

Eric Oldfield

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2872286/publications.pdf>

Version: 2024-02-01

200
papers

13,788
citations

15504

65
h-index

25787

108
g-index

221
all docs

221
docs citations

221
times ranked

12540
citing authors

#	ARTICLE	IF	CITATIONS
1	Mycobacterial membrane protein Large 3 α -like family proteins in bacteria, protozoa, fungi, plants, and animals: A bioinformatics and structural investigation. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 776-790.	2.6	3
2	In Vivo Efficacy of SQ109 against <i>Leishmania donovani</i> , <i>Trypanosoma</i> spp. and <i>Toxoplasma gondii</i> and In Vitro Activity of SQ109 Metabolites. <i>Biomedicines</i> , 2022, 10, 670.	3.2	4
3	A Structural and Bioinformatics Investigation of a Fungal Squalene Synthase and Comparisons with Other Membrane Proteins. <i>ACS Omega</i> , 2022, 7, 22601-22612.	3.5	2
4	Terpene Cyclases and Prenyltransferases: Structures and Mechanisms of Action. <i>ACS Catalysis</i> , 2021, 11, 290-303.	11.2	13
5	Structure, <i>In Vivo</i> Detection, and Antibacterial Activity of Metabolites of SQ109, an Anti-Infective Drug Candidate. <i>ACS Infectious Diseases</i> , 2021, 7, 2492-2507.	3.8	13
6	Immuno-antibiotics: targeting microbial metabolic pathways sensed by unconventional T cells. <i>Immunotherapy Advances</i> , 2021, 1, .	3.0	3
7	A polymeric approach toward resistance-resistant antimicrobial agent with dual-selective mechanisms of action. <i>Science Advances</i> , 2021, 7, .	10.3	50
8	Editor's Note: Relates to: "Immuno-antibiotics: targeting microbial metabolic pathways sensed by unconventional T cells". <i>Immunotherapy Advances</i> , 2021, 1, .	3.0	0
9	SQ109 inhibits proliferation of <i>Leishmania donovani</i> by disruption of intracellular Ca ²⁺ homeostasis, collapsing the mitochondrial electrochemical potential ($\Delta\psi_m$) and affecting acidocalcisomes. <i>Parasitology Research</i> , 2020, 119, 649-657.	1.6	23
10	Discovery of Prenyltransferase Inhibitors with <i>In Vitro</i> and <i>In Vivo</i> Antibacterial Activity. <i>ACS Infectious Diseases</i> , 2020, 6, 2979-2993.	3.8	14
11	COVID-19 and Other Pandemics: How Might They Be Prevented?. <i>ACS Infectious Diseases</i> , 2020, 6, 1563-1566.	3.8	16
12	<i>Mycobacterium tuberculosis</i> releases an antacid that remodels phagosomes. <i>Nature Chemical Biology</i> , 2019, 15, 889-899.	8.0	53
13	<i>Aspergillus flavus</i> squalene synthase as an antifungal target: Expression, activity, and inhibition. <i>Biochemical and Biophysical Research Communications</i> , 2019, 512, 517-523.	2.1	11
14	A Structural Change in Butyrophilin upon Phosphoantigen Binding Underlies Phosphoantigen-Mediated $\text{V}\beta 9\text{V}\beta 2\text{A}^{\text{T}}$ Cell Activation. <i>Immunity</i> , 2019, 50, 1043-1053.e5.	14.3	94
15	Complex structures of MoeN5 with substrate analogues suggest sequential catalytic mechanism. <i>Biochemical and Biophysical Research Communications</i> , 2019, 511, 800-805.	2.1	4
16	Discovery of Lipophilic Bisphosphonates That Target Bacterial Cell Wall and Quinone Biosynthesis. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2564-2581.	6.4	18
17	Farnesyl Pyrophosphate Synthase as a Target for Drug Development: Discovery of Natural-Product-Derived Inhibitors and Their Activity in Pancreatic Cancer Cells. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 10867-10896.	6.4	19
18	Catalytic Role of Conserved Asparagine, Glutamine, Serine, and Tyrosine Residues in Isoprenoid Biosynthesis Enzymes. <i>ACS Catalysis</i> , 2018, 8, 4299-4312.	11.2	19

