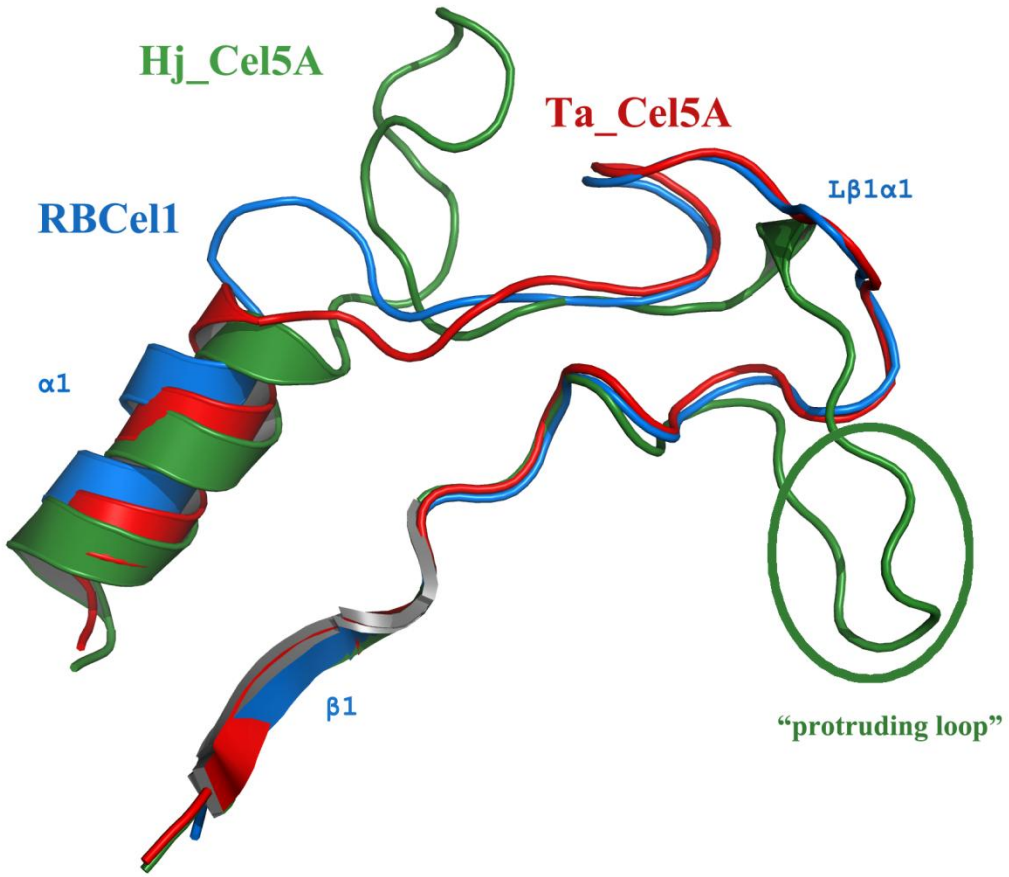
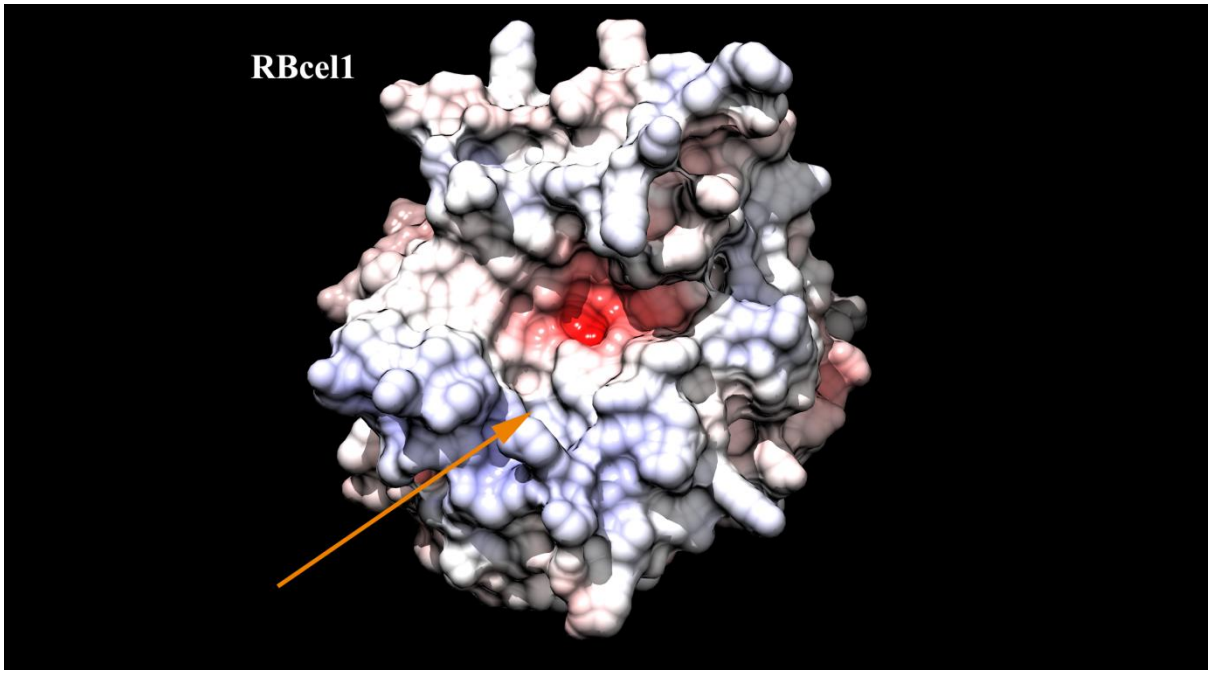
