

Dataset S6: Design of neutral probe set. Two carboxylic acids were included as close analogs. Crystal structures of Mac1 in complex with neutral probe set hits. PanDDA event maps are shown for ligands (contoured at 2σ). Protein-ligand hydrogen bonds are shown with dashed black lines. Hydrogen bonds between ligands and the Lys11 backbone nitrogen of a symmetry mate are highlighted with purple spheres/dashes.

D.1



