Jindrich Fanfrlik

List of Publications by Year
in descending order

94 papers	3,412 citations	147801 31 h-index	149698 56 g-index
97 all docs	97 docs citations	97 times ranked	3224 citing authors

#	Article	IF	Citations
1	Halogen bond tunability I: the effects of aromatic fluorine substitution on the strengths of halogen-bonding interactions involving chlorine, bromine, and iodine. Journal of Molecular Modeling, 2011, 17, 3309-3318.	1.8	374
2	Semiempirical Quantum Chemical PM6 Method Augmented by Dispersion and H-Bonding Correction Terms Reliably Describes Various Types of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2009, 5, 1749-1760.	5.3	312
3	Halogen bond tunability II: the varying roles of electrostatic and dispersion contributions to attraction in halogen bonds. Journal of Molecular Modeling, 2013, 19, 4651-4659.	1.8	190
4	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	2.1	134
5	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	6.4	132
6	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	13.8	124
7	A Reliable Docking/Scoring Scheme Based on the Semiempirical Quantum Mechanical PM6-DH2 Method Accurately Covering Dispersion and H-Bonding: HIV-1 Protease with 22 Ligands. Journal of Physical Chemistry B, 2010, 114, 12666-12678.	2.6	116
8	Inorganic Polyhedral Metallacarborane Inhibitors of HIV Protease: A New Approach to Overcoming Antiviral Resistance. Journal of Medicinal Chemistry, 2008, 51, 4839-4843.	6.4	90
9	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	3.4	85
10	Semiempirical Quantum Mechanical Method PM6-DH2X Describes the Geometry and Energetics of CK2-Inhibitor Complexes Involving Halogen Bonds Well, While the Empirical Potential Fails. Journal of Physical Chemistry B, 2011, 115, 8581-8589.	2.6	80
11	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	2.8	80
12	5-Substituted Pyrimidine and 7-Substituted 7-Deazapurine dNTPs as Substrates for DNA Polymerases in Competitive Primer Extension in the Presence of Natural dNTPs. ACS Chemical Biology, 2016, 11, 3165-3171.	3.4	63
13	7â€Arylâ€7â€deazaadenine 2â€²â€Deoxyribonucleoside Triphosphates (dNTPs): Better Substrates for DNA Polymerases than dATP in Competitive Incorporations. Angewandte Chemie - International Edition, 2014, 53, 7552-7555.	13.8	61
14	Structural Basis for Inhibition of Cathepsin B Drug Target from the Human Blood Fluke, Schistosoma mansoni. Journal of Biological Chemistry, 2011, 286, 35770-35781.	3.4	60
15	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. Journal of Physical Chemistry B, 2013, 117, 5950-5962.	2.6	60
16	The Structure-Based Design of SARS-CoV-2 nsp14 Methyltransferase Ligands Yields Nanomolar Inhibitors. ACS Infectious Diseases, 2021, 7, 2214-2220.	3.8	57
17	The SQM/COSMO filter: reliable native pose identification based on the quantum-mechanical description of proteinâ€“ligand interactions and implicit COSMO solvation. Chemical Communications, 2016, 52, 3312-3315.	4.1	55
18	Interpretation of Protein/Ligand Crystal Structure using QM/MM Calculations: Case of HIV-1 Protease/Metallacarborane Complex. Journal of Physical Chemistry B, 2008, 112, 15094-15102.	2.6	52

