James Spencer

List of Publications by Year
in descending order

104 papers	8,771 citations	109137 35 h-index	45213 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.	4.6	4,130
2	Î²-Lactamases and Î²-Lactamase Inhibitors in the 21st Century. Journal of Molecular Biology, 2019, 431, 3472-3500.	2.0	517
3	Metallo-Î²-lactamases:â€‰ Novel Weaponry for Antibiotic Resistance in Bacteria. Accounts of Chemical Research, 2006, 39, 721-728.	7.6	361
4	Structural basis of metallo-Î²-lactamase, serine-Î²-lactamase and penicillin-binding protein inhibition by cyclic boronates. Nature Communications, 2016, 7, 12406.	5.8	202
5	Overexpression, Purification, and Characterization of the Cloned Metallo-Î²-Lactamase L1 from <i>Stenotrophomonas maltophilia</i>. Antimicrobial Agents and Chemotherapy, 1998, 42, 921-926.	1.4	181
6	Balancing mcr-1 expression and bacterial survival is a delicate equilibrium between essential cellular defence mechanisms. Nature Communications, 2017, 8, 2054.	5.8	157
7	Bicyclic Boronate VNRX-5133 Inhibits Metallo- and Serine-Î²-Lactamases. Journal of Medicinal Chemistry, 2019, 62, 8544-8556.	2.9	139
8	Antibiotic Recognition by Binuclear Metallo-Î²-Lactamases Revealed by X-ray Crystallography#. Journal of the American Chemical Society, 2005, 127, 14439-14444.	6.6	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.	3.3	122
10	Rhodanine hydrolysis leads to potent thioenolate mediated metallo-Î²-lactamase inhibition. Nature Chemistry, 2014, 6, 1084-1090.	6.6	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.	1.6	107
12	Assay Platform for Clinically Relevant Metallo-Î²-lactamases. Journal of Medicinal Chemistry, 2013, 56, 6945-6953.	2.9	100
13	Bisthiazolidines: A Substrate-Mimicking Scaffold as an Inhibitor of the NDM-1 Carbapenemase. ACS Infectious Diseases, 2015, 1, 544-554.	1.8	100
14	A general reaction mechanism for carbapenem hydrolysis by mononuclear and binuclear metallo-Î²-lactamases. Nature Communications, 2017, 8, 538.	5.8	98
15	Cyclic Boronates Inhibit All Classes of Î²-Lactamases. Antimicrobial Agents and Chemotherapy, 2017, 61, .	1.4	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.	2.0	88
17	Novel Mechanism of Hydrolysis of Therapeutic Î²-Lactams byStenotrophomonas maltophilia L1 Metallo-Î²-lactamase. Journal of Biological Chemistry, 2001, 276, 33638-33644.	1.6	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.	7.2	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.	6.6	76
20	Penicillin-derived inhibitors that simultaneously target both metallo- and serine-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1299-1304.	1.0	74
21	NMR-filtered virtual screening leads to non-metal chelating metallo-Î²-lactamase inhibitors. Chemical Science, 2017, 8, 928-937.	3.7	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.	2.0	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.	1.4	57
24	A New Approach to the Inhibition of Metallo-Î²-lactamases. Angewandte Chemie - International Edition, 2006, 45, 1022-1026.	7.2	54
25	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
26	Structural and Kinetic Studies of the Potent Inhibition of Metallo-Î²-lactamases by 6-Phosphonomethylpyridine-2-carboxylates. Biochemistry, 2018, 57, 1880-1892.	1.2	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.	2.0	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.	0.4	45
29	Molecular Basis of Class A Î²-Lactamase Inhibition by Relebactam. Antimicrobial Agents and Chemotherapy, 2019, 63, .	1.4	45
30	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	2.8	44
31	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	2.2	43
32	Exploring the Role of Residue 228 in Substrate and Inhibitor Recognition by VIM Metallo-Î²-lactamases. Biochemistry, 2015, 54, 3183-3196.	1.2	41
33	In Silico Fragment-Based Design Identifies Subfamily B1 Metallo-Î²-lactamase Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1255-1260.	2.9	40
34	Structural/mechanistic insights into the efficacy of nonclassical Î²â€lactamase inhibitors against extensively drug resistant <i>Stenotrophomonas maltophilia</i> clinical isolates. Molecular Microbiology, 2017, 106, 492-504.	1.2	39
35	Imitation of Î²-lactam binding enables broad-spectrum metallo-Î²-lactamase inhibitors. Nature Chemistry, 2022, 14, 15-24.	6.6	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.	2.9	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.	3.7	36
38	Domain Behavior during the Folding of a Thermostable Phosphoglycerate Kinase. Biochemistry, 1996, 35, 15740-15752.	1.2	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.	2.0	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.	1.0	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.	2.5	34
43	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. Nature Communications, 2021, 12, 4461.	5.8	34
44	Structural Basis for the Role of Asp-120 in Metallo-Î²-lactamases[,]. Biochemistry, 2007, 46, 10664-10674.	1.2	31
45	Crystal structures of VIMâ€1 complexes explain active site heterogeneity in VIMâ€class metalloâ€Î²â€lactamases. FEBS Journal, 2019, 286, 169-183.	2.2	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.	1.4	29
47	Crystallographic analyses of isoquinoline complexes reveal a new mode of metallo-Î²-lactamase inhibition. Chemical Communications, 2017, 53, 5806-5809.	2.2	29
48	Detecting RNA base methylations in single cells by in situ hybridization. Nature Communications, 2018, 9, 655.	5.8	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.	7.2	27
50	Mechanistic Insights into Î²-Lactamase-Catalysed Carbapenem Degradation Through Product Characterisation. Scientific Reports, 2019, 9, 13608.	1.6	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.	7.2	27
52	Natural variants modify Klebsiella pneumoniae carbapenemase (KPC) acylâ€“enzyme conformational dynamics to extend antibiotic resistance. Journal of Biological Chemistry, 2021, 296, 100126.	1.6	27
53	Cyclobutanone Mimics of Intermediates in Metalloâ€Î²â€Lactamase Catalysis. Chemistry - A European Journal, 2018, 24, 5734-5737.	1.7	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.	3.7	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.	1.2	22
56	Crystal Structures of Pseudomonas aeruginosa GIM-1: Active-Site Plasticity in Metallo-Î²-Lactamases. Antimicrobial Agents and Chemotherapy, 2013, 57, 848-854.	1.4	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.	1.4	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.	0.4	22
59	Chromophoreâ€Linked Substrate (CLS405): Probing Metalloâ€Î²â€Lactamase Activity and Inhibition. ChemMedChem, 2013, 8, 1923-1929.	1.6	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.	7.2	20
61	Cyclic boronates as versatile scaffolds for KPC-2 Î²-lactamase inhibition. RSC Medicinal Chemistry, 2020, 11, 491-496.	1.7	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.	1.5	19
63	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	5.5	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.	1.2	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.	1.4	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.	2.5	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.	1.8	16
68	Assay for drug discovery: Synthesis and testing of nitrocefin analogues for use as Î²-lactamase substrates. Analytical Biochemistry, 2015, 486, 75-77.	1.1	15
69	Antimicrobial Resistance Conferred by OXA-48 Î²-Lactamases: Towards a Detailed Mechanistic Understanding. Antimicrobial Agents and Chemotherapy, 2021, 65, .	1.4	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.	1.4	14
71	Mixing and matching genes of marine and terrestrial origin in the biosynthesis of the mupirocin antibiotics. Chemical Science, 2020, 11, 5221-5226.	3.7	14
72	Faropenem reacts with serine and metallo-Î²-lactamases to give multiple products. European Journal of Medicinal Chemistry, 2021, 215, 113257.	2.6	14

