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Refereed Publications, 31 Dec 2025

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GIDEON DAVIES. Refereed[†] Publications

2026 Shaded

431.	Burchill, L., <i>et al.</i> Bridging a Gap in Marine Sulfur Cycling: Discovery of a D-Cysteinolic Acid Degradation Pathway <i>J Am Chem Soc.</i> 2025 147, 47934-47941 https://doi.org/10.1021/jacs.5c11066
430.	Sharma, M., Pudlo, N., Järvå, M., Kaur, A., John, A., Burchill, L., Lingford, J.P., Epa, R., Abayakoon, P., Scott, N.E., Turkenburg, J.P., Davies, G.J., Martens, E.C., Goddard-Borger, E.D., and Williams, S.J. Sulfoglycolysis sustains <i>Eubacterium rectale</i> in low-fiber diets <i>J Biol Chem.</i> 2025 301, Article 108320. https://doi.org/10.1016/j.jbc.2025.108320
429.	Ruijgrok, G., Offen, W.A., Pickles, I.B., Raju, D., Patsos, T., de Boer, C., Ofman, T., Rompa, J., van Oord, D., Dodson, E.J., Beekers, A., Voskuilen, T., Ferrari, M., Wu, L., Janssen, A.P.A., Codée, J.D.C., Howell, L., Davies, G.J., and Overkleeft, H.S. Bespoke activity-based probes reveal that the <i>Pseudomonas aeruginosa</i> endoglycosidase, PslG, is an endo- β -glucanase <i>J Am Chem Soc.</i> 2025 147, 8578–8586. https://doi.org/10.1021/jacs.4c16806
428.	Roth, C., Moroz, O.V., Miranda, S.A.D., Jahn, L., Blagova, E.V., Lebedev, A.A., Segura, D.R., Stringer, M.A., Friis, E.P., Davies, G.J., and Wilson, K.S. Structures of α -galactosaminidases from the CAZy GH114 family and homologs defining a new GH191 family of glycosidases <i>Acta Crystallogr.</i> 2025 D81, 234-251. https://doi.org/10.1107/S2059798325002864
427.	Radchenko, Y., Aerts, J.M.F.G., Davies, G.J., Codée, J.D.C., Overkleeft, H.S. (2025). Activity-Based Profiling of Retaining Glycosidases in Disease Diagnosis and Their Application in Drug Discovery. In Handbook of Experimental Pharmacology. (Berlin, Heidelberg: Springer Berlin Heidelberg), pp. 1-16. https://doi.org/10.1007/164_2025_743
426.	Pickles, I.B., Correa, T.L.R., Overkleeft, H.S., and Davies, G.J. Activity-based probes for dynamic characterisation of polysaccharide-degrading enzymes <i>Biochem. J.</i> 2025a 482, 939-954. https://doi.org/10.1042/bcj20253060
425.	Pickles, I.B., Chen, Y., Moroz, O., Brown, H.A., de Boer, C., Armstrong, Z., McGregor, N.G.S., Artola, M., Codée, J.D.C., Koropatkin, N.M., Overkleeft, H.S., and Davies, G.J. Precision activity-based α -amylase probes for dissection and annotation of linear and branched-chain starch degrading enzymes <i>Angew Chemie Int Ed.</i> 2025b e202415219. https://doi.org/10.1002/anie.202415219
424.	Males, A., Moroz, O.V., <i>et al.</i> Expansion of the diversity of Dispersin scaffolds <i>Acta Crystallogr.</i> 2025 D81, 130-146. https://doi.org/10.1107/S205979832500110X
423.	Cairo, J.P.L.F., <i>et al.</i> Signal-strapping: a protein-sequence search method for the discovery of metalloproteins <i>Nature Commun.</i> 2025 16, Article number 9244. https://doi.org/10.1038/s41467-025-64309-x
422.	Burchill, L., Sharma, M., Soler, N.M., Goddard-Borger, E.D., Davies, G.J., and Williams, S.J. Structure, kinetics, and mechanism of <i>Pseudomonas putida</i> sulfoquinovose dehydrogenase, the first enzyme in the sulfoglycolytic Entner-Doudoroff pathway <i>Biochemical J.</i> 2025 482, 57-72. https://doi.org/10.1042/BCJ20240605

[†] Gideon Davies has 16 unrefereed book chapters that are not included in this list.

