

# Peter J Tonge

## List of Publications by Citations

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214  
papers

8,007  
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50  
h-index

79  
g-index

231  
ext. papers

8,860  
ext. citations

6  
avg, IF

6.01  
L-index

#	Paper	IF	Citations
214	Drug-target residence time: critical information for lead optimization. <i>Current Opinion in Chemical Biology</i> , <b>2010</b> , 14, 467-74	9.7	325
213	The isoniazid-NAD adduct is a slow, tight-binding inhibitor of InhA, the Mycobacterium tuberculosis enoyl reductase: adduct affinity and drug resistance. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2003</b> , 100, 13881-6	11.5	253
212	Drug discovery using chemical systems biology: repositioning the safe medicine Comtan to treat multi-drug and extensively drug resistant tuberculosis. <i>PLoS Computational Biology</i> , <b>2009</b> , 5, e1000423	5	234
211	Inhibitors of FabI, an enzyme drug target in the bacterial fatty acid biosynthesis pathway. <i>Accounts of Chemical Research</i> , <b>2008</b> , 41, 11-20	24.3	210
210	High affinity InhA inhibitors with activity against drug-resistant strains of Mycobacterium tuberculosis. <i>ACS Chemical Biology</i> , <b>2006</b> , 1, 43-53	4.9	210
209	Inhibition of InhA, the enoyl reductase from Mycobacterium tuberculosis, by triclosan and isoniazid. <i>Biochemistry</i> , <b>2000</b> , 39, 7645-50	3.2	200
208	Structural basis and mechanism of enoyl reductase inhibition by triclosan. <i>Journal of Molecular Biology</i> , <b>1999</b> , 290, 859-65	6.5	179
207	Observation of excited-state proton transfer in green fluorescent protein using ultrafast vibrational spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 2864-5	16.4	174
206	Probing the ground state structure of the green fluorescent protein chromophore using Raman spectroscopy. <i>Biochemistry</i> , <b>2000</b> , 39, 4423-31	3.2	150
205	A machine learning-based method to improve docking scoring functions and its application to drug repurposing. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 408-19	6.1	138
204	A slow, tight binding inhibitor of InhA, the enoyl-acyl carrier protein reductase from Mycobacterium tuberculosis. <i>Journal of Biological Chemistry</i> , <b>2010</b> , 285, 14330-7	5.4	126
203	Novel trisubstituted benzimidazoles, targeting Mtb FtsZ, as a new class of antitubercular agents. <i>Journal of Medicinal Chemistry</i> , <b>2011</b> , 54, 374-81	8.3	125
202	Drug-Target Kinetics in Drug Discovery. <i>ACS Chemical Neuroscience</i> , <b>2018</b> , 9, 29-39	5.7	120
201	Marine natural products from the Turkish sponge <i>Agelas oroides</i> that inhibit the enoyl reductases from <i>Plasmodium falciparum</i> , <i>Mycobacterium tuberculosis</i> and <i>Escherichia coli</i> . <i>Bioorganic and Medicinal Chemistry</i> , <b>2007</b> , 15, 6834-45	3.4	114
200	Roles of tyrosine 158 and lysine 165 in the catalytic mechanism of InhA, the enoyl-ACP reductase from <i>Mycobacterium tuberculosis</i> . <i>Biochemistry</i> , <b>1999</b> , 38, 13623-34	3.2	103
199	An alternate proton acceptor for excited-state proton transfer in green fluorescent protein: rewiring GFP. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 1227-35	16.4	99
198	Ultrafast structural dynamics in BLUF domains: transient infrared spectroscopy of AppA and its mutants. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 15556-64	16.4	99

197	Slow-onset inhibition of the FabI enoyl reductase from <i>Francisella tularensis</i> : residence time and in vivo activity. <i>ACS Chemical Biology</i> , <b>2009</b> , 4, 221-31	4.9	98
196	Targeting FtsZ for antituberculosis drug discovery: noncytotoxic taxanes as novel antituberculosis agents. <i>Journal of Medicinal Chemistry</i> , <b>2006</b> , 49, 463-6	8.3	95
195	Light-driven decarboxylation of wild-type green fluorescent protein. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 6919-26	16.4	95
194	Translating slow-binding inhibition kinetics into cellular and in vivo effects. <i>Nature Chemical Biology</i> , <b>2015</b> , 11, 416-23	11.7	94
193	Isotopic Labeling and Normal-Mode Analysis of a Model Green Fluorescent Protein Chromophore. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 6056-6066	3.4	93
192	Inhibition of the bacterial enoyl reductase FabI by triclosan: a structure-reactivity analysis of FabI inhibition by triclosan analogues. <i>Journal of Medicinal Chemistry</i> , <b>2004</b> , 47, 509-18	8.3	92
191	Ultrafast Excited and Ground-State Dynamics of the Green Fluorescent Protein Chromophore in Solution. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 4587-4598	2.8	91
190	Structure-activity studies of the inhibition of FabI, the enoyl reductase from <i>Escherichia coli</i> , by triclosan: kinetic analysis of mutant Fabs. <i>Biochemistry</i> , <b>2003</b> , 42, 4406-13	3.2	90
189	Structure of acyl carrier protein bound to FabI, the FASII enoyl reductase from <i>Escherichia coli</i> . <i>Journal of Biological Chemistry</i> , <b>2006</b> , 281, 39285-39293	5.4	87
188	Noninvasive Determination of 2-[ <sup>18</sup> F]-Fluoroisonicotinic Acid Hydrazide Pharmacokinetics by Positron Emission Tomography in Mycobacterium tuberculosis-Infected Mice. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2013</b> , 57, 678-678	5.9	78
187	Crystal structure of Mycobacterium tuberculosis MenB, a key enzyme in vitamin K2 biosynthesis. <i>Journal of Biological Chemistry</i> , <b>2003</b> , 278, 42352-60	5.4	75
186	Synthesis and spectroscopic studies of model red fluorescent protein chromophores. <i>Organic Letters</i> , <b>2002</b> , 4, 1523-6	6.2	75
185	Synthesis and SAR studies of 1,4-benzoxazine MenB inhibitors: novel antibacterial agents against Mycobacterium tuberculosis. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2010</b> , 20, 6306-9	2.9	74
184	Proton relay reaction in green fluorescent protein (GFP): Polarization-resolved ultrafast vibrational spectroscopy of isotopically edited GFP. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 22009-18	3.4	69
183	Forces, bond lengths, and reactivity: fundamental insight into the mechanism of enzyme catalysis. <i>Biochemistry</i> , <b>1992</b> , 31, 9122-5	3.2	69
182	<i>Staphylococcus aureus</i> FabI: inhibition, substrate recognition, and potential implications for in vivo essentiality. <i>Structure</i> , <b>2012</b> , 20, 802-13	5.2	68
181	Direct inhibitors of InhA are active against Mycobacterium tuberculosis. <i>Science Translational Medicine</i> , <b>2015</b> , 7, 269ra3	17.5	66
180	Discovery of anti-TB agents that target the cell-division protein FtsZ. <i>Future Medicinal Chemistry</i> , <b>2010</b> , 2, 1305-23	4.1	66

