Sunghwan Kim

List of Publications by Year
in descending order

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	Database resources of the national center for biotechnology information. Nucleic Acids Research, 2022, 50, D20-D26.	14.5	887
2	Plant Reactome and PubChem: The Plant Pathway and (Bio)Chemical Entity Knowledgebases. Methods in Molecular Biology, 2022, 2443, 511-525.	0.9	7
3	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
4	PubChem in 2021: new data content and improved web interfaces. Nucleic Acids Research, 2021, 49, D1388-D1395.	14.5	2,146
5	Teaching Cheminformatics through a Collaborative Intercollegiate Online Chemistry Course (OLCC). Journal of Chemical Education, 2021, 98, 416-425.	2.3	12
6	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2021, 49, D10-D17.	14.5	545
7	Predicting drug-metagenome interactions: Variation in the microbial Î²-glucuronidase level in the human gut metagenomes. PLoS ONE, 2021, 16, e0244876.	2.5	15
8	Discovering and Summarizing Relationships Between Chemicals, Genes, Proteins, and Diseases in PubChem. Frontiers in Research Metrics and Analytics, 2021, 6, 689059.	1.9	14
9	Exploring Chemical Information in PubChem. Current Protocols, 2021, 1, e217.	2.9	42
10	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
11	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2020, 48, D9-D16.	14.5	381
12	Public Chemical Databases. , 2019, , 628-639.		4
13	PUG-View: programmatic access to chemical annotations integrated in PubChem. Journal of Cheminformatics, 2019, 11, 56.	6.1	23
14	Database resources of the National Center for Biotechnology Information. Nucleic Acids Research, 2019, 47, D23-D28.	14.5	502
15	PubChem 2019 update: improved access to chemical data. Nucleic Acids Research, 2019, 47, D1102-D1109.	14.5	2,217
16	Finding Potential Multitarget Ligands Using PubChem. Methods in Molecular Biology, 2018, 1825, 63-91.	0.9	17
17	Programmatic Retrieval of Small Molecule Information from PubChem Using PUG-REST. Methods in Pharmacology and Toxicology, 2018, , 1.	0.2	2
18	An update on PUG-REST: RESTful interface for programmatic access to PubChem. Nucleic Acids Research, 2018, 46, W563-W570.	14.5	69

#	Article	IF	Citations
19	PubChem chemical structure standardization. Journal of Cheminformatics, 2018, 10, 36.	6.1	83
20	Literature information in PubChem: associations between PubChem records and scientific articles. Journal of Cheminformatics, 2016, 8, 32.	6.1	58
21	Getting the most out of PubChem for virtual screening. Expert Opinion on Drug Discovery, 2016, 11, 843-855.	5.0	98
22	Similar compounds versus similar conformers: complementarity between PubChem 2-D and 3-D neighboring sets. Journal of Cheminformatics, 2016, 8, 62.	6.1	14
23	PubChem Substance and Compound databases. Nucleic Acids Research, 2016, 44, D1202-D1213.	14.5	3,471
24	PubChem structureâ€“activity relationship (SAR) clusters. Journal of Cheminformatics, 2015, 7, 33.	6.1	16
25	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
26	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
27	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
28	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
29	PubChem3D: conformer ensemble accuracy. Journal of Cheminformatics, 2013, 5, 1.	6.1	96
30	Effects of multiple conformers per compound upon 3-D similarity search and bioassay data analysis. Journal of Cheminformatics, 2012, 4, 28.	6.1	19
31	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.	2.6	7
32	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
33	PubChem3D: Similar conformers. Journal of Cheminformatics, 2011, 3, 13.	6.1	28
34	PubChem3D: Shape compatibility filtering using molecular shape quadrupoles. Journal of Cheminformatics, 2011, 3, 25.	6.1	8
35	PubChem3D: Biologically relevant 3-D similarity. Journal of Cheminformatics, 2011, 3, 26.	6.1	19
36	PubChem3D: a new resource for scientists. Journal of Cheminformatics, 2011, 3, 32.	6.1	121

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37	PubChem3D: Conformer generation. Journal of Cheminformatics, 2011, 3, 4.	6.1	37
38	PubChem3D: Diversity of shape. Journal of Cheminformatics, 2011, 3, 9.	6.1	14
39	Vertical detachment energies of anionic thymidine: Microhydration effects. Journal of Chemical Physics, 2010, 133, 144305.	3.0	11
40	Hydration of the Lowest Triplet States of the DNA/RNA Pyrimidines. Journal of Chemical Theory and Computation, 2010, 6, 930-939.	5.3	7
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	Conformations of Allyl Amine:â€‰ Theory vs Experiment. Journal of Physical Chemistry A, 2008, 112, 2120-2124.	2.5	9
43	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
44	Microhydration of cytosine and its radical anion: Cytosineâ^™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2007, 126, 064301.	3.0	52
45	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
46	Hydrogen-Atom Abstraction from the Adenineâ^'Uracil Base Pairâ€. Journal of Physical Chemistry A, 2007, 111, 6806-6812.	2.5	11
47	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	3.0	58
48	Effects of microsolvation on uracil and its radical anion: Uracilâ^™(H2O)n (n=1â€“5). Journal of Chemical Physics, 2006, 125, 144305.	3.0	41
49	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	3.0	6
50	Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861.	2.8	23
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	Conformational stabilization of phthalan: physical origin of tiny ring-puckering barrier. Journal of Molecular Structure, 2002, 609, 159-167.	3.6	9
59	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