

Kim Baldridge

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

241
papers

25,604
citations

49
h-index

159
g-index

276
ext. papers

27,003
ext. citations

7.7
avg, IF

6.2
L-index

#	Paper	IF	Citations
241	General atomic and molecular electronic structure system. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1347-1363	3.5	17180
240	The structure of the chromophore within DsRed, a red fluorescent protein from coral. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000 , 97, 11990-5	11.5	509
239	Ab initio reaction paths and direct dynamics calculations. <i>The Journal of Physical Chemistry</i> , 1989 , 93, 5107-5119		309
238	Proton-catalyzed, silane-fueled Friedel-Crafts coupling of fluoroarenes. <i>Science</i> , 2011 , 332, 574-7	33.3	248
237	Structure/energy correlation of bowl depth and inversion barrier in corannulene derivatives: combined experimental and quantum mechanical analysis. <i>Journal of the American Chemical Society</i> , 2001 , 123, 517-25	16.4	246
236	Synthesis and dynamics of the corannulene nucleus. <i>Journal of the American Chemical Society</i> , 1992 , 114, 1921-1923	16.4	213
235	Algorithms and accuracy requirements for computing reaction paths by the method of steepest descent. <i>The Journal of Physical Chemistry</i> , 1988 , 92, 1476-1488		182
234	First principles implementation of solvent effects without outlying charge error. <i>Journal of Chemical Physics</i> , 1997 , 106, 6622-6633	3.9	177
233	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 2030-48	6.4	149
232	Potentially aromatic metallocycles. <i>Journal of the American Chemical Society</i> , 1988 , 110, 4204-4208	16.4	136
231	Induced-fit catalysis of corannulene bowl-to-bowl inversion. <i>Nature Chemistry</i> , 2014 , 6, 222-8	17.6	122
230	Multiethynyl corannulenes: synthesis, structure, and properties. <i>Journal of the American Chemical Society</i> , 2008 , 130, 10729-39	16.4	118
229	Synthesis and Characterization of the First Corannulene Cyclophane. <i>Journal of the American Chemical Society</i> , 1996 , 118, 2754-2755	16.4	118
228	Synthesis of fluoranthenes and indenocorannulenes: elucidation of chiral stereoisomers on the basis of static molecular bowls. <i>Journal of the American Chemical Society</i> , 2006 , 128, 6870-84	16.4	117
227	Bond alternation in triannelated benzenes: dissection of cyclic .pi. from Mills-Nixon effects. <i>Journal of the American Chemical Society</i> , 1992 , 114, 9583-9587	16.4	116
226	Synthesis and characterization of open and sandwich-type polyoxometalates reveals visible-light-driven water oxidation via POM-photosensitizer complexes. <i>Green Chemistry</i> , 2012 , 14, 1680 ¹⁰		114
225	Hexahapto Metal Coordination to Curved Polyaromatic Hydrocarbon Surfaces: The First Transition Metal Corannulene Complex. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4781-4782	16.4	114

