Klaus R. Liedl

List of Publications by Year
in descending order

327	9,587	38742 50	74163 75
papers	citations	h-index	g-index

356	356	356	10708
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Paratope states in solution improve structure prediction and docking. Structure, 2022, 30, 430-440.e3.	3.3	8
2	Explicit solvation thermodynamics in ionic solution: extending grid inhomogeneous solvation theory to solvation free energy of saltâ€“water mixtures. Journal of Computer-Aided Molecular Design, 2022, 36, 101-116.	2.9	8
3	Impact of different protonation states on virtual screening performance against cruzain. Chemical Biology and Drug Design, 2022, 99, 703-716.	3.2	1
4	CDR loop interactions can determine heavy and light chain pairing preferences in bispecific antibodies. MAbs, 2022, 14, 2024118.	5.2	4
5	Comparing Antibody Interfaces to Inform Rational Design of New Antibody Formats. Frontiers in Molecular Biosciences, 2022, 9, 812750.	3.5	4
6	Broadly neutralizing antibodies target a haemagglutinin anchor epitope. Nature, 2022, 602, 314-320.	27.8	78
7	Calcium current modulation by the Î³1 subunit depends on alternative splicing of CaV1.1. Journal of General Physiology, 2022, 154, .	1.9	4
8	Essential role of a conserved aspartate for the enzymatic activity of plasmanylethanolamine desaturase. Cellular and Molecular Life Sciences, 2022, 79, 214.	5.4	2
9	Grid inhomogeneous solvation theory for cross-solvation in rigid solvents. Journal of Chemical Physics, 2022, 156, .	3.0	3
10	Nanobody Paratope Ensembles in Solution Characterized by MD Simulations and NMR. International Journal of Molecular Sciences, 2022, 23, 5419.	4.1	6
11	Increase of Radiative Forcing through Midinfrared Absorption by Stable CO₂ Dimers?. Journal of Physical Chemistry A, 2022, 126, 2966-2975.	2.5	3
12	Borylated Cymantrenes and Tromancenium Salts with Unusual Reactivity. Organometallics, 2022, 41, 1464-1473.	2.3	2
13	Hydration thermodynamics of cytosolic phospholipase A2 GIVA predict its membrane-associated parts and its highly hydrated binding site. Journal of Biomolecular Structure and Dynamics, 2021, 39, 953-959.	3.5	1
14	Conformational flexibility correlates with glucose tolerance for point mutations in Î²-glucosidases â€“ a computational study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1621-1634.	3.5	10
15	Conformational Ensembles of Antibodies Determine Their Hydrophobicity. Biophysical Journal, 2021, 120, 143-157.	0.5	23
16	Ensembles in solution as a new paradigm for antibody structure prediction and design. MAbs, 2021, 13, 1923122.	5.2	19
17	Inverse relation between structural flexibility and IgE reactivity of Cor a 1 hazelnut allergens. Scientific Reports, 2021, 11, 4173.	3.3	14
18	Structural determinants of voltage-gating properties in calcium channels. ELife, 2021, 10, .	6.0	18

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19	CACNA1I gain-of-function mutations differentially affect channel gating and cause neurodevelopmental disorders. Brain, 2021, 144, 2092-2106.	7.6	26
20	Conformational Shifts of Stacked Heteroaromatics: Vacuum vs. Water Studied by Machine Learning. Frontiers in Chemistry, 2021, 9, 641610.	3.6	1
21	Mutation of Framework Residue H71 Results in Different Antibody Paratope States in Solution. Frontiers in Immunology, 2021, 12, 630034.	4.8	17
22	X-Entropy: A Parallelized Kernel Density Estimator with Automated Bandwidth Selection to Calculate Entropy. Journal of Chemical Information and Modeling, 2021, 61, 1533-1538.	5.4	16
