

# 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	<sup>1</sup> H, <sup>13</sup> C and <sup>15</sup> N chemical shift referencing in biomolecular NMR. <i>Journal of Biomolecular NMR</i> , 1995, 6, 135-140.	2.8	2,216
2	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
3	A Cholesterol Biosynthesis Inhibitor Blocks <i>Staphylococcus aureus</i> Virulence. <i>Science</i> , 2008, 319, 1391-1394.	12.6	422
4	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
5	Terpene Biosynthesis: Modularity Rules. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1124-1137.	13.8	286
6	Multitarget Drug Discovery for Tuberculosis and Other Infectious Diseases. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 3126-3139.	6.4	205
7	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
8	Bisphosphonates target multiple sites in both cis- and trans-prenyltransferases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 10022-10027.	7.1	173
9	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
10	Lipophilic Bisphosphonates as Dual Farnesyl/Geranylgeranyl Diphosphate Synthase Inhibitors: An X-ray and NMR Investigation. <i>Journal of the American Chemical Society</i> , 2009, 131, 5153-5162.	13.7	159
11	Chemical shifts and three-dimensional protein structures. <i>Journal of Biomolecular NMR</i> , 1995, 5, 217-25.	2.8	157
12	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
13	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
14	The Mevalonate Pathway Is a Druggable Target for Vaccine Adjuvant Discovery. <i>Cell</i> , 2018, 175, 1059-1073.e21.	28.9	148
15	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
16	<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
17	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
18	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 [C17O-] and [13CO]-labeled species. <i>Biochemistry</i> , 1991, 30, 2333-2347.	2.5	132

#	ARTICLE	IF	CITATIONS
19	Diterpene cyclases and the nature of the isoprene fold. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2417-2432.	2.6	131
20	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
21	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
22	Targeting Isoprenoid Biosynthesis for Drug Discovery: Bench to Bedside. <i>Accounts of Chemical Research</i> , 2010, 43, 1216-1226.	15.6	119
23	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
24	Quantitative Structure-Activity Relationships for $\text{I}^{\text{31}}$ T Cell Activation by Bisphosphonates. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 375-384.	6.4	114
25	CHEMICALSHIFTS INAMINOACIDS, PEPTIDES,ANDPROTEINS: From Quantum Chemistry to Drug Design. <i>Annual Review of Physical Chemistry</i> , 2002, 53, 349-378.	10.8	112
26	A Detailed NMR-Based Model for CO on Pt Catalysts in an Electrochemical Environment: $\Delta$ 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
27	Anab InitioQuantum Chemical Investigation of Carbon-13 NMR Shielding Tensors in Glycine, Alanine, Valine, Isoleucine, Serine, and Threonine: $\Delta$ Comparisons between Helical and Sheet Tensors, and the Effects of $\text{I}^{\text{1}}$ on Shielding $\Delta$ . <i>Journal of the American Chemical Society</i> , 1997, 119, 11951-11958.	13.7	109
28	Activity of Bisphosphonates against <i>Trypanosoma brucei</i> rhodesiense. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 2904-2914.	6.4	101
29	Resistance-resistant antibiotics. <i>Trends in Pharmacological Sciences</i> , 2014, 35, 664-674.	8.7	101
30	Natural-abundance carbon-13 nuclear magnetic resonance studies in 20-mm sample tubes. Numerous single-carbon resonances of hen egg-white lysozyme. <i>Biochemistry</i> , 1973, 12, 1335-1341.	2.5	100