421.	Thaler, M., Ofman, T.P., Kok, K., Heming, J.J.A., Moran, E., Pickles, I., Leijts, A.A., an den Nieuwendijk, A.M.C.H.v., van den Berg, R.J.B.H.N., Ruijgrok, G., Armstrong, Z., Salgado-Benvindo, C., Ninaber, D.K., Snijder, E.J., van Boeckel, C.A.A., Artola, M., Davies, G.J., Overkleeft, H.S., and Hemert, M.J.v. Epi-cyclophellitol cyclosulfate, a mechanism-based ER α -glucosidase II inhibitor, blocks replication of SARS-CoV-2 and other coronaviruses <i>ACS Central Science</i> . 2024 <i>10</i> , 1594–1608. https://doi.org/10.1021/acscentsci.4c00506
420.	Su, Q., Louwerse, M., Lammers, R.F., Maurits, E., Janssen, M., Boot, R.G., Borlandelli, V., Offen, W.A., Linzel, D., Schröder, S.P., Davies, G.J., Overkleeft, H.S., Artola, M., and Aerts, J.M.F.G. Selective Labelling of GBA2 in Cells with Fluorescent β -D-Arabinofuranosyl Cyclitol Aziridines <i>Chem Sci</i> . 2024 <i>15</i> , 15212-15220 https://doi.org/10.1039/D3SC06146A
419.	Scott, C., McGregor, N., Leadbeater, D., Oates, N., Hoßbach, J., Abood, A., Setchfield, A., Dowle, A., Overkleeft, H., Davies, G.J., and Bruce, N. <i>Parascedosporium putredinis</i> NO1 tailors its secretome for different lignocellulosic substrates <i>Microbiology Spectrum</i> . 2024 <i>12</i> , e03943-03923. https://doi.org/10.1128/spectrum.03943-23
418.	Rajagopal, B.S., Yates, N., Smith, J., Paradisi, A., Tetard-Jones, C., Willats, W.G.T., Marcus, S., Knox, J.P., Firdaus-Raih, M., Henrissat, B., Davies, G.J., Walton, P.H., Parkin, A., and Hemsworth, G.R. Structural Dissection of Two Redox Proteins from the Shipworm Symbiont <i>Teredinibacter turnerae</i> . <i>IUCR J</i> . 2024 <i>11</i> , 260-274. https://doi.org/10.1107/S2052252524001386
417.	Ofman, T.P., Heming, J.J.A., Nin-Hill, A., Küllmer, F., Moran, E., Bennett, M., Steneker, R., Klein, A.-M., Ruijgrok, G., Kok, K., Armstrong, Z.W.B., Aerts, J.M.F.G., van der Marel, G.A., Rovira, C., Davies, G.J., Artola, M., Codée, J.D.C., and Overkleeft, H.S. Conformational and Electronic Variations in 1,2- and 1,6-Cyclophellitols and Their Impact on Retaining α -Glucosidase Inhibition <i>Chemistry - A European Journal</i> . 2024 e202400723. https://doi.org/10.1002/chem.202400723
416.	Liu, Y., Bineva-Todd, G., Meek, R.W., Mazo, L., Piniello, B., Moroz, O., Burnap, S.A., Begum, N., Ohara, A., Roustan, C., Tomita, S., Kjaer, S., Polizzi, K., Struwe, W.B., Rovira, C., Davies, G.J., and Schumann, B. A Bioorthogonal Precision Tool for human N-acetylglucosaminyltransferase V <i>J Am Chem Soc</i> . 2024 <i>146</i> , 26707–26718. https://doi.org/10.1021/jacs.4c05955
415.	Li, Z., Pickles, I., Sharma, M., Melling, B., Pallasdies, L., Codée, J., Williams, S., Overkleeft, H., and Davies, G. Detection of sulfoquinovosidase activity in cell lysates using activity-based probes <i>Angew Chemie Int Ed</i> . 2024 e202401358. https://doi.org/10.1002/anie.202401358
414.	Koemans, T., Bennett, M., Ferraz, M.J., Armstrong, Z., Artola, M., Aerts, J.M.F.G., Codée, J.D.C., Overkleeft, H.S., and Davies, G.J. Structure-Guided Design of C3-Branched Swainsonine as Potent and Selective Human Golgi α -Mannosidase (GMII) Inhibitor <i>Chem Commun</i> . 2024 <i>60</i> , 11734-11737 https://doi.org/10.1039/D4CC04514A
413.	Chen, Y., van den Nieuwendijk, A.M.C.H., Wu, L., Moran, E., Skoulikopoulou, F., Riet, V.v., Overkleeft, H.S., Davies, G.J., and Armstrong, Z. The molecular basis for inhibition of heparanases and β -glucuronidases by siastatin B <i>J Am Chem Soc</i> . 2024 <i>146</i> , 125–133. https://doi.org/10.1021/jacs.3c04162
412.	Caseiro, C., McGregor, N.G.S., Alves, V.D., Carvalho, A.L., Romão, M.J., Davies, G.J., Fontes, C.M.G.A., and Bule, P. Family GH157 enzyme exhibits broad linkage tolerance and a dual endo / exo- β - glucanase activity on β -glucans <i>International Journal of Biological Macromolecules</i> . 2024 <i>282</i> , Article 137402. https://doi.org/10.1016/j.ijbiomac.2024.137402