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73	Cysteine Methylation Controls Radical Generation in the Cfr Radical AdoMet rRNA Methyltransferase. PLoS ONE, 2013, 8, e67979.	1.1	12
74	Identification of Potent DNA Gyrase Inhibitors Active against <i>Mycobacterium tuberculosis</i>. Journal of Chemical Information and Modeling, 2022, 62, 1680-1690.	2.5	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.	0.6	11
76	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	1.5	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.	2.2	10
78	Multiscale Workflow for Modeling Ligand Complexes of Zinc Metalloproteins. Journal of Chemical Information and Modeling, 2021, 61, 5658-5672.	2.5	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.	1.8	9
80	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	5.5	9
81	Molecular basis of non-mutational derepression of ramA in Klebsiella pneumoniae. Journal of Antimicrobial Chemotherapy, 2014, 69, 2681-2689.	1.3	8
82	Arginine-containing peptides as potent inhibitors of VIM-2 metallo-Î²-lactamase. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 2228-2238.	1.1	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.	1.4	8
84	The Bristol Sponge Microbiome Collection: A Unique Repository of Deep-Sea Microorganisms and Associated Natural Products. Antibiotics, 2020, 9, 509.	1.5	8
85	A multiscale approach to predict the binding mode of metallo betaâ€lactamase inhibitors. Proteins: Structure, Function and Bioinformatics, 2022, 90, 372-384.	1.5	8
86	Studies on the Reactions of Biapenem with VIM Metallo Î²-Lactamases and the Serine Î²-Lactamase KPC-2. Antibiotics, 2022, 11, 396.	1.5	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, .	1.6	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.	1.6	6
89	Green fluorescent carbon dots as targeting probes for LEDâ€dependent bacterial killing. Nano Select, 2022, 3, 662-672.	1.9	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, , .	2.5	5

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91	Inhibition of <i>Mycobacterium tuberculosis</i><scp>InhA</scp> by 3â€nitropropanoic acid. Proteins: Structure, Function and Bioinformatics, 2022, 90, 898-904.	1.5	5
92	A New Mechanism for Î²â€Lactamases: Class D Enzymes Degrade 1Î²â€Methyl Carbapenems through Lactone Formation. Angewandte Chemie, 2018, 130, 1296-1299.	1.6	4
93	The Molecular Basis of Antibiotic Action and Resistance. Journal of Molecular Biology, 2019, 431, 3367-3369.	2.0	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.	1.6	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.	1.6	3
96	Simulations of Shikimate Dehydrogenase from <i>Mycobacterium tuberculosis</i> in Complex with 3-Dehydroshikimate and NADPH Suggest Strategies for <i>Mtb</i>SDH Inhibition. Journal of Chemical Information and Modeling, 2019, 59, 1422-1433.	2.5	3
97	Crystal Structure of DIM-1, an Acquired Subclass B1 Metallo-Î²-Lactamase from Pseudomonas stutzeri. PLoS ONE, 2015, 10, e0140059.	1.1	3
98	Cladobotric Acids: Metabolites from Cultures of <i>Cladobotryum</i> sp., Semisynthetic Analogues and Antibacterial Activity. Journal of Natural Products, 2022, 85, 572-580.	1.5	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, , .	1.8	2
100	Fast Identification and Quantification of Uropathogenic <i>E. coli</i> through Cluster Analysis. ACS Biomaterials Science and Engineering, 2022, 8, 242-252.	2.6	1
101	Discovery of novel and potent InhA inhibitors by an <i>in silico</i> screening and pharmacokinetic prediction. Future Medicinal Chemistry, 2022, 14, 717-729.	1.1	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, .	7.2	0
104	Imaging rRNA Methylation in Bacteria by MR-FISH. Methods in Molecular Biology, 2019, 2038, 89-107.	0.4	0