Tim Clark

List of Publications by Year in Descending Order

431 papers	23,277 citations	61 h-index	141 g-index
469 ext. papers	25,450 ext. citations	6.2 avg, IF	7.19 L-index

#	Paper	IF	Citations
431	N-Terminus to Arginine Side-Chain Cyclization of Linear Peptidic Neuropeptide Y Y Receptor Ligands Results in Picomolar Binding Constants. *Journal of Medicinal Chemistry*, **2021**, 64, 16746-16769	8.3	0
430	Dibenzodiazepinone-type muscarinic receptor antagonists conjugated to basic peptides: Impact of the linker moiety and unnatural amino acids on MR selectivity. *European Journal of Medicinal Chemistry*, **2021**, 213, 113159	6.8	2
429	Titelbild: An Electrically Conducting Three-Dimensional Iron□Catecholate Porous Framework (Angew. Chem. 33/2021). *Angewandte Chemie*, **2021**, 133, 17893-17893	3.6	
428	Comprehensive Computational Investigation of the Barton-Kellogg Reaction for Both Alkyl and Aryl Systems. *Journal of Organic Chemistry*, **2021**, 86, 7515-7528	4.2	2
427	The Detosylation of Chiral 1,2-Bis(tosylamides). *Journal of Organic Chemistry*, **2021**, 86, 9163-9180	4.2	2
426	An Electrically Conducting Three-Dimensional Iron□Catecholate Porous Framework. *Angewandte Chemie*, **2021**, 133, 18213-18220	3.6	1
425	Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal-Organic Framework Architectures. *Angewandte Chemie - International Edition*, **2021**, 60, 5519-5526	16.4	23
424	Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal□Organic Framework Architectures. *Angewandte Chemie*, **2021**, 133, 5579-5586	3.6	3
423	Pre-Planarized Triphenylamine-Based Linear Mixed-Valence Charge-Transfer Systems. *Angewandte Chemie - International Edition*, **2021**, 60, 6771-6777	16.4	5
422	The Cascade Reactions of Indigo with Propargyl Substrates for Heterocyclic and Photophysical Diversity. *Chemistry - A European Journal*, **2021**, 27, 3708-3721	4.8	3
421	The □hole revisited. *Physical Chemistry Chemical Physics*, **2021**, 23, 16458-16468	3.6	9
420	An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework. *Angewandte Chemie - International Edition*, **2021**, 60, 18065-18072	16.4	5
419	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. *Angewandte Chemie - International Edition*, **2020**, 59, 16104-16113	16.4	14
418	A combined activation mechanism for the glucagon receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 15414-15422	11.5	13
417	Perylene-Monoimides: Singlet Fission Down-Conversion Competes with Up-Conversion by Geminate Triplet-Triplet Recombination. *Journal of Physical Chemistry A*, **2020**, 124, 5727-5736	2.8	12
416	Panchromatic light funneling through the synergy in hexabenzocoronene-(metallo)porphyrin-fullerene assemblies to realize the separation of charges. *Chemical Science*, **2020**, 11, 7123-7132	9.4	3
415	EMPIRE: a highly parallel semiempirical molecular orbital program: 3: Born-Oppenheimer molecular dynamics. *Journal of Molecular Modeling*, **2020**, 26, 43	2	5

414	Understanding and Controlling Short- and Long-Range Electron/Charge-Transfer Processes in Electron Donor-Acceptor Conjugates. *Journal of the American Chemical Society*, **2020**, 142, 7898-7911	16.4	23
413	Tautomeric Equilibria of Nucleobases in the Hachimoji Expanded Genetic Alphabet. *Journal of Chemical Theory and Computation*, **2020**, 16, 2766-2777	6.4	9
412	Photoactive preorganized subphthalocyanine-based molecular tweezers for selective complexation of fullerenes. *Chemical Science*, **2020**, 11, 3448-3459	9.4	4
411	Regioselective convergent synthesis of 2-arylidene thiazolo[3,2-]pyrimidines as potential anti-chikungunya agents.. *RSC Advances*, **2020**, 10, 5191-5195	3.7	3