224	Through-space interactions between face-to-face, center-to-edge oriented arenes: importance of polar-pi effects. <i>Organic and Biomolecular Chemistry</i> , 2003 , 1, 157-62	3.9	106
223	X-Ray Diffraction Evidence for a Cyclohexatriene Motif in the Molecular Structure of Tris(bicyclo[2.1.1]hexeno)benzene: Bond Alternation after the Refutation of the Mills-Nixon Theory. <i>Angewandte Chemie International Edition in English</i> , 1995 , 34, 1454-1456		106
222	The Silabenzenes: Structure, Properties, and Aromaticity. <i>Organometallics</i> , 2000 , 19, 1477-1487	3.8	105
221	Molecular spur gears comprising triptycene rotators and bibenzimidazole-based stators. <i>Journal of the American Chemical Society</i> , 2012 , 134, 1528-35	16.4	101
220	Flexibility and molecular recognition in the immune system. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003 , 100, 92-7	11.5	101
219	Mechanism of photocatalytic hydrogen generation by a polypyridyl-based cobalt catalyst in aqueous solution. <i>Inorganic Chemistry</i> , 2015 , 54, 646-57	5.1	94
218	A simple model system for the study of carbohydrate--aromatic interactions. <i>Journal of the American Chemical Society</i> , 2007 , 129, 2890-900	16.4	94
217	Transition state structure, barrier height, and vibrational frequencies for the reaction $Cl+CH_4 \rightarrow H_3+HCl$. <i>Journal of Chemical Physics</i> , 1989 , 90, 7137-7142	3.9	93
216	C-F activation of fluorobenzene by silylium carboranes: evidence for incipient phenyl cation reactivity. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 7519-22	16.4	86
215	Uncatalyzed peptide bond formation in the gas phase. <i>The Journal of Physical Chemistry</i> , 1992 , 96, 8340-8351		85
214	Synthesis and Characterization of Trisbicyclo[2.1.1]hexabenzene, a Highly Strained Bicycloannelated Benzene. <i>Journal of the American Chemical Society</i> , 1995 , 117, 2102-2103	16.4	84
213	Correlation of Empirical (TMS) and Absolute NMR Chemical Shifts Predicted by ab Initio Computations. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 4038-4042	2.8	83
212	Modulating the Lewis acidity of boron using a photoswitch. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 5034-7	16.4	82
211	Through-space interactions between parallel-offset arenes at the van der Waals distance: 1,8-diarylbiophenylene syntheses, structure and QM computations. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 2686-94	3.6	81
210	Synthesis and Quantum Mechanical Structure of sym-Pentamethylcorannulene and Decamethylcorannulene. <i>Journal of the American Chemical Society</i> , 1999 , 121, 7439-7440	16.4	79
209	Tunable star-shaped triphenylamine fluorophores for fluorescence quenching detection and identification of nitro-aromatic explosives. <i>Chemical Communications</i> , 2013 , 49, 780-2	5.8	78
208	Molecular design, chemical synthesis, kinetic studies, calculations, and biological studies of novel enediynes equipped with triggering, detection, and deactivating devices. Model dynamycin A epoxide and cis-diol systems. <i>Journal of the American Chemical Society</i> , 1993 , 115, 7944-7953	16.4	78
207	Synthesis and properties of sym-pentasubstituted derivatives of corannulene. <i>Organic Letters</i> , 2003 , 5, 713-6	6.2	77

206	Effect of molecular packing on corannulene-based materials electroluminescence. <i>Journal of the American Chemical Society</i> , 2011 , 133, 14002-9	16.4	74
205	The Structure of Hexabenzotriphenylene and the Problem of Overcrowded D _{3h} Polycyclic Aromatic Compounds. <i>Journal of the American Chemical Society</i> , 1999 , 121, 727-733	16.4	73
204	Synthesis of 2,6-diarylphenyldimethylsilyl cations: polar-pi distribution of cation character. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 1719-22	16.4	69
203	Corannulene-based fullerene fragments C ₂₀ H ₁₀ -C ₅₀ H ₁₀ : when does a buckybowl become a buckytube?. <i>Theoretical Chemistry Accounts</i> , 1997 , 97, 67-71	1.9	66
202	Isochorismate pyruvate lyase: a pericyclic reaction mechanism?. <i>Journal of the American Chemical Society</i> , 2005 , 127, 15002-3	16.4	65
201	Dodecamethoxy- and hexaoxotricyclobutabenzene: synthesis and characterization. <i>Journal of the American Chemical Society</i> , 2006 , 128, 10032-3	16.4	65
200	Reversible phase transitions in a buckybowl monolayer. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 1966-9	16.4	64
199	d ⁸ rhodium and iridium complexes of corannulene. <i>Journal of the American Chemical Society</i> , 2006 , 128, 10644-5	16.4	64
198	Corannulylene Pentapetalae. <i>Journal of the American Chemical Society</i> , 2019 , 141, 5402-5408	16.4	63
197	Thiophene-fused bowl-shaped polycyclic aromatics with a dibenzo[a,g]corannulene core for organic field-effect transistors. <i>Chemical Communications</i> , 2015 , 51, 1681-4	5.8	63
196	Structural, optical, and electrochemical properties of three-dimensional push-pull corannulenes. <i>Journal of Organic Chemistry</i> , 2012 , 77, 11014-26	4.2	60
195	Corannulene derivatives as non-fullerene acceptors in solution-processed bulk heterojunction solar cells. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 20515-20519	13	56
194	Intramolecular halogen stabilization of silylium ions directs gearing dynamics. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7828-9	16.4	50
193	Rearrangement of Iridabenzvalenes to Iridabenzenes and/or β -Cyclopentadienyliridium(I) Complexes: Experimental and Computational Analysis of the Influence of Silyl Ring Substituents and Phosphine Ligands. <i>Organometallics</i> , 2007 , 26, 3957-3968	3.8	50
192	QMView: a computational chemistry three-dimensional visualization tool at the interface between molecules and mankind. <i>Journal of Molecular Graphics</i> , 1995 , 13, 63-6, 61		49
191	Synthesis of trioxatricornan and derivatives. Useful keystones for the construction of rigid molecular cavities. <i>Journal of Organic Chemistry</i> , 1992 , 57, 61-69	4.2	47
190	Steric isotope effects gauged by the bowl-inversion barrier in selectively deuterated pentaarylcorannulenes. <i>Journal of the American Chemical Society</i> , 2008 , 130, 1583-91	16.4	46
189	Stereoselective coordination of C ₅ -symmetric corannulene derivatives with an enantiomerically pure [Rh(I)(nbd*)] metal complex. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 865-7	16.4	45

