Synthesis, Crystal Structure Analysis, Computational Modelling and Evaluation of Anti-Cervical Cancer Activity of Novel 1,5-Dicyclooctyl Thiocarbohydrazone

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Supplementary Fig. S1 FT-IR spectrum of compound **3.**

Supplementary Fig. S2 ^{1}H-NMR spectrum of compound **3.**

Supplementary Fig. S3 ^{13}C-NMR spectrum of compound **3.**

Supplementary Fig. S4 Plausible reaction mechanism of synthesized compound **3.**

Supplementary Fig. S5 Colour coding of neighbouring molecules with respect to the central molecule (black colour).

Supplementary Fig. S6 Optimized structure of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.

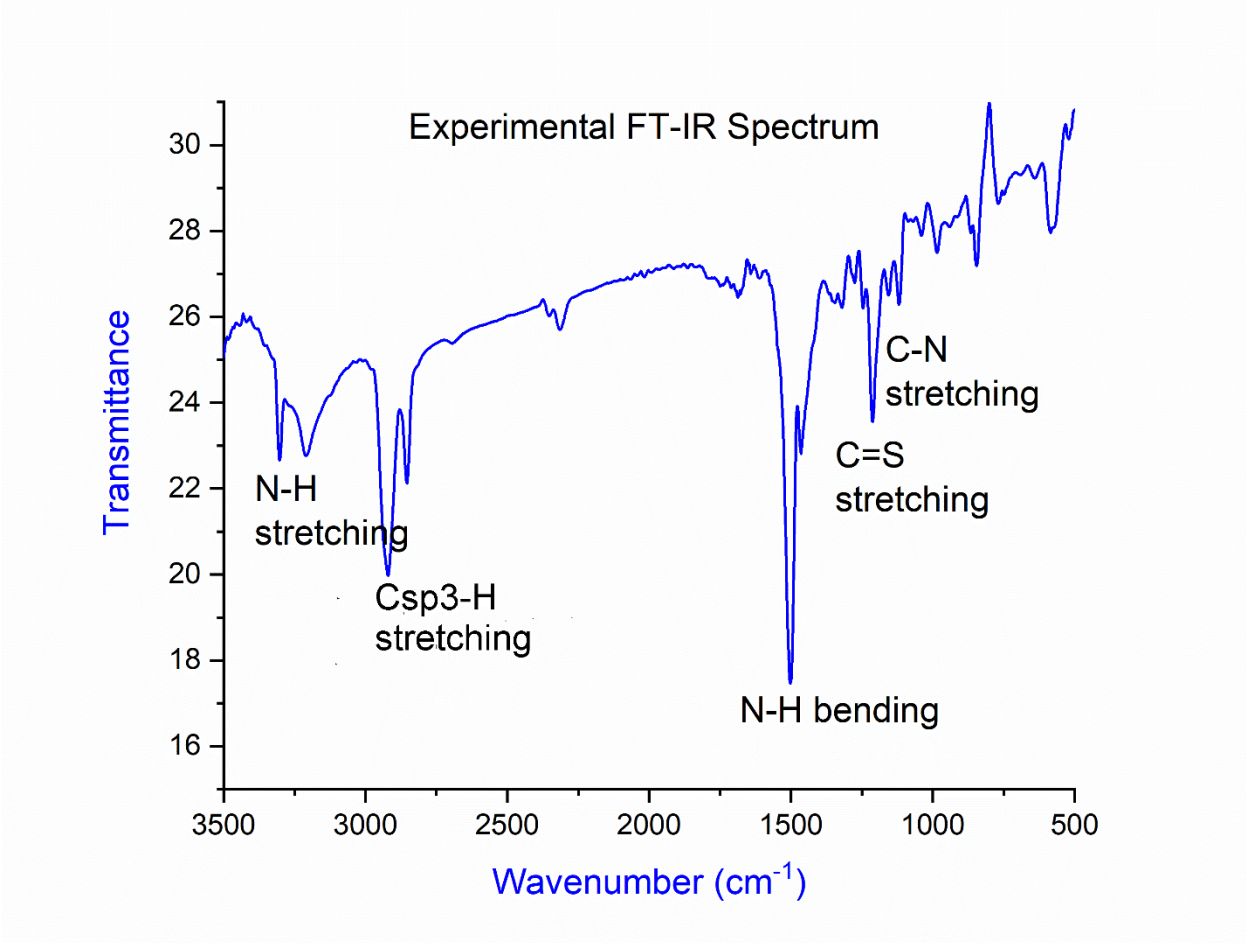
Supplementary Fig. S7 Theoretical FT- IR spectrum of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.

