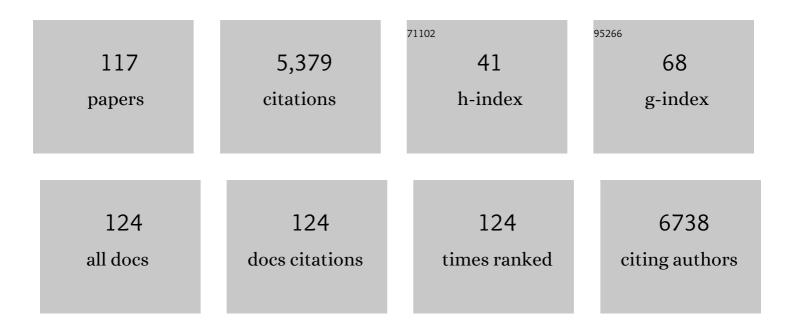
Olaf Wiest

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	EP300 Selectively Controls the Enhancer Landscape of <i>MYCN</i> -Amplified Neuroblastoma. Cancer Discovery, 2022, 12, 730-751.	9.4	64
2	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
3	Front Cover: Rational Design and Identification of Harmineâ€Inspired, <i>N</i> â€Heterocyclic DYRK1A Inhibitors Employing a Functional Genomic In Vivo <i>Drosophila</i> Model System (ChemMedChem) Tj ETQq1	1 03728431	4 ngBT ∕Over
4	Automated fitting of transition state force fields for biomolecular simulations. PLoS ONE, 2022, 17, e0264960.	2.5	5
5	Microsecond timescale MD simulations at the transition state of <i>Pm</i> HMGR predict remote allosteric residues. Chemical Science, 2021, 12, 6413-6418.	7.4	7
6	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
7	A Phosphine-Mediated Dearomative Skeletal Rearrangement of Dianiline Squaraine Dyes. Organic Letters, 2021, 23, 2853-2857.	4.6	5
8	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
9	Production of Proteins of the SARS-CoV-2 Proteome for Drug Discovery. ACS Omega, 2021, 6, 19983-19994.	3.5	6
10	HSP90 inhibitors reduce cholesterol storage in Niemann-Pick type C1 mutant fibroblasts. Journal of Lipid Research, 2021, 62, 100114.	4.2	6
11	Design, Synthesis, and Evaluation of a Luminescent Cholesterol Mimic. Journal of Organic Chemistry, 2021, 86, 1612-1621.	3.2	2
12	Proofreading experimentally assigned stereochemistry through Q2MM predictions in Pd-catalyzed allylic aminations. Nature Communications, 2021, 12, 6719.	12.8	5
13	Regioselective Alkylation of Pyridinium Riboses. European Journal of Organic Chemistry, 2020, 2020, 446-449.	2.4	1
14	Transition State Force Field for the Asymmetric Redox-Relay Heck Reaction. Journal of the American Chemical Society, 2020, 142, 9700-9707.	13.7	15
15	Molecular Analysis of Membrane Targeting by the C2 Domain of the E3 Ubiquitin Ligase Smurf1. Biomolecules, 2020, 10, 229.	4.0	13
16	Chemical genomics reveals histone deacetylases are required for core regulatory transcription. Nature Communications, 2019, 10, 3004.	12.8	107
17	2-Hydroxypropyl-β-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
18	Rapid virtual screening of enantioselective catalysts using CatVS. Nature Catalysis, 2019, 2, 41-45.	34.4	81