188	Ionization of corannulene and 1,6-dimethylcorannulene: photoelectron spectra, electrochemistry, charge transfer bands and ab initio computations. <i>Tetrahedron Letters</i> , 2000 , 41, 4519-4522	2	45
187	Quantum mechanical designs toward planar delocalized cyclooctatetraene: a new target for synthesis. <i>Journal of the American Chemical Society</i> , 2001 , 123, 1755-9	16.4	45
186	Extended Corannulenes: Aromatic Bowl/Sheet Hybridization. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10792-6	16.4	44
185	Theoretical Studies of Silicon Chemistry. <i>Annual Review of Physical Chemistry</i> , 1987 , 38, 211-252	15.7	44
184	C?F Activation of Fluorobenzene by Silylium Carboranes: Evidence for Incipient Phenyl Cation Reactivity. <i>Angewandte Chemie</i> , 2010 , 122, 7681-7684	3.6	41
183	New perspectives on polyoxometalate catalysts: alcohol oxidation with Zn/Sb-polyoxotungstates. <i>Chemistry - A European Journal</i> , 2012 , 18, 13293-8	4.8	40
182	A Framework for the Design and Reuse of Grid Workflows. <i>Lecture Notes in Computer Science</i> , 2005 , 120-133	1.3	40
181	The Nature of the Long Bond in 3,8-Dichloro-1,1,2,2-tetraphenylcyclobuta[b]naphthene. <i>Journal of the American Chemical Society</i> , 1998 , 120, 6167-6168	16.4	40
180	Balancing steric and electronic factors in push-pull benzenes: an ab initio study on the molecular structure of 1,3,5-triamino-2,4,6-trinitrobenzene and related compounds. <i>Journal of the American Chemical Society</i> , 1993 , 115, 10782-10785	16.4	40
179	Synthesis, structure and properties of decakis(phenylthio)corannulene. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 53-5	3.9	39
178	Large Induced Interface Dipole Moments without Charge Transfer: Buckybowls on Metal Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2805-2809	6.4	39
177	Pentaindenocorannulene: Properties, Assemblies, and C Complex. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 14648-14652	16.4	39
176	Synthesis, structure, and dynamics of endo-(starphenylene)chromium tricarbonyl derivatives: observation of metal-arene migration and hindered metal-tripod rotation. <i>Journal of the American Chemical Society</i> , 1993 , 115, 6138-6142	16.4	38
175	Cobalt complexes of tetradentate, bipyridine-based macrocycles: their structures, properties and photocatalytic proton reduction. <i>Dalton Transactions</i> , 2016 , 45, 1737-45	4.3	37
174	Competition between π -arene and lone-pair halogen coordination of silylium ions?. <i>Journal of the American Chemical Society</i> , 2011 , 133, 11844-6	16.4	37
173	Ab Initio Density Functional vs Hartree Fock Predictions for the Structure of [18]Annulene: Evidence for Bond Localization and Diminished Ring Currents in Bicycloannulated [18]Annulenes. <i>Angewandte Chemie International Edition in English</i> , 1997 , 36, 745-748		37
172	Optical Absorption and Computational Studies of [Ni]-Bacteriochlorophyll-a. New Insight into Charge Distribution between Metal and Ligands. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3937-3944	16.4	37
171	Long C?C single bonds in anthracene dimers: The structure of bi(anthracene-9,10-dimethylene) photodimer is redetermined. <i>Tetrahedron Letters</i> , 1995 , 36, 845-848	2	36

