N Arul Murugan

List of Publications by Year
in descending order

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128 papers	2,897 citations	172207 29 h-index	243296 44 g-index
132 all docs	132 docs citations	132 times ranked	3817 citing authors

#	Article	IF	Citations
1	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. Science Advances, 2020, 6, eabb8097.	4.7	138
2	A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid Î² Aggregates. Scientific Reports, 2016, 6, 23668.	1.6	90
3	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16453-16458.	3.3	84
4	AÎ² plaque-selective NIR fluorescence probe to differentiate Alzheimer's disease from tauopathies. Biosensors and Bioelectronics, 2017, 98, 54-61.	5.3	83
5	Cross-interaction of tau PET tracers with monoamine oxidase B: evidence from in silico modelling and in vivo imaging. European Journal of Nuclear Medicine and Molecular Imaging, 2019, 46, 1369-1382.	3.3	74
6	Computational investigation on Andrographis paniculata phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4415-4426.	2.0	73
7	Identification of Dihydrofuro[3,4-d]pyrimidine Derivatives as Novel HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties. Journal of Medicinal Chemistry, 2019, 62, 1484-1501.	2.9	70
8	Different Positron Emission Tomography Tau Tracers Bind to Multiple Binding Sites on the Tau Fibril: Insight from Computational Modeling. ACS Chemical Neuroscience, 2018, 9, 1757-1767.	1.7	69
9	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. Physical Chemistry Chemical Physics, 2011, 13, 12506.	1.3	64
10	Antioxidant Berberine-Derivative Inhibits Multifaceted Amyloid Toxicity. IScience, 2020, 23, 101005.	1.9	63
11	Demystifying the solvatochromic reversal in Brookerâ€™s merocyanine dye. Physical Chemistry Chemical Physics, 2011, 13, 1290-1292.	1.3	55
12	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357.	1.2	52
13	Conformations, structural transitions and visible near-infrared absorption spectra of four-, five- and six-coordinated Cu(<scp>ii</scp>) aqua complexes. Physical Chemistry Chemical Physics, 2009, 11, 508-519.	1.3	51
14	Investigation of the Binding Profiles of AZD2184 and Thioflavin T with Amyloid-Î²(1â€“42) Fibril by Molecular Docking and Molecular Dynamics Methods. Journal of Physical Chemistry B, 2015, 119, 11560-11567.	1.2	48
15	Searching for target-specific and multi-targeting organics for Covid-19 in the Drugbank database with a double scoring approach. Scientific Reports, 2020, 10, 19125.	1.6	47
16	Optimization of N-Substituted Oseltamivir Derivatives as Potent Inhibitors of Group-1 and -2 Influenza A Neuraminidases, Including a Drug-Resistant Variant. Journal of Medicinal Chemistry, 2018, 61, 6379-6397.	2.9	46
17	Structure-based drug repurposing: Traditional and advanced AI/ML-aided methods. Drug Discovery Today, 2022, 27, 1847-1861.	3.2	46
18	Solvent Dependence of Structure, Charge Distribution, and Absorption Spectrum in the Photochromic Merocyanineâ€“Spiropyran Pair. Journal of Physical Chemistry B, 2011, 115, 4025-4032.	1.2	43