179	Targeting InhA, the FASII enoyl-ACP reductase: SAR studies on novel inhibitor scaffolds. <i>Current Topics in Medicinal Chemistry</i> , <b>2012</b> , 12, 672-93	3	64
178	Synthesis and in vitro antimycobacterial activity of B-ring modified diaryl ether InhA inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2008</b> , 18, 3029-33	2.9	64
177	Ground state isomerization of a model green fluorescent protein chromophore. <i>FEBS Letters</i> , <b>2003</b> , 549, 35-8	3.8	64
176	Mechanism-based inhibitors of MenE, an acyl-CoA synthetase involved in bacterial menaquinone biosynthesis. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2008</b> , 18, 5963-6	2.9	63
175	Role of glutamate 144 and glutamate 164 in the catalytic mechanism of enoyl-CoA hydratase. <i>Biochemistry</i> , <b>1999</b> , 38, 9508-16	3.2	60
174	FtsZ: a novel target for tuberculosis drug discovery. <i>Current Topics in Medicinal Chemistry</i> , <b>2007</b> , 7, 527-43		57
173	Enoyl-coenzyme A hydratase-catalyzed exchange of the alpha-protons of coenzyme A thiol esters: a model for an enolized intermediate in the enzyme-catalyzed elimination?. <i>Biochemistry</i> , <b>1994</b> , 33, 14733-42	3.2	56
172	Mechanism and inhibition of saFabI, the enoyl reductase from <i>Staphylococcus aureus</i> . <i>Biochemistry</i> , <b>2008</b> , 47, 4228-36	3.2	55
171	Structure and mechanism of MbtI, the salicylate synthase from <i>Mycobacterium tuberculosis</i> . <i>Biochemistry</i> , <b>2007</b> , 46, 954-64	3.2	54
170	Radiosynthesis and bioimaging of the tuberculosis chemotherapeutics isoniazid, rifampicin and pyrazinamide in baboons. <i>Journal of Medicinal Chemistry</i> , <b>2010</b> , 53, 2882-91	8.3	53
169	Ultrafast vibrational spectroscopy of the flavin chromophore. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 20107-10	3.4	53
168	Crystal structures of <i>Mycobacterium tuberculosis</i> KasA show mode of action within cell wall biosynthesis and its inhibition by thiolactomycin. <i>Structure</i> , <b>2009</b> , 17, 1004-13	5.2	51
167	Electronic rearrangement induced by substrate analog binding to the enoyl-CoA hydratase active site: evidence for substrate activation. <i>Biochemistry</i> , <b>1994</b> , 33, 12635-43	3.2	51
166	Rational optimization of drug-target residence time: insights from inhibitor binding to the <i>Staphylococcus aureus</i> FabI enzyme-product complex. <i>Biochemistry</i> , <b>2013</b> , 52, 4217-28	3.2	50
165	Excited state dynamics in the green fluorescent protein. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2009</b> , 205, 1-11	4.7	50
164	A structural and energetic model for the slow-onset inhibition of the <i>Mycobacterium tuberculosis</i> enoyl-ACP reductase InhA. <i>ACS Chemical Biology</i> , <b>2014</b> , 9, 986-93	4.9	49
163	Unlocking the Secrets of Enzyme Power Using Raman Spectroscopy. <i>Accounts of Chemical Research</i> , <b>1995</b> , 28, 8-13	24.3	49
162	Targeting fatty acid biosynthesis for the development of novel chemotherapeutics against <i>Mycobacterium tuberculosis</i> : evaluation of A-ring-modified diphenyl ethers as high-affinity InhA inhibitors. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2007</b> , 51, 3562-7	5.9	48

