

Supplementary Materials

Article

Biochemical and Computational Approach of Selected Phytocompounds from *Tinospora crispa* in the Management of COVID-19

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32 **Figure Legends:**

33 **Figure S1.** 2D and 3D interactions of Benzeneethanamine (A) and Camphenol (B) with the active site of
34 SARS-CoV-2 M^{pro} (PDB ID: 6W63)

35 **Figure S2.** 2D and 3D interactions of Strophanthidin (C) and Retinal (D) with the active site of SARS-CoV-
36 2 M^{pro} (PDB ID: 6W63)

37 **Figure S3.** 2D and 3D interactions of Trans-geranylgeraniol (E) and 3,4-Dihydroxymandelic acid (F) with
38 the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

39 **Figure S4.** 2D and 3D interactions of Imidazolidin-4-one, 2-imino-1-(4-methoxy-6-dimethylamino-1,3,5-
40 triazin-2-yl) (G) and Retinol (F) with the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

41 **Figure S5.** 2D and 3D interactions of alpha-Santalol (I) and Santalol, E-cis, epi-.beta.- (J) with the active site
42 of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

43 **Figure S6.** 2D and 3D interactions of spiro [4.5]dec-6-en-1-ol, 2,6,10,10-tetramethyl (K) and 3.beta.-
44 Hydroxy-5-cholen-24-oic acid (L) with the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

45 **Figure S7.** 2D and 3D interactions of Phosphonoacetic acid, 3TMS derivative (M) and Nordazepam, TMS
46 derivative (N) with the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

47 **Figure S8.** 2D and 3D interactions of 2,6-Dihydroxybenzoic acid, 3TMS derivative (O) and aR-Turmerone
48 (P) with the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

49 **Figure S9.** 2D and 3D interactions of (Z)-.gamma.-Atlantone (Q) and Verbenyl angelate, cis- (R) with the
50 active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

51 **Figure S10.** 2D and 3D interactions of Tumerone (S) and Dibutyl phthalate (T) with the active site of SARS-
52 CoV-2 M^{pro} (PDB ID: 6W63)

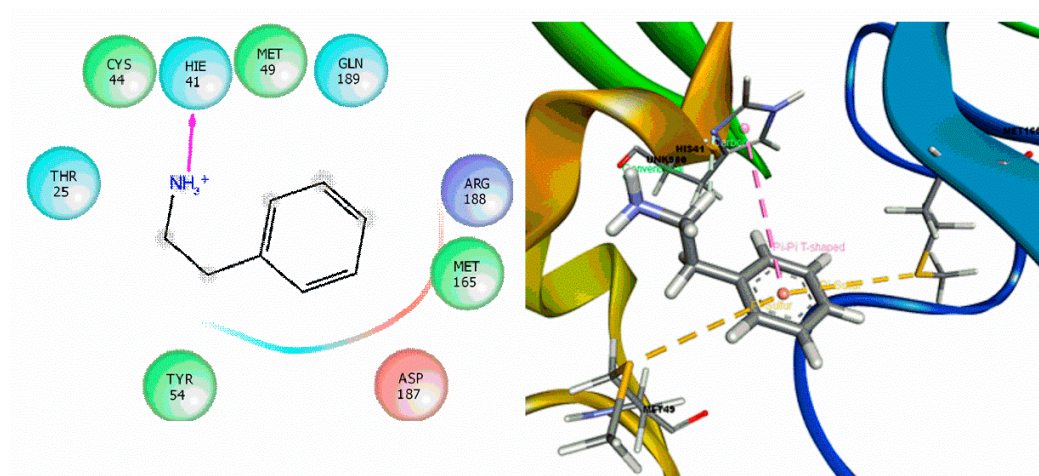
53 **Figure S11.** 2D and 3D interactions of (-)-Globulol (U) and Androstan-17-one, 3-ethyl-3-hydroxy-, (5.alpha)
54 (V) with the active site of SARS-CoV-2 M^{pro} (PDB ID: 6W63)

55 **Figure S12.** 2D and 3D interactions of Yangambin (W) with the active site of SARS-CoV-2 M^{pro} (PDB ID:
56 6W63)

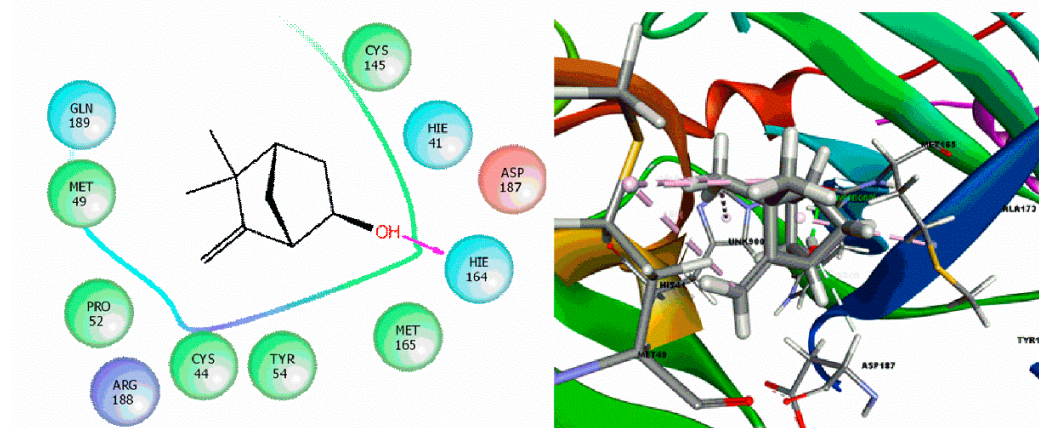
57 **Figure S13.** 2D and 3D interactions of Nelfinavir (X) and Lopinavir (Y) with the active site of SARS-CoV-
58 2M^{pro} (PDB ID: 6W63).

59

FIGURE S1.



A



B

FIGURE S2.

