David I Roper

List of Publications by Year in descending order

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#	Article	lF	CITATIONS
1	Bacterial cell wall assembly: still an attractive antibacterial target. Trends in Biotechnology, 2011, 29, 167-173.	9.3	230
2	Enzymatic Ketonization of 2-Hydroxymuconate: Specificity and Mechanism Investigated by the Crystal Structures of Two Isomerasesâ€. Biochemistry, 1996, 35, 792-802.	2.5	148
3	Vancomycin resistance in enterococci: reprogramming of the d-Ala–d-Ala ligases in bacterial peptidoglycan biosynthesis. Chemistry and Biology, 2000, 7, R109-R119.	6.0	127
4	Phospho-MurNAc-Pentapeptide Translocase (MraY) as a Target for Antibacterial Agents and Antibacterial Proteins. Infectious Disorders - Drug Targets, 2006, 6, 85-106.	0.8	119
5	Asymmetric triplex metallohelices with high and selective activity against cancer cells. Nature Chemistry, 2014, 6, 797-803.	13.6	115
6	Understanding the mechanism of ice binding by type III antifreeze proteins. Journal of Molecular Biology, 2001, 305, 875-889.	4.2	113
7	CO2 directly modulates connexin 26 by formation of carbamate bridges between subunits. ELife, 2013, 2, e01213.	6.0	103
8	Mechanisms of Incorporation for <scp>D</scp> -Amino Acid Probes That Target Peptidoglycan Biosynthesis. ACS Chemical Biology, 2019, 14, 2745-2756.	3.4	101
9	Crystal Structure of Penicillin Binding Protein 4 (dacB) fromEscherichia coli, both in the Native Form and Covalently Linked to Various Antibioticsâ€. Biochemistry, 2006, 45, 783-792.	2.5	84
10	FtsZ Polymer-bundling by the Escherichia coli ZapA Orthologue, YgfE, Involves a Conformational Change in Bound GTP. Journal of Molecular Biology, 2007, 369, 210-221.	4.2	83
11	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
12	<i>In vitro</i> Reconstitution of Peptidoglycan Assembly from the Gram-Positive Pathogen <i>Streptococcus pneumoniae</i> . ACS Chemical Biology, 2013, 8, 2688-2696.	3.4	74
13	The Escherichia coli C homoprotocatechuate degradative operon: hpc gene order, direction of transcription and control of expression. Molecular Genetics and Genomics, 1993, 237-237, 241-250.	2.4	72
14	IFN-Î ³ Enhances Production of Nitric Oxide from Macrophages via a Mechanism That Depends on Nucleotide Oligomerization Domain-2. Journal of Immunology, 2006, 176, 4804-4810.	0.8	72
15	Nod1 Signaling Overcomes Resistance of S. pneumoniae to Opsonophagocytic Killing. PLoS Pathogens, 2007, 3, e118.	4.7	72
16	The physico-chemical characterization of a boiling stable antifreeze protein from a perennial grass (Lolium perenne). Archives of Biochemistry and Biophysics, 2003, 410, 238-245.	3.0	70
17	Characterization of tRNA-dependent Peptide Bond Formation by MurM in the Synthesis of Streptococcus pneumoniae Peptidoglycan. Journal of Biological Chemistry, 2008, 283, 6402-6417.	3.4	70
18	The molecular basis of vancomycin resistance in clinically relevant Enterococci: Crystal structure of D-alanyl-D-lactate ligase (VanA). Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 8921-8925.	7.1	63

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19	Analysis of SMALP co-extracted phospholipids shows distinct membrane environments for three classes of bacterial membrane protein. Scientific Reports, 2019, 9, 1813.	3.3	61
20	Inhibition of D-Ala:D-Ala ligase through a phosphorylated form of the antibiotic D-cycloserine. Nature Communications, 2017, 8, 1939.	12.8	59
21	Structure/Function Studies on a S-Adenosyl-I-methionine-dependent Uroporphyrinogen III C Methyltransferase (SUMT), a Key Regulatory Enzyme of Tetrapyrrole Biosynthesis. Journal of Molecular Biology, 2004, 344, 419-433.	4.2	56
22	Subcloning and nucleotide sequence of the 3,4-dihydroxyphenylacetate (homoprotocatechuate) 2,3-dioxygenase gene fromEscherichia coliC. FEBS Letters, 1990, 275, 53-57.	2.8	53