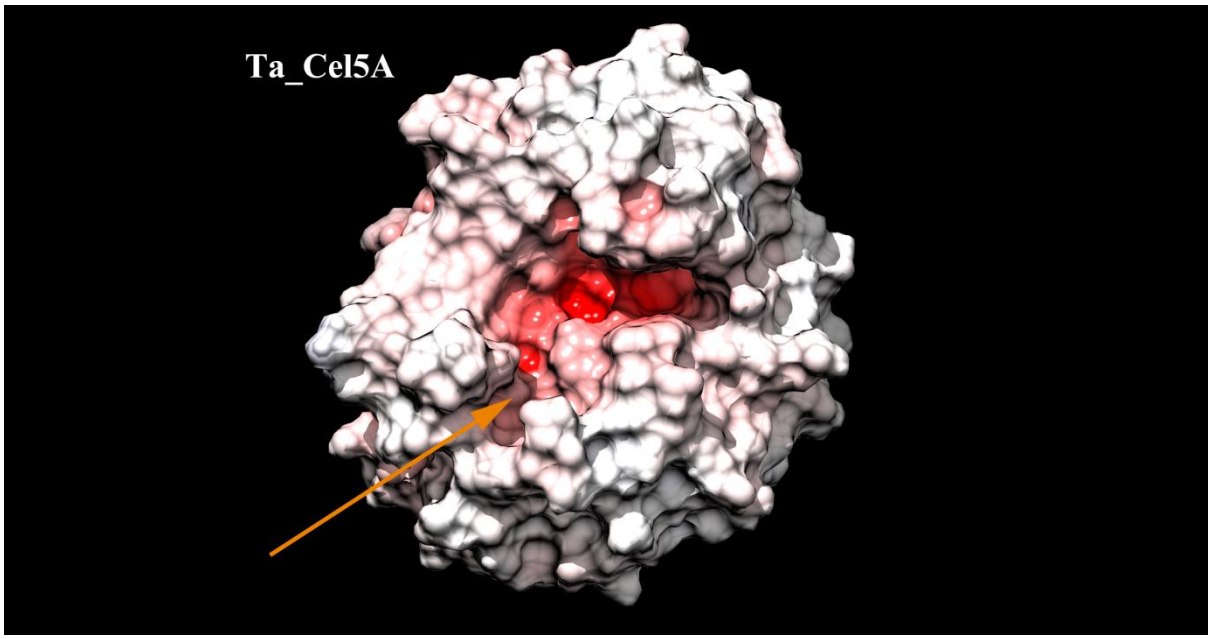
Supplementary Material