410	Modulating the dynamics of Förster resonance energy transfer and singlet fission by variable molecular spacers. *Nanoscale*, **2020**, 12, 23061-23068	7.7	1
409	Singlet Fission in Pyrene-Fused Azaacene Dimers. *Angewandte Chemie*, **2020**, 132, 1129-1133	3.6	3
408	Resonance-Enhanced Charge Delocalization in Carbazole-Oligoyne-Oxadiazole Conjugates. *Journal of the American Chemical Society*, **2020**, 142, 18769-18781	16.4	6
407	Solvent-Dependent Singlet Fission in Diketopyrrolopyrrole Dimers: A Mediating Charge Transfer versus a Trapping Symmetry-Breaking Charge Separation. *Advanced Energy Materials*, **2020**, 10, 2001496	21.8	14
406	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. *Angewandte Chemie*, **2020**, 132, 16238-16247	3.6	3
405	Synergie von elektrostatischen und □Wechselwirkungen f□ die Verwirklichung von k□nstlichen photosynthetischen Modellsystemen auf Nano-Ebene. *Angewandte Chemie*, **2020**, 132, 18946-18955	3.6	0
404	Synergy of Electrostatic and □Interactions in the Realization of Nanoscale Artificial Photosynthetic Model Systems. *Angewandte Chemie - International Edition*, **2020**, 59, 18786-18794	16.4	3
403	Models of necessity. *Beilstein Journal of Organic Chemistry*, **2020**, 16, 1649-1661	2.5	2
402	Singlet Fission in Pyrene-Fused Azaacene Dimers. *Angewandte Chemie - International Edition*, **2020**, 59, 1113-1117	16.4	15
401	Universal Activation Index for Class A GPCRs. *Journal of Chemical Information and Modeling*, **2019**, 59, 3938-3945	6.1	4
400	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. *Journal of Molecular Modeling*, **2019**, 25, 156	2	2
399	Metadynamics simulations of ligand binding to GPCRs. *Current Opinion in Structural Biology*, **2019**, 55, 129-137	8.1	11
398	Tuning electron transfer in supramolecular nano-architectures made of fullerenes and porphyrins. *Nanoscale*, **2019**, 11, 10782-10790	7.7	10
397	Pentacenes: A Molecular Ruler for Singlet Fission. *Trends in Chemistry*, **2019**, 1, 11-21	14.8	23

396	Carbon Nanodots for Charge-Transfer Processes. *Accounts of Chemical Research*, **2019**, 52, 955-963	24.3	53
395	Davydov splitting and singlet fission in excitonically coupled pentacene dimers. *Chemical Science*, **2019**, 10, 3854-3863	9.4	40
394	Interaction of Radicals with Holes. *Journal of Physical Chemistry A*, **2019**, 123, 3326-3333	2.8	6
393	Varying the Interpentacene Electronic Coupling to Tune Singlet Fission. *Journal of the American Chemical Society*, **2019**, 141, 6191-6203	16.4	42
392	Chromophore Multiplication To Enable Exciton Delocalization and Triplet Diffusion Following Singlet Fission in Tetrameric Pentacene. *Angewandte Chemie - International Edition*, **2019**, 58, 15263-15267	16.4	14
391	Chromophore Multiplication To Enable Exciton Delocalization and Triplet Diffusion Following Singlet Fission in Tetrameric Pentacene. *Angewandte Chemie*, **2019**, 131, 15407-15411	3.6	6
390	Switching on and off Interlayer Correlations and Porosity in 2D Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2019**, 141, 12570-12581	16.4	75
389	Explicit Inclusion of Polarizing Electric Fields in and Hole Interactions. *Journal of Physical Chemistry A*, **2019**, 123, 10123-10130	2.8	16
388	Size-Dependent Local Ordering in Melanin Aggregates and Its Implication on Optical Properties. *Journal of Physical Chemistry A*, **2019**, 123, 9403-9412	2.8	2
387	Basal Histamine H Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. *Chemistry - A European Journal*, **2019**, 25, 14613-14624	4.8	7