170	Partial bond localization in the crystal structure of trisbicyclo[2.2.1]heptabenzene and its effect on Cr-arene dynamics. <i>Tetrahedron Letters</i> , 1995 , 36, 4389-4392	2	36
169	A theoretical study of fluorine atom and fluoride ion attack on methane and silane. <i>Journal of the American Chemical Society</i> , 1985 , 107, 4415-4419	16.4	35
168	Symmetry and polar-effects on the dynamics of enshrouded aryl-alkyne molecular rotors. <i>Chemical Science</i> , 2010 , 1, 102	9.4	34
167	Ring selectivity and migratory aptitude of Cp*Ru ⁺ complexation to acecorannulene. <i>Chemical Communications</i> , 2004 , 950-1	5.8	34
166	Synthesis and full characterization of an iridium B-H activation intermediate of the monocarba-closo-dodecaborate anion. <i>Chemical Communications</i> , 2016 , 53, 176-179	5.8	33
165	Kristallographischer Nachweis der Cyclohexatrien-Struktur von Tris(bicyclo[2.1.1]hexeno)benzol: Bindungslängenalternanz nach Widerlegung der Mills-Nixon-Theorie. <i>Angewandte Chemie</i> , 1995 , 107, 1575-1577	3.6	33
164	Optical Properties of Phthalocyanine and Naphthalocyanine Compounds. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 870-7	6.4	32
163	Stereoselectivity and expanded substrate scope of an engineered PLP-dependent aldolase. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 6824-6	16.4	32
162	Direct experimental evaluation of charge scheme performance by a molecular charge-meter. <i>Journal of the American Chemical Society</i> , 2004 , 126, 5897-905	16.4	30
161	Ground state gas and solution phase conformational dynamics of polar processes: Furfural systems. <i>Journal of Chemical Physics</i> , 2000 , 113, 7519-7529	3.9	29
160	Accurate ab initio anharmonic force field and heat of formation for silane. <i>Molecular Physics</i> , 1999 , 97, 945-953	1.7	29
159	Intramolecular C _H insertion vs. Friedel-Crafts coupling induced by silyl cation-promoted C _H activation. <i>Organic Chemistry Frontiers</i> , 2015 , 2, 1018-1021	5.2	28
158	Surface-assisted bowl-in-bowl stacking of nonplanar aromatic hydrocarbons. <i>Chemical Communications</i> , 2011 , 47, 7995-7	5.8	28
157	Synthesis and crystal structure of a silyl-stabilized allyl cation formed by disruption of an arene by a protonation-hydrosilylation sequence. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 3787-90	16.4	28
156	An -Symmetric 5-Fold Interlocked [2]Catenane. <i>Journal of the American Chemical Society</i> , 2020 , 142, 10267-10277	6.1	27
155	Boronic esters of corannulene: potential building blocks toward icosahedral supramolecules. <i>Organic Chemistry Frontiers</i> , 2015 , 2, 626-633	5.2	27
154	Experimental and computational investigation of the uncatalyzed rearrangement and elimination reactions of isochorismate. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2043-51	16.4	27
153	Application of grid computing to parameter sweeps and optimizations in molecular modeling. <i>Future Generation Computer Systems</i> , 2005 , 21, 27-35	7.5	27

