

XChem EcMurE



Libraries:

- China extracts
- Atomwise

Tested at 2 final concentrations:

- 60 and 30 mM

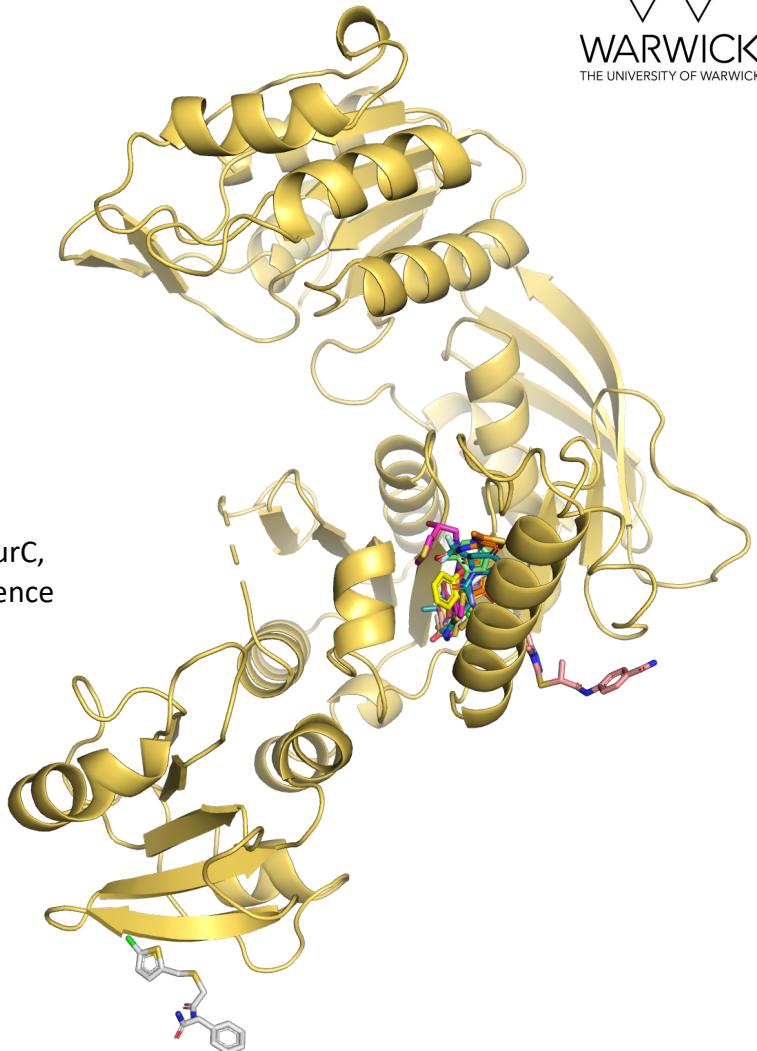
Results:

- Natural extracts were not very soluble and didn't have any hits
- 60 mM gave more hits than 30 mM

Compound ID	Confidence	Site
Z225695112	High	Crystal contact
Z224156390	High	Allosteric
Z1720524522	High	Allosteric
Z915722616	High	Allosteric
Z25112280	High	Allosteric
Z652877744	Medium	Allosteric
Z1275565768	High	Allosteric
Z1216046212	Medium	Allosteric
Z1532460536	Low	Allosteric

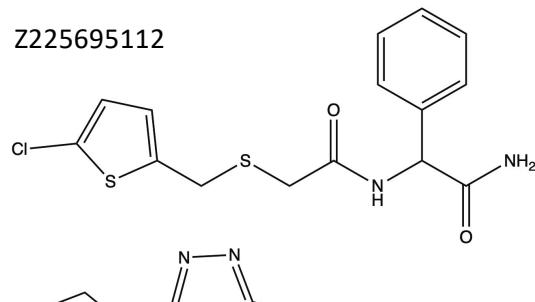
Next:

- Activity assays
- Binding assays (SPR): MurE, MurC, MurD in the presence and absence of ADP/AMPPNP

