James Spencer

List of Publications by Year in descending order

104 papers	8,771 citations	109311 35 h-index	45310 90 g-index
110 all docs	110 docs citations	110 times ranked	9303 citing authors

#	Article	IF	Citations
1	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
2	Î²-Lactamases and Î²-Lactamase Inhibitors in the 21st Century. Journal of Molecular Biology, 2019, 431, 3472-3500.	4.2	517
3	Metallo-Î²-lactamases:â€‰ Novel Weaponry for Antibiotic Resistance in Bacteria. Accounts of Chemical Research, 2006, 39, 721-728.	15.6	361
4	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
5	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
6	Balancing mcr-1 expression and bacterial survival is a delicate equilibrium between essential cellular defence mechanisms. Nature Communications, 2017, 8, 2054.	12.8	157
7	Bicyclic Boronate VNRX-5133 Inhibits Metallo- and Serine-Î²-Lactamases. Journal of Medicinal Chemistry, 2019, 62, 8544-8556.	6.4	139
8	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
9	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
10	Rhodanine hydrolysis leads to potent thioenolate mediated metallo-Î²-lactamase inhibition. Nature Chemistry, 2014, 6, 1084-1090.	13.6	110
11	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
12	Assay Platform for Clinically Relevant Metallo-Î²-lactamases. Journal of Medicinal Chemistry, 2013, 56, 6945-6953.	6.4	100
13	Bisthiazolidines: A Substrate-Mimicking Scaffold as an Inhibitor of the NDM-1 Carbapenemase. ACS Infectious Diseases, 2015, 1, 544-554.	3.8	100
14	A general reaction mechanism for carbapenem hydrolysis by mononuclear and binuclear metallo-Î²-lactamases. Nature Communications, 2017, 8, 538.	12.8	98
15	Cyclic Boronates Inhibit All Classes of Î²-Lactamases. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	94
16	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
17	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
18	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

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19	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
20	Penicillin-derived inhibitors that simultaneously target both metallo- and serine-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1299-1304.	2.2	74
21	NMR-filtered virtual screening leads to non-metal chelating metallo-Î²-lactamase inhibitors. Chemical Science, 2017, 8, 928-937.	7.4	63
22	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
23	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
24	A New Approach to the Inhibition of Metallo-Î²-lactamases. Angewandte Chemie - International Edition, 2006, 45, 1022-1026.	13.8	54
25	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	7.4	54
26	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
27	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
28	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
29	Molecular Basis of Class A Î²-Lactamase Inhibition by Relebactam. Antimicrobial Agents and Chemotherapy, 2019, 63, .	3.2	45
30	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	6.0	44
31	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	4.1	43
32	Exploring the Role of Residue 228 in Substrate and Inhibitor Recognition by VIM Metallo-Î²-lactamases. Biochemistry, 2015, 54, 3183-3196.	2.5	41
33	In Silico Fragment-Based Design Identifies Subfamily B1 Metallo-Î²-lactamase Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1255-1260.	6.4	40
34	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
35	Imitation of Î²-lactam binding enables broad-spectrum metallo-Î²-lactamase inhibitors. Nature Chemistry, 2022, 14, 15-24.	13.6	39
36	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

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37	Studying the active-site loop movement of the SÃ£o Paolo metallo-Î²-lactamase-1. Chemical Science, 2015, 6, 956-963.	7.4	36
38	Domain Behavior during the Folding of a Thermostable Phosphoglycerate Kinase. Biochemistry, 1996, 35, 15740-15752.	2.5	35
39	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
40	Structure of a kinetic protein folding intermediate by equilibrium amide exchange. Nature Structural Biology, 1997, 4, 801-804.	9.7	34
41	Profiling interactions of vaborbactam with metallo-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1981-1984.	2.2	34
42	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
43	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. Nature Communications, 2021, 12, 4461.	12.8	34
44	Structural Basis for the Role of Asp-120 in Metallo-Î²-lactamases[,]. Biochemistry, 2007, 46, 10664-10674.	2.5	31
45	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
46	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
47	Crystallographic analyses of isoquinoline complexes reveal a new mode of metallo-Î²-lactamase inhibition. Chemical Communications, 2017, 53, 5806-5809.	4.1	29
48	Detecting RNA base methylations in single cells by in situ hybridization. Nature Communications, 2018, 9, 655.	12.8	28
49	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
50	Mechanistic Insights into Î²-Lactamase-Catalysed Carbapenem Degradation Through Product Characterisation. Scientific Reports, 2019, 9, 13608.	3.3	27
51	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
52	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
53	Cyclobutanone Mimics of Intermediates in Metalloâ€Î²â€Lactamase Catalysis. Chemistry - A European Journal, 2018, 24, 5734-5737.	3.3	25
54	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