31	An Experimental and Quantum Chemical Investigation of CO Binding to Heme Proteins and Model Systems: $\Delta$ A Unified Model Based on $^{13}\text{C}$ , $^{17}\text{O}$ , and $^{57}\text{Fe}$ Nuclear Magnetic Resonance and $^{57}\text{Fe}$ Mössbauer and Infrared Spectroscopies. <i>Journal of the American Chemical Society</i> , 1998, 120, 4784-4797.	13.7	100
32	Solid-State NMR, Mössbauer, Crystallographic, and Density Functional Theory Investigation of $\text{Fe}^{\text{2}}$ and $\text{Fe}^{\text{3}}$ O <sub>2</sub> Analogue Metalloporphyrins and Metalloproteins $\Delta$ . <i>Journal of the American Chemical Society</i> , 1999, 121, 3829-3844.	13.7	99
33	$^{57}\text{Fe}$ Mössbauer Isomer Shifts of Heme Protein Model Systems: $\Delta$ Electronic Structure Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 7829-7839.	13.7	97
34	Nuclear Magnetic Resonance Shifts in Paramagnetic Metalloporphyrins and Metalloproteins. <i>Journal of the American Chemical Society</i> , 2002, 124, 13911-13920.	13.7	94
35	A Structural Change in Butyrophilin upon Phosphoantigen Binding Underlies Phosphoantigen-Mediated $\text{V}^{\text{39}}$ $\text{V}^{\text{2}}$ $\Delta$ Cell Activation. <i>Immunity</i> , 2019, 50, 1043-1053.e5.	14.3	94
36	Structure of ( <i>i&gt;E&lt;/i&gt;)-4-Hydroxy-3-methyl-but-2-enyl Diphosphate Reductase, the Terminal Enzyme of the Non-Mevalonate Pathway. <i>Journal of the American Chemical Society</i>, 2008, 130, 17206-17207.</i>	13.7	91

#	ARTICLE	IF	CITATIONS
37	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
38	Thermodynamics of Bisphosphonates Binding to Human Bone: A Two-Site Model. <i>Journal of the American Chemical Society</i> , 2009, 131, 8374-8375.	13.7	90
39	Correlation between <sup>15</sup> N NMR chemical shifts in proteins and secondary structure. <i>Journal of Biomolecular NMR</i> , 1994, 4, 341-8.	2.8	89
40	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
41	Solid-State NMR, Crystallographic, and Computational Investigation of Bisphosphonates and Farnesyl Diphosphate Synthase-Bisphosphonate Complexes. <i>Journal of the American Chemical Society</i> , 2006, 128, 14485-14497.	13.7	89
42	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
43	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
44	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
45	<sup>31</sup> 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
46	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
47	The Farnesyl-diphosphate/Geranylgeranyl-diphosphate Synthase of <i>Toxoplasma gondii</i> Is a Bifunctional Enzyme and a Molecular Target of Bisphosphonates. <i>Journal of Biological Chemistry</i> , 2007, 282, 30804-30816.	3.4	82
48	Chemical shifts in proteins: a shielding trajectory analysis of the fluorine nuclear magnetic resonance spectrum of the <i>Escherichia coli</i> 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
49	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
50	Indirect Stimulation of Human $\hat{V}^3\hat{V}^2$ T Cells through Alterations in Isoprenoid Metabolism. <i>Journal of Immunology</i> , 2011, 187, 5099-5113.	0.8	79
51	Predicting Chemical Shifts in Proteins: Structure Refinement of Valine Residues by Using an Initial and Empirical Geometry Optimizations. <i>Journal of the American Chemical Society</i> , 1997, 119, 11941-11950.	13.7	78
52	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
53	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
54	Determination of rotational mobilities of backbone and side-chain carbons of poly( <sup>13</sup> -benzyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td and nuclear Overhauser enhancements. <i>Biochemistry</i> , 1973, 12, 3428-3433.	2.5	75

#	ARTICLE	IF	CITATIONS
55	19F Nuclear Magnetic Resonance Chemical Shifts of Fluorine Containing Aliphatic Amino Acids in Proteins: A Study on Lactobacillus casei Dihydrofolate Reductase Containing (2S,4S)-5-Fluoroleucine. Journal of the American Chemical Society, 1996, 118, 8700-8706.	13.7	74