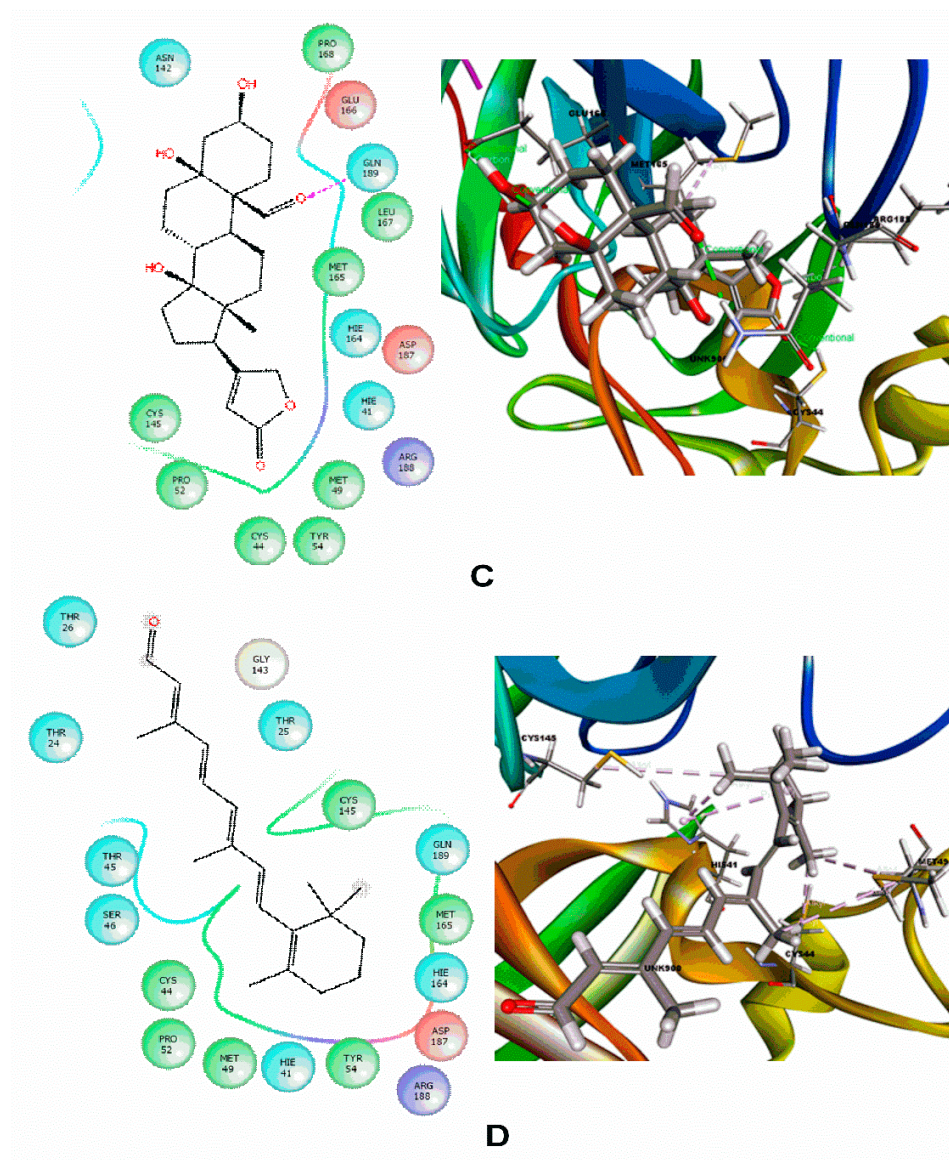


FIGURE S3.

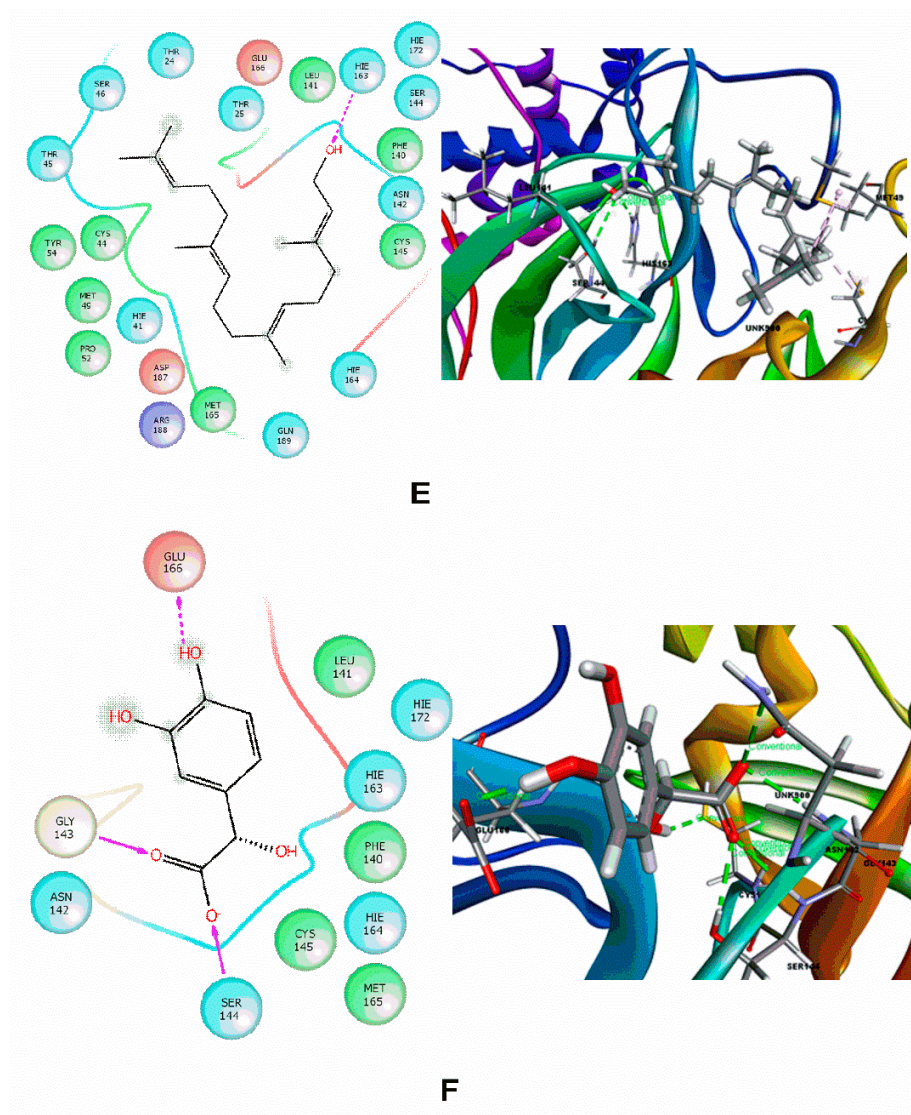


FIGURE S4.

