Supplementary Information

For

Synthesis, Structural Characterization, Biological and *In silico* Evaluation of Halogenated Schiff Bases as Potential Multifunctional Agents

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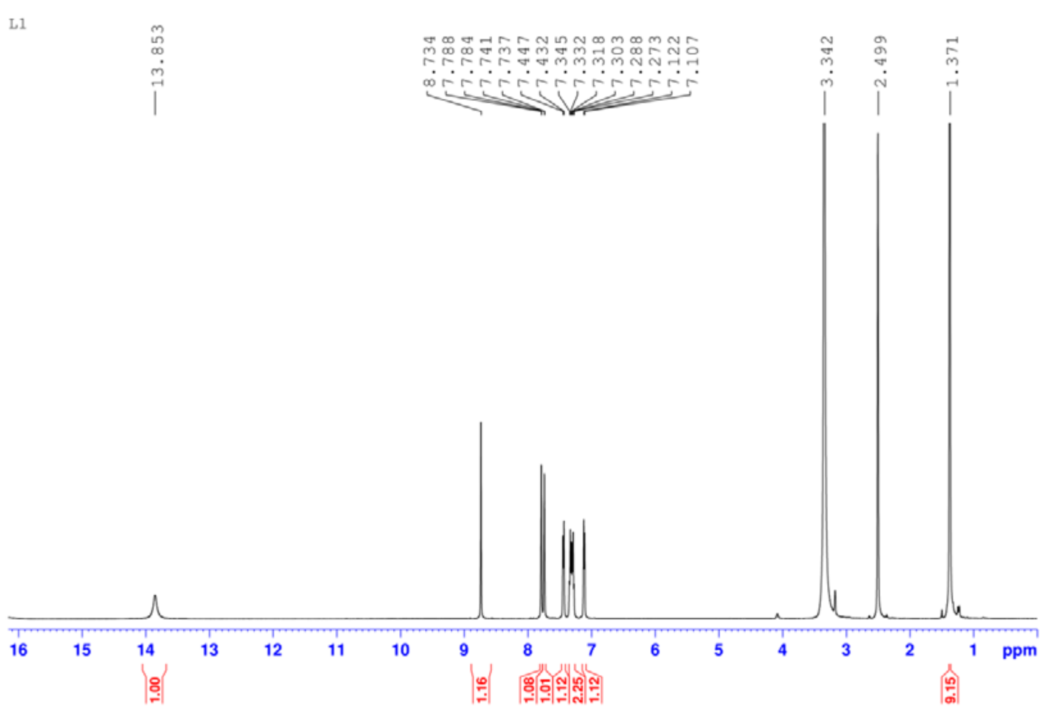

Figure S1: ^{1}H NMR spectrum of **SB1** obtained at room temperature using (500 MHz, DMSO-d_6)

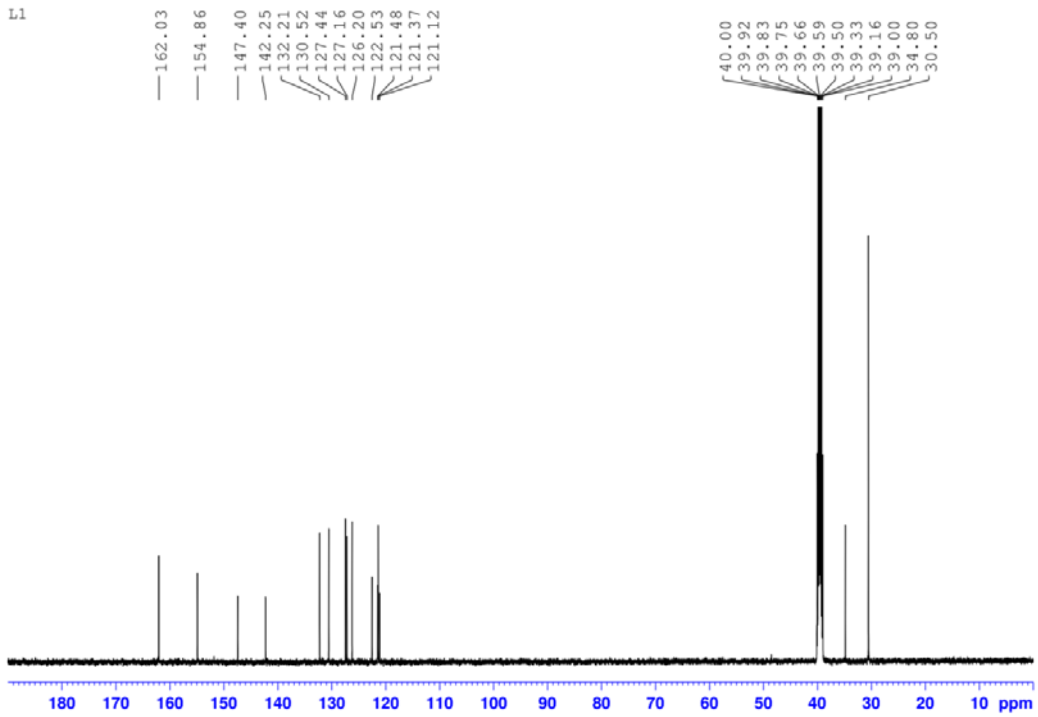

Figure S2: ^{13}C NMR spectrum of **SB1** obtained at room temperature using (125 MHz, DMSO-d_6)

