

Figure S5. Actual ligands in our crystal structures in comparison to related known substrates.

Chloramphenicol (Cm): MW, 323 Da; electroneutral; and size: ~260 Å³. N-dodecyl-N,N-dimethylamine-N-oxide (LDAO): MW, 229 Da; positively charged; and size: ~235 Å³. Deoxycholate (Dxc): MW, 391 Da; negatively charged; and size: ~360 Å³. Potential homologues are selected from a previous report [17].