



Supplementary Figure 1. Binding pattern of CsA (compound 1) in the CypA/calceurin complex. A) A 3D diagram and B) a 2D diagram are depicted (PDB code: 1MF8). The docking process of **1** to the CypA/calceurin complex was modeled using Flare and the resulting diagram was analyzed using the Discovery Studio Visualizer. CsA binds to the CypA/calceurin complex via two parts of the ligand, and the red dotted line on (B) shows demarcation of CsA by CypA and calcineurin. P1, P2, P9, and P10 of CsA, as shown in Figure 4, mainly interact with CypA, whereas P4, P5, and P6 interact with calcineurin.