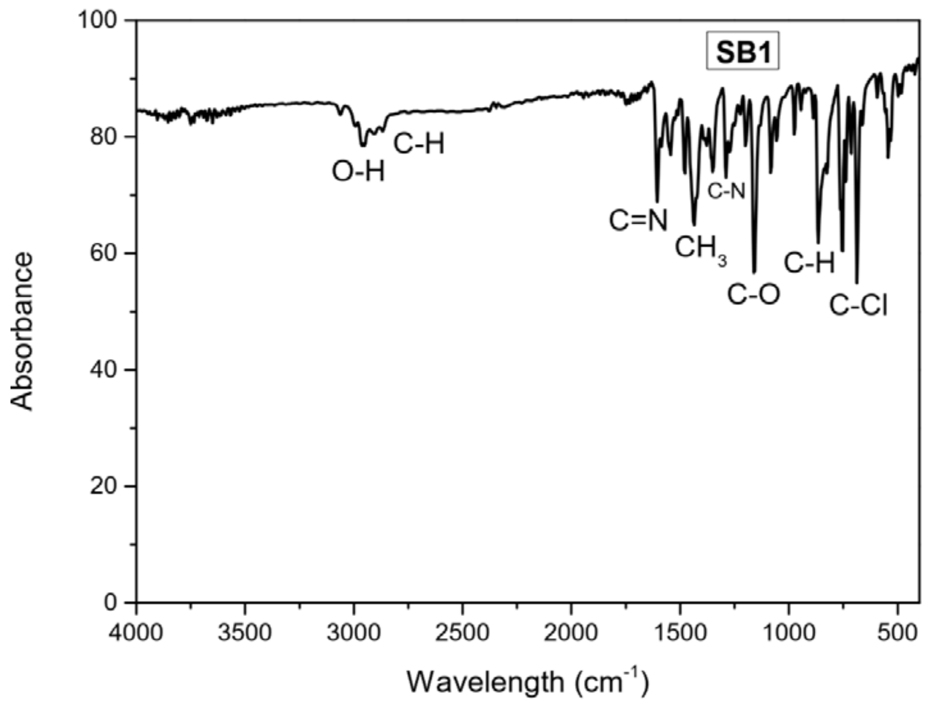

Figure S3: FTIR spectrum of **SB1** obtained in solid state at room temperature using ATR method

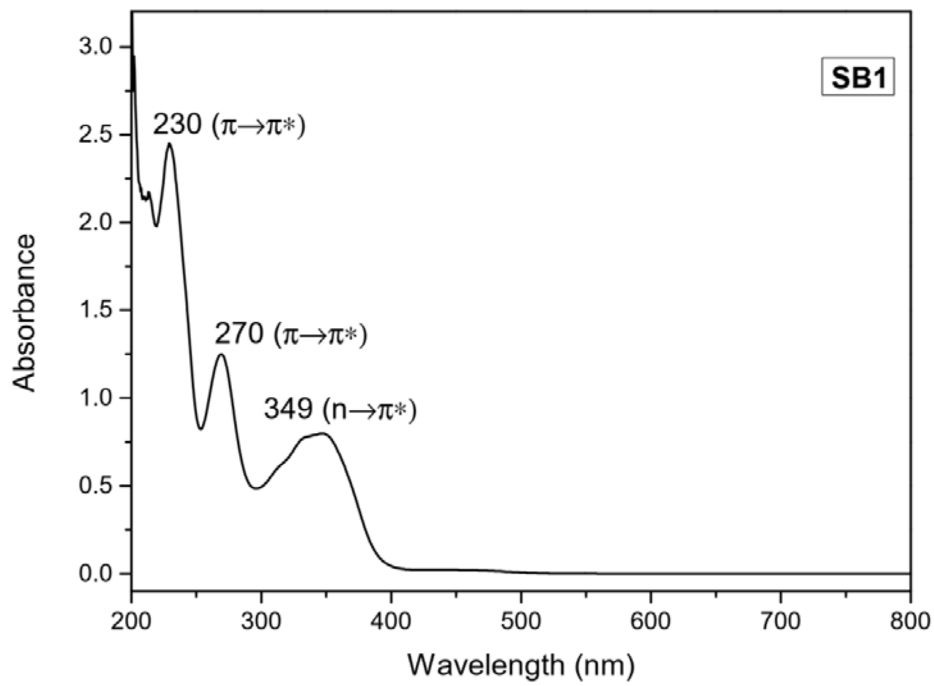

Figure S4: UV-Vis Spectrum of **SB1** obtained at room temperature using DMSO (10^{-3}M) solution

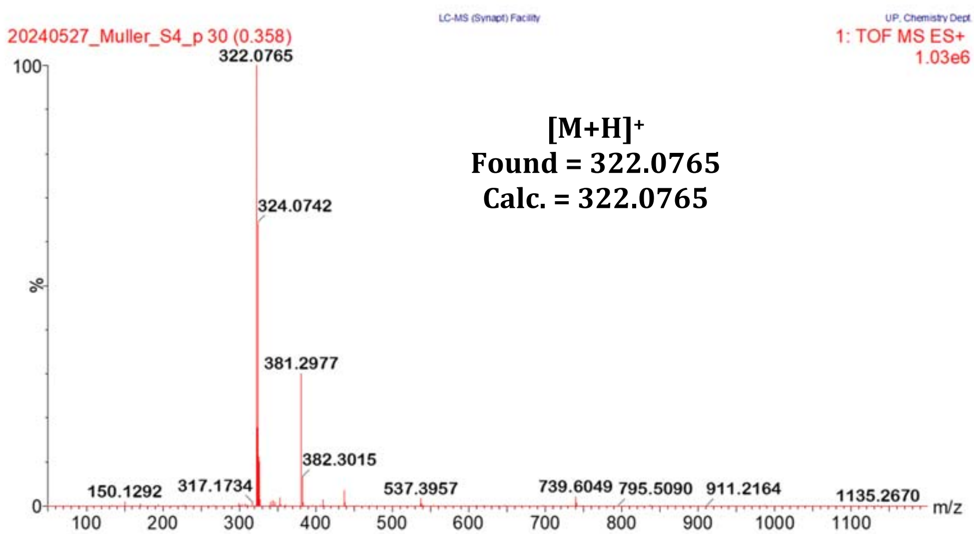

Figure S5: Mass spectrum of **SB1** obtained at room temperature using HRMS in DMSO solution

