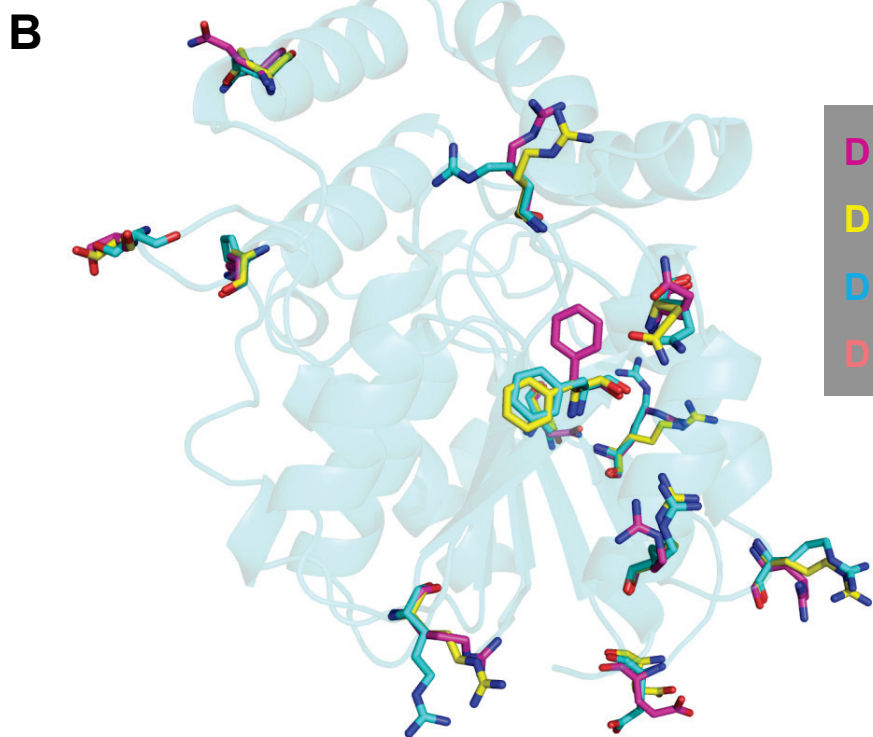


D14-GR24

D14-GR24

D14-lactone



D14 apo (PDB 4IH9, mol-A)

D14 apo (PDB 4IH9, mol-B)

D14 apo (PDB 3VXK)

D14/D-ring (PDB 3WIO)

Supplementary information, Figure S2 A group of flexible charged surface residues adopts different conformations in six different D14 crystal structures. **A.** Structure overlay of the two complexes found in the D14/GR24 complex structure (grey and cyan) with the structure of D14 bound to a GR24 hydrolysis intermediate (PDB 4IHA²⁴, magenta). **B.** Structure overlay of three D14 apo complexes (PDB 4IH9²⁴, magenta and yellow, and 3VXK²⁶, cyan) or D14 bound to the D-ring GR24 hydrolysis product (PDB 3WIO²⁶, pink). Transparent ribbon presentations with conformationally dynamic surface residues shown in stick presentation.