161	H-Bonding in Alcohols Is Reflected in the C-H Bond Strength: Variation of C-D Vibrational Frequency and Fractionation Factor. <i>Journal of the American Chemical Society</i> , <b>2000</b> , 122, 11660-11669	16.4	48
160	Fourier-transform infra-red studies of the alkaline isomerization of mitochondrial cytochrome c and the ionization of carboxylic acids. <i>Biochemical Journal</i> , <b>1989</b> , 258, 599-605	3.8	48
159	Noninvasive determination of 2-[18F]-fluoroisonicotinic acid hydrazide pharmacokinetics by positron emission tomography in Mycobacterium tuberculosis-infected mice. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2012</b> , 56, 6284-90	5.9	47
158	Lysine 190 is the catalytic base in MenF, the menaquinone-specific isochorismate synthase from Escherichia coli: implications for an enzyme family. <i>Biochemistry</i> , <b>2007</b> , 46, 946-53	3.2	47
157	Length of the acyl carbonyl bond in acyl-serine proteases correlates with reactivity. <i>Biochemistry</i> , <b>1990</b> , 29, 10723-7	3.2	45
156	Stable analogues of OSB-AMP: potent inhibitors of MenE, the o-succinylbenzoate-CoA synthetase from bacterial menaquinone biosynthesis. <i>ChemBioChem</i> , <b>2012</b> , 13, 129-36	3.8	44
155	Photoexcitation of the blue light using FAD photoreceptor AppA results in ultrafast changes to the protein matrix. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 16893-900	16.4	43
154	Proteins in action: femtosecond to millisecond structural dynamics of a photoactive flavoprotein. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 16168-74	16.4	42
153	Mechanism of the intramolecular Claisen condensation reaction catalyzed by MenB, a crotonase superfamily member. <i>Biochemistry</i> , <b>2011</b> , 50, 9532-44	3.2	41
152	Raman study of the polarizing forces promoting catalysis in 4-chlorobenzoate-CoA dehalogenase. <i>Biochemistry</i> , <b>1997</b> , 36, 10192-9	3.2	41
151	Evidence for electrophilic catalysis in the 4-chlorobenzoyl-CoA dehalogenase reaction: UV, Raman, and 13C-NMR spectral studies of dehalogenase complexes of benzoyl-CoA adducts. <i>Biochemistry</i> , <b>1995</b> , 34, 13881-8	3.2	41
150	Time-dependent diaryl ether inhibitors of InhA: structure-activity relationship studies of enzyme inhibition, antibacterial activity, and in vivo efficacy. <i>ChemMedChem</i> , <b>2014</b> , 9, 776-91	3.7	40
149	Rational design of broad spectrum antibacterial activity based on a clinically relevant enoyl-acyl carrier protein (ACP) reductase inhibitor. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 15987-6005	5.4	39
148	Positron Emission Tomography Imaging with 2-[F]- p-Aminobenzoic Acid Detects Staphylococcus aureus Infections and Monitors Drug Response. <i>ACS Infectious Diseases</i> , <b>2018</b> , 4, 1635-1644	5.5	38
147	CoA Adducts of 4-Oxo-4-Phenylbut-2-enoates: Inhibitors of MenB from the M. tuberculosis Menaquinone Biosynthesis Pathway. <i>ACS Medicinal Chemistry Letters</i> , <b>2011</b> , 2, 818-823	4.3	38
146	Evaluating the Contribution of Transition-State Destabilization to Changes in the Residence Time of Triazole-Based InhA Inhibitors. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 3417-3429	16.4	37
145	Ultrafast dynamics of protein proton transfer on short hydrogen bond potential energy surfaces: S65T/H148D GFP. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 1452-3	16.4	37
144	Development of modern InhA inhibitors to combat drug resistant strains of Mycobacterium tuberculosis. <i>Current Topics in Medicinal Chemistry</i> , <b>2007</b> , 7, 489-98	3	37

143	Structure of hexadienoyl-CoA bound to enoyl-CoA hydratase determined by transferred nuclear Overhauser effect measurements: mechanistic predictions based on the X-ray structure of 4-(chlorobenzoyl)-CoA dehalogenase. <i>Biochemistry</i> , <b>1997</b> , 36, 2211-20	3.2	36
142	Resonance Raman and Fourier transform infrared spectroscopic studies of the acyl carbonyl group in [3-(5-methyl-2-thienyl)acryloyl]chymotrypsin: evidence for artifacts in the spectra obtained by both techniques. <i>Biochemistry</i> , <b>1991</b> , 30, 4790-5	3.2	36
141	Determination of [ <sup>11</sup> C]rifampin pharmacokinetics within Mycobacterium tuberculosis-infected mice by using dynamic positron emission tomography bioimaging. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2015</b> , 59, 5768-74	5.9	35
140	FTIR studies of hydrogen bonding between $\pi$ -unsaturated esters and alcohols. <i>Journal of Molecular Structure</i> , <b>1996</b> , 379, 135-142	3.4	34
139	Ultrafast infrared spectroscopy of an isotope-labeled photoactivatable flavoprotein. <i>Biochemistry</i> , <b>2011</b> , 50, 1321-8	3.2	33
138	Vibrationally resolved photoabsorption spectroscopy of red fluorescent protein chromophore anions. <i>Physical Review Letters</i> , <b>2003</b> , 90, 118103	7.4	32
137	BLUF domain function does not require a metastable radical intermediate state. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 4605-15	16.4	31
136	A virtual screen discovers novel, fragment-sized inhibitors of Mycobacterium tuberculosis InhA. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 645-59	6.1	30
135	Slow onset inhibition of bacterial beta-ketoacyl-acyl carrier protein synthases by thiolactomycin. <i>Journal of Biological Chemistry</i> , <b>2010</b> , 285, 6161-9	5.4	30
134	Insight through molecular mechanics Poisson-Boltzmann surface area calculations into the binding affinity of triclosan and three analogues for FabI, the E. coli enoyl reductase. <i>Journal of Medicinal Chemistry</i> , <b>2006</b> , 49, 4574-80	8.3	29
133	Critical role of reverse transcriptase in the inhibitory mechanism of CNI-H0294 on HIV-1 nuclear translocation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1996</b> , 93, 11859-64	11.5	29
132	Excited state structure and dynamics of the neutral and anionic flavin radical revealed by ultrafast transient mid-IR to visible spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 5810-8	3.4	28
131	Gas-phase absorption properties of DsRed model chromophores. <i>Physical Chemistry Chemical Physics</i> , <b>2003</b> , 5, 3021-3026	3.6	28
130	Rational Modulation of the Induced-Fit Conformational Change for Slow-Onset Inhibition in Mycobacterium tuberculosis InhA. <i>Biochemistry</i> , <b>2015</b> , 54, 4683-91	3.2	27
129	Thiolactomycin-based $\beta$ -ketoacyl-AcpM synthase A (KasA) inhibitors: fragment-based inhibitor discovery using transient one-dimensional nuclear overhauser effect NMR spectroscopy. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 6045-52	5.4	27
128	Substituted diphenyl ethers as a broad-spectrum platform for the development of chemotherapeutics for the treatment of tularaemia. <i>Journal of Antimicrobial Chemotherapy</i> , <b>2009</b> , 64, 1052-61	5.1	27
127	Stereoselectivity of enoyl-CoA hydratase results from preferential activation of one of two bound substrate conformers. <i>Chemistry and Biology</i> , <b>2002</b> , 9, 1247-55		27
126	Synthesis of crotonyl-oxyCoA: a mechanistic probe of the reaction catalyzed by enoyl-CoA hydratase. <i>Journal of the American Chemical Society</i> , <b>2001</b> , 123, 506-7	16.4	27