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19	Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867.	1.0	41
20	Color modeling of protein optical probes. Physical Chemistry Chemical Physics, 2012, 14, 1107-1112.	1.3	40
21	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181.	1.2	40
22	Relation between Nonlinear Optical Properties of Pushâ€“Pull Molecules and Metric of Charge Transfer Excitations. Journal of Chemical Theory and Computation, 2015, 11, 4182-4188.	2.3	39
23	Advanced Glycation End Products Modulate Structure and Drug Binding Properties of Albumin. Molecular Pharmaceutics, 2015, 12, 3312-3322.	2.3	39
24	Toward Fully Nonempirical Simulations of Optical Band Shapes of Molecules in Solution: A Case Study of Heterocyclic Ketoimine Difluoroborates. Journal of Physical Chemistry A, 2015, 119, 5145-5152.	1.1	39
25	On/off-switchable LSPR nano-immunoassay for troponin-T. Scientific Reports, 2017, 7, 44027.	1.6	36
26	Cyclic Dipeptide-Based Ambidextrous Supergelators: Minimalistic Rational Design, Structure-Gelation Studies, and In Situ Hydrogelation. Biomacromolecules, 2017, 18, 3581-3590.	2.6	36
27	The Culprit Is in the Cave: The Core Sites Explain the Binding Profiles of Amyloid-Specific Tracers. Journal of Physical Chemistry Letters, 2016, 7, 3313-3321.	2.1	35
28	Structure-Based Optimization of N-Substituted Oseltamivir Derivatives as Potent Anti-Influenza A Virus Agents with Significantly Improved Potency against Oseltamivir-Resistant N1-H274Y Variant. Journal of Medicinal Chemistry, 2018, 61, 9976-9999.	2.9	35
29	A Review on Parallel Virtual Screening Softwares for High-Performance Computers. Pharmaceuticals, 2022, 15, 63.	1.7	34
30	Improved Binding Affinity of Omicronâ€™s Spike Protein for the Human Angiotensin-Converting Enzyme 2 Receptor Is the Key behind Its Increased Virulence. International Journal of Molecular Sciences, 2022, 23, 3409.	1.8	34
31	Artificial intelligence in virtual screening: Models versus experiments. Drug Discovery Today, 2022, 27, 1913-1923.	3.2	33
32	Twoâ€Photon Solvatochromism II: Experimental and Theoretical Study of Solvent Effects on the Twoâ€Photon Absorption Spectrum of Reichardtâ€™s Dye. ChemPhysChem, 2013, 14, 3731-3739.	1.0	32
33	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77.	2.1	29
34	Computational Insight into the Binding Profile of the Second-Generation PET Tracer PI2620 with Tau Fibrils. ACS Chemical Neuroscience, 2020, 11, 900-908.	1.7	29
35	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF₂) Core Complex. Journal of Physical Chemistry B, 2016, 120, 2323-2332.	1.2	28
36	Role of Dynamic Flexibility in Computing Solvatochromic Properties of Dyeâ^'Solvent Systems: o-Betaine in Water. Journal of Physical Chemistry A, 2009, 113, 2572-2577.	1.1	27

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37	Association Dynamics and Linear and Nonlinear Optical Properties of an N-Acetylaladanamide Probe in a POPC Membrane. Journal of the American Chemical Society, 2013, 135, 13590-13597.	6.6	27
38	Acetylene-sourced CVD-synthesised catalytically active graphene for electrochemical biosensing. Biosensors and Bioelectronics, 2017, 89, 496-504.	5.3	27
39	Progress in electronics and photonics with nanomaterials. Vacuum, 2017, 146, 304-307.	1.6	27
40	Development of an Efficient Gâ€Quadruplexâ€Stabilised Thrombinâ€Binding Aptamer Containing a Threeâ€Carbon Spacer Molecule. ChemBioChem, 2017, 18, 755-763.	1.3	26
41	Solvatochromic shift of phenol blue in water from a combined Carâ€“Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and <scp>ZINDO</scp> approach. Journal of Chemical Physics, 2010, 132, 234508.	1.2	25
42	Promising two-photon probes for in vivo detection of Î² amyloid deposits. Chemical Communications, 2014, 50, 11694-11697.	2.2	25
43	Investigation into Biological Environments through (Non)linear Optics: A Multiscale Study of Laurdan Derivatives. Journal of Chemical Theory and Computation, 2016, 12, 6169-6181.	2.3	25
44	Cryptic Sites in Tau Fibrils Explain the Preferential Binding of the AV-1451 PET Tracer toward Alzheimerâ€™s Tauopathy. ACS Chemical Neuroscience, 2021, 12, 2437-2447.	1.7	24
45	Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Carâ€“Parrinello Molecular Dynamics Investigation. Journal of Physical Chemistry A, 2009, 113, 4833-4839.	1.1	23
46	One- and Two-Photon Absorption of a Spiropyranâ€“Merocyanine System: Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2015, 119, 1515-1522.	1.2	23
47	Revealing Spectral Features in Two-Photon Absorption Spectrum of Hoechst 33342: A Combined Experimental and Quantum-Chemical Study. Journal of Physical Chemistry B, 2013, 117, 12013-12019.	1.2	22
48	Studies on an on/off-switchable immunosensor for troponin T. Biosensors and Bioelectronics, 2015, 73, 100-107.	5.3	22
49	Modeling solvatochromism of Nile red in water. International Journal of Quantum Chemistry, 2011, 111, 1521-1530.	1.0	21
50	Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358.	1.2	20
51	Pressure Induced Orientational Ordering inp-Terphenyl. Journal of Physical Chemistry B, 2005, 109, 1433-1440.	1.2	19
52	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263.	2.3	19
53	Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. Journal of Physical Chemistry B, 2014, 118, 1715-1725.	1.2	19
54	High Pressure Phase of Biphenyl at Room Temperature:â€‰ A Monte Carlo Study. Journal of Physical Chemistry B, 2004, 108, 4178-4184.	1.2	18

