

Full list of publications – Jürgen Brem

Peer-reviewed publications

2025

91. Z. Wang, G. Cao, M.P. Collier, X. Qiu, S. Broadway-Stringer, D. Šaman, J.Z.Y. Ng, N. Sen, A.J. Azad, C. Hooper, J. Zimmermann, M.A. McDonough, **J. Brem**, P. Rabe, H. Song, T. Reid Alderson, C.J. Schofield, J.R. Bolla, K. Djinovic-Carugo, D.O. Fürst, B. Warscheid, M.T. Degiacomi, T.M. Allison, G.K.A. Hochberg, C.V. Robinson, K. Gehmlich, J.L.P. Benesch, *Nature Communications*, 2025, 16(1):4090, “Filamin C dimerisation is regulated by HSPB7”
90. Z. Ling, A.J. Macdonald Farley, A. Lankapalli, Y. Zhang, S. Premchand-Branker, K. Cook, A. Baran, C. Gray-Hammerton, C. Orbegoza Rubio, E. Suna, J. Mathias, **J. Brem**, K. Sands, M. Nieto-Rosado, M. Mykolaivna Trush, N. Naznin Rakhi, W. Martins, Y. Zhou, C.J. Schofield, T. Walsh, *Engineering*, 2024, 38:124-132, “The Triple Combination of Meropenem, Avibactam, and a Metallo- β -Lactamase Inhibitor Optimizes Antibacterial Coverage Against Different β -Lactamase Producers”.
89. M. de Munnik, P.A. Lang, K. Calvopiña, P. Rabe, **J. Brem**, C.J. Schofield, *Communications Biology*, 2024, 2024, 7(1):1173, “Biochemical and crystallographic studies of L,D-transpeptidase 2 from *Mycobacterium tuberculosis* with its natural monomer substrate”.

2024

88. P.A. Lang, M. de Munnik, A.O. Oluwole, T.D.W. Claridge, C.V. Robinson, **J. Brem**, C.J. Schofield, *Chembiochem*, 2024, 25(22):e202400280, “How Clavulanic Acid Inhibits Serine β -Lactamases”.
87. M. Bielinski, L.R. Henderson, Y. Yosaatmadja, L.P. Swift, H.T. Baddock, M.J. Bowen, **J. Brem**, P.S. Jones, S.P. McElroy, A. Morrison, M. Speake, S. van Boeckel, E. van Doornmalen, J. van Groningen, H. van den Hurk, O. Gileadi, J.A. Newman, P.J. McHugh, C.J. Schofield, *Chemical Science*, 2024, 15(21):8227-8241, “Cell-active small molecule inhibitors validate the SNM1A DNA repair nuclease as a cancer target”.

2023

86. C. Chen, Y. Xu, P. Oelschlaeger, **J. Brem**, L. Liu, D. Wang, H. Sun, K.-W. Yang, *Chemical Communications*, 2023, 59(60): 9227-9230, “A dual covalent binder for labelling and inhibiting serine and metallo-carbapenemases”.
85. M. Munnik, P.A. Lang, F.D.D. Anton, M. Cacho, R.H. Bates, **J. Brem**, B. Rodríguez Miquel, C.J. Schofield, *Chemical Science*, 2023, 14(26):7262-7278, “L,D-transpeptidase Ldt_{Mt2} of *Mycobacterium tuberculosis* Reveals Novel Classes of Covalently Reacting Inhibitors”.
84. A. Baran, J. Kuzmins, J. Kuzmins, J. Kuznecovs, A.J.M. Farley, T. Panduwawala, A. Parkova, P.A. Donets, **J. Brem**, E. Suna, C.J. Schofield, K. Shubin, *Organic Process Research & Development*, 2023, 27(4), 692-706, “Optimized Synthesis of Indole Carboxylate Metallo- β -Lactamase Inhibitor EBL-3183”.

2022

83. P.A. Lang, R. Raj, A. Tumber, C.T. Lohans, P. Rabe, C.V. Robinson, **J. Brem**, C.J. Schofield, *Proceedings of the National Academy of Sciences (PNAS)*, 2022, 119(18):e2117310119, “Studies on enmetazobactam clarify mechanisms of widely used β -lactamase inhibitors”. **Co-corresponding author**
82. A. Lucic, T.R. Malla, K. Calvopiña, C.L. Tooke, **J. Brem**, M.A. McDonough, J. Spencer, C.J. Schofield, *Antibiotics*, 2022, 11(3):396, “Studies on the Reactions of Biapenem with VIM Metallo β -Lactamases and the Serine β -Lactamase KPC-2”

81. **J. Brem**, T. Panduwawala, J.U. Hansen, J. Hewitt, E. Liepins, P. Donets, L. Espina, A.J.M. Farley, K. Shubin, G.G. Campillos, P. Kiuru, S. Shishodia, D. Krahm, R.K. Leśniak, J.S. Adrian, K. Calvopiña, M.-C. Turrientes, M.E. Kavanagh, D. Lubriks, P. Hinchliffe, G.W. Langley, A.F. Aboklaish, A. Eneroth, M. Backlund, A.G. Baran, E.I. Nielsen, M. Speake, J. Kuka, J. Robinson, S. Grinberga, L. Robinson, M.A. McDonough, A.M. Rydzik, T.M. Leissing, J.C. Jimenez-Castellanos, M.B. Avison, S.D. Silva Pinto, A.D. Pannifer, M. Martjuga, E. Widlake, M. Priede, I. Hopkins Navratilova, M. Gniadkowski, A.K. Belfrage, P. Brandt, J. Yli-Kauhaluoma, E. Bacque, M.G.P. Page, F. Björkling, J.M. Tyrrell, J. Spencer, P.A. Lang, P. Baranczewski, R. Cantón, S.P. McElroy, P.S. Jones, F. Baquero, E. Suna, A. Morrison, T.R. Walsh, C.J. Schofield, *Nature Chemistry*, 2022, 14(1):15-24, "Imitation of β -lactam binding enables broad-spectrum metallo- β -lactamase inhibitors". **First and co-corresponding author**

