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	Bornâ^'Oppenheimer ab Initio QM/MM Dynamics Simulations of Na+and K+in Water:Â From Structure Making to Structure Breaking Effects. Journal of Physical Chemistry A, 1998, 102, 10340-10347.	2.5	218
2	Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091.	4.9	198
3	How To Optimize Shape-Based Virtual Screening: Choosing the Right Query and Including Chemical Information. Journal of Chemical Information and Modeling, 2009, 49, 678-692.	5.4	178
4	A QM/MM simulation method applied to the solution of Li+ in liquid ammonia. Chemical Physics, 1996, 211, 313-323.	1.9	175
5	Prediction of the structure of human Janus kinase 2 (JAK2) comprising the two carboxy-terminal domains reveals a mechanism for autoregulation. Protein Engineering, Design and Selection, 2001, 14, 27-37.	2.1	154
6	On the Surprising Kinetic Stability of Carbonic Acid (H2CO3). Angewandte Chemie - International Edition, 2000, 39, 891-894.	13.8	152
7	CACNA1D De Novo Mutations in Autism Spectrum Disorders Activate Cav1.3 L-Type Calcium Channels. Biological Psychiatry, 2015, 77, 816-822.	1.3	147
8	Influenza neuraminidase: A druggable target for natural products. Natural Product Reports, 2012, 29, 11-36.	10.3	146
9	Identification of Novel Functional Inhibitors of Acid Sphingomyelinase. PLoS ONE, 2011, 6, e23852.	2.5	145
10	Heteroaromatic Ï€-Stacking Energy Landscapes. Journal of Chemical Information and Modeling, 2014, 54, 1371-1379.	5.4	144
11	Solvation of Ca2+in Water Studied by Bornâ^'Oppenheimer ab Initio QM/MM Dynamics. Journal of Physical Chemistry A, 1997, 101, 6299-6309.	2.5	140
12	Carbonic Acid in the Gas Phase and Its Astrophysical Relevance. Science, 1998, 279, 1332-1335.	12.6	125
13	Antiviral Potential and Molecular Insight into Neuraminidase Inhibiting Diarylheptanoids from Alpinia katsumadai. Journal of Medicinal Chemistry, 2010, 53, 778-786.	6.4	114
14	Characterization of the Vitamin E-Binding Properties of Human Plasma Afamin. Biochemistry, 2002, 41, 14532-14538.	2.5	103
15	Qualitative prediction of bloodâ€“brain barrier permeability on a large and refined dataset. Journal of Computer-Aided Molecular Design, 2011, 25, 1095-1106.	2.9	97
16	DPPC-cholesterol phase diagram using coarse-grained Molecular Dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2846-2857.	2.6	95
17	Toward elimination of discrepancies between theory and experiment: The rate constant of the atmospheric conversion of SO3 to H2SO4. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 8874-8878.	7.1	91
18	The Protein Data Bank (PDB), Its Related Services and Software Tools as Key Components for In Silico Guided Drug Discovery. Journal of Medicinal Chemistry, 2008, 51, 7021-7040.	6.4	91

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19	The hydration shell structure of Li+ investigated by Bornâ€“Oppenheimer ab initio QM/MM dynamics. Chemical Physics Letters, 1998, 286, 56-64.	2.6	89
20	A critical analysis of electronic density functionals for structural, energetic, dynamic, and magnetic properties of hydrogen fluoride clusters. Journal of Computational Chemistry, 1997, 18, 1695-1719.	3.3	85
21	Towards the Experimental Decomposition Rate of Carbonic Acid (H2CO3) in Aqueous Solution. Chemistry - A European Journal, 2002, 8, 66-73.	3.3	84
22	Reactivity and Regioselectivity of Hydroxyl Radical Addition to Halogenated Ethenes. Journal of Physical Chemistry A, 1998, 102, 1583-1594.	2.5	81
23	The optimal tunneling path for the proton transfer in malonaldehyde. Journal of Chemical Physics, 2002, 117, 1962-1966.	3.0	80
24	Broadly neutralizing antibodies target a haemagglutinin anchor epitope. Nature, 2022, 602, 314-320.	27.8	78
25	A challenging system: Free energy prediction for factor Xa. Journal of Computational Chemistry, 2011, 32, 1743-1752.	3.3	75
26	Dispersion dominated halogenâ€“Ï€ interactions: energies and locations of minima. Physical Chemistry Chemical Physics, 2010, 12, 14941.	2.8	73
