



## Supplementary information, Fig. S3. Two-dimensional ligand-interaction diagrams of NAMPT bound to NAT or NAT-5r.

**a** Left panel, NAT and its adjacent residues within 4Å in the crystal structure. Right panel, the predicted preferable binding mode of NAT-5r and adjacent residues within 4Å. H-bond interactions are shown as yellow dash lines. **b** A surface display for the NATs-binding in an internal region of the NAMPT enzyme. NAT and NAT-5r are shown as sticks in orange and cyan, respectively.