Olaf Wiest

List of Publications by Year
in descending order

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117 papers	5,379 citations	71102 41 h-index	95266 68 g-index
124 all docs	124 docs citations	124 times ranked	6738 citing authors

#	Article	IF	Citations
1	A molecular mechanism of artemisinin resistance in Plasmodium falciparum malaria. Nature, 2015, 520, 683-687.	27.8	485
2	Toward Selective Histone Deacetylase Inhibitor Design:Â Homology Modeling, Docking Studies, and Molecular Dynamics Simulations of Human Class I Histone Deacetylases. Journal of Medicinal Chemistry, 2005, 48, 6936-6947.	6.4	205
3	Direct Visible-Light-Excited Asymmetric Lewis Acid Catalysis of Intermolecular [2+2] Photocycloadditions. Journal of the American Chemical Society, 2017, 139, 9120-9123.	13.7	203
4	Mechanism, Reactivity, and Selectivity in Palladium-Catalyzed Redox-Relay Heck Arylations of Alkenyl Alcohols. Journal of the American Chemical Society, 2014, 136, 1960-1967.	13.7	187
5	Histone deacetylase inhibitor treatment dramatically reduces cholesterol accumulation in Niemann-Pick type C1 mutant human fibroblasts. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 5620-5625.	7.1	175
6	On the Function of the 14 Ã… Long Internal Cavity of Histone Deacetylase-Like Protein:â€‰ Implications for the Design of Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 3409-3417.	6.4	140
7	Synergy of Combining Sonolysis and Photocatalysis in the Degradation and Mineralization of Chlorinated Aromatic Compounds. Environmental Science & Technology, 2003, 37, 1926-1932.	10.0	117
8	Structural Origin of Selectivity in Class II-Selective Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 2898-2906.	6.4	112
9	Discovery of selective small-molecule HDAC6 inhibitor for overcoming proteasome inhibitor resistance in multiple myeloma. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13162-13167.	7.1	112
10	Prediction of Enantioselectivity in Rhodium Catalyzed Hydrogenations. Journal of the American Chemical Society, 2009, 131, 410-411.	13.7	110
11	Theoretical Studies of Mixed-Valence Transition Metal Complexes for Molecular Computing. Journal of Physical Chemistry A, 2003, 107, 285-291.	2.5	109
12	Synthesis and Conformationâ^'Activity Relationships of the Peptide Isosteres of FK228 and Largazole. Journal of the American Chemical Society, 2009, 131, 2900-2905.	13.7	107
13	Chemical genomics reveals histone deacetylases are required for core regulatory transcription. Nature Communications, 2019, 10, 3004.	12.8	107
14	Investigating the Nature of Palladium Chain-Walking in the Enantioselective Redox-Relay Heck Reaction of Alkenyl Alcohols. Journal of Organic Chemistry, 2014, 79, 11841-11850.	3.2	95
15	Sonolysis of 2,4-Dichlorophenoxyacetic Acid in Aqueous Solutions. Evidence forâ€¢OH-Radical-Mediated Degradation. Journal of Physical Chemistry A, 2001, 105, 3176-3181.	2.5	93
16	Hydroxyl Radical's Role in the Remediation of a Common Herbicide, 2,4-Dichlorophenoxyacetic Acid (2,4-D). Journal of Physical Chemistry A, 2004, 108, 10925-10933.	2.5	90
17	Visible-Light-Activated Asymmetric Î²-Câ€“H Functionalization of Acceptor-Substituted Ketones with 1,2-Dicarbonyl Compounds. Journal of the American Chemical Society, 2017, 139, 17245-17248.	13.7	85
18	The cytoplasmic prolyl-tRNA synthetase of the malaria parasite is a dual-stage target of febrifugine and its analogs. Science Translational Medicine, 2015, 7, 288ra77.	12.4	82