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19	pHP-Tethered N-Acyl Carbamate: A Photocage for Nicotinamide. Organic Letters, 2018, 20, 2547-2550.	4.6	10
20	Mechanistic Study of the Nickel-Catalyzed α,β-Coupling of Saturated Ketones. ACS Catalysis, 2018, 8, 1740-1747.	11.2	14
21	Revisiting the Stereodetermining Step in Enantioselective Iridium-Catalyzed Imine Hydrogenation. ACS Catalysis, 2018, 8, 615-623.	11.2	38
22	Application of Q2MM to predictions in stereoselective synthesis. Chemical Communications, 2018, 54, 8294-8311.	4.1	37
23	Hydrogenation catalyst generates cyclic peptide stereocentres in sequence. Nature Chemistry, 2018, 10, 968-973.	13.6	24
24	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
25	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
26	Diastereoselective Synthesis of Highly Substituted Tetrahydrofurans by Pd-Catalyzed Tandem Oxidative Cyclization–Redox Relay Reactions Controlled by Intramolecular Hydrogen Bonding. Journal of Organic Chemistry, 2017, 82, 57-75.	3.2	11
27	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
28	Visible-Light-Activated Asymmetric β-C–H Functionalization of Acceptor-Substituted Ketones with 1,2-Dicarbonyl Compounds. Journal of the American Chemical Society, 2017, 139, 17245-17248.	13.7	85
29	Protein dynamics and structural waters in bromodomains. PLoS ONE, 2017, 12, e0186570.	2.5	17
30	Prediction of Stereochemistry using Q2MM. Accounts of Chemical Research, 2016, 49, 996-1005.	15.6	76
31	Anomeric Effects in Sulfamides. Journal of Physical Chemistry A, 2016, 120, 3677-3682.	2.5	9
32	Mechanism and Selectivity in the Pd-Catalyzed Difunctionalization of Isoprene. Journal of Organic Chemistry, 2016, 81, 7604-7611.	3.2	13
33	Single-Flask Multicomponent Synthesis of Highly Substituted α-Pyrones via a Sequential Enolate Arylation and Alkenylation Strategy. Organic Letters, 2016, 18, 5724-5727.	4.6	17
34	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
35	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
36	Stereoselectivity in (Acyloxy)borane-Catalyzed Mukaiyama Aldol Reactions. Journal of Organic Chemistry, 2016, 81, 5314-5321.	3.2	11

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37	Singleâ€Flask Multicomponent Palladiumâ€Catalyzed α,Ĵ³â€Coupling of Ketone Enolates: Facile Preparation of Complex Carbon Scaffolds. Angewandte Chemie - International Edition, 2015, 54, 11822-11825.	13.8	20
38	Design and synthesis of a crosslinker for studying intracellular steroid trafficking pathways. Bioorganic and Medicinal Chemistry, 2015, 23, 3843-3851.	3.0	5
39	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
40	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
41	A nickel-catalyzed \hat{I}_{\pm}, \hat{I}^2 -coupling of saturated ketones. Tetrahedron Letters, 2015, 56, 3468-3472.	1.4	4
42	Relative reactivity of alkenyl alcohols in the palladium-catalyzed redox-relay Heck reaction. Tetrahedron, 2015, 71, 6513-6518.	1.9	24
43	A molecular mechanism of artemisinin resistance in Plasmodium falciparum malaria. Nature, 2015, 520, 683-687.	27.8	485
44	Variable Active Site Loop Conformations Accommodate the Binding of Macrocyclic Largazole Analogues to HDAC8. Biochemistry, 2015, 54, 2126-2135.	2.5	55
45	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
46	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
47	Stereoselectivity in Asymmetric Catalysis: The Case of Ruthenium-Catalyzed Ketone Hydrogenation. Journal of Chemical Theory and Computation, 2014, 10, 2427-2435.	5.3	27
48	Inhibition and Mechanism of HDAC8 Revisited. Journal of the American Chemical Society, 2014, 136, 11636-11643.	13.7	51
49	Palladium-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions. Organic Letters, 2014, 16, 3970-3973.	4.6	36
50	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
51	Computational Studies on the Mechanism of the Copperâ€Catalyzed sp ³ â€CH Crossâ€Dehydrogenative Coupling Reaction. ChemPlusChem, 2013, 78, 943-951.	2.8	42
52	Synthesis and HDAC inhibitory activity of isosteric thiazoline-oxazole largazole analogs. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6025-6028.	2.2	29
53	Development of carbamate-tethered coumarins as phototriggers for caged nicotinamide. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6321-6324.	2.2	14
54	Treatment of Niemann–Pick Type C Disease by Histone Deacetylase Inhibitors. Neurotherapeutics, 2013, 10, 688-697.	4.4	49