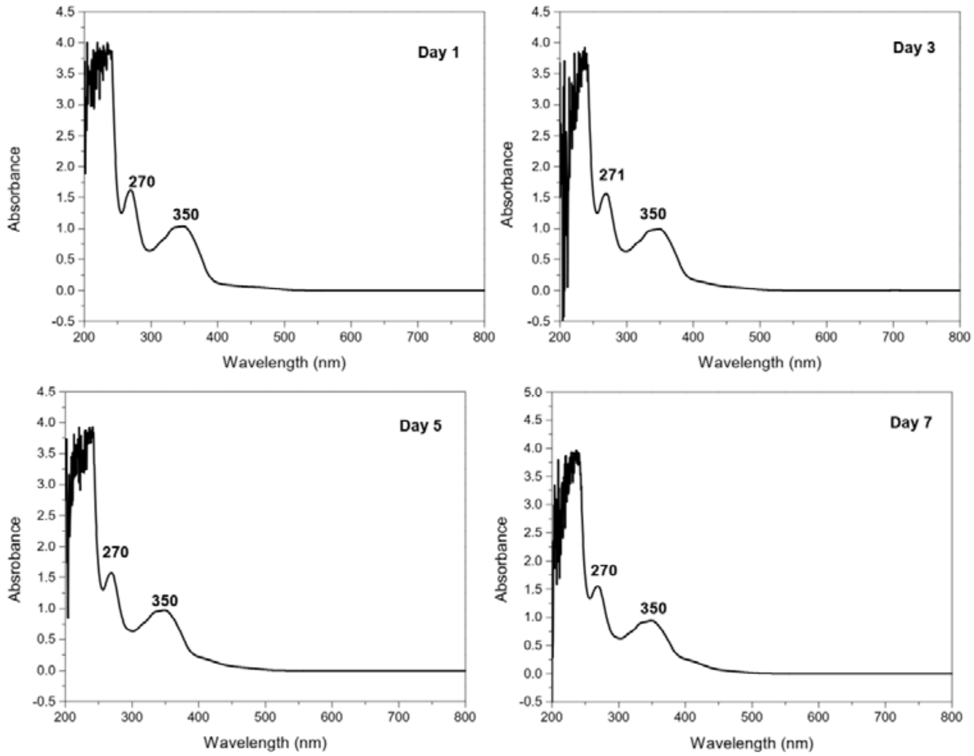

Figure S6: UV-vis spectra of 30 µM solutions of **SB1** recorded as a function of time in KH_2PO_4 buffer (50 mM pH 7.5). **SB1** was present with a final concentration of 10% (v/v) DMSO.

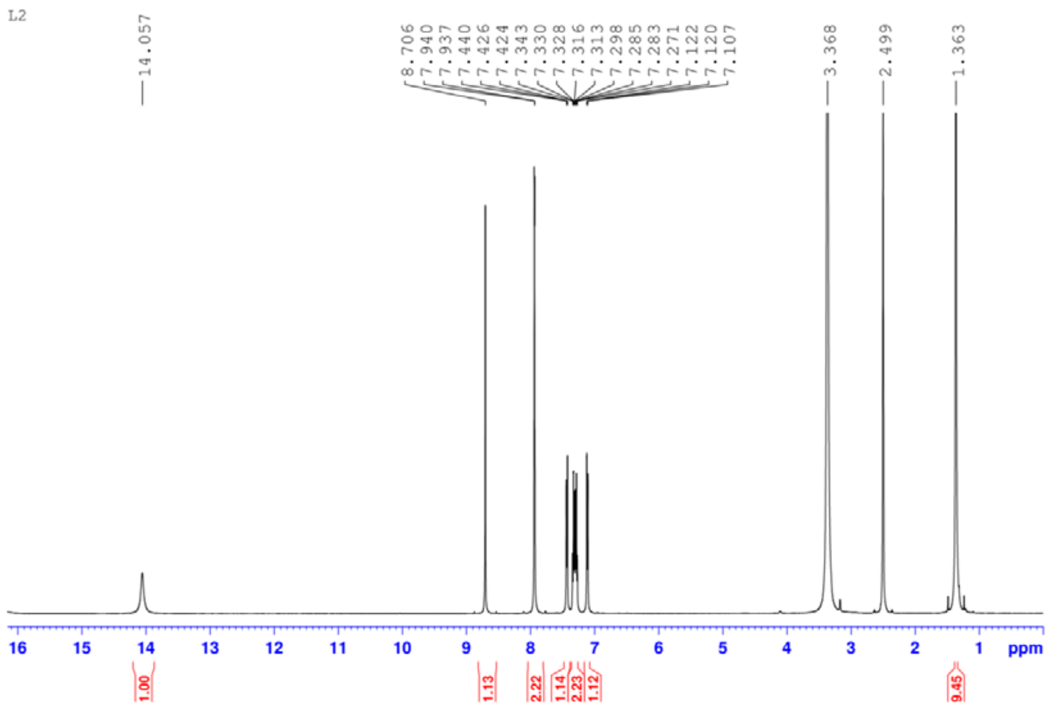

Figure S7: ^{1}H NMR spectrum of **SB2** obtained at room temperature using (500 MHz, DMSO-d_6)

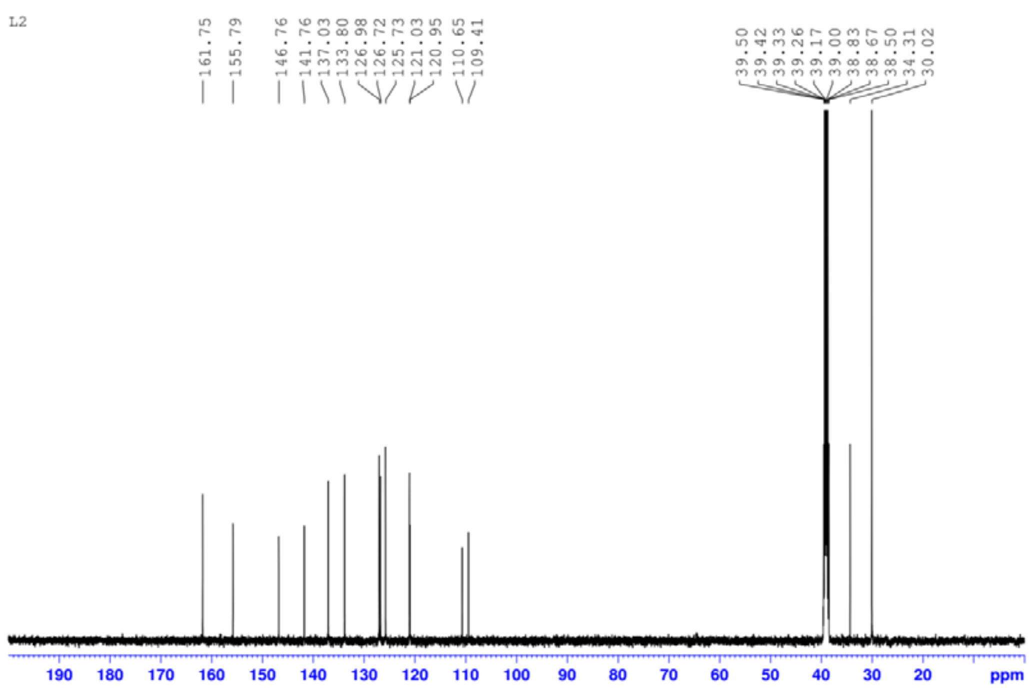

Figure S8: ^{13}C NMR spectrum of **SB2** obtained at room temperature using (125 MHz, DMSO-d_6)