23	pyPolyBuilder: Automated Preparation of Molecular Topologies and Initial Configurations for Molecular Dynamics Simulations of Arbitrary Supramolecules. Journal of Chemical Information and Modeling, 2021, 61, 1539-1544.	5.4	8
24	Shark Antibody Variable Domains Rigidify Upon Affinity Maturationâ€”Understanding the Potential of Shark Immunoglobulins as Therapeutics. Frontiers in Molecular Biosciences, 2021, 8, 639166.	3.5	9
25	Correcting cisâ€transâ€transgressions in macromolecular structure models. FEBS Journal, 2021, , .	4.7	1
26	Implementation of the Freely Jointed Chain Model to Assess Kinetics and Thermodynamics of Thermosensitive Coilâ€“Globule Transition by Markov States. Journal of Physical Chemistry B, 2021, 125, 4898-4909.	2.6	4
27	Pore mutation N617D in the skeletal muscle DHPR blocks Ca2+ influx due to atypical high-affinity Ca2+ binding. ELife, 2021, 10, .	6.0	5
28	Structure and Zeatin Binding of the Peach Allergen Pru p 1. Journal of Agricultural and Food Chemistry, 2021, 69, 8120-8129.	5.2	10
29	Germline-Dependent Antibody Paratope States and Pairing Specific VH-VL Interface Dynamics. Frontiers in Immunology, 2021, 12, 675655.	4.8	11
30	Inhibitors of Fumarylacetoacetate Hydrolase Domain Containing Protein 1 (FAHD1). Molecules, 2021, 26, 5009.	3.8	0
31	Energy penalties enhance flexible receptor docking in a model cavity. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	17
32	Ion-pair interactions between voltage-sensing domain IV and pore domain I regulate CaV1.1 gating. Biophysical Journal, 2021, 120, 4429-4441.	0.5	3
33	A Lightâ€Triggerable Nanoparticle Library for the Controlled Release of Nonâ€Coding RNAs. Angewandte Chemie - International Edition, 2020, 59, 1985-1991.	13.8	24
34	V_Hâ€V_L interdomain dynamics observed by computer simulations and NMR. Proteins: Structure, Function and Bioinformatics, 2020, 88, 830-839.	2.6	28
35	The interplay of VSCF/VCI calculations and matrix-isolation IR spectroscopy â€“ Mid infrared spectrum of CH3CH2F and CD3CD2F. Journal of Molecular Spectroscopy, 2020, 367, 111224.	1.2	22
36	Alphaâ€Carbonic Acid Revisited: Carbonic Acid Monomethyl Ester as a Solid and its Conformational Isomerism in the Gas Phase. Chemistry - A European Journal, 2020, 26, 285-305.	3.3	9

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37	Thermosensitive Hydration of Four Acrylamide-Based Polymers in Coil and Globule Conformations. Journal of Physical Chemistry B, 2020, 124, 9745-9756.	2.6	10
38	N-Heterocyclic Carbene Gold(I) Complexes: Mechanism of the Ligand Scrambling Reaction and Their Oxidation to Gold(III) in Aqueous Solutions. Inorganic Chemistry, 2020, 59, 15312-15323.	4.0	27
39	Solvation Thermodynamics in Different Solvents: Waterâ€“Chloroform Partition Coefficients from Grid Inhomogeneous Solvation Theory. Journal of Chemical Information and Modeling, 2020, 60, 3843-3853.	5.4	11
40	Replacement of the Cobalt Center of Vitamin B₁₂ by Nickel: Nibalamin and Nibyric Acid Prepared from Metalâ€Free B₁₂â€...Ligands Hydrogenobalamin and Hydrogenobyric Acid. Angewandte Chemie - International Edition, 2020, 59, 20129-20136.	13.8	18
41	On the synergy of matrix-isolation infrared spectroscopy and vibrational configuration interaction computations. Theoretical Chemistry Accounts, 2020, 139, 174.	1.4	3
42	Polarizable and non-polarizable force fields: Protein folding, unfolding, and misfolding. Journal of Chemical Physics, 2020, 153, 185102.	3.0	26
43	Local and Global Rigidification Upon Antibody Affinity Maturation. Frontiers in Molecular Biosciences, 2020, 7, 182.	3.5	29