56	Polyoxometalates Functionalized by Bisphosphonate Ligands: Synthesis, Structural, Magnetic, and Spectroscopic Characterizations and Activity on Tumor Cell Lines. Inorganic Chemistry, 2012, 51, 7921-7931.	4.0	74
57	Inhibition of Geranylgeranyl Diphosphate Synthase by Bisphosphonates: A Crystallographic and Computational Investigation. Journal of Medicinal Chemistry, 2008, 51, 5594-5607.	6.4	73
58	Vacuolar proton pyrophosphatase activity and pyrophosphate (PPi) in Toxoplasma gondii as possible chemotherapeutic targets. Biochemical Journal, 2000, 349, 737-745.	3.7	72
59	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. Journal of the American Chemical Society, 1994, 116, 5307-5314.	13.7	71
60	Iron-57 NMR Chemical Shifts and Mössbauer Quadrupole Splittings in Metalloporphyrins, Ferrocyclochromec, and Myoglobins: A Density Functional Theory Investigation. Journal of Physical Chemistry A, 1998, 102, 2342-2350.	2.5	71
61	Tetra- to Dodecanuclear Oxomolybdate Complexes with Functionalized Bisphosphonate Ligands: Activity in Killing Tumor Cells. Chemistry - A European Journal, 2010, 16, 13741-13748.	3.3	70
62	Chemical shifts in proteins: an ab initio study of carbon-13 nuclear magnetic resonance chemical shielding in glycine, alanine, and valine residues. Journal of the American Chemical Society, 1993, 115, 9768-9773.	13.7	69
63	Predicting Carbon-13 Nuclear Magnetic Resonance Chemical Shielding Tensors in Zwitterionic L-Threonine and L-Tyrosine via Quantum Chemistry. Journal of the American Chemical Society, 1994, 116, 7784-7786.	13.7	67
64	Mechanism of action and inhibition of dehydrosqualene synthase. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21337-21342.	7.1	66
65	Organometallic mechanism of action and inhibition of the 4Fe-4S isoprenoid biosynthesis protein GcpE (IspG). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 11189-11193.	7.1	66
66	Experimental, Hartree-Fock, and Density Functional Theory Investigations of the Charge Density, Dipole Moment, Electrostatic Potential, and Electric Field Gradients in L-Asparagine Monohydrate. Journal of the American Chemical Society, 2000, 122, 4708-4717.	13.7	65
67	Mössbauer Quadrupole Splittings and Electronic Structure in Heme Proteins and Model Systems: A Density Functional Theory Investigation. Journal of the American Chemical Society, 2002, 124, 13921-13930.	13.7	65
68	Density Functional Study of Cobalt-59 Nuclear Magnetic Resonance Chemical Shifts and Shielding Tensor Elements in Co(III) Complexes. Journal of the American Chemical Society, 1997, 119, 8065-8069.	13.7	64
69	Squalene Synthase As a Target for Chagas Disease Therapeutics. PLoS Pathogens, 2014, 10, e1004114.	4.7	64
70	Correlation between the Knight Shift of Chemisorbed CO and the Fermi Level Local Density of States at Clean Platinum Catalyst Surfaces. Journal of the American Chemical Society, 1999, 121, 2996-3003.	13.7	63
71	Lipophilic Pyridinium Bisphosphonates: Potent T Cell Stimulators. Angewandte Chemie - International Edition, 2010, 49, 1136-1138.	13.8	63
72	Chemical Shifts of Carbonyl Carbons in Peptides and Proteins. Journal of the American Chemical Society, 1994, 116, 11485-11488.	13.7	62

#	ARTICLE	IF	CITATIONS
73	Solid-State NMR, Crystallographic and Density Functional Theory Investigation of Fe <sup>2+</sup> CO and Fe <sup>3+</sup> CO Analogue Metalloporphyrins and Metalloproteins. <i>Journal of the American Chemical Society</i> , 1999, 121, 3818-3828.	13.7	61
74	Activity of Nitrogen-Containing and Non-Nitrogen-Containing Bisphosphonates on Tumor Cell Lines. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 5804-5814.	6.4	61
75	Inhibition of the Fe <sub>4</sub> S <sub>4</sub> -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
