A molecular modeling investigation of the therapeutic potential of marine compounds as DPP-4 inhibitors

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SUPPLEMENTARY MATERIALS

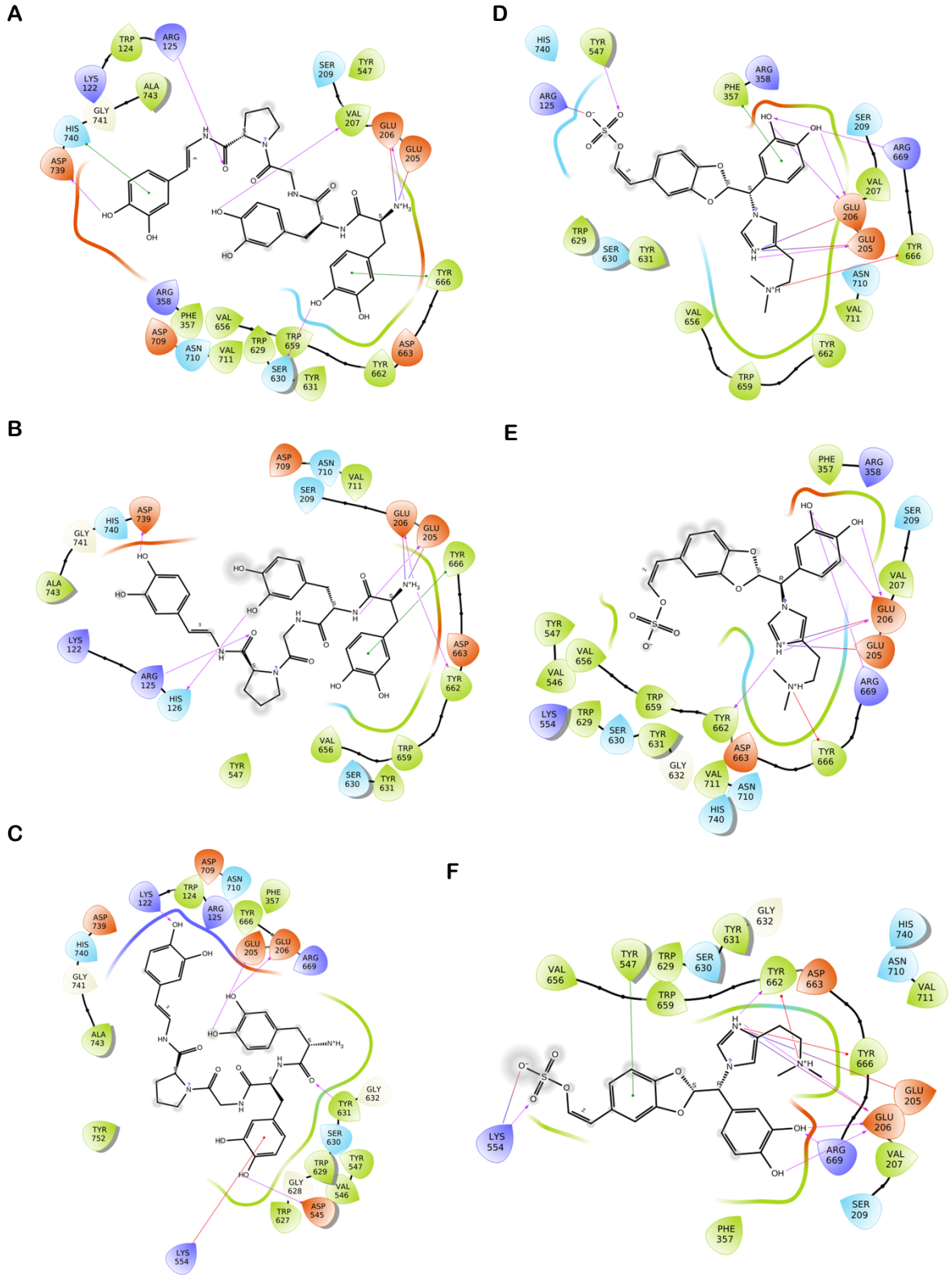

Figure S1. Ligand interaction diagram of DPP-4 residues that interact with the docked ligand in complexes: **(A)** 5I7U-CMNPD13046; **(B)** 5T4E-CMNPD13046; **(C)** 6B1E-CMNPD13046; **(D)** 5I7U-CMNPD17868; **(E)** 5T4E-CMNPD17868; **(F)** 6B1E_CMNPD17868 .

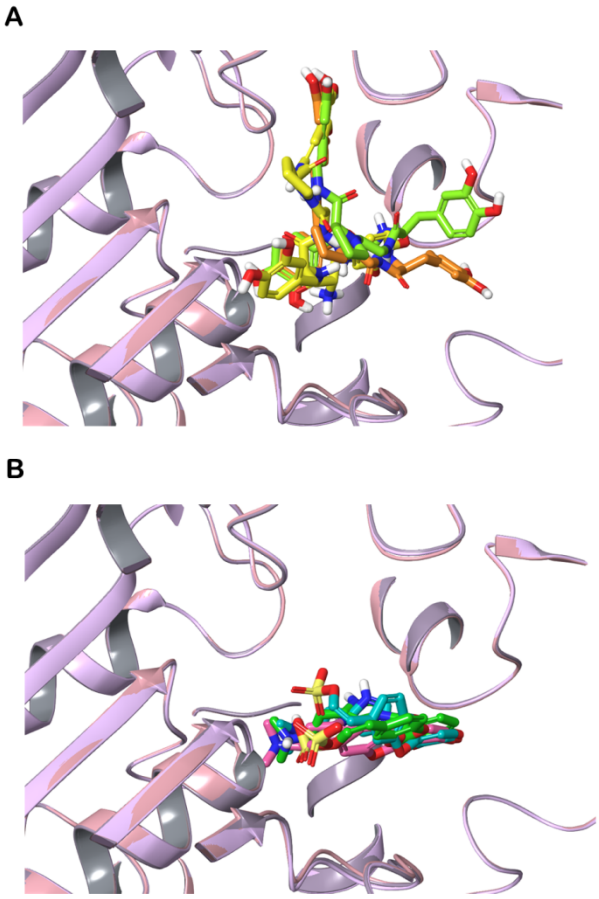

Figure S2. Superimposition of the docked ligands in the active site of DPP-4. **(A)** 6B1E-CMNPD13046 (orange), 5I7U-CMNPD13046 (green), and 5T4E-CMNPD13046 (yellow); **(B)** 6B1E-CMNPD17868 (cyan), 5I7U-CMNPD17868 (green), 5T4E-CMNPD17868 (pink).