44	Profiling selectivity of chagasin mutants towards cysteine proteases cruzain or cathepsin L through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	3.5	1
45	T-Cell Receptor CDR3 Loop Conformations in Solution Shift the Relative VÎ±-VÎ² Domain Distributions. Frontiers in Immunology, 2020, 11, 1440.	4.8	17
46	Decomposing anharmonicity and mode-coupling from matrix effects in the IR spectra of matrix-isolated carbon dioxide and methane. Physical Chemistry Chemical Physics, 2020, 22, 17932-17947.	2.8	9
47	Two CaV3.3 (CACNA1I) Gain-of-Function Mutations Linked to Epilepsy and Intellectual Disability Affect Gating Properties and the Window Current. Biophysical Journal, 2020, 118, 106a.	0.5	0
48	Polyreactive Broadly Neutralizing B cells Are Selected to Provide Defense against Pandemic Threat Influenza Viruses. Immunity, 2020, 53, 1230-1244.e5.	14.3	61
49	Antibodies exhibit multiple paratope states influencing VHâ€“VL domain orientations. Communications Biology, 2020, 3, 589.	4.4	38
50	In silico Design of Phl p 6 Variants With Altered Fold-Stability Significantly Impacts Antigen Processing, Immunogenicity and Immune Polarization. Frontiers in Immunology, 2020, 11, 1824.	4.8	8
51	Replacement of the Cobalt Center of Vitamin B₁₂ by Nickel: Nibalamin and Nibyric Acid Prepared from Metalâ€Free B₁₂â€...Ligands Hydrogenobalamin and Hydrogenobyric Acid. Angewandte Chemie, 2020, 132, 20304-20311.	2.0	2
52	Surprisingly Fast Interface and Elbow Angle Dynamics of Antigen-Binding Fragments. Frontiers in Molecular Biosciences, 2020, 7, 609088.	3.5	11
53	The intermolecular anthracene-transfer in a regiospecific antipodal C₆₀difunctionalization. Organic and Biomolecular Chemistry, 2020, 18, 4090-4103.	2.8	1
54	Ni[B 2 (SO 4) 4] and Co[B 2 (SO 4) 4]: Unveiling Systematic Trends in Phyllosilicate Analogue Borosulfates. Chemistry - A European Journal, 2020, 26, 17405-17415.	3.3	12

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55	Macrocycle Cell Permeability Measured by Solvation Free Energies in Polar and Apolar Environments. Journal of Chemical Information and Modeling, 2020, 60, 3508-3517.	5.4	15
56	Dynamics Rationalize Proteolytic Susceptibility of the Major Birch Pollen Allergen Bet v 1. Frontiers in Molecular Biosciences, 2020, 7, 18.	3.5	6
57	T-Cell Receptor Variable Î² Domains Rigidify During Affinity Maturation. Scientific Reports, 2020, 10, 4472.	3.3	20
58	STACKED â€“ <u>S</u>olvation <u>T</u>heory of <u>A</u>romatic <u>C</u>omplexes as <u>K</u>ey for <u>E</u>stimating <u>D</u>rug Binding. Journal of Chemical Information and Modeling, 2020, 60, 2304-2313.	5.4	10
59	Protein-Protein Binding as a Two-Step Mechanism: Preselection of Encounter Poses during the Binding of BPTI and Trypsin. Biophysical Journal, 2020, 119, 652-666.	0.5	22
60	Local Unfolding Relates to Proteolytic Susceptibility of the Major Birch Pollen Allergen Bet v 1. Biophysical Journal, 2020, 118, 502a.	0.5	0
61	Biophysical classification of a CACNA1D de novo mutation as a high-risk mutation for a severe neurodevelopmental disorder. Molecular Autism, 2020, 11, 4.	4.9	33
62	Catalytic Site pK_a Values of Aspartic, Cysteine, and Serine Proteases: Constant pH MD Simulations. Journal of Chemical Information and Modeling, 2020, 60, 3030-3042.	5.4	44
63	Antibody CDR loops as ensembles in solution vs. canonical clusters from X-ray structures. MAbs, 2020, 12, 1744328.	5.2	34
64	pH-Induced Local Unfolding of the Phl p 6 Pollen Allergen From cpH-MD. Frontiers in Molecular Biosciences, 2020, 7, 603644.	3.5	5
65	Charge Anisotropy of Nitrogen: Where Chemical Intuition Fails. Journal of Chemical Theory and Computation, 2020, 16, 4443-4453.	5.3	8