2021

80. A. Butryn, P.S. Simon, P. Aller, P. Hinchliffe, R.N. Massad, G. Leen, C.L. Tooke, I. Bogacz, In-Sik Kim, A. Bhowmick, A.S. Brewster, N.E. Devenish, **J. Brem**, J.J.A.G. Kamps, P.A. Lang, P. Rabe, D. Axford, J.H. Beale, B. Davy, A. Ebrahim, J. Orlans, S.L.S. Storm, T. Zhou, S. Owada, R. Tanaka, K. Tono, G. Evans, R.L. Owen, F.A. Houle, N.K. Sauter, C.J. Schofield, J. Spencer, V.K. Yachandra, J. Yano, J.F. Kern, A.M. Orville, *Nature communications*, 2021, 12(1):4461, "An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography".

79. H. Newman, A. Krajnc, D. Bellini, C.J. Eyermann, G.A. Boyle, N.G. Paterson, K.E. McAuley, R. Lesniak, M. Gangar, F.v. Delft, **J. Brem**, K. Chibale, C.J. Schofield, C.G. Dowson, *Journal of Medicinal Chemistry*, 2021, 64(15):11379-11394, "High-Throughput Crystallography Reveals Boron-Containing Inhibitors of a Penicillin-Binding Protein with Di- and Tricovaleent Binding Modes".

78. Y.-C. Xiao, X.-P. Chen, J. Deng, Y.-H. Yan, K.-R. Zhu, G. Li, J.-L. Yu, **J. Brem**, F. Chen, C.J. Schofield, G.-B. Li, *Chemical Communications*, 2021, 57(62):7709-7712, "Design and enantioselective synthesis of 3-(α -acrylic acid) benzoxaboroles to combat carbapenemase resistance".

77. P. Rabe, J.J.A.G. Kamps, K.D. Sutherlin, J.D.S. Linyard, P. Aller, C.C. Pham, H. Makita, I. Clifton, M.A. McDonough, T.M. Leissing, D. Shutin, P.A. Lang, A. Butryn, **J. Brem**, S. Gul, F.D. Fuller, In-Sik Kim, M.H. Cheah, T. Fransson, A. Bhowmick, I.D. Young, L. O'Riordan, A.S. Brewster, I. Pettinati, M. Doyle, Y. Joti, S. Owada, K. Tono, A. Batyuk, M.S. Hunter, R. Alonso-Mori, U. Bergmann, R.L. Owen, N.K. Sauter, T.D.W. Claridge, C.V. Robinson, V.K. Yachandra, J. Yano, J.F. Kern, A.M. Orville, C.J. Schofield, *Science Advances*, 2021, 7(34):eabh0250, "A X-ray free-electron laser studies reveal correlated motion during isopenicillin N synthase catalysis".

76. A.J.M. Farley, Y. Ermolovich, K. Calvopina, P. Rabe, T. Panduwawala, **J. Brem**, F. Björkling, C.J. Schofield, *ACS Infectious Diseases*, 2021, 7(6):1809-1817, "Structural Basis of Metallo- β -lactamase Inhibition by N-Sulfamoylpyrrole-2-carboxylates".

75. A. Lucic, P. Hinchliffe, T.R. Malla, C.L. Tooke, **J. Brem**, K. Calvopiña, C.T. Lohans, P. Rabe, M.A. McDonough, T. Armistead, A.M. Orville, J. Spencer, C.J. Schofield, *European Journal of Medicinal Chemistry*, 2021, 215:113257, "Faropenem reacts with serine and metallo- β -lactamases to give multiple products".

74. P.A. Lang, T.M. Leissing, M.G.P. Page, C. Schofield **J. Brem**, 2020, *Antimicrobial Agents and Chemotherapy*, 2021, 65(2):e02073-20, "Structural Investigations of the Inhibition of Escherichia coli AmpC β -Lactamase by Diazabicyclooctanes". **Corresponding author**.