#	ARTICLE	IF	CITATIONS
19	Alkynyl-containing phenylthiazoles: Systemically active antibacterial agents effective against methicillin-resistant <i>Staphylococcus aureus</i> (MRSA). <i>European Journal of Medicinal Chemistry</i> , 2018, 148, 195-209.	5.5	36
20	Remarkable similarity in <i>Plasmodium falciparum</i> and <i>Plasmodium vivax</i> geranylgeranyl diphosphate synthase dynamics and its implication for antimalarial drug design. <i>Chemical Biology and Drug Design</i> , 2018, 91, 1068-1077.	3.2	5
21	Head and Middle and Tail cis Prenyl Transferases: Structure of Isosesquilandulyl Diphosphate Synthase. <i>Angewandte Chemie</i> , 2018, 130, 691-695.	2.0	5
22	Head and Middle and Tail cis Prenyl Transferases: Structure of Isosesquilandulyl Diphosphate Synthase. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 683-687.	13.8	24
23	The Mevalonate Pathway Is a Druggable Target for Vaccine Adjuvant Discovery. <i>Cell</i> , 2018, 175, 1059-1073.e21.	28.9	148
24	Bisphosphonate-Generated ATP-Analogs Inhibit Cell Signaling Pathways. <i>Journal of the American Chemical Society</i> , 2018, 140, 7568-7578.	13.7	27
25	Structure-activity relationship investigation of coumarin-chalcone hybrids with diverse side-chains as acetylcholinesterase and butyrylcholinesterase inhibitors. <i>Molecular Diversity</i> , 2018, 22, 893-906.	3.9	17
26	Phenylthiazole Antibacterial Agents Targeting Cell Wall Synthesis Exhibit Potent Activity in Vitro and in Vivo against Vancomycin-Resistant Enterococci. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 2425-2438.	6.4	46
27	Spectroscopic and Computational Investigations of Ligand Binding to IspH: Discovery of Non-diphosphate Inhibitors. <i>ChemBioChem</i> , 2017, 18, 914-920.	2.6	10
28	Anticancer Activity of Polyoxometalate-Bisphosphonate Complexes: Synthesis, Characterization, In Vitro and In Vivo Results. <i>Inorganic Chemistry</i> , 2017, 56, 7558-7565.	4.0	44
29	Head and Head Prenyl Synthases in Pathogenic Bacteria. <i>ChemBioChem</i> , 2017, 18, 985-991.	2.6	6
30	Pulsed Electron Paramagnetic Resonance Insights into the Ligand Environment of Copper in <i>Drosophila</i> Lysyl Oxidase. <i>Biochemistry</i> , 2017, 56, 3770-3779.	2.5	5
31	Combining V β 9V γ 2 T Cells with a Lipophilic Bisphosphonate Efficiently Kills Activated Hepatic Stellate Cells. <i>Frontiers in Immunology</i> , 2017, 8, 1381.	4.8	13
32	Structure and Function of a Head-Middle-Prenyltransferase: Lavandulyl Diphosphate Synthase. <i>Angewandte Chemie</i> , 2016, 128, 4799-4802.	2.0	9
33	Moenomycin Biosynthesis: Structure and Mechanism of Action of the Prenyltransferase MoeN5. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4716-4720.	13.8	19
34	Structure and Function of a Head-Middle-Prenyltransferase: Lavandulyl Diphosphate Synthase. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4721-4724.	13.8	32
35	Titelbild: Structure and Function of a Head-Middle-Prenyltransferase: Lavandulyl Diphosphate Synthase (<i>Angew. Chem.</i> 15/2016). <i>Angewandte Chemie</i> , 2016, 128, 4689-4689.	2.0	2
36	Chemical Exchange Saturation Transfer (CEST) Agents: Quantum Chemistry and MRI. <i>Chemistry - A European Journal</i> , 2016, 22, 264-271.	3.3	14

#	ARTICLE	IF	CITATIONS
37	Bacterial Cell Growth Inhibitors Targeting Undecaprenyl Diphosphate Synthase and Undecaprenyl Diphosphate Phosphatase. <i>ChemMedChem</i> , 2016, 11, 2311-2319.	3.2	20
38	Structure, Function, and Inhibition of <i>Staphylococcus aureus</i> Heptaprenyl Diphosphate Synthase. <i>ChemMedChem</i> , 2016, 11, 1915-1923.	3.2	23
39	Dynamic Structure and Inhibition of a Malaria Drug Target: Geranylgeranyl Diphosphate Synthase. <i>Biochemistry</i> , 2016, 55, 5180-5190.	2.5	8
40	Isoprenoid Biosynthesis Inhibitors Targeting Bacterial Cell Growth. <i>ChemMedChem</i> , 2016, 11, 2205-2215.	3.2	37
41	A Highly Efficient Single-Chain Metal-Organic Nanoparticle Catalyst for Alkyne-Azide "Click" Reactions in Water and in Cells. <i>Journal of the American Chemical Society</i> , 2016, 138, 11077-11080.	13.7	190
42	Inhibition of <i>Leishmania mexicana</i> Growth by the Tuberculosis Drug SQ109. <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 6386-6389.	3.2	21
43	Moenomycin Biosynthesis: Structure and Mechanism of Action of the Prenyltransferase MoeN5. <i>Angewandte Chemie</i> , 2016, 128, 4794-4798.	2.0	3
44	Structure and Function of Four Classes of the 4Fe-4S Protein, IspH. <i>Biochemistry</i> , 2016, 55, 4119-4129.	2.5	14
45	Structures of Trypanosome Vacuolar Soluble Pyrophosphatases: Antiparasitic Drug Targets. <i>ACS Chemical Biology</i> , 2016, 11, 1362-1371.	3.4	15
46	Titelbild: Structures of Iridoid Synthase from <i>Cantharanthus roseus</i> with Bound NAD ⁺ , NADPH, or NAD ⁺ /10-Oxogeranial: Reaction Mechanisms (<i>Angew. Chem.</i> 51/2015). <i>Angewandte Chemie</i> , 2015, 127, 15517-15517.	2.0	0
47	Structures of Iridoid Synthase from <i>Cantharanthus roseus</i> with Bound NAD ⁺ , NADPH, or NAD ⁺ /10-Oxogeranial: Reaction Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 15478-15482.	13.8	21
48	Polyoxomolybdate Bisphosphonate Heterometallic Complexes: Synthesis, Structure, and Activity on a Breast Cancer Cell Line. <i>Chemistry - A European Journal</i> , 2015, 21, 10537-10547.	3.3	43
49	Antiinfectives targeting enzymes and the proton motive force. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E7073-82.	7.1	138
50	IspH-RPS1 and IspH-UbiA: Rosetta stone proteins. <i>Chemical Science</i> , 2015, 6, 6813-6822.	7.4	6
51	Farnesyl Diphosphate Synthase Inhibitors With Unique Ligand-Binding Geometries. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 349-354.	2.8	20
52	SQ109, a New Drug Lead for Chagas Disease. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 1950-1961.	3.2	51
53	Antibacterial Drug Leads: DNA and Enzyme Multitargeting. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 1215-1227.	6.4	48
54	In Vitro and in Vivo Activity of Multitarget Inhibitors against <i>Trypanosoma brucei</i> . <i>ACS Infectious Diseases</i> , 2015, 1, 388-398.	3.8	5