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55	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
56	Computational Exploration of Zinc Binding Groups for HDAC Inhibition. Journal of Organic Chemistry, 2013, 78, 5051-5055.	3.2	51
57	The Increasingly Complex Mechanism of HMG-CoA Reductase. Accounts of Chemical Research, 2013, 46, 2416-2426.	15.6	47
58	Synthesis, Photophysical, Photochemical, and Computational Studies of Coumarin-Labeled Nicotinamide Derivatives. Journal of Organic Chemistry, 2012, 77, 2756-2762.	3.2	26
59	Molecular Modeling of the Reaction Pathway and Hydride Transfer Reactions of HMG-CoA Reductase. Biochemistry, 2012, 51, 7983-7995.	2.5	31
60	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
61	Structures and conformations of heteroatomâ€bridged calixarenes. Journal of Physical Organic Chemistry, 2011, 24, 1157-1165.	1.9	17
62	Striking a Balance to Control Stereochemistry. Science, 2011, 333, 1831-1832.	12.6	2
63	Application of Q2MM to Stereoselective Reactions. Current Organic Chemistry, 2010, 14, 1629-1645.	1.6	19
64	On the inhibition of histone deacetylase 8. Bioorganic and Medicinal Chemistry, 2010, 18, 4103-4110.	3.0	75
65	Mild and Efficient Desymmetrization of Diynes via Hydroamination: Application to the Synthesis of (±)-Monomorine I. Journal of Organic Chemistry, 2010, 75, 1325-1328.	3.2	35
66	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
67	Prediction of Enantioselectivity in Rhodium Catalyzed Hydrogenations. Journal of the American Chemical Society, 2009, 131, 410-411.	13.7	110
68	Selectivity in the Electron Transfer Catalyzed Dielsâ~'Alder Reaction of (R)-α-Phellandrene and 4-Methoxystyrene. Journal of Organic Chemistry, 2008, 73, 7909-7915.	3.2	26
69	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
70	Structural Origin of Selectivity in Class II-Selective Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 2898-2906.	6.4	112
71	Development of a Q2MM Force Field for the Silver(I) atalyzed Hydroamination of Alkynes. Advanced Synthesis and Catalysis, 2007, 349, 2647-2654.	4.3	13
72	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

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73	Explicit and implicit solvation of radical ions: the cycloreversion of CPD dimers. Tetrahedron, 2006, 62, 6490-6500.	1.9	11
74	Structure and Reactivity of Radical Ions: New Twists on Old Concepts. Chemistry - A European Journal, 2006, 12, 7018-7026.	3.3	29
75	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
76	Computational Studies of DNA Photolyase. Journal of Physical Chemistry A, 2005, 109, 7001-7012.	2.5	61
77	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
78	Chiral Diamineâ^'Silver(I)â^'Alkene Complexes:  A Quantum Chemical and NMR Study. Organometallics, 2005, 24, 3737-3745.	2.3	10
79	Syntheses of Conformationally Constricted Molecules as Potential NAALADase/PSMA Inhibitors. Organic Letters, 2004, 6, 1805-1808.	4.6	36
80	Toward an Artificial Oxidative DNA Photolyase. Journal of Organic Chemistry, 2004, 69, 543-548.	3.2	19
81	Design, Synthesis, and Evaluation of a Biomimetic Artificial Photolyase Model. Journal of Organic Chemistry, 2004, 69, 8183-8185.	3.2	29
82	On the Function of the 14 à Long Internal Cavity of Histone Deacetylase-Like Protein:  Implications for the Design of Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 3409-3417.	6.4	140
83	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
84	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
85	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
86	Conformational and SAR analysis of NAALADase and PSMA inhibitors. Bioorganic and Medicinal Chemistry, 2003, 11, 4455-4461.	3.0	19
87	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
88	Radical-Induced Oxidative Transformation of Quinoline. Journal of Physical Chemistry A, 2003, 107, 427-433.	2.5	25
89	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
90	Theoretical Studies of Mixed-Valence Transition Metal Complexes for Molecular Computing. Journal of Physical Chemistry A, 2003, 107, 285-291.	2.5	109

