James Spencer

List of Publications by Year in descending order

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104 papers	8,771 citations	109321 35 h-index	45317 90 g-index
110 all docs	110 docs citations	110 times ranked	9303 citing authors

#	Article	IF	Citations
1	Green fluorescent carbon dots as targeting probes for LEDâ€dependent bacterial killing. Nano Select, 2022, 3, 662-672.	3.7	5
2	A multiscale approach to predict the binding mode of metallo betaâ€lactamase inhibitors. Proteins: Structure, Function and Bioinformatics, 2022, 90, 372-384.	2.6	8
3	Inhibition of Mycobacterium tuberculosis <scp>InhA</scp> by 3â€nitropropanoic acid. Proteins: Structure, Function and Bioinformatics, 2022, 90, 898-904.	2.6	5
4	Imitation of Î²-lactam binding enables broad-spectrum metallo-Î²-lactamase inhibitors. Nature Chemistry, 2022, 14, 15-24.	13.6	39
5	Cladobotric Acids: Metabolites from Cultures of Cladobotryum sp., Semisynthetic Analogues and Antibacterial Activity. Journal of Natural Products, 2022, 85, 572-580.	3.0	3
6	Identification of Potent DNA Gyrase Inhibitors Active against Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2022, 62, 1680-1690.	5.4	12
7	Studies on the Reactions of Biapenem with VIM Metallo Î²-Lactamases and the Serine Î²-Lactamase KPC-2. Antibiotics, 2022, 11, 396.	3.7	8
8	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	11.2	9
9	Fast Identification and Quantification of Uropathogenic E. coli through Cluster Analysis. ACS Biomaterials Science and Engineering, 2022, 8, 242-252.	5.2	1
10	Discovery of novel and potent InhA inhibitors by an in silico screening and pharmacokinetic prediction. Future Medicinal Chemistry, 2022, 14, 717-729.	2.3	1
11	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	2.8	11
12	Natural variants modify Klebsiella pneumoniae carbapenemase (KPC) acylâ€“enzyme conformational dynamics to extend antibiotic resistance. Journal of Biological Chemistry, 2021, 296, 100126.	3.4	27
13	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein**. Angewandte Chemie - International Edition, 2021, 60, 7098-7110.	13.8	77
14	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein**. Angewandte Chemie, 2021, 133, 7174-7186.	2.0	6
15	Frontispiz: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein. Angewandte Chemie, 2021, 133, .	2.0	7
16	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	6.0	44
17	Frontispiece: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
18	Faropenem reacts with serine and metallo-Î²-lactamases to give multiple products. European Journal of Medicinal Chemistry, 2021, 215, 113257.	5.5	14

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19	Antimicrobial Resistance Conferred by OXA-48 Î²-Lactamases: Towards a Detailed Mechanistic Understanding. Antimicrobial Agents and Chemotherapy, 2021, 65, .	3.2	15
20	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. Nature Communications, 2021, 12, 4461.	12.8	34
21	2-Mercaptomethyl Thiazolidines (MMTZs) Inhibit All Metallo-Î²-Lactamase Classes by Maintaining a Conserved Binding Mode. ACS Infectious Diseases, 2021, 7, 2697-2706.	3.8	16
22	Identification and Phenotypic Characterization of Hsp90 Phosphorylation Sites That Modulate Virulence Traits in the Major Human Fungal Pathogen Candida albicans. Frontiers in Cellular and Infection Microbiology, 2021, 11, 637836.	3.9	9
