

# 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	Aurora kinase inhibitors: Progress towards the clinic. <i>Investigational New Drugs</i> , 2012, 30, 2411-2432.	2.6	201
2	Interaction of Carboranes with Biomolecules: Formation of Dihydrogen Bonds. <i>ChemPhysChem</i> , 2006, 7, 1100-1105.	2.1	134
3	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 7132-7141.	6.4	132
4	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 10139-10142.	13.8	124
5	Metallacarboranes and their interactions: theoretical insights and their applicability. <i>Chemical Society Reviews</i> , 2012, 41, 3445.	38.1	117
6	Inorganic Polyhedral Metallacarborane Inhibitors of HIV Protease: A New Approach to Overcoming Antiviral Resistance. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 4839-4843.	6.4	90
7	Substrate binding and specificity of rhomboid intramembrane protease revealed by substrate-peptide complex structures. <i>EMBO Journal</i> , 2014, 33, 2408-2421.	7.8	87
8	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. <i>ACS Chemical Biology</i> , 2013, 8, 2484-2492.	3.4	85
9	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. <i>ChemPlusChem</i> , 2013, 78, 921-931.	2.8	80
10	Efficiency of a second-generation HIV-1 protease inhibitor studied by molecular dynamics and absolute binding free energy calculations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 279-293.	2.6	60
11	Structural Basis for Inhibition of Cathepsin B Drug Target from the Human Blood Fluke, <i>Schistosoma mansoni</i> . <i>Journal of Biological Chemistry</i> , 2011, 286, 35770-35781.	3.4	60
12	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5950-5962.	2.6	60
13	Calcium Binding to Calmodulin by Molecular Dynamics with Effective Polarization. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3964-3969.	4.6	60
14	The SQM/COSMO filter: reliable native pose identification based on the quantum-mechanical description of protein-ligand interactions and implicit COSMO solvation. <i>Chemical Communications</i> , 2016, 52, 3312-3315.	4.1	55
15	Structure-Aided Design of Novel Inhibitors of HIV Protease Based on a Benzodiazepine Scaffold. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 10130-10135.	6.4	53
16	Interpretation of Protein/Ligand Crystal Structure using QM/MM Calculations: Case of HIV-1 Protease/Metallacarborane Complex. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15094-15102.	2.6	52
17	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 118-129.	1.2	52
18	Digestive $\alpha$ -amylases of the flour moth <i>Ephesia kuehniella</i> adaptation to alkaline environment and plant inhibitors. <i>FEBS Journal</i> , 2009, 276, 3531-3546.	4.7	51

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19	Chalcogen Bonding in Protein-Ligand Complexes: PDB Survey and Quantum Mechanical Calculations. <i>ChemPhysChem</i> , 2018, 19, 2540-2548.	2.1	50
20	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. <i>European Journal of Medicinal Chemistry</i> , 2015, 89, 189-197.	5.5	49
21	Thermodynamic and structural analysis of HIV-1 protease resistance to darunavir: Analysis of heavily mutated patient-derived HIV-1 proteases. <i>FEBS Journal</i> , 2014, 281, 1834-1847.	4.7	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. <i>Journal of Physical Chemistry B</i> , 2007, 111, 10012-10022.	2.6	47
23	QM/MM Calculations Reveal the Different Nature of the Interaction of Two Carborane-Based Sulfamide Inhibitors of Human Carbonic Anhydrase II. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16096-16104.	2.6	47
24	Unusual Binding Mode of an HIV-1 Protease Inhibitor Explains its Potency against Multi-drug-resistant Virus Strains. <i>Journal of Molecular Biology</i> , 2002, 324, 739-754.	4.2	46
25	Inhibition of Human Serine Racemase, an Emerging Target for Medicinal Chemistry. <i>Current Drug Targets</i> , 2011, 12, 1037-1055.	2.1	46
26	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. <i>ACS Chemical Biology</i> , 2015, 10, 1637-1642.	3.4	45
27	Quantum Mechanics-Based Scoring Rationalizes the Irreversible Inactivation of Parasitic <i>Schistosoma mansoni</i> Cysteine Peptidase by Vinyl Sulfone Inhibitors. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14973-14982.	2.6	43
28	SQM/COSMO Scoring Function at the DFTB3-D3H4 Level: Unique Identification of Native Protein-Ligand Poses. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 127-132.	5.4	40
29	Interaction of heteroboranes with biomolecules : Part 2. The effect of various metal vertices and exo-substitutions. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2085-2093.	2.8	39
30	Chalcogen and Pnictogen Bonds in Complexes of Neutral Icosahedral and Bicapped Square-Antiprismatic Heteroboranes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1388-1395.	2.5	39