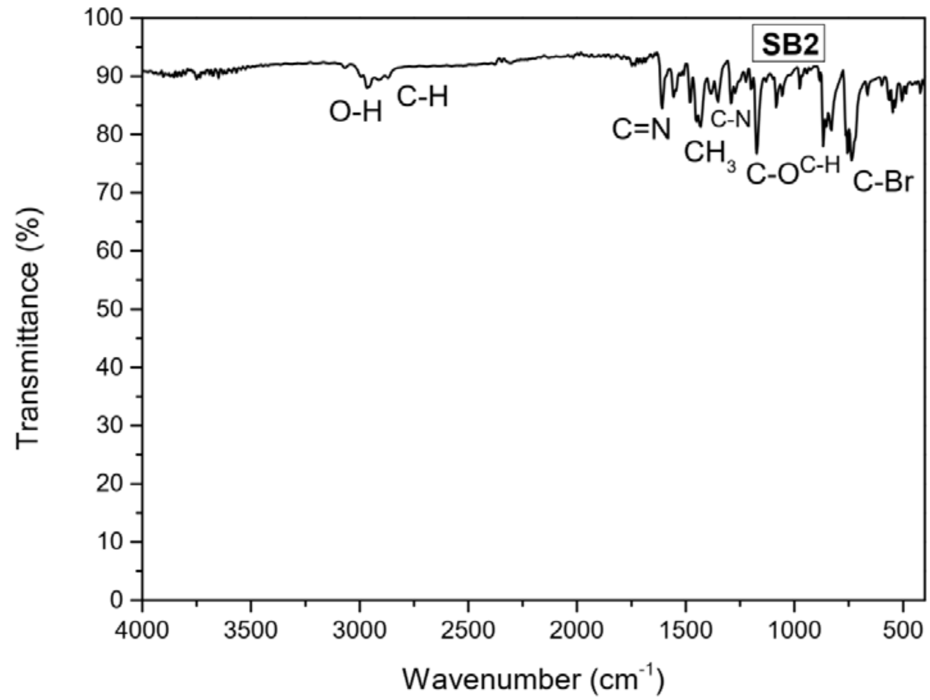

Figure S9: FTIR spectrum of **SB2** obtained in solid state at room temperature using ATR method

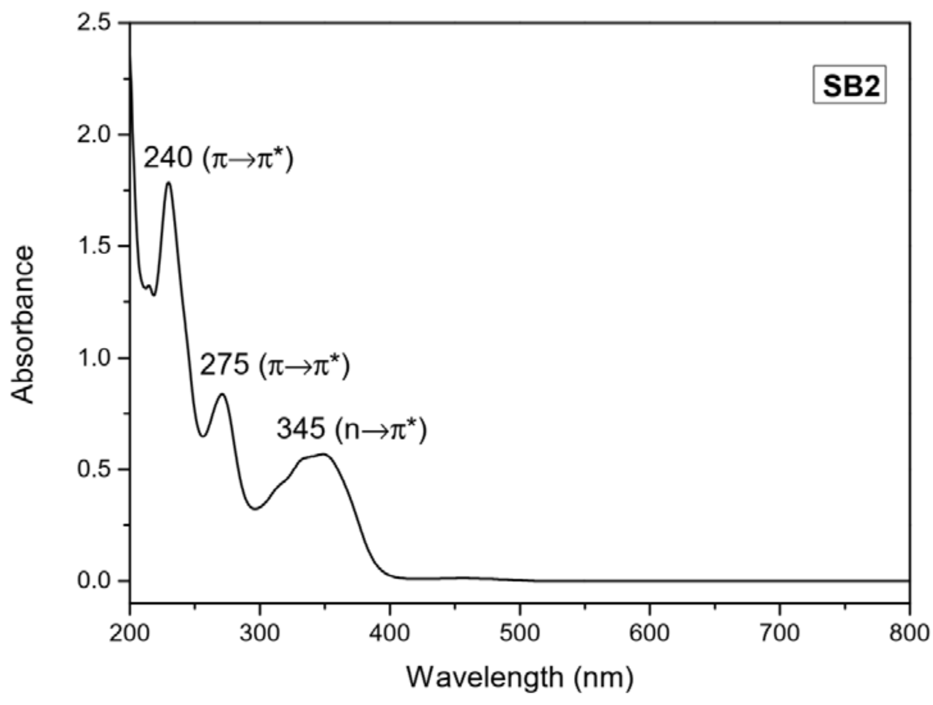

Figure S10: UV-Vis Spectrum of **SB2** obtained at room temperature using DMSO (10^{-3}M) solution

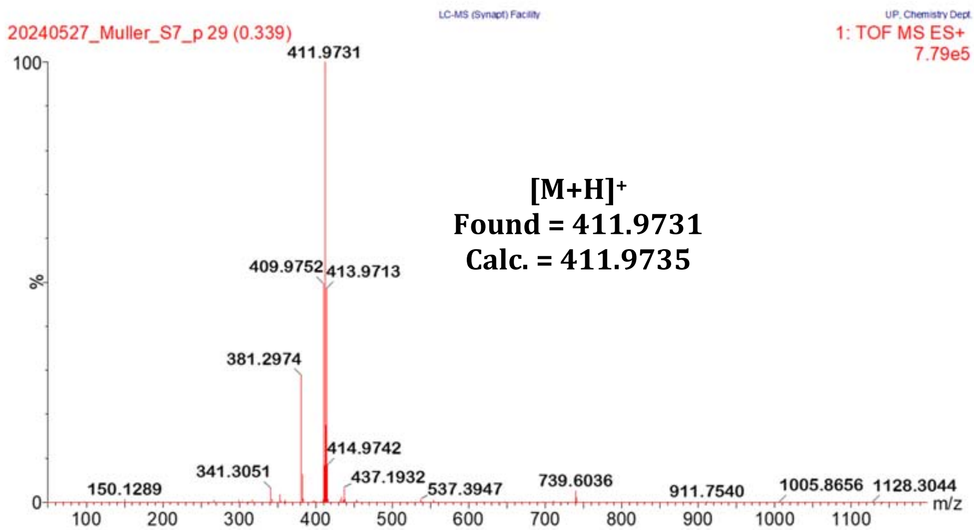

Figure S11: Mass spectrum of **SB2** obtained at room temperature using HRMS in DMSO solution