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55	Modeling Solvatochromism of a Quinolinium Betaine Dye in Water Solvent Using Sequential Hybrid QM/MM and Semicontinuum Approach. Journal of Physical Chemistry B, 2011, 115, 1056-1061.	1.2	18
56	Density Functional Restrictedâ€“Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271.	2.3	18
57	Destabilization of amyloid fibrils on interaction with MoS₂-based nanomaterials. RSC Advances, 2019, 9, 1613-1624.	1.7	18
58	Mechanistic Insight into the Binding Profile of DCVJ and Î±-Synuclein Fibril Revealed by Multiscale Simulations. ACS Chemical Neuroscience, 2019, 10, 610-617.	1.7	18
59	Naphthalene Monoimide Derivative Ameliorates Amyloid Burden and Cognitive Decline in a Transgenic Mouse Model of Alzheimer's Disease. Advanced Therapeutics, 2021, 4, 2000225.	1.6	18
60	Inflammation-sensitive in situ smart scaffolding for regenerative medicine. Nanoscale, 2016, 8, 17213-17222.	2.8	17
61	Recent trends in computational tools and data-driven modeling for advanced materials. Materials Advances, 2022, 3, 4069-4087.	2.6	17
62	Free Energy Landscape for Alpha-Helix to Beta-Sheet Interconversion in Small Amyloid Forming Peptide under Nanoconfinement. Journal of Physical Chemistry B, 2018, 122, 9654-9664.	1.2	16
63	Effect of Familial Mutations on the Interconversion of Î±-Helix to Î²-Sheet Structures in an Amyloid-Forming Peptide: Insight from Umbrella Sampling Simulations. ACS Chemical Neuroscience, 2019, 10, 1347-1354.	1.7	16
64	Hybrid density functionalâ€“molecular mechanics calculations for core-electron binding energies of glycine in water solution. Physical Chemistry Chemical Physics, 2013, 15, 244-254.	1.3	15
65	Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. Journal of Physical Chemistry C, 2015, 119, 653-664.	1.5	15
66	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. Molecules, 2017, 22, 1643.	1.7	15
67	Structure, Energetics, and Dynamics of Pedal-Like Motion in Stilbene from Molecular Simulation and ab Initio Calculations. Journal of Physical Chemistry B, 2004, 108, 17403-17411.	1.2	14
68	Thermal behavior of disordered phase of caffeine molecular crystal: Insights from Monte Carlo simulation studies. Journal of Chemical Physics, 2009, 130, 204514.	1.2	14
69	Solvent Dependence of Conformational Distribution, Molecular Geometry, and Electronic Structure in Adenosine. Journal of Physical Chemistry B, 2009, 113, 1012-1021.	1.2	14
70	NMR Spinâ€“Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. Chemistry - A European Journal, 2012, 18, 11677-11684.	1.7	14
71	Solvent Dependence on Conformational Transition, Dipole Moment, and Molecular Geometry of 1,2-Dichloroethane: Insight from Carâ€“Parrinello Molecular Dynamics Calculations. Journal of Physical Chemistry B, 2008, 112, 14673-14677.	1.2	13
72	Elucidating the Mechanism of Zn²⁺ Sensing by a Bipyridine Probe Based on Two-Photon Absorption. Journal of Physical Chemistry B, 2016, 120, 9067-9075.	1.2	13