2020

73. P.A. Lang, A. Parkova, T.M. Leissing, K. Calvopiña, R. Cain, A. Krajnc, T.D. Panduwawala, J. Philippe, C.W.G. Fishwick, P. Trapencieris, M.G.P. Page, C.J. Schofield, **J. Brem**, 2020, *Biomolecules*, 10(6),

899, "Bicyclic Boronates as Potent Inhibitors of AmpC, the Class C β -Lactamase from *Escherichia coli*". **Corresponding author.**

72. A.M. Rydzik, **J. Brem**, S.A. Chandler, J.L.P. Benesch, T.D.W. Claridge, C.J. Schofield, 2020, RSC Medicinal Chemistry, 11, 387-391, "Monitoring protein-metal binding by ^{19}F NMR – a case study with the New Delhi metallo- β -lactamase 1". **Co-first author.**

71. L.Tselepis, G.W. Langley, A.F. Aboklaish, E. Widlake, D.E. Jackson, T.R. Walsh, C.J. Schofield, **J. Brem**, J.M. Tyrrell, 2020, International Journal of Antimicrobial Agents, 56(1), 105925, "In vitro efficacy of Imipenem-Relebactam and Cefepime-AAI101 against a global collection of ESBL-positive and carbapenemase-producing Enterobacteriaceae". **Co-corresponding author.**

70. C.L. Tooke, P. Hinchliffe, A. Krajnc, A.J. Mulholland, **J. Brem**, C.J. Schofield, J. Spencer, 2020, RSC Medicinal Chemistry, 11, 491-496, "Cyclic boronates as versatile scaffolds for KPC-2 β -lactamase inhibition".

69. A. Parkova, A. Lucic, A. Krajnc, **J. Brem**, K. Calvopina, G. Langley G, M.A. McDonough, P. Trapencieris, C.J. Schofield, 2019, ACS Infectious Diseases, 6(6), 1398-1404, "Broad Spectrum β -lactamase Inhibition by a Thioether Substituted Bicyclic Boronate".

2019

68. A. Krajnc, **J. Brem**, P. Hinchliffe, K. Calvopiña, T.D. Panduwawal, P.A. Lang, J.J.A.G. Kamps, J.M. Tyrrell, E. Widlake, B.G. Saward, T.R. Walsh, J. Spencer, C.J. Schofield, 2019, Journal of Medicinal Chemistry, 62 (18), 8544-8556, "Bicyclic Boronate VNRX-5133 Inhibits Metallo- and Serine- β -Lactamases".

67. C.T. Lohans, E.L. Freeman, E. van Groesen, C. L. Tooke, P. Hinchliffe, J. Spencer, **J. Brem**, C. J. Schofield, 2019, Scientific Reports, 9:13608, "Mechanistic insights into β -Lactamase-catalysed carbapenem Degradation through product characterisation".

66. E. Z. A. Nagy, S. D. Tork, P. A. Lang, A. Filip, F. D. Irimie, L. Poppe, M. I. Toşa, C. J. Schofield, **J. Brem**, C. Paizs, L. C. Bencze, 2019, ACS Catalysis, 9, 8825-8834, "Mapping the Hydrophobic Substrate Binding Site of Phenylalanine Ammonia Lyase from *Petroselinum crispum*".

65. M. Munnik, C. T. Lohans, P. A. Lang, G. W. Langley, T. R. Malla, A. Tumber, C. J. Schofield, **J. Brem**, 2019, Chemical Communications, 2019, 55, 10214-10217, "Targeting the *Mycobacterium tuberculosis* transpeptidase Ldt_{Mt2} with cysteine-reactive inhibitors including ebselen" **Co-corresponding author**

64. C. L. Tooke, P. Hinchliffe, P. A. Lang, A. J. Mulholland, **J. Brem**, C. J. Schofield, J. Spencer, 2019, Antimicrobial Agents and Chemotherapy, 63(10), e00564-19, "Molecular Basis of Class A β -lactamase Inhibition by Relebactam".

63. M. Munnik, C. T. Lohans, G. W. Langley, C. Bon, **J. Brem**, C. J. Schofield, 2019, ChemBioChem, Accepted Articles, "A Fluorescence-based Assay for Screening β -Lactams Targeting the *Mycobacterium tuberculosis* Transpeptidase Ldt_{Mt2}".

62. E. Groesen, C. T. Lohans, **J. Brem**, K.M.J. Aertker, T. D. W. Claridge. C. J. Schofield, 2019. Chemistry A European Journal, 2019, 25(51): 11837-11841, " ^{19}F -NMR Monitoring of Reversible Protein Post-Translational Modifications: Class D β -Lactamase Carbamylation and Inhibition".

61. G. W. Langley, R. Cainc, J. M. Tyrrell, P. Hinchliffe, K. Calvopiña, C. Tooke, E. Widlake, C. G. Dowson, J. Spencer, T. R. Walsh, C. J. Schofield, **J. Brem**, 2019. Bioorganic & Medicinal Chemistry Letters, 29(15), 1981-1984, "Profiling Interactions of Vaborbactam with Metallo- β -Lactamases", **Co-corresponding author.**

60. A. Krajnc, P.A. Lang, T.D. Panduwawala, **J. Brem**, C.J. Schofield, 2019. Current Opinion in Chemical Biology, 50, 101-110, "Will morphing boron-based inhibitors beat the β -lactamases?". **Co-first author.**

59. S.T. Cahill, J.M. Tyrrell, I.H. Navratilova, K. Calvopiña, S.W. Robinson, C.T. Lohans, M.A. McDonough, R. Cain, C.W.G. Fishwick, M.B. Avison, T.R. Walsh, C.J. Schofield, **J. Brem**, 2019, *Biochimica et Biophysica Acta (BBA) - General Subjects*, 1863(4), 742-748, "Studies on the inhibition of AmpC and other β -lactamases by cyclic boronates". **Co-corresponding author**
58. C.T. Lohans, H.T.H. Chan, T.R. Malla, K. Kumar, J.J.A.G. Kamps, D.J.B. McArd, E. van Groesen, M. de Munnik, C.L. Tooke, J. Spencer, R.S. Paton, **J. Brem**, C.J. Schofield, 2018, *Angewandte Chemie International Edition*, 58(7), 1990-1994, "Non-Hydrolytic β -Lactam Antibiotic Fragmentation by L,D-Transpeptidases and Serine β -Lactamase Cysteine Variants".
57. R. Salimraj, P. Hinchliffe, M. Kosmopoulou, J.M. Tyrrell, **J. Brem**, S.S. van Berkel, A. Verma, R.J. Owens, M.A. McDonough, T.R. Walsh, C.J. Schofield, J. Spencer, 2018, *FEBS Journal*, 286(1), 169-183, "Crystal Structures of VIM-1 Complexes Explain Active Site Heterogeneity in VIM-Class Metallo- β -Lactamases".