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410.	Arumapperuma, T., Lee, M., Sharma, M., Zhang, Y., Snow, A., Lingford, J., Goddard-Borger, E., Davies, G.J., and Williams, S. Capture-and-release of a sulfoquinovose-binding protein on sulfoquinovose-modified agarose <i>OrgBioMol Chem</i> . 2024 <i>22</i> , 3237-3244 https://doi.org/10.1039/D4OB00307A
409.	Artola, M., Aerts, J.M.F.G., van der Marel, G.A., Rovira, C., Codée, J.D.C., Davies, G.J., and Overkleeft, H.S. From mechanism-based retaining glycosidase inhibitors to activity-based glycosidase profiling <i>J Am Chem Soc</i> . 2024 <i>146</i> , 24729–24741. https://doi.org/10.1021/jacs.4c08840
408.	Walton, P.H., Davies, G.J., Diaz, D.E., and Franco-Cairo, J.P. The Histidine Brace: Nature's Copper Alternative to Haem? <i>FEBS Lett</i> . 2023 <i>597</i> , 485-494. https://doi.org/10.1002/1873-3468.14579
407.	van der Gracht, D., Rowland, R.J., Roig-Zamboni, V., Ferraz, M.J., Geurink, P.P., Aerts, J.M.F.G., Sulzenbacher, G., Davies, G.J., Overkleeft, H.S., and Artola, M. Fluorescence Polarisation Activity-Based Protein Profiling in the Identification of Deoxynojirimycin-type Inhibitors selective for Lysosomal Retaining Alpha- and Beta-Glucosidases <i>Chem Sci</i> . 2023 <i>14</i> , 9136-9144 https://doi.org/10.1039/D3SC01021J
406.	Snow, A.J.D., Sharma, M., Abayakoon, P., Williams, S.J., Blaza, J.N., and Davies, G.J. Structure and mechanism of sulfofructose transaldolase, a key enzyme in sulfoquinovose metabolism <i>Structure</i> . 2023 <i>31</i> , 244-252.e244. https://doi.org/10.1016/j.str.2023.01.010
405.	Sharma, M., Kaur, A., Soler, N.M., Lingford, J.P., Epa, R., Goddard-Borger, E.D., Davies, G.J., and Williams, S.J. Defining the molecular architecture, metal dependence, and distribution of metal-dependent class II sulfofructose-1-phosphate aldolases <i>J Biol Chem</i> . 2023 <i>299</i> , 105338. https://doi.org/10.1016/j.jbc.2023.105338
404.	Pengthaisong, S., Piniello, B., Davies, G.J., Rovira, C., and Cairns, J.R.K. Reaction mechanism of glycoside hydrolase family 116 utilizes perpendicular protonation <i>ACS Catalysis</i> 2023 <i>13</i> , 5850–5863. https://doi.org/10.1021/acscatal.3c00620
403.	Moroz, O.V., Blagova, E., Lebedev, A.A., Skov, L.K., Pache, R.A., Schnorr, K.M., Kiemer, L., Friis, E.P., Nymand-Grarup, S., Ming, L., Ye, L., Klausen, M., Cohn, M.T., Schmidt, E.G.W., Davies, G.J., and Wilson, K.S. Module walking using an SH3-like cell wall binding domain leads to a new GH family of muramidases <i>Acta Crystallogr</i> . 2023 <i>D79</i> , 706-720. https://doi.org/10.1107/S2059798323005004
402.	McGregor, N.G.S., de Boer, C., Foucart, Q.P.O., Beenakker, T., Offen, W.A., Codée, J.D.C., Willems, L.I., Overkleeft, H.S., and Davies, G.J. A multiplexing activity-based protein profiling platform for dissection of a native bacterial xyloglucan-degrading system <i>ACS Central Science</i> . 2023 <i>9</i> , 2306–2314. https://doi.org/10.1021/acscentsci.3c00831
401.	Males, A., Kok, K., Nin-Hill, A., Beukel, S.v.d., Beenakker, T.J.M., van der Marel, G.A., Codée, J.D.C., Overkleeft, H.S., Rovira, C., Davies, G.J., and Artola, M. Cyclosulfamidate Mannose-Configured Cyclitol Allows Specific Allele-Dependent Inhibition of GH47 α -D-Mannosidases Through a Bump-Hole Strategy <i>Chem Sci</i> . 2023 <i>14</i> , 13581–13586. https://doi.org/10.1039/d3sc05016e