76	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
77	Phosphonosulfonates Are Potent, Selective Inhibitors of Dehydrosqualene Synthase and Staphyloxanthin Biosynthesis in <i>Staphylococcus aureus</i> . <i>Journal of Medicinal Chemistry</i> , 2009, 52, 976-988.	6.4	59
78	Ab Initio Studies of Amide-15N Chemical Shifts in Dipeptides: Applications to Protein NMR Spectroscopy. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16423-16428.	2.9	58
79	Bisphosphonates as Inhibitors of <i>Trypanosoma cruzi</i> Hexokinase. <i>Journal of Biological Chemistry</i> , 2007, 282, 12377-12387.	3.4	57
80	An Experimental and Theoretical Investigation of the Chemical Shielding Tensors of <sup>13</sup> 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
81	Protein Structure Refinement Using <sup>13</sup> C Chemical Shift Tensors. <i>Journal of the American Chemical Society</i> , 2009, 131, 985-992.	13.7	54
82	<i>Mycobacterium tuberculosis</i> releases an antacid that remodels phagosomes. <i>Nature Chemical Biology</i> , 2019, 15, 889-899.	8.0	53
83	Isoprenoid Biosynthesis as a Drug Target: 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
84	Lipophilic Bisphosphonates Are Potent Inhibitors of <i>Plasmodium</i> Liver-Stage Growth. <i>Antimicrobial Agents and Chemotherapy</i> , 2010, 54, 2987-2993.	3.2	52
85	SQ109, a New Drug Lead for Chagas Disease. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 1950-1961.	3.2	51
86	Computation of Through-Space <sup>19</sup> F- <sup>19</sup> F Scalar Couplings via Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2000, 122, 12164-12168.	13.7	50
87	Bioorganometallic Chemistry with IspG and IspH: Structure, Function, and Inhibition of the [Fe <sub>4</sub> S <sub>4</sub> ] Proteins Involved in Isoprenoid Biosynthesis. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4294-4310.	13.8	50
88	A polymeric approach toward resistance-resistant antimicrobial agent with dual-selective mechanisms of action. <i>Science Advances</i> , 2021, 7, .	10.3	50
89	Photoaffinity Antigens for Human T Cells. <i>Journal of Immunology</i> , 2008, 181, 7738-7750.	0.8	49
90	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

#	ARTICLE	IF	CITATIONS
91	Antibacterial Drug Leads: DNA and Enzyme Multitargeting. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 1215-1227.	6.4	48
92	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
93	A combination therapy for KRAS-driven lung adenocarcinomas using lipophilic bisphosphonates and rapamycin. <i>Science Translational Medicine</i> , 2014, 6, 263ra161.	12.4	47
94	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
95	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
96	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
97	Structure, function and inhibition of ent-kaurene synthase from <i>Bradyrhizobium japonicum</i> . <i>Scientific Reports</i> , 2014, 4, 6214.	3.3	44
98	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
99	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
100	Undecaprenyl Diphosphate Synthase Inhibitors: Antibacterial Drug Leads. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 5693-5701.	6.4	43
101	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
102	Cytochrome P450: An Investigation of the Mössbauer 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
103	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
104	Farnesyl Diphosphate Synthase Inhibitors from <i>In Silico</i> Screening. <i>Chemical Biology and Drug Design</i> , 2013, 81, 742-748.	3.2	42
105	Quantum chemical studies of protein structure. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2005, 360, 1347-1361.	4.0	40
106	Structures of a potent phenylalkyl bisphosphonate inhibitor bound to farnesyl and geranylgeranyl diphosphate synthases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 431-439.	2.6	40