Supplementary Fig. S8 ^{1}H and ^{13}C NMR correlation diagram of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.

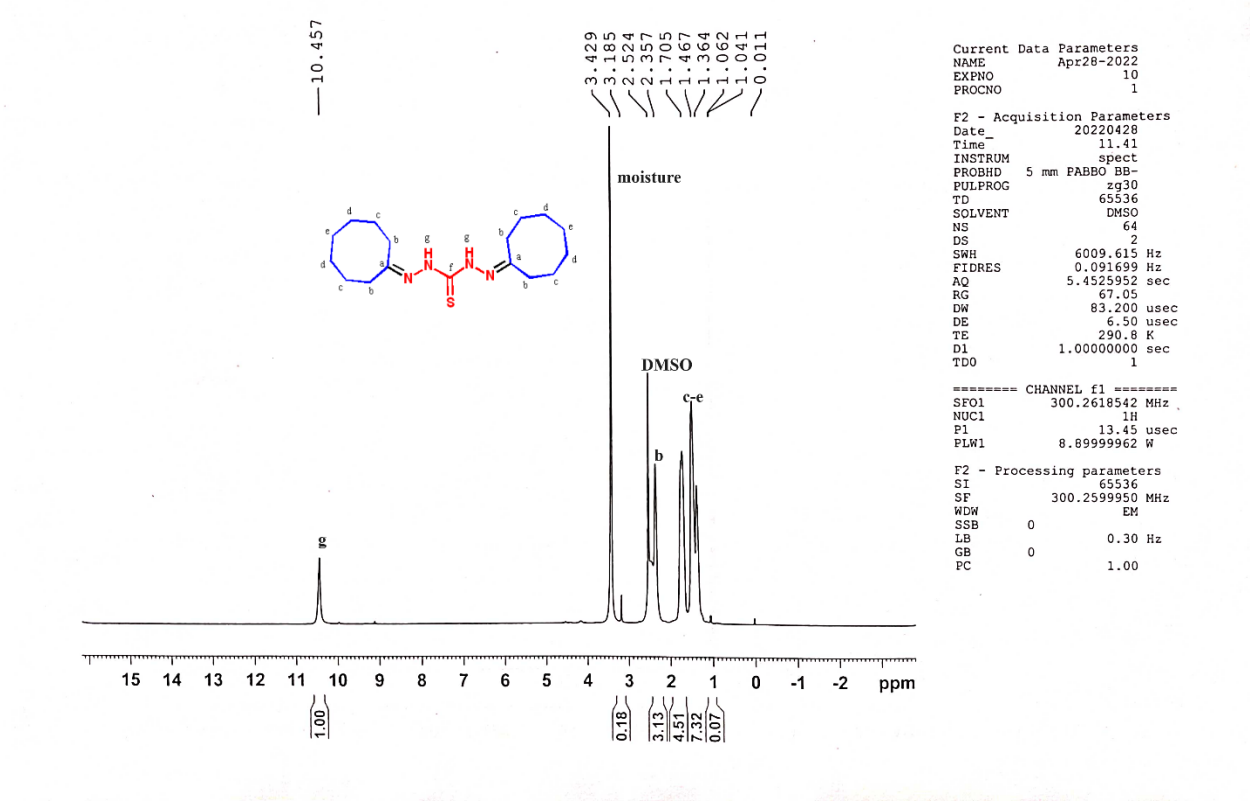
Supplementary Fig. S9 The correlation diagram of UV- Vis spectra of compound **3** using DFT/B3LYP/B3WP91/PBE-PBE/6-311++G (d, p) level of theory.

Supplementary Fig. S10 The MEP diagram of compound **3** using DFT/B3LYP /6-311++G (d, p) level of theory.