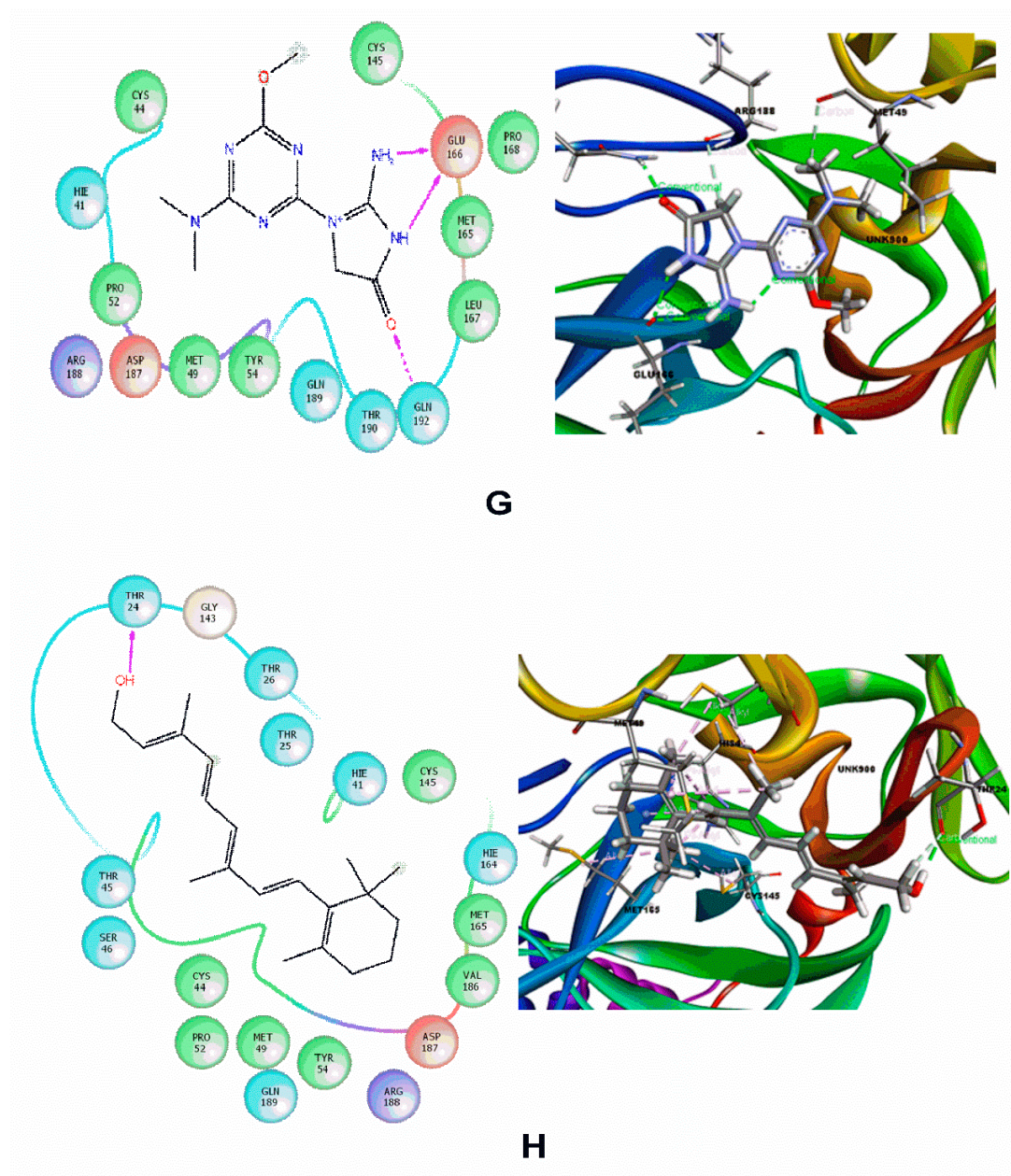


FIGURE S5.

