

## Supplementary Data

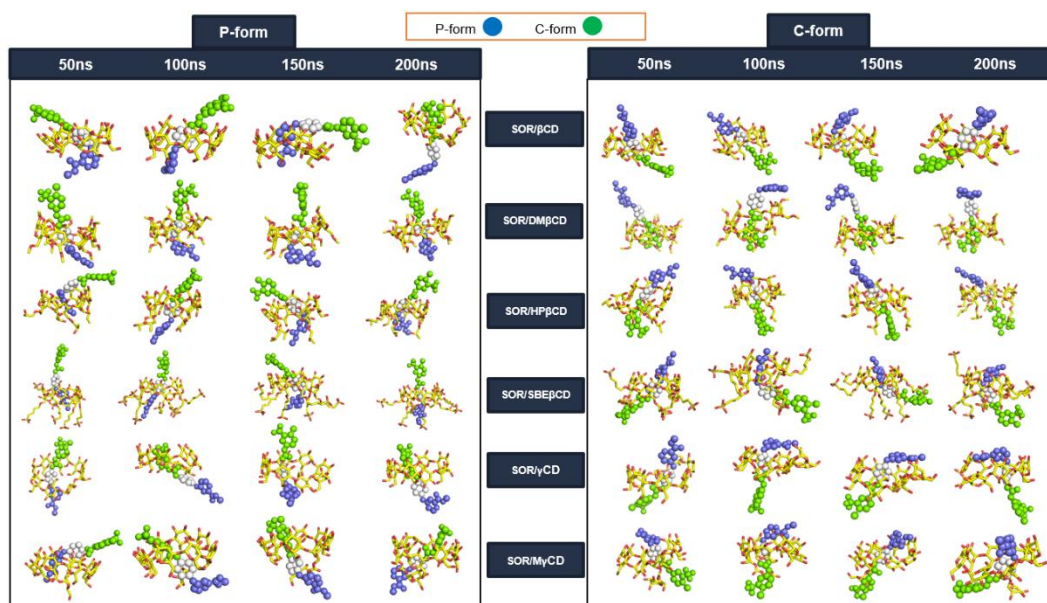


Figure S1. MD1 snapshots of all simulated complexes, taken at 50ns, 100ns, 150ns, and 200ns.

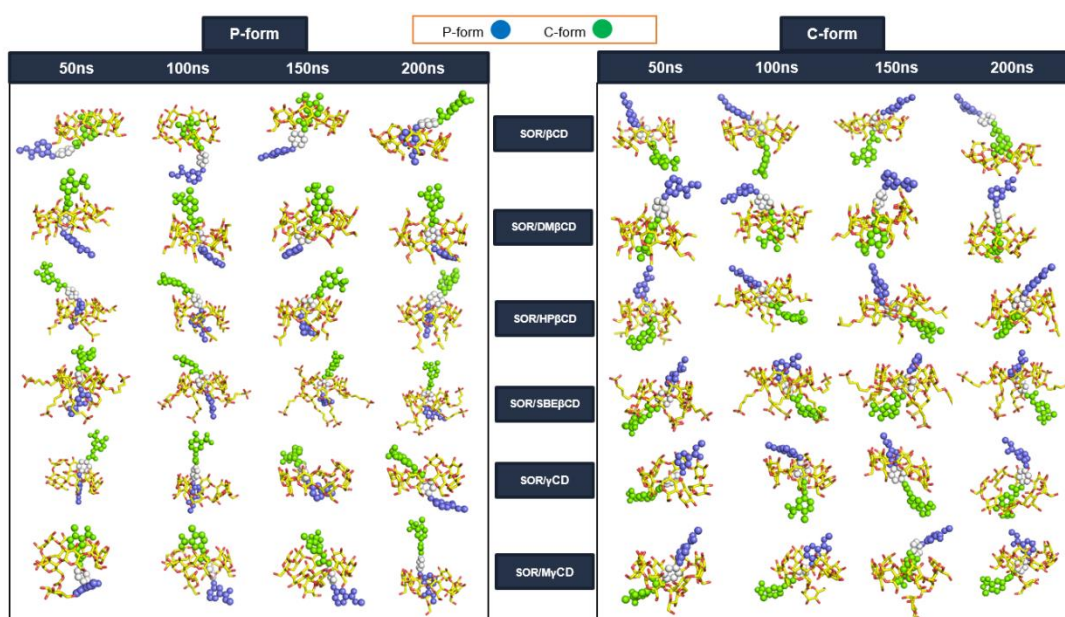


Figure S2. MD2 snapshots of all simulated complexes, taken at 50ns, 100ns, 150ns, and 200ns.

