Martin Lepsik

List of Publications by Year
in descending order

87	2,951	136740	182168
papers	citations	32 h-index	51 g-index

92	92	92	3774
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Aurora kinase inhibitors: Progress towards the clinic. Investigational New Drugs, 2012, 30, 2411-2432.	1.2	201
2	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	1.0	134
3	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	2.9	132
4	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	7.2	124
5	Metallacarboranes and their interactions: theoretical insights and their applicability. Chemical Society Reviews, 2012, 41, 3445.	18.7	117
6	Inorganic Polyhedral Metallacarborane Inhibitors of HIV Protease: A New Approach to Overcoming Antiviral Resistance. Journal of Medicinal Chemistry, 2008, 51, 4839-4843.	2.9	90
7	Substrate binding and specificity of rhomboid intramembrane protease revealed by substrateâ€“peptide complex structures. EMBO Journal, 2014, 33, 2408-2421.	3.5	87
8	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
9	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	1.3	80
10	Efficiency of a second-generation HIV-1 protease inhibitor studied by molecular dynamics and absolute binding free energy calculations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 279-293.	1.5	60
11	Structural Basis for Inhibition of Cathepsin B Drug Target from the Human Blood Fluke, Schistosoma mansoni. Journal of Biological Chemistry, 2011, 286, 35770-35781.	1.6	60
12	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. Journal of Physical Chemistry B, 2013, 117, 5950-5962.	1.2	60
13	Calcium Binding to Calmodulin by Molecular Dynamics with Effective Polarization. Journal of Physical Chemistry Letters, 2014, 5, 3964-3969.	2.1	60
14	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.	2.2	55
15	Structure-Aided Design of Novel Inhibitors of HIV Protease Based on a Benzodiazepine Scaffold. Journal of Medicinal Chemistry, 2012, 55, 10130-10135.	2.9	53
16	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.	1.2	52
17	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.	0.8	52
18	Digestive Î±â€amylases of the flour moth Ephestiaâ€ƒkuehniellaâ€“ adaptation to alkaline environment and plant inhibitors. FEBS Journal, 2009, 276, 3531-3546.	2.2	51

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19	Chalcogen Bonding in Proteinâ^'Ligand Complexes: PDB Survey and Quantum Mechanical Calculations. ChemPhysChem, 2018, 19, 2540-2548.	1.0	50
20	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	2.6	49
21	Thermodynamic and structural analysis of <scp>HIV</scp> protease resistance to darunavirÂâ€“Âanalysis of heavily mutated patientâ€derived <scp>HIV</scp>â€1 proteases. FEBS Journal, 2014, 281, 1834-1847.	2.2	48
22	Binding of Calcium and Other Metal Ions to the EF-Hand Loops of Calmodulin Studied by Quantum Chemical Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 10012-10022.	1.2	47
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.	1.2	47
24	Unusual Binding Mode of an HIV-1 Protease Inhibitor Explains its Potency against Multi-drug-resistant Virus Strains. Journal of Molecular Biology, 2002, 324, 739-754.	2.0	46
25	Inhibition of Human Serine Racemase, an Emerging Target for Medicinal Chemistry. Current Drug Targets, 2011, 12, 1037-1055.	1.0	46
26	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	1.6	45
27	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.	1.2	43
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.	2.5	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.	1.3	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.	1.1	39
31	Structural Integrity of the B24 Site in Human Insulin Is Important for Hormone Functionality*. Journal of Biological Chemistry, 2013, 288, 10230-10240.	1.6	38
32	Discovery of N²-(4-Amino-cyclohexyl)-9-cyclopentyl-N⁶-(4-morpholin-4-ylmethyl-phenyl)-9H-purine-2,6 as a Potent FLT3 Kinase Inhibitor for Acute Myeloid Leukemia with FLT3 Mutations. Journal of Medicinal Chemistry, 2018, 61, 3855-3869.	2.9	36
33	General and Modular Strategy for Designing Potent, Selective, and Pharmacologically Compliant Inhibitors of Rhomboid Proteases. Cell Chemical Biology, 2017, 24, 1523-1536.e4.	2.5	35
34	Bâ€“Hâ‹¯Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	1.3	32
35	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.	2.6	32
36	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.	1.1	31