#	ARTICLE	IF	CITATIONS
55	Oxa, Thia, Heterocycle, and Carborane Analogues of SQ109: Bacterial and Protozoal Cell Growth Inhibitors. <i>ACS Infectious Diseases</i> , 2015, 1, 215-221.	3.8	31
56	Tuberculosis Terpene Targets. <i>Chemistry and Biology</i> , 2015, 22, 437-438.	6.0	4
57	Atomic-Resolution Structures of Discrete Stages on the Reaction Coordinate of the [Fe ₄ S ₄] Enzyme IspG (GcpE). <i>Journal of Molecular Biology</i> , 2015, 427, 2220-2228.	4.2	14
58	<i>In Vitro</i> and <i>In Vivo</i> Investigation of the Inhibition of <i>Trypanosoma brucei</i> Cell Growth by Lipophilic Bisphosphonates. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 7530-7539.	3.2	13
59	Antagonism screen for inhibitors of bacterial cell wall biogenesis uncovers an inhibitor of undecaprenyl diphosphate synthase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 11048-11053.	7.1	83
60	A Molecular Dynamics Investigation of <i>Mycobacterium tuberculosis</i> Prenyl Synthases: Conformational Flexibility and Implications for Computer-aided Drug Discovery. <i>Chemical Biology and Drug Design</i> , 2015, 85, 756-769.	3.2	14
61	Crystal structures of ligand-bound octaprenyl pyrophosphate synthase from <i>Escherichia coli</i> reveal the catalytic and chain-length determining mechanisms. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 37-45.	2.6	22
62	Squalene Synthase As a Target for Chagas Disease Therapeutics. <i>PLoS Pathogens</i> , 2014, 10, e1004114.	4.7	64
63	Taxodione and arenarone inhibit farnesyl diphosphate synthase by binding to the isopentenyl diphosphate site. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E2530-9.	7.1	34
64	Structural and thermodynamic basis of the inhibition of <i>Leishmania major</i> farnesyl diphosphate synthase by nitrogen-containing bisphosphonates. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 802-810.	2.5	20
65	Resistance-resistant antibiotics. <i>Trends in Pharmacological Sciences</i> , 2014, 35, 664-674.	8.7	101
66	Structural and Functional Analysis of <i>Bacillus subtilis</i> YisP Reveals a Role of Its Product in Biofilm Production. <i>Chemistry and Biology</i> , 2014, 21, 1557-1563.	6.0	44
67	A combination therapy for KRAS-driven lung adenocarcinomas using lipophilic bisphosphonates and rapamycin. <i>Science Translational Medicine</i> , 2014, 6, 263ra161.	12.4	47
68	Multitarget Drug Discovery for Tuberculosis and Other Infectious Diseases. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 3126-3139.	6.4	205
69	Undecaprenyl Diphosphate Synthase Inhibitors: Antibacterial Drug Leads. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 5693-5701.	6.4	43
70	Structure and Inhibition of Tuberculosinol Synthase and Decaprenyl Diphosphate Synthase from <i>Mycobacterium tuberculosis</i> . <i>Journal of the American Chemical Society</i> , 2014, 136, 2892-2896.	13.7	37
71	Dronedarone, an Amiodarone Analog with Improved Anti- <i>Leishmania mexicana</i> Efficacy. <i>Antimicrobial Agents and Chemotherapy</i> , 2014, 58, 2295-2303.	3.2	33
72	Biorganometallic Chemistry with IspG and IspH: Structure, Function, and Inhibition of the [Fe ₄ S ₄] Proteins Involved in Isoprenoid Biosynthesis. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4294-4310.	13.8	50