152	Bond Fixation in a [14]Annulene: Synthesis, Characterization, and ab Initio Computations of Furan Adducts of Dimethyldihydropyrene. <i>Journal of the American Chemical Society</i> , 1996 , 118, 2907-2911	16.4	27
151	Synthesis of Bioconjugated sym-pentasubstituted corannulenes: experimental and theoretical investigations of supramolecular architectures. <i>Bioconjugate Chemistry</i> , 2014 , 25, 115-28	6.3	26
150	Extended Corannulenes: Aromatic Bowl/Sheet Hybridization. <i>Angewandte Chemie</i> , 2015 , 127, 10942-10946	16.4	26
149	Synthesis, structure, and isomerization of decapentynylcorannulene: enediyne cyclization/interconversion of C(40)R(10) isomers. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12612-3	16.4	26
148	Multiple versus single pathways in electron transfer in proteins: Influence of protein dynamics and hydrogen bonds. <i>Journal of Chemical Physics</i> , 2003 , 119, 3550-3558	3.9	26
147	The crystal structure of a heptiptycene-chlorobenzene clathrate. <i>Tetrahedron Letters</i> , 1995 , 36, 2419-2422	16.4	26
146	Of graphs and graphenes: molecular design and chemical studies of aromatic compounds. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 5436-8	16.4	25
145	Baskets, covered baskets, and basket balls: corannulene based cyclophanes as fullerene mimics. <i>Tetrahedron</i> , 2001 , 57, 3737-3742	2.4	25
144	Quadruple anionic buckybowls by solid-state chemistry of corannulene and cesium. <i>Journal of the American Chemical Society</i> , 2013 , 135, 12857-60	16.4	24
143	Exploring biomolecular machines: energy landscape control of biological reactions. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2006 , 361, 1439-43	5.8	24
142	Pentaindenocorannulene: Properties, Assemblies, and C60 Complex. <i>Angewandte Chemie</i> , 2016 , 128, 14868-14872	3.6	24
141	Theoretical studies of disilabenzenes. <i>Journal of Organometallic Chemistry</i> , 1984 , 271, 369-379	2.3	23
140	Molecular nesting in co-crystals of tetrabenzoquadranulene and C60: application of the sphere in a cone model. <i>Chemical Communications</i> , 2012 , 48, 9882-4	5.8	22
139	The Central Bond Length in 1,2-Diarylethanes. <i>Journal of the American Chemical Society</i> , 1995 , 117, 4479-4482	16.4	22
138	Theoretical investigation of the binding process of corannulene on a Cu(111) surface. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8864-72	2.8	21
137	Directing power of cyclobutenoid annulations on the double bonds of planar cyclooctatetraenes. <i>Journal of the American Chemical Society</i> , 2002 , 124, 5514-7	16.4	21
136	Substituted silabenzenes. <i>Organometallics</i> , 1988 , 7, 144-155	3.8	21
135	Buckybowl superatom states: a unique route for electron transport?. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 6114-21	3.6	20

- 134 Interconversion and Reactions of In- and Out-Isomers of a Triarylphosphine-Containing Cyclophane. *Journal of the American Chemical Society*, **1999**, 121, 12082-12087 16.4 20
- 133 Canastanes: Ab Initio Quantum Mechanical Prediction of New Curved Polynuclear Aromatic Hydrocarbon Motif. *Journal of the American Chemical Society*, **1999**, 121, 5332-5333 16.4 20
- 132 Structure-property relationships of curved aromatic materials from first principles. *Accounts of Chemical Research*, **2014**, 47, 3310-20 24.3 19
- 131 Opal: SimpleWeb Services Wrappers for Scientific Applications **2006**, 19
- 130 Parameter scan of an effective group difference pseudopotential using grid computing. *New Generation Computing*, **2004**, 22, 137-146 0.9 19
- 129 Mutual control of axial and equatorial ligands: model studies with [Ni]-bacteriochlorophyll-a. *Journal of the American Chemical Society*, **2002**, 124, 8406-15 16.4 19
- 128 Chemomentum - UNICORE 6 Based Infrastructure for Complex Applications in Science and Technology. *Lecture Notes in Computer Science*, **2008**, 82-93 0.9 19
- 127 Electron transport and optical properties of curved aromatics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 1-12 7.9 18
- 126 Efficient discovery of fluorescent chemosensors based on a biarylpyridine scaffold. *Organic Letters*, **2010**, 12, 940-3 6.2 18
- 125 Transition Metal Complexes of a Monocarpa-closo-dodecaborate Ligand via B π Activation. *European Journal of Inorganic Chemistry*, **2017**, 2017, 4420-4424 2.3 17
- 124 Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, **2014**, 35, 611-21 3.5 17
- 123 Reactions of a metallacyclobutene complex with alkenes. *Journal of the American Chemical Society*, **2008**, 130, 10093-5 16.4 17
- 122 Structure of centrally bound angular-(terphenylene)chromium tricarbonyl. *Journal of the American Chemical Society*, **1992**, 114, 369-371 16.4 16
- 121 Versatile hydrochromic fluorescent materials based on a 1,8-naphthalimide integrated fluorophore-receptor system. *Journal of Materials Chemistry C*, **2019**, 7, 7399-7410 7.1 15
- 120 On the Origins of Nonradiative Excited State Relaxation in Aryl Sulfoxides Relevant to Fluorescent Chemosensing. *Journal of the American Chemical Society*, **2016**, 138, 15889-15895 16.4 15
- 119 Trifluoromethyl/Perfluoroalkyl Corannulenes: Directed Synthesis and Photophysical Characterization. *European Journal of Organic Chemistry*, **2017**, 2017, 875-879 3.2 15
- 118 Pentagonal tiling with buckybowl: pentamethylcorannulene on Cu(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 13365-9 3.6 15
- 117 Chemistry at the alkyne-carbene intersection: a metallacyclobutene- β -vinylcarbene equilibration. *Journal of the American Chemical Society*, **2013**, 135, 8826-9 16.4 15

