upon 3-D similarity search and bioassay data analysis. Journal of Cheminformatics, 2012, 4, 28.	6.1	19
29	Finding Potential Multitarget Ligands Using PubChem. Methods in Molecular Biology, 2018, 1825, 63-91.	0.9	17
30	PubChem structureâ€“activity relationship (SAR) clusters. Journal of Cheminformatics, 2015, 7, 33.	6.1	16
31	Density Functional Calculations, Structure, and Vibrational Frequencies of 2-Cyclopenten-1-one in Its S0, S1(n,Ï€*), T1(n,Ï€*), and T2(Ï€,Ï€*) Statesâ€. Journal of Physical Chemistry A, 2003, 107, 10655-10659.	2.5	15
32	Predicting drug-metagenome interactions: Variation in the microbial Î²-glucuronidase level in the human gut metagenomes. PLoS ONE, 2021, 16, e0244876.	2.5	15
33	Ultraviolet absorption spectra, structure, vibrations, and theoretical calculations of 2-fluoro- and 3-fluoropyridine in their electronic excited states. Chemical Physics Letters, 2011, 514, 214-219.	2.6	14
34	PubChem3D: Diversity of shape. Journal of Cheminformatics, 2011, 3, 9.	6.1	14
35	Similar compounds versus similar conformers: complementarity between PubChem 2-D and 3-D neighboring sets. Journal of Cheminformatics, 2016, 8, 62.	6.1	14
36	Discovering and Summarizing Relationships Between Chemicals, Genes, Proteins, and Diseases in PubChem. Frontiers in Research Metrics and Analytics, 2021, 6, 689059.	1.9	14

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37	Teaching Cheminformatics through a Collaborative Intercollegiate Online Chemistry Course (OLCC). Journal of Chemical Education, 2021, 98, 416-425.	2.3	12
38	The molecular structure and conformation of bicyclo[3.3.1]nonan-9-one: ab initio and DFT calculations. Computational and Theoretical Chemistry, 2002, 619, 113-120.	1.5	11
39	Hydrogen-Atom Abstraction from the Adenineâ˜'Uracil Base Pairâ€. Journal of Physical Chemistry A, 2007, 111, 6806-6812.	2.5	11
40	Structures and Energetics of the Deprotonated Adenineâ˜'Uracil Base Pair, Including Proton-Transferred Systems. Journal of Physical Chemistry B, 2008, 112, 3545-3551.	2.6	11
41	Spectroscopic investigations and potential energy surfaces of the ground and excited electronic states of 1,3-benzodioxan. Journal of Chemical Physics, 2009, 131, 044302.	3.0	11
42	Vertical detachment energies of anionic thymidine: Microhydration effects. Journal of Chemical Physics, 2010, 133, 144305.	3.0	11
43	PubChem Periodic Table and Element pages: improving access to information on chemical elements from authoritative sources. Chemistry Teacher International, 2021, 3, 57-65.	1.7	11
44	Conformational stabilization of phthalan: physical origin of tiny ring-puckering barrier. Journal of Molecular Structure, 2002, 609, 159-167.	3.6	9
45	Conformations of Allyl Amine:â€‰ Theory vs Experiment. Journal of Physical Chemistry A, 2008, 112, 2120-2124.	2.5	9
46	Infrared, Raman, and Ultraviolet Absorption Spectra and Theoretical Calculations and Structure of 2,6-Difluoropyridine in Its Ground and Excited Electronic States. Journal of Physical Chemistry A, 2013, 117, 13596-13604.	2.5	9
47	PubChem3D: Shape compatibility filtering using molecular shape quadrupoles. Journal of Cheminformatics, 2011, 3, 25.	6.1	8
48	Theoretical molecular structures for weakly bound complexes HXâ‹¯Â·SO3 (X=F, Cl, Br): ab initio and DFT calculations. Chemical Physics Letters, 2002, 358, 121-129.	2.6	7
49	Hydration of the Lowest Triplet States of the DNA/RNA Pyrimidines. Journal of Chemical Theory and Computation, 2010, 6, 930-939.	5.3	7
50	Structures, Energetics, and Aromaticities of the Tetrasilacyclobutadiene Dianion and Related Compounds: (Si4H4)2â€“, (Si4H4)2â€“Â·2Li+, [Si4(SiH3)4]2â€“Â·2Li+, [Si4(SiH3)4]2â€“Â·2Na+, and [Si4(SiH3)4]2â€“Â·2K+. Journal of Physical Chemistry A, 2011, 115, 5478-5487.	2.7	7
51	Plant Reactome and PubChem: The Plant Pathway and (Bio)Chemical Entity Knowledgebases. Methods in Molecular Biology, 2022, 2443, 511-525.	0.9	7
52	Theoretical molecular structures for partially bonded complexes of trimethylamine with SO2 and SO3: ab initio and density functional theory calculations. Computational and Theoretical Chemistry, 2002, 594, 147-156.	1.5	6
53	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	3.0	6
54	Infrared, Raman, and ultraviolet absorption spectra and theoretical calculations and structure of 2,3,5,6-tetrafluoropyridine in its ground and excited electronic states. Chemical Physics, 2015, 456, 28-33.	1.9	4

#	Article	IF	Citations
55	Public Chemical Databases. , 2019, , 628-639.		4
56	Molecular structures of 2,3-diaza-1,3-butadiene and 2,3-diphospha-1,3-butadiene: ab initio and DFT calculations. Computational and Theoretical Chemistry, 2004, 685, 185-189.	1.5	3
57	Molecular structures of gauche and trans conformers for oxalyl chlorofluoride: ab initio and DFT calculations. Computational and Theoretical Chemistry, 2004, 711, 67-71.	1.5	2
58	Programmatic Retrieval of Small Molecule Information from PubChem Using PUG-REST. Methods in Pharmacology and Toxicology, 2018, , 1.	0.2	2
59	Fluorescence excitation and ultraviolet absorption spectra and theoretical calculations for benzocyclobutane: Vibrations and structure of its excited S1(Ï€,Ï€*) electronic state. Journal of Chemical Physics, 2014, 140, 034305.	3.0	1