#	ARTICLE	IF	CITATIONS
73	Inhibition of the 4Fe-4S proteins IspG and IspH: an EPR, ENDOR and HYSCORE investigation. <i>Chemical Science</i> , 2014, 5, 1642-1649.	7.4	14
74	Insights into the Binding of Pyridines to the Iron-Sulfur Enzyme IspH. <i>Journal of the American Chemical Society</i> , 2014, 136, 7926-7932.	13.7	20
75	Structure, function and inhibition of ent-kaurene synthase from <i>Bradyrhizobium japonicum</i> . <i>Scientific Reports</i> , 2014, 4, 6214.	3.3	44
76	Insights into TIM-Barrel Prenyl Transferase Mechanisms: Crystal Structures of PcrB from <i>Bacillus subtilis</i> and <i>Staphylococcus aureus</i> . <i>ChemBioChem</i> , 2013, 14, 195-199.	2.6	10
77	Structures of Fluoro, Amino, and Thiol Inhibitors Bound to the [Fe ₄ S ₄] Protein IspH. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2118-2121.	13.8	25
78	Farnesyl Diphosphate Synthase Inhibitors from <i>In Silico</i> Screening. <i>Chemical Biology and Drug Design</i> , 2013, 81, 742-748.	3.2	42
79	Chemo-Immunotherapeutic Antimalarials Targeting Isoprenoid Biosynthesis. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 423-427.	2.8	35
80	Isoprenoid Biosynthesis: Ferraoxetane or Allyl Anion Mechanism for IspH Catalysis?. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6522-6525.	13.8	17
81	Characterization of Potential Drug Targets Farnesyl Diphosphate Synthase and Geranylgeranyl Diphosphate Synthase in <i>Schistosoma mansoni</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2013, 57, 5969-5976.	3.2	9
82	Antibacterial drug leads targeting isoprenoid biosynthesis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 123-128.	7.1	129
83	Isoprenoid Biosynthesis: Ferraoxetane or Allyl Anion Mechanism for IspH Catalysis?. <i>Angewandte Chemie</i> , 2013, 125, 6650-6653.	2.0	4
84	Structure, function and inhibition of the two- and three-domain 4Fe-4S IspG proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 8558-8563.	7.1	29
85	Lipophilic analogs of zoledronate and risedronate inhibit <i>Plasmodium</i> geranylgeranyl diphosphate synthase (GGPPS) and exhibit potent antimalarial activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4058-4063.	7.1	61
86	Discovery of acetylene hydratase activity of the iron-sulphur protein IspH. <i>Nature Communications</i> , 2012, 3, 1042.	12.8	34
87	Are Free Radicals Involved in IspH Catalysis? An EPR and Crystallographic Investigation. <i>Journal of the American Chemical Society</i> , 2012, 134, 11225-11234.	13.7	45
88	Head-to-Head Prenyl Transferases: Anti-Infective Drug Targets. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 4367-4372.	6.4	19
89	HIV-1 Integrase Inhibitor-Inspired Antibacterials Targeting Isoprenoid Biosynthesis. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 402-406.	2.8	16
90	Insights into the Mechanism of the Antibiotic-Synthesizing Enzyme MoeO5 from Crystal Structures of Different Complexes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4157-4160.	13.8	16

#	ARTICLE	IF	CITATIONS
91	Back Cover: Insights into the Mechanism of the Antibiotic-Synthesizing Enzyme MoeO5 from Crystal Structures of Different Complexes (<i>Angew. Chem. Int. Ed.</i> 17/2012). <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4240-4240.	13.8	0
92	Dual Dehydrosqualene/Squalene Synthase Inhibitors: Leads for Innate Immune System-Based Therapeutics. <i>ChemMedChem</i> , 2012, 7, 561-564.	3.2	18
93	Polyoxometalates Functionalized by Bisphosphonate Ligands: Synthesis, Structural, Magnetic, and Spectroscopic Characterizations and Activity on Tumor Cell Lines. <i>Inorganic Chemistry</i> , 2012, 51, 7921-7931.	4.0	74
94	Terpene Biosynthesis: Modularity Rules. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1124-1137.	13.8	286
95	Pyridine Inhibitor Binding to the 4Fe-4S Protein A. aeolicus IspH (LytB): A HYSORE Investigation. <i>Journal of the American Chemical Society</i> , 2011, 133, 6525-6528.	13.7	35
96	An ENDOR and HYSORE Investigation of a Reaction Intermediate in IspG (GcpE) Catalysis. <i>Journal of the American Chemical Society</i> , 2011, 133, 8400-8403.	13.7	33
97	Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligand-Bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target. <i>Chemical Biology and Drug Design</i> , 2011, 77, 412-420.	3.2	38
98	Non-Bisphosphonate Inhibitors of Isoprenoid Biosynthesis Identified via Computer-Aided Drug Design. <i>Chemical Biology and Drug Design</i> , 2011, 78, 323-332.	3.2	49
99	Indirect Stimulation of Human $\text{V}\alpha 2\text{V}\beta 2$ T Cells through Alterations in Isoprenoid Metabolism. <i>Journal of Immunology</i> , 2011, 187, 5099-5113.	0.8	79
100	Tetra- to Dodecanuclear Oxomolybdate Complexes with Functionalized Bisphosphonate Ligands: Activity in Killing Tumor Cells. <i>Chemistry - A European Journal</i> , 2010, 16, 13741-13748.	3.3	70
101	Lipophilic Pyridinium Bisphosphonates: Potent $\text{V}\alpha 3\text{V}\beta 1$ T Cell Stimulators. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1136-1138.	13.8	63
102	Diterpene cyclases and the nature of the isoprene fold. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2417-2432.	2.6	131
103	Mechanism of action and inhibition of dehydrosqualene synthase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 21337-21342.	7.1	66
104	Lipophilic Bisphosphonates Are Potent Inhibitors of Plasmodium Liver-Stage Growth. <i>Antimicrobial Agents and Chemotherapy</i> , 2010, 54, 2987-2993.	3.2	52
105	Organometallic mechanism of action and inhibition of the 4Fe-4S isoprenoid biosynthesis protein GcpE (IspG). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 11189-11193.	7.1	66
106	Bioorganometallic mechanism of action, and inhibition, of IspH. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 4522-4527.	7.1	86
107	Inhibition of the Fe_4S_4 -Cluster-Containing Protein IspH (LytB): Electron Paramagnetic Resonance, Metallacycles, and Mechanisms. <i>Journal of the American Chemical Society</i> , 2010, 132, 6719-6727.	13.7	61
108	Targeting Isoprenoid Biosynthesis for Drug Discovery: Bench to Bedside. <i>Accounts of Chemical Research</i> , 2010, 43, 1216-1226.	15.6	119