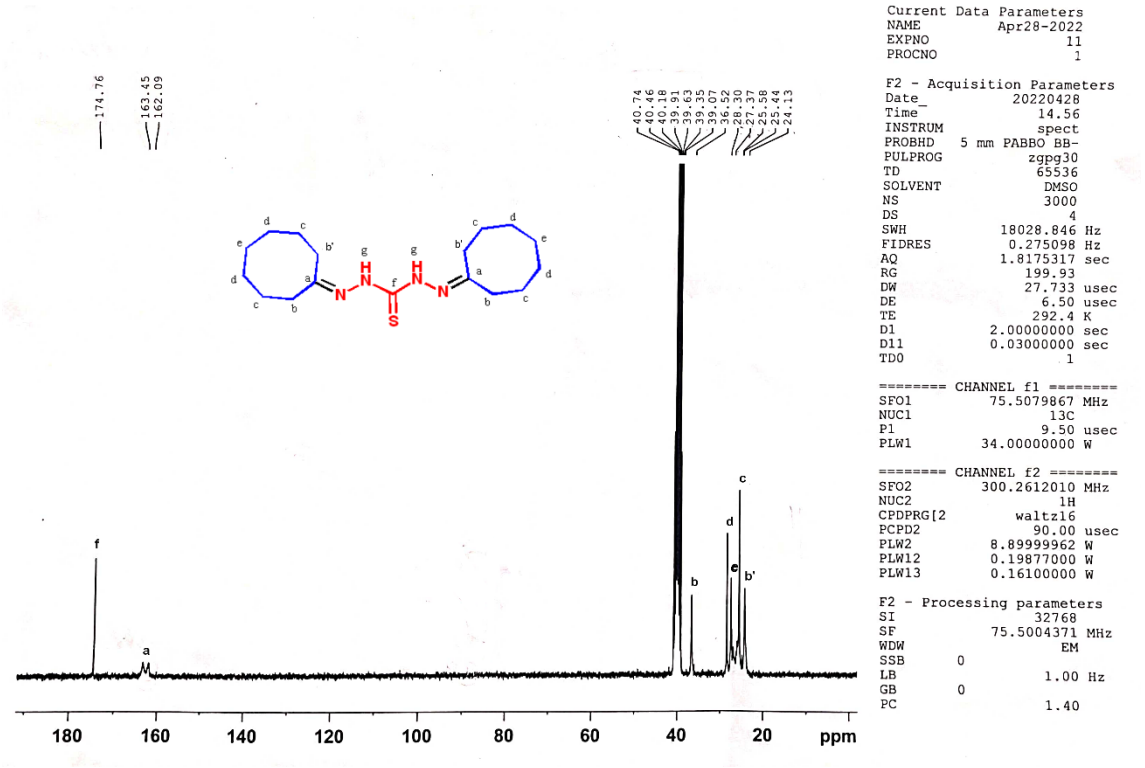
Supplementary Fig. S11 The Histograms of compound **3** with protein tyrosine-protein phosphatase 4XR8(A) and 7VZE (B) found number of distinct conformational clusters 12 and 10 with binding energies out of 50 runs using a RMSD-tolerance of 2.0 Å.