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19	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. Current Computer-Aided Drug Design, 2013, 9, 118-129.	1.2	52
20	Chalcogen Bonding in Proteinâ^'Ligand Complexes: PDB Survey and Quantum Mechanical Calculations. ChemPhysChem, 2018, 19, 2540-2548.	2.1	50
21	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	5.5	49
22	Transferable scoring function based on semiempirical quantum mechanical PM6-DH2 method: CDK2 with 15 structurally diverse inhibitors. Journal of Computer-Aided Molecular Design, 2011, 25, 223-235.	2.9	48
23	QM/MM Calculations Reveal the Different Nature of the Interaction of Two Carborane-Based Sulfamide Inhibitors of Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2013, 117, 16096-16104.	2.6	47
24	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	3.4	45
25	Quantum Mechanics-Based Scoring Rationalizes the Irreversible Inactivation of Parasitic Schistosoma mansoni Cysteine Peptidase by Vinyl Sulfone Inhibitors. Journal of Physical Chemistry B, 2013, 117, 14973-14982.	2.6	43
26	Stimuli-Responsive Nanoparticles Based on Interaction of Metallacarborane with Poly(ethylene oxide). Macromolecules, 2009, 42, 4829-4837.	4.8	40
27	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. ChemPhysChem, 2016, 17, 3373-3376.	2.1	40
28	SQM/COSMO Scoring Function at the DFTB3-D3H4 Level: Unique Identification of Native Proteinâ€"Ligand Poses. Journal of Chemical Information and Modeling, 2017, 57, 127-132.	5.4	40
29	Interaction of heteroboranes with biomolecules : Part 2. The effect of various metal vertices and exo-substitutions. Physical Chemistry Chemical Physics, 2007, 9, 2085-2093.	2.8	39
30	Chalcogen and Pnicogen Bonds in Complexes of Neutral Icosahedral and Bicapped Square-Antiprismatic Heteroboranes. Journal of Physical Chemistry A, 2015, 119, 1388-1395.	2.5	39
31	Bâ€"Hâ‹Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	2.8	32
32	Explicit treatment of active-site waters enhances quantum mechanical/implicit solvent scoring: Inhibition of CDK2 by new pyrazolo[1,5-a]pyrimidines. European Journal of Medicinal Chemistry, 2017, 126, 1118-1128.	5.5	32
33	Interactions of Boranes and Carboranes with Aromatic Systems: CCSD(T) Complete Basis Set Calculations and DFT-SAPT Analysis of Energy Components. Journal of Physical Chemistry A, 2010, 114, 11304-11311.	2.5	31
34	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€...IIâ€"Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	2.1	29
35	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie, 2014, 126, 10303-10306.	2.0	26
36	Structural Basis for Inhibition of Mycobacterial and Human Adenosine Kinase by 7-Substituted 7-(Het)aryl-7-deazaadenine Ribonucleosides. Journal of Medicinal Chemistry, 2014, 57, 8268-8279.	6.4	26

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37	The properties of substituted 3D-aromatic neutral carboranes: the potential for Ïƒ-hole bonding. Physical Chemistry Chemical Physics, 2015, 17, 20814-20821.	2.8	26
38	Binary twinned-icosahedral [B₂₁H₁₈]^{â^'} interacts with cyclodextrins as a precedent for its complexation with other organic motifs. Physical Chemistry Chemical Physics, 2017, 19, 11748-11752.	2.8	26
39	A systematic examination of classical and multi-center bonding in heteroborane clusters. Physical Chemistry Chemical Physics, 2018, 20, 4666-4675.	2.8	26
40	Ligand Conformational and Solvation/Desolvation Free Energy in Proteinâ^'Ligand Complex Formation. Journal of Physical Chemistry B, 2011, 115, 4718-4724.	2.6	24
41	Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse Proteinâ€“Ligand Complexes in Cognate Docking. ACS Omega, 2017, 2, 4022-4029.	3.5	22
42	Unraveling the anti-influenza effect of flavonoids: Experimental validation of luteolin and its congeners as potent influenza endonuclease inhibitors. European Journal of Medicinal Chemistry, 2020, 208, 112754.	5.5	21
43	IDD388 Polyhalogenated Derivatives as Probes for an Improved Structure-Based Selectivity of AKR1B10 Inhibitors. ACS Chemical Biology, 2016, 11, 2693-2705.	3.4	19
44	Biomimetic Macrocyclic Inhibitors of Human Cathepsin D: Structureâ€“Activity Relationship and Binding Mode Analysis. Journal of Medicinal Chemistry, 2020, 63, 1576-1596.	6.4	19
45	Carborane-Based Carbonic Anhydrase Inhibitors: Insight into CAII/CAIX Specificity from a High-Resolution Crystal Structure, Modeling, and Quantum Chemical Calculations. BioMed Research International, 2014, 2014, 1-9.	1.9	18
46	Pnictogen bonding in pyrazineâ€¢PnX5 (Pn = P, As, Sb and X = F, Cl, Br) complexes. Journal of Molecular Modeling, 2017, 23, 328.	1.8	18
47	Substrate Specificity, Inhibitor Selectivity and Structure-Function Relationships of Aldo-Keto Reductase 1B15: A Novel Human Retinaldehyde Reductase. PLoS ONE, 2015, 10, e0134506.	2.5	17
48	Dihalogen and Pnictogen Bonding in Crystalline Icosahedral Phosphaboranes. Crystals, 2018, 8, 390.	2.2	16
49	Icosahedral Carbaboranes with Peripheral Hydrogenâ€“Chalcogenide Groups: Structures from Gas Electron Diffraction and Chemical Shielding in Solution. Chemistry - A European Journal, 2019, 25, 2313-2321.	3.3	16
50	Structural Basis of the Interaction of Cyclinâ€Dependent Kinaseâ€...2 with Roscovitine and Its Analogues Having Bioisosteric Central Heterocycles. ChemPhysChem, 2017, 18, 785-795.	2.1	14
51	A novel stibacarbaborane cluster with adjacent antimony atoms exhibiting unique pnictogen bond formation that dominates its crystal packing. Dalton Transactions, 2017, 46, 13714-13719.	3.3	14
52	Faceâ€Fusion of Icosahedral Boron Hydride Increases Affinity to Î³â€Cyclodextrin: closo , closo â€[B 21 H 18] â^' as an Anion with Very Low Free Energy of Dehydration. ChemPhysChem, 2020, 21, 971-976.	2.1	14
53	Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of SÂ·Â·Â·O chalcogen bonds. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	13
54	Theoretical insight into the stabilization of triazole fungicides via their interactions with dications. International Journal of Mass Spectrometry, 2014, 359, 38-43.	1.5	12