#	ARTICLE	IF	CITATIONS
109	Protein Structure Refinement Using ^{13}C Chemical Shift Tensors. Journal of the American Chemical Society, 2009, 131, 985-992.	13.7	54
110	Thermodynamics of Bisphosphonates Binding to Human Bone: A Two-Site Model. Journal of the American Chemical Society, 2009, 131, 8374-8375.	13.7	90
111	Lipophilic Bisphosphonates as Dual Farnesyl/Geranylgeranyl Diphosphate Synthase Inhibitors: An X-ray and NMR Investigation. Journal of the American Chemical Society, 2009, 131, 5153-5162.	13.7	159
112	Phosphonosulfonates Are Potent, Selective Inhibitors of Dehydroqualene Synthase and Staphyloxanthin Biosynthesis in <i>Staphylococcus aureus</i> . Journal of Medicinal Chemistry, 2009, 52, 976-988.	6.4	59
113	Structures of a potent phenylalkyl bisphosphonate inhibitor bound to farnesyl and geranylgeranyl diphosphate synthases. Proteins: Structure, Function and Bioinformatics, 2008, 73, 431-439.	2.6	40
114	Bisphosphonate inhibitors of ATP-mediated HIV-1 reverse transcriptase catalyzed excision of chain-terminating 3'-azido, 3'-deoxythymidine: A QSAR investigation. Bioorganic and Medicinal Chemistry, 2008, 16, 8959-8967.	3.0	22
115	A Cholesterol Biosynthesis Inhibitor Blocks <i>Staphylococcus aureus</i> Virulence. Science, 2008, 319, 1391-1394.	12.6	422
116	Inhibition of Geranylgeranyl Diphosphate Synthase by Bisphosphonates: A Crystallographic and Computational Investigation. Journal of Medicinal Chemistry, 2008, 51, 5594-5607.	6.4	73
117	Bisphosphonate Inhibition of a <i>Plasmodium</i> Farnesyl Diphosphate Synthase and a General Method for Predicting Cell-Based Activity from Enzyme Data. Journal of Medicinal Chemistry, 2008, 51, 7827-7833.	6.4	38
118	Structure of (E)-4-Hydroxy-3-methyl-but-2-enyl Diphosphate Reductase, the Terminal Enzyme of the Non-Mevalonate Pathway. Journal of the American Chemical Society, 2008, 130, 17206-17207.	13.7	91
119	Photoaffinity Antigens for Human $\text{CD}4^+$ T Cells. Journal of Immunology, 2008, 181, 7738-7750.	0.8	49
120	The Farnesyl-diphosphate/Geranylgeranyl-diphosphate Synthase of <i>Toxoplasma gondii</i> Is a Bifunctional Enzyme and a Molecular Target of Bisphosphonates. Journal of Biological Chemistry, 2007, 282, 30804-30816.	3.4	82
121	Bisphosphonates as Inhibitors of <i>Trypanosoma cruzi</i> Hexokinase. Journal of Biological Chemistry, 2007, 282, 12377-12387.	3.4	57
122	Bisphosphonates target multiple sites in both cis- and trans-prenyltransferases. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 10022-10027.	7.1	173
123	A Solid State ^{13}C NMR, Crystallographic, and Quantum Chemical Investigation of Phenylalanine and Tyrosine Residues in Dipeptides and Proteins. Journal of the American Chemical Society, 2007, 129, 7385-7392.	13.7	15
124	Activity of Sulfonium Bisphosphonates on Tumor Cell Lines. Journal of Medicinal Chemistry, 2007, 50, 6067-6079.	6.4	15
125	^{13}C NMR spectroscopy of carbon nanohorns. Physical Review B, 2006, 73, .	3.2	36
126	Activity of Nitrogen-Containing and Non-Nitrogen-Containing Bisphosphonates on Tumor Cell Lines. Journal of Medicinal Chemistry, 2006, 49, 5804-5814.	6.4	61