27	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
28	Toward Elimination of Discrepancies between Theory and Experiment:â€‰ Double Proton Transfer in Dimers of Carboxylic Acids. Journal of the American Chemical Society, 1998, 120, 12595-12600.	13.7	72
29	Automated Docking of Ligands to Antibodies: Methods and Applications. Methods, 2000, 20, 280-291.	3.8	72
30	The ground-state tunneling splitting of various carboxylic acid dimers. Journal of Chemical Physics, 2004, 120, 631-637.	3.0	71
31	Has the Dimer of Carbonic Acid a Lower Energy Than Its Constituents Water and Carbon Dioxide?. Journal of the American Chemical Society, 1997, 119, 3782-3784.	13.7	70
32	The Impact of Nitration on the Structure and Immunogenicity of the Major Birch Pollen Allergen Bet v 1.0101. PLoS ONE, 2014, 9, e104520.	2.5	70
33	Investigation of Cu2+ Hydration and the Jahnâ€“Teller Effect in Solution by QM/MM Monte Carlo Simulations. Journal of Physical Chemistry A, 1999, 103, 11387-11393.	2.5	69
34	Water-Mediated Proton Transfer:Â A Mechanistic Investigation on the Example of the Hydration of Sulfur Oxides. Journal of Physical Chemistry A, 2001, 105, 5137-5145.	2.5	69
35	Modeling Anhydrous and Aqua Copper(II) Amino Acid Complexes:Â A New Molecular Mechanics Force Field Parametrization Based on Quantum Chemical Studies and Experimental Crystal Data. Inorganic Chemistry, 2003, 42, 2268-2279.	4.0	69
36	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

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37	Enthalpic and Entropic Contributions to Hydrophobicity. Journal of Chemical Theory and Computation, 2016, 12, 4600-4610.	5.3	68
38	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
39	Matched Molecular Pair Analysis: Significance and the Impact of Experimental Uncertainty. Journal of Medicinal Chemistry, 2014, 57, 3786-3802.	6.4	62
40	Polyreactive Broadly Neutralizing B cells Are Selected to Provide Defense against Pandemic Threat Influenza Viruses. Immunity, 2020, 53, 1230-1244.e5.	14.3	61
41	Asymmetric arginine dimethylation of RelA provides a repressive mark to modulate TNFÎ±/NF-Î²B response. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4326-4331.	7.1	60
42	Stabilizing of a Globular Protein by a Highly Complex Water Network: A Molecular Dynamics Simulation Study on Factor Xa. Journal of Physical Chemistry B, 2010, 114, 7405-7412.	2.6	59
43	Predictions of rate constants and estimates for tunneling splittings of concerted proton transfer in small cyclic water clusters. Journal of Chemical Physics, 1998, 109, 2672-2679.	3.0	57
44	Conformationally Induced Changes in the Electronic Structures of Some Flexible Benzenes. A Molecular Orbital Model. Journal of the American Chemical Society, 1998, 120, 12573-12582.	13.7	57
45	B-DNA's BIâ†' BIIConformer Substate Dynamics Is Coupled with Water Migration. Journal of Physical Chemistry B, 1998, 102, 8934-8940.	2.6	57
46	Evaporation cycle experiments â€" A simulation of salt-induced peptide synthesis under possible prebiotic conditions. Origins of Life and Evolution of Biospheres, 1993, 23, 167-176.	1.9	56
47	A gatekeeper helix determines the substrate specificity of SjÃ¶grenâ€"Larsson Syndrome enzyme fatty aldehyde dehydrogenase. Nature Communications, 2014, 5, 4439.	12.8	55
48	Peptidic Macrocycles - Conformational Sampling and Thermodynamic Characterization. Journal of Chemical Information and Modeling, 2018, 58, 982-992.	5.4	55
49	Double hydrogen tunneling revisited: The breakdown of experimental tunneling criteria. Journal of Chemical Physics, 2004, 120, 11650-11657.	3.0	54
50	One Concept, Three Implementations of 3D Pharmacophore-Based Virtual Screening: Distinct Coverage of Chemical Search Space. Journal of Chemical Information and Modeling, 2010, 50, 1241-1247.	5.4	54
51	Charge Anisotropy: Where Atomic Multipoles Matter Most. Journal of Chemical Theory and Computation, 2014, 10, 4488-4496.	5.3	54