125	Asparagine deprivation mediated by Salmonella asparaginase causes suppression of activation-induced T cell metabolic reprogramming. <i>Journal of Leukocyte Biology</i> , <b>2016</b> , 99, 387-98	6.5	26
124	Involvement of glycine 141 in substrate activation by enoyl-CoA hydratase. <i>Biochemistry</i> , <b>2001</b> , 40, 1725-33	3.2	26
123	Direct observation of the titration of substrate carbonyl groups in the active site of alpha-chymotrypsin by resonance Raman spectroscopy. <i>Biochemistry</i> , <b>1989</b> , 28, 6701-9	3.2	26
122	Infrared spectroscopy reveals multi-step multi-timescale photoactivation in the photoconvertible protein archetype dronpa. <i>Nature Chemistry</i> , <b>2018</b> , 10, 845-852	17.6	25
121	Photoactivation of the BLUF Protein PixD Probed by the Site-Specific Incorporation of Fluorotyrosine Residues. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 14638-14648	16.4	25
120	Substrate recognition by E ketoacyl-ACP synthases. <i>Biochemistry</i> , <b>2011</b> , 50, 10678-86	3.2	25
119	Inhibiting enoyl-ACP reductase (FabI) across pathogenic microorganisms by linear sesquiterpene lactones from Anthemis auriculata. <i>Phytomedicine</i> , <b>2008</b> , 15, 1125-9	6.5	25
118	Characterizing septum inhibition in Mycobacterium tuberculosis for novel drug discovery. <i>Tuberculosis</i> , <b>2008</b> , 88, 420-9	2.6	25
117	Mechanism and inhibition of the FabV enoyl-ACP reductase from Burkholderia mallei. <i>Biochemistry</i> , <b>2010</b> , 49, 1281-9	3.2	24
116	Femtosecond to Millisecond Dynamics of Light Induced Allostery in the Avena sativa LOV Domain. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 1010-1019	3.4	23
115	Structural basis for the recognition of mycolic acid precursors by KasA, a condensing enzyme and drug target from Mycobacterium tuberculosis. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 34190-34204	5.4	23
114	Potential of lichen secondary metabolites against Plasmodium liver stage parasites with FAS-II as the potential target. <i>Journal of Natural Products</i> , <b>2013</b> , 76, 1064-70	4.9	23
113	Medium-chain acyl-coenzyme A dehydrogenase bound to a product analogue, hexadienoyl-coenzyme A: effects on reduction potential, pK(a), and polarization. <i>Biochemistry</i> , <b>2000</b> , 39, 13982-92	3.2	23
112	Stereospecificity of the Reaction Catalyzed by Enoyl-CoA Hydratase. <i>Journal of the American Chemical Society</i> , <b>2000</b> , 122, 3987-3994	16.4	23
111	Active site heterogeneity in dimethyl sulfoxide reductase from Rhodobacter capsulatus revealed by Raman spectroscopy. <i>Biochemistry</i> , <b>2001</b> , 40, 440-8	3.2	23
110	Mechanism of MenE inhibition by acyl-adenylate analogues and discovery of novel antibacterial agents. <i>Biochemistry</i> , <b>2015</b> , 54, 6514-6524	3.2	22
109	Structural and functional studies of fatty acyl adenylate ligases from E. coli and L. pneumophila. <i>Journal of Molecular Biology</i> , <b>2011</b> , 406, 313-24	6.5	22
108	Mechanism and inhibition of the FabI enoyl-ACP reductase from Burkholderia pseudomallei. <i>Journal of Antimicrobial Chemotherapy</i> , <b>2011</b> , 66, 564-73	5.1	22