#	ARTICLE	IF	CITATIONS
127	Solid-State NMR, Crystallographic, and Computational Investigation of Bisphosphonates and Farnesyl Diphosphate Synthase ^â Bisphosphonate Complexes. <i>Journal of the American Chemical Society</i> , 2006, 128, 14485-14497.	13.7	89
128	Enthalpy versus Entropy-Driven Binding of Bisphosphonates to Farnesyl Diphosphate Synthase. <i>Journal of the American Chemical Society</i> , 2006, 128, 3524-3525.	13.7	42
129	Isoprenoid Biosynthesis as a Drug Target:Â Bisphosphonate Inhibition of <i>Escherichia coli</i> K12 Growth and Synergistic Effects of Fosmidomycin. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 7331-7341.	6.4	52
130	Amiodarone Has Intrinsic Anti- <i>Trypanosoma cruzi</i> Activity and Acts Synergistically with Posaconazole. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 892-899.	6.4	162
131	Structural Studies of $\sqrt{3} \times \sqrt{2}$ T Cell Phosphoantigens. <i>Chemistry and Biology</i> , 2006, 13, 985-992.	6.0	23
132	Pyridinium-1-yl Bisphosphonates Are Potent Inhibitors of Farnesyl Diphosphate Synthase and Bone Resorption. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 2957-2963.	6.4	77
133	Structure and mechanism of the farnesyl diphosphate synthase from <i>Trypanosoma cruzi</i> : Implications for drug design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 80-88.	2.6	123
134	Quantum chemical studies of protein structure. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2005, 360, 1347-1361.	4.0	40
135	A Crystallographic Investigation of Phosphoantigen Binding to Isopentenyl Pyrophosphate/Dimethylallyl Pyrophosphate Isomerase. <i>Journal of the American Chemical Society</i> , 2005, 127, 536-537.	13.7	12
136	Crystallization and preliminary X-ray diffraction study of the farnesyl diphosphate synthase from <i>Trypanosoma brucei</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1863-1866.	2.5	14
137	Synthesis of chiral phosphoantigens and their activity in $\hat{I}3\hat{T}$ T cell stimulation. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 4471-4477.	2.2	20
138	Cytochrome P450:Â An Investigation of the MÃssbauer Spectra of a Reaction Intermediate and an Fe(IV)O Model System. <i>Journal of the American Chemical Society</i> , 2004, 126, 4470-4471.	13.7	42
139	Quantitative Structure ^â Activity Relationships for $\hat{I}3\hat{T}$ T Cell Activation by Bisphosphonates. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 375-384.	6.4	114
140	Effects of Bisphosphonates on the Growth of <i>Entamoeba histolytica</i> and <i>Plasmodium</i> Species in Vitro and in Vivo. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 175-187.	6.4	155
141	Farnesyl Pyrophosphate Synthase Is an Essential Enzyme in <i>Trypanosoma brucei</i> . <i>Journal of Biological Chemistry</i> , 2003, 278, 17075-17083.	3.4	79
142	Quantitative Structure ^â Activity Relations for $\hat{I}3\hat{T}$ T Cell Activation by Phosphoantigens. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 4868-4874.	6.4	32
143	57Fe MÃssbauer Isomer Shifts of Heme Protein Model Systems:â€% Electronic Structure Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 7829-7839.	13.7	97
144	MÃssbauer Quadrupole Splittings and Electronic Structure in Heme Proteins and Model Systems:Â A Density Functional Theory Investigation. <i>Journal of the American Chemical Society</i> , 2002, 124, 13921-13930.	13.7	65

#	ARTICLE	IF	CITATIONS
145	Carbon-13 NMR Shielding in the Twenty Common Amino Acids: Comparisons with Experimental Results in Proteins. <i>Journal of the American Chemical Society</i> , 2002, 124, 5486-5495.	13.7	90
146	CHEMICALSHIFTS INAMINOACIDS, PEPTIDES,ANDPROTEINS: From Quantum Chemistry to Drug Design. <i>Annual Review of Physical Chemistry</i> , 2002, 53, 349-378.	10.8	112
147	Inhibition of Geranylgeranyl Diphosphate Synthase by Bisphosphonates and Diphosphates: A Potential Route to New Bone Antiresorption and Antiparasitic Agents. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 2185-2196.	6.4	89
148	Nuclear Magnetic Resonance Shifts in Paramagnetic Metalloporphyrins and Metalloproteins. <i>Journal of the American Chemical Society</i> , 2002, 124, 13911-13920.	13.7	94
149	Activity of Bisphosphonates against <i>Trypanosoma brucei</i> rhodesiense. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 2904-2914.	6.4	101
150	Magic-angle spinning ³¹ P NMR spectroscopy of condensed phosphates in parasitic protozoa: visualizing the invisible. <i>FEBS Letters</i> , 2002, 523, 207-212.	2.8	32
151	NMR evidence of a spatially resolved oscillation in the Ef-LDOS in a nanoscale platinum electrocatalyst. <i>Chemical Physics Letters</i> , 2002, 361, 183-188.	2.6	6
152	Theoretical Investigation of ¹⁹ F NMR Chemical Shielding Tensors in Fluorobenzenes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8098-8104.	2.5	36
153	Bisphosphonates Inhibit the Growth of <i>Trypanosoma brucei</i> , <i>Trypanosoma cruzi</i> , <i>Leishmania donovani</i> , <i>Toxoplasma gondii</i> , and <i>Plasmodium falciparum</i> : A Potential Route to Chemotherapy. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 909-916.	6.4	312
154	An Experimental and Theoretical Investigation of the Chemical Shielding Tensors of ¹³ C of Alanine, Valine, and Leucine Residues in Solid Peptides and in Proteins in Solution. <i>Journal of the American Chemical Society</i> , 2001, 123, 10362-10369.	13.7	54
155	Electronic Properties at a Metal-Solution Interface as Viewed by Solid-State NMR. <i>ACS Symposium Series</i> , 2001, , 26-39.	0.5	2
156	Bisphosphonates Are Potent Inhibitors of <i>Trypanosoma cruzi</i> Farnesyl Pyrophosphate Synthase. <i>Journal of Biological Chemistry</i> , 2001, 276, 33930-33937.	3.4	134
157	Vacuolar proton pyrophosphatase activity and pyrophosphate (PPi) in <i>Toxoplasma gondii</i> as possible chemotherapeutic targets. <i>Biochemical Journal</i> , 2000, 349, 737-745.	3.7	72
158	³¹ P NMR Spectroscopy of <i>Trypanosoma brucei</i> , <i>Trypanosoma cruzi</i> , and <i>Leishmania major</i> . <i>Journal of Biological Chemistry</i> , 2000, 275, 28356-28362.	3.4	85
159	Expression of doubly labeled <i>Saccharomyces cerevisiae</i> iso-1 ferricytochrome c and ¹ H, ¹³ C and ¹⁵ N chemical shift assignments by multidimensional NMR. <i>FEBS Letters</i> , 2000, 482, 25-30.	2.8	7
160	Experimental, Hartree-Fock, and Density Functional Theory Investigations of the Charge Density, Dipole Moment, Electrostatic Potential, and Electric Field Gradients in Asparagine Monohydrate. <i>Journal of the American Chemical Society</i> , 2000, 122, 4708-4717.	13.7	65
161	A Detailed NMR-Based Model for CO on Pt Catalysts in an Electrochemical Environment: Shifts, Relaxation, Back-Bonding, and the Fermi-Level Local Density of States. <i>Journal of the American Chemical Society</i> , 2000, 122, 1123-1129.	13.7	111
162	Computation of Through-Space ¹⁹ F- ¹⁹ F Scalar Couplings via Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2000, 122, 12164-12168.	13.7	50

