Martin Lepsik

List of Publications by Year
in descending order

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87 papers	2,951 citations	136950 32 h-index	182427 51 g-index
92 all docs	92 docs citations	92 times ranked	3774 citing authors

#	Article	IF	Citations
1	In Vitro Evolution Reveals Noncationic Proteinâ€“RNA Interaction Mediated by Metal Ions. Molecular Biology and Evolution, 2022, 39, .	8.9	13
2	Engineering the Ligand Specificity of the Human Galectinâ€1 by Incorporation of Tryptophan Analogues. ChemBioChem, 2022, , .	2.6	2
3	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.	5.2	5
4	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
5	Multipodal insulin mimetics built on adamantane or proline scaffolds. Bioorganic Chemistry, 2021, 107, 104548.	4.1	3
6	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
7	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.	5.2	3
8	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.	6.4	10
9	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
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	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	2.1	4
12	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
13	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. Journal of Molecular Recognition, 2020, 33, e2842.	2.1	2
14	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.	4.1	19
15	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.	3.4	21
16	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.	5.5	6
17	When Additive Molecular Dynamics Fails: Quantum Effects in Calcium-Dependent Lectin/Carbohydrate Complex. Biophysical Journal, 2019, 116, 144a.	0.5	0
18	Capturing a dynamically interacting inhibitor by paramagnetic NMR spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 5661-5673.	2.8	21

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19	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.	6.4	36
20	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.	2.1	10
21	Micellization: Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Nonâ€Amphiphilic Structures (Adv. Theory Simul. 1/2018). Advanced Theory and Simulations, 2018, 1, 1870003.	2.8	4
22	Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Nonâ€Amphiphilic Structures. Advanced Theory and Simulations, 2018, 1, 1700002.	2.8	13
23	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€...IIâ€"Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	2.1	29
24	Synthesis of Î±â€Branched Acyclic Nucleoside Phosphonates as Potential Inhibitors of Bacterial Adenylate Cyclases. ChemMedChem, 2018, 13, 199-206.	3.2	7
25	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.	2.4	5
26	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.	7.1	27
27	Chalcogen Bonding in Proteinâ^'Ligand Complexes: PDB Survey and Quantum Mechanical Calculations. ChemPhysChem, 2018, 19, 2540-2548.	2.1	50
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	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
30	Bâ€"Hâ‹Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	2.8	32
31	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
32	General and Modular Strategy for Designing Potent, Selective, and Pharmacologically Compliant Inhibitors of Rhomboid Proteases. Cell Chemical Biology, 2017, 24, 1523-1536.e4.	5.2	35
33	Structural characterization of CAS SH3 domain selectivity and regulation reveals new CAS interaction partners. Scientific Reports, 2017, 7, 8057.	3.3	14
34	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
35	The Role of Cysteine Residues in Catalysis of Phosphoenolpyruvate Carboxykinase from Mycobacterium tuberculosis. PLoS ONE, 2017, 12, e0170373.	2.5	0
36	Myristoylation drives dimerization of matrix protein from mouse mammary tumor virus. Retrovirology, 2016, 13, 2.	2.0	6

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37	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
38	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.	3.0	24
39	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
40	The Development of a Versatile Trifunctional Scaffold for Biological Applications. European Journal of Organic Chemistry, 2015, 2015, 3689-3701.	2.4	23
41	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
42	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
43	A Î³-cyclodextrin duplex connected with two disulfide bonds: synthesis, structure and inclusion complexes. Organic and Biomolecular Chemistry, 2015, 13, 2980-2985.	2.8	15
44	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
45	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	3.4	45
46	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
47	Role of Mason-Pfizer Monkey Virus CA-NC Spacer Peptide-Like Domain in Assembly of Immature Particles. Journal of Virology, 2014, 88, 14148-14160.	3.4	15
48	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
49	Calcium Binding to Calmodulin by Molecular Dynamics with Effective Polarization. Journal of Physical Chemistry Letters, 2014, 5, 3964-3969.	4.6	60
50	Substrate binding and specificity of rhomboid intramembrane protease revealed by substrateâ€“peptide complex structures. EMBO Journal, 2014, 33, 2408-2421.	7.8	87
51	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie, 2014, 126, 10303-10306.	2.0	26
52	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
53	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.	4.7	48
54	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

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55	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
56	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
57	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
58	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
59	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	3.4	85
60	Preparation and Separation of Telechelic Carboraneâ€Containing Poly(ethylene glycol)s. ChemPlusChem, 2013, 78, 528-535.	2.8	11
61	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	2.8	80
62	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
63	Structural Integrity of the B24 Site in Human Insulin Is Important for Hormone Functionality*. Journal of Biological Chemistry, 2013, 288, 10230-10240.	3.4	38
64	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
65	Aurora kinase inhibitors: Progress towards the clinic. Investigational New Drugs, 2012, 30, 2411-2432.	2.6	201
66	Structure-Aided Design of Novel Inhibitors of HIV Protease Based on a Benzodiazepine Scaffold. Journal of Medicinal Chemistry, 2012, 55, 10130-10135.	6.4	53
67	Modulation of HIV-1 Gag NC/p1 cleavage efficiency affects protease inhibitor resistance and viral replicative capacity. Retrovirology, 2012, 9, 29.	2.0	13
68	Metallacarboranes and their interactions: theoretical insights and their applicability. Chemical Society Reviews, 2012, 41, 3445.	38.1	117
69	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
70	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
71	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
72	Inhibition of Human Serine Racemase, an Emerging Target for Medicinal Chemistry. Current Drug Targets, 2011, 12, 1037-1055.	2.1	46

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73	Medicinal Application ofÂCarboranes. , 2011, , 41-70.		12
74	Thiocyanation of closo-Dodecaborate B12H122â^'. A Novel Synthetic Route and Theoretical Elucidation of the Reaction Mechanism. Inorganic Chemistry, 2010, 49, 5040-5048.	4.0	13
75	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
76	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
77	Digestive Î±â€amylases of the flour moth Ephestiaâ€ƒkuehniellaâ€“ adaptation to alkaline environment and plant inhibitors. FEBS Journal, 2009, 276, 3531-3546.	4.7	51
78	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	6.4	132
79	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
80	Enzymatic and structural analysis of the I47A mutation contributing to the reduced susceptibility to HIV protease inhibitor lopinavir. Protein Science, 2008, 17, 1555-1564.	7.6	24
81	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
82	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
83	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.	2.6	47
84	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. ChemPhysChem, 2006, 7, 1100-1105.	2.1	134
85	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.	2.6	60
86	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.	6.4	22
87	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.	4.2	46