107	NMR chemical shifts and structure refinement in proteins. <i>Journal of Biomolecular NMR</i> , 1993, 3, 607-612.	2.8	38
108	Bisphosphonate Inhibition of a <i>Plasmodium</i> Farnesyl Diphosphate Synthase and a General Method for Predicting Cell-Based Activity from Enzyme Data. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7827-7833.	6.4	38

#	ARTICLE	IF	CITATIONS
109	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
110	Structure and Inhibition of Tuberculosin 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
111	Isoprenoid Biosynthesis Inhibitors Targeting Bacterial Cell Growth. <i>ChemMedChem</i> , 2016, 11, 2205-2215.	3.2	37
112	Theoretical Investigation of <sup>19</sup> F NMR Chemical Shielding Tensors in Fluorobenzenes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8098-8104.	2.5	36
113	<sup>13</sup> C NMR spectroscopy of carbon nanohorns. <i>Physical Review B</i> , 2006, 73, .	3.2	36
114	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
115	Pyridine Inhibitor Binding to the 4Fe-4S Protein A. <i>aeolicus</i> LspH (LytB): A HYSORE Investigation. <i>Journal of the American Chemical Society</i> , 2011, 133, 6525-6528.	13.7	35
116	Chemo-Immunotherapeutic Antimalarials Targeting Isoprenoid Biosynthesis. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 423-427.	2.8	35
117	Discovery of acetylene hydratase activity of the iron-sulphur protein LspH. <i>Nature Communications</i> , 2012, 3, 1042.	12.8	34
118	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
119	An ENDOR and HYSORE Investigation of a Reaction Intermediate in LspG (GcpE) Catalysis. <i>Journal of the American Chemical Society</i> , 2011, 133, 8400-8403.	13.7	33
120	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
121	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
122	Quantitative Structure-Activity Relations for <sup>31</sup> P T Cell Activation by Phosphoantigens. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 4868-4874.	6.4	32
123	Magic-angle spinning <sup>31</sup> P NMR spectroscopy of condensed phosphates in parasitic protozoa: visualizing the invisible. <i>FEBS Letters</i> , 2002, 523, 207-212.	2.8	32
124	Structure and Function of a Head-Middle-Prenyltransferase: Lavandulyl Diphosphate Synthase. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4721-4724.	13.8	32
125	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
126	Structure, function and inhibition of the two- and three-domain 4Fe-4S LspG proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 8558-8563.	7.1	29



#	ARTICLE	IF	CITATIONS
127	Carbon-13 $\alpha$ -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
128	Evaluating $^{19}\text{F}$ 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
129	Bisphosphonate-Generated ATP-Analogs Inhibit Cell Signaling Pathways. <i>Journal of the American Chemical Society</i> , 2018, 140, 7568-7578.	13.7	27
130	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
131	Structures of Fluoro, Amino, and Thiol Inhibitors Bound to the $[\text{Fe}_4\text{S}_4]$ Protein IspH. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2118-2121.	13.8	25
132	$\alpha$ -Head-to-Middle- and $\alpha$ -Head-to-Tail-Prenyl Transferases: Structure of Isosesquilandulyl Diphosphate Synthase. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 683-687.	13.8	24
133	Structural Studies of $^{32}\text{P}$ T Cell Phosphoantigens. <i>Chemistry and Biology</i> , 2006, 13, 985-992.	6.0	23
134	Structure, Function, and Inhibition of <i>Staphylococcus aureus</i> Heptaprenyl Diphosphate Synthase. <i>ChemMedChem</i> , 2016, 11, 1915-1923.	3.2	23
135	SQ109 inhibits proliferation of <i>Leishmania donovani</i> by disruption of intracellular $\text{Ca}^{2+}$ homeostasis, collapsing the mitochondrial electrochemical potential ( $\Delta\psi_m$ ) and affecting acidocalcisomes. <i>Parasitology Research</i> , 2020, 119, 649-657.	1.6	23
