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Electronic Supplementary Information (ESI)

Computational approaches to predict binding interactions between mammalian tyrosinases and (S)-(+)-decursin and its analogues as potent inhibitors

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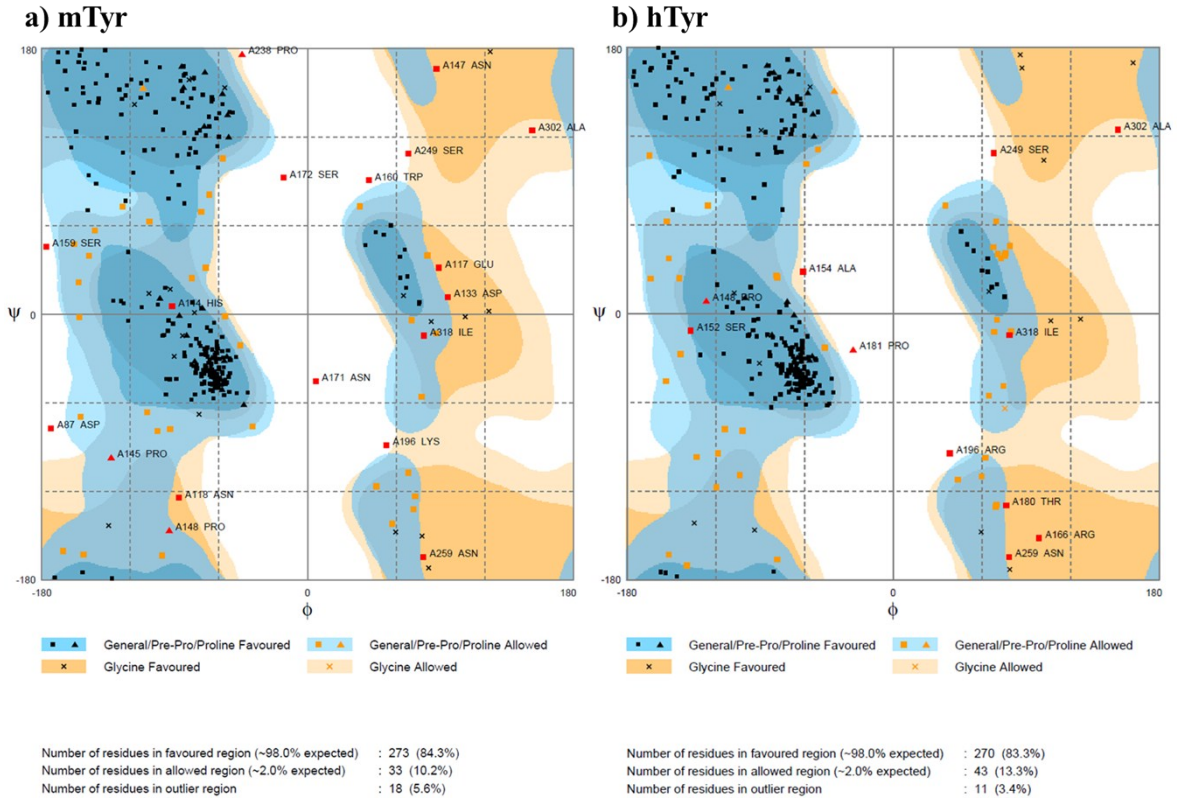

Fig. S1 Ramanchandran plot of the psi/phi distribution of the a) mTyr and b) hTyr homology model as obtained by RAMPAGE. (a) 94.5% residues are in favored and allowed regions and 5.6% residues are in outlier region. (b) 96.6% residues are in favored and allowed regions and 3.4% residues are in outlier region.

