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	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
2	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
3	Transformation of various multicenter bondings within bicapped-square antiprismatic motifs: Z-rearrangement. Dalton Transactions, 2021, 50, 12098-12106.	3.3	4
4	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
5	The Structure-Based Design of SARS-CoV-2 nsp14 Methyltransferase Ligands Yields Nanomolar Inhibitors. ACS Infectious Diseases, 2021, 7, 2214-2220.	3.8	57
6	Thiaborane Icosahedral Barrier Increased by the Functionalization of all Terminal Hydrogens in closo-1-SB11H11. Inorganic Chemistry, 2021, 60, 8428-8431.	4.0	1
7	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
8	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
9	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
10	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
11	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
12	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	2.1	4
13	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
14	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
15	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. Journal of Molecular Recognition, 2020, 33, e2842.	2.1	2
16	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
17	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
18	Chalcogen Bonding due to the Exo-Substitution of Icosahedral Dicarbaborane. Molecules, 2019, 24, 2657.	3.8	6

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19	Thiaboranes on Both Sides of the Icosahedral Barrier: Retaining and Breaking the Barrier with Carbon Functionalities. ChemPlusChem, 2019, 84, 822-827.	2.8	4
20	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
21	Thiaborane clusters with an exoskeletal Bâ€“H group. Chemical Communications, 2019, 55, 3375-3378.	4.1	1
22	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
23	Investigation of Thiaborane closoâ€“nido Conversion Pathways Promoted by N-Heterocyclic Carbenes. Inorganic Chemistry, 2019, 58, 2471-2482.	4.0	6
24	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
25	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
26	A systematic examination of classical and multi-center bonding in heteroborane clusters. Physical Chemistry Chemical Physics, 2018, 20, 4666-4675.	2.8	26
27	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€…IIâ€“Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	2.1	29
28	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
29	Sâ‹¯N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. Chemical Physics, 2018, 500, 37-44.	1.9	12
30	Dihalogen and Pnictogen Bonding in Crystalline Icosahedral Phosphaboranes. Crystals, 2018, 8, 390.	2.2	16
31	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
32	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
33	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
34	Chalcogen Bonding in Proteinâˆ’Ligand Complexes: PDB Survey and Quantum Mechanical Calculations. ChemPhysChem, 2018, 19, 2540-2548.	2.1	50
35	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
36	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

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37	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
38	Bâ€“Hâ‹¯Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	2.8	32
39	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
40	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
41	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
42	Mimicking of cyproconazole behavior in the presence of Cu and Zn. Rapid Communications in Mass Spectrometry, 2017, 31, 2043-2050.	1.5	8
43	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
44	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
45	The Interplay between Various Ïƒ- and Ï€-Hole Interactions of Trigonal Boron and Trigonal Pyramidal Arsenic Triiodides. Crystals, 2017, 7, 225.	2.2	6
46	IDD388 Polyhalogenated Derivatives as Probes for an Improved Structure-Based Selectivity of AKR1B10 Inhibitors. ACS Chemical Biology, 2016, 11, 2693-2705.	3.4	19
47	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. ChemPhysChem, 2016, 17, 3373-3376.	2.1	40
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
56	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
57	The properties of substituted 3D-aromatic neutral carboranes: the potential for ĭf-hole bonding. Physical Chemistry Chemical Physics, 2015, 17, 20814-20821.	2.8	26
58	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	3.4	45
59	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
60	Structural and Functional Studies of Phosphoenolpyruvate Carboxykinase from Mycobacterium tuberculosis. PLoS ONE, 2015, 10, e0120682.	2.5	7
61	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
62	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie, 2014, 126, 10303-10306.	2.0	26
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	3.4	85
72	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	2.8	80

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73	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
74	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
75	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
76	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
77	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
78	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
79	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
80	Ligand Conformational and Solvation/Desolvation Free Energy in Proteinâ^'Ligand Complex Formation. Journal of Physical Chemistry B, 2011, 115, 4718-4724.	2.6	24
81	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
82	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
83	Inhibition of human purine nucleoside phosphorylase by tenofovir phosphate congeners. Collection of Czechoslovak Chemical Communications, 2010, 75, 1249-1257.	1.0	3
84	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
85	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
86	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
87	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
88	Stimuli-Responsive Nanoparticles Based on Interaction of Metallacarborane with Poly(ethylene oxide). Macromolecules, 2009, 42, 4829-4837.	4.8	40
89	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	6.4	132
90	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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91	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
92	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
93	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	2.1	134
94	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