23	Discovery of SARS-CoV-2 M‹sup›pro‹/sup› peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	7.4	54
24	2-Mercaptomethyl-thiazolidines use conserved aromaticâ€“S interactions to achieve broad-range inhibition of metallo-Î²-lactamases. Chemical Science, 2021, 12, 2898-2908.	7.4	24
25	Crystallography and QM/MM Simulations Identify Preferential Binding of Hydrolyzed Carbapenem and Penem Antibiotics to the L1 Metallo-Î²-Lactamase in the Imine Form. Journal of Chemical Information and Modeling, 2021, , .	5.4	5
26	Multiscale Workflow for Modeling Ligand Complexes of Zinc Metalloproteins. Journal of Chemical Information and Modeling, 2021, 61, 5658-5672.	5.4	10
27	Discovery of New and Potent InhA Inhibitors as Antituberculosis Agents: Structure-Based Virtual Screening Validated by Biological Assays and X-ray Crystallography. Journal of Chemical Information and Modeling, 2020, 60, 226-234.	5.4	34
28	The Bristol Sponge Microbiome Collection: A Unique Repository of Deep-Sea Microorganisms and Associated Natural Products. Antibiotics, 2020, 9, 509.	3.7	8
29	Resistance to the â€œlast resortâ€•antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. Chemical Communications, 2020, 56, 6874-6877.	4.1	10
30	Mixing and matching genes of marine and terrestrial origin in the biosynthesis of the mupirocin antibiotics. Chemical Science, 2020, 11, 5221-5226.	7.4	14
31	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	11.2	19
32	Cyclic boronates as versatile scaffolds for KPC-2 Î²-lactamase inhibition. RSC Medicinal Chemistry, 2020, 11, 491-496.	3.9	20
33	Molecular Basis of Class A Î²-Lactamase Inhibition by Relebactam. Antimicrobial Agents and Chemotherapy, 2019, 63, .	3.2	45
34	An Efficient Computational Assay for Î²-Lactam Antibiotic Breakdown by Class A Î²-Lactamases. Journal of Chemical Information and Modeling, 2019, 59, 3365-3369.	5.4	16
35	The Molecular Basis of Antibiotic Action and Resistance. Journal of Molecular Biology, 2019, 431, 3367-3369.	4.2	4
36	Bicyclic Boronate VNRX-5133 Inhibits Metallo- and Serine-Î²-Lactamases. Journal of Medicinal Chemistry, 2019, 62, 8544-8556.	6.4	139

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37	Mechanistic Insights into Î²-Lactamase-Catalysed Carbapenem Degradation Through Product Characterisation. Scientific Reports, 2019, 9, 13608.	3.3	27
38	Profiling interactions of vaborbactam with metallo-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1981-1984.	2.2	34
39	Exploitation of Antibiotic Resistance as a Novel Drug Target: Development of a Î²-Lactamase-Activated Antibacterial Prodrug. Journal of Medicinal Chemistry, 2019, 62, 4411-4425.	6.4	38
40	Simulations of Shikimate Dehydrogenase from Mycobacterium tuberculosis in Complex with 3-Dehydroshikimate and NADPH Suggest Strategies for MtbSDH Inhibition. Journal of Chemical Information and Modeling, 2019, 59, 1422-1433.	5.4	3
41	Î²-Lactamases and Î²-Lactamase Inhibitors in the 21st Century. Journal of Molecular Biology, 2019, 431, 3472-3500.	4.2	517
42	Nonâ€Hydrolytic Î²â€Lactam Antibiotic Fragmentation by <scp>l,d</scp>â€Transpeptidases and Serine Î²â€Lactamase Cysteine Variants. Angewandte Chemie, 2019, 131, 2012-2016.	2.0	4
43	Nonâ€Hydrolytic Î²â€Lactam Antibiotic Fragmentation by <scp>l,d</scp>â€Transpeptidases and Serine Î²â€Lactamase Cysteine Variants. Angewandte Chemie - International Edition, 2019, 58, 1990-1994.	13.8	27