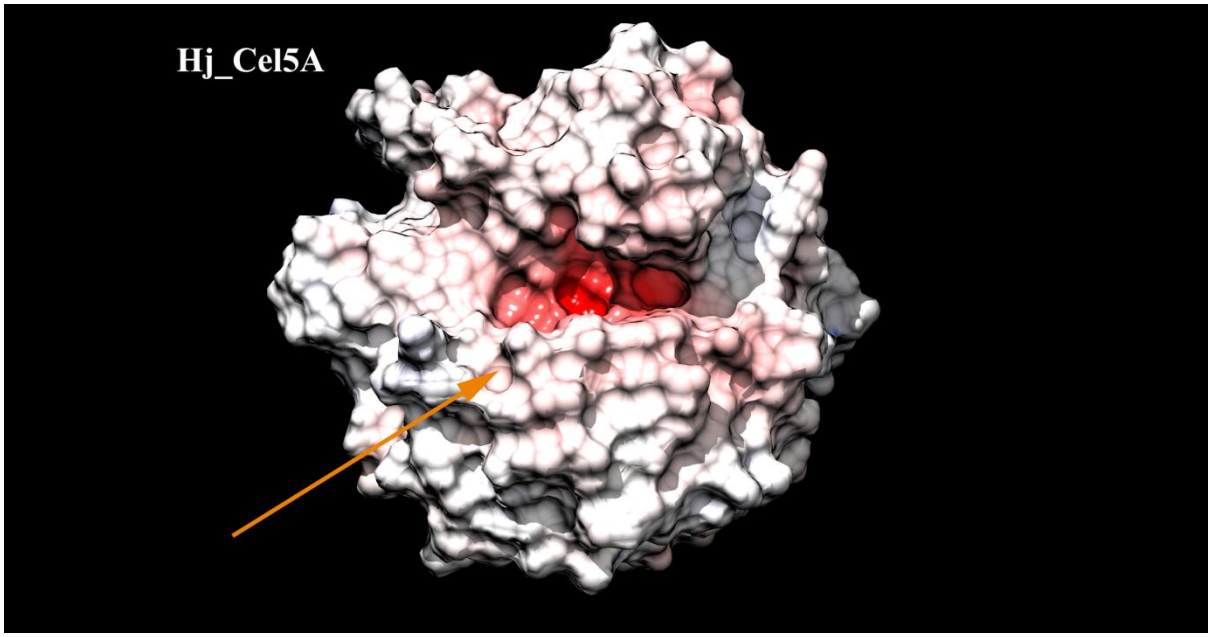
Supplementary Figure S1. Superposition of the $L_{\beta1\alpha1}$ loops of RBCel1, Ta_Cel5A, and Hj_Cel5A. The Cα traces are blue for RBCel1, red for Ta_Cel5A, and green for Hj_Cel5A.