52	Molecular dynamics simulation studies of novel Î²-lactamase inhibitor. Journal of Molecular Graphics and Modelling, 2017, 74, 143-152.	2.4	53
53	Dangers of counterpoise corrected hypersurfaces. Advantages of basis set superposition improvement. Journal of Chemical Physics, 1998, 108, 3199-3204.	3.0	51
54	Backbone Flexibility Controls the Activity and Specificity of a Proteinâ^'Protein Interface: Specificity in Snake Venom Metalloproteases. Journal of the American Chemical Society, 2010, 132, 10330-10337.	13.7	51

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55	Why Are Copper(II) Amino Acid Complexes Not Planar in Their Crystal Structures? An ab Initio and Molecular Mechanics Study. Inorganic Chemistry, 1999, 38, 2764-2774.	4.0	50
56	Spectroscopic Observation of Matrixâ€Isolated Carbonic Acid Trapped from the Gas Phase. Angewandte Chemie - International Edition, 2011, 50, 1939-1943.	13.8	50
57	Structure of the Major Apple Allergen MalÂdÂ1. Journal of Agricultural and Food Chemistry, 2017, 65, 1606-1612.	5.2	50
58	Cleavage Entropy as Quantitative Measure of Protease Specificity. PLoS Computational Biology, 2013, 9, e1003007.	3.2	49
59	CDR-H3 loop ensemble in solution â€“ conformational selection upon antibody binding. MAbs, 2019, 11, 1077-1088.	5.2	49
60	Identification of PPARgamma Partial Agonists of Natural Origin (I): Development of a Virtual Screening Procedure and In Vitro Validation. PLoS ONE, 2012, 7, e50816.	2.5	48
61	Salt induced peptide formation: on the selectivity of the copper induced peptide formation under possible prebiotic conditions. Inorganica Chimica Acta, 1995, 228, 207-214.	2.4	47
62	An accurate semiclassical method to predict ground-state tunneling splittings. Journal of Chemical Physics, 2002, 117, 1967-1974.	3.0	47
63	Coilâ€“Globule Transition Thermodynamics of Poly(N-isopropylacrylamide). Journal of Physical Chemistry B, 2019, 123, 8838-8847.	2.6	45
64	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
65	Reaction-Path Dynamics of Hydroxyl Radical Reactions with Ethane and Haloethanes. Journal of Physical Chemistry A, 1997, 101, 4245-4253.	2.5	43
66	About the Stability of Sulfurous Acid (H2SO3) and Its Dimer. Chemistry - A European Journal, 2002, 8, 5644-5651.	3.3	43
67	Development of Anti-Viral Agents Using Molecular Modeling and Virtual Screening Techniques. Infectious Disorders - Drug Targets, 2011, 11, 64-93.	0.8	43
68	Molecular Docking Studies of Natural Cholinesterase-Inhibiting Steroidal Alkaloids fromSarcococcasaligna. Journal of Medicinal Chemistry, 2003, 46, 5087-5090.	6.4	42
69	Reciprocal regulation of PKA and Rac signaling. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8531-8536.	7.1	42
70	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
71	Complex of B-DNA with Polyamides Freezes DNA Backbone Flexibility. Journal of the American Chemical Society, 2001, 123, 5044-5049.	13.7	41
72	Interaction mechanisms of a melatonergic inhibitor in the melatonin synthesis pathway. Journal of Molecular Liquids, 2016, 221, 507-517.	4.9	39

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73	Structure, Reaction Enthalpies, Entropies, and Free Energies of Cationâ"Molecule Complexes. A Theoretical Study by Means of the ab Initio Complete Basis Set CBS-Q Method. Journal of Physical Chemistry A, 1998, 102, 771-777.	2.5	38
74	Quantitative Analysis of the Structural Requirements for Blockade of the N-Methyl-d-aspartate Receptor at the Phencyclidine Binding Site. Journal of Medicinal Chemistry, 1998, 41, 393-400.	6.4	38
75	Cooperative effects on the formation of intercalation sites. Nucleic Acids Research, 2004, 32, 4696-4703.	14.5	38
76	Computer-Guided Approach to Access the Anti-influenza Activity of Licorice Constituents. Journal of Natural Products, 2014, 77, 563-570.	3.0	38
77	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
78	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
79	Antibodies exhibit multiple paratope states influencing VHâ€"VL domain orientations. Communications Biology, 2020, 3, 589.	4.4	38