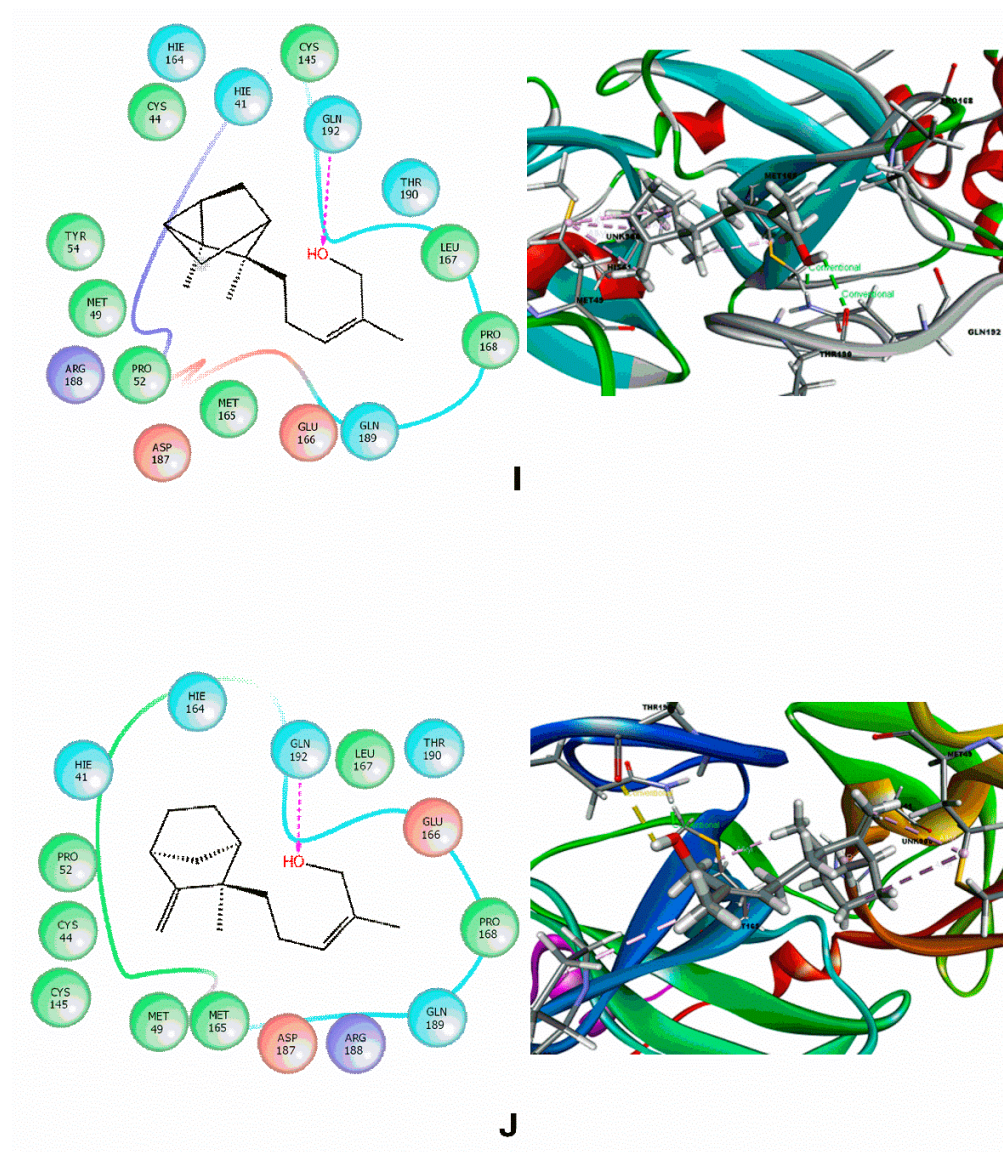


FIGURE S6.

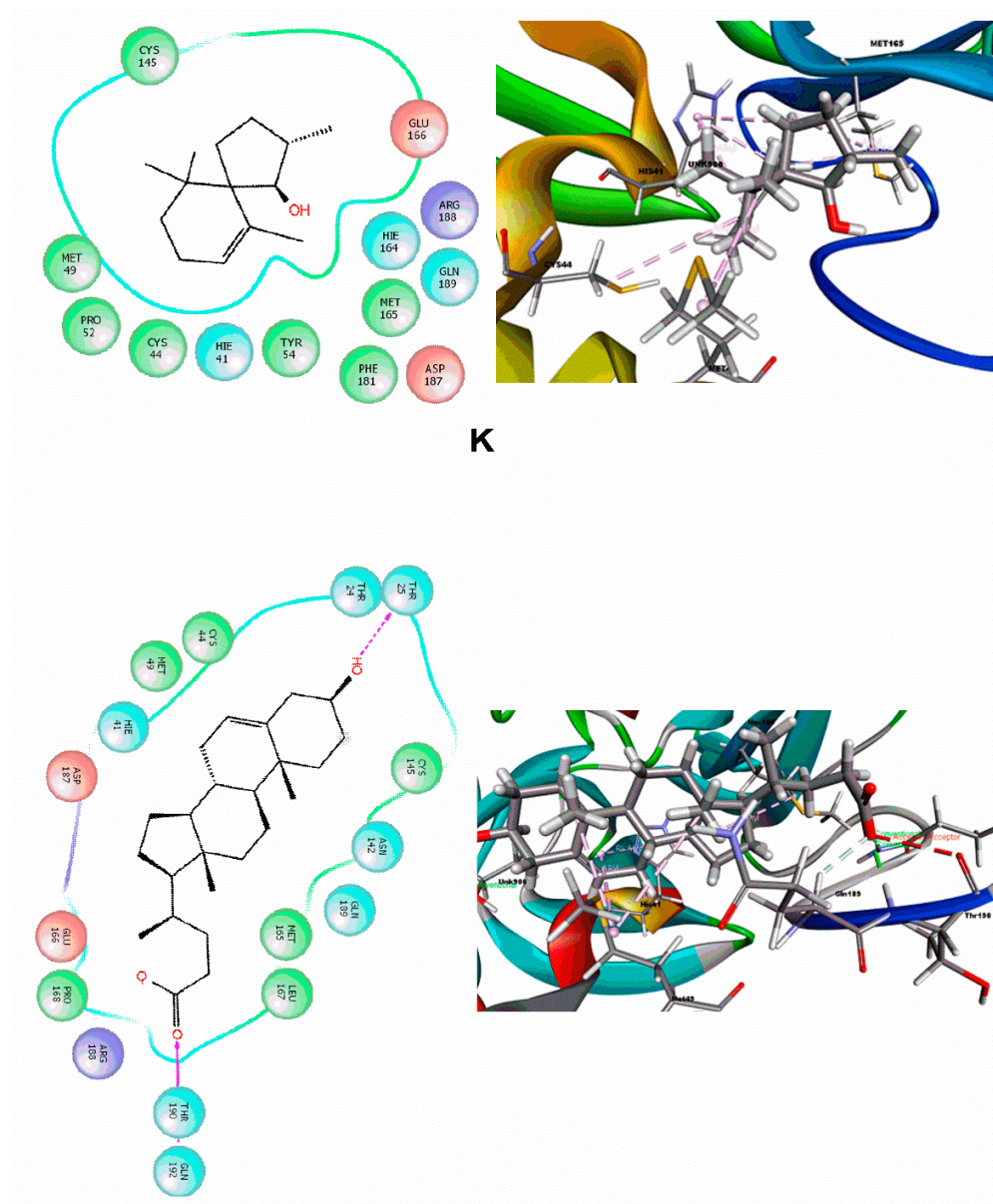


FIGURE S7.