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37	Human insulin analogues modified at the B26 site reveal a hormone conformation that is undetected in the receptor complex. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2765-2774.	2.5	29
38	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€…Iiâ€“Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	1.0	29
39	Affinity switching of the LEDGF/p75 IBD interactome is governed by kinase-dependent phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7053-E7062.	3.3	27
40	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie, 2014, 126, 10303-10306.	1.6	26
41	The properties of substituted 3D-aromatic neutral carboranes: the potential for Ïƒ-hole bonding. Physical Chemistry Chemical Physics, 2015, 17, 20814-20821.	1.3	26
42	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.	1.3	26
43	Enzymatic and structural analysis of the I47A mutation contributing to the reduced susceptibility to HIV protease inhibitor lopinavir. Protein Science, 2008, 17, 1555-1564.	3.1	24
44	Synthesis, structural characterization, docking, lipophilicity and cytotoxicity of 1-[(1R)-1-(6-fluoro-1,3-benzothiazol-2-yl)ethyl]-3-alkyl carbamates, novel acetylcholinesterase and butyrylcholinesterase pseudo-irreversible inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 1560-1572.	1.4	24
45	The Development of a Versatile Trifunctional Scaffold for Biological Applications. European Journal of Organic Chemistry, 2015, 2015, 3689-3701.	1.2	23
46	A Phenylnorstatine Inhibitor Binding to HIV-1 Protease:Â Geometry, Protonation, and Subsiteâ^'Pocket Interactions Analyzed at Atomic Resolution. Journal of Medicinal Chemistry, 2004, 47, 2030-2036.	2.9	22
47	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.	1.6	22
48	Mutations at hypothetical binding site 2 in insulin and insulin-like growth factors 1 and 2 result in receptor- and hormone-specific responses. Journal of Biological Chemistry, 2019, 294, 17371-17382.	1.6	21
49	Capturing a dynamically interacting inhibitor by paramagnetic NMR spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 5661-5673.	1.3	21
50	Biomimetic Macrocyclic Inhibitors of Human Cathepsin D: Structureâ€“Activity Relationship and Binding Mode Analysis. Journal of Medicinal Chemistry, 2020, 63, 1576-1596.	2.9	19
51	A rapid synthesis of low-nanomolar divalent LecA inhibitors in four linear steps from <scp>d</scp>-galactose pentaacetate. Chemical Communications, 2020, 56, 8822-8825.	2.2	19
52	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.	0.9	18
53	exo-Substituent effects in halogenated icosahedral (B12H122â€“) and octahedral (B6H62â€“) closo-borane skeletons: chemical reactivity studied by experimental and quantum chemical methods. Collection of Czechoslovak Chemical Communications, 2009, 74, 1-27.	1.0	16
54	Role of Mason-Pfizer Monkey Virus CA-NC Spacer Peptide-Like Domain in Assembly of Immature Particles. Journal of Virology, 2014, 88, 14148-14160.	1.5	15