#	ARTICLE	IF	CITATIONS
163	The Chemical Nature of Hydrogen Bonding in Proteins via NMR: J -Couplings, Chemical Shifts, and AIM Theory. <i>Journal of the American Chemical Society</i> , 2000, 122, 12835-12841.	13.7	422
164	Solid-State NMR, Mössbauer, Crystallographic, and Density Functional Theory Investigation of Fe ²⁺ O ₂ and Fe ²⁺ O ₂ Analogue Metalloporphyrins and Metalloproteins. <i>Journal of the American Chemical Society</i> , 1999, 121, 3829-3844.	13.7	99
165	<i>Trypanosoma cruzi</i> Contains Major Pyrophosphate Stores, and Its Growth in Vitro and in Vivo Is Blocked by Pyrophosphate Analogs. <i>Journal of Biological Chemistry</i> , 1999, 274, 33609-33615.	3.4	134
166	Determination of order parameters and correlation times in proteins: a comparison between Bayesian, Monte Carlo and simple graphical methods. <i>Journal of Biomolecular NMR</i> , 1999, 13, 133-137.	2.8	8
167	Correlation between the Knight Shift of Chemisorbed CO and the Fermi Level Local Density of States at Clean Platinum Catalyst Surfaces. <i>Journal of the American Chemical Society</i> , 1999, 121, 2996-3003.	13.7	63
168	Solid-State NMR, Crystallographic and Density Functional Theory Investigation of Fe ²⁺ CO and Fe ²⁺ CO Analogue Metalloporphyrins and Metalloproteins. <i>Journal of the American Chemical Society</i> , 1999, 121, 3818-3828.	13.7	61
169	Nitrogen-Containing Bisphosphonates as Carbocation Transition State Analogs for Isoprenoid Biosynthesis. <i>Biochemical and Biophysical Research Communications</i> , 1999, 263, 754-758.	2.1	153
170	NMR and Quantum Chemistry of Proteins and Model Systems. <i>ACS Symposium Series</i> , 1999, , 40-62.	0.5	4
171	Carbonyl Complexes of Iron(II), Ruthenium(II), and Osmium(II) 5,10,15,20-Tetraphenylporphyrinates: A Comparative Investigation by X-ray Crystallography, Solid-State NMR Spectroscopy, and Density Functional Theory. <i>Journal of the American Chemical Society</i> , 1998, 120, 11323-11334.	13.7	76
172	An Experimental and Density Functional Theoretical Investigation of Iron-57 Mössbauer Quadrupole Splittings in Organometallic and Heme-Model Compounds: Applications to Carbonmonoxy-Heme Protein Structure. <i>Journal of the American Chemical Society</i> , 1998, 120, 3144-3151.	13.7	85
173	An Experimental and Quantum Chemical Investigation of CO Binding to Heme Proteins and Model Systems: A Unified Model Based on ¹³ C, ¹⁷ O, and ⁵⁷ Fe Nuclear Magnetic Resonance and ⁵⁷ Fe Mössbauer and Infrared Spectroscopies. <i>Journal of the American Chemical Society</i> , 1998, 120, 4784-4797.	13.7	100
174	Iron-57 NMR Chemical Shifts and Mössbauer Quadrupole Splittings in Metalloporphyrins, Ferrocyclochromec, and Myoglobins: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2342-2350.	2.5	71
175	Assignment and Analysis of Fluorine Nuclear Magnetic Resonance Spectra of 4-Fluorotryptophan Myoglobins and Hemoglobins. <i>Biochemistry</i> , 1997, 36, 3590-3599.	2.5	26
176	Predicting Chemical Shifts in Proteins: Structure Refinement of Valine Residues by Using ab Initio and Empirical Geometry Optimizations. <i>Journal of the American Chemical Society</i> , 1997, 119, 11941-11950.	13.7	78
177	Density Functional Study of Cobalt-59 Nuclear Magnetic Resonance Chemical Shifts and Shielding Tensor Elements in Co(III) Complexes. <i>Journal of the American Chemical Society</i> , 1997, 119, 8065-8069.	13.7	64
178	Ab Initio Quantum Chemical Investigation of Carbon-13 NMR Shielding Tensors in Glycine, Alanine, Valine, Isoleucine, Serine, and Threonine: Comparisons between Helical and Sheet Tensors, and the Effects of π Ion Shielding. <i>Journal of the American Chemical Society</i> , 1997, 119, 11951-11958.	13.7	109
179	¹⁹ F Nuclear Magnetic Resonance Chemical Shifts of Fluorine Containing Aliphatic Amino Acids in Proteins: Studies on <i>Lactobacillus casei</i> Dihydrofolate Reductase Containing (2S,4S)-5-Fluoroisoleucine. <i>Journal of the American Chemical Society</i> , 1996, 118, 8700-8706.	13.7	74
180	Ab Initio Studies of Amide- ¹⁵ N Chemical Shifts in Dipeptides: Applications to Protein NMR Spectroscopy. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16423-16428.	2.9	58