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55	Sâ‹¯N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. Chemical Physics, 2018, 500, 37-44.	1.9	12
56	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2362-2371.	2.8	12
57	The non-planarity of the benzene molecule in the X-ray structure of the chelated bismuth(iii) heteroboroxine complex is not supported by quantum mechanical calculations. Dalton Transactions, 2016, 45, 462-465.	3.3	10
58	Nuclear Magnetic Shielding of Monoboranes: Calculation and Assessment of ¹¹B NMR Chemical Shifts in Planar BX₃ and in Tetrahedral [BX₄]^{â¯'} Systems. Journal of Physical Chemistry A, 2017, 121, 9631-9637.	2.5	10
59	Synthesis of nucleosides and dNTPs bearing oligopyridine ligands linked through an octadiyne tether, their incorporation into DNA and complexation with transition metal cations. Organic and Biomolecular Chemistry, 2013, 11, 78-89.	2.8	9
60	Druggable Hot Spots in the Schistosomiasis Cathepsin B1 Target Identified by Functional and Binding Mode Analysis of Potent Vinyl Sulfone Inhibitors. ACS Infectious Diseases, 2021, 7, 1077-1088.	3.8	9
61	Azanitrile Inhibitors of the SmCB1 Protease Target Are Lethal to Schistosoma mansoni: Structural and Mechanistic Insights into Chemotype Reactivity. ACS Infectious Diseases, 2021, 7, 189-201.	3.8	9
62	Chalcogens act as inner and outer heteroatoms in borane cages with possible consequences for Ïƒ-hole interactions. CrystEngComm, 2016, 18, 8982-8987.	2.6	8
63	Mimicking of cyproconazole behavior in the presence of Cu and Zn. Rapid Communications in Mass Spectrometry, 2017, 31, 2043-2050.	1.5	8
64	Complexation and stability of the fungicide penconazole in the presence of zinc and copper ions. Rapid Communications in Mass Spectrometry, 2020, 34, e8714.	1.5	8
65	Structural and Thermodynamic Analysis of the Resistance Development to Pimodivir (VX-787), the Clinical Inhibitor of Cap Binding to PB2 Subunit of Influenza A Polymerase. Molecules, 2021, 26, 1007.	3.8	8
66	Synthesis of Analogues of Acyclic Nucleoside Diphosphates Containing a (Phosphonomethyl)phosphanyl Moiety and Studies of Their Phosphorylation. European Journal of Organic Chemistry, 2009, 2009, 1082-1092.	2.4	7
67	On the reliability of the corrected semiempirical quantum chemical method (PM6-DH2) for assigning the protonation states in HIV-1 protease/inhibitor complexes. Collection of Czechoslovak Chemical Communications, 2011, 76, 457-479.	1.0	7
68	Synthesis of closo-1,2-H₂C₂B₈Me₈ and 1,2-H₂C₂B₈Me₇X (X = I and OTf) Dicarbaboranes and Their Rearrangement Reactions. Inorganic Chemistry, 2019, 58, 2865-2871.	4.0	7
69	Structural and Functional Studies of Phosphoenolpyruvate Carboxykinase from Mycobacterium tuberculosis. PLoS ONE, 2015, 10, e0120682.	2.5	7
70	The Interplay between Various Ïƒ- and Ï€-Hole Interactions of Trigonal Boron and Trigonal Pyramidal Arsenic Triiodides. Crystals, 2017, 7, 225.	2.2	6
71	Quantitative syntheses of permethylated closo-1,10-R₂C₂B₈Me₈ (R = H, Me) carboranes. Egg-shaped hydrocarbons on the Frontier between inorganic and organic chemistry. RSC Advances, 2018, 8, 38238-38244.	3.6	6
72	Methyl camouflage in the ten-vertex closo-dicarbaborane(10) series. Isolation of closo-1,6-R₂C₂B₈Me₈ (R = H and Me) and their monosubstituted analogues. Dalton Transactions, 2018, 47, 11070-11076.	3.3	6