Supplementary Fig. S1 FT-IR spectrum of compound **3.**

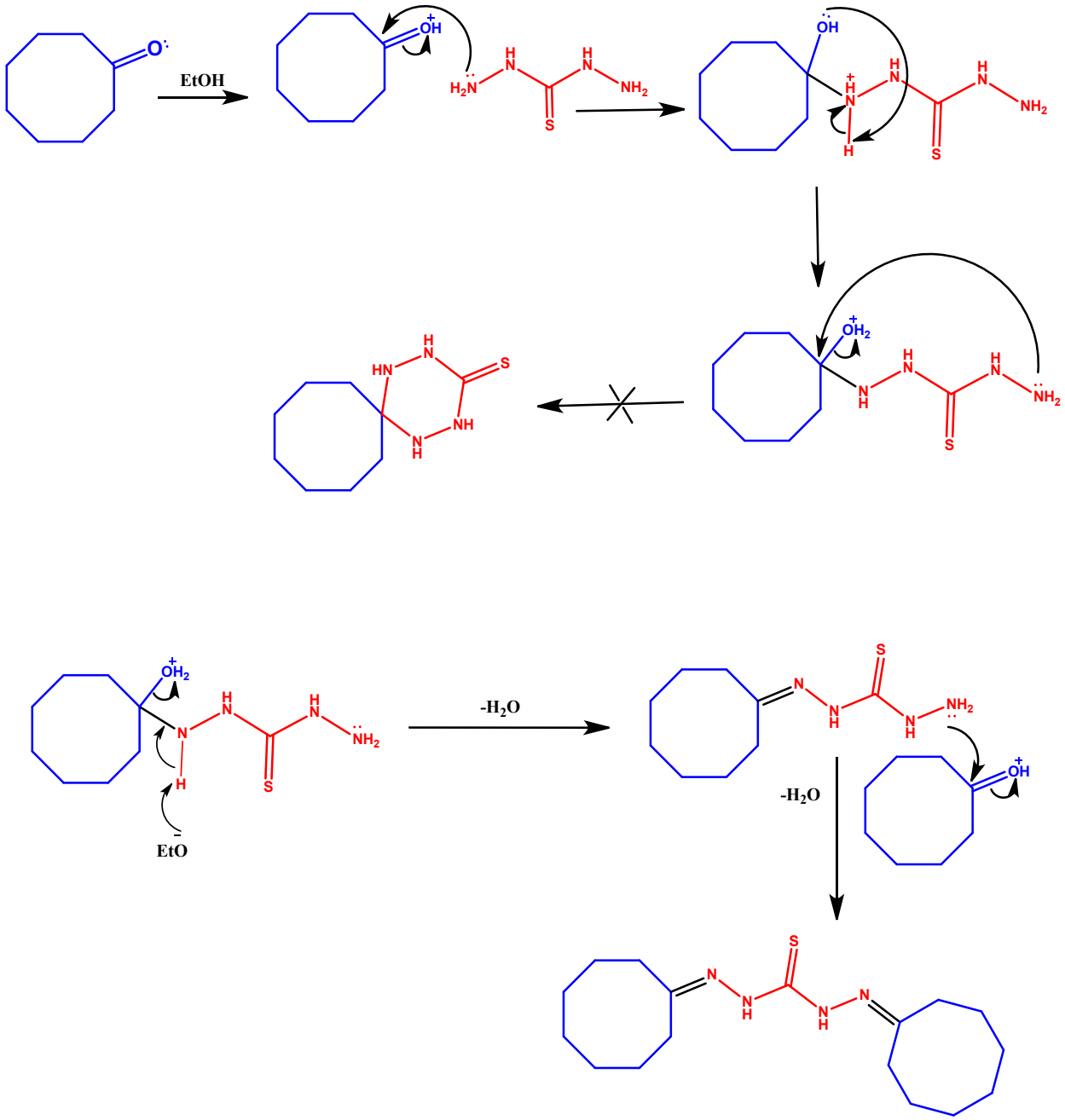


Supplementary Fig. S2 ^{1}H-NMR spectrum of compound **3.**

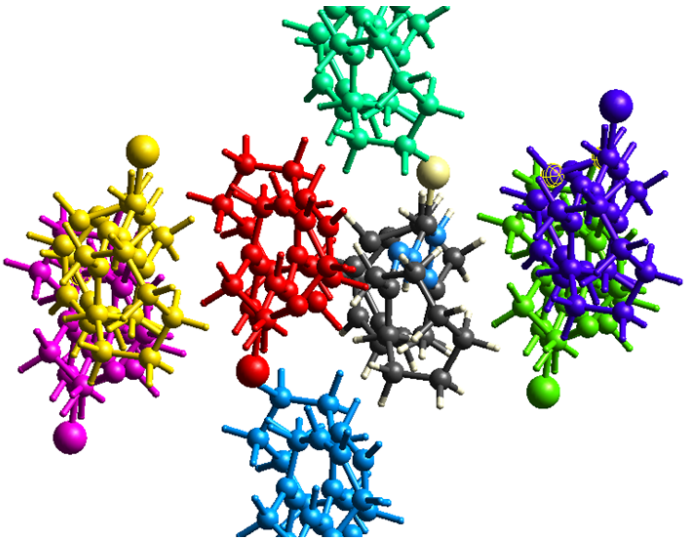


Supplementary Fig. S3 ^{13}C-NMR spectrum of compound **3.**

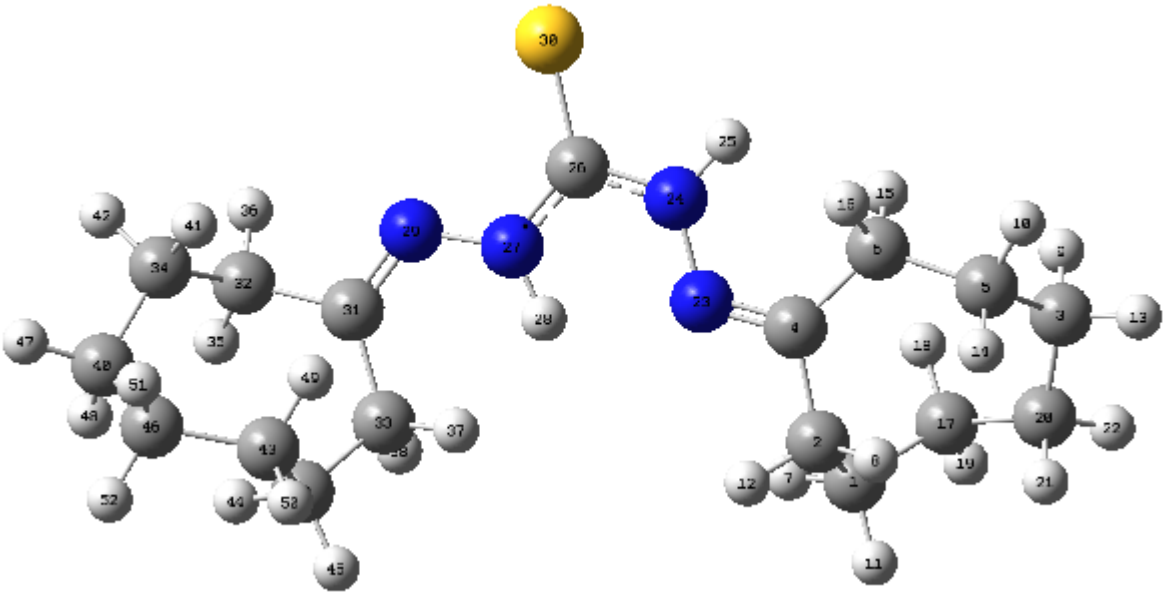
UV λ_{max} (Methanol): 285 nm, **FT-IR using KBr pellets (cm^{-1}):** 3302 and 3215 (-NH stretching), 2926 and 2849 (-CH_2 stretching), 1506 (N-H bending), 1460 (C-N stretching), 1219 (-C=S stretching) & 1113 (C-N bending), ^{1}H-NMR (DMSO-d_6, 300 MHz) δ (ppm): 1.041-1.705 (m for 20H on C_c-C_e), 2.357 (s for 4H on C_b) & 10.457 [s for 2H on N-H (denoted by g)]. ^{13}C-NMR (DMSO-d_6, 75 MHz) δ (ppm): 24.13, 25.44, 27.37, 28.30, 36.52, 162.09 & 174.76.



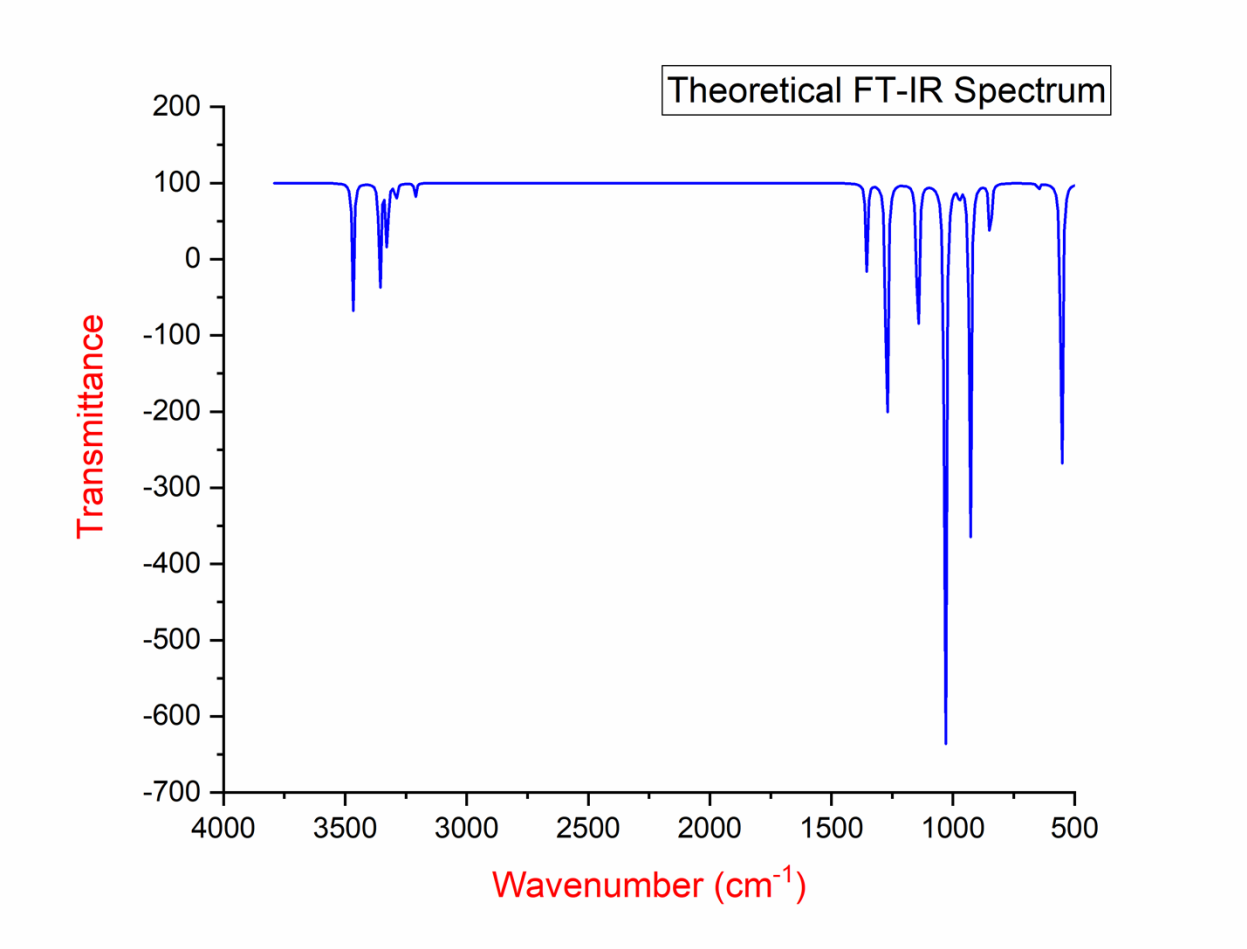
Supplementary Fig. S4 Plausible reaction mechanism of synthesized compound **3.**



