

Supplementary data

Figure S1. MM3 free energy maps derived from population analysis of a MD simulation of the extended repeating unit **E-D-A-[C]-B-E-D** (30 ns / 700 K). a, β -D-Galp-(1 \rightarrow 4)- β -D-Glcp; b, β -D-Glcp-(1 \rightarrow 3)- β -D-Galf; c, β -D-Galf-(1 \rightarrow 3)- α -D-Galp; d, α -D-Glcp-(1 \rightarrow 6)- α -D-Galp; e, α -D-Galp-(1 \rightarrow 3)- β -D-Galp. Iso-energy contours have been plotted at regular intervals of 1 kcal/mole up to 10 kcal/mole above the global minimum in each map.

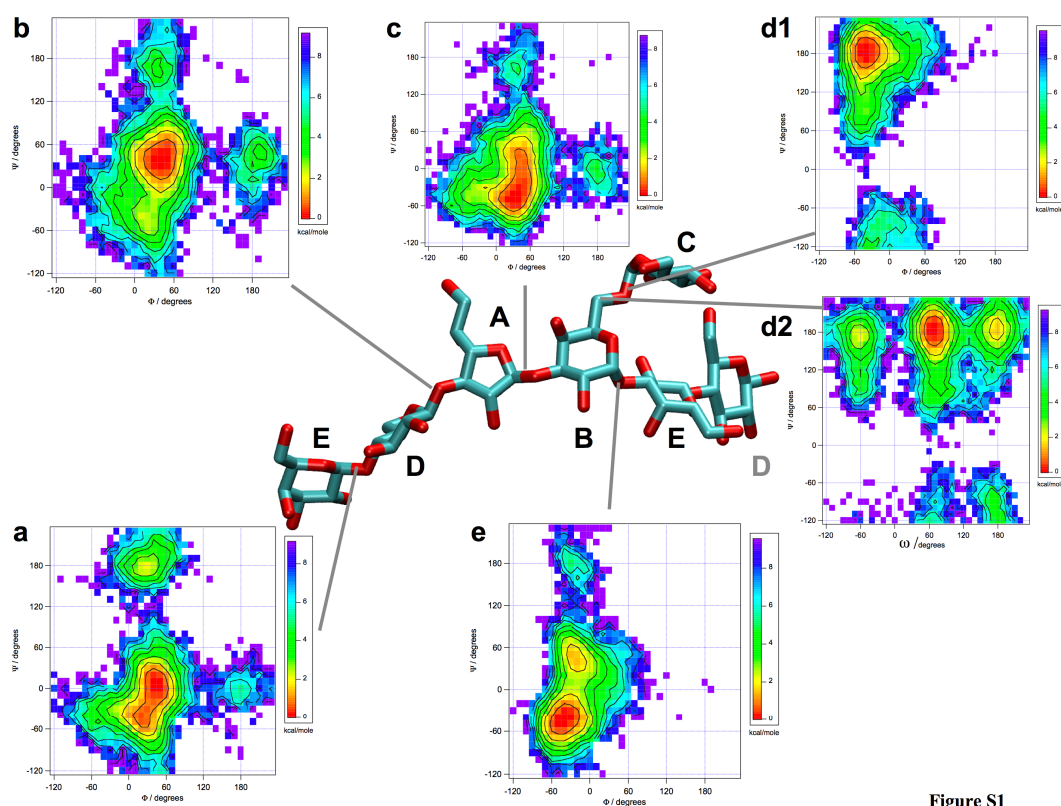


Figure S1