2018

56. I. Pettinati, P. Grzechnik, C. Ribeiro de Almeida, **J. Brem**, M.A. McDonough, S. Dhir, N.J. Proudfoot, C.J. Schofield, 2018, *eLife Sciences*, e39865A, "Biosynthesis of histone messenger RNA employs a specific 3' end endonuclease".
55. Z. Dong, M. S. Markoulides, D. Stepanovs, A. M. Rydzik, A. El-Hussein, C.A.M. Bon, J.J.A.G. Kamps, K.-D. Umland, P. M. Collins, S.T. Cahill, D.Y. Wang, T.D.W. Claridge, **J. Brem**, Michael A. McDonough, Christopher J. Schofield, 2018, *Bioorganic & Medicinal Chemistry*, 26 (11), 2928-2936, "Structure activity relationship studies on rhodanines and derived enethiol inhibitors of metallo- β -lactamases"
54. Z. Chen, Y.-C. Pu, Z.-J. Yu, C.-U. Wu, **J. Brem**, M.A. McDonough, C.J. Schofield, G.-B. Li, Y. Wu, 2018, *Organic Chemistry Frontiers*, 5, 1288-1292, "Rh(III)-Catalyzed Directed C-H Carbenoid Coupling Reveals Aromatic Bisphosphonates Inhibiting Metallo- and Serine- β -Lactamases".
53. M.I. Abboud, M. Kosmopoulou, A.P. Krismanich, J.W. Johnson, P. Hinchliffe, **J. Brem**, T.D.W. Claridge, J. Spencer, C.J. Schofield, G.I. Dmitrienko, 2018, *Chemistry A - European Journal*, 24(22), 5734-5737, "Cyclobutanone Mimics of Intermediates in Metallo- β -Lactamase Catalysis".
52. C.T. Lohans, E. van Groesen, K. Kumar, C.L. Tooke, J. Spencer, R.S. Paton, **J. Brem**, C.J. Schofield, 2018, *Angewandte Chemie International Edition*, 57(5), 1282-1285, "A New Mechanism for β -Lactamases: Class D Enzymes Degrade 1 β -Methyl Carbapenems via Lactone Formation".
51. R. Cain, **J. Brem**,* D. Zollman, M.A. McDonough, R.M. Johnson, J. Spencer, A. Makena, M.I. Abboud, S. Cahill, S.Y. Lee, P. McHugh, C.J. Schofield, C.W.G. Fishwick, 2018, *Journal of Medicinal Chemistry*, 61(3), 1255-1260, "In silico fragment based design identifies subfamily B1 metallo- β -lactamase inhibitors"; ***Co-first author**.

2017

50. M.I. Abboud, P. Hinchliffe, **J. Brem**, R. Macsics, I. Pfeffer, A. Makena, K.-D. Umland, A.M. Rydzik, G.-B. Li, J. Spencer, T.D.W. Claridge, C.J. Schofield, 2017, *Angewandte Chemie International Edition*, 56 (14), 3862-3866, "¹⁹F-NMR Reveals the Role of Mobile Loops in Product and Inhibitor Binding by the São Paulo Metallo- β -Lactamase".
49. C.T. Lohans, **J. Brem**,* C.J. Schofield, 2017, *Antimicrobial Agents and Chemotherapy*, 61(12), e01224-17, "New Delhi metallo- β -lactamase 1 catalyses avibactam and aztreonam hydrolysis"; **Co-corresponding author**.

