



Supplemental Figure 2. CA-4948 affinity for murine IRAK-4. (a) Structural formula of CA-4948. (b) Binding mode of CA-4948 to human IRAK-4 (PDBID: 7C2V (35,36), visualized with Maestro (37). Ribbon structures shown. (c) Binding mode with ribbon structure for residues 182-203 hidden for clarity. (d) Uniprot IRAK-4 sequence alignment of 7C2V to Q8R4K2 (42) (homo sapiens to mus musculus). (e) Energy-based homology model of murine IRAK-4. Residues that were only sidechain mutations are shown in cyan (note ribbon structure of ALA263). Red residues indicate those that had to be built (i.e. unstructured regions without defined structure in the crystal template). CA-4948 from 7C2V (homo sapiens) crystal structure superimposed.