Supporting Information

Madej et al. 10.1073/pnas.1400336111

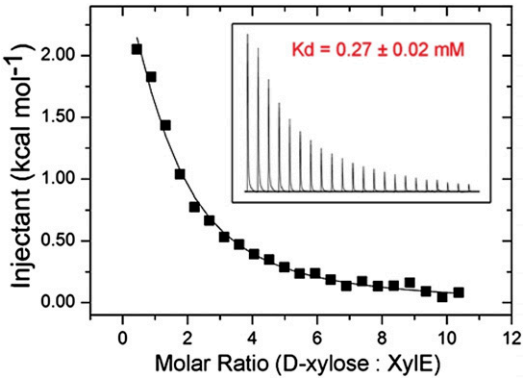

Fig. S1. The binding affinity between D-xylose and XylE with D27N mutant measured by isothermal titration calorimetry.

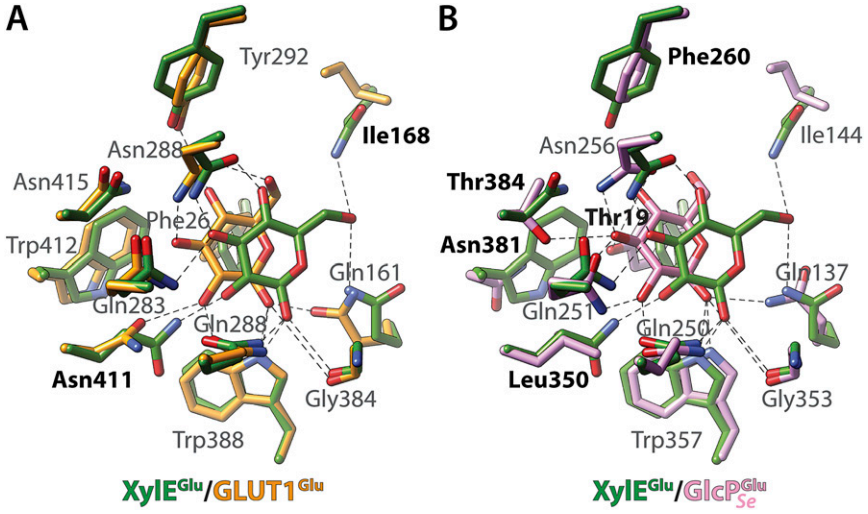

Fig. S2. Comparison of the sugar binding sites. (*A*) The X-ray structure of XylE with bound D-glucose (PDB ID code 4GBZ; green) is aligned to the comparative model GLUT1 with docked D-glucose (orange). Labels are shown for GLUT1, bold font indicates important differences in GLUT1 (N411, I168) compared with XylE. (*B*) The X-ray structure of XylE (same as in *A*; green) is aligned to the comparative model of $GlcP_{Se}$ in occluded conformation with docked D-glucose (pink). Labels are shown for $GlcP_{Se}$, bold font indicates important differences in $GlcP_{Se}$ (Thr19, L350, N381, T384) compared with GLUT1. Broken lines indicate polar contacts to the ligand. See Fig. 4 for comparison.

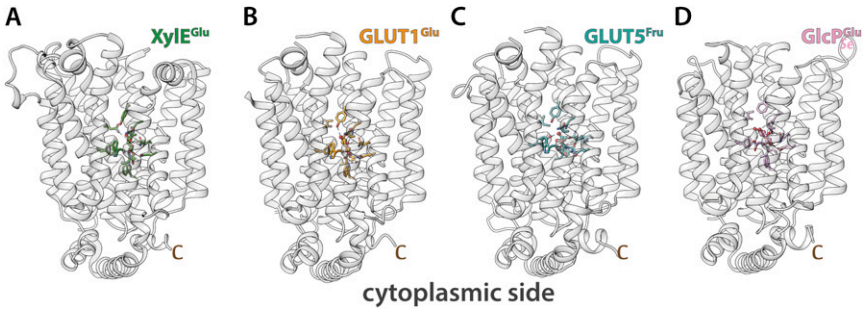

Fig. S3. Orientation of the sugar binding sites. (*A*) X-ray structure of XylE with bound D-glucose (PDB ID code 4GBZ). (*B*) Comparative model of GLUT1 and (*C*) comparative model of GLUT5 with docked ligands. (*D*) Comparative model of $GlcP_{Se}$ in occluded conformation with docked D-glucose. Residues providing polar contacts to the ligand are shown as stick model, and the respective ligands are indicated as ball-and-stick model.

Table S1. Modeling and refinement statistics

Modeling and refinement	GLUT1	GLUT5	$GlcP_{Se}$
Identity to XylE (%)	28.0	22.2	31.9
Total residues	468	501	467
Modeled residues	438	456	439
Completeness (%)	93.6	91.0	94.0
Z-DOPE	−0.343	−0.293	−0.668
Ramachandran plot			
Favored (%)	95.8	94.8	96.3
Outliers (%)	0.7	2.7	0.9

Other Supporting Information Files

Dataset S1 (DOCX)