

Supplementary Information

Unravelling the molecular interaction of diselenodipropionic acid (DSePA) with human serum albumin (HSA)

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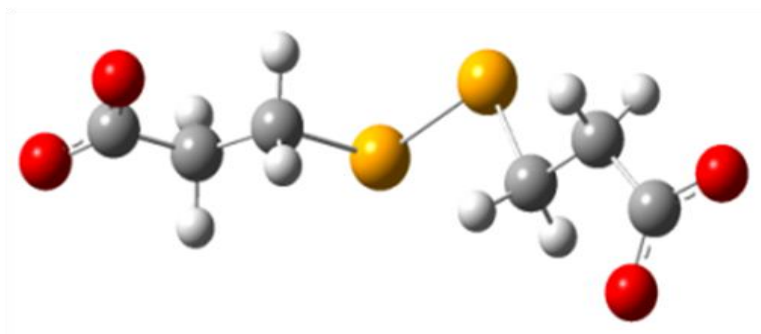


Figure S11: Optimized structures of DSePA in water by using density functional theory (DFT) employing B3LYP as exchange-correlation functional and also basis set at 6-31+G(d,p), respectively.

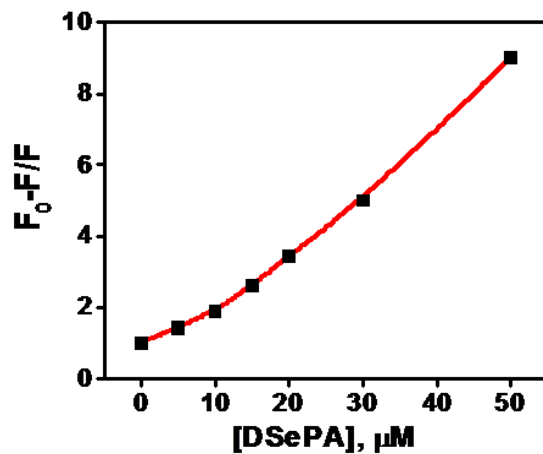


Figure SI2: The linear fit of $(F_0 - F)/F$ against $[\text{DSePA}]$ for complexes of HSA with different concentrations of DSePA (5-50 μM) at pH 7 phosphate buffer solution.

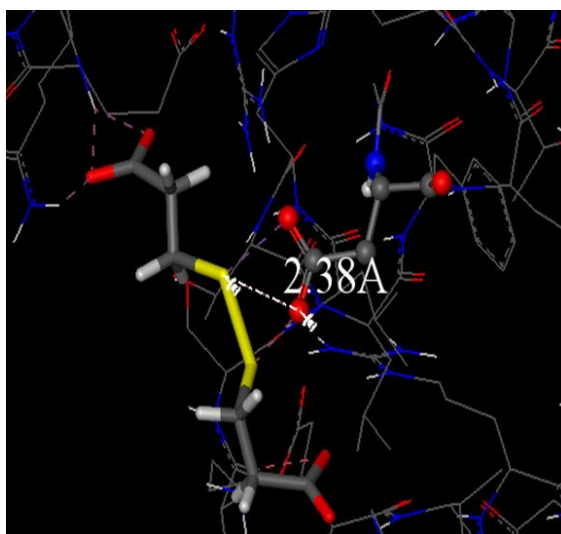


Figure SI3: Schematic representation displaying amino acids in domain IA pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between Se of DSePA and Asp72 amino acid in domain IA pocket of HSA.

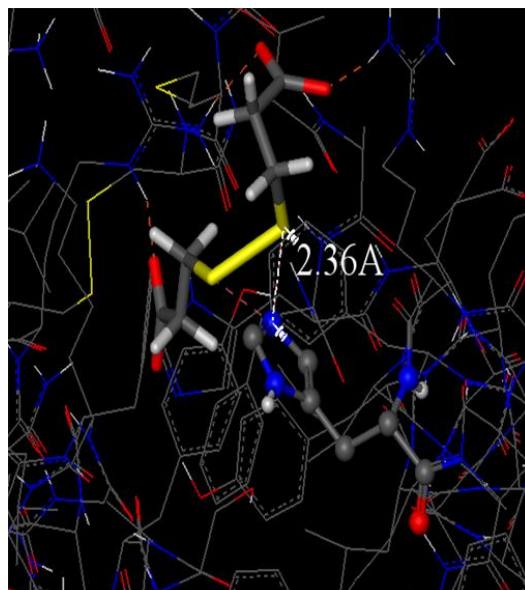


Figure S14: Schematic representation displaying amino acids in domain IB pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between Se of DSePA and His146 amino acid in domain IB pocket of HSA.