107	Thiolactomycin-Based Inhibitors of Bacterial $\beta$ Ketoacyl-ACP Synthases with in Vivo Activity. <i>Journal of Medicinal Chemistry</i> , <b>2016</b> , 59, 5377-90	8.3	22
106	Complete Proton Transfer Cycle in GFP and Its T203V and S205V Mutants. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 9303-7	16.4	21
105	Localized electron polarization in a substrate analog binding to the active site of enoyl-CoA hydratase: Raman spectroscopic and conformational analyses of rotamers of hexadienoyl thioesters. <i>Biospectroscopy</i> , <b>1995</b> , 1, 387-394		21
104	Ultrafast Structural Dynamics of BlsA, a Photoreceptor from the Pathogenic Bacterium. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 220-224	6.4	20
103	4-Hydroxycinnamoyl-CoA: an ionizable probe of the active site of the medium chain acyl-CoA dehydrogenase. <i>Biochemistry</i> , <b>2000</b> , 39, 92-101	3.2	20
102	Molecular structures of cis- and trans-S-Ethyl thiocrotonate. A combined vibrational spectroscopic and ab initio SCF-MO study. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1994</b> , 90, 3491		20
101	Correlating Drug-Target Kinetics and Pharmacodynamics: Long Residence Time Inhibitors of the FabI Enoyl-ACP Reductase. <i>Chemical Science</i> , <b>2016</b> , 7, 5945-5954	9.4	19
100	An ordered water channel in Staphylococcus aureus FabI: unraveling the mechanism of substrate recognition and reduction. <i>Biochemistry</i> , <b>2015</b> , 54, 1943-55	3.2	18
99	A Methyl 4-Oxo-4-phenylbut-2-enoate with Activity against MRSA that Inhibits MenB in the Bacterial Menaquinone Biosynthesis Pathway. <i>ACS Infectious Diseases</i> , <b>2016</b> , 2, 329-340	5.5	18
98	The Francisella tularensis FabI enoyl-acyl carrier protein reductase gene is essential to bacterial viability and is expressed during infection. <i>Journal of Bacteriology</i> , <b>2013</b> , 195, 351-8	3.5	18
97	Markedly different acyl papain structures deacylate at similar rates: resonance Raman spectroscopic and kinetic evidence. <i>Journal of the American Chemical Society</i> , <b>1991</b> , 113, 4297-4303	16.4	18
96	Discovery of a cofactor-independent inhibitor of InhA. <i>Life Science Alliance</i> , <b>2018</b> , 1, e201800025	5.8	18
95	Mechanism of the AppABLUF Photocycle Probed by Site-Specific Incorporation of Fluorotyrosine Residues: Effect of the Y21 pKa on the Forward and Reverse Ground-State Reactions. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 926-935	16.4	17
94	Protein photochromism observed by ultrafast vibrational spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 11954-9	3.4	17
93	Antitubercular activity of 1,2,3-triazolyl fatty acid derivatives. <i>European Journal of Medicinal Chemistry</i> , <b>2017</b> , 125, 842-852	6.8	17
92	Vibrational assignment of the ultrafast infrared spectrum of the photoactivatable flavoprotein AppA. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 10722-9	3.4	17
91	Ultrafast transient mid IR to visible spectroscopy of fully reduced flavins. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 17642-8	3.6	17
90	Synthesis of 4-phenoxybenzamide adenine dinucleotide as NAD analogue with inhibitory activity against enoyl-ACP reductase (InhA) of Mycobacterium tuberculosis. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2007</b> , 17, 4588-91	2.9	17



89	Time-Resolved Emission Spectra of Green Fluorescent Protein. <i>Photochemistry and Photobiology</i> , <b>2006</b> , 82, 373	3.6	17
88	Variation in LOV Photoreceptor Activation Dynamics Probed by Time-Resolved Infrared Spectroscopy. <i>Biochemistry</i> , <b>2018</b> , 57, 620-630	3.2	16
87	Antibacterial Activity and Mode of Action of a Sulfonamide-Based Class of Oxaborole Leucyl-tRNA-Synthetase Inhibitors. <i>ACS Infectious Diseases</i> , <b>2019</b> , 5, 1231-1238	5.5	15
86	Structure of the Yersinia pestis FabV enoyl-ACP reductase and its interaction with two 2-pyridone inhibitors. <i>Structure</i> , <b>2012</b> , 20, 89-100	5.2	15
85	Ultrafast Electronic and Vibrational Dynamics of Stabilized A State Mutants of the Green Fluorescent Protein (GFP): Snipping the Proton Wire. <i>Chemical Physics</i> , <b>2008</b> , 350, 193-200	2.3	15
84	A quantitative mechanistic PK/PD model directly connects Btk target engagement and efficacy. <i>Chemical Science</i> , <b>2017</b> , 8, 3434-3443	9.4	14
83	Quantifying the Interactions between Biomolecules: Guidelines for Assay Design and Data Analysis. <i>ACS Infectious Diseases</i> , <b>2019</b> , 5, 796-808	5.5	14
82	Elucidation of the protonation states of the catalytic residues in mtKasA: implications for inhibitor design. <i>Biochemistry</i> , <b>2011</b> , 50, 5743-56	3.2	14
81	Fatty Acid Biosynthesis and Oxidation <b>2010</b> , 231-275		14
80	Crystal structure and Raman studies of dsFP483, a cyan fluorescent protein from <i>Discosoma striata</i> . <i>Journal of Molecular Biology</i> , <b>2008</b> , 378, 871-86	6.5	14
79	A novel interaction linking the FAS-II and phthiocerol dimycocerosate (PDIM) biosynthetic pathways. <i>Journal of Biological Chemistry</i> , <b>2008</b> , 283, 31719-25	5.4	14
78	Femtosecond stimulated Raman study of the photoactive flavoprotein AppABLUF. <i>Chemical Physics Letters</i> , <b>2017</b> , 683, 365-369	2.5	13
77	Probing mechanisms of resistance to the tuberculosis drug isoniazid: Conformational changes caused by inhibition of InhA, the enoyl reductase from <i>Mycobacterium tuberculosis</i> . <i>Protein Science</i> , <b>2007</b> , 16, 1617-27	6.3	13
76	A Raman-active competitive inhibitor of OMP decarboxylase. <i>Bioorganic Chemistry</i> , <b>2006</b> , 34, 59-65	5.1	13
75	Effect of mutagenesis on the stereochemistry of enoyl-CoA hydratase. <i>Biochemistry</i> , <b>2002</b> , 41, 12883-90	3.2	13
74	Chemistry of enzyme-substrate complexes revealed by resonance Raman spectroscopy. <i>Chemical Society Reviews</i> , <b>1990</b> , 19, 293-316	58.5	13
73	The biodistribution of 5-[ <sup>18</sup> F]fluoropyrazinamide in <i>Mycobacterium tuberculosis</i> -infected mice determined by positron emission tomography. <i>PLoS ONE</i> , <b>2017</b> , 12, e0170871	3.7	13
72	Pharmacokinetic-pharmacodynamic models that incorporate drug-target binding kinetics. <i>Current Opinion in Chemical Biology</i> , <b>2019</b> , 50, 120-127	9.7	12