48. K. Calvopiña, P. Hinchliffe, **J. Brem**, K.J. Heesom, S. Johnson, R. Cain, C.T. Lohans, C.W.G. Fishwick, C.J. Schofield, J. Spencer, M.B. Avison, 2017, *Molecular Microbiology*, 106(3), 492–504, “Structural/mechanistic insights into the efficacy of non-classical β -lactamase inhibitors against extensively drug resistant *Stenotrophomonas maltophilia* clinical isolates.”
47. C.T. Lohans, D.Y. Wang, C. Jorgensen, S.T. Cahill ST, I.J. Clifton, M.A. McDonough, H.P. Oswin, J. Spencer, C. Domene, T.D.W. Claridge, **J. Brem**,* C.J. Schofield., 2017, *Organic and Biomolecular Chemistry*, 15(28), 6024-6032, “ ^{13}C -Carbamylation as a mechanistic probe for the inhibition of class D β -lactamases by avibactam and halide ions”; **Co-corresponding author**.
46. G.-B. Li, **J. Brem**,* R. Lesniak, M. I. Abboud, C. T. Lohans, I. J. Clifton, S.-Y. Yang, J.-C. Jimenez-Castellanos, M. B. Avison, J. Spencer, M. A. McDonough, C. J. Schofield*, 2017, *Chemical Communications*, 53, 5806-5809, “Crystallographic Analyses of Isoquinoline Complexes Reveal a New Mode of Metallo- β -Lactamase Inhibition”; **Co-first author**.
45. S. T. Cahill, R. Cain, D. Y. Wang, C. T. Lohans, D. W. Wareham, H. P. Oswin, J. Mohammed, J. Spencer, C. W. G. Fishwick, M. A. McDonough, C. J. Schofield, **J. Brem**, 2017, *Antimicrobial Agents and Chemotherapy*, 61(4), e02260-16, “Cyclic Boronates Inhibit All Classes of β -Lactamase”, **Corresponding author**.
44. P. Hinchliffe, Q. E. Yang, E. Portal, T. Young, H. Li, C. L. Tooke, M. J. Carvalho, N. G. Paterson, **J. Brem**, P. R. Niumsup, U. Tansawai, L. Lei, M. Li, Z. Shen, Y. Wang, C. J. Schofield, A. J. Mulholland, J. Shen, N. Fey, T. R. Walsh, J. Spencer, 2017, *Scientific Reports*, 7, 39392, “Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1”.
43. G.-B. Li, M. I. Abboud, **J. Brem**, H. Someya, C. T. Lohans, S.-Y. Yang, J. Spencer, D. W. Wareham, M. A. McDonough, C. J. Schofield, 2017, *Chemical Science*, 8, 928-937, “NMR-filtered virtual screening leads to non-metal chelating metallo- β -lactamase inhibitors”
42. A. Abuhammad, M. A. McDonough, **J. Brem**, A. Makena, S. Johnson, C. J. Schofield, E. F. Garman, 2017, *Crystal Growth & Design*, 17, 913–924, “To Cross-Seed or Not To Cross-Seed”: A Pilot Study Using Metallo- β -lactamases”.

2016

41. **J. Brem**, R. Cain, S. Cahill, M. A. McDonough, I. J. Clifton, J.-C. Jiménez-Castellanos, M. B. Avison, J. Spencer, C. W. G. Fishwick, C. J. Schofield, 2016, *Nature Communications*, 7:12406, “Structural basis of metallo- β -lactamase, serine- β -lactamase and penicillin-binding protein inhibition by cyclic boronates”. **First author**
40. D. Y. Wang, M. I. Abboud, M. S. Markoulides, **J. Brem**, C. J. Schofield, 2016, *Future Medicinal Chemistry*, 8, 1063-1084, “The road to avibactam: the first clinically useful non- β -lactam working somewhat like a β -lactam”.
39. S. T. Cahill, H. Tarhonskaya, A. M. Rydzik, E. Flashman, M. A. McDonough, C. J. Schofield, **J. Brem**, 2016, *Journal of Inorganic Biochemistry*, 163, 185–193 “Use of ferrous iron by metallo- β -lactamases”. **Co-corresponding author**.
38. R. Salimraj, L. Zhang, P. Hinchliffe, E. M. H. Wellington, **J. Brem**, C. J. Schofield, W. H. Gaze, J. Spencer, 2016, *Antimicrobial Agents and Chemotherapy*, 60(10), 5828-5840, “Structural and Biochemical Characterization of Rm3, a SubClass B3 Metallo- β -Lactamase Identified from a Functional Metagenomic Study.”

37. M. I. Abboud, C. Damblon, **J. Brem**, N. Smargiasso, P. Mercuri, B. Gilbert, A. M. Rydzik, T. D. W. Claridge, C. J. Schofield, J.-M. Frère, 2016, *Antimicrobial Agents and Chemotherapy*, 60(10), 5655-5662, "Interaction of Avibactam with Class B Metallo- β -lactamases".
36. K. Calvopiña, K.-D. Umland, A. M. Rydzik, P. Hinchliffe, **J. Brem**, J. Spencer, C. J. Schofield, M. B. Avison, 2016, *Antimicrobial Agents and Chemotherapy*, 60(7), 4170-4175, "Sideromimic Modification of Lactivicin Dramatically Increases Potency against Extensively Drug-Resistant *Stenotrophomonas maltophilia* Clinical Isolates."
35. S.Y. Lee, **J. Brem**, I. Pettinati, T. D. W. Claridge, O. Gileadi, C. J. Schofield, P. J. McHugh, 2016, *Chemical Communications*, 52, 6727-6730, "Cephalosporins inhibit human metallo- β -lactamase fold DNA repair nucleases SNM1A and SNM1B/Apollo".
34. A. Khan, R. Lesniak, **J. Brem**, A.M. Rydzik, H. Choi, I.K.H. Leung, M.A. McDonough, C.J. Schofield, T.D.W. Claridge, 2016, *Medicinal Chemistry Communication*, 7, 873-880. "Development and application of ligand-based NMR screening assays for γ -butyrobetaine hydroxylase."
33. I. Pettinati, **J. Brem**, S.Y. Lee, P.J. McHugh, C.J. Schofield, 2016, *Trends in Biochemical Sciences*, 41, 338–355. "The Chemical Biology of Human Metallo- β -Lactamase Fold Proteins."
32. J.W. Betts, L.M. Phee, M.H.F. Abdul Momin, K. Umland, **J. Brem**, C.J. Schofield, D.W. Wareham, 2016, *Medicinal Chemistry Communication*, 7, 190. "In-vitro and in-vivo Activity of ML302F: A Thioenolate Inhibitor of VIM-subfamily Metallo β -lactamases."
31. J.J.A.G. Kamps, A. Khan, H. Choi, R.K. Lesniak, **J. Brem**, A.M. Rydzik, M.A. McDonough, C.J. Schofield, T.D.W. Claridge, J. Mecinović, 2015, *Chemistry - A European Journal*, 22, 1270–1276. "Cation- π Interactions Contribute to Substrate Recognition in γ -Butyrobetaine Hydroxylase Catalysis."
30. A. Makena, A.Ö. Düzgün, **J. Brem**, M.A. McDonough, A.M. Rydzik, M.I. Abboud, A. Saral, A.Ç. Çiçek, C. Sandalli, C.J. Schofield, 2015, *Antimicrobial Agents and Chemotherapy*, 60(3), 1377–1384. "Comparison of Verona Integron-Borne Metallo- β -lactamase Variants Reveals Differences in Stability and Inhibition Profiles."