(a)

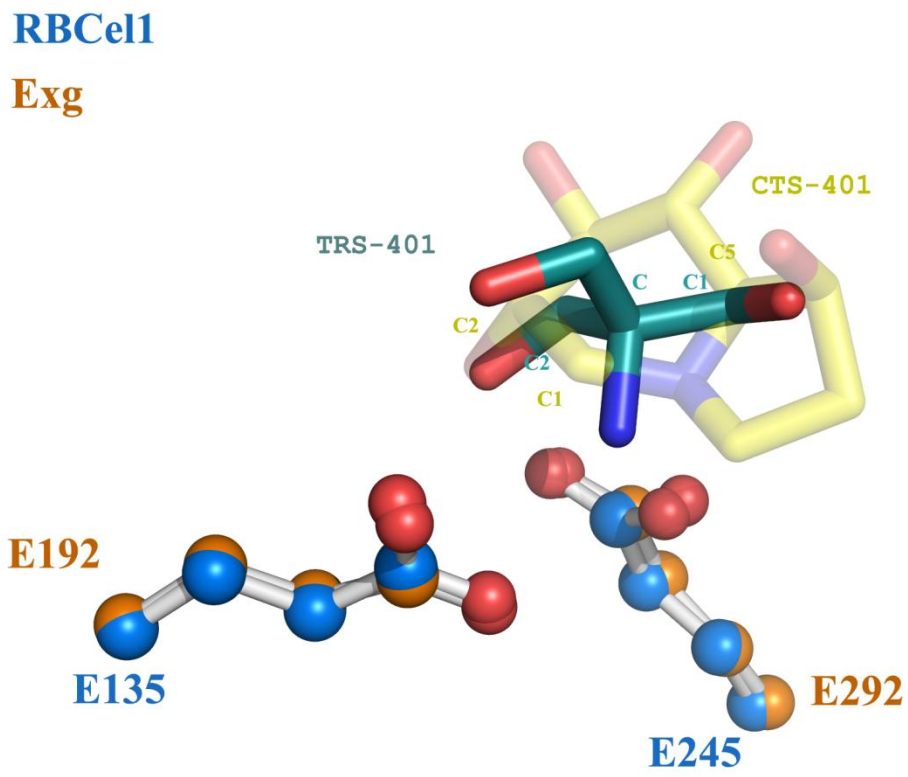


(b)

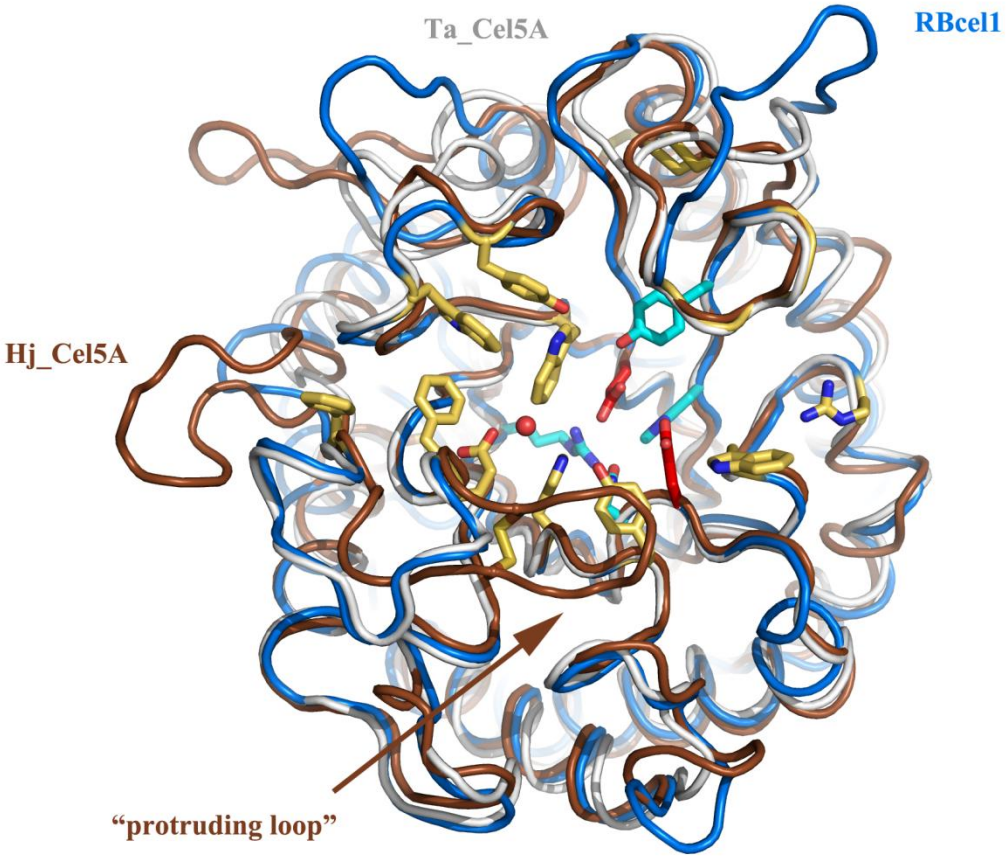


(c)