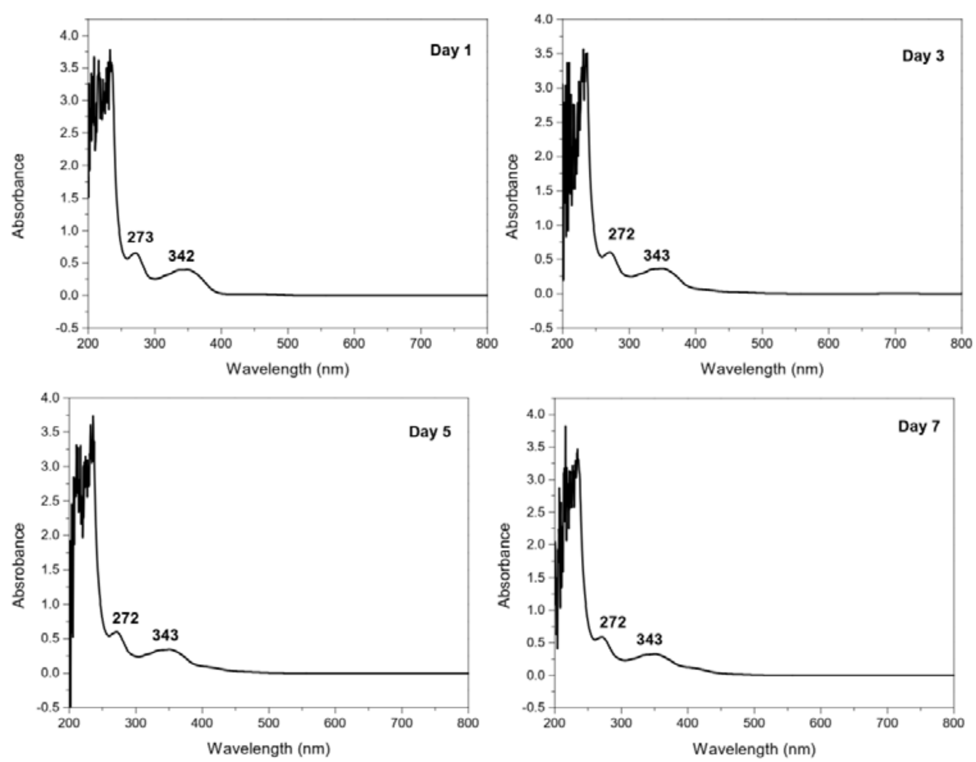

Figure S12: UV-vis spectra of 30 μM solutions of **SB2** recorded as a function of time in KH_2PO_4 buffer (50 mM pH 7.5). **SB2** was present with a final concentration of 10% (v/v) DMSO.

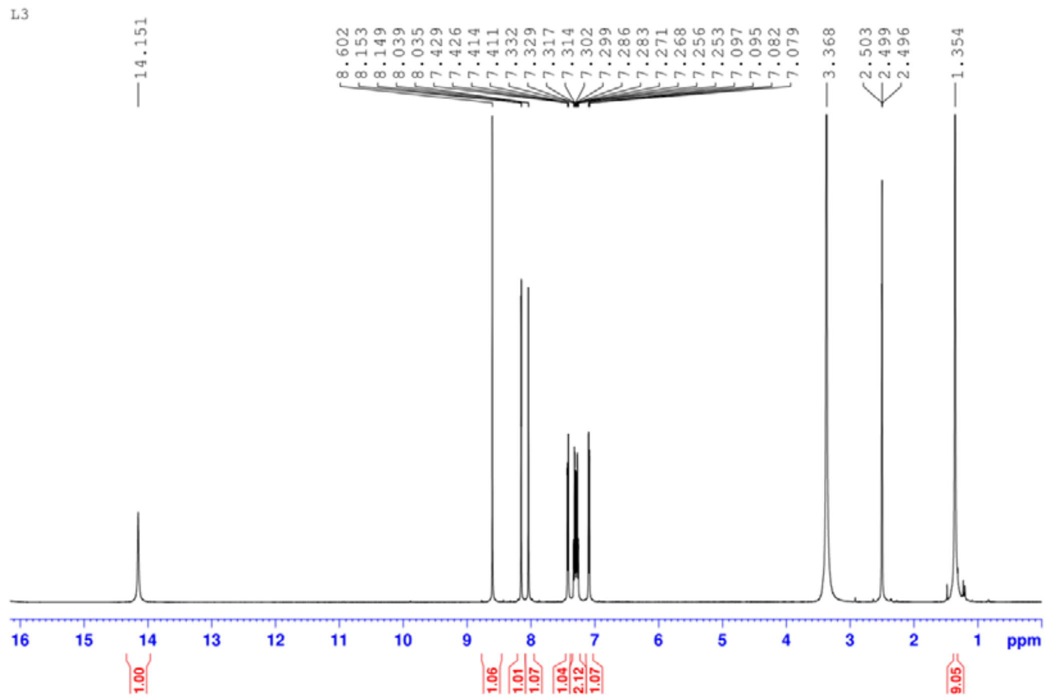

Figure S13: ^1H NMR spectrum of **SB3** obtained at room temperature using (500 MHz, DMSO-d_6)