71	Substituted diphenyl ethers as a novel chemotherapeutic platform against Burkholderia pseudomallei. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2014</b> , 58, 1646-51	5.9	12
70	The Burkholderia pseudomallei enoyl-acyl carrier protein reductase FabI1 is essential for in vivo growth and is the target of a novel chemotherapeutic with efficacy. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2014</b> , 58, 931-5	5.9	12
69	Unraveling the Mechanism of a LOV Domain Optogenetic Sensor: A Glutamine Lever Induces Unfolding of the J <sub>H</sub> Helix. <i>ACS Chemical Biology</i> , <b>2020</b> , 15, 2752-2765	4.9	12
68	Computer-aided identification, synthesis, and biological evaluation of novel inhibitors for botulinum neurotoxin serotype A. <i>Bioorganic and Medicinal Chemistry</i> , <b>2015</b> , 23, 5489-95	3.4	11
67	Functional dynamics of a single tryptophan residue in a BLUF protein revealed by fluorescence spectroscopy. <i>Scientific Reports</i> , <b>2020</b> , 10, 2061	4.9	11
66	Structure-kinetic relationships that control the residence time of drug-target complexes: insights from molecular structure and dynamics. <i>Current Opinion in Chemical Biology</i> , <b>2018</b> , 44, 101-109	9.7	11
65	Probing hydrogen-bonding interactions in the active site of medium-chain acyl-CoA dehydrogenase using Raman spectroscopy. <i>Biochemistry</i> , <b>2003</b> , 42, 11846-56	3.2	11
64	Structure/function of medium chain acyl-CoA dehydrogenase: the importance of substrate polarization. <i>Archives of Biochemistry and Biophysics</i> , <b>1999</b> , 370, 16-21	4.1	11
63	Site-Specific Protein Dynamics Probed by Ultrafast Infrared Spectroscopy of a Noncanonical Amino Acid. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 9592-9597	3.4	10
62	Evidence from Raman spectroscopy that InhA, the mycobacterial enoyl reductase, modulates the conformation of the NADH cofactor to promote catalysis. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 6425-31	16.4	10
61	Procatalytic ligand strain. Ionization and perturbation of 8-nitroxanthine at the urate oxidase active site. <i>Biochemistry</i> , <b>2005</b> , 44, 11440-6	3.2	10
60	Stereoselective Synthesis, Docking, and Biological Evaluation of Difluoroindanediol-Based MenE Inhibitors as Antibiotics. <i>Organic Letters</i> , <b>2016</b> , 18, 6384-6387	6.2	10
59	Electron transfer quenching in light adapted and mutant forms of the AppA BLUF domain. <i>Faraday Discussions</i> , <b>2015</b> , 177, 293-311	3.6	9
58	Substrate recognition by the human fatty-acid synthase. <i>Journal of Biological Chemistry</i> , <b>2005</b> , 280, 42613-8	3.8	9
57	Stereospecific <sup>1</sup> H and <sup>13</sup> C NMR Assignments of Crotonyl CoA and Hexadienoyl CoA: Conformational Analysis and Comparison with Protein-CoA Complexes. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 9988-9994	16.4	9
56	CNS Anticancer Drug Discovery and Development: 2016 conference insights. <i>CNS Oncology</i> , <b>2017</b> , 6, 167-177	11.7	8
55	Deacylation and reacylation for a series of acyl cysteine proteases, including acyl groups derived from novel chromophoric substrates. <i>Biochemistry</i> , <b>1996</b> , 35, 12487-94	3.2	8
54	A [(32)P]NAD(+)-based method to identify and quantitate long residence time enoyl-acyl carrier protein reductase inhibitors. <i>Analytical Biochemistry</i> , <b>2015</b> , 474, 40-9	3.1	7

