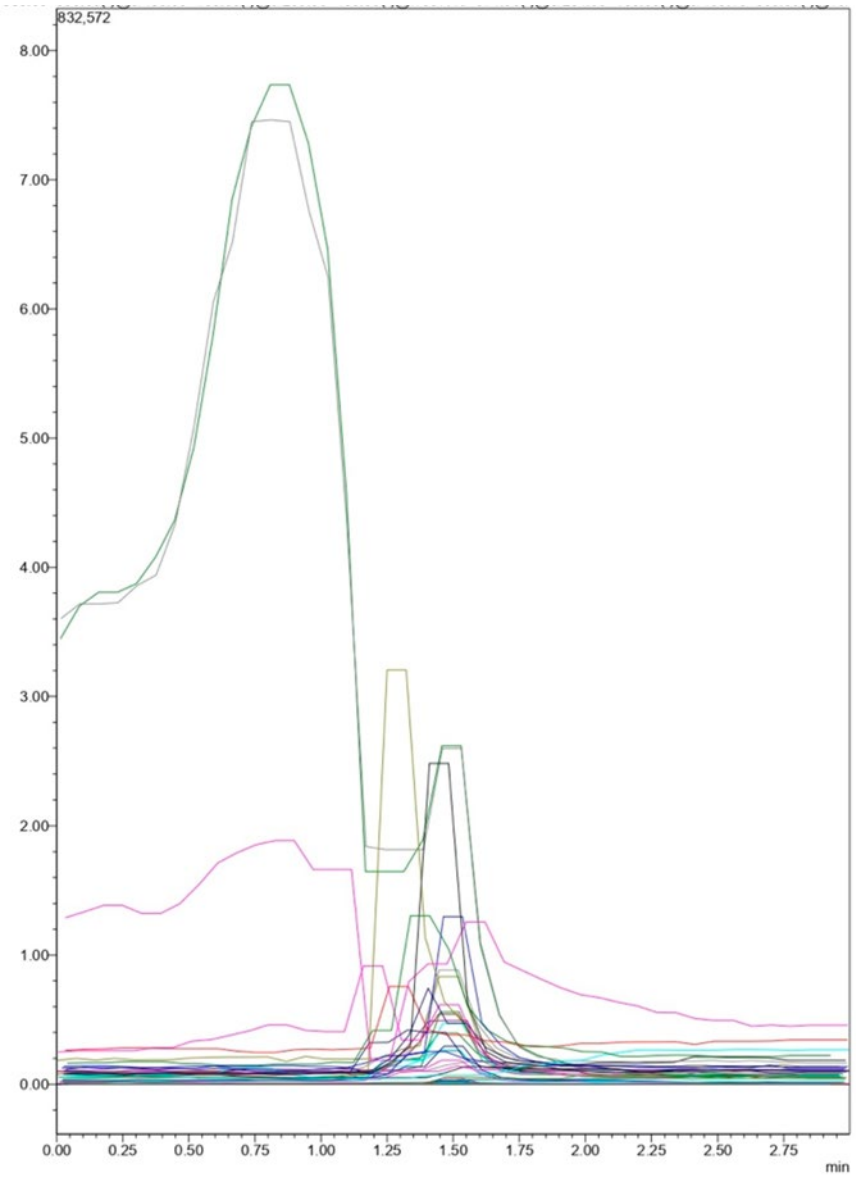


Figure S1. Selected fragments derive from the molecular weight of the polyphenol minus one (due to ESI- ionization) and their subsequent fragmentation in MS/MS experiment.