80	New Insights into the Dynamics of Concerted Proton Tunneling in Cyclic Water and Hydrogen Fluoride Clusters. Journal of Physical Chemistry A, 1997, 101, 4707-4716.	2.5	37
81	Theoretical Prediction of Hydrogen Bond Strength for Use in Molecular Modeling. Journal of Chemical Information and Modeling, 2009, 49, 2067-2076.	5.4	37
82	Identification of FAH Domain-containing Protein 1 (FAHD1) as Oxaloacetate Decarboxylase. Journal of Biological Chemistry, 2015, 290, 6755-6762.	3.4	37
83	Different electrostatic descriptors in comparative molecular field analysis: A comparison of molecular electrostatic and coulomb potentials. Journal of Computational Chemistry, 1996, 17, 1296-1308.	3.3	36
84	New High-Pressure Gallium Borate Ga₂B₃O₇(OH) with Photocatalytic Activity. Inorganic Chemistry, 2016, 55, 676-681.	4.0	36
85	C5-Methylation of Cytosine in B-DNA Thermodynamically and Kinetically Stabilizes BI. Journal of the American Chemical Society, 2003, 125, 14990-14991.	13.7	35
86	On the Formation of the Sulfonate Ion from Hydrated Sulfur Dioxide. Journal of Physical Chemistry A, 2004, 108, 3859-3864.	2.5	35
87	Ligand Binding Modulates the Structural Dynamics and Compactness of the Major Birch Pollen Allergen. Biophysical Journal, 2014, 107, 2972-2981.	0.5	35
88	Ab initio calculations concerning the reaction mechanism of the copper(II) catalyzed glycine condensation in aqueous sodium chloride solution. Chemical Physics Letters, 1992, 197, 181-186.	2.6	34
89	Novel neuraminidase inhibitors: identification, biological evaluation and investigations of the binding mode. Future Medicinal Chemistry, 2011, 3, 437-450.	2.3	34
90	Antibody CDR loops as ensembles in solution vs. canonical clusters from X-ray structures. MAbs, 2020, 12, 1744328.	5.2	34

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91	Unexpected B II Conformer Substate Population in Unoriented Hydrated Films of the d(CGCGAATTCGCG) 2 Dodecamer and of Native B-DNA from Salmon Testes. Biophysical Journal, 1999, 77, 398-409.	0.5	33
92	Raman Spectroscopic Study of the Phase Transition of Amorphous to Crystalline Î²â€Carbonic Acid. Angewandte Chemie - International Edition, 2009, 48, 2690-2694.	13.8	33
93	Matrix Isolation Studies of Carbonic Acidâ€"The Vapor Phase above the Î²-Polymorph. Journal of the American Chemical Society, 2013, 135, 7732-7737.	13.7	33
94	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
95	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
96	Antipneumococcal activity of neuraminidase inhibiting artocarpin. International Journal of Medical Microbiology, 2015, 305, 289-297.	3.6	32
97	Elbow Flexibility and Ligand-Induced Domain Rearrangements in Antibody Fab NC6.8: Large Effects of a Small Hapten. Biophysical Journal, 2000, 79, 614-628.	0.5	31
98	Simulation ofEcoRI Dodecamer Netropsin Complex Confirms Class I Complexation Mode. Journal of the American Chemical Society, 2000, 122, 3927-3931.	13.7	31
99	A Novel Paramagnetic Relaxation Enhancement Tag for Nucleic Acids: A Tool to Study Structure and Dynamics of RNA. ACS Chemical Biology, 2013, 8, 2697-2706.	3.4	31
100	The fumarylacetoacetate hydrolase (FAH) superfamily of enzymes: multifunctional enzymes from microbes to mitochondria. Biochemical Society Transactions, 2018, 46, 295-309.	3.4	30
101	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
102	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
103	Large Curvature Tunneling Effects Reveal Concerted Hydrogen Exchange Rates in Cyclic Hydrogen Fluoride Clusters Comparable to Carboxylic Acid Dimers. Journal of the American Chemical Society, 1998, 120, 404-412.	13.7	29
104	Local and Global Rigidification Upon Antibody Affinity Maturation. Frontiers in Molecular Biosciences, 2020, 7, 182.	3.5	29
105	Gas-phase acidities of HM(=X)XH (Mî—»C, Si; Xî—»O, S) acids calculated by ab initio molecular orbital methods at the G2 level of theory. Chemical Physics Letters, 1996, 263, 379-384.	2.6	28
