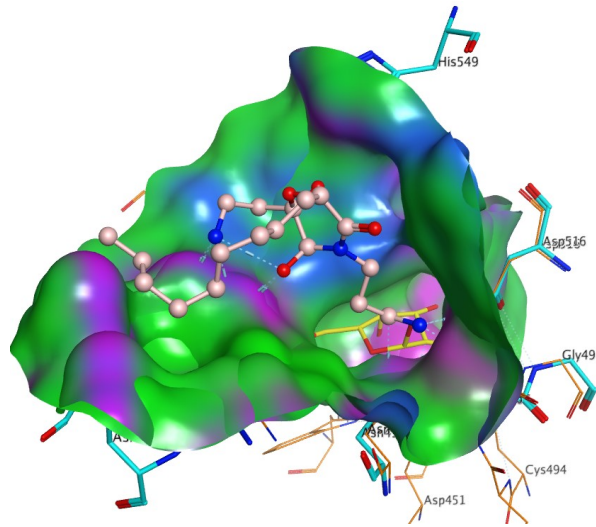
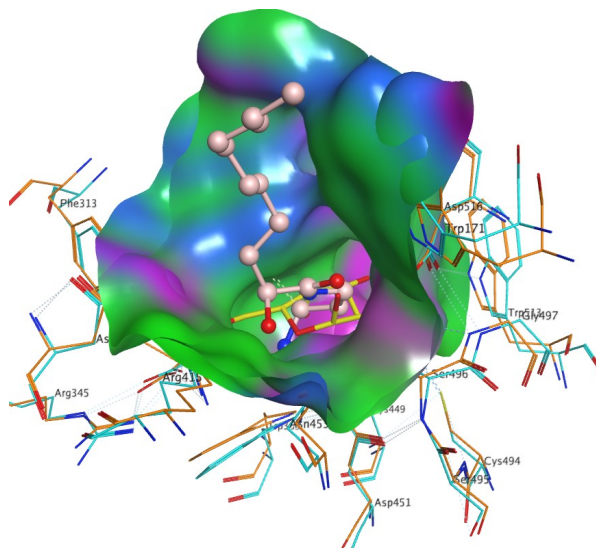


(a)



(b)



(c)

Figure S1. 3D-superposition of the α -PsGal active site with galactose and spermidine residue of monachomycalin B (**a**), tetra-substituted morpholinone derivative of monanchocidine A (**b**) and monosubstituted diaminopropane of normonanchocidine A (**c**). Parts of guanidine alkaloids are shown as "ball and stick" with grey color, galactose shown as "stick" with yellow color. The molecular surface close to the ligands is shown in pink (H-bonding), green (hydrophobic) and blue (mild polar).