386	Propagation of Holes and Electrons in Metal-Organic Frameworks. *Journal of Chemical Information and Modeling*, **2019**, 59, 5057-5064	6.1	4
385	Combining Zinc Phthalocyanines, Oligo(p-Phenylenevinylenes), and Fullerenes to Impact Reorganization Energies and Attenuation Factors. *ChemPhysChem*, **2019**, 20, 2806-2815	3.2	3
384	Opposing Electronic and Nuclear Quantum Effects on Hydrogen Bonds in H O and D O. *ChemPhysChem*, **2019**, 20, 2461-2465	3.2	12
383	Synthesis and Density Functional Theory Studies of Azirinyl and Oxiranyl Functionalized Isoindigo and (3,3')-3,3'-(ethane-1,2-diylidene)bis(indolin-2-one) Derivatives. *Molecules*, **2019**, 24,	4.8	1
382	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I **2019**, 25, 1		1
381	Influence of the heavy-atom effect on singlet fission: a study of platinum-bridged pentacene dimers. *Chemical Science*, **2019**, 10, 11130-11140	9.4	13
380	A Fluorescent Benzo[g]isoquinoline-Based HIF Prolyl Hydroxylase Inhibitor for Cellular Imaging. *ChemMedChem*, **2019**, 14, 94-99	3.7	2
379	A Self-Assembled Unit Comprising 12 Squaraine Dyes Built Up from Two Star-Shaped Hexasquarainyl-Benzene Molecules. *Chemistry - A European Journal*, **2019**, 25, 2831-2839	4.8	5

378	Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. *Angewandte Chemie*, **2018**, 130, 2610-2615	3.6	6
377	Molecular Mechanisms of Biased and Probe-Dependent Signaling at CXC-Motif Chemokine Receptor CXCR3 Induced by Negative Allosteric Modulators. *Molecular Pharmacology*, **2018**, 93, 309-322	4.3	8
376	A water-soluble, bay-functionalized perylenediimide derivative - correlating aggregation and excited state dynamics. *Nanoscale*, **2018**, 10, 2317-2326	7.7	8
375	Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. *Angewandte Chemie - International Edition*, **2018**, 57, 2580-2585	16.4	34
374	Tuning the Carbon Nanotube Selectivity: Optimizing Reduction Potentials and Distortion Angles in Perylenediimides. *Journal of the American Chemical Society*, **2018**, 140, 5427-5433	16.4	12
373	Binding, Thermodynamics, and Selectivity of a Non-peptide Antagonist to the Melanocortin-4 Receptor. *Frontiers in Pharmacology*, **2018**, 9, 560	5.6	7
372	Evidence for Charge-Transfer Mediation in the Primary Events of Singlet Fission in a Weakly Coupled Pentacene Dimer. *CheM*, **2018**, 4, 1092-1111	16.2	74
371	The coulombic □hole model describes bonding in CXIY complexes completely. *Physical Chemistry Chemical Physics*, **2018**, 20, 22849-22855	3.6	40
370	1D Chains of Diruthenium Tetracarbonyl Sawhorse Complexes. *European Journal of Inorganic Chemistry*, **2018**, 2018, 54-61	2.3	4
369	A perspective on quantum mechanics and chemical concepts in describing noncovalent interactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 30076-30082	3.6	96
368	A Feynman dispersion correction: a proof of principle for MNDO. *Journal of Molecular Modeling*, **2018**, 24, 338	2	7
367	Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 16544-16552	16.4	72
366	Solvatochromic covalent organic frameworks. *Nature Communications*, **2018**, 9, 3802	17.4	100
365	The □Hole Coulombic Interpretation of Trihalide Anion Formation. *ChemPhysChem*, **2018**, 19, 3044-3049	3.2	35
364	On bond-critical points in QTAIM and weak interactions. *Journal of Molecular Modeling*, **2018**, 24, 142	2	56
363	Dispersion and polar flattening: noble gas-halogen complexes. *Journal of Molecular Modeling*, **2018**, 24, 172	2	2
362	Directional Charge-Carrier Transport in Oriented Benzodithiophene Covalent Organic Framework Thin Films. *ACS Nano*, **2017**, 11, 2706-2713	16.7	90