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19	Rapid virtual screening of enantioselective catalysts using CatVS. Nature Catalysis, 2019, 2, 41-45.	34.4	81
20	Prediction of Stereochemistry using Q2MM. Accounts of Chemical Research, 2016, 49, 996-1005.	15.6	76
21	On the inhibition of histone deacetylase 8. Bioorganic and Medicinal Chemistry, 2010, 18, 4103-4110.	3.0	75
22	Density functional theory calculations of pericyclic reaction transition structures. Topics in Current Chemistry, 1996, , 1-24.	4.0	74
23	Metal-Templated Design: Enantioselective Hydrogen-Bond-Driven Catalysis Requiring Only Parts-per-Million Catalyst Loading. Journal of the American Chemical Society, 2016, 138, 8774-8780.	13.7	71
24	Rate Enhancement and Enantioselectivity of the Jacobsen-Katsuki Epoxidation: The Significance of the Sixth Coordination Site. Angewandte Chemie - International Edition, 2001, 40, 2073-2076.	13.8	67
25	EP300 Selectively Controls the Enhancer Landscape of MYCN-Amplified Neuroblastoma. Cancer Discovery, 2022, 12, 730-751.	9.4	64
26	Development of a Q2MM Force Field for the Asymmetric Rhodium Catalyzed Hydrogenation of Enamides. Journal of Chemical Theory and Computation, 2008, 4, 1313-1323.	5.3	63
27	Computational Studies of DNA Photolyase. Journal of Physical Chemistry A, 2005, 109, 7001-7012.	2.5	61
28	Biasing Mixed-Valence Transition Metal Complexes in Search of Bistable Complexes for Molecular Computing. Journal of Physical Chemistry B, 2003, 107, 9624-9628.	2.6	60
29	Variable Active Site Loop Conformations Accommodate the Binding of Macrocyclic Largazole Analogues to HDAC8. Biochemistry, 2015, 54, 2126-2135.	2.5	55
30	Ab Initio Studies of the Radical Cation Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 1999, 121, 6730-6736.	13.7	53
31	Coordination chemistry of manganeseâ€“salen complexes studied by electrospray tandem mass spectrometry: the significance of axial ligands. International Journal of Mass Spectrometry, 2000, 195-196, 351-362.	1.5	53
32	Ni-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions: Catalyst Identification and Optimization. Journal of the American Chemical Society, 2015, 137, 7019-7022.	13.7	53
33	Isotope Effects and the Mechanism of an Electron-Transfer-Catalyzed Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 2002, 124, 11552-11559.	13.7	52
34	Computational Exploration of Zinc Binding Groups for HDAC Inhibition. Journal of Organic Chemistry, 2013, 78, 5051-5055.	3.2	51
35	Inhibition and Mechanism of HDAC8 Revisited. Journal of the American Chemical Society, 2014, 136, 11636-11643.	13.7	51
36	Computational Explorations of Vinylcyclopropaneâ^'Cyclopentene Rearrangements and Competing Diradical Stereoisomerizations. Journal of Organic Chemistry, 2000, 65, 3259-3268.	3.2	50

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37	Treatment of Niemannâ€“Pick Type C Disease by Histone Deacetylase Inhibitors. Neurotherapeutics, 2013, 10, 688-697.	4.4	49
38	Mechanism of Hydroxyl Radical-Induced Breakdown of the Herbicide 2,4-Dichlorophenoxyacetic Acid (2,4-D). Chemistry - A European Journal, 2003, 9, 5379-5387.	3.3	48
39	The Increasingly Complex Mechanism of HMG-CoA Reductase. Accounts of Chemical Research, 2013, 46, 2416-2426.	15.6	47
40	Radical cation Diels-Alder reaction of indoles and exocyclic dienes. Tetrahedron Letters, 1993, 34, 6391-6394.	1.4	43
41	Electron-Transfer-Induced Diels-Alder Reactions of Indole and Exocyclic Dienes: Synthesis and Quantum-Chemical Studies. Chemistry - A European Journal, 1999, 5, 2859-2865.	3.3	43
42	Pericyclic Reactions of Radical Cations. European Journal of Organic Chemistry, 2001, 2001, 1429-1439.	2.4	42
43	Computational Studies on the Mechanism of the Copperâ€Catalyzed sp³â€ï£¿H Crossâ€Dehydrogenative Coupling Reaction. ChemPlusChem, 2013, 78, 943-951.	2.8	42
44	Synthesis and Structure of {Î·5-C5H5Cr}2{Î¼-Î·6:Î·6-(Î¼-1,2-C3H6-1,2-C2B4H4)}. An Unusual 24-Electron Triple-Decker Sandwich Complex Containing a Metal-Stabilized, Planar Tetraborabenzene. Inorganic Chemistry, 1998, 37, 608-609.	4.0	41
45	Understanding Rate Acceleration and Stereoinduction of an Asymmetric Giese Reaction Mediated by a Chiral Rhodium Catalyst. Journal of the American Chemical Society, 2017, 139, 8062-8065.	13.7	41
46	Ab Initio Studies of [1,5]-H Shifts:Â Pentadiene and Beyond. Journal of Organic Chemistry, 2000, 65, 2331-2336.	3.2	40
47	DFT Study of the [2 + 2] Cycloreversion of Uracil Dimer Anion Radical:Â Waters Matter. Journal of the American Chemical Society, 2001, 123, 2693-2694.	13.7	39
48	Revisiting the Stereodetermining Step in Enantioselective Iridium-Catalyzed Imine Hydrogenation. ACS Catalysis, 2018, 8, 615-623.	11.2	38
49	Structure and [2+2] Cycloreversion of the Cyclobutane Radical Cation. Journal of Physical Chemistry A, 1999, 103, 7907-7911.	2.5	37
50	Application of Q2MM to predictions in stereoselective synthesis. Chemical Communications, 2018, 54, 8294-8311.	4.1	37
51	Syntheses of Conformationally Constricted Molecules as Potential NAALADase/PSMA Inhibitors. Organic Letters, 2004, 6, 1805-1808.	4.6	36
52	Palladium-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions. Organic Letters, 2014, 16, 3970-3973.	4.6	36
53	Mild and Efficient Desymmetrization of Diynes via Hydroamination: Application to the Synthesis of (Â±)-Monomorine I. Journal of Organic Chemistry, 2010, 75, 1325-1328.	3.2	35
54	Ab Initio Studies of the Ring-Opening Reaction of the Cyclobutene Radical Cation. Journal of the American Chemical Society, 1997, 119, 5713-5719.	13.7	34