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73	Recognition of G-quadruplex topology through hybrid binding with implications in cancer theranostics. Theranostics, 2020, 10, 10394-10414.	4.6	13
74	Pressure-Induced Ordering in Adamantane: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2005, 109, 2014-2020.	1.2	12
75	pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. Journal of Chemical Theory and Computation, 2013, 9, 3660-3669.	2.3	12
76	Solvent-Dependent Conformational States of a [2]Rotaxane-Based Molecular Machine: A Molecular Dynamics Perspective. Journal of Physical Chemistry C, 2013, 117, 25059-25068.	1.5	12
77	Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. Journal of Chemical Theory and Computation, 2014, 10, 778-788.	2.3	12
78	Structureâ€“Activity Relationship Exploration of NNIBP Tolerant Region I Leads to Potent HIV-1 NNRTIs. ACS Infectious Diseases, 2020, 6, 2225-2234.	1.8	12
79	An unexpected role of an extra phenolic hydroxyl on the chemical reactivity and bioactivity of catechol or gallol modified hyaluronic acid hydrogels. Polymer Chemistry, 2021, 12, 2987-2991.	1.9	12
80	Identification of C5-NH₂ Modified Oseltamivir Derivatives as Novel Influenza Neuraminidase Inhibitors with Highly Improved Antiviral Activities and Favorable Druggability. Journal of Medicinal Chemistry, 2021, 64, 17992-18009.	2.9	12
81	Combining (Non)linear Optical and Fluorescence Analysis of DiD To Enhance Lipid Phase Recognition. Journal of Chemical Theory and Computation, 2018, 14, 5350-5359.	2.3	11
82	Molecular Architectonics of Cyclic Dipeptide Amphiphiles and Their Application in Drug Delivery. ACS Applied Bio Materials, 2020, 3, 3413-3422.	2.3	11
83	Differences in first neighbor orientation behind the anomalies in the low and high density trans-1,2-dichloroethene liquid. Journal of Chemical Physics, 2012, 136, 124514.	1.2	10
84	Integrative approaches in HIV â€1 nonâ€nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328.	6.2	10
85	Unusual binding-site-specific photophysical properties of a benzothiazole-based optical probe in amyloid beta fibrils. Physical Chemistry Chemical Physics, 2018, 20, 20334-20339.	1.3	10
86	Unraveling the Unbinding Pathways of Products Formed in Catalytic Reactions Involved in SIRT1â€“3: A Random Acceleration Molecular Dynamics Simulation Study. Journal of Chemical Information and Modeling, 2019, 59, 4100-4115.	2.5	10
87	Applying polypharmacology approach for drug repurposing for SARS-CoV2. Journal of Chemical Sciences, 2022, 134, 57.	0.7	10
88	Orientational Melting and Reorientational Motion in a Cubane Molecular Crystal: A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 23955-23962.	1.2	9
89	The impact of the heteroatom in a five-membered ring on the photophysical properties of difluoroborates. Dyes and Pigments, 2019, 170, 107481.	2.0	9
90	Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Proteinâ€“Inhibitor Complexes in Relevance to Developing Parkinsonâ€™s Therapeutics. International Journal of Molecular Sciences, 2020, 21, 7648.	1.8	9

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91	High-Pressure Study of Adamantane:Â Variable Shape Simulations up to 26 GPa. Journal of Physical Chemistry B, 2005, 109, 17296-17303.	1.2	8
92	1,2-Dichloroethane in Haloalkane Dehalogenase Protein and in Water Solvent: A Case Study of the Confinement Effect on Structural and Dynamical Properties. Journal of Physical Chemistry B, 2009, 113, 3257-3263.	1.2	8
93	Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4766-4774.	2.3	8
94	Simulations of Light Absorption of Carbon Particles in Nanoaerosol Clusters. Journal of Physical Chemistry A, 2014, 118, 1879-1886.	1.1	8
95	Atomic level simulations of the interaction of asphaltene with quartz surfaces: role of chemical modifications and aqueous environment. Materials and Structures/Materiaux Et Constructions, 2017, 50, 1.	1.3	8
96	Effect of Alzheimer Familial Chromosomal Mutations on the Amyloid Fibril Interaction with Different PET Tracers: Insight from Molecular Modeling Studies. ACS Chemical Neuroscience, 2017, 8, 2655-2666.	1.7	8
97	Thiopheneâ€Based Dual Modulators of AÎ² and Tau Aggregation. ChemBioChem, 2021, 22, 3348-3357.	1.3	8
98	Solvent Polarity-Induced Conformational Unlocking of Asparagine. Journal of Physical Chemistry A, 2012, 116, 11702-11708.	1.1	7
99	Synthesis, spectral characterization and DFT analysis for the validation of 2, 6 diaryl -piperidin-4-ones as potential sunscreens and UV filters. Journal of Molecular Structure, 2015, 1099, 560-566.	1.8	7
100	Multistep Modeling Strategy To Improve the Binding Affinity Prediction of PET Tracers to AÎ²₄₂: Case Study with Styrylbenzoxazole Derivatives. ACS Chemical Neuroscience, 2016, 7, 1698-1705.	1.7	7
101	Multiscale Modeling of Two-Photon Probes for Parkinsonâ€™s Diagnostics Based on Monoamine Oxidase B Biomarker. Journal of Chemical Information and Modeling, 2020, 60, 3854-3863.	2.5	7
102	Molecular basis for stereoselective transport of fenoterol by the organic cation transporters 1 and 2. Biochemical Pharmacology, 2022, 197, 114871.	2.0	7
103	Temperature-induced dynamical conformational disorder in 4-vinyl benzoic acid molecular crystals: A molecular simulation study. Journal of Chemical Physics, 2005, 123, 094508.	1.2	6
104	Investigations into conformational transitions and solvation structure of a 7-piperidino-5,9-methanobenzo[8] annulene in water. Physical Chemistry Chemical Physics, 2008, 10, 6135.	1.3	6
105	Pressure dependence of crystal structure and molecular packing in anthracene. Molecular Physics, 2009, 107, 1689-1695.	0.8	6
106	In silicomodeling and experimental evidence of coagulant protein interaction with precursors for nanoparticle functionalization. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1182-1190.	2.0	6
107	Data-driven approach towards identifying dyesensitizer molecules for higher power conversion efficiency in solar cells. New Journal of Chemistry, 2022, 46, 4395-4405.	1.4	6
108	Studies of pH-Sensitive Optical Properties of the deGFP1 Green Fluorescent Protein Using a Unique Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 3492-3502.	2.3	5