361	Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. *Journal of Chemical Information and Modeling*, **2017**, 57, 298-310	6.1	8

360	Trifluoromethyl: An Amphiphilic Noncovalent Bonding Partner. *ChemPhysChem*, **2017**, 18, 772-784	3.2	39
359	Identification of the Beer Component Hordenine as Food-Derived Dopamine D2 Receptor Agonist by Virtual Screening a 3D Compound Database. *Scientific Reports*, **2017**, 7, 44201	4.9	20
358	Differences between G-Protein-Stabilized Agonist-GPCR Complexes and their Nanobody-Stabilized Equivalents. *Angewandte Chemie - International Edition*, **2017**, 56, 9008-9012	16.4	13
357	Differences between G-Protein-Stabilized Agonist□GPCR Complexes and their Nanobody-Stabilized Equivalents. *Angewandte Chemie*, **2017**, 129, 9136-9140	3.6	4
356	An Efficient Metadynamics-Based Protocol To Model the Binding Affinity and the Transition State Ensemble of G-Protein-Coupled Receptor Ligands. *Journal of Chemical Information and Modeling*, **2017**, 57, 1210-1217	6.1	77
355	Radical Arylation of Anilines and Pyrroles via Aryldiazotates. *Chemistry - A European Journal*, **2017**, 23, 9647-9656	4.8	20
354	Accurate Intermolecular Potential for the C Dimer: The Performance of Different Levels of Quantum Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 274-285	6.4	14
353	Charge-Gating Dibenzothiophene-S,S-dioxide Bridges in Electron Donor□Bridge□Acceptor Conjugates. *Journal of Physical Chemistry C*, **2017**, 121, 13557-13569	3.8	16
352	Unified model for singlet fission within a non-conjugated covalent pentacene dimer. *Nature Communications*, **2017**, 8, 15171	17.4	143
351	Odd-Electron Bonds. *ChemPhysChem*, **2017**, 18, 2766-2771	3.2	13
350	On the feasibility of reactions through the fullerene wall: a theoretical study of NH@C. *Physical Chemistry Chemical Physics*, **2017**, 19, 17199-17209	3.6	4
349	Investigating allosteric effects on the functional dynamics of □2-adrenergic ternary complexes with enhanced-sampling simulations. *Chemical Science*, **2017**, 8, 4019-4026	9.4	20
348	Choosing the right nanoparticle size □designing novel ZnO electrode architectures for efficient dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2017**, 5, 7516-7522	13	8
347	Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. *ChemPlusChem*, **2017**, 82, 163	2.8	
346	Computational approaches and sigma-hole interactions: general discussion. *Faraday Discussions*, **2017**,	3.6	9
345	Beyond the halogen bond: general discussion. *Faraday Discussions*, **2017**, 203, 227-244	3.6	1
344	Solid-state chemistry and applications: general discussion. *Faraday Discussions*, **2017**, 203, 459-483	3.6	1
343	Polarization, donor-acceptor interactions, and covalent contributions in weak interactions: a clarification. *Journal of Molecular Modeling*, **2017**, 23, 297	2	30

342	Mediating Reductive Charge Shift Reactions in Electron Transport Chains. *Journal of the American Chemical Society*, **2017**, 139, 17474-17483	16.4	28
341	Charge Transport in Organic Materials: Norm-Conserving Imaginary Time Propagation with Local Ionization Energy as the External Potential. *Journal of Chemical Theory and Computation*, **2017**, 13, 6308-6316	6.4	3
340	The hpCADD NDDO Hamiltonian: Parametrization. *Journal of Chemical Information and Modeling*, **2017**, 57, 1907-1922	6.1	11
339	Halogen bonds and □holes. *Faraday Discussions*, **2017**, 203, 9-27	3.6	76
338	Highly Regioselective Alkylation of Hexabenzocoronenes: Fundamental Insights into the Covalent Chemistry of Graphene. *Angewandte Chemie - International Edition*, **2017**, 56, 12184-12190	16.4	25