23	Surfactant-free purification of membrane protein complexes from bacteria: application to the staphylococcal penicillin-binding protein complex PBP2/PBP2a. Nanotechnology, 2014, 25, 285101.	2.6	53
24	Anticancer metallohelices: nanomolar potency and high selectivity. Chemical Science, 2016, 7, 951-958.	7.4	53
25	Crystal Structures of Penicillin-Binding Protein 3 (PBP3) from Methicillin-Resistant Staphylococcus aureus in the Apo and Cefotaximeâ€Bound Forms. Journal of Molecular Biology, 2012, 423, 351-364.	4.2	48
26	Sansanmycin natural product analogues as potent and selective anti-mycobacterials that inhibit lipid I biosynthesis. Nature Communications, 2017, 8, 14414.	12.8	43
27	Design and synthesis of new hydroxyethylamines as inhibitors of d-alanyl-d-lactate ligase (VanA) and d-alanyl-d-alanine ligase (DdlB). Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1376-1379.	2.2	41
28	A De Novo Designed Inhibitor ofD-Ala-D-Ala Ligase fromE. coli. Angewandte Chemie - International Edition, 2005, 44, 6403-6406.	13.8	40
29	Crystal Structure and Functional Assignment of YfaU, a Metal Ion Dependent Class II Aldolase from <i>Escherichia coli</i> K12. Biochemistry, 2008, 47, 9955-9965.	2.5	38
30	Structural Characterisation of the Insecticidal Toxin XptA1, Reveals a 1.15ÂMDa Tetramer with a Cage-like Structure. Journal of Molecular Biology, 2007, 366, 1558-1568.	4.2	37
31	Expression, purification and characterisation of soluble ClfT and the identification of a novel galactofuranosyltransferase Rv3782 involved in priming ClfT-mediated galactan polymerisation in Mycobacterium tuberculosis. Protein Expression and Purification, 2008, 58, 332-341.	1.3	37
32	Tetramerization of ZapA is required for FtsZ bundling. Biochemical Journal, 2013, 449, 795-802.	3.7	37
33	Mutational Analysis of the Substrate Specificity of <i>Escherichia coli</i> Penicillin Binding Protein 4. Biochemistry, 2009, 48, 2675-2683.	2.5	35
34	Core Steps of Membrane-Bound Peptidoglycan Biosynthesis: Recent Advances, Insight and Opportunities. Antibiotics, 2015, 4, 495-520.	3.7	35
35	In vitro characterization of the antivirulence target of Gram-positive pathogens, peptidoglycan O-acetyltransferase A (OatA). PLoS Pathogens, 2017, 13, e1006667.	4.7	35
36	Mutations in the DNA Mismatch Repair Proteins MutS and MutL of Oxazolidinone-Resistant or -Susceptible Enterococcus faecium. Antimicrobial Agents and Chemotherapy, 2003, 47, 3061-3066.	3.2	34

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37	Carbohydrate scaffolds as glycosyltransferase inhibitors with in vivo antibacterial activity. Nature Communications, 2015, 6, 7719.	12.8	34
38	Specificity Determinants for Lysine Incorporation in Staphylococcus aureus Peptidoglycan as Revealed by the Structure of a MurE Enzyme Ternary Complex. Journal of Biological Chemistry, 2013, 288, 33439-33448.	3.4	33
39	The N-Terminal Domain of Human Topoisomerase Ilα Is a DNA-Dependent ATPase. Biochemistry, 1998, 37, 16997-17004.	2.5	32
40	Circular Dichroism Spectroscopy for the Study of Protein–Ligand Interactions. , 2005, 305, 343-364.		32
41	Fluorescent reagents for in vitro studies of lipid-linked steps of bacterial peptidoglycan biosynthesis: derivatives of UDPMurNAc-pentapeptide containing d-cysteine at position 4 or 5. Molecular BioSystems, 2006, 2, 484.	2.9	32
42	Insights into bacterial cell division from a structure of EnvC bound to the FtsX periplasmic domain. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 28355-28365.	7.1	32
43	Allosteric Activation in Bacillus stearothermophilus Lactate Dehydrogenase Investigated by an X-ray Crystallographic Analysis of a Mutant Designed to Prevent Tetramerization of the Enzyme. Journal of Molecular Biology, 1994, 238, 615-625.	4.2	29
44	The Mechanics of FtsZ Fibers. Biophysical Journal, 2012, 102, 731-738.	0.5	29
45	Structure and Mechanism of HpcH: A Metal Ion Dependent Class II Aldolase from the Homoprotocatechuate Degradation Pathway of Escherichia coli. Journal of Molecular Biology, 2007, 373, 866-876.	4.2	28