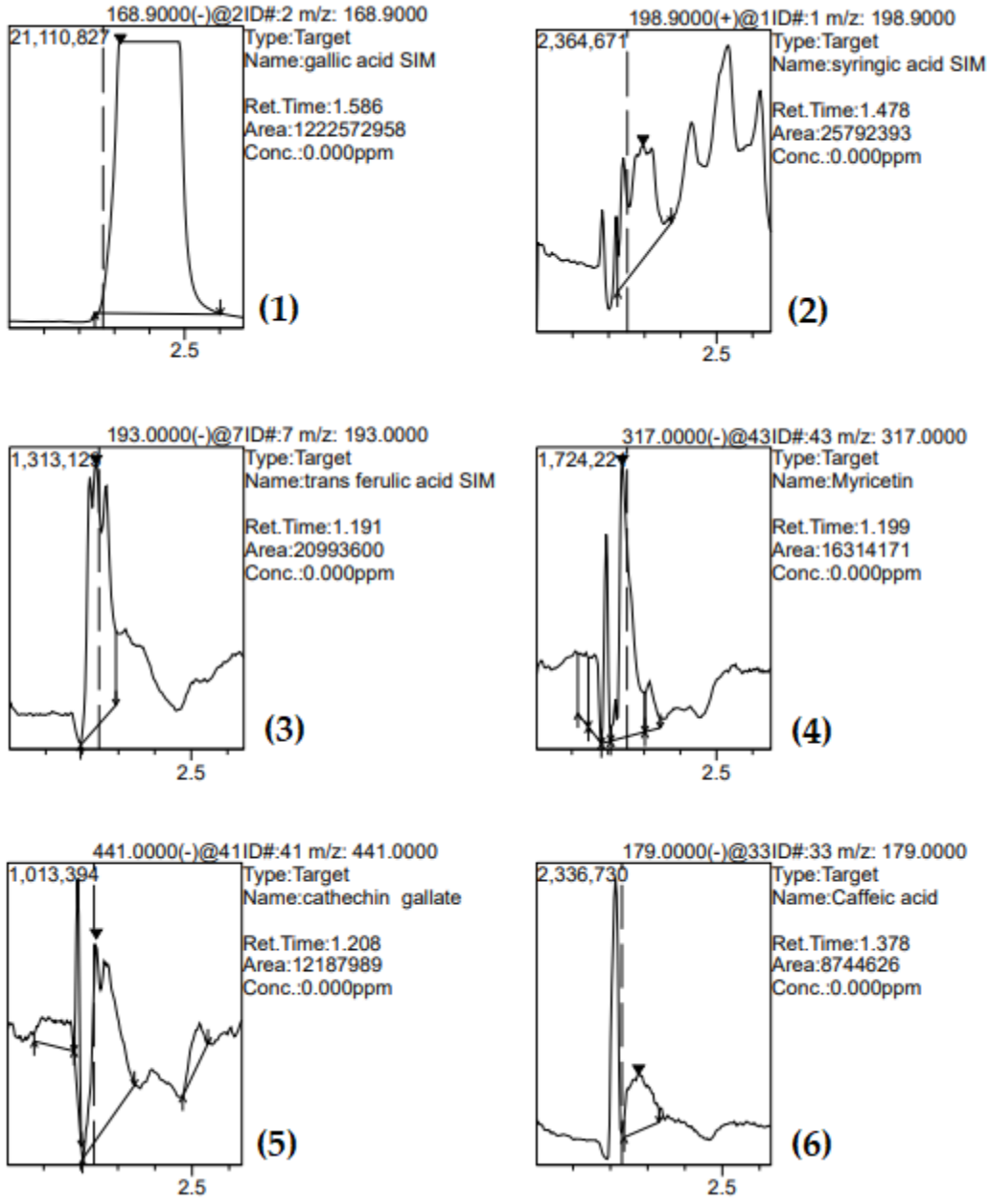


Figure S2. Screening of polyphenols from *A. halimus* ethanolic extract (AHEE) using LC-MS/MS. **(1)** Gallic acid, **(2)** Syringic acid, **(3)** *trans*-Ferulic acid, **(4)** Myricetin, **(5)** Catechin gallate, **(6)** Caffeic acid, **(7)** Chlorogenic acid, **(8)** Arbutin, **(9)** Trimethoxyflavone.