31	Structural Integrity of the B24 Site in Human Insulin Is Important for Hormone Functionality*. <i>Journal of Biological Chemistry</i> , 2013, 288, 10230-10240.	3.4	38
32	Discovery of $N^{2,6}$ -(4-Amino-cyclohexyl)-9-cyclopentyl- $N^{9H}$ -purine-2,6 as a Potent FLT3 Kinase Inhibitor for Acute Myeloid Leukemia with FLT3 Mutations. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 3855-3869.	6.4	36
33	General and Modular Strategy for Designing Potent, Selective, and Pharmacologically Compliant Inhibitors of Rhomboid Proteases. <i>Cell Chemical Biology</i> , 2017, 24, 1523-1536.e4.	5.2	35
34	B $\cdots$ H $\cdots$ F: a nonclassical hydrogen bond or dispersion contact?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18194-18200.	2.8	32
35	Explicit treatment of active-site waters enhances quantum mechanical/implicit solvent scoring: Inhibition of CDK2 by new pyrazolo[1,5-a]pyrimidines. <i>European Journal of Medicinal Chemistry</i> , 2017, 126, 1118-1128.	5.5	32
36	Interactions of Boranes and Carboranes with Aromatic Systems: CCSD(T) Complete Basis Set Calculations and DFT-SAPT Analysis of Energy Components. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11304-11311.	2.5	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. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2765-2774.	2.5	29
38	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydrase Inhibitor Complexes. <i>ChemPhysChem</i> , 2018, 19, 873-879.	2.1	29
39	Affinity switching of the LEDGF/p75 IBD interactome is governed by kinase-dependent phosphorylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7053-E7062.	7.1	27
40	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. <i>Angewandte Chemie</i> , 2014, 126, 10303-10306.	2.0	26
41	The properties of substituted 3D-aromatic neutral carboranes: the potential for $\pi$ -hole bonding. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20814-20821.	2.8	26
42	Binary twinned-icosahedral $[B_{21}H_{18}]^{+}$ interacts with cyclodextrins as a precedent for its complexation with other organic motifs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11748-11752.	2.8	26
43	Enzymatic and structural analysis of the I47A mutation contributing to the reduced susceptibility to HIV protease inhibitor lopinavir. <i>Protein Science</i> , 2008, 17, 1555-1564.	7.6	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. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 1560-1572.	3.0	24
45	The Development of a Versatile Trifunctional Scaffold for Biological Applications. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3689-3701.	2.4	23
46	A Phenylnorstatine Inhibitor Binding to HIV-1 Protease: Geometry, Protonation, and Subsite Pocket Interactions Analyzed at Atomic Resolution. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 2030-2036.	6.4	22
47	Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse Protein-Ligand Complexes in Cognate Docking. <i>ACS Omega</i> , 2017, 2, 4022-4029.	3.5	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. <i>Journal of Biological Chemistry</i> , 2019, 294, 17371-17382.	3.4	21
49	Capturing a dynamically interacting inhibitor by paramagnetic NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5661-5673.	2.8	21
50	Biomimetic Macrocyclic Inhibitors of Human Cathepsin D: Structure-Activity Relationship and Binding Mode Analysis. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 1576-1596.	6.4	19
51	A rapid synthesis of low-nanomolar divalent LecA inhibitors in four linear steps from $\alpha$ -D-galactose pentaacetate. <i>Chemical Communications</i> , 2020, 56, 8822-8825.	4.1	19
52	Carborane-Based Carbonic Anhydrase Inhibitors: Insight into CAII/CAIX Specificity from a High-Resolution Crystal Structure, Modeling, and Quantum Chemical Calculations. <i>BioMed Research International</i> , 2014, 2014, 1-9.	1.9	18
53	exo-Substituent effects in halogenated icosahedral ( $B_{12}H_{12}^{+}$ ) and octahedral ( $B_6H_6^{+}$ ) closo-borane skeletons: chemical reactivity studied by experimental and quantum chemical methods. <i>Collection of Czechoslovak Chemical Communications</i> , 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. <i>Journal of Virology</i> , 2014, 88, 14148-14160.	3.4	15

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55	A $\beta$ -cyclodextrin duplex connected with two disulfide bonds: synthesis, structure and inclusion complexes. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2980-2985.	2.8	15
56	Enzymatic activity and immunoreactivity of Aca s 4, an alpha-amylase allergen from the storage mite <i>Acarus siro</i> . <i>BMC Biochemistry</i> , 2012, 13, 3.	4.4	14