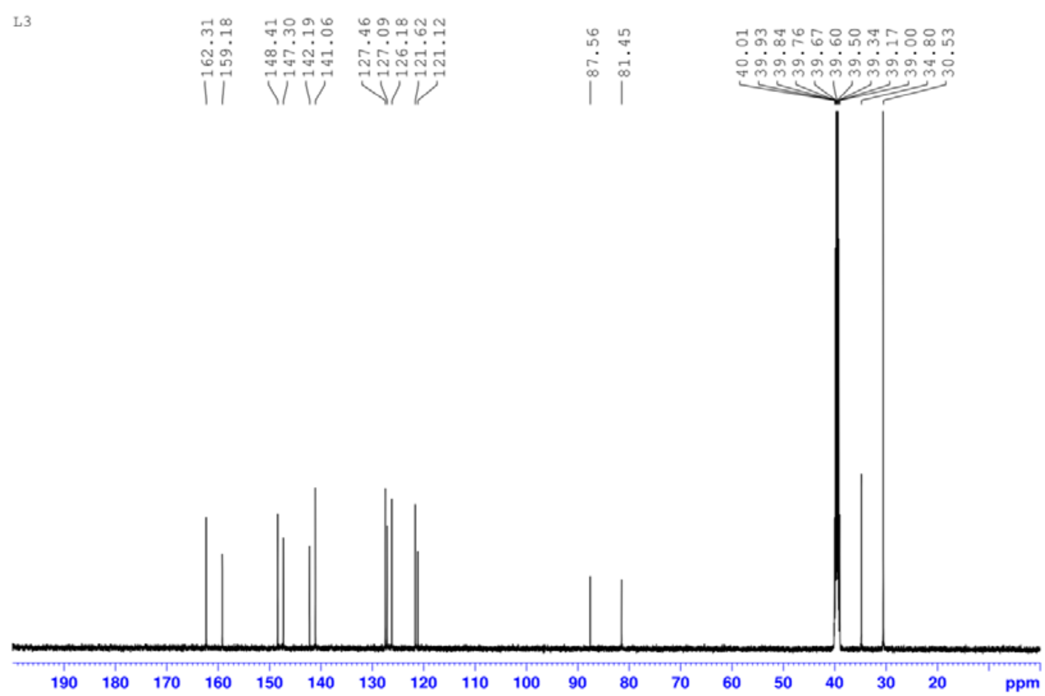

Figure S14: ^{13}C NMR spectrum of **SB3** obtained at room temperature using (125 MHz, DMSO-d_6)

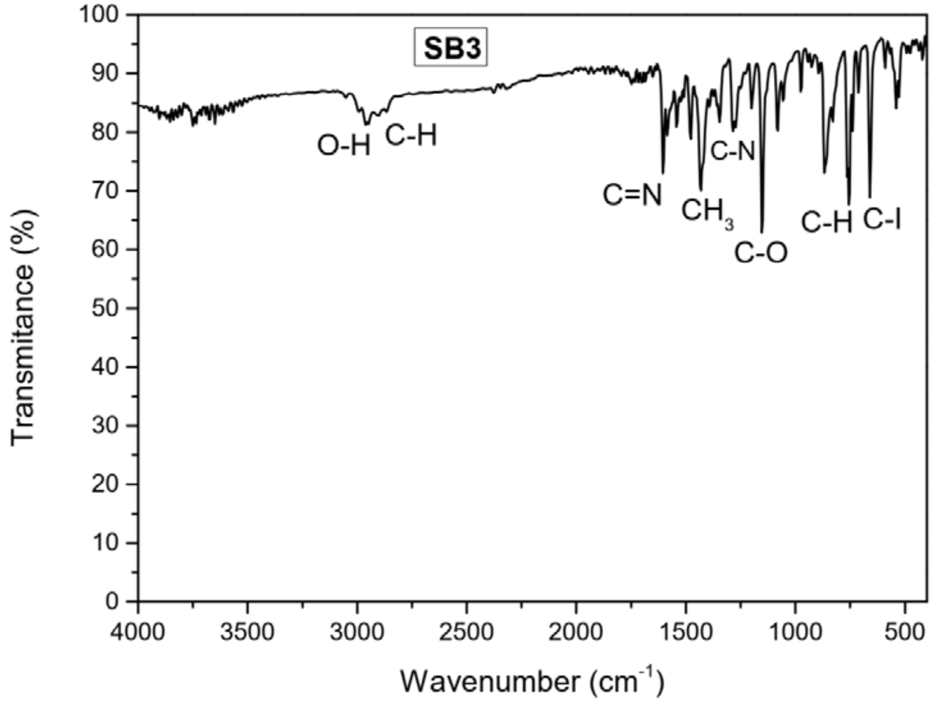

Figure S15: FTIR spectrum of **SB3** obtained in solid state at room temperature using ATR method

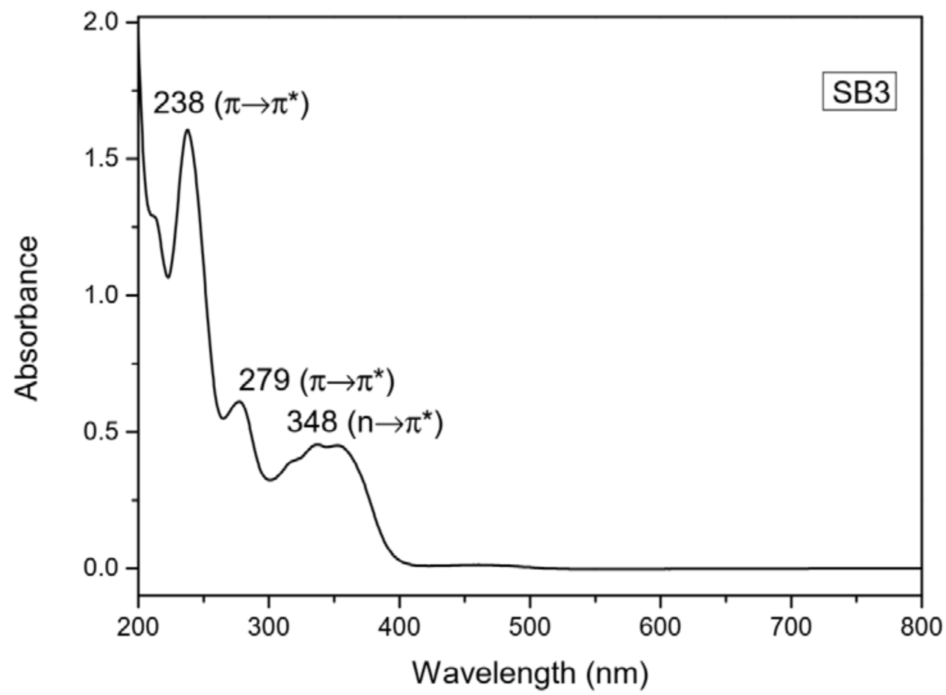

Figure S16: UV-Vis Spectrum of **SB3** obtained at room temperature using DMSO (10^{-3}M) solution