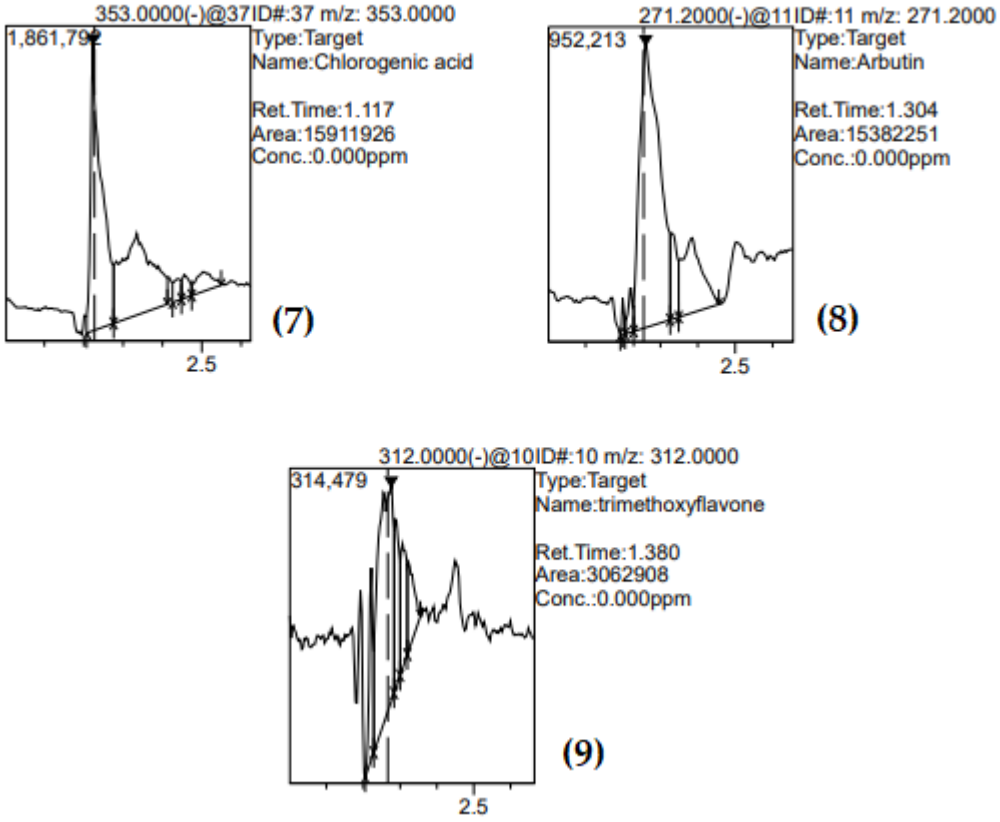


Figure S2. *Cont.*

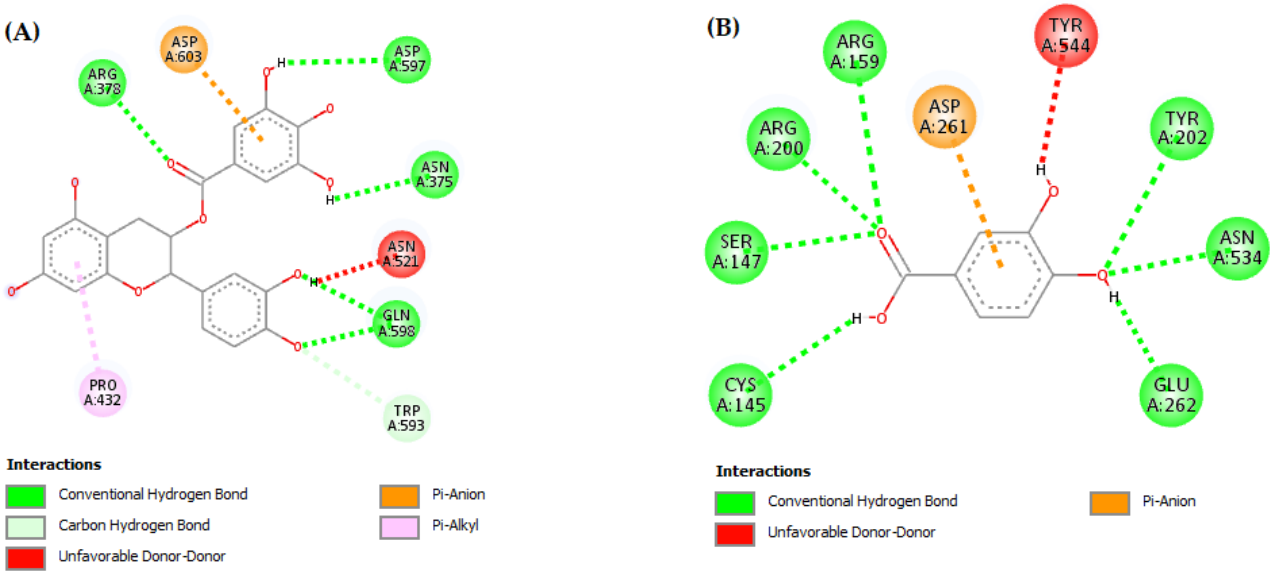


Figure S3. 2D binding interactions of the potent inhibitor from AHEE, Catechin gallate (**A**), and the native ligand, Protocatechuic acid (**B**), against Lipoxygenase protein **(PDB ID: 1N8Q)**