2015

29. **J. Brem**, S.S.v. Berkel, D. Zollman, S.Y. Lee, O. Gileadi, P.J. McHugh, T.R. Walsh, M.A. McDonough, C.J. Schofield, 2015, *Antimicrobial Agents and Chemotherapy*, 60(1), 142-150. "Structural basis of metallo- β -lactamase inhibition by captopril stereoisomers." **First author**
28. M.M. González, M. Kosmopoulou, M.F. Mojica, V. Castillo, P. Hinchliffe, I. Pettinati, **J. Brem**, C.J. Schofield, G. Mahler, R.A. Bonomo, L.I. Llarrull, J. Spencer, A.J. Vila, 2015, *ACS Infectious Diseases*, 1, 544. "Bisthiazolidines: A Substrate-Mimicking Scaffold as an Inhibitor of the NDM-1 Carbapenemase."
27. A. Ghavami,* G. Labbé,* **J. Brem**,* V.J. Goodfellow, L. Marrone, C.A. Tanner, D.T. King, M. Lam, N.C.J. Strynadka, D.R. Pillai, S. Siemann, J. Spencer, C.J. Schofield G.I. Dmitrienko, 2015, *Analytical Biochemistry*, 486, 75. "Assay for drug discovery: Synthesis and testing of nitrocefin analogues for use as β -lactamase substrates." ***The contribution of these authors should be considered equal.**
26. I Pettinati, **J. Brem**, .A. McDonough, C.J. Schofield, 2015, *Human Molecular Genetics*, 24, 2458. "Crystal structure of human persulfide dioxygenase: structural basis of ethylmalonic encephalopathy".
25. **J. Brem**, W.B. Struwe, A.M. Rydzik, H. Tarhonskaya, I. Pfeffer, E. Flashman, S.S. van Berkel, J. Spencer, T.D.W. Claridge, M.A. McDonough, J.L.P. Benesch, C.J. Schofield, 2015, *Chemical Science*, 6, 956. "Studying the active-site loop movement of the São Paulo metallo- β -lactamase-1." **First author**

2014

24. A. Abuhammad, M.A. McDonough, **J. Brem**, C.J. Schofield, E. Garman, 2014, *Acta Crystallographica Section A: Foundations and Advances*, **A70**, C1144. "From one seed a whole handful": homologous proteins as seeds in crystallisation.
23. A. Makena, **J. Brem**, I. Pfeffer R.E. Geffen, S.E. Wilkins, H. Tarhonskaya, E. Flashman, L.M. Phee, D.W. Wareham, C.J. Schofield, 2014, *Journal of Antimicrobial and Chemotherapy*, **70**, 463. "Biochemical characterization of New Delhi metallo- β -lactamase variants reveals differences in protein stability."
22. **J. Brem**, S.S. van Berkel, W. Aik, A.M. Rydzik, M.B. Avison, I. Pettinati, K.D. Umland, A. Kawamura, J. Spence, T.D. Claridge, M.A. McDonough, C.J. Schofield, 2014, *Nature Chemistry*, **6**, 1084. "Rhodanine hydrolysis leads to potent thioenolate mediated metallo- β -lactamase inhibition". **First author**
21. A.M. Rydzik, **J. Brem**, W.B. Struwe, G.T. Kochan, J.L.P. Benesch, C.J. Schofield, 2014, *Bioorganic and Medicinal Chemistry Letters*, **21**, 4954. "Ejection of structural zinc leads to inhibition of γ -butyrobetaine hydroxylase."
20. A.M. Rydzik, * **J. Brem**,* S.S. van Berkel, I. Pfeffer, A. Makena, T.D.W. Claridge, C.J. Schofield, C.J., 2014, *Angewandte Chemie*, **53**, 3129. "Monitoring conformational changes in the NDM-1 metallo- β -lactamase by ^{19}F NMR spectroscopy." ***The contribution of these authors should be considered equal.**
19. B. Nagy, N. Dima, C. Paizs, **J. Brem**, F. D. Irimie, M. I. Toşa, 2014, *Tetrahedron: Asymmetry*, **25**, 1316. "New chemo-enzymatic approaches for the synthesis of (*R*)- and (*S*)-bufuralol."