106	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
107	V_Hâ€V_L interdomain dynamics observed by computer simulations and NMR. Proteins: Structure, Function and Bioinformatics, 2020, 88, 830-839.	2.6	28
108	Influence of Backbone Conformations of Human Carbonic Anhydrase II on Carbon Dioxide Hydration:â€‰ Hydration Pathways and Binding of Bicarbonate. Journal of the American Chemical Society, 2003, 125, 8921-8927.	13.7	28

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109	Helix Morphology Changes in B-DNA Induced By Spontaneous B_Iâ‡ŒB_{II}Substate Interconversion. Journal of Biomolecular Structure and Dynamics, 1999, 17, 223-235.	3.5	27
110	About the Kinetic Feasibility of the Lipscomb Mechanism in Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2003, 107, 12013-12020.	2.6	27
111	Toward elimination of discrepancies between theory and experiment: The gas-phase reaction of N2O5 with H2O. Physical Chemistry Chemical Physics, 2003, 5, 487-495.	2.8	27
112	Mechanism of the Cisâ^'Trans Isomerization of Bis(glycinato)copper(II). Journal of Physical Chemistry B, 2004, 108, 2098-2102.	2.6	27
113	DNA Minor Groove Pharmacophores Describing Sequence Specific Properties. Journal of Chemical Information and Modeling, 2007, 47, 1580-1589.	5.4	27
114	Dynamic Regulation of Phenylalanine Hydroxylase by Simulated Redox Manipulation. PLoS ONE, 2012, 7, e53005.	2.5	27
115	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
116	Significance of Ligand Tails for Interaction with the Minor Groove of B-DNA. Biophysical Journal, 2001, 81, 1588-1599.	0.5	26
117	Indirect Readout of thetrp-Repressorâ^'Operator Complex by B-DNA's Backbone Conformation Transitionsâ€. Biochemistry, 2002, 41, 4088-4095.	2.5	26
118	The structure, modelling and dynamics of 2,7-diisopropoxy-1,8-diarylnaphthalenes. Perkin Transactions II RSC, 2002, , 1510-1519.	1.1	26
119	The ground state tunneling splitting of the 2-pyridone2-hydroxypyridine dimer. Chemical Physics, 2003, 292, 47-52.	1.9	26
120	Local structural order in carbonic acid polymorphs: Raman and FTâ€IR spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 108-115.	2.5	26
121	Polarizable and non-polarizable force fields: Protein folding, unfolding, and misfolding. Journal of Chemical Physics, 2020, 153, 185102.	3.0	26
122	CACNA1I gain-of-function mutations differentially affect channel gating and cause neurodevelopmental disorders. Brain, 2021, 144, 2092-2106.	7.6	26
123	Ligand-induced domain movement in an antibody fab: molecular dynamics studies confirm the unique domain movement observed experimentally for fab NC6.8 upon complexation and reveal its segmental flexibility 1 1Edited by I. Wilson. Journal of Molecular Biology, 1998, 278, 301-306.	4.2	25
124	On the competing hydrations of sulfur dioxide and sulfur trioxide in our atmosphere. Chemical Communications, 2000, , 999-1000.	4.1	25
125	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	5.4	25
126	CaB₂S₄O₁₆: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, 16773-16781.	3.3	25

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127	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
128	Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658.	2.5	25
129	Application of multivariate data analysis methods to comparative molecular field analysis (CoMFA) data: proton affinities and pKa prediction for nucleic acids components. Journal of Computer-Aided Molecular Design, 1999, 13, 611-623.	2.9	24
130	Hydration of Hydroxypyrrole Influences Binding of ImHpPyPy-Î²-Dp Polyamide to DNA. Journal of the American Chemical Society, 2003, 125, 1088-1095.	13.7	24
131	Daunomycin Intercalation Stabilizes Distinct Backbone Conformations of DNA. Journal of Biomolecular Structure and Dynamics, 2004, 21, 713-724.	3.5	24
132	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 104-120.	3.5	24
133	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