53	A quick method for purifying bile salt-activated lipases. <i>Biotechnology Letters</i> , <b>1996</b> , 10, 523		7
52	Characterization of trans- and cis-5-methylthienylacryloyl chymotrypsin using Raman difference spectroscopy, NMR, and kinetics: carbonyl environment and reactivity. <i>Journal of the American Chemical Society</i> , <b>1993</b> , 115, 8757-8762	16.4	7
51	Vibrational spectroscopy of flavoproteins. <i>Methods in Enzymology</i> , <b>2019</b> , 620, 189-214	1.7	6
50	Diacyltransferase Activity and Chain Length Specificity of Mycobacterium tuberculosis PapA5 in the Synthesis of Alkyl Diol Lipids. <i>Biochemistry</i> , <b>2015</b> , 54, 5457-68	3.2	6
49	Correlating Drug-Target Residence Time and Post-antibiotic Effect: Insight into Target Vulnerability. <i>ACS Infectious Diseases</i> , <b>2020</b> , 6, 629-636	5.5	6
48	Structural Basis for the Regulation of Biofilm Formation and Iron Uptake in by the Blue-Light-Using Photoreceptor, BIsA. <i>ACS Infectious Diseases</i> , <b>2020</b> , 6, 2592-2603	5.5	6
47	Rationalizing the Binding Kinetics for the Inhibition of the Burkholderia pseudomallei FabI1 Enoyl-ACP Reductase. <i>Biochemistry</i> , <b>2017</b> , 56, 1865-1878	3.2	5
46	Radiosynthesis and biological evaluation of a novel enoyl-ACP reductase inhibitor for Staphylococcus aureus. <i>European Journal of Medicinal Chemistry</i> , <b>2014</b> , 88, 66-73	6.8	5
45	Rotational Isomerism in CH <sub>3</sub> CH <sub>2</sub> C(:S)SR (R = CH <sub>3</sub> , CH <sub>2</sub> CH <sub>3</sub> ): a Combined Vibrational Spectroscopic and ab Initio Study. <i>The Journal of Physical Chemistry</i> , <b>1994</b> , 98, 3592-3600		5
44	Resonance Raman and absorption spectroscopic characterization of the chemically engineered enzyme thiolsubtilisin; comparison with a natural thiolenzyme. <i>Journal of Molecular Liquids</i> , <b>1989</b> , 42, 195-212	6	5
43	Striking changes observed in key acyl-enzyme linkages by resonance Raman experiments near 77 K. <i>Journal of the American Chemical Society</i> , <b>1989</b> , 111, 1496-1497	16.4	5
42	Positron Emission Tomography Imaging of Infection Using a Nitro-Prodrug Analogue of 2-[F]-Aminobenzoic Acid. <i>ACS Infectious Diseases</i> , <b>2020</b> , 6, 2249-2259	5.5	5
41	Excited State Vibrations of Isotopically Labeled FMN Free and Bound to a Light-Oxygen-Voltage (LOV) Protein. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 7152-7165	3.4	5
40	Excited State Resonance Raman of Flavin Mononucleotide: Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 6171-6179	2.8	5
39	Selectivity of Pyridone- and Diphenyl Ether-Based Inhibitors for the Yersinia pestis FabV Enoyl-ACP Reductase. <i>Biochemistry</i> , <b>2016</b> , 55, 2992-3006	3.2	5
38	Radiolabelling and positron emission tomography of PT70, a time-dependent inhibitor of InhA, the Mycobacterium tuberculosis enoyl-ACP reductase. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2015</b> , 25, 4782-4786	2.9	4
37	Ultrafast proton transfer in the green fluorescent protein: Analysing the instantaneous emission at product state wavelengths. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2012</b> , 234, 21-26	4.7	4
36	Personalized Combined Organic Spectroscopy Problems Online and in the Lab. <i>Journal of Chemical Education</i> , <b>2001</b> , 78, 1208	2.4	4