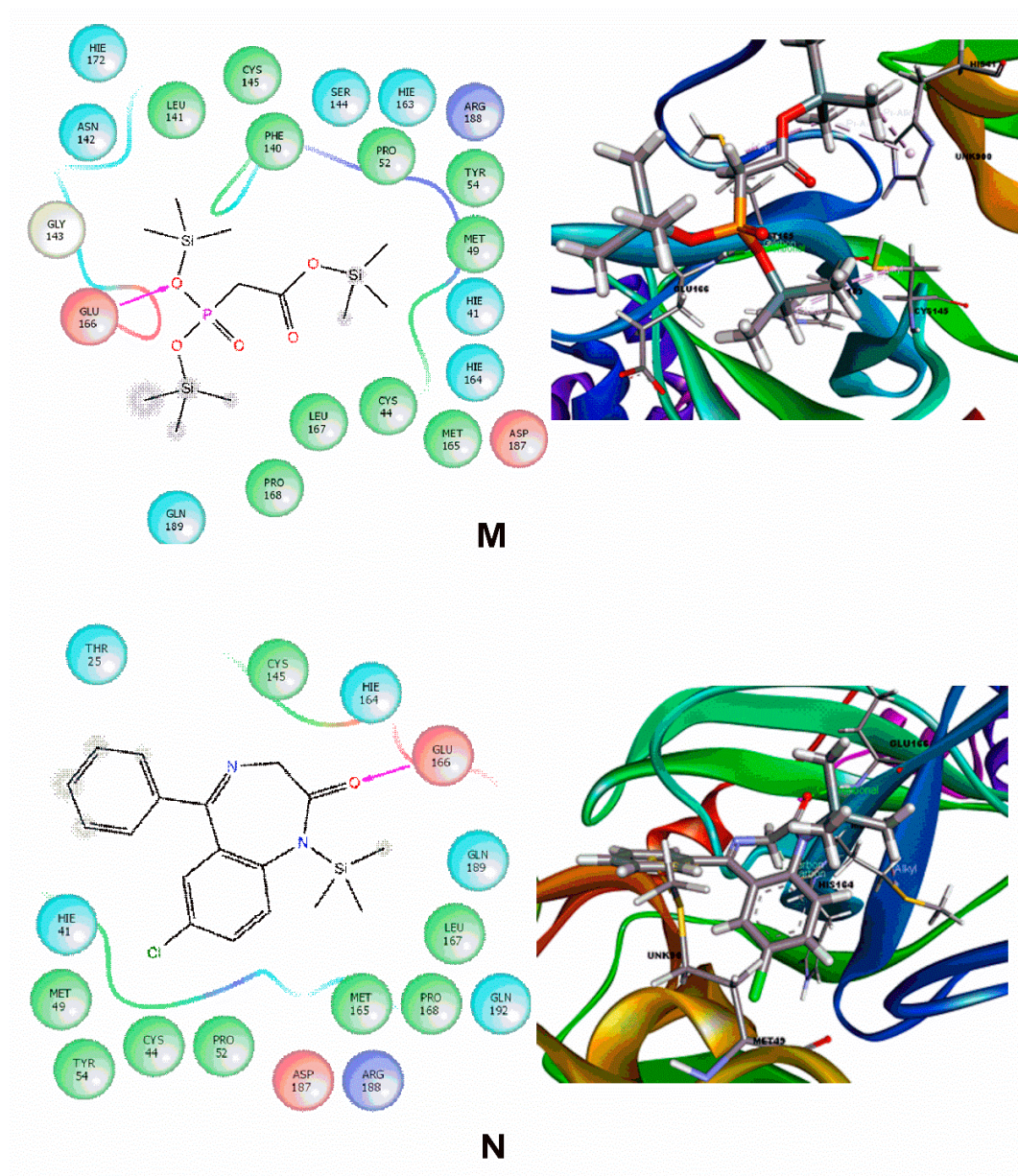


FIGURE S8.