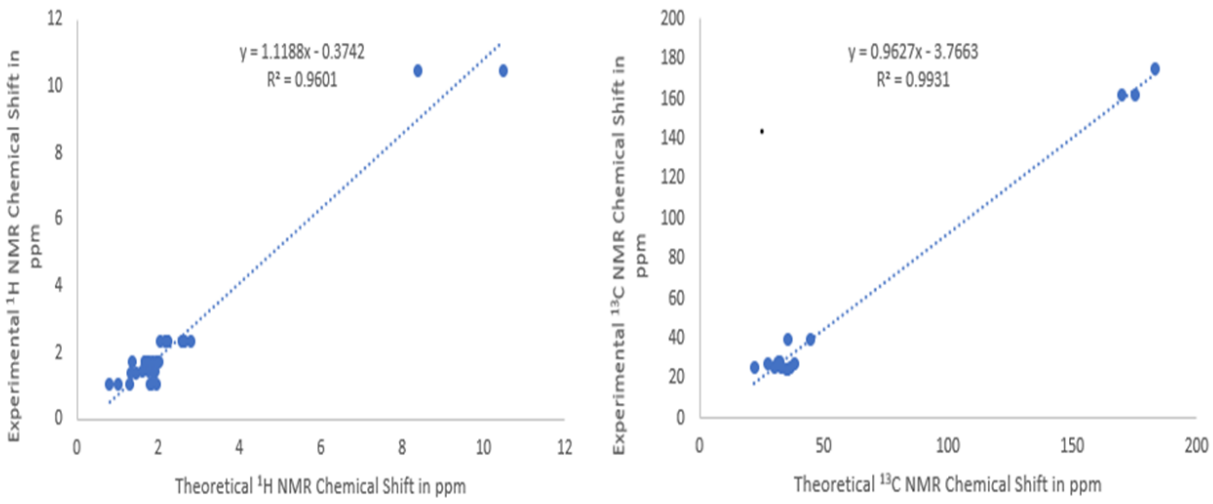
Supplementary Fig. S5 A collection of molecules surrounds the central molecule (black colour).