35	Formulation studies of InhA inhibitors and combination therapy to improve efficacy against Mycobacterium tuberculosis. <i>Tuberculosis</i> , <b>2016</b> , 101, 8-14	2.6	4
34	Identification of the vibrational marker of tyrosine cation radical using ultrafast transient infrared spectroscopy of flavoprotein systems. <i>Photochemical and Photobiological Sciences</i> , <b>2021</b> , 20, 369-378	4.2	4
33	Structure-Based Design, Synthesis, and Biological Evaluation of Non-Acyl Sulfamate Inhibitors of the Adenylate-Forming Enzyme MenE. <i>Biochemistry</i> , <b>2019</b> , 58, 1918-1930	3.2	3
32	Complete Proton Transfer Cycle in GFP and Its T203V and S205V Mutants. <i>Angewandte Chemie</i> , <b>2015</b> , 127, 9435-9439	3.6	3
31	Molecular structure of S-ethylthioacrylate Combined vibrational spectroscopic and abinitioSCF-MO study. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1997</b> , 93, 3619-3624		3
30	Observation of carbonyl stretch vibrations in acyl-chymotrypsins by using Fourier transform infrared spectroscopy. <i>Biochemical Society Transactions</i> , <b>1985</b> , 13, 929-930	5.1	3
29	The Catalytic Mechanism of MenB, the 1,4-Dihydroxynaphthoyl-CoA Synthase from Mycobacterium Tuberculosis. <i>FASEB Journal</i> , <b>2006</b> , 20, A41	0.9	3
28	Exploring the chemical space of 1,2,3-triazolyl triclosan analogs for discovery of new antileishmanial chemotherapeutic agents. <i>RSC Medicinal Chemistry</i> , <b>2021</b> , 12, 120-128	3.5	3
27	Ring current effects in the active site of medium-chain Acyl-CoA dehydrogenase revealed by NMR spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 8424-32	16.4	2
26	Rotational isomerism in CH <sub>3</sub> C(S)SCH <sub>3</sub> and CH <sub>3</sub> C(S)SCH <sub>2</sub> CH <sub>3</sub> : a combined vibrational spectroscopic and ab initio study. <i>Journal of Molecular Structure</i> , <b>1994</b> , 323, 59-69	3.4	2
25	Rotational isomers of N-( $\beta$ -phenylpropionyl)alanine ethyl dithioester: a Raman spectroscopic and MO study. <i>Journal of Molecular Structure</i> , <b>1994</b> , 324, 113-122	3.4	2
24	Synthesis of chromophoric dipeptides as substrates for papain. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>1995</b> , 5, 2381-2384	2.9	2
23	Multiple forms of thioacetyl coenzyme A binding to citrate synthase. Resonance Raman evidence. <i>Journal of the American Chemical Society</i> , <b>1992</b> , 114, 8738-8739	16.4	2
22	Ultraviolet resonance Raman spectroscopy of a highly specific acyl-papain. <i>Biochemical Society Transactions</i> , <b>1985</b> , 13, 930-931	5.1	2
21	Pharmacokinetic and Pharmacodynamics Relationships <b>2017</b> , 195-207		2
20	CHAPTER 4:Narrow Spectrum Antibacterial Agents. <i>RSC Drug Discovery Series</i> ,76-102	0.6	2
19	Impact of Target Turnover on the Translation of Drug-Target Residence Time to Time-Dependent Antibacterial Activity. <i>ACS Infectious Diseases</i> , <b>2021</b> , 7, 2755-2763	5.5	2
18	Ultrafast excited and ground-state isomerization dynamics of the Green Fluorescent Protein chromophore in solution. <i>Springer Series in Chemical Physics</i> , <b>2005</b> , 610-612	0.3	1

17	Ultrafast Protein Dynamics Probed by Site Specific Transient IR Spectroscopy <b>2020</b> ,		1
16	N/C Terminal Relocation, Truncation, and Native Chemical Ligation; Accessing the Chromophore of Green Fluorescent Protein. <i>FASEB Journal</i> , <b>2006</b> , 20, A965	0.9	1
15	A Long Residence Time Enoyl-Reductase Inhibitor Explores an Extended Binding Region with Isoenzyme-Dependent Tautomer Adaptation and Differential Substrate-Binding Loop Closure. <i>ACS Infectious Diseases</i> , <b>2021</b> , 7, 746-758	5.5	0
14	The Kinetics and Thermodynamics of Staphylococcus aureus FabI Inhibition. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2015</b> , 295-311	0.4	
13	Transient IR study of Blue Light Sensing Proteins. <i>EPJ Web of Conferences</i> , <b>2013</b> , 41, 07009	0.3	
12	FACILE CHARACTERIZATION OF THE SPECTRA OF cis AND trans PHOTOISOMERS IN A MIXTURE OF ACYL-ENZYMES BY RAMAN DIFFERENCE SPECTROSCOPY. <i>Photochemistry and Photobiology</i> , <b>1994</b> , 60, 432-434	3.6	
11	Resonance Raman spectroscopic and kinetic consequences of a nitrogen ... sulphur enzyme-substrate contact in a series of dithioacylpapains. <i>Biophysical Journal</i> , <b>1992</b> , 63, 191-6	2.9	
10	Comparative Structural and Biochemical Studies of Chorismate Binding Enzymes, MenF, EntC and MbtI. <i>FASEB Journal</i> , <b>2006</b> , 20, A463	0.9	
9	Ultrafast Photoreactions in the Green Fluorescent Protein Studied Through Time Resolved Vibrational Spectroscopy. <i>Springer Series in Chemical Physics</i> , <b>2007</b> , 468-470	0.3	
8	The Kinetic Studies of saFabI, the Enoyl ACP Reductase From Staphylococcus aureus. <i>FASEB Journal</i> , <b>2007</b> , 21, A999	0.9	
7	Targeting the Enoyl-Reductase Enzyme (FabI): Modern Drug Discovery Effects to Combat Tularemia. <i>FASEB Journal</i> , <b>2008</b> , 22, 791.6	0.9	
6	Investigation of Menaquinone Biosynthesis in Mycobacterium Tuberculosis: Catalytic Mechanism and Inhibition Studies of MenB. <i>FASEB Journal</i> , <b>2008</b> , 22, 611.15	0.9	
5	Ultrafast Vibrational Dynamics in the AppA Blue Light Sensing Protein. <i>Springer Series in Chemical Physics</i> , <b>2009</b> , 538-540	0.3	
4	Mechanism and Inhibition of the Dihydroxynaphthoyl-CoA Synthase MenB from Mycobacterium Tuberculosis. <i>FASEB Journal</i> , <b>2010</b> , 24, 463.11	0.9	
3	Imaging the Distribution of Carbon-11 Labeled Rifampicin, Isoniazid and Pyrazinamide in Baboons using PET. <i>FASEB Journal</i> , <b>2010</b> , 24, 907.7	0.9	
2	Residence Time and in vivo Antibacterial Activity - A Critical Aspect of Lead Compound Optimization. <i>FASEB Journal</i> , <b>2010</b> , 24, 680.3	0.9	
1	Slow Onset Inhibitors of Bacterial Fatty Acid Biosynthesis: Residence Time, In Vivo Activity and In Vivo Imaging. <i>FASEB Journal</i> , <b>2010</b> , 24, 71.3	0.9	