136	Bisphosphonate inhibitors of ATP-mediated HIV-1 reverse transcriptase catalyzed excision of chain-terminating 3-azido, 3-deoxythymidine: A QSAR investigation. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 8959-8967.	3.0	22
137	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
138	Structures of Iridoid Synthase from <i>Cantharanthus roseus</i> with Bound $\text{NAD}^+$ , $\text{NADPH}$ , or $\text{NAD}^{10}\text{Oxogeranial}$ : Reaction Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 15478-15482.	13.8	21
139	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
140	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
141	Synthesis of chiral phosphoantigens and their activity in $^{32}\text{P}$ T cell stimulation. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 4471-4477.	2.2	20
142	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
143	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
144	Farnesyl Diphosphate Synthase Inhibitors With Unique Ligand-Binding Geometries. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 349-354.	2.8	20

#	ARTICLE	IF	CITATIONS
145	Bacterial Cell Growth Inhibitors Targeting Undecaprenyl Diphosphate Synthase and Undecaprenyl Diphosphate Phosphatase. <i>ChemMedChem</i> , 2016, 11, 2311-2319.	3.2	20
146	Head-to-Head Prenyl Tranferases: Anti-Infective Drug Targets. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 4367-4372.	6.4	19
147	Moenomycin Biosynthesis: Structure and Mechanism of Action of the Prenyltransferase MoeN5. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4716-4720.	13.8	19
148	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
149	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
150	Dual Dehydroisqualene/Squalene Synthase Inhibitors: Leads for Innate Immune System-Based Therapeutics. <i>ChemMedChem</i> , 2012, 7, 561-564.	3.2	18
151	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
152	Isoprenoid Biosynthesis: Ferraoxetane or Allyl Anion Mechanism for IspH Catalysis?. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6522-6525.	13.8	17
153	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
154	HIV-1 Integrase Inhibitor-Inspired Antibacterials Targeting Isoprenoid Biosynthesis. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 402-406.	2.8	16
155	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
156	COVID-19 and Other Pandemics: How Might They Be Prevented?. <i>ACS Infectious Diseases</i> , 2020, 6, 1563-1566.	3.8	16
157	A Solid State <sup>13</sup> C NMR, Crystallographic, and Quantum Chemical Investigation of Phenylalanine and Tyrosine Residues in Dipeptides and Proteins. <i>Journal of the American Chemical Society</i> , 2007, 129, 7385-7392.	13.7	15
158	Activity of Sulfonium Bisphosphonates on Tumor Cell Lines. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 6067-6079.	6.4	15
159	Structures of Trypanosome Vacuolar Soluble Pyrophosphatases: Antiparasitic Drug Targets. <i>ACS Chemical Biology</i> , 2016, 11, 1362-1371.	3.4	15
160	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
161	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
162	Atomic-Resolution Structures of Discrete Stages on the Reaction Coordinate of the [Fe <sub>4</sub> S <sub>4</sub> ] Enzyme IspG (GcpE). <i>Journal of Molecular Biology</i> , 2015, 427, 2220-2228.	4.2	14

#	ARTICLE	IF	CITATIONS
163	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
164	Chemical Exchange Saturation Transfer (CEST) Agents: Quantum Chemistry and MRI. <i>Chemistry - A European Journal</i> , 2016, 22, 264-271.	3.3	14
165	Structure and Function of Four Classes of the 4Fe-4S Protein, IspH. <i>Biochemistry</i> , 2016, 55, 4119-4129.	2.5	14
166	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