57	Structural characterization of CAS SH3 domain selectivity and regulation reveals new CAS interaction partners. <i>Scientific Reports</i> , 2017, 7, 8057.	3.3	14
58	Thiocyanation of closo-Dodecaborate B <sub>12</sub> H <sub>12</sub> 2 <sup>-</sup> . A Novel Synthetic Route and Theoretical Elucidation of the Reaction Mechanism. <i>Inorganic Chemistry</i> , 2010, 49, 5040-5048.	4.0	13
59	Modulation of HIV-1 Gag NC/p1 cleavage efficiency affects protease inhibitor resistance and viral replicative capacity. <i>Retrovirology</i> , 2012, 9, 29.	2.0	13
60	Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Non-Amphiphilic Structures. <i>Advanced Theory and Simulations</i> , 2018, 1, 1700002.	2.8	13
61	In Vitro Evolution Reveals Noncationic Protein-RNA Interaction Mediated by Metal Ions. <i>Molecular Biology and Evolution</i> , 2022, 39, .	8.9	13
62	Medicinal Application of Carboranes. , 2011, , 41-70.		12
63	SQM/COSMO Scoring Function: Reliable Quantum-Mechanical Tool for Sampling and Ranking in Structure-Based Drug Design. <i>ChemPlusChem</i> , 2020, 85, 2362-2371.	2.8	12
64	Preparation and Separation of Telechelic Carborane-Containing Poly(ethylene glycol)s. <i>ChemPlusChem</i> , 2013, 78, 528-535.	2.8	11
65	Imidazo[1,2- <i>bc</i> ]pyrimidin-5(6 <i>H</i> )-one as a novel core of cyclin-dependent kinase 2 inhibitors: Synthesis, activity measurement, docking, and quantum mechanical scoring. <i>Journal of Molecular Recognition</i> , 2018, 31, e2720.	2.1	10
66	3 <i>H</i> -Pyrazolo[4,3- <i>fi</i> ]quinoline-Based Kinase Inhibitors Inhibit the Proliferation of Acute Myeloid Leukemia Cells In Vivo. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 10981-10996.	6.4	10
67	Atomic resolution crystal structure of Sapp2p, a secreted aspartic protease from <i>Candida parapsilosis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 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. <i>ACS Infectious Diseases</i> , 2021, 7, 1077-1088.	3.8	9
69	Azanitrile Inhibitors of the SmCB1 Protease Target Are Lethal to <i>Schistosoma mansoni</i> : Structural and Mechanistic Insights into Chemotype Reactivity. <i>ACS Infectious Diseases</i> , 2021, 7, 189-201.	3.8	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. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 457-479.	1.0	7
71	Synthesis of $\beta$ -Branched Acyclic Nucleoside Phosphonates as Potential Inhibitors of Bacterial Adenylate Cyclases. <i>ChemMedChem</i> , 2018, 13, 199-206.	3.2	7
72	Myristoylation drives dimerization of matrix protein from mouse mammary tumor virus. <i>Retrovirology</i> , 2016, 13, 2.	2.0	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. <i>European Journal of Medicinal Chemistry</i> , 2019, 177, 212-220.	5.5	6
74	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 118-129.	1.2	5
75	Interface Interactions of the Bowmanâ€Birk Inhibitor BTCl in a Ternary Complex with Trypsin and Chymotrypsin Evaluated by Semiempirical Quantum Mechanical Calculations. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 5203-5211.	2.4	5
76	Highly potent inhibitors of cathepsin K with a differently positioned cyanohyrazide warhead: structural analysis of binding mode to mature and zymogen-like enzymes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 515-526.	5.2	5
77	Noncovalent Interactions of Heteroboranes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 219-239.	0.6	4
78	Micellization: Nonclassical Hydrophobic Effect in Micellization: Molecular Arrangement of Nonâ€Amphiphilic Structures (Adv. Theory Simul. 1/2018). <i>Advanced Theory and Simulations</i> , 2018, 1, 1870003.	2.8	4
79	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. <i>ChemPlusChem</i> , 2020, 85, 2361-2361.	2.8	4
80	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. <i>ChemPhysChem</i> , 2020, 21, 2599-2604.	2.1	4
81	Multipodal insulin mimetics built on adamantane or proline scaffolds. <i>Bioorganic Chemistry</i> , 2021, 107, 104548.	4.1	3
82	Structural determinants for subnanomolar inhibition of the secreted aspartic protease Sapp1p from <i>Candida parapsilosis</i> . <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 914-921.	5.2	3
83	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. <i>Journal of Molecular Recognition</i> , 2020, 33, e2842.	2.1	2
84	Engineering the Ligand Specificity of the Human Galectinâ€1 by Incorporation of Tryptophan Analogues. <i>ChemBioChem</i> , 2022, , .	2.6	2
85	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 10139-10142.	13.8	1
86	The Role of Cysteine Residues in Catalysis of Phosphoenolpyruvate Carboxykinase from <i>Mycobacterium tuberculosis</i> . <i>PLoS ONE</i> , 2017, 12, e0170373.	2.5	0
87	When Additive Molecular Dynamics Fails: Quantum Effects in Calcium-Dependent Lectin/Carbohydrate Complex. <i>Biophysical Journal</i> , 2019, 116, 144a.	0.5	0