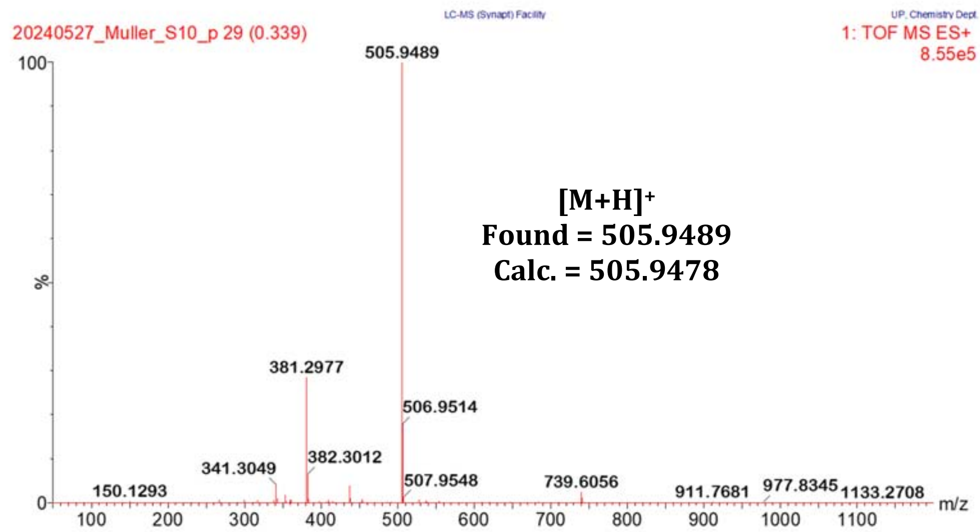

Figure S17: Mass spectrum of **SB3** obtained at room temperature using HRMS in DMSO solution

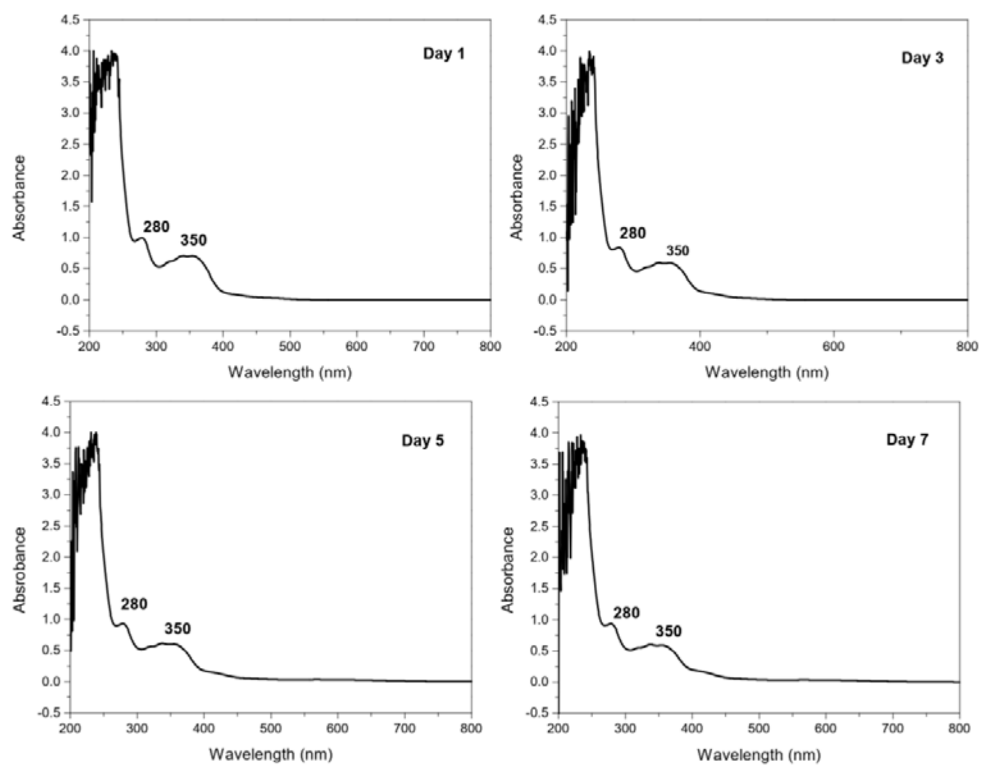

Figure S18: UV-vis spectra of 30 μM solutions of **SB3** recorded as a function of time in KH_2PO_4 buffer (50 mM pH 7.5). **SB3** was present with a final concentration of 10% (v/v) DMSO.