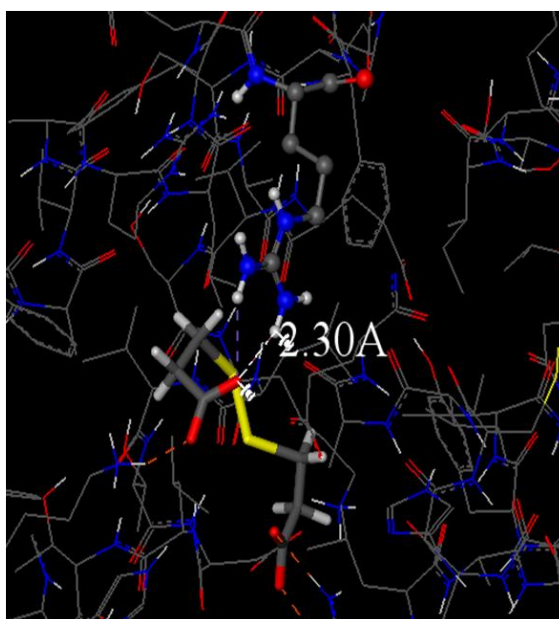


Figure SI5: Schematic representation displaying amino acids in domain IIA pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between carboxylate ion of DSePA and Arg222 amino acid in domain IIA pocket of HSA.

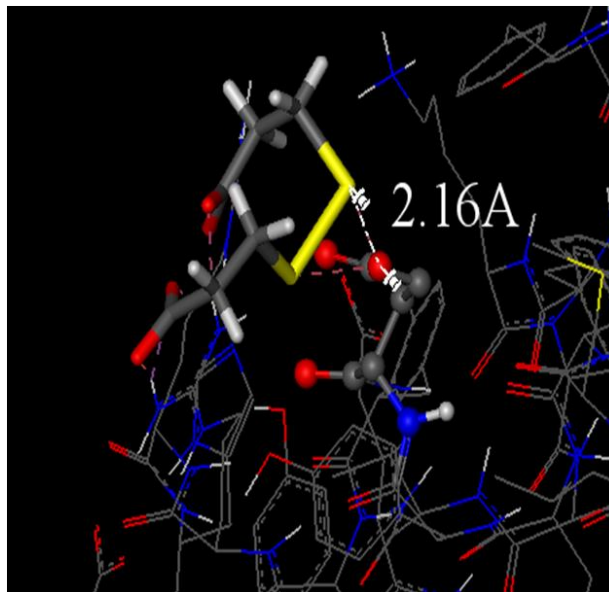


Figure SI6: Schematic representation displaying amino acids in domain IIB pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between Se of DSePA and Glu333 amino acid in domain IIB pocket of HSA.

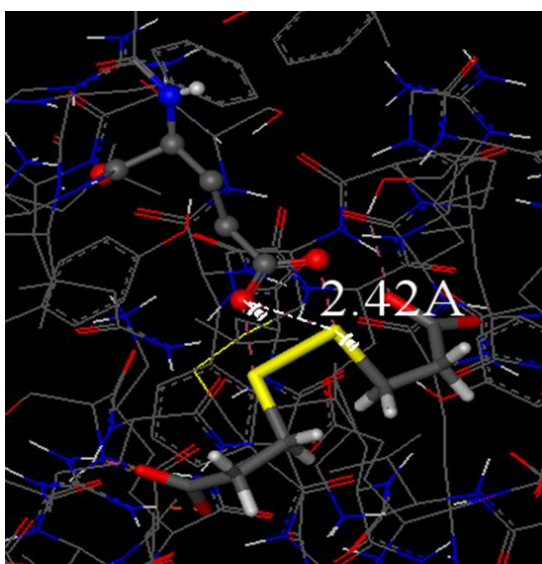


Figure SI7: Schematic representation displaying amino acids in domain IIIA pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between Se of DSePA and Glu400 amino acid in domain IIIA pocket of HSA.