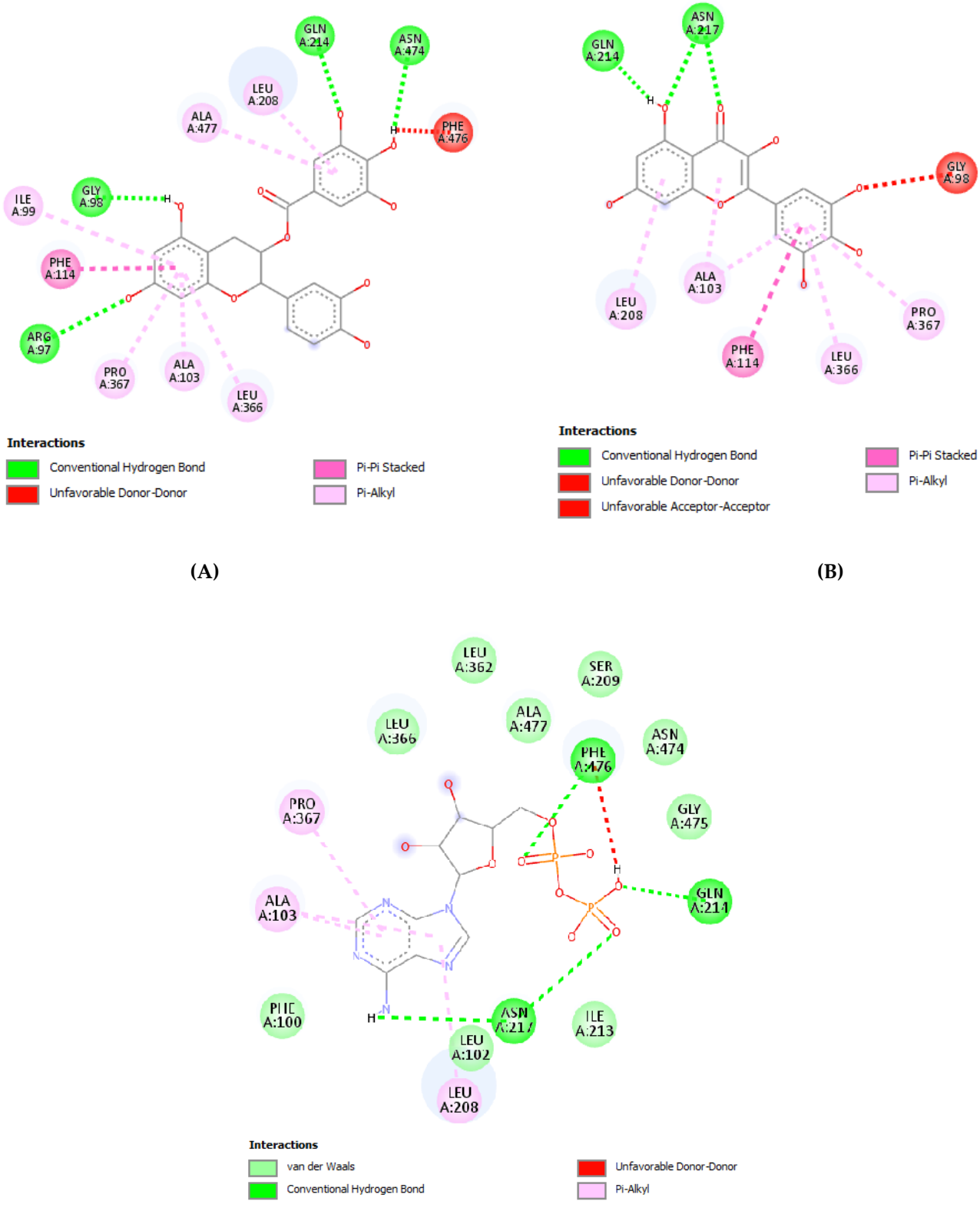


Figure S4. 2D binding interactions of the potent inhibitors from AHEE, Catechin gallate (**A**), Mericetin (**B**), and the native ligand, Warfarin (**C**), against CYP450 protein **(PDB ID: 1OG5)**