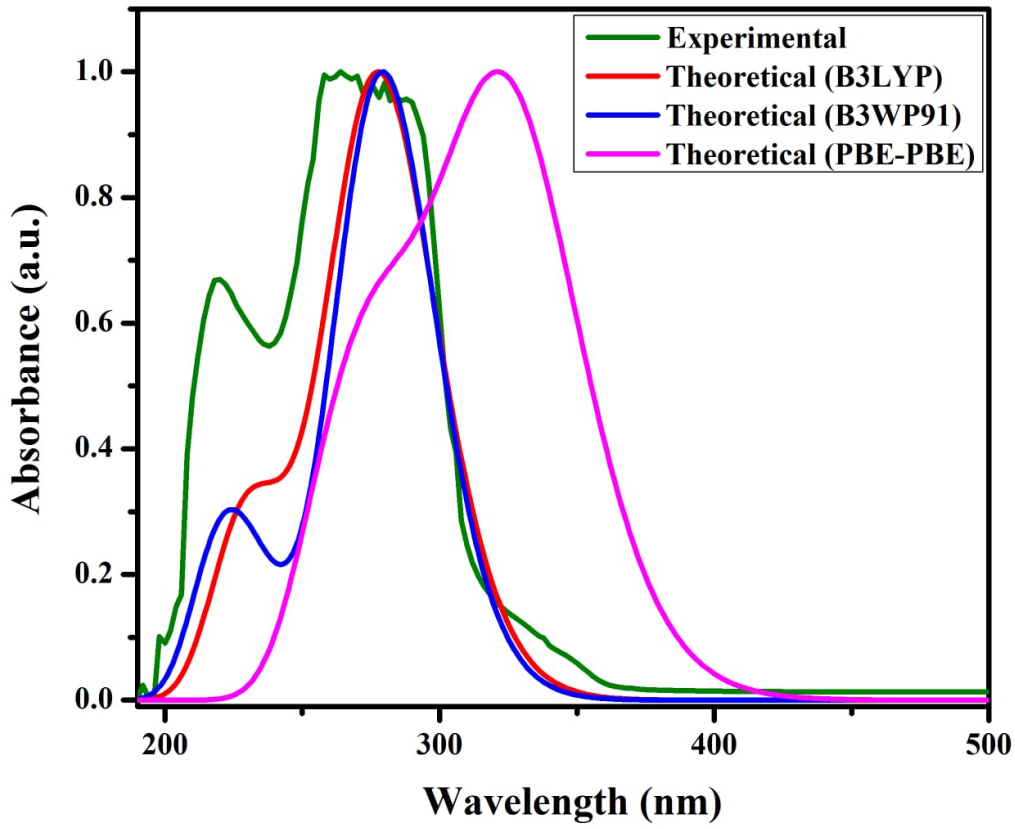
Supplementary Fig. S6 Optimized structure of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.



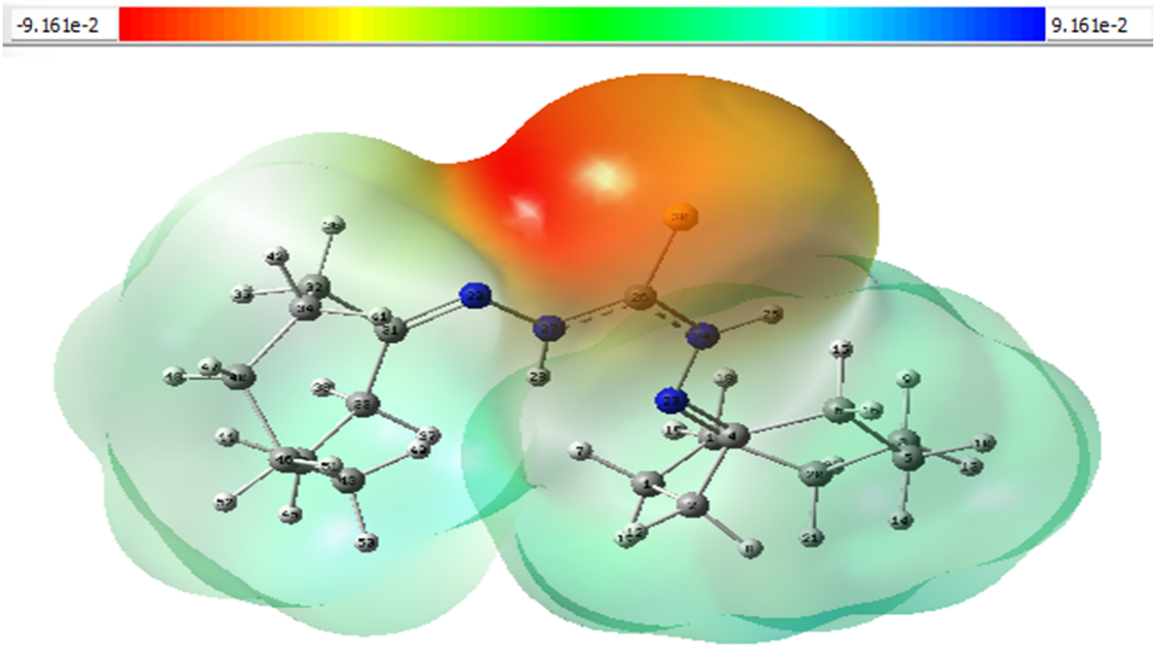
Supplementary Fig. S7 Theoretical FT- IR spectrum of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.