134	Chlorophyllâ€Derived Yellow Phyllobilins of Higher Plants as Mediumâ€Responsive Chiral Photoswitches. Angewandte Chemie - International Edition, 2016, 55, 15760-15765.	13.8	24
135	A Lightâ€Triggerable Nanoparticle Library for the Controlled Release of Nonâ€Coding RNAs. Angewandte Chemie - International Edition, 2020, 59, 1985-1991.	13.8	24
136	Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. PLoS ONE, 2015, 10, e0140713.	2.5	24
137	Comparative docking studies on ligand binding to the multispecific antibodies IgE-La2 and IgE-Lb4. Journal of Computer-Aided Molecular Design, 1996, 10, 305-320.	2.9	23
138	Nonoriented d(CGCGAATTCGCG)2Dodecamer Persists in the B-Form Even at Low Water Activity. Journal of the American Chemical Society, 2000, 122, 716-717.	13.7	23
139	A QM-MM interface between CHARMM and TURBOMOLE: Implementation and application to systems in bulk phase and biologically active systems. Journal of Computational Chemistry, 2003, 24, 1240-1249.	3.3	23
140	Entropy from State Probabilities: Hydration Entropy of Cations. Journal of Physical Chemistry B, 2013, 117, 6466-6472.	2.6	23
141	Substrate-Driven Mapping of the Degradome by Comparison of Sequence Logos. PLoS Computational Biology, 2013, 9, e1003353.	3.2	23
142	Complementary assays helping to overcome challenges for identifying neuraminidase inhibitors. Future Virology, 2015, 10, 77-88.	1.8	23
143	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
144	Localization of Millisecond Dynamics: Dihedral Entropy from Accelerated MD. Journal of Chemical Theory and Computation, 2016, 12, 3449-3455.	5.3	23

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145	Conformational Ensembles of Antibodies Determine Their Hydrophobicity. Biophysical Journal, 2021, 120, 143-157.	0.5	23
146	Hydrogen transitions between (HF)n Cnh structures (n=2â^'5) via Dnh transition states as models for hydrogen tunneling in hydrogen fluoride clusters. Chemical Physics Letters, 1995, 246, 455-462.	2.6	22
147	Structure and gas-phase acidity of oxalic acid and its disila derivative. A theoretical study by means of the DFT quantum theoretical method. Journal of the Chemical Society Perkin Transactions II, 1996, , 1743.	0.9	22
148	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
149	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
150	Dynamics of DNA:â€‰ BI and BII Phosphate Backbone Transitions. Journal of Physical Chemistry B, 2004, 108, 2470-2476.	2.6	21
151	Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins. Scientific Reports, 2017, 7, 11901.	3.3	21
152	Structure and acidity of carbamic acid, and its thio, dithio and sila dervatives. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2375.	1.7	20
153	The role of water in B-DNAs BI to BII conformer substates interconversion: a combined study by calorimetry, FT-IR spectroscopy and computer simulation. Chemical Physics, 2000, 258, 391-404.	1.9	20
154	Sulfurous acid (H2SO3) on Io?. Icarus, 2004, 169, 242-249.	2.5	20
155	Specificity of a proteinâ€“protein interface: Local dynamics direct substrate recognition of effector caspases. Proteins: Structure, Function and Bioinformatics, 2014, 82, 546-555.	2.6	20
156	Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling, 2017, 57, 345-354.	5.4	20
157	T-Cell Receptor Variable Î² Domains Rigidify During Affinity Maturation. Scientific Reports, 2020, 10, 4472.	3.3	20
158	Comparative Molecular Field Analysis of Haptens Docked to the Multispecific Antibody IgE(Lb4). Journal of Medicinal Chemistry, 1996, 39, 3882-3888.	6.4	19
159	BIâ‡Œ BIISubstate Transitions Induce Changes in the Hydration of B-DNA, Potentially Mediating Signal Transduction from the Minor to Major Groove. Journal of Physical Chemistry B, 2001, 105, 10379-10387.	2.6	19
160	Reactions of HOCl + HCl +nH2O and HOCl + HBr +nH2O. Journal of Physical Chemistry A, 2002, 106, 7850-7857.	2.5	19
161	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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