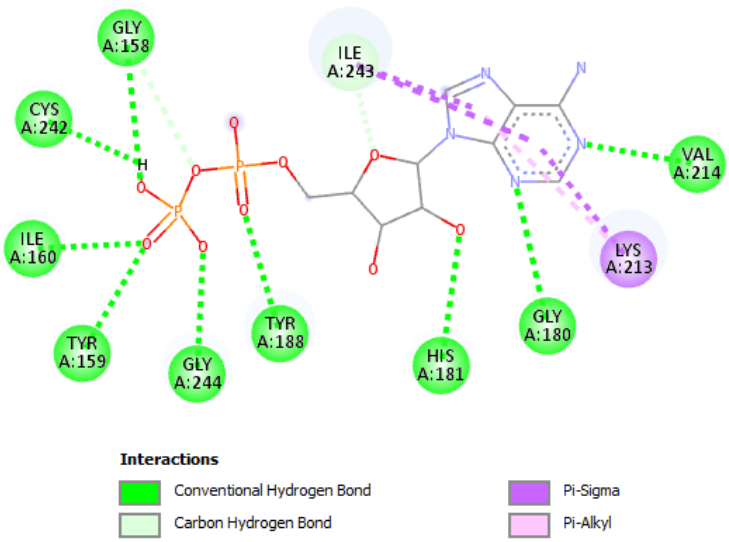
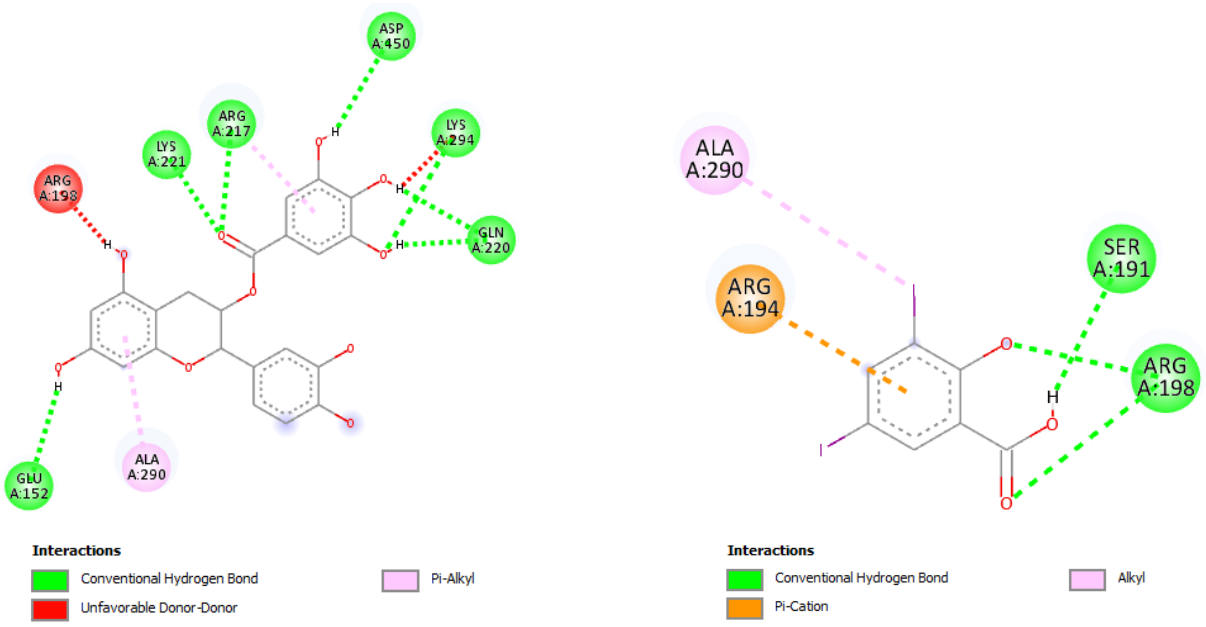


Figure S5. 2D binding interactions of Adenosine-5'-diphosphate (native ligand), against NADPH Oxidase protein **(PDB ID: 2CDU), * Our analysis revealed that none of the identified compounds in AHEE can inhibit the activity of NADPH Oxidase.**



(A) **(B)**

Figure S6. 2D binding interactions of the potent inhibitor from AHEE, Catechin gallate (**A**), 3,5-Diiodosalicylic Acid (native ligand) (**B**), against Bovine Serum Albumin (BSA) protein **(PDB ID: 4JK4)**, *** All the identified components were found to be potent inhibitors of BSA protein.**