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Refereed Publications, 22 May 2025

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GIDEON DAVIES. Refereed[†] Publications

2025 Shaded

429.	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
428.	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
427.	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
426.	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
425.	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> 2025b bcj-2025-3060_C, accepted for publication.
424.	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> 2025a e202415219. https://doi.org/10.1002/anie.202415219
423.	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
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
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 10, 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

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

	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
411.	Bhosale, S., Kandalkar, S., Gilormini, P.-A., Akintola, O., Rowland, R.J., Adabala, P.J.P., King, D., Deen, M.C., Xi, K., Davies, G.J., Voadlo, D.J., and Bennet, A.J. Tunable mechanism-based carbasugar ligands that form a transient covalent intermediate that stabilizes glycoside hydrolases <i>ACS Catalysis.</i> 2024 <i>14</i> , 14769–14779. https://doi.org/10.1021/acscatal.4c04549
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 22, 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 146, 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 597, 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 14, 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 31, 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 299, 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 13, 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., Nyman-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 D79, 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 9, 2306–2314. https://doi.org/10.1021/acscentsci.3c00831
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400.	Lipsh-Sokolik, R., Khersonsky, O., Schröder, S.P., Hoch, S.-Y., Davies, G.J., Overkleeft, H.S., and Fleishman, 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., Alhifithi, 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 <i>14</i> , 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 <i>21</i> , 7813-7820. https://doi.org/10.1039/D3OB01261A
397.	Kolaczowski, B.M., Moroz, O.V., Blagova, E., Davies, G.J., Möller, M.S., Meyer, A.S., Westh, P., Jensen, K., Wilson, K.S., and Krogh, K.B.R.M. Structural and functional characterization of a multi-domain GH92 α -1,2-mannosidase from <i>Neobacillus novalis</i> <i>Acta Crystallographica.</i> 2023 <i>D</i> <i>79</i> , 387-400. https://doi.org/10.1107/S2059798323001663
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 <i>146</i> , 125-133. https://doi.org/10.1021/jacs.3c11126
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