337	Effect of Structure and Disorder on the Charge Transport in Defined Self-Assembled Monolayers of Organic Semiconductors. *ACS Nano*, **2017**, 11, 8747-8757	16.7	16
336	The □hole revisited. *Physical Chemistry Chemical Physics*, **2017**, 19, 32166-32178	3.6	222
335	Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. *ChemPlusChem*, **2017**, 82, 204-211	2.8	7
334	G-Protein coupled receptors: answers from simulations. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 1071-1078	2.5	12
333	Simulation of charge transport in organic semiconductors: A time-dependent multiscale method based on nonequilibrium Green's functions. *Physical Review Materials*, **2017**, 1,	3.2	12
332	Identification of Two Distinct Sites for Antagonist and Biased Agonist Binding to the Human Chemokine Receptor CXCR3. *Angewandte Chemie - International Edition*, **2016**, 55, 15277-15281	16.4	19
331	Structure-guided development of heterodimer-selective GPCR ligands. *Nature Communications*, **2016**, 7, 12298	17.4	65
330	Identification of Two Distinct Sites for Antagonist and Biased Agonist Binding to the Human Chemokine Receptor CXCR3. *Angewandte Chemie*, **2016**, 128, 15503-15507	3.6	6
329	A Three-Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. *Angewandte Chemie*, **2016**, 128, 8140-8144	3.6	10
328	Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks. *Nature Chemistry*, **2016**, 8, 310-316	17.6	338
327	20D-dynamic representation of protein sequences. *Genomics*, **2016**, 107, 16-23	4.3	16
326	From benzodithiophene to diethoxy-benzodithiophene covalent organic frameworks □structural investigations. *CrystEngComm*, **2016**, 18, 4295-4302	3.3	18
325	Using carbon nanodots as inexpensive and environmentally friendly sensitizers in mesoscopic solar cells. *Nanoscale Horizons*, **2016**, 1, 220-226	10.8	40

324	Comparative MD Simulations Indicate a Dual Role for Arg1323.50 in Dopamine-Dependent D2R Activation. *PLoS ONE*, **2016**, 11, e0146612	3.7	8
323	DNA-Dye-Conjugates: Conformations and Spectra of Fluorescence Probes. *PLoS ONE*, **2016**, 11, e0160229	3.7	3
322	A Three-Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. *Angewandte Chemie - International Edition*, **2016**, 55, 8008-12	16.4	32
321	Synchronized Offset Stacking: A Concept for Growing Large-Domain and Highly Crystalline 2D Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2016**, 138, 16703-16710	16.4	135
320	Can Simulations and Modeling Decipher NMR Data for Conformational Equilibria? Arginine-Vasopressin. *Journal of Chemical Information and Modeling*, **2016**, 56, 1798-807	6.1	8
319	Strongly Directing Substituents in the Radical Arylation of Substituted Benzenes. *Journal of Organic Chemistry*, **2016**, 81, 9785-9791	4.2	14
318	Facile C(sp(2))-C(sp(2)) bond cleavage in oxalic acid-derived radicals. *Journal of the American Chemical Society*, **2015**, 137, 3248-52	16.4	10
317	Amphiphilic perylene-calix[4]arene hybrids: synthesis and tunable self-assembly. *Journal of the American Chemical Society*, **2015**, 137, 3308-17	16.4	42
316	Mathematical modeling and physical reality in noncovalent interactions. *Journal of Molecular Modeling*, **2015**, 21, 52	2	199
315	Thermochromic and solvatochromic properties of Lindqvist polyoxometalates. *Chemical Communications*, **2015**, 51, 13702-5	5.8	16
314	On-off switch of charge-separated states of pyridine-vinylene-linked porphyrin-C conjugates detected by EPR. *Chemical Science*, **2015**, 6, 5994-6007	9.4	21