167	<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
168	Combining $\sqrt{39}\sqrt{2}$ T Cells with a Lipophilic Bisphosphonate Efficiently Kills Activated Hepatic Stellate Cells. <i>Frontiers in Immunology</i> , 2017, 8, 1381.	4.8	13
169	Terpene Cyclases and Prenyltransferases: Structures and Mechanisms of Action. <i>ACS Catalysis</i> , 2021, 11, 290-303.	11.2	13
170	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
171	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
172	<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
173	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
174	Spectroscopic and Computational Investigations of Ligand Binding to IspH: Discovery of Non-diphosphate Inhibitors. <i>ChemBioChem</i> , 2017, 18, 914-920.	2.6	10
175	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
176	Structure and Function of a $\alpha$ -Head- $\beta$ -Middle- $\gamma$ -Prenyltransferase: Lavandulyl Diphosphate Synthase. <i>Angewandte Chemie</i> , 2016, 128, 4799-4802.	2.0	9
177	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
178	Dynamic Structure and Inhibition of a Malaria Drug Target: Geranylgeranyl Diphosphate Synthase. <i>Biochemistry</i> , 2016, 55, 5180-5190.	2.5	8
179	Expression of doubly labeled <i>Saccharomyces cerevisiae</i> iso-1 ferricytochrome c and $^1\text{H}$ , $^{13}\text{C}$ and $^{15}\text{N}$ chemical shift assignments by multidimensional NMR. <i>FEBS Letters</i> , 2000, 482, 25-30.	2.8	7
180	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

#	ARTICLE	IF	CITATIONS
181	IspHâ€“RPS1 and IspHâ€“UbiA: â€œRosetta stoneâ€•proteins. <i>Chemical Science</i> , 2015, 6, 6813-6822.	7.4	6
182	Headâ€œtoâ€•Head Prenyl Synthases in Pathogenic Bacteria. <i>ChemBioChem</i> , 2017, 18, 985-991.	2.6	6
183	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
184	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
185	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
186	â€œHeadâ€œtoâ€•Middleâ€•and â€œHeadâ€œtoâ€•Tailâ€•cis â€•Prenyl Transferases: Structure of Isosesquilavandulyl Diphosphate Synthase. <i>Angewandte Chemie</i> , 2018, 130, 691-695.	2.0	5
187	NMR and Quantum Chemistry of Proteins and Model Systems. <i>ACS Symposium Series</i> , 1999, , 40-62.	0.5	4
188	Isoprenoid Biosynthesis: Ferraoxetane or Allyl Anion Mechanism for IspH Catalysis?. <i>Angewandte Chemie</i> , 2013, 125, 6650-6653.	2.0	4
189	Tuberculosis Terpene Targets. <i>Chemistry and Biology</i> , 2015, 22, 437-438.	6.0	4
190	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
191	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
192	Moenomycin Biosynthesis: Structure and Mechanism of Action of the Prenyltransferase MoeN5. <i>Angewandte Chemie</i> , 2016, 128, 4794-4798.	2.0	3
193	Immuno-antibiotics: targeting microbial metabolic pathways sensed by unconventional T cells. <i>Immunotherapy Advances</i> , 2021, 1, .	3.0	3
194	Mycobacterial membrane protein Large 3â€•like<scp>â€•family</scp> 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
195	Electronic Properties at a Metal-Solution Interface as Viewed by Solid-State NMR. <i>ACS Symposium Series</i> , 2001, , 26-39.	0.5	2
196	Titelbild: Structure and Function of a â€œHeadâ€œtoâ€•Middleâ€•Prenyltransferase: Lavandulyl Diphosphate Synthase ( <i>Angew. Chem.</i> 15/2016). <i>Angewandte Chemie</i> , 2016, 128, 4689-4689.	2.0	2
197	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
198	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

#	ARTICLE	IF	CITATIONS
199	Titelbild: Structures of Iridoid Synthase from <i>Cantharanthus roseus</i> with Bound NAD <sup>+</sup> , NADPH, or NAD <sup>+</sup> /10-Oxogeraniol: Reaction Mechanisms (Angew. Chem. 51/2015). <i>Angewandte Chemie</i> , 2015, 127, 15517-15517.	2.0	0
200	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