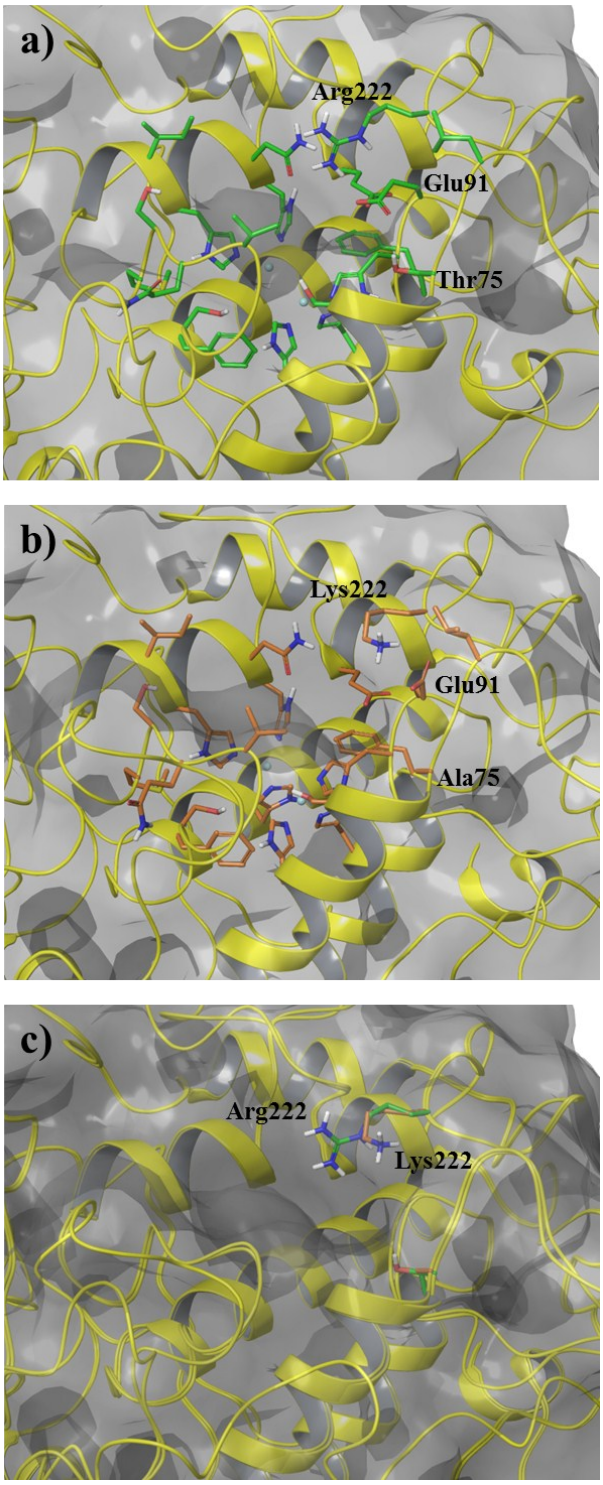

Fig. S2 Comparison of a) mTyr and b) hTyr binding site. Residue side chains around the binding site are displayed on mTyr(green) and hTyr(orange) binding site. Residues which are different except Glu91 between the mTyr and hTyr are indicated in bold. c) mTyr (green) and hTyr (orange) structure is superimposed for comparing different residues between the structures.