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73	Chalcogen Bonding due to the Exo-Substitution of Icosahedral Dicarbaborane. Molecules, 2019, 24, 2657.	3.8	6
74	Investigation of Thiaborane closoâ€“nido Conversion Pathways Promoted by N-Heterocyclic Carbenes. Inorganic Chemistry, 2019, 58, 2471-2482.	4.0	6
75	Nature of Binding in Planar Halogenâ€“Benzene Assemblies and Their Possible Visualization in Scanning Probe Microscopy. Journal of Physical Chemistry C, 2019, 123, 8379-8386.	3.1	6
76	Bromination Mechanism of closoâ€1,2â€C₂B₁₀H₁₂ and the Structure of the Resulting 9â€Brâ€closoâ€1,2â€C₂B₁₀H₁₁ Determined by Gas Electron Diffraction. ChemPlusChem, 2020, 85, 2606-2610.	2.8	6
77	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. Current Computer-Aided Drug Design, 2013, 9, 118-129.	1.2	5
78	A theoretical analysis of the structure and properties of B₂₆H₃₀ isomers. Consequences to the laser and semiconductor doping capabilities of large borane clusters. Physical Chemistry Chemical Physics, 2019, 21, 12916-12923.	2.8	5
79	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
80	Outerly functionalized and non-functionalized boron clusters intercalated into layered hydroxides with different modes of binding: materials for superacid storage. Dalton Transactions, 2018, 47, 11669-11679.	3.3	4
81	Thiaboranes on Both Sides of the Icosahedral Barrier: Retaining and Breaking the Barrier with Carbon Functionalities. ChemPlusChem, 2019, 84, 822-827.	2.8	4
82	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2361-2361.	2.8	4
83	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	2.1	4
84	Transformation of various multicenter bondings within bicapped-square antiprismatic motifs: Z-rearrangement. Dalton Transactions, 2021, 50, 12098-12106.	3.3	4
85	Inhibition of human purine nucleoside phosphorylase by tenofovir phosphate congeners. Collection of Czechoslovak Chemical Communications, 2010, 75, 1249-1257.	1.0	3
86	Electrophilic Methylation of Decaborane(14): Selective Synthesis of Tetramethylated and Heptamethylated Decaboranes and Their Conjugated Bases. Inorganic Chemistry, 2020, 59, 10540-10547.	4.0	3
87	The Influence of Halogenated Hypercarbon on Crystal Packing in the Series of 1-Ph-2-X-1,2-dicarba-closo-dodecaboranes (X = F, Cl, Br, I). Molecules, 2020, 25, 1200.	3.8	3
88	Hydration Gibbs Energies of Nucleic Acid Bases Determined by Gibbs Energy Perturbation, Continuous and Hybrid Approaches. Collection of Czechoslovak Chemical Communications, 2005, 70, 1756-1768.	1.0	3
89	The Ï€ Complex of the Hydronium Ion Frozen on the Pathway of Electrophilic Aromatic Substitution. European Journal of Organic Chemistry, 2016, 2016, 4473-4475.	2.4	2
90	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. Journal of Molecular Recognition, 2020, 33, e2842.	2.1	2

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91	Various types of non-covalent interactions contributing towards crystal packing of halogenated diphospha-dicarbaborane with an open pentagonal belt. New Journal of Chemistry, 2018, 42, 10481-10483.	2.8	1
92	Thiaborane clusters with an exoskeletal Bâ€“H group. Chemical Communications, 2019, 55, 3375-3378.	4.1	1
93	Thiaborane Icosahedral Barrier Increased by the Functionalization of all Terminal Hydrogens in closo-1-SB11H11. Inorganic Chemistry, 2021, 60, 8428-8431.	4.0	1
94	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	13.8	1