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55	Palladium-catalyzed enantioselective Heck alkenylation of trisubstituted allylic alkenols: a redox-relay strategy to construct vicinal stereocenters. Chemical Science, 2017, 8, 2277-2282.	7.4	33
56	Modular synthesis and biological activity of pyridyl-based analogs of the potent Class I Histone Deacetylase Inhibitor Largazole. Bioorganic and Medicinal Chemistry, 2015, 23, 5061-5074.	3.0	32
57	Molecular Modeling of the Reaction Pathway and Hydride Transfer Reactions of HMG-CoA Reductase. Biochemistry, 2012, 51, 7983-7995.	2.5	31
58	Design, Synthesis, and Evaluation of a Biomimetic Artificial Photolyase Model. Journal of Organic Chemistry, 2004, 69, 8183-8185.	3.2	29
59	Structure and Reactivity of Radical Ions: New Twists on Old Concepts. Chemistry - A European Journal, 2006, 12, 7018-7026.	3.3	29
60	Synthesis and HDAC inhibitory activity of isosteric thiazoline-oxazole largazole analogs. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6025-6028.	2.2	29
61	Stereoselectivity in Asymmetric Catalysis: The Case of Ruthenium-Catalyzed Ketone Hydrogenation. Journal of Chemical Theory and Computation, 2014, 10, 2427-2435.	5.3	27
62	Symmetry, Radical Ions, and Butadienes:Â Exploring the Limits of Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 8236-8240.	2.5	26
63	Selectivity in the Electron Transfer Catalyzed Dielsâ"Alder Reaction of (R)-Î±-Phellandrene and 4-Methoxystyrene. Journal of Organic Chemistry, 2008, 73, 7909-7915.	3.2	26
64	Synthesis, Photophysical, Photochemical, and Computational Studies of Coumarin-Labeled Nicotinamide Derivatives. Journal of Organic Chemistry, 2012, 77, 2756-2762.	3.2	26
65	Radical-Induced Oxidative Transformation of Quinoline. Journal of Physical Chemistry A, 2003, 107, 427-433.	2.5	25
66	Relative reactivity of alkenyl alcohols in the palladium-catalyzed redox-relay Heck reaction. Tetrahedron, 2015, 71, 6513-6518.	1.9	24
67	Hydrogenation catalyst generates cyclic peptide stereocentres in sequence. Nature Chemistry, 2018, 10, 968-973.	13.6	24
68	The Vinylcyclopropane Radical Cation Rearrangement and Related Reactions on the C5H8â€¢+Hypersurface. Journal of the American Chemical Society, 1999, 121, 11531-11537.	13.7	23
69	Mechanistic Pathways of the Hydroxyl Radical Reactions of Quinoline. 2. Computational Analysis of Hydroxyl Radical Attack at C Atoms. Journal of Physical Chemistry A, 2005, 109, 2829-2835.	2.5	23
70	Singleâ€Flask Multicomponent Palladiumâ€Catalyzed Î±,Î³â€Coupling of Ketone Enolates: Facile Preparation of Complex Carbon Scaffolds. Angewandte Chemie - International Edition, 2015, 54, 11822-11825.	13.8	20
71	Conformational and SAR analysis of NAALADase and PSMA inhibitors. Bioorganic and Medicinal Chemistry, 2003, 11, 4455-4461.	3.0	19
72	Toward an Artificial Oxidative DNA Photolyase. Journal of Organic Chemistry, 2004, 69, 543-548.	3.2	19