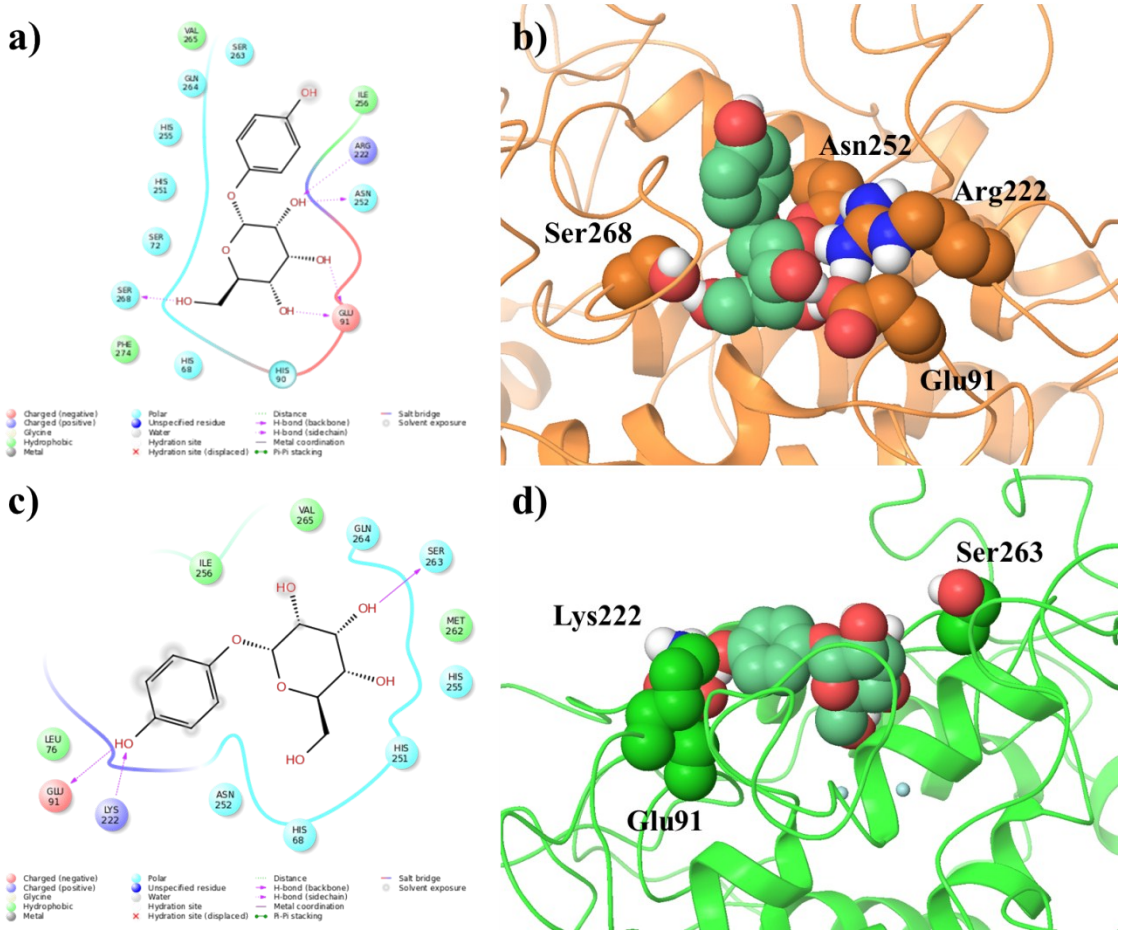

Fig. S3 Binding mode of arbutin in mTyr and hTyr. Ligand interaction diagram of arbutin with a) mTyr and c) hTyr is displayed. Binding pose of arbutin in b) mTyr and d) hTyr structure is displayed. Residues which form hydrogen bond with the arbutin is indicated in bold and shown in CPK model.

