

Supplementary Information to

Complementing machine learning-based structure predictions with native mass spectrometry

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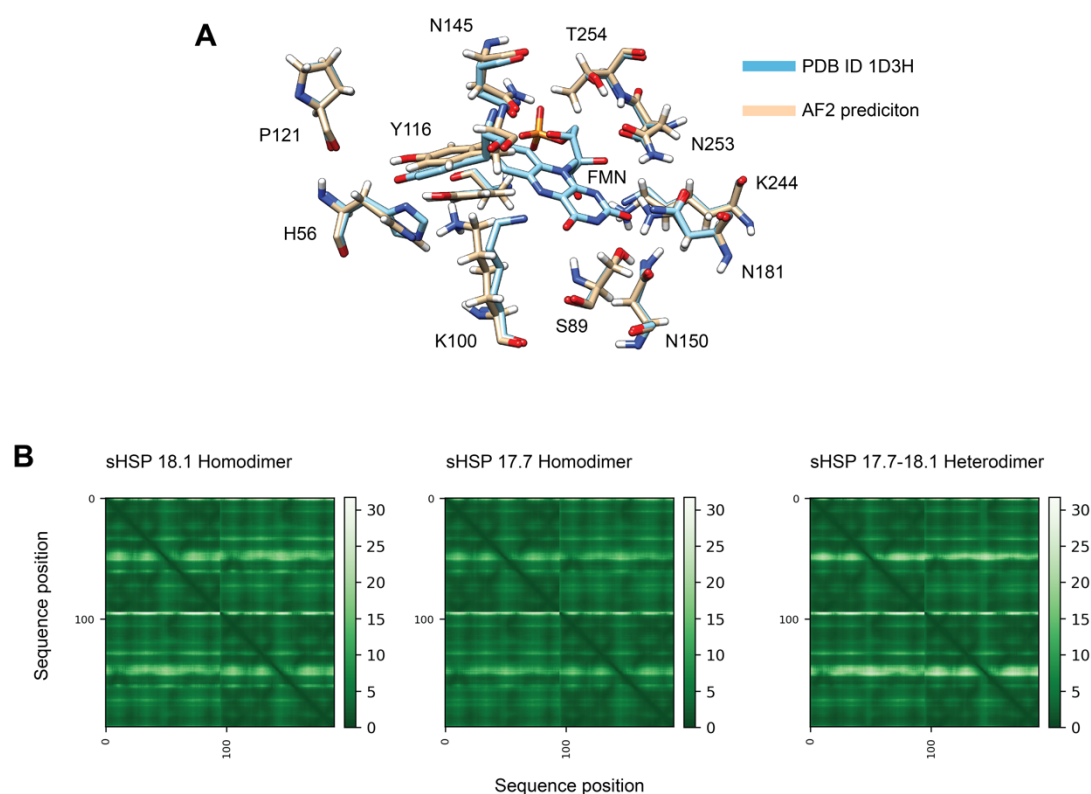


Figure S1. (A) Overlay of the residues that line the FMN binding pocket in human DHODH. The side-chain orientations in the AF2 prediction of apo-DHODH (gold) agree closely with the X-ray structure for holo-DHODH (blue), except for a 30° rotation of the imidazole moiety of H56 and the orientation of the terminal amine group of K100. (B) The PAE plots for the top-scoring predictions of homodimeric sHSP18.1 and sHSP17.7 as well as the 17.7-18.1-heterodimer show no significant differences.