66	Sodium-induced population shift drives activation of thrombin. Scientific Reports, 2020, 10, 1086.	3.3	8
67	Zinc Substitution of Cobalt in Vitaminâ€…B12: Zincobyric acid and Zincobalamin as Luminescent Structural B12â€Mimics. Angewandte Chemie - International Edition, 2019, 58, 14568-14572.	13.8	25
68	Zinc Substitution of Cobalt in Vitaminâ€…B12: Zincobyric acid and Zincobalamin as Luminescent Structural B12â€Mimics. Angewandte Chemie, 2019, 131, 14710-14714.	2.0	4
69	Solvation Free Energy as a Measure of Hydrophobicity: Application to Serine Protease Binding Interfaces. Journal of Chemical Theory and Computation, 2019, 15, 5872-5882.	5.3	42
70	Die HydrogenobyrsÃureâ€Struktur enthÃ¼llt den Corrinâ€Liganden als entatisches Zustandsmodul zur Steigerung der KatalyseaktivitÃt von B₁₂â€Cofaktoren. Angewandte Chemie, 2019, 131, 10869-10873.	2.0	8
71	Novel Dual Ligands Targeting Sigma1 Receptor and Acetylcholinesterase Endowed with Antioxidant Properties. Proceedings (mdpi), 2019, 22, .	0.2	0
72	Toward Elimination of Discrepancies between Theory and Experiment: Anharmonic Rotationalâ€“Vibrational Spectrum of Water in Solid Noble Gas Matrices. Journal of Physical Chemistry A, 2019, 123, 8234-8242.	2.5	9

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73	pH-Dependent Protonation of the Phl p 6 Pollen Allergen Studied by NMR and cpH-aMD. Journal of Chemical Theory and Computation, 2019, 15, 5716-5726.	5.3	10
74	Molecular Dynamics Gives New Insights into the Glucose Tolerance and Inhibition Mechanisms on Î²-Glucosidases. Molecules, 2019, 24, 3215.	3.8	17
75	Hydration of Aromatic Heterocycles as an Adversary of Ï€-Stacking. Journal of Chemical Information and Modeling, 2019, 59, 4209-4219.	5.4	11
76	Benzimidazole inhibitors of the major cysteine protease of Trypanosoma brucei. Future Medicinal Chemistry, 2019, 11, 1537-1551.	2.3	7
77	Coilâ€“Globule Transition Thermodynamics of Poly(N-isopropylacrylamide). Journal of Physical Chemistry B, 2019, 123, 8838-8847.	2.6	45
78	CDR-H3 loop ensemble in solution â€“ conformational selection upon antibody binding. MAbs, 2019, 11, 1077-1088.	5.2	49
79	The Hydrogenobyric Acid Structure Reveals the Corrin Ligand as an Entatic State Module Empowering B₁₂ Cofactors for Catalysis. Angewandte Chemie - International Edition, 2019, 58, 10756-10760.	13.8	30
80	Mechanism of Olefin Metathesis with Neutral and Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes. Journal of the American Chemical Society, 2019, 141, 8264-8276.	13.7	38
81	Structure Modelling of CaV1.1 Reveals Functional Trans-Domain Interactions Involved in Voltage Sensing. Biophysical Journal, 2019, 116, 112a.	0.5	0
82	Conformational selection of allergen-antibody complexesâ€”surface plasticity of paratopes and epitopes. Protein Engineering, Design and Selection, 2019, 32, 513-523.	2.1	17
83	Antibody humanizationâ€”the Influence of the antibody framework on the CDR-H3 loop ensemble in solution. Protein Engineering, Design and Selection, 2019, 32, 411-422.	2.1	17
84	Transitions of CDR-L3 Loop Canonical Cluster Conformations on the Micro-to-Millisecond Timescale. Frontiers in Immunology, 2019, 10, 2652.	4.8	18
85	Understanding Structureâ€“Activity Relationships for Trypanosomal Cysteine Protease Inhibitors by Simulations and Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 137-148.	5.4	17
86	Toward novel inhibitors against KdsB: a highly specific and selective broad-spectrum bacterial enzyme. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1326-1345.	3.5	30