44	Crystal structures of VIMâ€1 complexes explain active site heterogeneity in VIMâ€class metalloâ€Î²â€lactamases. FEBS Journal, 2019, 286, 169-183.	4.7	30
45	Imaging rRNA Methylation in Bacteria by MR-FISH. Methods in Molecular Biology, 2019, 2038, 89-107.	0.9	0
46	Structural and Kinetic Studies of the Potent Inhibition of Metallo-Î²-lactamases by 6-Phosphonomethylpyridine-2-carboxylates. Biochemistry, 2018, 57, 1880-1892.	2.5	49
47	A New Mechanism for Î²â€Lactamases: Class D Enzymes Degrade 1Î²â€Methyl Carbapenems through Lactone Formation. Angewandte Chemie, 2018, 130, 1296-1299.	2.0	4
48	Detecting RNA base methylations in single cells by in situ hybridization. Nature Communications, 2018, 9, 655.	12.8	28
49	In Silico Fragment-Based Design Identifies Subfamily B1 Metallo-Î²-lactamase Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1255-1260.	6.4	40
50	The economic burden of occupational non-melanoma skin cancer due to solar radiation. Journal of Occupational and Environmental Hygiene, 2018, 15, 481-491.	1.0	45
51	A New Mechanism for Î²â€Lactamases: Class D Enzymes Degrade 1Î²â€Methyl Carbapenems through Lactone Formation. Angewandte Chemie - International Edition, 2018, 57, 1282-1285.	13.8	27
52	Cyclobutanone Mimics of Intermediates in Metalloâ€Î²â€Lactamase Catalysis. Chemistry - A European Journal, 2018, 24, 5734-5737.	3.3	25
53	Multiscale Simulations of Clavulanate Inhibition Identify the Reactive Complex in Class A Î²-Lactamases and Predict the Efficiency of Inhibition. Biochemistry, 2018, 57, 3560-3563.	2.5	17
54	Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1. Scientific Reports, 2017, 7, 39392.	3.3	107

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55	Cyclic Boronates Inhibit All Classes of Î²-Lactamases. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	94
56	¹⁹Fâ€NMR Reveals the Role of Mobile Loops in Product and Inhibitor Binding by the SÃ£o Paulo Metalloâ€Î²â€Lactamase. Angewandte Chemie - International Edition, 2017, 56, 3862-3866.	13.8	20
57	¹⁹Fâ€NMR Reveals the Role of Mobile Loops in Product and Inhibitor Binding by the SÃ£o Paulo Metalloâ€Î²â€Lactamase. Angewandte Chemie, 2017, 129, 3920-3924.	2.0	3
58	Crystallographic analyses of isoquinoline complexes reveal a new mode of metallo-Î²-lactamase inhibition. Chemical Communications, 2017, 53, 5806-5809.	4.1	29
59	NMR-filtered virtual screening leads to non-metal chelating metallo-Î²-lactamase inhibitors. Chemical Science, 2017, 8, 928-937.	7.4	63
60	A general reaction mechanism for carbapenem hydrolysis by mononuclear and binuclear metallo-Î²-lactamases. Nature Communications, 2017, 8, 538.	12.8	98
61	Structural/mechanistic insights into the efficacy of nonclassical Î²â€lactamase inhibitors against extensively drug resistant Stenotrophomonas maltophilia clinical isolates. Molecular Microbiology, 2017, 106, 492-504.	2.5	39
62	Balancing mcr-1 expression and bacterial survival is a delicate equilibrium between essential cellular defence mechanisms. Nature Communications, 2017, 8, 2054.	12.8	157
63	¹³C-Carbamylation as a mechanistic probe for the inhibition of class D Î²-lactamases by avibactam and halide ions. Organic and Biomolecular Chemistry, 2017, 15, 6024-6032.	2.8	19
64	1.12â€…Ã… resolution crystal structure of the catalytic domain of the plasmid-mediated colistin resistance determinant MCR-2. Acta Crystallographica Section F, Structural Biology Communications, 2017, 73, 443-449.	0.8	22
