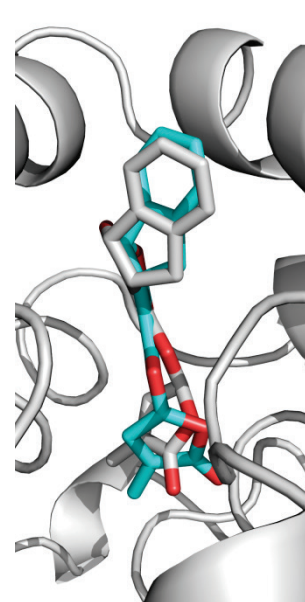
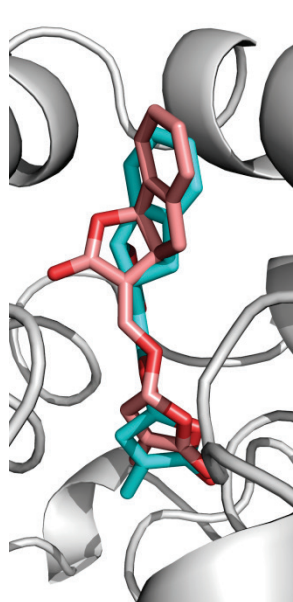


A

Stereo-isomer	Grid score (sum)	Grid score (VdW)	Grid score (es)	Internal energy
5DS	-39.7	-34.4	-5.3	2.8
Ent-5DS	-15.5	-16.3	0.8	2.2
4DO	-22.6	-20.4	-2.3	1.7
Ent-4DO	0.04	2.2	-2.1	3.2

B**GR24 model**
5DS-GR24**GR24 model**
ent5DS-GR24**GR24 model**
4DO-GR24**GR24 model**
ent4DO-GR24

Supplementary information, Figure S7 Unbiased computational docking of GR24 stereoisomers in the D14 LBP. (A) Docking scores for the four different GR24 stereoisomers. The Grid score (kcal/mole) indicates the energy component of Van-der-Waals (VdW) and electrostatic (es) interactions between ligand and pocket residues, and the internal energy (kcal/mole) the energy of the ligand geometry (i.e., angles, bond length and clashes within the ligand itself). **(B)** Docked structures overlaid with the density-based structure model of GR24.