87	The fumarylacetoacetate hydrolase (FAH) superfamily of enzymes: multifunctional enzymes from microbes to mitochondria. Biochemical Society Transactions, 2018, 46, 295-309.	3.4	30
88	Cu[B₂(SO₄)₄] and Cu[B(SO₄)₂(HSO₄)]â€”Two Silicate Analogue Borosulfates Differing in their Dimensionality: A Comparative Study of Stability and Acidity. Angewandte Chemie - International Edition, 2018, 57, 9548-9552.	13.8	28
89	Peptidic Macrocycles - Conformational Sampling and Thermodynamic Characterization. Journal of Chemical Information and Modeling, 2018, 58, 982-992.	5.4	55
90	Pyroâ€Phyllobilins: Elusive Chlorophyll Catabolites Lacking a Critical Carboxylate Function of the Natural Chlorophylls. Chemistry - A European Journal, 2018, 24, 2987-2998.	3.3	11

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91	Cobaltocenylidene: A Mesoionic Metalloceno Carbene, Stabilized in a Gold(III) Complex. Chemistry - A European Journal, 2018, 24, 3165-3169.	3.3	17
92	Highly Electrophilic, Catalytically Active and Redoxâ€Responsive Cobaltoceniumyl and Ferrocenyl Triazolylidene Coinage Metal Complexes. Chemistry - A European Journal, 2018, 24, 3742-3753.	3.3	67
93	An unexpected switch in peptide binding mode: from simulation to substrate specificity. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4072-4084.	3.5	7
94	Low frequency vibrational anharmonicity and nuclear spin effects of Clâ€“(H2) and Clâ€“(D2). Journal of Chemical Physics, 2018, 149, 174310.	3.0	9
95	Cu[B₂(SO₄)₄] und Cu[B(SO₄)₂(HSO₄)] â€“ zwei silicatanaloge Borosulfate unterschiedlicher DimensionalitÃt: Vergleich von StabilitÃt und AziditÃt. Angewandte Chemie, 2018, 130, 9693-9697.	2.0	12
96	Structural basis for the bi-functionality of human oxaloacetate decarboxylase FAHD1. Biochemical Journal, 2018, 475, 3561-3576.	3.7	13
97	Phase Diagram of a Stratum Corneum Lipid Mixture. Journal of Physical Chemistry B, 2018, 122, 10505-10521.	2.6	13
98	Identification of dual Sigma1 receptor modulators/acetylcholinesterase inhibitors with antioxidant and neurotrophic properties, as neuroprotective agents. European Journal of Medicinal Chemistry, 2018, 158, 353-370.	5.5	14
99	Electrostatic recognition in substrate binding to serine proteases. Journal of Molecular Recognition, 2018, 31, e2727.	2.1	13
100	Novel Types of Hypermodified Fluorescent Phyllobilins from Breakdown of Chlorophyll in Senescent Leaves of Grapevine (Vitis vinifera). Chemistry - A European Journal, 2018, 24, 17268-17279.	3.3	15
101	Innentitelbild: Cu[B2 (SO4)4] und Cu[B(SO4)2 (HSO4)] - zwei silicatanaloge Borosulfate unterschiedlicher DimensionalitÃt: Vergleich von StabilitÃt und AziditÃt (Angew. Chem. 30/2018). Angewandte Chemie, 2018, 130, 9330-9330.	2.0	0
102	Discovery of Retinoic Acid-Related Orphan Receptor Î³t Inverse Agonists via Docking and Negative Image-Based Screening. ACS Omega, 2018, 3, 6259-6266.	3.5	10
103	Characterizing the Diversity of the CDR-H3 Loop Conformational Ensembles in Relationship to Antibody Binding Properties. Frontiers in Immunology, 2018, 9, 3065.	4.8	73
104	High-pressure synthesis and crystal structure of In₃B₅O₁₂. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 69-76.	0.7	6
105	Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling, 2017, 57, 345-354.	5.4	20
106	Structure of the Major Apple Allergen MalÂdÂ1. Journal of Agricultural and Food Chemistry, 2017, 65, 1606-1612.	5.2	50
107	Carbonic acid monoethyl ester as a pure solid and its conformational isomerism in the gas-phase. RSC Advances, 2017, 7, 22222-22233.	3.6	11