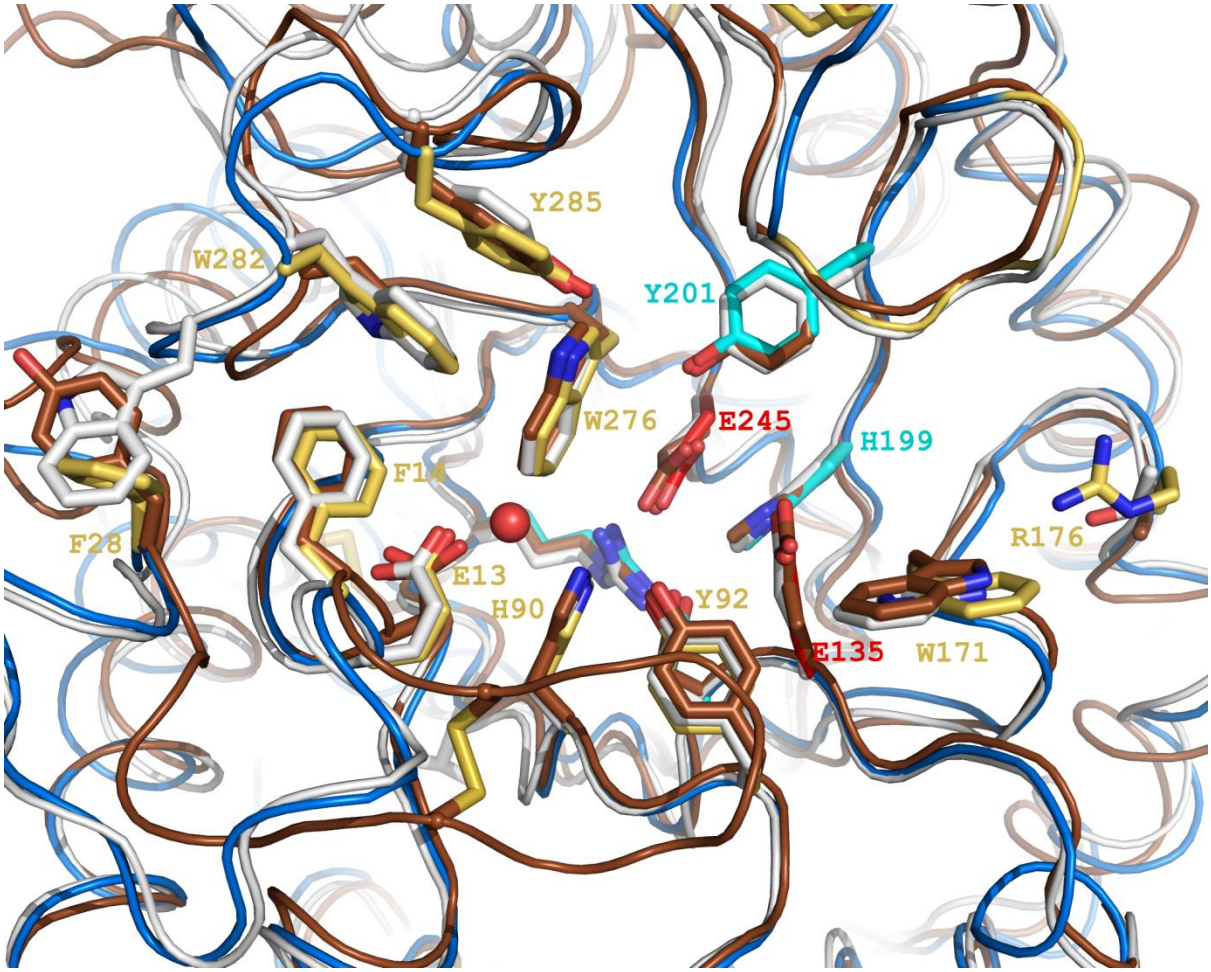
Supplementary Figure S2. Electrostatic potential displayed on the solvent-accessible surface of RBcel1 (a), Ta_Cel5A (b) and Hj_Cel5A (c). The figures were generated with the Delphi web server (Smith *et al.*, 2012) and Chimera (Pettersen *et al.*, 2004) using a 1.4 Å probe radius. Electrostatic surface potentials are colored in red (-15 kT), white (neutral), and blue (+15 kT). The orange arrows point to the small cavity connected to the main crescent-shaped cleft.



Supplementary Figure S3. Superposition of catalytic glutamates of RBcel1 and Exg complexed with TRIS and castanospermine, respectively. The TRIS and castanospermine molecule are depicted as stick model in green and yellow, respectively.



(a)



(b)

Supplementary Figure S4. Comparison of RBcel1, Ta_Cel5A, and Hj_Cel5A structures. (a) Superposition of the Cα traces of the three proteins. (b) Close-up view of the substrate binding clefts. The side chains of residues lining the substrate binding cleft are shown in yellow (substrate binding residues), cyan (conserved residues), and red (catalytic residues).