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Supplementary Information

ThermoFMN - A Thermofluor Assay Developed for Ligand-Screening as an Alternative Strategy for Drug Discovery

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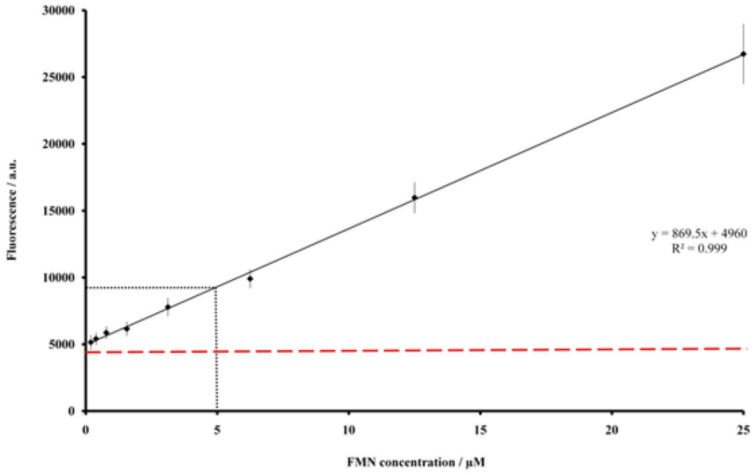

Figure S1. Fluorescence intensity versus FMN concentration. Data was fit to the equation $y = k\varphi I_0 \varepsilon bx$, where the intensity of emitted light, y, is described by the relationship where φ is the quantum efficiency, I_0 is the incident radiant power, ε is the molar absorptivity, b is the path length of the cell, and x is the FMN molar concentration.[1] The level of background noise of was estimated in 4960 a.u. close to the measured fluorescence signal of empty wells (red). Two times signal-to-noise ratio is found for concentrations around 5 μmol L^{-1}.

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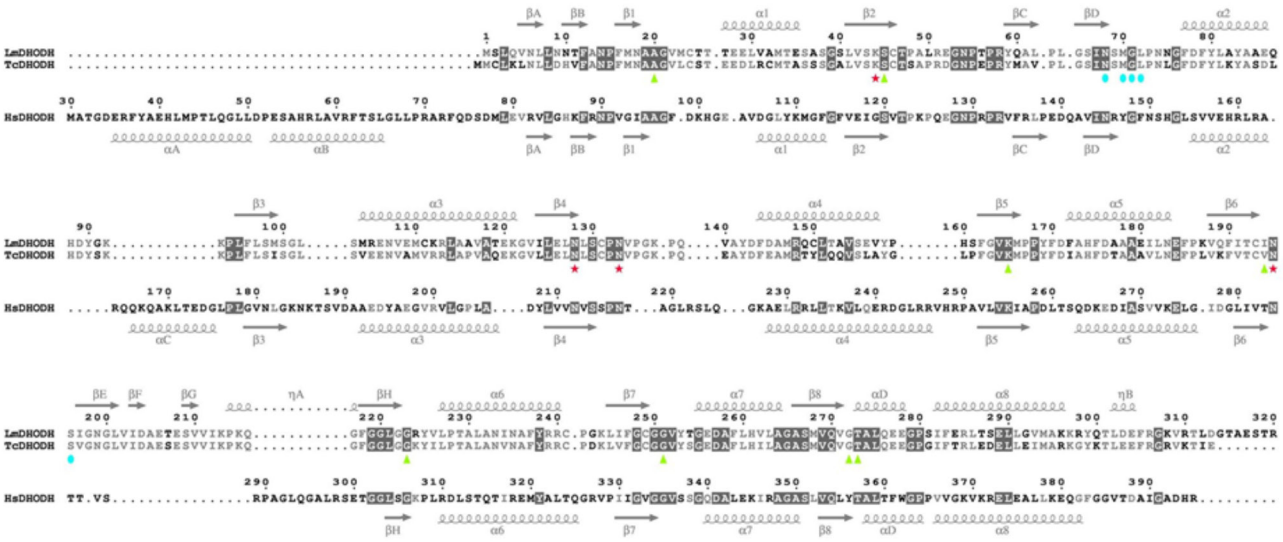

Figure S2. Structure-based sequence alignment of selected DHODHs proteins: LmDHODH (PDB ID 3GYE), TcDHODH (PDB ID 3C3N), and HsDHODH (PDB ID 1D3G). Residue numbering is based on LmDHODH and HsDHODH. Residues that are fully conserved are highlighted in dark gray box. Residues highly, little or non-conserved are colored in white, light gray and black, respectively. Secondary structures of LmDHODH (top) and HsDHODH (bottom) are also labeled. Residues that directly bind orotate, FMN, and both, are indicated by cyan filled circules, lime green triangles, and red stars, respectively. The structural alignment was performed using COOT and graphically displayed using ESPript.[2,3]

References

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