108	Ag[B(SO₄)₂] â€“ Synthesis, Crystal Structure, and Characterization of the First Preciousâ€Metal Borosulfate. European Journal of Inorganic Chemistry, 2017, 2017, 3981-3989.	2.0	19

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109	Molecular dynamics simulation studies of novel Î²-lactamase inhibitor. Journal of Molecular Graphics and Modelling, 2017, 74, 143-152.	2.4	53
110	Crystal structure of Pla l 1 reveals both structural similarity and allergenic divergence within the Ole e 1â€“like protein family. Journal of Allergy and Clinical Immunology, 2017, 140, 277-280.	2.9	14
111	CaB₂S₄O₁₆: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, 16773-16781.	3.3	25
112	Mechanisms Responsible for Ï‰ -Pore Currents in Ca v Calcium Channel Voltage-Sensing Domains. Biophysical Journal, 2017, 113, 1485-1495.	0.5	16
113	Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins. Scientific Reports, 2017, 7, 11901.	3.3	21
114	Frontispiece: CaB₂S₄O₁₆: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, .	3.3	0
115	High-Pressure Synthesis and Characterization of the Ammonium Yttrium Borate (NH4)YB8O14. Inorganic Chemistry, 2017, 56, 14291-14299.	4.0	9
116	Gaining in pan-affinity towards sigma 1 and sigma 2 receptors. SAR studies on arylalkylamines. Bioorganic and Medicinal Chemistry, 2017, 25, 11-19.	3.0	15
117	Molecular Connectivity Predefines Polypharmacology: Aliphatic Rings, Chirality, and sp3 Centers Enhance Target Selectivity. Frontiers in Pharmacology, 2017, 8, 552.	3.5	16
118	Discovery and Characterization of Diazenylaryl Sulfonic Acids as Inhibitors of Viral and Bacterial Neuraminidases. Frontiers in Microbiology, 2017, 8, 205.	3.5	13
119	Determinants of Macromolecular Specificity from Proteomics-De rived Peptide Substrate Data. Current Protein and Peptide Science, 2017, 18, 905-913.	1.4	1
120	Conformational Flexibility Differentiates Naturally Occurring Bet v 1 Isoforms. International Journal of Molecular Sciences, 2017, 18, 1192.	4.1	18
121	Prediction of blood:air and fat:air partition coefficients of volatile organic compounds for the interpretation of data in breath gas analysis. Journal of Breath Research, 2016, 10, 017103.	3.0	15
122	Asymmetric arginine dimethylation of RelA provides a repressive mark to modulate TNFÎ±/NF-Î°B response. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4326-4331.	7.1	60
123	Orthorhombic HPâ€REOF (RE = Pr, Nd, Sm â€“ Gd) â€“ Highâ€Pressure Syntheses and Singleâ€Crystal Structures (RE = Nd, Sm, Eu). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 1134-1142.	1.2	11
124	DPPC-cholesterol phase diagram using coarse-grained Molecular Dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2846-2857.	2.6	95
125	Chlorophyllâ€Derived Yellow Phyllobilins of Higher Plants as Mediumâ€Responsive Chiral Photoswitches. Angewandte Chemie - International Edition, 2016, 55, 15760-15765.	13.8	24
126	Enthalpic and Entropic Contributions to Hydrophobicity. Journal of Chemical Theory and Computation, 2016, 12, 4600-4610.	5.3	68

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127	Interaction mechanisms of a melatonergic inhibitor in the melatonin synthesis pathway. Journal of Molecular Liquids, 2016, 221, 507-517.	4.9	39
128	Von Chlorophyll abstammende gelbe Phyllobiline hÃ¶herer Pflanzen als umgebungsgesteuerte, chirale Photoschalter. Angewandte Chemie, 2016, 128, 15992-15997.	2.0	4
129	Innentitelbild: Von Chlorophyll abstammende gelbe Phyllobiline hÃ¶herer Pflanzen als umgebungsgesteuerte, chirale Photoschalter (Angew. Chem. 51/2016). Angewandte Chemie, 2016, 128, 15912-15912.	2.0	0