313	A push-pull unsymmetrical subphthalocyanine dimer. *Chemical Science*, **2015**, 6, 5571-5577	9.4	15
312	Carboxylate Ion Pairing with Alkali-Metal Ions for β-Lactoglobulin and Its Role on Aggregation and Interfacial Adsorption. *Journal of Physical Chemistry B*, **2015**, 119, 5505-17	3.4	28
311	Template-dependent photochemical reactivity of molecular metal oxides. *Chemistry - A European Journal*, **2015**, 21, 8716-9	4.8	39
310	Carbon Nanodots: Supramolecular Electron Donor-Acceptor Hybrids Featuring Perylenediimides. *Angewandte Chemie - International Edition*, **2015**, 54, 8292-7	16.4	66
309	A carbon-carbon hybrid - immobilizing carbon nanodots onto carbon nanotubes. *Chemical Science*, **2015**, 6, 6878-6885	9.4	36
308	Synthesis of dibenzo[c,e][1,2]diazocines□ new group of eight-membered cyclic azo compounds. *Tetrahedron Letters*, **2015**, 56, 316-320	2	3
307	Correct electrostatic treatment of noncovalent interactions: the importance of polarization. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 169-177	7.9	87

306	Tuning the reorganization energy of electron transfer in supramolecular ensembles--metalloporphyrin, oligophenylenevinylenes, and fullerene--and the impact on electron transfer kinetics. *Nanoscale*, **2015**, 7, 2597-608	7.7	44
305	Molecular wires--impact of π-conjugation and implementation of molecular bottlenecks. *Chemical Society Reviews*, **2015**, 44, 988-98	58.5	78
304	A multi-agent quantum Monte Carlo model for charge transport: Application to organic field-effect transistors. *Journal of Chemical Physics*, **2015**, 143, 044114	3.9	10
303	Simulating charge transport in flexible systems. *Perspectives in Science*, **2015**, 6, 58-65	0.8	3
302	Cubic C8 : An Observable Allotrope of Carbon?. *ChemPhysChem*, **2015**, 16, 2165-71	3.2	5
301	Kohlenstoff-Nanopunkte: supramolekulare Elektronendonor-Akzeptor-Hybride mit Perylendiimiden. *Angewandte Chemie*, **2015**, 127, 8410-8415	3.6	9
300	The Electronic Structure of Amorphous Carbon Nanodots. *Journal of Physical Chemistry B*, **2015**, 119, 7258-65	3.4	47
299	EMPIRE: a highly parallel semiempirical molecular orbital program: 2: periodic boundary conditions. *Journal of Molecular Modeling*, **2015**, 21, 144	2	23
298	π-Hole bonding: a physical interpretation. *Topics in Current Chemistry*, **2015**, 358, 19-42		117
297	In Silico Adoption of an Orphan Nuclear Receptor NR4A1. *PLoS ONE*, **2015**, 10, e0135246	3.7	5
296	Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. *Journal of Molecular Modeling*, **2014**, 20, 2159	2	12
295	Carbon nanodots: toward a comprehensive understanding of their photoluminescence. *Journal of the American Chemical Society*, **2014**, 136, 17308-16	16.4	282
294	Indentation and self-healing mechanisms of a self-assembled monolayer--a combined experimental and modeling study. *Journal of the American Chemical Society*, **2014**, 136, 10718-27	16.4	29
293	Integrating metalloporphycenes into p-type NiO-based dye-sensitized solar cells. *Chemical Communications*, **2014**, 50, 11339-42	5.8	21
292	Fullerene van der Waals oligomers as electron traps. *Journal of the American Chemical Society*, **2014** , 136, 10890-3	16.4	38
291	Driving forces for the self-assembly of graphene oxide on organic monolayers. *Nanoscale*, **2014**, 6, 11344-50	7.7	11
290	EMPIRE: a highly parallel semiempirical molecular orbital program: 1: self-consistent field calculations. *Journal of Molecular Modeling*, **2014**, 20, 2331	2	42
289	Quantum-mechanics-based molecular interaction fields for 3D-QSAR. *Journal of Cheminformatics*, **2014**, 6, O10	8.6	0