46	The Extracellular Domain of Two-component System Sensor Kinase VanS from Streptomyces coelicolor Binds Vancomycin at a Newly Identified Binding Site. Scientific Reports, 2020, 10, 5727.	3.3	27
47	The Crystal Structure of HpcE, a Bifunctional Decarboxylase/Isomerase with a Multifunctional Fold. Biochemistry, 2002, 41, 2982-2989.	2.5	26
48	Crystal Structures of Penicillin-Binding Proteins 4 and 5 from Haemophilus influenzae. Journal of Molecular Biology, 2010, 396, 634-645.	4.2	26
49	Identification of a Novel Inhibition Site in Translocase MraY Based upon the Site of Interaction with Lysis Protein E from Bacteriophage ϕX174. ChemBioChem, 2014, 15, 1300-1308.	2.6	26
50	Prospects for novel inhibitors of peptidoglycan transglycosylases. Bioorganic Chemistry, 2014, 55, 16-26.	4.1	26
51	Pseudomonas aeruginosa MurE amide ligase: enzyme kinetics and peptide inhibitor. Biochemical Journal, 2009, 421, 263-272.	3.7	25
52	Structure of dual BON-domain protein DolP identifies phospholipid binding as a new mechanism for protein localisation. ELife, 2020, 9, .	6.0	25
53	Structural basis of lipopolysaccharide maturation by the O-antigen ligase. Nature, 2022, 604, 371-376.	27.8	25
54	Sequence of the hpcC and hpcG genes of the meta-fission homoprotocatechuic acid pathway of Escherichia coli C: nearly 40% amino-acid identity with the analogous enzymes of the catechol pathway. Gene, 1995, 156, 47-51.	2.2	23

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55	Refinement ofHaemophilus influenzaediaminopimelic acid epimerase (DapF) at 1.75â€Ã resolution suggests a mechanism for stereocontrol during catalysis. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 397-400.	2.5	23
56	The pH Dependence of Polymerization and Bundling by the Essential Bacterial Cytoskeltal Protein FtsZ. PLoS ONE, 2011, 6, e19369.	2.5	23
57	Active membrane transport and receptor proteins from bacteria. Biochemical Society Transactions, 2005, 33, 867-872.	3.4	22
58	Full-length structure of the major autolysin LytA. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1373-1381.	2.5	22
59	Metallohelices that kill Gram-negative pathogens using intracellular antimicrobial peptide pathways. Chemical Science, 2019, 10, 9708-9720.	7.4	22
60	SMA-PAGE: A new method to examine complexes of membrane proteins using SMALP nano-encapsulation and native gel electrophoresis. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1437-1445.	2.6	22
61	The Pneumococcal Divisome: Dynamic Control of Streptococcus pneumoniae Cell Division. Frontiers in Microbiology, 2021, 12, 737396.	3.5	22
62	Purification, nucleotide sequence and some properties of a bifunctional isomerase/decarboxylase from the homoprotocatechuate degradative pathway of Escherichia coli C. FEBS Journal, 1993, 217, 575-580.	0.2	21
63	Structure of the diaminopimelate epimerase DapF fromMycobacterium tuberculosis. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 383-387.	2.5	21
64	Substrate and Stereochemical Control of Peptidoglycan Cross-Linking by Transpeptidation by Escherichia coliPBP1B. Journal of the American Chemical Society, 2020, 142, 5034-5048.	13.7	21
65	Preliminary crystallographic analysis of 4-oxalocrotonate tautomerase reveals the oligomeric structure of the enzyme. Journal of Molecular Biology, 1994, 243, 799-801.	4.2	17
66	Structure and Mechanism of HpcG, a Hydratase in the Homoprotocatechuate Degradation Pathway of Escherichia coli. Journal of Molecular Biology, 2007, 370, 899-911.	4.2	17
67	Nano-encapsulated Escherichia coli Divisome Anchor ZipA, and in Complex with FtsZ. Scientific Reports, 2019, 9, 18712.	3.3	16
68	Purification, some properties and nucleotide sequence of 5-carboxymethyl-2-hydroxymuconate isomerase ofEscherichia coliC. FEBS Letters, 1990, 266, 63-66.	2.8	15