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55	A Î³-cyclodextrin duplex connected with two disulfide bonds: synthesis, structure and inclusion complexes. Organic and Biomolecular Chemistry, 2015, 13, 2980-2985.	1.5	15
56	Enzymatic activity and immunoreactivity of Aca s 4, an alpha-amylase allergen from the storage mite Acarus siro. BMC Biochemistry, 2012, 13, 3.	4.4	14
57	Structural characterization of CAS SH3 domain selectivity and regulation reveals new CAS interaction partners. Scientific Reports, 2017, 7, 8057.	1.6	14
58	Thiocyanation of closo-Dodecaborate B12H122â^'. A Novel Synthetic Route and Theoretical Elucidation of the Reaction Mechanism. Inorganic Chemistry, 2010, 49, 5040-5048.	1.9	13
59	Modulation of HIV-1 Gag NC/p1 cleavage efficiency affects protease inhibitor resistance and viral replicative capacity. Retrovirology, 2012, 9, 29.	0.9	13
60	Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Nonâ€Amphiphilic Structures. Advanced Theory and Simulations, 2018, 1, 1700002.	1.3	13
61	In Vitro Evolution Reveals Noncationic Proteinâ€“RNA Interaction Mediated by Metal Ions. Molecular Biology and Evolution, 2022, 39, .	3.5	13
62	Medicinal Application ofÂCarboranes. , 2011, , 41-70.		12
63	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2362-2371.	1.3	12
64	Preparation and Separation of Telechelic Carboraneâ€Containing Poly(ethylene glycol)s. ChemPlusChem, 2013, 78, 528-535.	1.3	11
65	Imidazo[1,2â€c]pyrimidinâ€5(6H)â€one as a novel core of cyclinâ€dependent kinase 2 inhibitors: Synthesis, activity measurement, docking, and quantum mechanical scoring. Journal of Molecular Recognition, 2018, 31, e2720.	1.1	10
66	3H-Pyrazolo[4,3-f]quinoline-Based Kinase Inhibitors Inhibit the Proliferation of Acute Myeloid Leukemia Cells In Vivo. Journal of Medicinal Chemistry, 2021, 64, 10981-10996.	2.9	10
67	Atomic resolution crystal structure of Sapp2p, a secreted aspartic protease fromCandida parapsilosis. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 2494-2504.	2.5	9
68	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.	1.8	9
69	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.	1.8	9
70	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
71	Synthesis of Î±â€Branched Acyclic Nucleoside Phosphonates as Potential Inhibitors of Bacterial Adenylate Cyclases. ChemMedChem, 2018, 13, 199-206.	1.6	7
72	Myristoylation drives dimerization of matrix protein from mouse mammary tumor virus. Retrovirology, 2016, 13, 2.	0.9	6

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73	Induction of rare conformation of oligosaccharide by binding to calcium-dependent bacterial lectin: X-ray crystallography and modelling study. European Journal of Medicinal Chemistry, 2019, 177, 212-220.	2.6	6
74	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.	0.8	5
75	Interface Interactions of the Bowmanâ€“Birk Inhibitor BTCI in a Ternary Complex with Trypsin and Chymotrypsin Evaluated by Semiempirical Quantum Mechanical Calculations. European Journal of Organic Chemistry, 2018, 2018, 5203-5211.	1.2	5
76	Highly potent inhibitors of cathepsin K with a differently positioned cyanohydrazide warhead: structural analysis of binding mode to mature and zymogen-like enzymes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 515-526.	2.5	5
77	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
78	Micellization: Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Nonâ€Amphiphilic Structures (Adv. Theory Simul. 1/2018). Advanced Theory and Simulations, 2018, 1, 1870003.	1.3	4
79	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2361-2361.	1.3	4
80	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	1.0	4
81	Multipodal insulin mimetics built on adamantane or proline scaffolds. Bioorganic Chemistry, 2021, 107, 104548.	2.0	3
82	Structural determinants for subnanomolar inhibition of the secreted aspartic protease Sapp1p from Candida parapsilosis. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 914-921.	2.5	3
83	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. Journal of Molecular Recognition, 2020, 33, e2842.	1.1	2
84	Engineering the Ligand Specificity of the Human Galectinâ€1 by Incorporation of Tryptophan Analogues. ChemBioChem, 2022, , .	1.3	2
85	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	7.2	1
86	The Role of Cysteine Residues in Catalysis of Phosphoenolpyruvate Carboxykinase from Mycobacterium tuberculosis. PLoS ONE, 2017, 12, e0170373.	1.1	0
87	When Additive Molecular Dynamics Fails: Quantum Effects in Calcium-Dependent Lectin/Carbohydrate Complex. Biophysical Journal, 2019, 116, 144a.	0.2	0