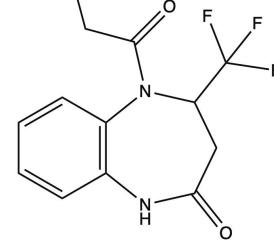


XChem EcMurE

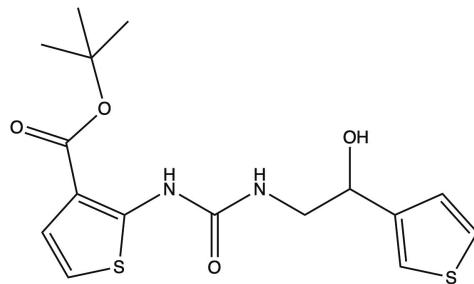
Z225695112



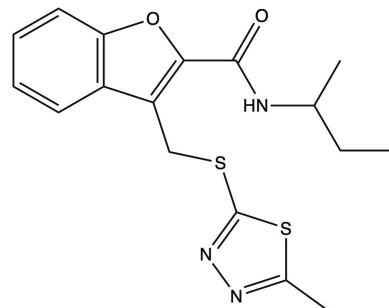
Z224156390



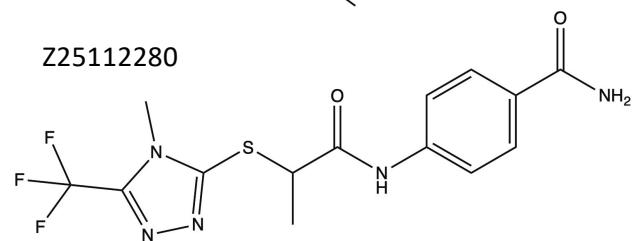
Z1720524522



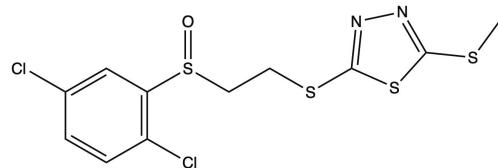
Z915722616



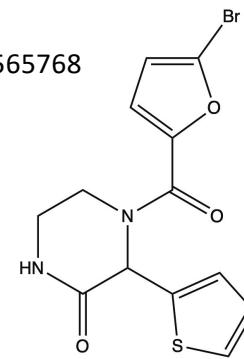