65	Sideromimic Modification of Lactivicin Dramatically Increases Potency against Extensively Drug-Resistant Stenotrophomonas maltophilia Clinical Isolates. Antimicrobial Agents and Chemotherapy, 2016, 60, 4170-4175.	3.2	16
66	Structural basis of metallo-Î²-lactamase, serine-Î²-lactamase and penicillin-binding protein inhibition by cyclic boronates. Nature Communications, 2016, 7, 12406.	12.8	202
67	Structural and Biochemical Characterization of Rm3, a Subclass B3 Metallo-Î²-Lactamase Identified from a Functional Metagenomic Study. Antimicrobial Agents and Chemotherapy, 2016, 60, 5828-5840.	3.2	22
68	Cross-class metallo-Î²-lactamase inhibition by bisthiazolidines reveals multiple binding modes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3745-54.	7.1	122
69	Emergence of plasmid-mediated colistin resistance mechanism MCR-1 in animals and human beings in China: a microbiological and molecular biological study. Lancet Infectious Diseases, The, 2016, 16, 161-168.	9.1	4,130
70	Role of Residues W228 and Y233 in the Structure and Activity of Metallo-Î²-Lactamase GIM-1. Antimicrobial Agents and Chemotherapy, 2016, 60, 990-1002.	3.2	8
71	Arginine-containing peptides as potent inhibitors of VIM-2 metallo-Î²-lactamase. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 2228-2238.	2.4	8
72	Bisthiazolidines: A Substrate-Mimicking Scaffold as an Inhibitor of the NDM-1 Carbapenemase. ACS Infectious Diseases, 2015, 1, 544-554.	3.8	100

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73	Assay for drug discovery: Synthesis and testing of nitrocefin analogues for use as Î²-lactamase substrates. Analytical Biochemistry, 2015, 486, 75-77.	2.4	15
74	Exploring the Role of Residue 228 in Substrate and Inhibitor Recognition by VIM Metallo-Î²-lactamases. Biochemistry, 2015, 54, 3183-3196.	2.5	41
75	Studying the active-site loop movement of the SÃ£o Paolo metallo-Î²-lactamase-1. Chemical Science, 2015, 6, 956-963.	7.4	36
76	Crystal Structure of DIM-1, an Acquired Subclass B1 Metallo-Î²-Lactamase from Pseudomonas stutzeri. PLoS ONE, 2015, 10, e0140059.	2.5	3
77	Rhodanine hydrolysis leads to potent thioenolate mediated metallo-Î²-lactamase inhibition. Nature Chemistry, 2014, 6, 1084-1090.	13.6	110
78	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	4.1	43
79	Molecular basis of non-mutational derepression of ramA in Klebsiella pneumoniae. Journal of Antimicrobial Chemotherapy, 2014, 69, 2681-2689.	3.0	8
80	Assay Platform for Clinically Relevant Metallo-Î²-lactamases. Journal of Medicinal Chemistry, 2013, 56, 6945-6953.	6.4	100
81	Chromophoreâ€Linked Substrate (CLS405): Probing Metalloâ€Î²â€Lactamase Activity and Inhibition. ChemMedChem, 2013, 8, 1923-1929.	3.2	21
82	Crystal Structures of Pseudomonas aeruginosa GIM-1: Active-Site Plasticity in Metallo-Î²-Lactamases. Antimicrobial Agents and Chemotherapy, 2013, 57, 848-854.	3.2	22
83	Cysteine Methylation Controls Radical Generation in the Cfr Radical AdoMet rRNA Methyltransferase. PLoS ONE, 2013, 8, e67979.	2.5	12
84	Crystal Structure of the Mobile Metallo-Î²-Lactamase AIM-1 from Pseudomonas aeruginosa: Insights into Antibiotic Binding and the Role of Gln157. Antimicrobial Agents and Chemotherapy, 2012, 56, 4341-4353.	3.2	57