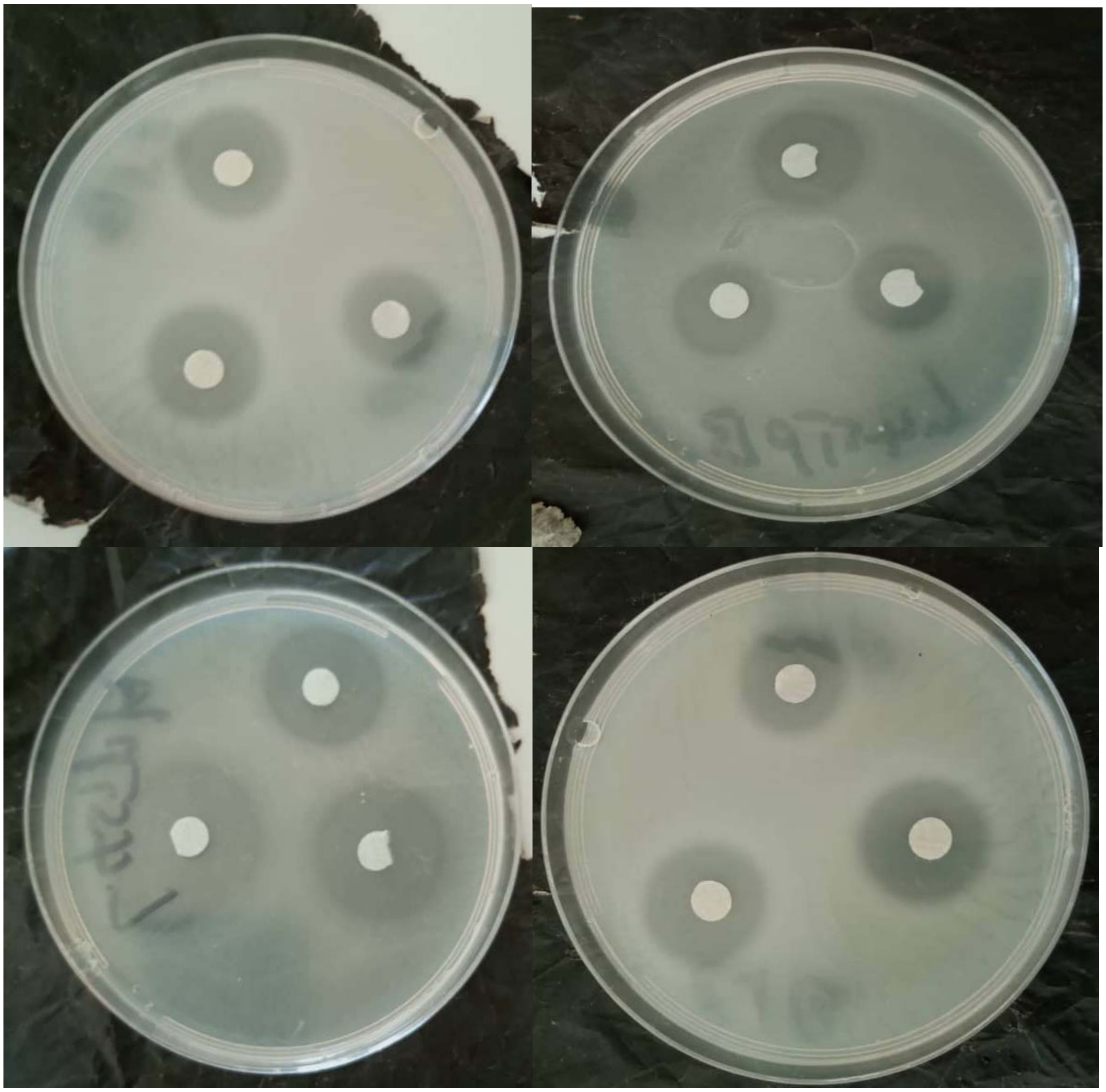

Figure S19: Representative Culture Plates showing the zone of Inhibitions

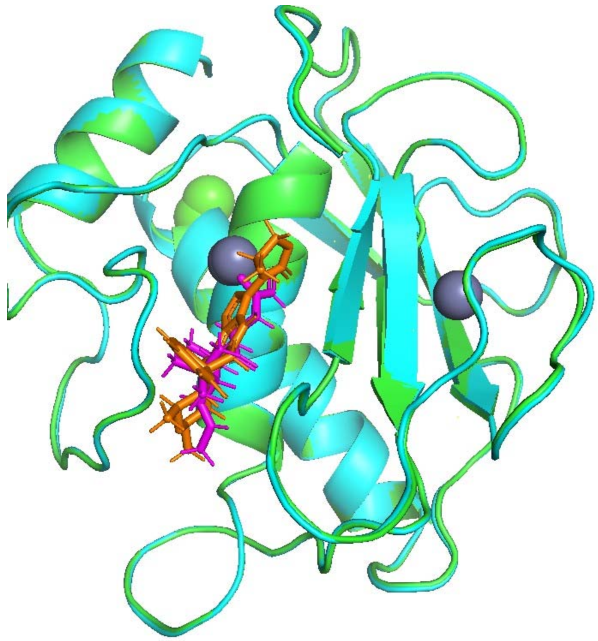

Figure S20: Validation of the docking protocol by superimposing the co-ligand (orange) and after redocking the same ligand (magenta), exhibiting an RMSD of 0.161 Å.

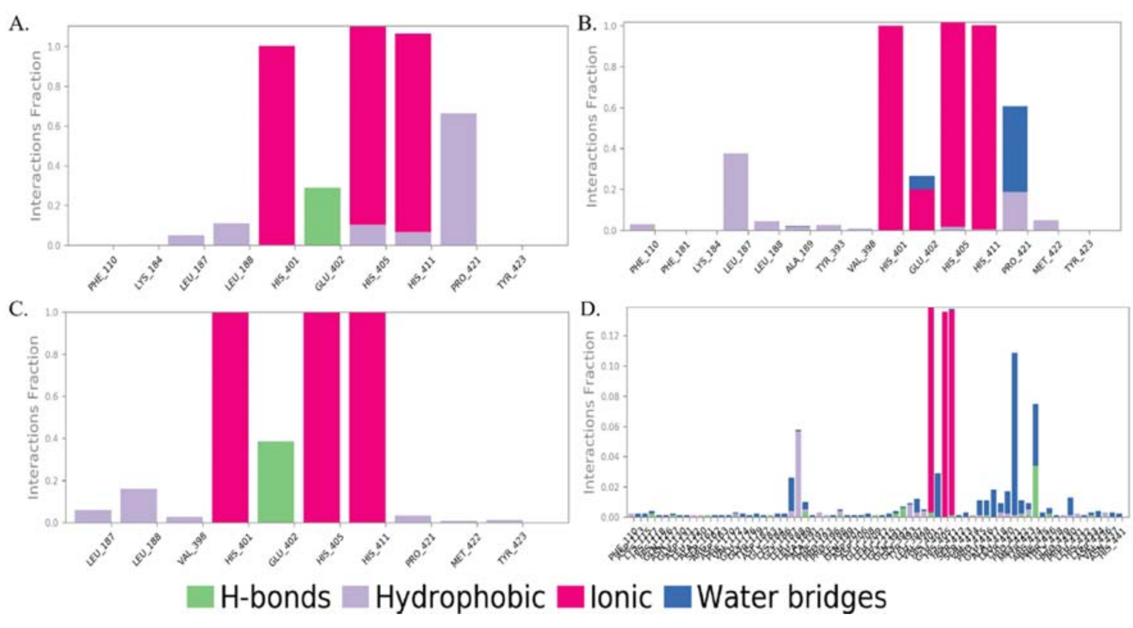

Figure S21: The binding interaction lifetime of the halogenated Schiff base compounds (SB1-SB3) and methylglyoxal at the active site of 1GKC during a simulation run at 150 ns. Figure S1A, B, C, and D present the complex formed by SB1, SB2, SB3, and methylglyoxal, respectively. The interactions include hydrogen bonds, water bridges, ionic bonds, and hydrophobic bonds.