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73	Acyclic or Long-Bond Intermediate in the Electron-Transfer-Catalyzed Dimerization of 4-Methoxystyrene. Journal of Organic Chemistry, 2006, 71, 8926-8933.	3.2	19
74	Application of Q2MM to Stereoselective Reactions. Current Organic Chemistry, 2010, 14, 1629-1645.	1.6	19
75	2-Hydroxypropyl-Î²-cyclodextrin is the active component in a triple combination formulation for treatment of Niemann-Pick C1 disease. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2019, 1864, 1545-1561.	2.4	19
76	Structures and conformations of heteroatomâ€bridged calixarenes. Journal of Physical Organic Chemistry, 2011, 24, 1157-1165.	1.9	17
77	Single-Flask Multicomponent Synthesis of Highly Substituted Î±-Pyrones via a Sequential Enolate Arylation and Alkenylation Strategy. Organic Letters, 2016, 18, 5724-5727.	4.6	17
78	Protein dynamics and structural waters in bromodomains. PLoS ONE, 2017, 12, e0186570.	2.5	17
79	Density functional theory studies of the methanol radical cation hypersurface. Computational and Theoretical Chemistry, 1996, 368, 39-48.	1.5	16
80	Substituent Effects in Pericyclic Reactions of Radical Cations:Â The Ring Opening of 3-Substituted Cyclobutene Radical Cations. Journal of Organic Chemistry, 2000, 65, 6708-6714.	3.2	16
81	Epoxide Formation by Ring Closure of the Cinnamyloxy Radical. Organic Letters, 2000, 2, 1251-1254.	4.6	15
82	Transition State Force Field for the Asymmetric Redox-Relay Heck Reaction. Journal of the American Chemical Society, 2020, 142, 9700-9707.	13.7	15
83	Electron Transfer Catalyzed [2 + 2] Cycloreversion of Benzene Dimers. Journal of Organic Chemistry, 1999, 64, 2860-2863.	3.2	14
84	Rehybridized 1,3-Butadiene Radical Cations:â€‰ How Far Will a Radical Cation Go To Maintain Conjugation?. Journal of Physical Chemistry A, 2002, 106, 3967-3974.	2.5	14
85	Development of carbamate-tethered coumarins as phototriggers for caged nicotinamide. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6321-6324.	2.2	14
86	Mechanistic Study of the Nickel-Catalyzed Î±,Î²-Coupling of Saturated Ketones. ACS Catalysis, 2018, 8, 1740-1747.	11.2	14
87	Quantum Mechanical Study of the Ring-Closing Reaction of the Hexatriene Radical Cation. Journal of Organic Chemistry, 2001, 66, 5808-5813.	3.2	13
88	Sterically Crowded Bicyclo[1.1.0]butane Radical Cations. Journal of Organic Chemistry, 2003, 68, 4549-4552.	3.2	13
89	Development of a Q2MM Force Field for the Silver(I)â€Catalyzed Hydroamination of Alkynes. Advanced Synthesis and Catalysis, 2007, 349, 2647-2654.	4.3	13
90	Evolution of Concise and Flexible Synthetic Strategies for Trichostatic Acid and the Potent Histone Deacetylase Inhibitor Trichostatin A. European Journal of Organic Chemistry, 2013, 2013, 162-172.	2.4	13