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91	Computational Studies of Molecular Electronic Devices. ACS Symposium Series, 2003, , 230-242.	0.5	1
92	Sterically Crowded Bicyclo[1.1.0]butane Radical Cations. Journal of Organic Chemistry, 2003, 68, 4549-4552.	3.2	13
93	Rehybridized 1,3-Butadiene Radical Cations:  How Far Will a Radical Cation Go To Maintain Conjugation?. Journal of Physical Chemistry A, 2002, 106, 3967-3974.	2.5	14
94	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
95	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
96	Sonolysis of 2,4-Dichlorophenoxyacetic Acid in Aqueous Solutions. Evidence for•OH-Radical-Mediated Degradation. Journal of Physical Chemistry A, 2001, 105, 3176-3181.	2.5	93
97	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
98	Quantum Mechanical Study of the Ring-Closing Reaction of the Hexatriene Radical Cation. Journal of Organic Chemistry, 2001, 66, 5808-5813.	3.2	13
99	Pericyclic Reactions of Radical Cations. European Journal of Organic Chemistry, 2001, 2001, 1429-1439.	2.4	42
100	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
101	Ion Chemistry of anti-o,o′-Dibenzene. Chemistry - A European Journal, 2000, 6, 4422-4430.	3.3	11
102	Coordination chemistry of manganese–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
103	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
104	Computational Explorations of Vinylcyclopropaneâ^'Cyclopentene Rearrangements and Competing Diradical Stereoisomerizations. Journal of Organic Chemistry, 2000, 65, 3259-3268.	3.2	50
105	Epoxide Formation by Ring Closure of the Cinnamyloxy Radical. Organic Letters, 2000, 2, 1251-1254.	4.6	15
106	Ab Initio Studies of [1,5]-H Shifts:Â Pentadiene and Beyond. Journal of Organic Chemistry, 2000, 65, 2331-2336.	3.2	40
107	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
108	Structure and [2+2] Cycloreversion of the Cyclobutane Radical Cation. Journal of Physical Chemistry A, 1999, 103, 7907-7911.	2.5	37

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109	Ab Initio Studies of the Radical Cation Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 1999, 121, 6730-6736.	13.7	53
110	Electron Transfer Catalyzed [2 + 2] Cycloreversion of Benzene Dimers. Journal of Organic Chemistry, 1999, 64, 2860-2863.	3.2	14
111	The Vinylcyclopropane Radical Cation Rearrangement and Related Reactions on the C5H8•+Hypersurface. Journal of the American Chemical Society, 1999, 121, 11531-11537.	13.7	23
112	Synthesis and Structure of {η5-C5H5Cr}2{μ-η6:η6-(μ-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
113	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
114	Density functional theory studies of the methanol radical cation hypersurface. Computational and Theoretical Chemistry, 1996, 368, 39-48.	1.5	16
115	Density functional theory calculations of pericyclic reaction transition structures. Topics in Current Chemistry, 1996, , 1-24.	4.0	74
116	Radical cation Diels-Alder reaction of indoles and exocyclic dienes. Tetrahedron Letters, 1993, 34, 6391-6394.	1.4	43
117	Selectivity in Radical Cation Cycloadditions. , 0, , 61-82.		0