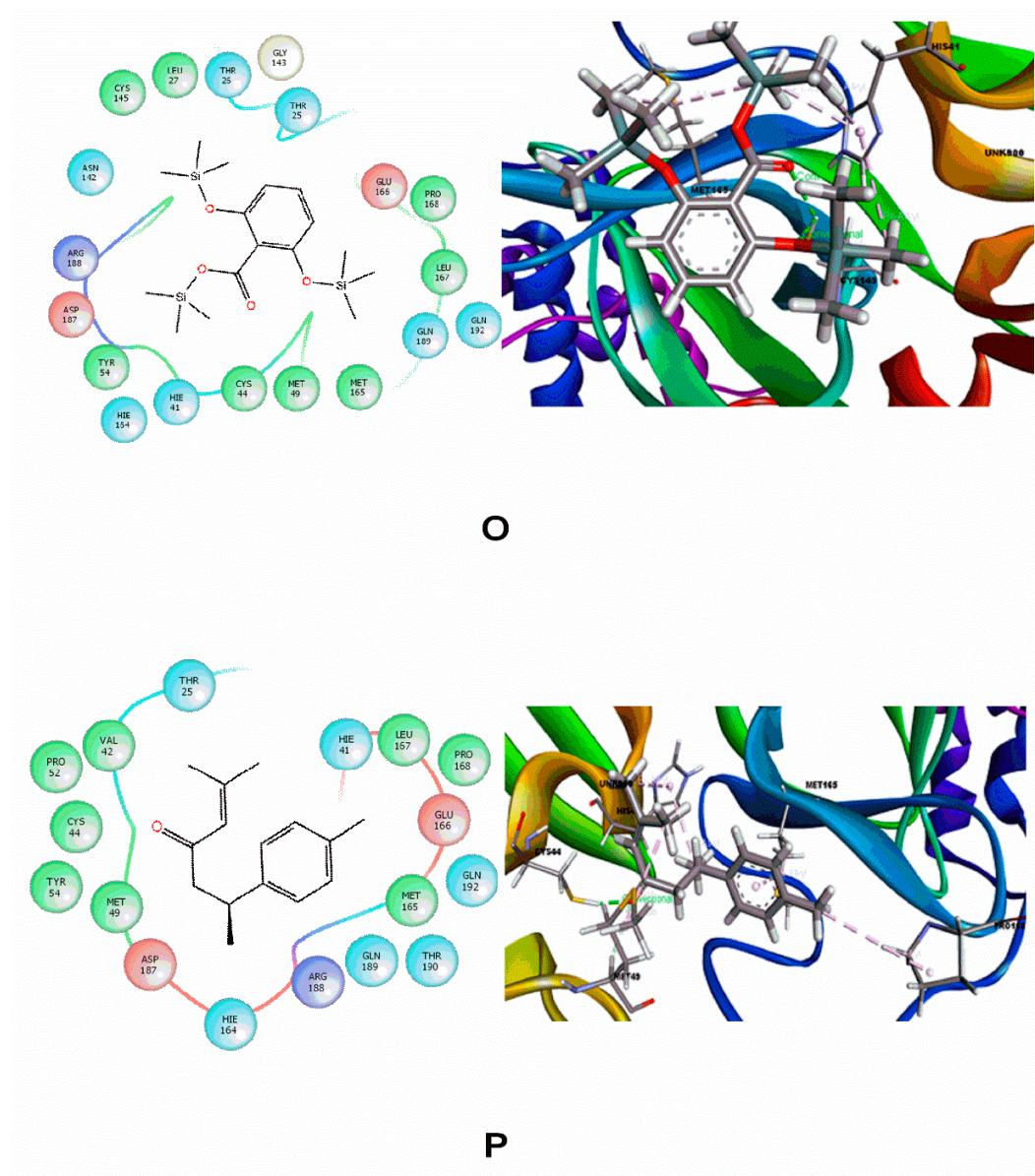


FIGURE S9.

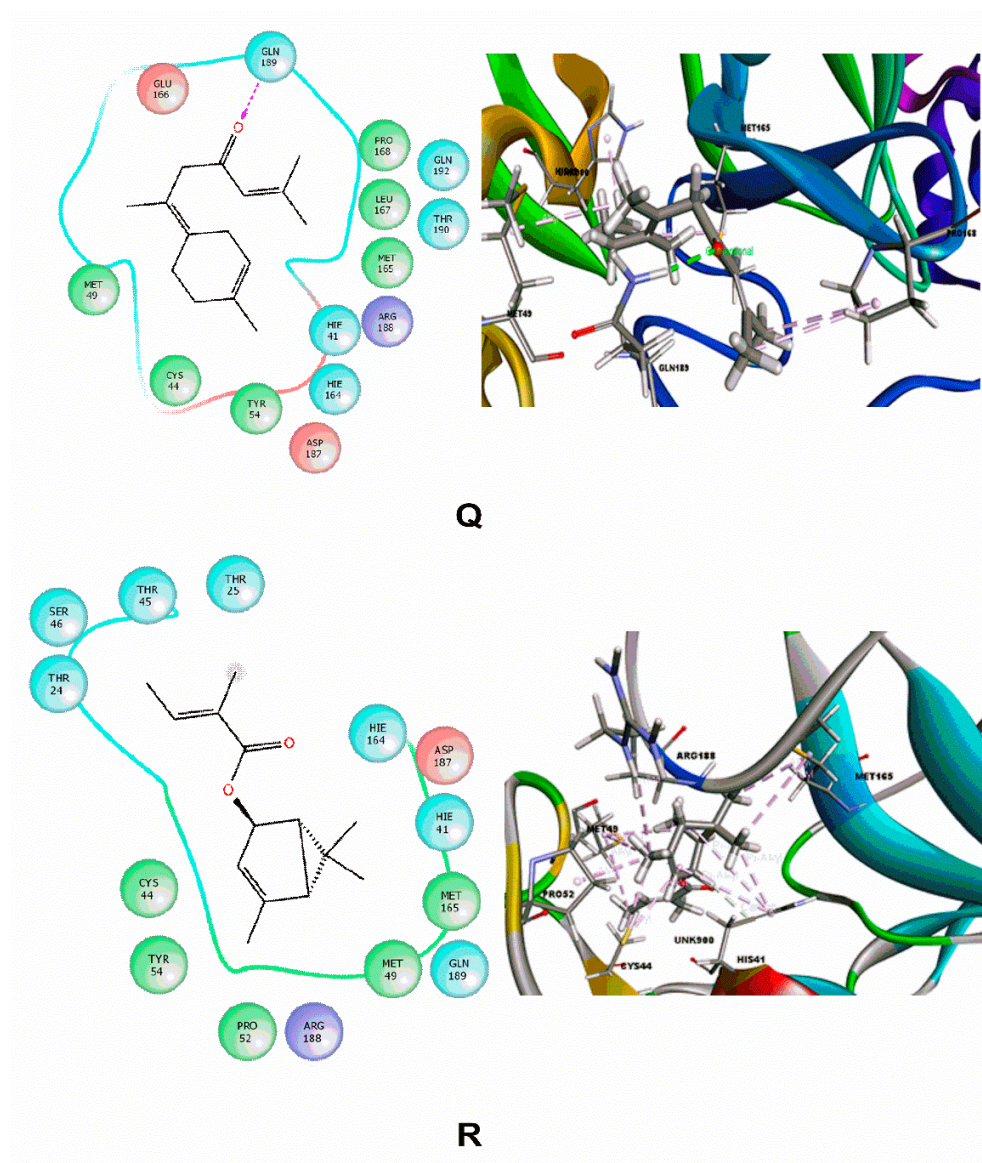


FIGURE S10.