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91	Mechanism and Selectivity in the Pd-Catalyzed Difunctionalization of Isoprene. Journal of Organic Chemistry, 2016, 81, 7604-7611.	3.2	13
92	Molecular Analysis of Membrane Targeting by the C2 Domain of the E3 Ubiquitin Ligase Smurf1. Biomolecules, 2020, 10, 229.	4.0	13
93	Ion Chemistry of anti-o,oâ€²-Dibenzene. Chemistry - A European Journal, 2000, 6, 4422-4430.	3.3	11
94	Substituent Effects in the Vinylcyclopropane Radical Cation Rearrangement: A Computational Road to a New Synthetic Tool. European Journal of Organic Chemistry, 2003, 2003, 1454-1462.	2.4	11
95	Explicit and implicit solvation of radical ions: the cycloreversion of CPD dimers. Tetrahedron, 2006, 62, 6490-6500.	1.9	11
96	Stereoselectivity in (Acyloxy)borane-Catalyzed Mukaiyama Aldol Reactions. Journal of Organic Chemistry, 2016, 81, 5314-5321.	3.2	11
97	Diastereoselective Synthesis of Highly Substituted Tetrahydrofurans by Pd-Catalyzed Tandem Oxidative Cyclizationâ€“Redox Relay Reactions Controlled by Intramolecular Hydrogen Bonding. Journal of Organic Chemistry, 2017, 82, 57-75.	3.2	11
98	Chiral Diamineâˆ’Silver(I)âˆ’Alkene Complexes:â€‰ A Quantum Chemical and NMR Study. Organometallics, 2005, 24, 3737-3745.	2.3	10
99	pHP-Tethered N-Acyl Carbamate: A Photocage for Nicotinamide. Organic Letters, 2018, 20, 2547-2550.	4.6	10
100	Anomeric Effects in Sulfamides. Journal of Physical Chemistry A, 2016, 120, 3677-3682.	2.5	9
101	Microsecond timescale MD simulations at the transition state of PmHMGR predict remote allosteric residues. Chemical Science, 2021, 12, 6413-6418.	7.4	7
102	Stereoselectivity Predictions for the Pd-Catalyzed 1,4-Conjugate Addition Using Quantum-Guided Molecular Mechanics. Journal of Organic Chemistry, 2021, 86, 5660-5667.	3.2	6
103	Production of Proteins of the SARS-CoV-2 Proteome for Drug Discovery. ACS Omega, 2021, 6, 19983-19994.	3.5	6
104	HSP90 inhibitors reduce cholesterol storage in Niemann-Pick type C1 mutant fibroblasts. Journal of Lipid Research, 2021, 62, 100114.	4.2	6
105	Design and synthesis of a crosslinker for studying intracellular steroid trafficking pathways. Bioorganic and Medicinal Chemistry, 2015, 23, 3843-3851.	3.0	5
106	A Phosphine-Mediated Dearomative Skeletal Rearrangement of Dianiline Squaraine Dyes. Organic Letters, 2021, 23, 2853-2857.	4.6	5
107	Inhibition of Histone Deacetylases 1, 2, and 3 Enhances Clearance of Cholesterol Accumulation in Niemann-Pick C1 Fibroblasts. ACS Pharmacology and Translational Science, 2021, 4, 1136-1148.	4.9	5
108	Proofreading experimentally assigned stereochemistry through Q2MM predictions in Pd-catalyzed allylic aminations. Nature Communications, 2021, 12, 6719.	12.8	5

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109	Automated fitting of transition state force fields for biomolecular simulations. PLoS ONE, 2022, 17, e0264960.	2.5	5
110	A nickel-catalyzed Î±,Î²-coupling of saturated ketones. Tetrahedron Letters, 2015, 56, 3468-3472.	1.4	4
111	Striking a Balance to Control Stereochemistry. Science, 2011, 333, 1831-1832.	12.6	2
112	Design, Synthesis, and Evaluation of a Luminescent Cholesterol Mimic. Journal of Organic Chemistry, 2021, 86, 1612-1621.	3.2	2
113	Rational Design and Identification of Harmineâ€Inspired, N â€Heterocyclic DYRK1A Inhibitors Employing a Functional Genomic In Vivo Drosophila Model System**. ChemMedChem, 2022, , .	3.2	2
114	Computational Studies of Molecular Electronic Devices. ACS Symposium Series, 2003, , 230-242.	0.5	1
115	Regioselective Alkylation of Pyridinium Riboses. European Journal of Organic Chemistry, 2020, 2020, 446-449.	2.4	1
116	Selectivity in Radical Cation Cycloadditions. , 0, , 61-82.		0
117	Front Cover: Rational Design and Identification of Harmineâ€Inspired, Nâ€Heterocyclic DYRK1A Inhibitors Employing a Functional Genomic In Vivo Drosophila Model System (ChemMedChem) Tj ETQq1 1 0.784314 rgBT /Ove	3.2	0