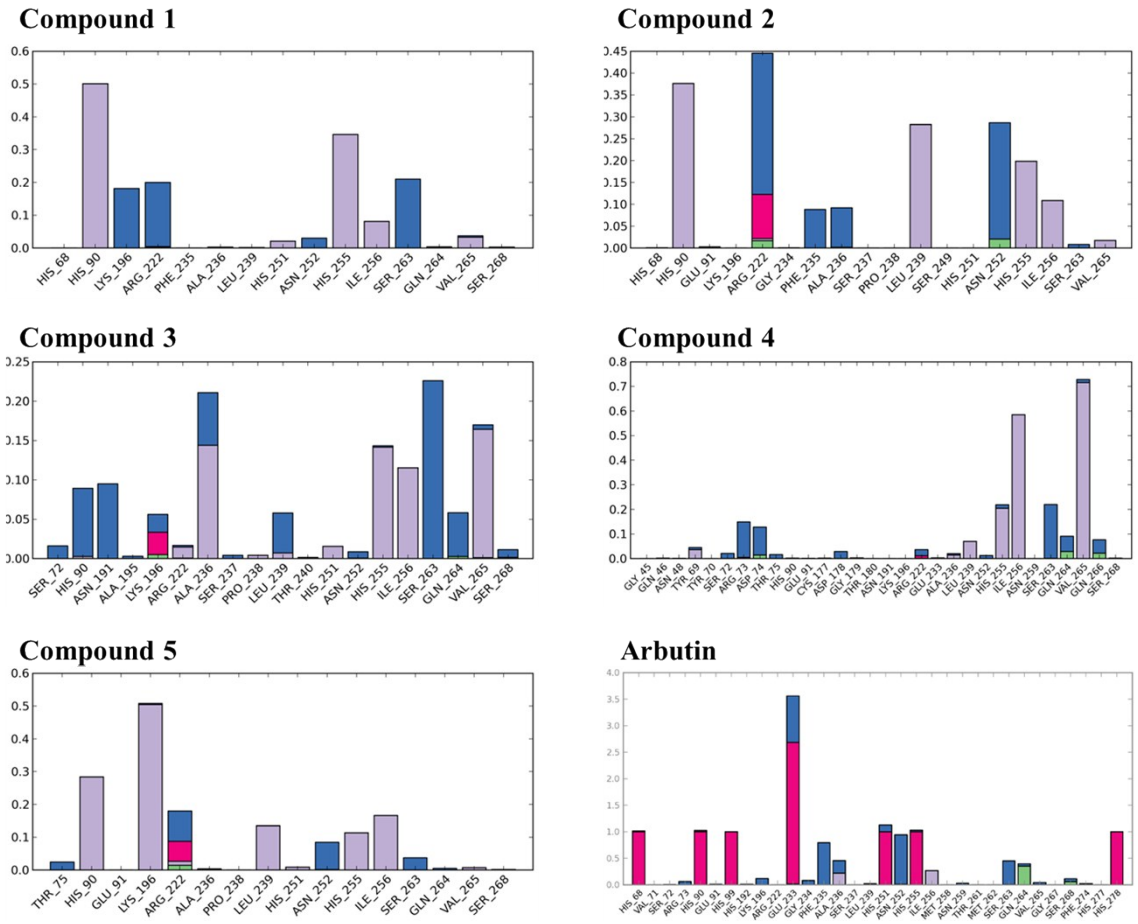

Fig. S4 Molecular dynamics simulations trajectory analyses of mTyr-inhibitor contacts. Protein-ligand contacts are categorized into four types: hydrogen bonds (green), hydrophobic (sky blue), ionic (magenta) and water bridges (blue). The stacked bar charts are normalized over the course of the trajectory.

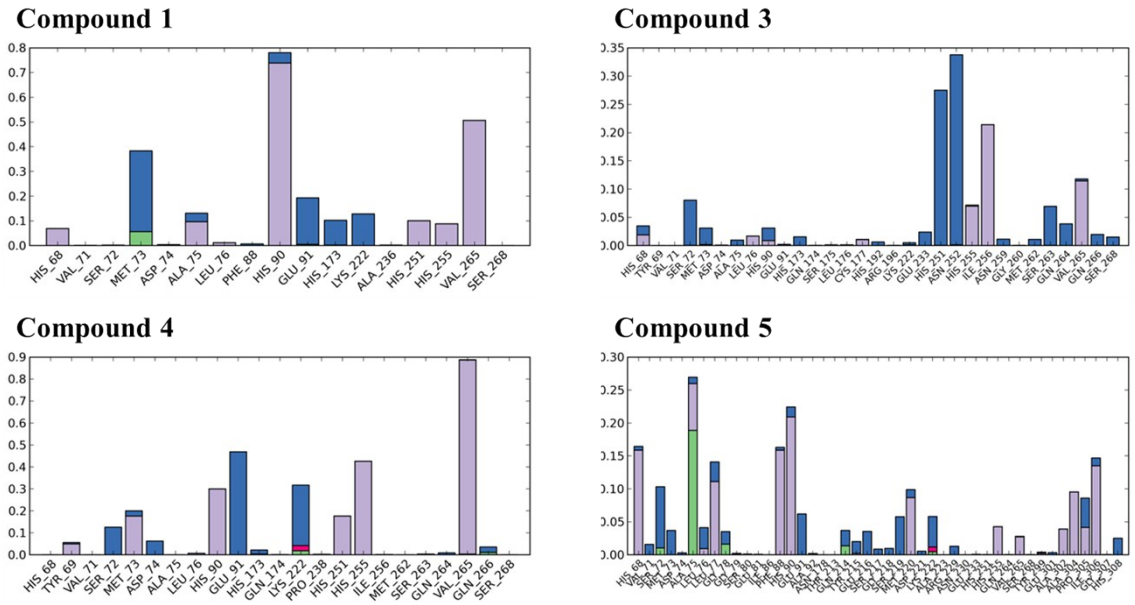

Fig. S5 Molecular dynamics simulations trajectory analyses of hTyr-inhibitor contacts. Protein-ligand contacts are categorized into four types: hydrogen bonds (green), hydrophobic (sky blue), ionic (magenta) and water bridges (blue). The stacked bar charts are normalized over the course of the trajectory.