400.	Lipsh-Sokolik, R., Khersonsky, O., Schröder, S.P., Hoch, S.-Y., Davies, G.J., Overkleeft, H.S., and Fleishmam, S.J. Modularly designed protein fragments combine into thousands of active and structurally diverse enzymes <i>Science</i> . 2023 379, 195-201. https://doi.org/10.1126/science.ade943
399.	Li, J., Sharma, M., Meek, R., Alhifhi, A., Armstrong, Z., Soler, N.M., Goddard-Borger, E.D., Blaza, J., Davies, G.J., and Williams, S.J. Molecular basis of sulfolactate synthesis by sulfolactaldehyde dehydrogenase from <i>Rhizobium leguminosarum</i> <i>Chem Sci</i> . 2023 14, 11429-11440 https://doi.org/10.1039/D3SC01594G
398.	Kuo, C.-L., Su, Q., van den Nieuwendijk, A.M.C.H., Beenakker, T.J.M., Offen, W.A., Willems, L.I., Boot, R.G., Sarris, A.J., Marques, A.R.A., Codée, J.D.C., van der Marel, G.A., Florea, B.I., Davies, G.J., Overkleeft, H.S., and Aerts, J.M.F.G. The Development of a Broad-Spectrum Retaining β -Exo-Galactosidase Activity-Based Probe <i>Org BioMol Chem</i> . 2023 21, 7813-7820. https://doi.org/10.1039/D3OB01261A
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396.	Kaur, A., Pickles, I.B., Sharma, M., Soler, N.M., Scott, N.E., Pidot, S.J., Goddard-Borger, E.D., Davies, G.J., and Williams, S.J. A widespread family of oxidoreductive sulfoquinovosidases at the gateway to sulfoquinovose catabolism <i>J Am Chem Soc</i> . 2023 146, 125-133. https://doi.org/10.1021/jacs.3c11126
395.	Doherty, G.G., Ler, G.J.M., Norbert Wimmer, Bernhardt, P.V., Ashmus, R.A., Vocadlo, D.J., Armstrong, Z.W.B., Davies, G.J., Marco MacCarana, Li, J.-p., Kayal, Y., and Ferro, V. Synthesis of Uronic Acid 1-Azasugars as Putative Inhibitors of α -Iduronidase, β -Glucuronidase and Heparanase <i>ChemBioChem</i> . 2023 24, e202200619. http://dx.doi.org/10.1002/cbic.202200619
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392.	Borlandelli, V., Offen, W.A., Moroz, O., Nin-Hill, A., McGregor, N., Binkhorst, L., Ishiwata, A., Armstrong, Z., Artola, M., Rovira, C., Davies, G.J., and Overkleeft, H.S. β -L-Arabinofuranocyclitol Aziridines are Cysteine-directed Broad-spectrum Inhibitors and Activity-based Probes for Retaining β -L-arabinofuranosidases <i>ACS Chemical Biology</i> . 2023b 8, 2564-2573. https://doi.org/10.1021/acschembio.3c00558
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388.	Walton, P.H., and Davies, G.J. Structural perturbations of substrate binding and oxidation state changes in a lytic polysaccharide monooxygenase <i>J Biol Inorg Chem</i> . 2022 27, 705-713. https://doi.org/10.1007/s00775-022-01966-z
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