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... that face special stereoelectronic challenges in effecting the hydrolysis of the glycosidic bond. In their Communication on page 10997 ff., C. Rovira, G. J. Davies, and co-workers use QM/MM calculations, supported by X-ray structures of the enzyme with ligands mimicking the substrate, transition state, and product, to show that the free-energy landscape of an isolated alpha-mannoside is shaped on-enzyme into a single conformational itinerary along the reaction coordinate.



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