130	Sequence diversity of NanA manifests in distinct enzyme kinetics and inhibitor susceptibility. Scientific Reports, 2016, 6, 25169.	3.3	14
131	Chlorophyll Catabolites in Fall Leaves of the Wych Elm Tree Present a Novel Glycosylation Motif. Chemistry - A European Journal, 2016, 22, 9498-9503.	3.3	23
132	Protease Inhibitors in View of Peptide Substrate Databases. Journal of Chemical Information and Modeling, 2016, 56, 1228-1235.	5.4	4
133	Kinetic barriers in the isomerization of substituted ureas: implications for computer-aided drug design. Journal of Computer-Aided Molecular Design, 2016, 30, 391-400.	2.9	10
134	Localization of Millisecond Dynamics: Dihedral Entropy from Accelerated MD. Journal of Chemical Theory and Computation, 2016, 12, 3449-3455.	5.3	23
135	Fold stability during endolysosomal acidification is a key factor for allergenicity and immunogenicity of the major birch pollen allergen. Journal of Allergy and Clinical Immunology, 2016, 137, 1525-1534.	2.9	69
136	Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases. Journal of Physical Chemistry B, 2016, 120, 299-308.	2.6	5
137	New High-Pressure Gallium Borate Ga₂B₃O₇(OH) with Photocatalytic Activity. Inorganic Chemistry, 2016, 55, 676-681.	4.0	36
138	Highâ€Pressure Synthesis of Cd(NH₃)₂[B₃O₅(NH₃)]₂: Pioneering the Way to the Substance Class of Ammine Borates. Angewandte Chemie - International Edition, 2015, 54, 6360-6363.	13.8	33
139	Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091.	4.9	198
140	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 104-120.	3.5	24
141	Independent Metrics for Protein Backbone and Side-Chain Flexibility: Time Scales and Effects of Ligand Binding. Journal of Chemical Theory and Computation, 2015, 11, 851-860.	5.3	24
142	Structure, Thermal Behavior, and Vibrational Spectroscopy of the Silver Borate AgB₃O₅. European Journal of Inorganic Chemistry, 2015, 2015, 527-533.	2.0	10
143	CACNA1D De Novo Mutations in Autism Spectrum Disorders Activate Cav1.3 L-Type Calcium Channels. Biological Psychiatry, 2015, 77, 816-822.	1.3	147
144	Unique Macrocycles in the Taiwan Traditional Chinese Medicine Database. Planta Medica, 2015, 81, 459-466.	1.3	6

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145	Antipneumococcal activity of neuraminidase inhibiting artocarpin. International Journal of Medical Microbiology, 2015, 305, 289-297.	3.6	32
146	Complementary assays helping to overcome challenges for identifying neuraminidase inhibitors. Future Virology, 2015, 10, 77-88.	1.8	23
147	Identification of FAH Domain-containing Protein 1 (FAHD1) as Oxaloacetate Decarboxylase. Journal of Biological Chemistry, 2015, 290, 6755-6762.	3.4	37
148	Strong Nonadditivity as a Key Structureâ€“Activity Relationship Feature: Distinguishing Structural Changes from Assay Artifacts. Journal of Chemical Information and Modeling, 2015, 55, 483-494.	5.4	38
149	Matched Peptides: Tuning Matched Molecular Pair Analysis for Biopharmaceutical Applications. Journal of Chemical Information and Modeling, 2015, 55, 2315-2323.	5.4	6
150	FAH Domain Containing Protein 1 (FAHD-1) Is Required for Mitochondrial Function and Locomotion Activity in C. elegans. PLoS ONE, 2015, 10, e0134161.	2.5	13
151	Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. PLoS ONE, 2015, 10, e0140713.	2.5	24
152	A Cross-Reactive Human Single-Chain Antibody for Detection of Major Fish Allergens, Parvalbumins, and Identification of a Major IgE-Binding Epitope. PLoS ONE, 2015, 10, e0142625.	2.5	12
153	Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658.	2.5	25
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