Z25112280



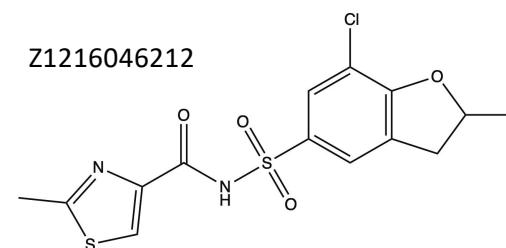
Z652877744



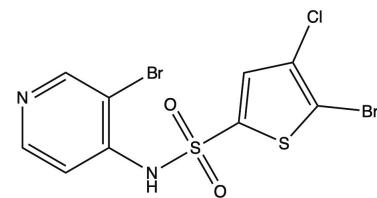
Z1275565768

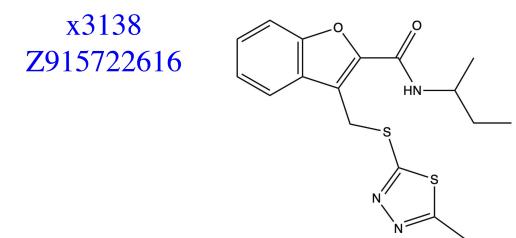
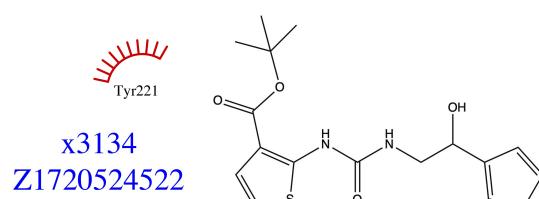
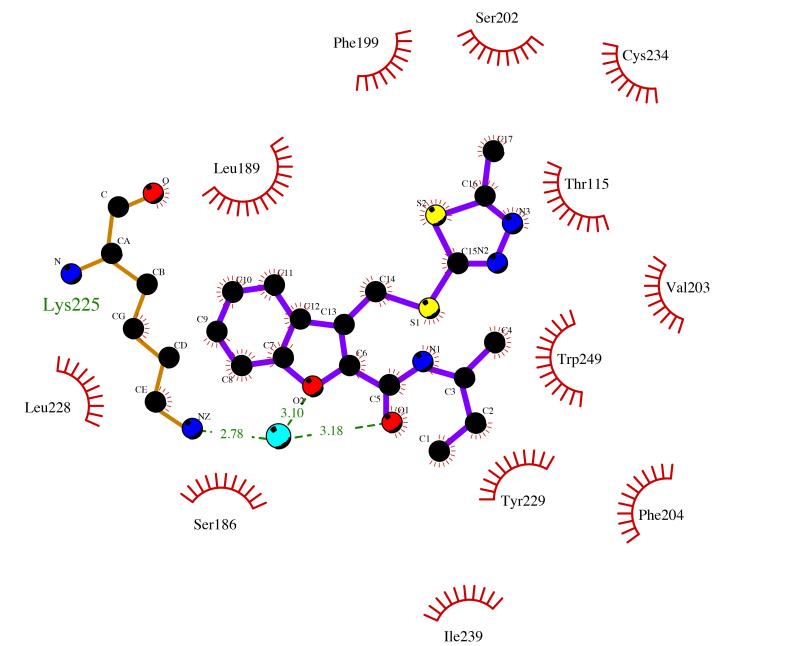
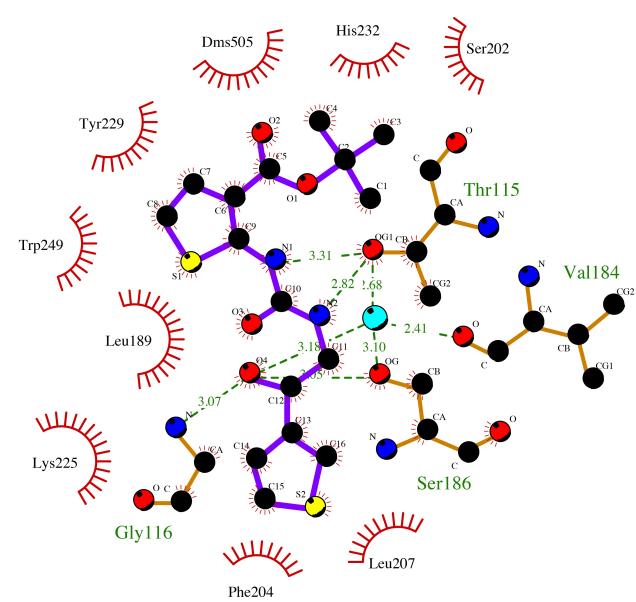
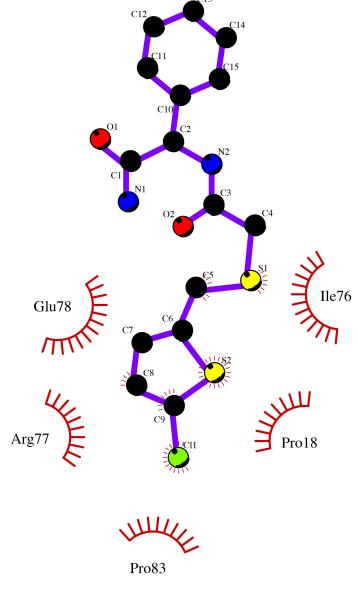