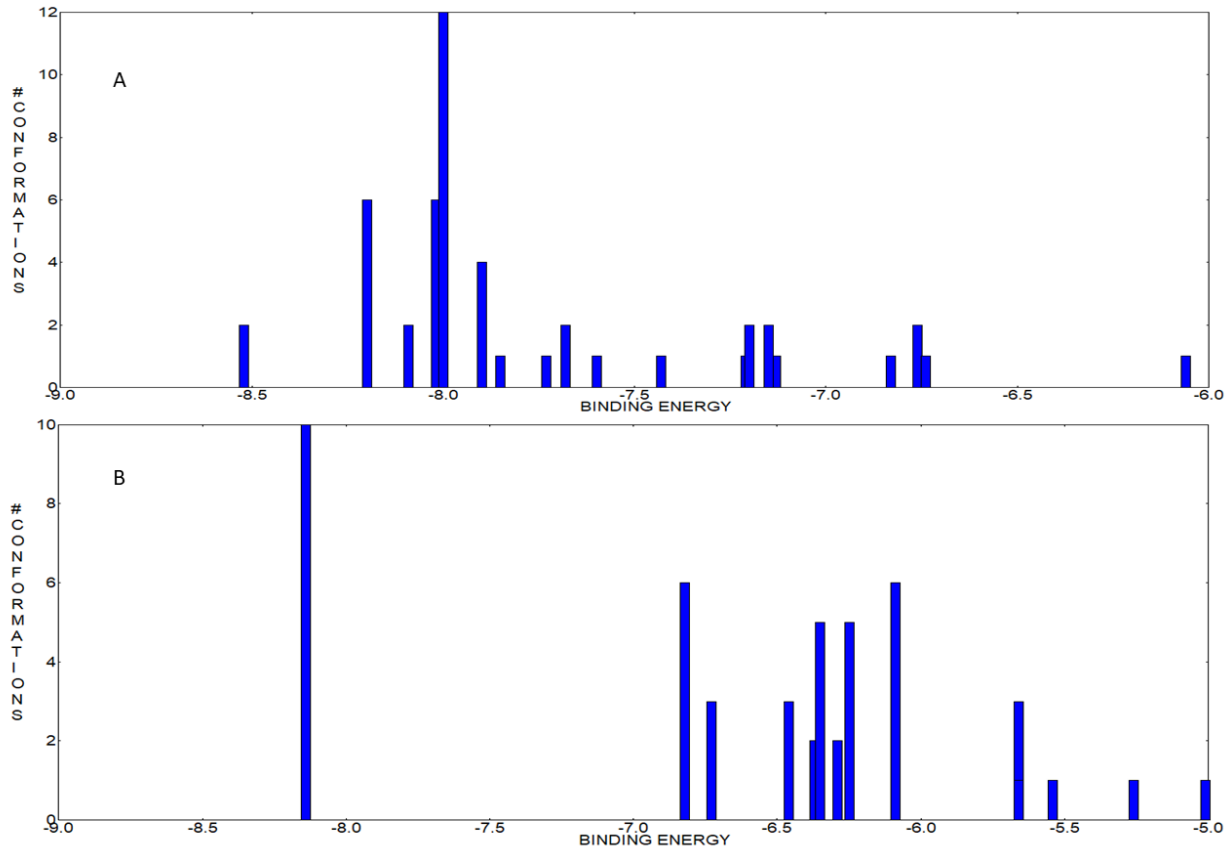
Supplementary Fig. S8 ^{1}H and ^{13}C NMR correlation diagram of compound **3** using DFT/B3LYP/6-311++G (d, p) level of theory.



Supplementary Fig. S9 The correlation diagram of UV- Vis spectra of compound **3** using DFT/B3LYP/B3WP91/PBE-PBE/6-311++G (d, p) level of theory.



Supplementary Fig. S10 The MEP diagram of compound **3** using DFT/B3LYP /6-311++G (d, p) level of theory



Supplementary Fig. S11 The Histograms of compound **3** with protein tyrosine-protein phosphatase 4XR8(A) and 7VZE (B) found number of distinct conformational clusters 12 and 10 with binding energies out of 50 runs using a RMSD-tolerance of 2.0 Å.