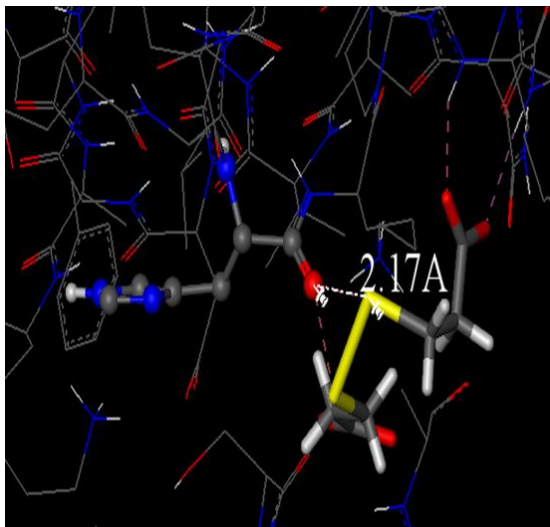
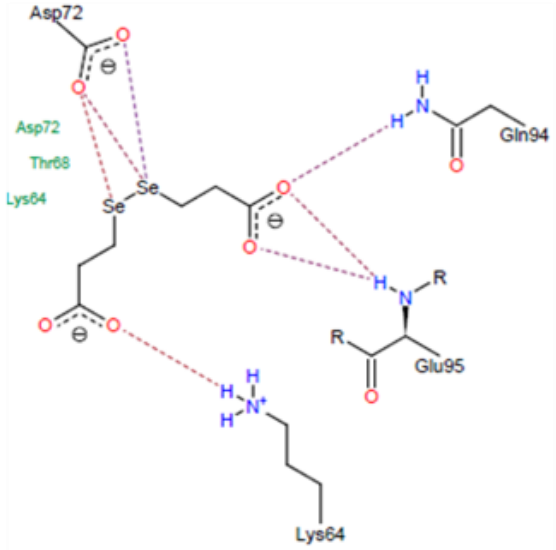
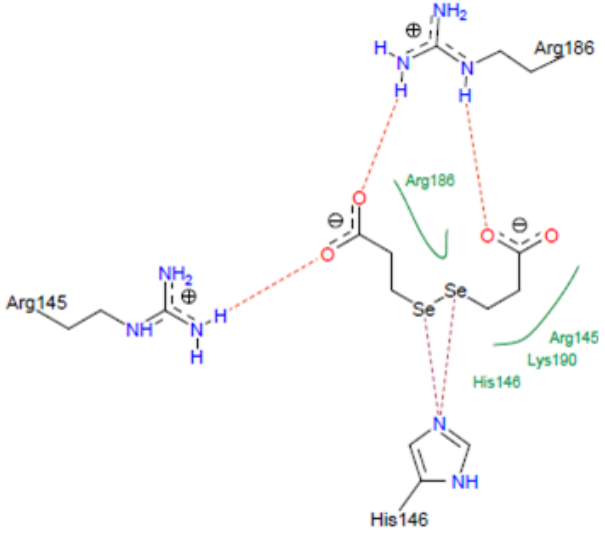
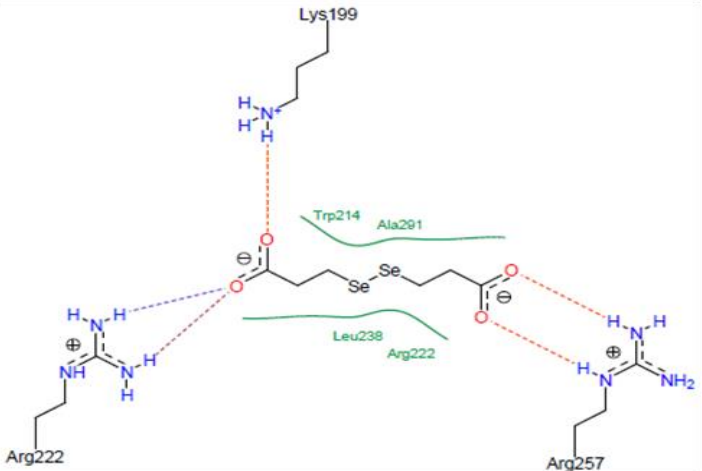
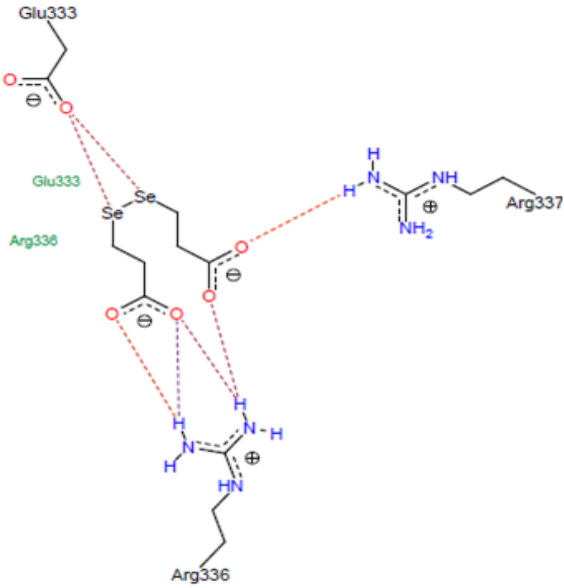
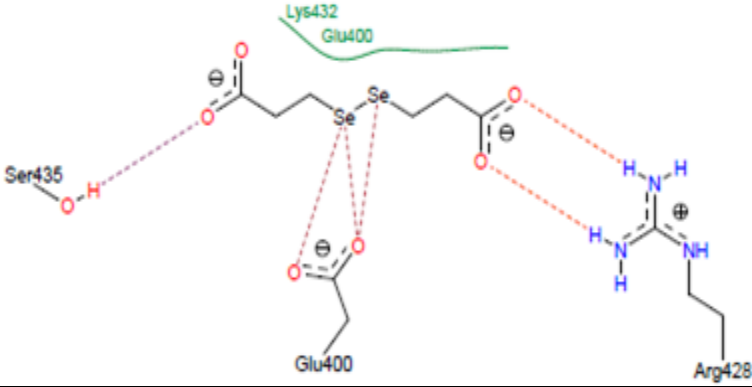
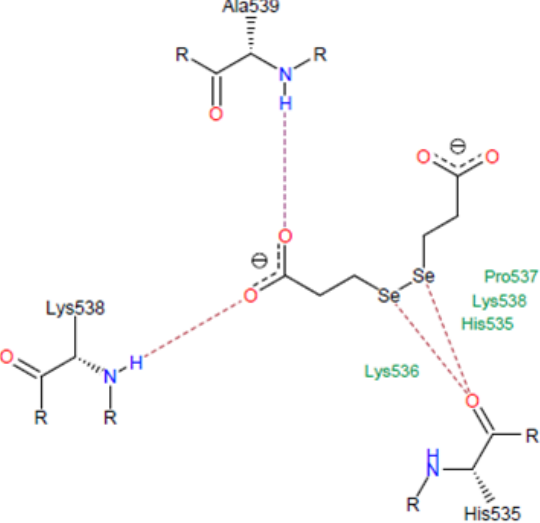


Figure SI8: Schematic representation displaying amino acids in domain IIIB pocket of HSA involved in hydrogen binding with DSePA. The measured hydrogen bond distance between Se of DSePA and His535 amino acid in domain IIIB pocket of HSA.

Table-1: Molecular docked structures of DSePA and amino acids of HSA at different domain sites and also their scoring pose and the standard free energy change (ΔG°) values.

HSA Domain Site	Schematic representation displaying amino acids in HSA involved in binding with DSePA	Score	ΔG° (kJ/mol)

<p>IA</p>		<p>-12</p>	<p>-13</p>
<p>IB</p>		<p>-20</p>	<p>-8</p>
<p>IIA</p>		<p>-21</p>	<p>-28</p>

<p>IIB</p>		<p>-13</p>	<p>-6</p>
<p>IIIA</p>		<p>-20</p>	<p>-1</p>
<p>IIB</p>		<p>-17</p>	<p>-8</p>