116	The transition state and barrier heights for the reaction $O(3P) + HCl \rightarrow OH + Cl$. <i>Chemical Physics Letters</i> , 1989 , 158, 189-192	2.5	15
115	Indenocorannulene-Based Materials: Effect of Solid-State Packing and Intermolecular Interactions on Optoelectronic Properties. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1220-1234	3.8	14
114	Synthesis of Modified Nucleoside Oligophosphates Simplified: Fast, Pure, and Protecting Group Free. <i>Journal of the American Chemical Society</i> , 2019 , 141, 15013-15017	16.4	14
113	Thermodynamic and computational studies on the binding of p53-derived peptides and peptidomimetic inhibitors to HDM2. <i>ChemBioChem</i> , 2009 , 10, 1360-8	3.8	14
112	Solvent, Isotope, and Substituent Effects on the Bimolecular Electron Transfer Reaction between Chlorine Oxide and Benzenes. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 13938-13947		14
111	Thermal decomposition of methanethiol and ethanethiol. <i>The Journal of Physical Chemistry</i> , 1987 , 91, 4145-4155		14
110	[3+3] Cyclocondensation of Disubstituted Biphenyl Dialdehydes: Access to Inherently Luminescent and Optically Active Hexa-substituted C-Symmetric and Asymmetric Trianglimine Macrocycles. <i>Journal of Organic Chemistry</i> , 2017 , 82, 2472-2480	4.2	13
109	Diastereoselective Monofluorocyclopropanation Using Fluoromethylsulfonium Salts. <i>Organic Letters</i> , 2019 , 21, 7174-7178	6.2	13
108	Chiral Atropisomeric Indenocorannulene Bowls: Critique of the Cahn-Ingold-Prelog Conception of Molecular Chirality. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6470-6474	16.4	13
107	Decakis(arylthio)corannulenes: Transferable Photochemical and Redox Parameters and Photovoltaic Device Performance. <i>European Journal of Organic Chemistry</i> , 2017 , 2017, 4338-4342	3.2	13
106	Diels-Alder reactions of 3,6-disubstituted 1,2,4,5-tetrazines. Synthesis and X-ray crystal structures of diazafluoranthene derivatives. <i>Organic and Biomolecular Chemistry</i> , 2009 , 7, 2082-92	3.9	13
105	Application of Structural Principles to the Design of Triptycene-Based Molecular Gears with Parallel Axes. <i>Chimia</i> , 2009 , 63, 201-204	1.3	13
104	General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 26191-26200	3.6	12
103	Von Graphen und Graphenen: molekulares Design und chemische Studien aromatischer Verbindungen. <i>Angewandte Chemie</i> , 2013 , 125, 5546-5548	3.6	12
102	Quantum chemical prediction of the ^{13}C NMR shifts in alkyl and chlorocorannulenes: correction of chlorine effects. <i>Theoretical Chemistry Accounts</i> , 2008 , 120, 95-106	1.9	12
101	Stereoselectivity and Expanded Substrate Scope of an Engineered PLP-Dependent Aldolase. <i>Angewandte Chemie</i> , 2006 , 118, 6978-6980	3.6	12
100	Modulation of fragmental charge transfer via hydrogen bonds. Direct measurement of electronic contributions. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 412-21	2.8	12
99	Stabilization of benzene versus oligoacetylenes: not another scale for aromaticity. <i>Journal of Physical Organic Chemistry</i> , 2004 , 17, 740-742	2.1	12

98	Multithreaded shared memory parallel implementation of the electronic structure code GAMESS. <i>Computer Physics Communications</i> , 2000 , 128, 55-66	4.2	12
97	Implementation and refinement of the modified-conductorlike screening quantum mechanical solvation model at the MP2 level. <i>Journal of Chemical Physics</i> , 2000 , 113, 7511-7518	3.9	12
96	Diindenocorannulenes: Curved Aromatics Blending Bowl-in-Bowl Assembly and Nanocarbon Material Properties. <i>European Journal of Organic Chemistry</i> , 2017 , 2017, 2801-2805	3.2	11
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