2013

18. R.B. Hamed, L. Henry, J.R. Gomez-Castellanos, A. Asghar, **J. Brem**, T.D.W. Claridge, C.J., 2013 *Organic and Biomolecular Chemistry*, **47**, 8191. "Stereoselective preparation of lipidated carboxymethyl-proline/pipecolic acid derivatives via coupling of engineered crotonases with an alkylmalonyl-CoA synthetase."
17. S.S. van Berkel, * **J. Brem**,* A.M. Rydzik, R. Salimraj, R. Cain, R., A. Verma, R.J. Owens, C.W. Fishwick, J. Spencer, C.J. Schofield, 2013, *Journal of Medicinal Chemistry*, **56(17)**, 6945-53. "Assay Platform for Clinically Relevant Metallo- β -lactamases." ***The contribution of these authors should be considered equal.**
16. A. Makena, S.S. van Berkel, C. Lejeune, R.J. Owens, A. Verma, R. Salimraj, J. Spencer, **J. Brem**,* C.J. Schofield, 2013, *ChemMedChem*, **8**, 1929. "Chromophore-linked substrate (CLS405): Probing metallo- β -lactamase activity and inhibition." ***Co-corresponding author.**
15. S.S. Berkel, J.E. Nettleship, I.K.H. Leung, **J. Brem**, H. Choi, D. I. Stuart, T.D.W. Claridge, M.A. McDonough, R.J. Owens, J. Ren, C.J. Schofield, 2013, *ACS Chemical Biology*, **8(10)**, 2112-2116. "Binding of (5*S*)-Penicilloic Acid to Penicillin Binding Protein 3."
14. D. Hapău, **J. Brem**, M. Moisă, M. I. Toşa, F. D. Irimie, V. Zaharia, 2013, *Journal of Molecular Catalysis B: Enzymatic*, **94**, 88. "Heterocycles 32. Efficient kinetic resolution of 1-(2-arylthiazol-4-yl) ethanol and their acetates using lipase B from *Candida antarctica*."
13. M. I. Toşa, **J. Brem**, A. Mantu, F. D. Irimie, C. Paizs, J. Rétey, 2013, *ChemCatChem*, **5(3)**, 779-783. "The Interaction of Nitrophenylalanines with Wild Type and Mutant 4-Methylideneimidazole-5-one-less Phenylalanine Ammonia Lyase."

2012

12. **J. Brem**, C.-L. Bencze, M.C. Turcu, C. Paizs, F.D. Irimie, L.T. Kanerva, 2012, *European Journal of Organic Chemistry*, 17, 3288. "Chemoenzymatic preparation of 1-heteroarylethanamines of low solubility." **First author**
11. M. Naghi, C.-L. Bencze, **J. Brem**, P. Csaba, F.D. Irimie, M.I. Toşa, 2012, *Tetrahedron: Asymmetry*, 23, 181. "Sequential enzymatic procedure for the preparation of enantiomerically pure 2-heteroaryl-2-hydroxyacetic acids."
10. **J. Brem**, M.C. Turcu, C. Paizs, K. Lundell, M.I. Toşa, F.D. Irimie, L.T. Kanerva, 2012, *Process Biochemistry*, 47, 119. "Immobilization to improve the properties of *Pseudomonas fluorescens* lipase for the kinetic resolution of 3-aryl-3-hydroxy esters." **First author**

2011

9. D. Hapău, **J. Brem**, V. Zaharia, 2011, *Tetrahedron: Asymmetry*, 22, 2165. "Heterocycles 30: Lipase catalyzed kinetic resolution of racemic 1-(2-aryl-4-methyl-thiazol-5-yl)ethanols."
8. **J. Brem**, M. Naghi, M.I. Toşa, Z. Boros, L. Poppe, F.D. Irimie, P. Csaba, 2011, *Tetrahedron: Asymmetry*, 22, 1672. "Lipase mediated sequential resolution of aromatic β -hydroxy esters using fatty acid derivatives." **First author**
7. **J. Brem**, S. Pilbák, C. Paizs, G. Bánóczy, F.D. Irimie, M.I. Toşa, L. Poppe, 2011, *Tetrahedron: Asymmetry*, 22, 916. "Lipase-catalyzed kinetic resolution of racemic 1-(10-ethyl-10H-phenothiazin-1,2, and 4-yl)ethanols and their acetates." **First author**
6. **J. Brem**, A. Liljeblad, C. Paizs, M.I. Toşa, F.D. Irimie, L.T. Kanerva, 2011, *Tetrahedron: Asymmetry*, 22, 315. "Lipases A and B from *Candida antarctica* in the enantioselective acylation of ethyl 3-heteroaryl-3-hydroxypropanoates: aspects on preparation and enantioference." **First author**

2010

- 5 **J. Brem**, M.I. Toşa, C. Paizs, A. Munceanu, D. Matković-Čalogović, F.D. Irimie, 2010, *Tetrahedron: Asymmetry*, 21, 1993. "Lipase-catalyzed kinetic resolution of racemic 1-(10-alkyl-10H-phenothiazin-3-yl)ethanols and their butanoates." **First author**
4. **J. Brem**, M.I. Toşa, C. Paizs, E. Vass, F.D. Irimie, 2010, *Tetrahedron: Asymmetry*, 21, 365. "Enzyme-catalysed synthesis of (*R*)- and (*S*)-3-hydroxy-3-(10-alkyl-10H-phenothiazin-3-yl)propionic acids." **First author**
3. C. Paizs, M.I. Toşa, C.-L. Bencze, **J. Brem**, F.D. Irimie, J. Rétey, 2010, *Heterocycles*, 82, 1217, "2-amino-3-(5-phenylfuran-2-yl)propionic acids and 5-phenylfuran-2-ylacrylic acids are novel substrates of phenylalanine ammonia-lyase."

