

# Saber Mirzaei

## List of Publications by Year in descending order

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29  
papers

281  
citations

933410

10  
h-index

996954

15  
g-index

30  
all docs

30  
docs citations

30  
times ranked

341  
citing authors

#	ARTICLE	IF	CITATIONS
1	Improving Performance of the SMD Solvation Model: Bondi Radii Improve Predicted Aqueous Solvation Free Energies of Ions and $pK_a$ Values of Thiols. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9498-9504.	2.5	37
2	Highly Selective Synthesis of Pillar[5]arene ( $n = 5, 6$ ). <i>Organic Letters</i> , 2018, 20, 6583-6586.	4.6	24
3	Conjugated Molecular Nanotubes. <i>Chemistry - A European Journal</i> , 2021, 27, 8642-8655.	3.3	23
4	Predicting the regioselectivity of nucleophilic addition to arynes using frontier molecular orbital contribution analysis. <i>Tetrahedron Letters</i> , 2017, 58, 3362-3365.	1.4	21
5	Comprehensive insights into the structure and coordination behavior of thiosemicarbazone ligands: a computational assessment of the E-Z interconversion mechanism during coordination. <i>New Journal of Chemistry</i> , 2015, 39, 9313-9324.	2.8	19
6	Regioselectivity in the Scholl Reaction: Mono and Double [7]Helicenes. <i>Organic Letters</i> , 2021, 23, 5170-5174.	4.6	17
7	The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites. <i>Journal of Molecular Modeling</i> , 2016, 22, 270.	1.8	12
8	Tubularenes. <i>Chemical Science</i> , 2020, 11, 8089-8094.	7.4	12
9	Mechanistic study of the hydrolytic degradation and protonation of temozolomide. <i>RSC Advances</i> , 2015, 5, 41112-41119.	3.6	11
10	Mechanism-Based Inactivation of Cytochrome P450 Enzymes: Computational Insights. <i>Chemical Research in Toxicology</i> , 2021, 34, 959-987.	3.3	11
11	Nonspherical anion sequestration by C-H hydrogen bonding. <i>Chemical Science</i> , 2022, 13, 2026-2032.	7.4	10
12	An electron-transfer induced conformational transformation: from non-cofacial $\pi$ - $\pi$ to cofacial $\pi$ - $\pi$ in cyclotetraveratrylene (CTTV) and formation of charge transfer complexes. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5712-5717.	2.8	9
13	Synthesis of Spiro[chromene-imidazo[1,2-a]pyridin]-3-imines via 6-exo-dig Cyclization Reaction. <i>Journal of Organic Chemistry</i> , 2021, 86, 13693-13701.	3.2	9
14	Mechanistic study of allopurinol oxidation using aldehyde oxidase, xanthine oxidase and cytochrome P450 enzymes. <i>RSC Advances</i> , 2016, 6, 109672-109680.	3.6	8
15	Molecular Actuators in Action: Electron-Transfer-Induced Conformation Transformation in Cofacially Arrayed Polyfluorenes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4233-4238.	4.6	7
16	Predicting the regioselectivity of arynes: a simple model based on orbital electronegativity. <i>New Journal of Chemistry</i> , 2019, 43, 1130-1133.	2.8	7
17	Electron-Transfer-Induced Self-Assembly of a Molecular Tweezer Platform. <i>Chemistry - A European Journal</i> , 2020, 26, 14085-14089.	3.3	7
18	Radially Oriented [5]Cyclo-meta-phenylenes. <i>Organic Letters</i> , 2021, 23, 87-92.	4.6	7

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19	An Electron-Rich Calix[4]arene-Based Receptor with Unprecedented Binding Affinity for Nitric Oxide. <i>Chemistry - A European Journal</i> , 2018, 24, 17439-17443.	3.3	6
20	Proton shuttle efficiency of bicarbonate: A theoretical study on tautomerization and CO <sub>2</sub> hydration. <i>Tetrahedron</i> , 2019, 75, 130693.	1.9	5
21	Ï-Extended dibenzo[ <i>g</i> , <i>p</i> ]chrysenes. <i>Organic Chemistry Frontiers</i> , 2021, 8, 2393-2401.	4.5	5
22	Rhodium-Catalyzed Regio- and Diastereoselective Hydroarylation of Allenes: An Unprecedented Ene Reaction. <i>ACS Catalysis</i> , 2021, 11, 14570-14574.	11.2	5
23	Angular ladder-type <i>meta</i> -phenylenes: synthesis and electronic structural analysis. <i>Organic Chemistry Frontiers</i> , 2020, 7, 3215-3222.	4.5	4
24	Redox-Induced Molecular Actuators: The Case of Oxy-Alternate Bridged Cyclotetraveratrylene. <i>Organic Letters</i> , 2019, 21, 7987-7991.	4.6	2
25	Conformational switch in the crystal states of a calix[4]arene. <i>CrystEngComm</i> , 2021, 23, 1906-1911.	2.6	2
26	Importance of Azo-Hydrazo Tautomerization in the Oxidative Degradation of Procarbazine by Cytochrome P450: Computational Insights. <i>ChemistrySelect</i> , 2018, 3, 6042-6049.	1.5	1
27	Modified Newman projections: A new representation of the Newman notations to convey conformational properties. <i>Educacion Quimica</i> , 2016, 27, 269-277.	0.1	0
28	Accessing highly electron-rich calix[n]arene (n = 4 and 8) derivatives from acid-catalyzed condensation of 1,3,5-tripropoxybenzene. <i>Tetrahedron Letters</i> , 2019, 60, 151215.	1.4	0
29	Decarboxylative Cyclization of Proline with <i>o</i> -Alkynylbenzaldehyde through an Unexploited Ï-Electrocyclization: A DFT Study. <i>Journal of Organic Chemistry</i> , 0, , .	3.2	0