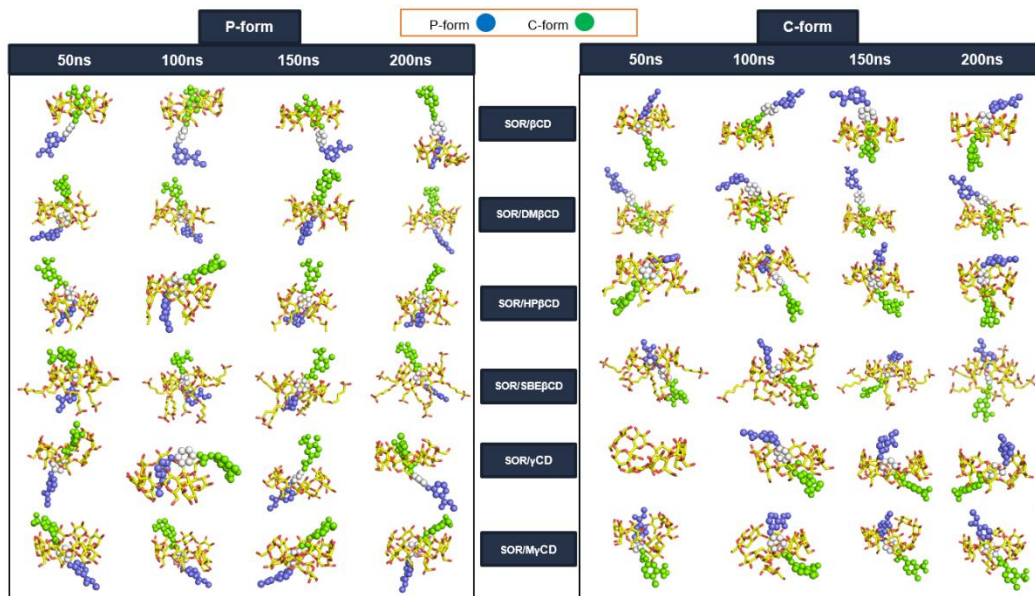


Figure S3. MD2 snapshots of all simulated complexes, taken at 50ns, 100ns, 150ns, and 200ns.

Table S1. Number of contacts and SASA values of all complexes. The data are expressed as mean  $\pm$  standard deviation,  $n = 3$ .

Complexes	Number of contacts		SASA ( $\text{\AA}^2$ )	
	P-form	C-form	P-form	C-form
<b>SOR/<math>\beta</math>CD</b>	35.06 $\pm$ 9.2	36.29 $\pm$ 9.3	338.92 $\pm$ 17.8	342.33 $\pm$ 21.2
<b>SOR/DM<math>\beta</math>CD</b>	49.33 $\pm$ 8.0	39.76 $\pm$ 7.8	329.15 $\pm$ 15.9	338.51 $\pm$ 20.9
<b>SOR/HP<math>\beta</math>CD</b>	46.12 $\pm$ 9.6	50 $\pm$ 9.6	296.47 $\pm$ 25.6	282.23 $\pm$ 19.4
<b>SOR/SBE<math>\beta</math>CD</b>	49.73 $\pm$ 9.8	54.29 $\pm$ 9.1	273.77 $\pm$ 27.9	250.44 $\pm$ 25.3
<b>SOR/<math>\gamma</math>CD</b>	37.89 $\pm$ 9.1	41.82 $\pm$ 9.3	337.96 $\pm$ 26.6	316.5 $\pm$ 26.9
<b>SOR/M<math>\gamma</math>CD</b>	42.59 $\pm$ 8.1	47.28 $\pm$ 8.6	310.35 $\pm$ 23.4	306.4 $\pm$ 22.7