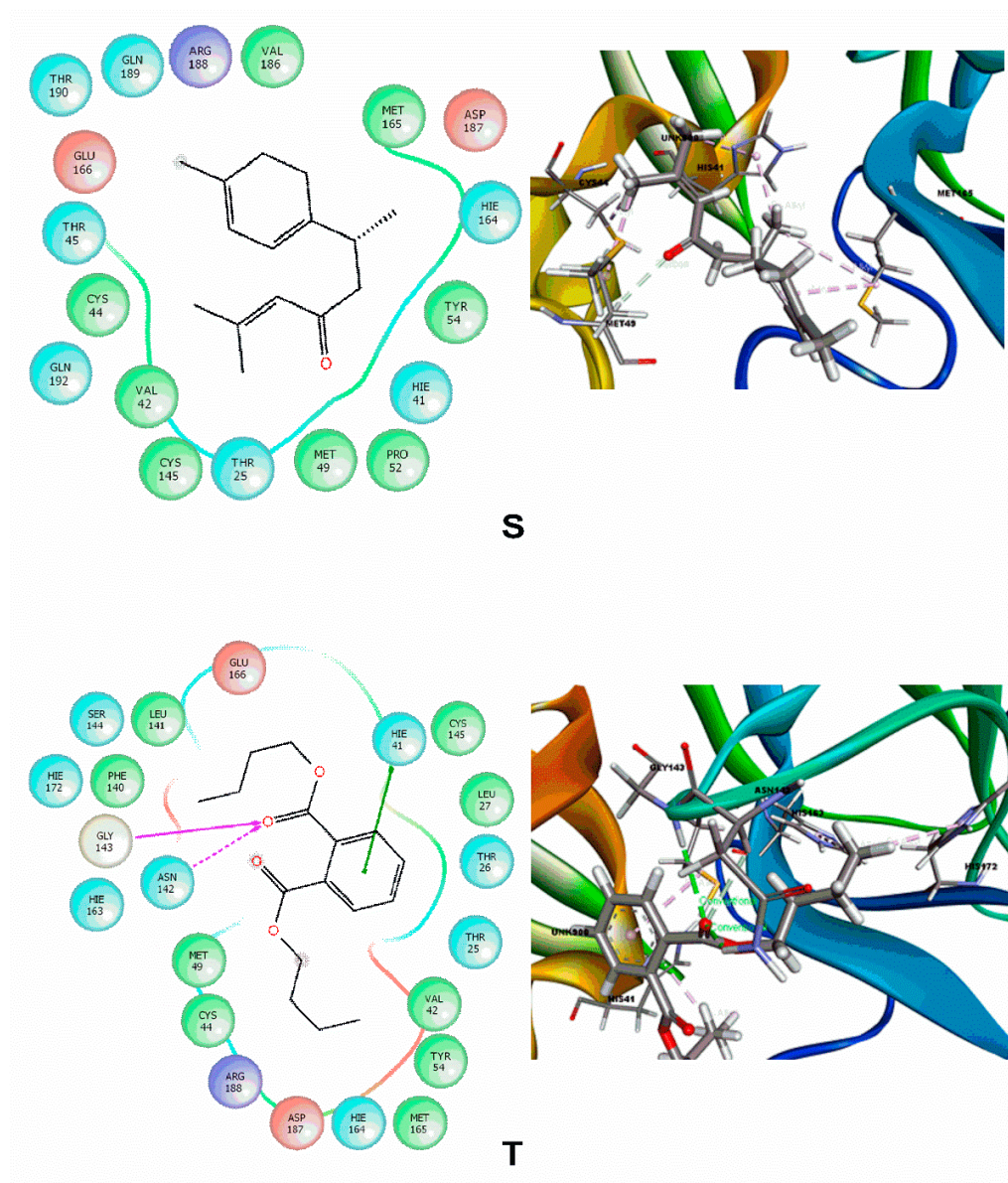


FIGURE S11.