69	Adenosine phosphonate inhibitors of lipid II: Alanyl tRNA ligase MurM from Streptococcus pneumoniae. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4654-4656.	2.2	15
70	Synthesis and in vitro enzyme activity of an oxa analogue of azi-DAP. Journal of the Chemical Society, Perkin Transactions 1, 2002, , 1029-1035.	1.3	14
71	Kinetic Characterization of Lipid II-Ala:Alanyl-tRNA Ligase (MurN) from Streptococcus pneumoniae using Semisynthetic Aminoacyl-lipid II Substrates. Journal of Biological Chemistry, 2008, 283, 34571-34579.	3.4	14
72	Substitutions in PBP2b from β-Lactam-resistant Streptococcus pneumoniae Have Different Effects on Enzymatic Activity and Drug Reactivity. Journal of Biological Chemistry, 2017, 292, 2854-2865.	3.4	14

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73	Inhibition of tRNA-dependent ligase MurM from Streptococcus pneumoniae by phosphonate and sulfonamide inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 3443-3455.	3.0	13
74	Diaryltriazenes as antibacterial agents against methicillin resistant Staphylococcus aureus (MRSA) and Mycobacterium smegmatis. European Journal of Medicinal Chemistry, 2017, 127, 223-234.	5.5	13
75	A Dynamic Network of Proteins Facilitate Cell Envelope Biogenesis in Gram-Negative Bacteria. International Journal of Molecular Sciences, 2021, 22, 12831.	4.1	13
76	A model of membrane contraction predicting initiation and completion of bacterial cell division. Integrative Biology (United Kingdom), 2013, 5, 778.	1.3	11
77	Adenosine Tetraphosphoadenosine Drives a Continuous ATP-Release Assay for Aminoacyl-tRNA Synthetases and Other Adenylate-Forming Enzymes. ACS Chemical Biology, 2013, 8, 2157-2163.	3.4	10
78	Reconstruction of diaminopimelic acid biosynthesis allows characterisation of Mycobacterium tuberculosis N-succinyl-L,L-diaminopimelic acid desuccinylase. Scientific Reports, 2016, 6, 23191.	3.3	10
79	In silico identification, synthesis and biological evaluation of novel tetrazole inhibitors of MurB. Chemical Biology and Drug Design, 2018, 91, 1101-1112.	3.2	10
80	Solution Structure and Interactions of theEscherichiacoliCell Division Activator Protein CedAâ€,‡. Biochemistry, 2005, 44, 6738-6744.	2.5	8
81	Crystallization and preliminary X-ray analysis of a <scp>D</scp> -alanyl- <scp>D</scp> -alanine ligase (EcDdlB) from <i>Escherichia coli</i> . Acta Crystallographica Section F: Structural Biology Communications, 2010, 66, 405-408.	0.7	8
82	Structural and mechanistic studies of theorf12gene product from the clavulanic acid biosynthesis pathway. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1567-1579.	2.5	8
83	The role of the jaw subdomain of peptidoglycan glycosyltransferases for lipid II polymerization. Cell Surface, 2018, 2, 54-66.	3.0	8
84	A molecular link between cell wall biosynthesis, translation fidelity, and stringent response in <i>Streptococcus pneumoniae</i> . Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	8
85	Synthetic Sansanmycin Analogues as Potent <i>Mycobacterium tuberculosis</i> Translocase I Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 17326-17345.	6.4	8
86	Indistinguishability and identifiability of kinetic models for the MurC reaction in peptidoglycan biosynthesis. Computer Methods and Programs in Biomedicine, 2011, 104, 70-80.	4.7	7
87	Beyond the Discovery Void: New Targets for Antibacterial Compounds. Science Progress, 2016, 99, 153-182.	1.9	7
88	Structure-based modeling and dynamics of MurM, a Streptococcus pneumoniae penicillin resistance determinant present at the cytoplasmic membrane. Structure, 2021, 29, 731-742.e6.	3.3	7
89	Expression, purification, crystallization and preliminary characterization of uridine 5′-diphospho-N-acetylmuramoylL-alanyl-D-glutamate:lysine ligase (MurE) fromStreptococcus pneumoniae110K/70. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 359-361.	2.5	6