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55	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
56	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
57	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
58	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
59	Chromophoreâ€Linked Substrate (CLS405): Probing Metalloâ€Î²â€Lactamase Activity and Inhibition. ChemMedChem, 2013, 8, 1923-1929.	3.2	21
60	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
61	Cyclic boronates as versatile scaffolds for KPC-2 Î²-lactamase inhibition. RSC Medicinal Chemistry, 2020, 11, 491-496.	3.9	20
62	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
63	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	11.2	19
64	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
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	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
67	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
68	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
69	Antimicrobial Resistance Conferred by OXA-48 Î²-Lactamases: Towards a Detailed Mechanistic Understanding. Antimicrobial Agents and Chemotherapy, 2021, 65, .	3.2	15
70	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
71	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
72	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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73	Cysteine Methylation Controls Radical Generation in the Cfr Radical AdoMet rRNA Methyltransferase. PLoS ONE, 2013, 8, e67979.	2.5	12
74	Identification of Potent DNA Gyrase Inhibitors Active against Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2022, 62, 1680-1690.	5.4	12
75	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
76	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	2.8	11
77	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
78	Multiscale Workflow for Modeling Ligand Complexes of Zinc Metalloproteins. Journal of Chemical Information and Modeling, 2021, 61, 5658-5672.	5.4	10
79	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
80	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	11.2	9
81	Molecular basis of non-mutational derepression of ramA in Klebsiella pneumoniae. Journal of Antimicrobial Chemotherapy, 2014, 69, 2681-2689.	3.0	8
82	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
83	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
84	The Bristol Sponge Microbiome Collection: A Unique Repository of Deep-Sea Microorganisms and Associated Natural Products. Antibiotics, 2020, 9, 509.	3.7	8
85	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
86	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
87	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
88	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
89	Green fluorescent carbon dots as targeting probes for LEDâ€dependent bacterial killing. Nano Select, 2022, 3, 662-672.	3.7	5
90	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

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91	Inhibition of Mycobacterium tuberculosis<scp>InhA</scp> by 3â€nitropropanoic acid. Proteins: Structure, Function and Bioinformatics, 2022, 90, 898-904.	2.6	5
92	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
93	The Molecular Basis of Antibiotic Action and Resistance. Journal of Molecular Biology, 2019, 431, 3367-3369.	4.2	4
94	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
95	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
96	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
97	Crystal Structure of DIM-1, an Acquired Subclass B1 Metallo-Î²-Lactamase from Pseudomonas stutzeri. PLoS ONE, 2015, 10, e0140059.	2.5	3
98	Cladobotric Acids: Metabolites from Cultures of Cladobotryum sp., Semisynthetic Analogues and Antibacterial Activity. Journal of Natural Products, 2022, 85, 572-580.	3.0	3
99	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
100	Fast Identification and Quantification of Uropathogenic E. coli through Cluster Analysis. ACS Biomaterials Science and Engineering, 2022, 8, 242-252.	5.2	1
101	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
102	Repurposing of Meropenem and Nadifloxacin for Treatment of Burn Patients?. Nature Precedings, 2009, , .	0.1	0
103	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
104	Imaging rRNA Methylation in Bacteria by MR-FISH. Methods in Molecular Biology, 2019, 2038, 89-107.	0.9	0