Govindan Subramanian

List of Publications by Year
in descending order

38 papers	1,302 citations	516215 16 h-index	344852 36 g-index
40 all docs	40 docs citations	40 times ranked	1291 citing authors

#	Article	IF	Citations
1	Computational Modeling of Î²-Secretase 1 (BACE-1) Inhibitors Using Ligand Based Approaches. Journal of Chemical Information and Modeling, 2016, 56, 1936-1949.	2.5	166
2	Are the Most Stable Fused Heterobicycles the Most Aromatic?. Angewandte Chemie International Edition in English, 1996, 35, 2638-2641.	4.4	165
3	Cationâˆ'Ï€ Interactions:â€‰ An Energy Decomposition Analysis and Its Implication in Î´-Opioid Receptorâˆ'Ligand Binding. Journal of the American Chemical Society, 2002, 124, 4832-4837.	6.6	131
4	Potent and Selective Indolomorphinan Antagonists of the Kappa-Opioid Receptor. Journal of Medicinal Chemistry, 2000, 43, 2759-2769.	2.9	106
5	Aromaticity of Annelated Borepins. Organometallics, 1997, 16, 2362-2369.	1.1	96
6	Molecular Docking Reveals a Novel Binding Site Model for Fentanyl at the Î¼-Opioid Receptor. Journal of Medicinal Chemistry, 2000, 43, 381-391.	2.9	92
7	Computational models to predict bloodâ€“brain barrier permeation and CNS activity. Journal of Computer-Aided Molecular Design, 2003, 17, 643-664.	1.3	69
8	Conformational Analysis and Automated Receptor Docking of Selective Arylacetamide-Based Îº-Opioid Agonists. Journal of Medicinal Chemistry, 1998, 41, 4777-4789.	2.9	56
9	Decisive Evidence for Nonclassical Bonding in Five-Vertexcloso-Boranes, X2B3H3, X = N, CH, P, SiH, BH-. Journal of the American Chemical Society, 1996, 118, 9988-9989.	6.6	51
10	Carbene Analogues of Boron Stabilized by Neighboring Bï£¿B Moieties: Doubly Aromatic Bishomotriboriranides. Angewandte Chemie International Edition in English, 1997, 36, 1469-1472.	4.4	50
11	The Remarkably Stabilized Trilithiocyclopropenium Ion, C3Li3+, and Its Relatives. Journal of the American Chemical Society, 1997, 119, 9504-9512.	6.6	35
12	A Diboracyclopropane with a Planar-Tetracoordinate Carbon Atom and a Triborabicyclobutane. Angewandte Chemie - International Edition, 2003, 42, 671-674.	7.2	29
13	Computational approaches for modeling human intestinal absorption and permeability. Journal of Molecular Modeling, 2006, 12, 577-589.	0.8	29
14	Haben die stabilsten anellierten Heterobicyclen auch den stÃrksten aromatischen Charakter?. Angewandte Chemie, 1996, 108, 2824-2827.	1.6	17
15	Exotic Structures of Si2B2H4. Journal of Physical Chemistry A, 1997, 101, 919-925.	1.1	17
16	Deciphering the Allosteric Binding Mechanism of the Human Tropomyosin Receptor Kinase A (hTrkA) Inhibitors. ACS Chemical Biology, 2019, 14, 1205-1216.	1.6	16
17	1,2-Diboretanides: Homoaromatic 2Ï€-Electron Compounds with High Inversion Barriers. Angewandte Chemie International Edition in English, 1996, 35, 1990-1992.	4.4	13
18	Internal conrotation and disrotation in H2BCH2BH2 and diborylmethane 1,3 H exchange. Journal of Computational Chemistry, 1997, 18, 1792-1803.	1.5	12

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19	Computational Modeling of Kinase Inhibitor Selectivity. ACS Medicinal Chemistry Letters, 2010, 1, 395-399.	1.3	11
20	Allosteric antagonist binding sites in class B GPCRs: corticotropin receptor 1. Journal of Computer-Aided Molecular Design, 2010, 24, 659-674.	1.3	11
21	Contrasting Structures of Pyramidal Carbocations and Their Silicon Analogues. Angewandte Chemie International Edition in English, 1993, 32, 865-867.	4.4	10
22	Skeletal Bonding incloso-1,5-X2B3Y3(X = N, CH, P, SiH; Y = NH2, CH3, H) Cages Is Dictated by Boron Substituents. Organometallics, 1998, 17, 1634-1636.	1.1	10
23	Connecting the conformational behavior of cyclic octadepsipeptides with their ionophoric property and membrane permeability. Organic and Biomolecular Chemistry, 2020, 18, 7110-7126.	1.5	9
24	4 Molecular Modeling of Opioid Receptor-Ligand Complexes. Progress in Medicinal Chemistry, 2002, 40, 107-135.	4.1	8
25	Ein Diboracyclopropan mit planar-tetrakoordiniertem Kohlenstoffatom und ein Triborabicyclobutan. Angewandte Chemie, 2003, 115, 695-698.	1.6	7
26	An integrated computational workflow for efficient and quantitative modeling of renin inhibitors. Bioorganic and Medicinal Chemistry, 2012, 20, 851-858.	1.4	7
27	1, 2â€Diboretanide: homoaromatische 2Ï€â€Elektronenâ€Verbindungen mit hohen Inversionsbarrieren. Angewandte Chemie, 1996, 108, 2123-2125.	1.6	6
28	Type 2 inhibitor leads of human tropomyosin receptor kinase (hTrkA). Bioorganic and Medicinal Chemistry Letters, 2019, 29, 126624.	1.0	5
29	Lead identification and characterization of hTrkA type 2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 126680.	1.0	5
30	In Pursuit of an Allosteric Human Tropomyosin Kinase A (hTrkA) Inhibitor for Chronic Pain. ACS Medicinal Chemistry Letters, 2021, 12, 1847-1852.	1.3	5
31	Integrated Approaches to Perform In Silico Drug Discovery. Current Drug Discovery Technologies, 2006, 3, 189-197.	0.6	4
32	Vergleich der Strukturen von pyramidalen Carbokationen und ihren Siliciumanaloga. Angewandte Chemie, 1993, 105, 921-923.	1.6	3
33	Comprehending renin inhibitorâ€™s binding affinity using structure-based approaches. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6667-6672.	1.0	3
34	Computational modeling and design of renin inhibitors. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 460-465.	1.0	3
35	In silico ligandâ€based modeling of <scp>hBACE</scp>â€1 inhibitors. Chemical Biology and Drug Design, 2018, 91, 817-827.	1.5	3
36	Synthetic inhibitor leads of human tropomyosin receptor kinase A (hTrkA). RSC Medicinal Chemistry, 2020, 11, 370-377.	1.7	1

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37	Computational approaches for modeling human intestinal absorption and permeability. , 0, , 577-589.		1
38	Integrated Web-Based ab initio Modeling Platform for G-protein Coupled Receptors. Letters in Drug Design and Discovery, 2011, 8, 159-171.	0.4	0