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109	Origin of the Absorption Band of Bromophenol Blue in Acidic and Basic pH: Insight from a Combined Molecular Dynamics and TD-DFT/MM Study. Journal of Physical Chemistry A, 2016, 120, 7175-7182.	1.1	5
110	Peptide-Based Antiviral Drugs. Advances in Experimental Medicine and Biology, 2021, 1322, 261-284.	0.8	5
111	DNA Minor Groove-Induced cisâ€“trans Isomerization of a Near-Infrared Fluorescent Probe. Biochemistry, 2021, 60, 2084-2097.	1.2	5
112	How Crucial Are Finite Temperature and Solvent Effects on Structure and Absorption Spectra of Si₁₀?. Journal of Physical Chemistry C, 2012, 116, 26618-26624.	1.5	4
113	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. Physical Chemistry Chemical Physics, 2013, 15, 2427.	1.3	4
114	Synthesis, characterization of (3E)-1-(6-chloro-2-methyl-4-phenyl quinolin-3-Yl)-3-aryl prop-2-en-1-ones through IR, NMR, single crystal X-ray diffraction and insights into their electronic structure using DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1010-1017.	2.0	4
115	Effect of Pressure on Pedal Motion in Stilbene Molecular Crystals and Its Dependence on the Crystallographic Site. Journal of Physical Chemistry B, 2005, 109, 12107-12114.	1.2	3
116	Role of Protonation State and Solvation on the pH Dependent Optical Properties of Bromocresol Green. Journal of Chemical Theory and Computation, 2014, 10, 3958-3968.	2.3	3
117	Discovery of biphenyl pyrazole scaffold for neurodegenerative diseases: A novel class of acetylcholinesterase-centered multitargeted ligands. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127370.	1.0	3
118	Assessment of Amyloid Forming Tendency of Peptide Sequences from Amyloid Beta and Tau Proteins Using Force-Field, Semi-Empirical, and Density Functional Theory Calculations. International Journal of Molecular Sciences, 2021, 22, 3244.	1.8	3
119	Solvation shell structure of cyclooctylpyranone in water solvent and its comparative structure, dynamics and dipole moment in HIV protease. Physical Chemistry Chemical Physics, 2009, 11, 6482.	1.3	2
120	Solvatochromism in a Pyridinium Cyclopentadienylide: Insights from a Sequential Carâ€“Parrinello QM/MM and TD-DFT/Semicontinuum Approach. Journal of Physical Chemistry B, 2014, 118, 7358-7366.	1.2	2
121	Exhibiting environment sensitive optical properties through multiscale modelling: A study of photoactivatable probes. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 425, 113672.	2.0	2
122	Organosulfur/Seleniumâ€Based Highly Fluorogenic Molecular Probes for Liveâ€Cell Nucleolus Imaging. Chemistry - an Asian Journal, 2022, 17, .	1.7	2
123	Near-infrared emissive cyanine probes for selective visualization of the physiological and pathophysiological modulation of albumin levels. Journal of Materials Chemistry B, 2022, 10, 3657-3666.	2.9	2
124	What does pressure decide to cook with orientationally disordered plastic phase of cubane: An orientational glass or crystal?. Journal of Chemical Physics, 2005, 123, 244514.	1.2	1
125	Al3+ induced planarization, conformational arrest and metallochromic shift in a pyrimidine dione dye: insight from integrated hybrid quantumâ€“classical calculations. Physical Chemistry Chemical Physics, 2012, 14, 2339.	1.3	1
126	Recent Advancements in Computing Reliable Binding Free Energies in Drug Discovery Projects. Challenges and Advances in Computational Chemistry and Physics, 2019, , 221-246.	0.6	1

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127	Spatial spin-charge separation in neutral endohedral metallofullerene: A combined restricted open-shell MP2 and Carâ€“Parrinello molecular dynamics study. Chemical Physics Letters, 2013, 557, 71-75.	1.2	0
128	Cover Image, Volume 8, Issue 1. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1356.	6.2	0