#	ARTICLE	IF	CITATIONS
181	Chemical shifts and three-dimensional protein structures. <i>Journal of Biomolecular NMR</i> , 1995, 5, 217-25.	2.8	157
182	¹ H, ¹³ C and ¹⁵ N chemical shift referencing in biomolecular NMR. <i>Journal of Biomolecular NMR</i> , 1995, 6, 135-140.	2.8	2,216
183	A Basis Size Dependence Study of Carbon-13 Nuclear Magnetic Resonance Spectroscopic Shielding in Alanyl and Valyl Fragments: Toward Protein Shielding Hypersurfaces. <i>Journal of the American Chemical Society</i> , 1995, 117, 9542-9546.	13.7	32
184	Protein Structure Refinement Using Carbon-13 Nuclear Magnetic Resonance Spectroscopic Chemical Shifts and Quantum Chemistry. <i>Journal of the American Chemical Society</i> , 1995, 117, 8823-8829.	13.7	43
185	Correlation between ¹⁵ N NMR chemical shifts in proteins and secondary structure. <i>Journal of Biomolecular NMR</i> , 1994, 4, 341-8.	2.8	89
186	Ab Initio Study of the Effects of Torsion Angles on Carbon-13 Nuclear Magnetic Resonance Chemical Shielding in N-Formyl-L-alanine Amide, N-Formyl-L-valine Amide, and Some Simple Model Compounds: Applications to Protein NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 1994, 116, 5307-5314.	13.7	71
187	Evaluating ¹⁹ F Chemical Shielding in Fluorobenzenes: Implications for Chemical Shifts in Proteins. <i>Journal of the American Chemical Society</i> , 1994, 116, 7453-7454.	13.7	28
188	Predicting Carbon-13 Nuclear Magnetic Resonance Chemical Shielding Tensors in Zwitterionic L-Threonine and L-Tyrosine via Quantum Chemistry. <i>Journal of the American Chemical Society</i> , 1994, 116, 7784-7786.	13.7	67
189	Fluorine-19 Nuclear Magnetic Resonance Spectroscopic Study of Fluorophenylalanine- and Fluorotryptophan-Labeled Avian Egg White Lysozymes. <i>Biochemistry</i> , 1994, 33, 5238-5245.	2.5	47
190	Chemical Shifts of Carbonyl Carbons in Peptides and Proteins. <i>Journal of the American Chemical Society</i> , 1994, 116, 11485-11488.	13.7	62
191	Computing nuclear magnetic resonance chemical shielding in large systems via multipole shielding polarizabilities. <i>Chemical Physics Letters</i> , 1993, 213, 211-216.	2.6	20
192	Methods for computing nuclear magnetic resonance chemical shielding in large systems. Multiple cluster and charge field approaches. <i>Chemical Physics Letters</i> , 1993, 205, 108-116.	2.6	85
193	Carbon-13 α -magic-angle sample-spinning nuclear magnetic resonance studies of human myelin, and model membrane systems. <i>Magnetic Resonance in Medicine</i> , 1993, 29, 168-178.	3.0	28
194	NMR chemical shifts and structure refinement in proteins. <i>Journal of Biomolecular NMR</i> , 1993, 3, 607-612.	2.8	38
195	Chemical shifts in proteins: an ab initio study of carbon-13 nuclear magnetic resonance chemical shielding in glycine, alanine, and valine residues. <i>Journal of the American Chemical Society</i> , 1993, 115, 9768-9773.	13.7	69
196	Chemical shifts in proteins: a shielding trajectory analysis of the fluorine nuclear magnetic resonance spectrum of the Escherichia coli galactose binding protein using a multipole shielding polarizability-local reaction field-molecular dynamics approach. <i>Journal of the American Chemical Society</i> , 1993, 115, 6851-6862.	13.7	80
197	Correlation of carbon-13 and oxygen-17 chemical shifts and the vibrational frequency of electrically perturbed carbon monoxide: a possible model for distal ligand effects in carbonmonoxyheme proteins. <i>Journal of the American Chemical Society</i> , 1991, 113, 2447-2451.	13.7	116
198	Distal and proximal ligand interactions in heme proteins: correlations between carbon-oxygen and iron-carbon vibrational frequencies, oxygen-17 and carbon-13 nuclear magnetic resonance chemical shifts, and oxygen-17 nuclear quadrupole coupling constants in [¹⁷ O] and [¹³ C]O-labeled species. <i>Biochemistry</i> , 1991, 30, 2333-2347.	2.5	132

#	ARTICLE	IF	CITATIONS
199	Determination of rotational mobilities of backbone and side-chain carbons of poly($\hat{1}^3$ -benzyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf and nuclear Overhauser enhancements. Biochemistry, 1973, 12, 3428-3433.	2.5	75
200	Natural-abundance carbon-13 nuclear magnetic resonance studies in 20-mm sample tubes. Numerous single-carbon resonances of hen egg-white lysozyme. Biochemistry, 1973, 12, 1335-1341.	2.5	100