85	The Basis for Carbapenem Hydrolysis by Class A Î²-Lactamases: A Combined Investigation using Crystallography and Simulations. Journal of the American Chemical Society, 2012, 134, 18275-18285.	13.7	76
86	Structural and Computational Investigations of VIM-7: Insights into the Substrate Specificity of VIM Metallo-Î²-Lactamases. Journal of Molecular Biology, 2011, 411, 174-189.	4.2	35
87	Crystal Structure of Serratia fonticola Sfh-I: Activation of the Nucleophile in Mono-Zinc Metallo-Î²-Lactamases. Journal of Molecular Biology, 2011, 411, 951-959.	4.2	48
88	Biochemical Characterization of Sfh-I, a Subclass B2 Metallo-Î²-Lactamase from Serratia fonticola UTAD54. Antimicrobial Agents and Chemotherapy, 2011, 55, 5392-5395.	3.2	14
89	Crystal Structure of the LasA Virulence Factor from Pseudomonas aeruginosa: Substrate Specificity and Mechanism of M23 Metallopeptidases. Journal of Molecular Biology, 2010, 396, 908-923.	4.2	58
90	High-level expression and reconstitution of active Cfr, a radical-SAM rRNA methyltransferase that confers resistance to ribosome-acting antibiotics. Protein Expression and Purification, 2010, 74, 204-210.	1.3	11

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91	Repurposing of Meropenem and Nadifloxacin for Treatment of Burn Patients?. Nature Precedings, 2009, , .	0.1	0
92	Kinetic Characterization of VIM-7, a Divergent Member of the VIM Metallo-Î²-Lactamase Family. Antimicrobial Agents and Chemotherapy, 2008, 52, 2905-2908.	3.2	29
93	Structural Basis for the Role of Asp-120 in Metallo-Î²-lactamases[,]. Biochemistry, 2007, 46, 10664-10674.	2.5	31
94	Metallo-Î²-lactamases:â€‰ Novel Weaponry for Antibiotic Resistance in Bacteria. Accounts of Chemical Research, 2006, 39, 721-728.	15.6	361
95	Crystal Structure of Pseudomonas aeruginosa SPM-1 Provides Insights into Variable Zinc Affinity of Metallo-Î²-lactamases. Journal of Molecular Biology, 2006, 357, 890-903.	4.2	88
96	A New Approach to the Inhibition of Metallo-Î²-lactamases. Angewandte Chemie - International Edition, 2006, 45, 1022-1026.	13.8	54
97	Antibiotic Recognition by Binuclear Metallo-Î²-Lactamases Revealed by X-ray Crystallography#. Journal of the American Chemical Society, 2005, 127, 14439-14444.	13.7	123
98	Penicillin-derived inhibitors that simultaneously target both metallo- and serine-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1299-1304.	2.2	74
99	Novel Mechanism of Hydrolysis of Therapeutic Î²-Lactams byStenotrophomonas maltophilia L1 Metallo-Î²-lactamase. Journal of Biological Chemistry, 2001, 276, 33638-33644.	3.4	85
100	Overexpression, Purification, and Characterization of the Cloned Metallo-Î²-Lactamase L1 from Stenotrophomonas maltophilia. Antimicrobial Agents and Chemotherapy, 1998, 42, 921-926.	3.2	181
101	Is the Structure of the N-Domain of Phosphoglycerate Kinase Affected by Isolation from the Intact Molecule?. Biochemistry, 1997, 36, 333-340.	2.5	22
102	Structure of a kinetic protein folding intermediate by equilibrium amide exchange. Nature Structural Biology, 1997, 4, 801-804.	9.7	34
103	Domain Behavior during the Folding of a Thermostable Phosphoglycerate Kinase. Biochemistry, 1996, 35, 15740-15752.	2.5	35
104	Penicillanic Acid Sulfones Inactivate the Extended-Spectrum Î²-Lactamase CTX-M-15 through Formation of a Serine-Lysine Cross-Link: an Alternative Mechanism of Î²-Lactamase Inhibition. MBio, 0, , .	4.1	2