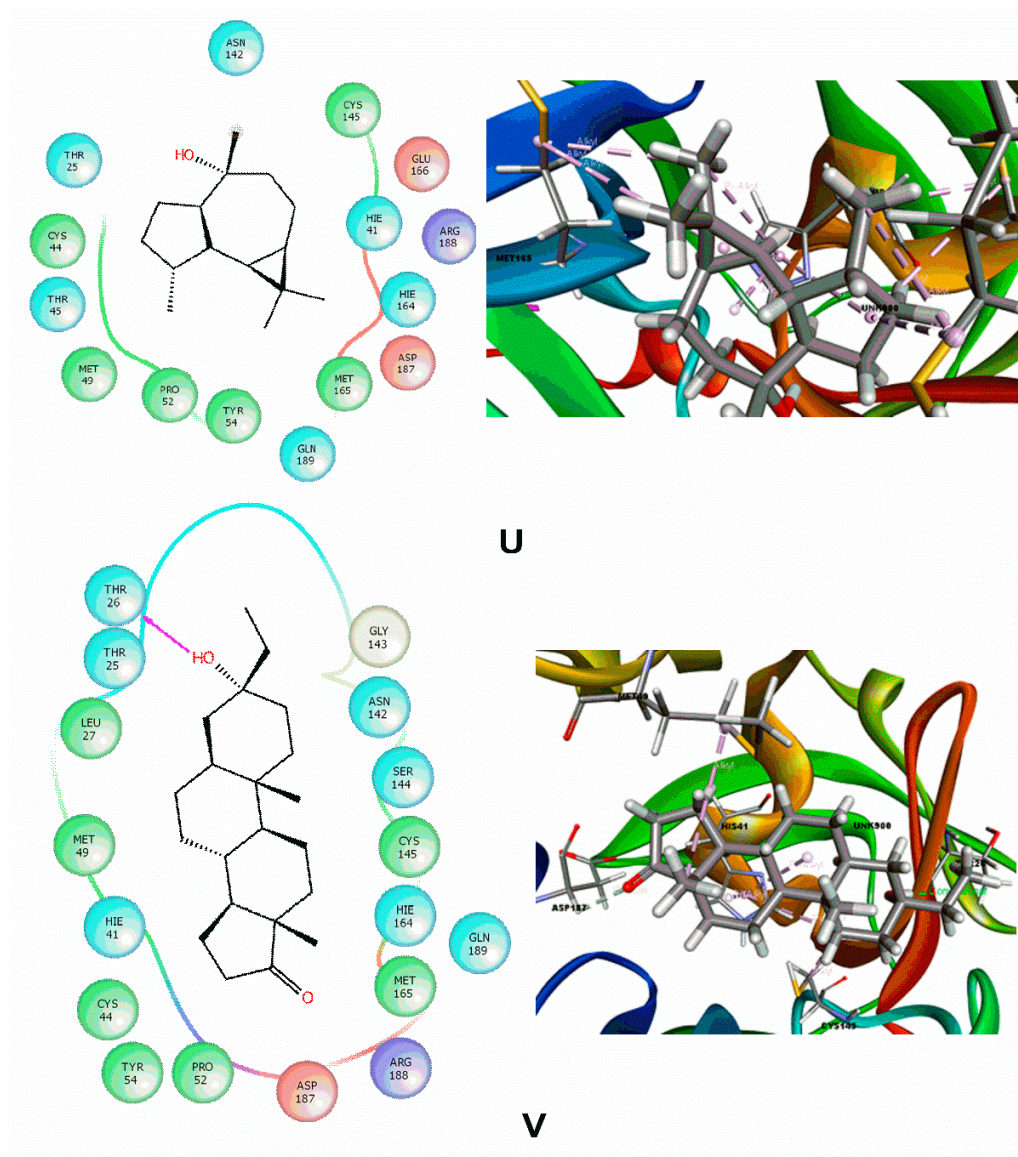


FIGURE S12.

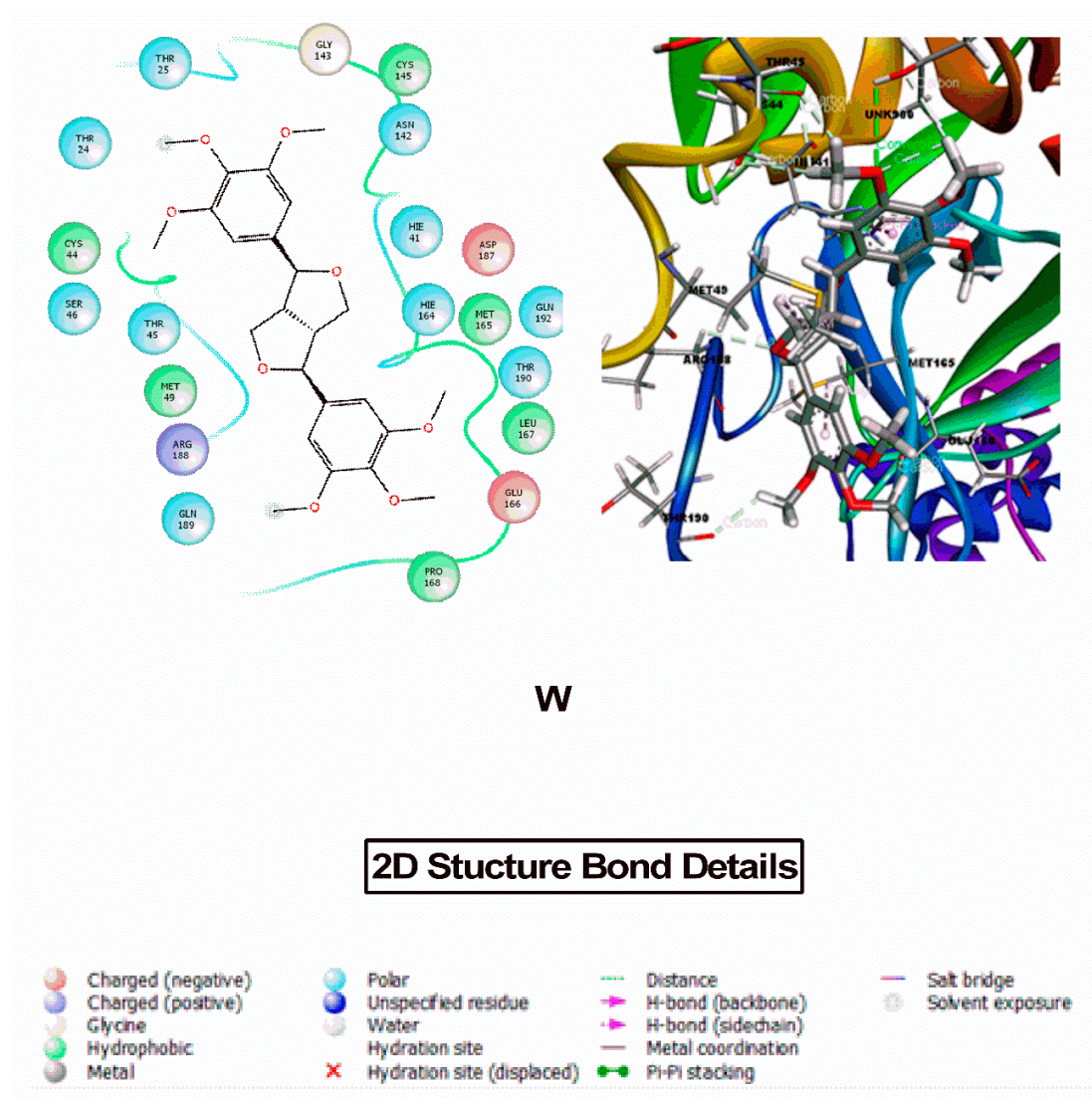


FIGURE S13.