288	Simulating "soft" electronics. *Journal of Cheminformatics*, **2014**, 6, O19	8.6	
287	Directional Electrostatic Bonding **2014**, 523-536		2
286	Active-state model of a dopamine D2 receptor-G□complex stabilized by aripiprazole-type partial agonists. *PLoS ONE*, **2014**, 9, e100069	3.7	26
285	Role of Polarization in Halogen Bonds. *Australian Journal of Chemistry*, **2014**, 67, 451	1.2	59
284	Conformation and dynamics of 8-Arg-vasopressin in solution. *Journal of Molecular Modeling*, **2014**, 20, 2485	2	10
283	Structure-based evolution of subtype-selective neurotensin receptor ligands. *ChemistryOpen*, **2014**, 3, 206-18	2.3	8
282	Multiply bonded metal(II) acetate (rhodium, ruthenium, and molybdenum) complexes with the trans-1,2-bis(N-methylimidazol-2-yl)ethylene ligand. *Inorganic Chemistry*, **2014**, 53, 12305-14	5.1	17
281	A molecular placeholder strategy to access a family of transition-metal-functionalized vanadium oxide clusters. *Chemistry - A European Journal*, **2014**, 20, 12269-73	4.8	61
280	Modeling charge transport in C60-based self-assembled monolayers for applications in field-effect transistors. *Journal of Chemical Physics*, **2014**, 140, 204702	3.9	14
279	Statistical properties of spectra of chloronaphthalenes. *Journal of Mathematical Chemistry*, **2013**, 51, 857-867	2.1	2
278	Probing charge transfer in benzodifuran-C60 dumbbell-type electron donor-acceptor conjugates: ground- and excited-state assays. *ChemPhysChem*, **2013**, 14, 2910-9	3.2	8
277	Economical and accurate protocol for calculating hydrogen-bond-acceptor strengths. *Journal of Chemical Information and Modeling*, **2013**, 53, 3262-72	6.1	14
276	Molecular dynamics simulations of liquid phase interfaces: understanding the structure of the glycerol/water-dodecane system. *Langmuir*, **2013**, 29, 11898-907	4	18
275	An unsymmetrical pentacene derivative with ambipolar behavior in organic thin-film transistors. *Chemical Communications*, **2013**, 49, 6725-7	5.8	22
274	Improving the charge transport in self-assembled monolayer field-effect transistors: from theory to devices. *Journal of the American Chemical Society*, **2013**, 135, 4893-900	16.4	61
273	Doped polycyclic aromatic hydrocarbons as building blocks for nanoelectronics: a theoretical study. *Journal of Organic Chemistry*, **2013**, 78, 1894-902	4.2	28
272	Directional Noncovalent Interactions: Repulsion and Dispersion. *Journal of Chemical Theory and Computation*, **2013**, 9, 2264-75	6.4	64
271	Precise control of intramolecular charge-transport: the interplay of distance and conformational effects. *Chemistry - A European Journal*, **2013**, 19, 7575-86	4.8	20

270	Quantum-dot-sensitized solar cells: understanding linker molecules through theory and experiment. *Langmuir*, **2013**, 29, 2434-8	4	39
269	Halogen bonding and other □hole interactions: a perspective. *Physical Chemistry Chemical Physics*, **2013**, 15, 11178-89	3.6	1186
268	Blending through-space and through-bond □□coupling in [2,2']-paracyclophane-oligophenylenevinylene molecular wires. *Journal of the American Chemical Society*, **2013**, 135, 10372-81	16.4	60
267	Quantum mechanics-based properties for 3D-QSAR. *Journal of Chemical Information and Modeling*, **2013**, 53, 1486-502	6.1	20
266	Phosphonate- and carboxylate-based self-assembled monolayers for organic devices: a theoretical study of surface binding on aluminum oxide with experimental support. *ACS Applied Materials & Interfaces*, **2013**, 5, 6073-80	9.5	85
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