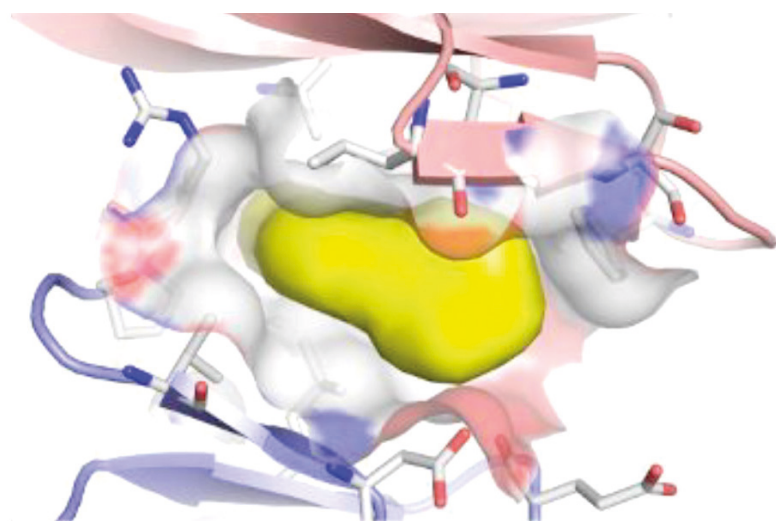
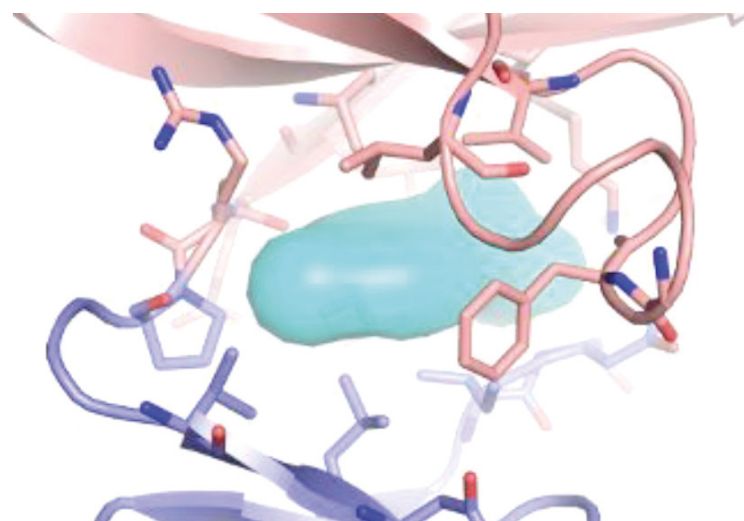


PACE™ Fragments-to-Leads Case Study

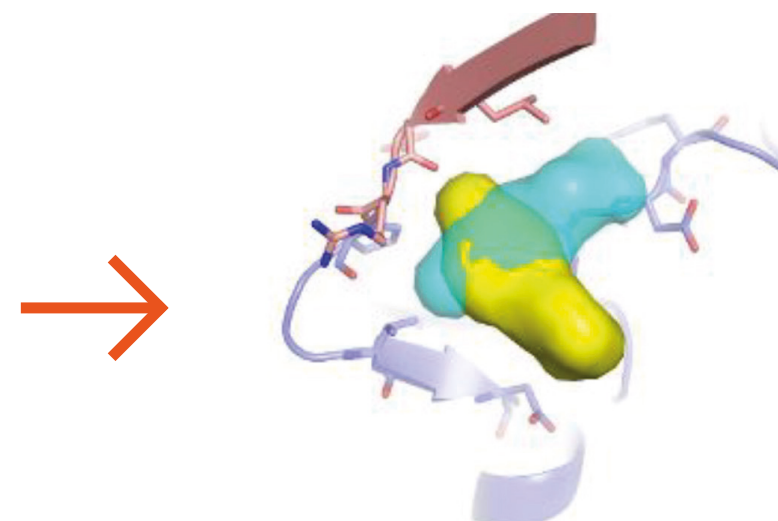
From the LCC Fragment Library, three distinct sub μ M fragments were confirmed for optimisation. SBDD-guided fragment optimisation resulted in the identification of a single-digit nM Lead compound in two DMTA cycles.



Fragment-1 bound to ATP site of PIM1



Fragment-4 bound to ATP site of PIM1



View from top, Animated Fragment-1 bound to ATP site of PIM1, with frag-4 overlayed