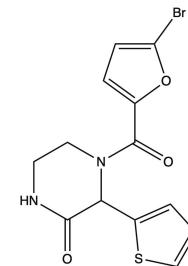
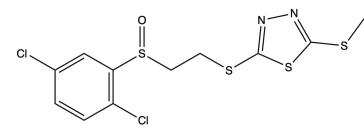
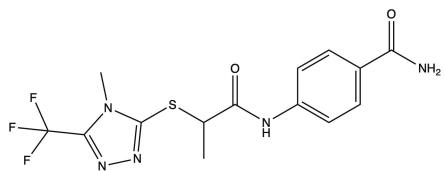
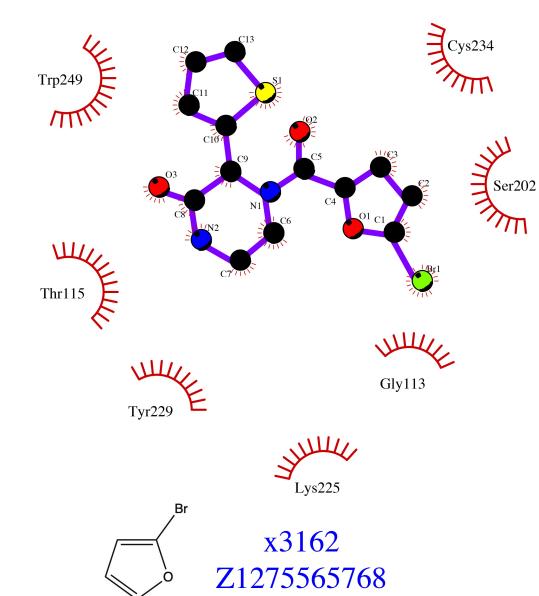
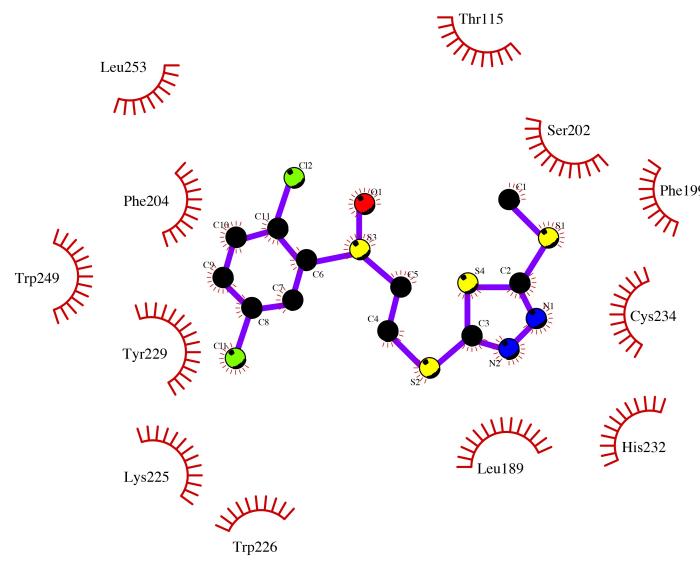
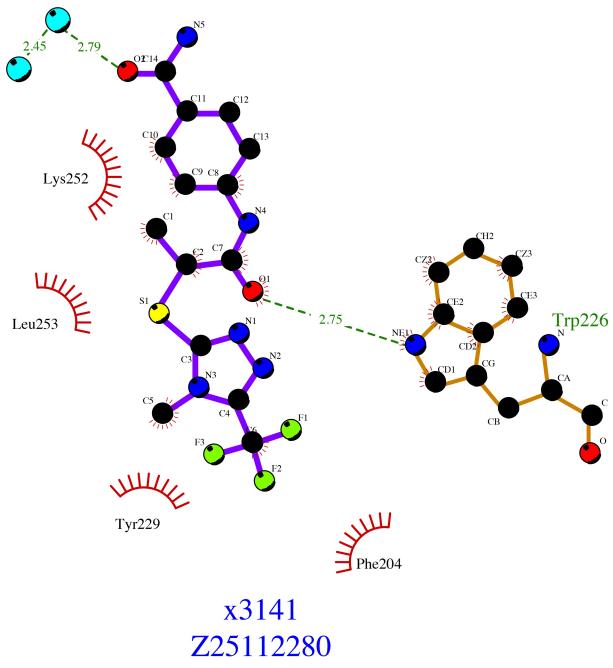
Z1216046212