2009

2. D. Sandu, I. Lingvay, S. Lányi, D.D. Micu, C.L. Popescu, **J. Brem**, C.-L. Bencze, C. Paizs, 2009, *Studia Universitatis Babes-Bolyai Chemia*, 4, 195. "The effect of electromagnetic fields on baker's yeast population dynamics, biocatalytic activity and selectivity. "
1. **J. Brem**, C. Paizs, M.I. Toşa, E. Vass, F.D. Irimie, 2009, *Tetrahedron: Asymmetry*, 20, 489-496. "Enzyme-catalysed synthesis of (*R*)- and (*S*)-3-heteroaryl-3-hydroxypropanoic acids and their derivatives." **First author**

Patents

1. **J. Brem**, S.v. Berkel, M.A. McDonough, C.J. Schofield, WO/2016/051133 A1 (WO, EP, US); *Beta Lactamase Inhibitors*.
2. **J. Brem**, A.M. Rydzik, M.A. McDonough, C.J. Schofield, A. Morrison, J. Hewitt, A. Pannifer, P. Jones, WO2017093727A1 (WO, EP, JP, CN, AU); *Inhibitors of metallo-beta-lactamases*.
3. **J. Brem**, C.J. Schofield, S.T. Cahill, K. Calvopina, P. Hinchcliffe, R. Cain, J. Spencer, C.W.G. Fishwick, M. B. Avison, WO2018211289 (WO, EP); *β -lactamase inhibitors*.
4. J. Gising, S. Lindstrom, D. Antonov, P. Brandt, A.K. Belfrage, **J. Brem**, C.J. Schofield., WO2018/215800 (WO, EP); *Inhibitors of metallo- β -lactamases (5/5 series)*.
5. T. Panduwawala, P. Brandt, D. Wang, M. Andaloussi, **J. Brem**, C.J. Schofield, WO2018/215799 (WO, EP); *Inhibitors of metallo- β -lactamases (Pyrrole / Imidazole series)*.
6. C. Schofield, **J. Brem**, T. Panduwawala, A. Farley, E. Suna, WO2022248887A1, 2-carboxyl-indole inhibitors of metallo-beta-lactamases

Book

“*Insight in pure and applied biocatalysis*”, C. Paizs, A. Katona, C.L. Bencze, **J. Brem**, 2015, Napoca Star, Cluj-Napoca.

Selected presentations and invited talks

15. Industry Academia Collaboration in AMR R&D: Does it Take Two to Tango?, 23rd September, Drug Discovery Conference 2022, Riga. (invited talk)
14. Inhibition of the bacterial metallo- β -lactamases, 25th August 2020, AMR Conference, Basel. (invited talk)
13. Enabling antibiotics to combat multidrug resistant bacteria, 12th November 2019, Pasteur Institute, France. (invited talk)
12. The Chemistry of β -Lactam Antibiotic Resistance, CDT Antibacterial Drug Discovery Briefing Day, 4th Jan 2018, Oxford, UK. (invited talk)
11. Tackling anti-microbial resistance, development of novel metallo- β -lactamase inhibitors, 6th Pharmaceutical Sciences World Congress, 21-24 May 2017. (invited talk)
10. HTS against bacterial metallo- and serine-beta lactamases, towards clinically useful inhibitors, 16-19th June 2017, 13th Beta lactamase meeting, Santo Stefano di Sessanio, in L'Aquila (IT) (invited talk).
9. Structural biology and assays enabling β -lactams that target, Mycobacterium tuberculosis, Open Lab TC241 GSK Tres Cantos Madrid, Spain, 20th November 2017 meeting (poster)
8. Dual serine and metallo- β -lactamase inhibitors: Enabling antibiotics to combat multidrug resistant bacteria Birmingham BSAC meeting, December 2017, oral presentations.
7. HTS against bacterial metallo-beta-lactamases, Towards clinically useful inhibitors, EFMC – ICMC, Manchester, 2016

6. Revealing the Structural Basis of Pan Metallo- β -Lactamase Inhibition by Captopril Stereoisomers, 17 September - 21 September 2015, ICAAC/ICC 2015 San Diego, USA. (oral presentation)
5. Assays for the development of broad spectrum metallo- β -lactamase inhibitors, 28 June – 1 July 2014, 12th Beta-Lactamase Meeting, Gran Canaria, Spain. (oral presentation).
4. Development of metallo- β -lactamase inhibitors, Seminar, 13 September 2013, Bristol, UK. (invited talk)
3. Towards broad spectrum metallo- β -lactamase inhibitors. 13-17 July 2013, UK Canada Antimicrobial resistance meeting, Waterloo, Canada. (oral presentation)
2. Metallo-beta-Lactamases: Structure and Inhibition, enGENEious, 25-26 June 2012, Oxford. (poster presentation)
1. Biocatalytic synthesis of benzofuran and benzothiophene based optically active heteroaryl- β -hydroxy-propanoic acid derivatives, 4th International congress on biocatalysis, 31 August - 4 September, 2008, Hamburg, Germany. (poster presentation).