90	Expression, purification and preliminary crystallographic analysis of 2,4-dihydroxy-hepta-2-ene-1,7-dioate aldolase (HpcH) fromEscherichia coliC. Acta Crystallographica Section F: Structural Biology Communications, 2005, 61, 821-824.	0.7	6

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91	Use of a codon alteration strategy in a novel approach to cloning theMycobacterium tuberculosisdiaminopimelic acid epimerase. FEMS Microbiology Letters, 2006, 262, 39-47.	1.8	6
92	Bacterial Cell Division: Experimental and Theoretical Approaches to the Divisome. Science Progress, 2015, 98, 313-345.	1.9	6
93	Biological Insights from a Simulation Model of the Critical FtsZ Accumulation Required for Prokaryotic Cell Division. Biochemistry, 2015, 54, 3803-3813.	2.5	6
94	The crystal structure and oligomeric form of Escherichia coli l , d -carboxypeptidase A. Biochemical and Biophysical Research Communications, 2018, 499, 594-599.	2.1	6
95	Plant peptidoglycan precursor biosynthesis: Conservation between moss chloroplasts and Gram-negative bacteria. Plant Physiology, 2022, 190, 165-179.	4.8	6
96	The structural consequences of exchanging tryptophan and tyrosine residues in B.stearothermophilus lactate dehydrogenase. Protein Engineering, Design and Selection, 1992, 5, 611-615.	2.1	5
97	Crystallization and preliminary X-ray characterization of VanA from Enterococcus faecium BM4147: towards the molecular basis of bacterial resistance to the glycopeptide antibiotic vancomycin. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1481-1483.	2.5	5
98	Structure-Guided Enhancement of Selectivity of Chemical Probe Inhibitors Targeting Bacterial Seryl-tRNA Synthetase. Journal of Medicinal Chemistry, 2019, 62, 9703-9717.	6.4	5
99	Preliminary crystallographic analysis of 5-carboxymethyl-2-hydroxymuconate isomerase from Escherichia coli. Journal of Molecular Biology, 1989, 210, 881-882.	4.2	4
100	Crystallization and preliminary X-ray analysis of a bifunctional enzyme: HHDD isomerase/OPET decarboxylase fromEscherichia coli. Acta Crystallographica Section D: Biological Crystallography, 1996, 52, 1036-1038.	2.5	4
101	Expression, purification, crystallization and preliminary characterization of an HHED aldolase homologue fromEscherichia coliK12. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 2191-2193.	2.5	3
102	Crystallization and preliminary X-ray analysis of a UDP-MurNAc-tripeptide <scp>D</scp> -alanyl- <scp>D</scp> -alanine-adding enzyme (PaMurF) from <i>Pseudomonas aeruginosa</i> . Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 503-505.	0.7	3
103	Observation of the time-course for peptidoglycan lipid intermediate II polymerization by Staphylococcus aureus monofunctional transglycosylase. Microbiology (United Kingdom), 2014, 160, 1628-1636.	1.8	3
104	Expression, purification and crystallization of 2-oxo-hept-4-ene-1,7-dioate hydratase (HpcG) fromEscherichiacoli C. Acta Crystallographica Section F: Structural Biology Communications, 2006, 62, 1010-1012.	0.7	2
105	Bacterial Lipid II Analogs: Novel In Vitro Substrates for Mammalian Oligosaccharyl Diphosphodolichol Diphosphatase (DLODP) Activities. Molecules, 2019, 24, 2135.	3.8	1
106	Expression, purification and crystallization of the cell-division protein YgfE fromEscherichia coli. Acta Crystallographica Section F: Structural Biology Communications, 2005, 61, 305-307.	0.7	0
107	Penicillin-Binding Protein 4. , 2013, , 3470-3473.		0
108	Specificity determinants for lysine revealed by theS. aureusMurE structure. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s332-s332.	0.3	0

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109	Structure and functional study of tRNA dependent Fem ligases inStaphylococcus aureus. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s336-s336.	0.3	0
110	Characterization of secondary structure and thermal stability by biophysical methods of the D-alanyl,D-alanine ligase B protein from Escherichia coli. Protein and Peptide Letters, 2022, 29, .	0.9	0