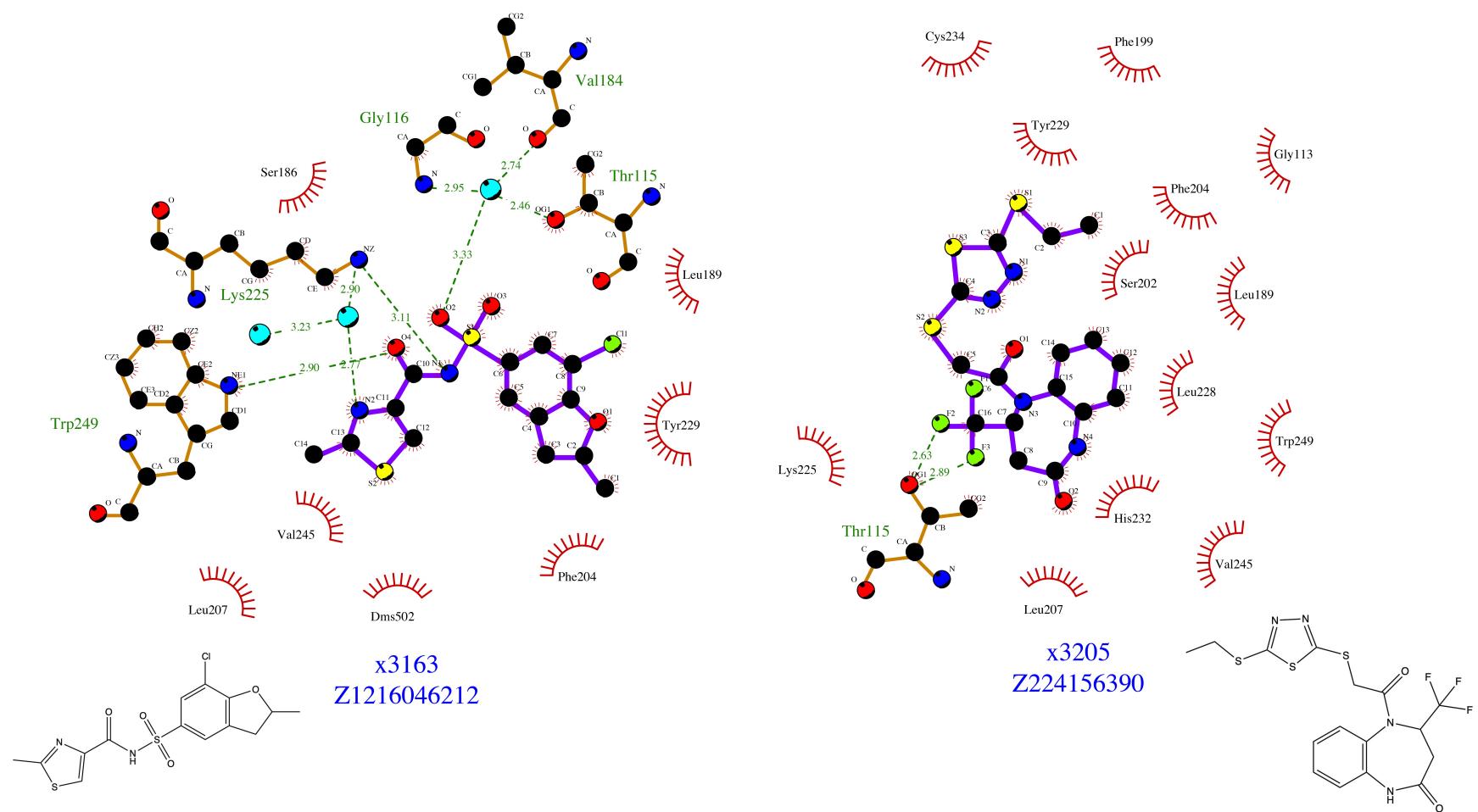


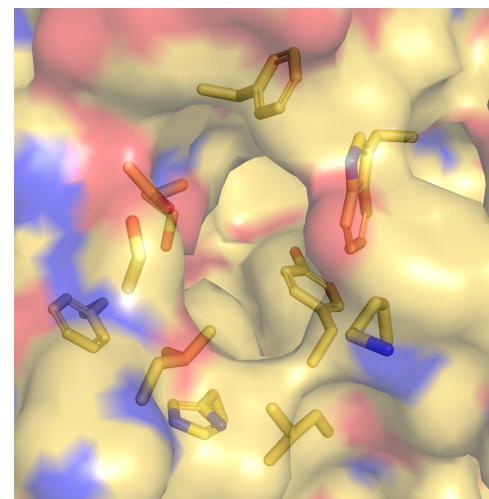
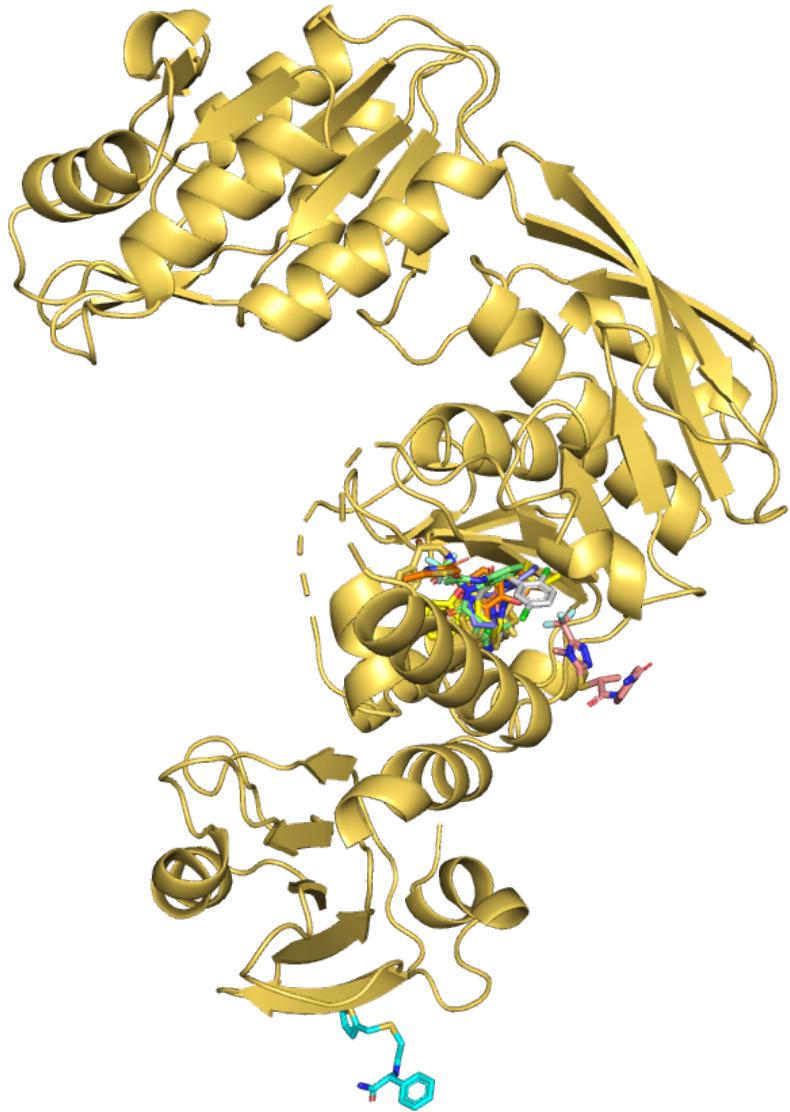
Z1532460536



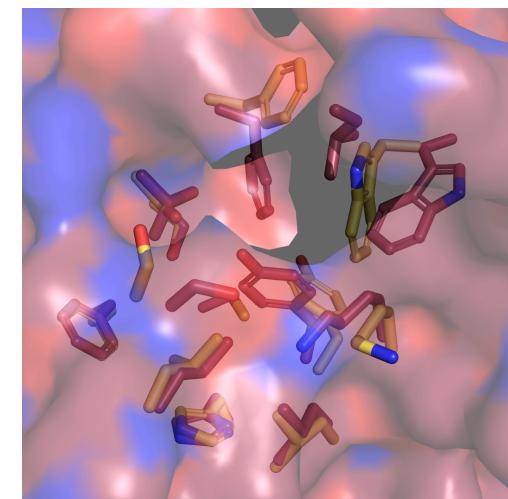








Pocket generated by the compound binding (ligand not shown)



Pocket region at the apo structure
(overlaid residues from a ligand-bound structure are coloured in yellow)