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Identification of potential benzoxazolinones as CYP1B1 inhibitors via molecular docking, dynamics, waterswap, and *In vitro* analysis

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Supplementary Information

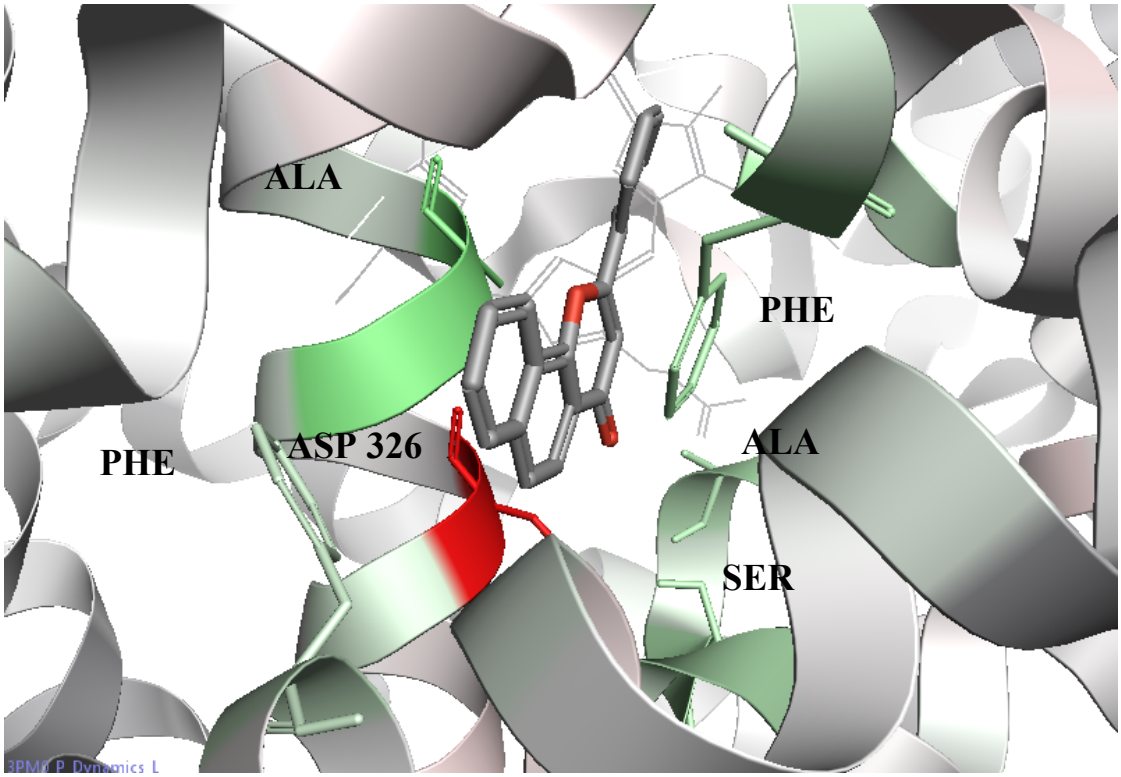

Figure S1. Binding free energy contribution diagram of ANF (co-crystal ligand) from WaterSwap analysis. The green color represents residues that are favorable to ligand interactions; the darker the green, the more favorable; red represents residues that are unfavorable to ligand binding

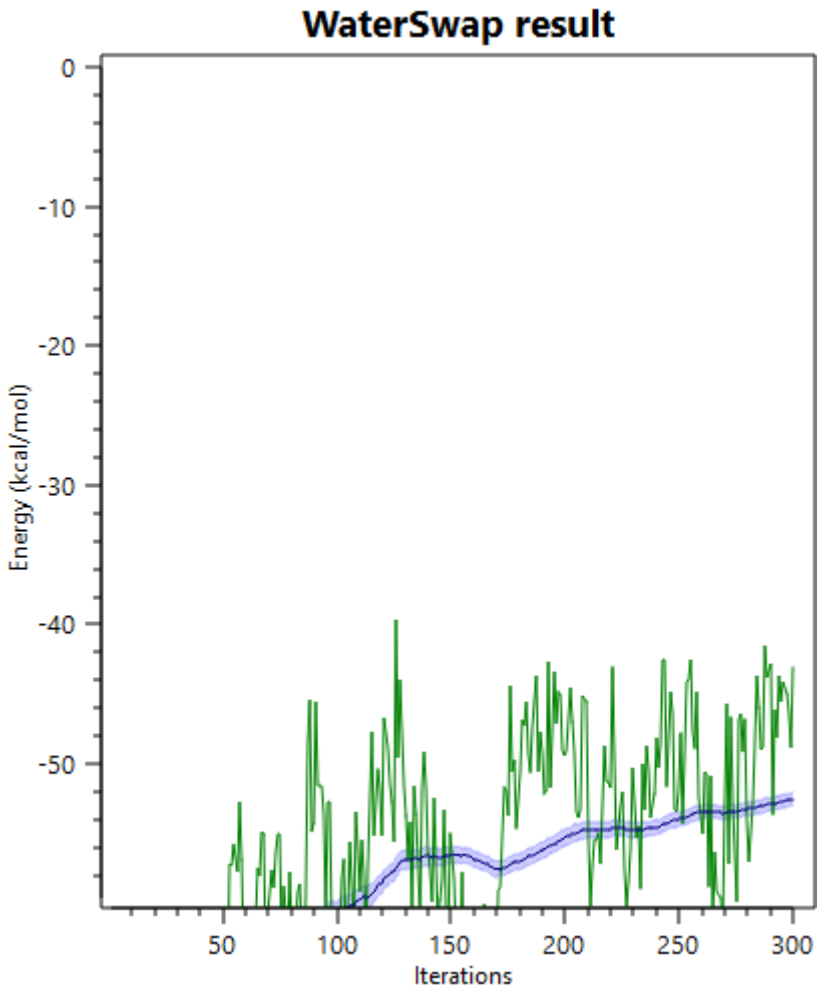

Figure S2. Consensus free energy values and iterations of the reference compound i.e. ANF