Supplementary Data

New 1,2,3-triazole-containing hybrids as antitumor candidates: Design, click-reaction synthesis, DFT calculations and molecular docking study

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I- DFT Calculations

Figure S1: Optimized structure of **4** and **5** derivatives at B3LYP /6-311++G(d,p) level of theory in the gas phase.

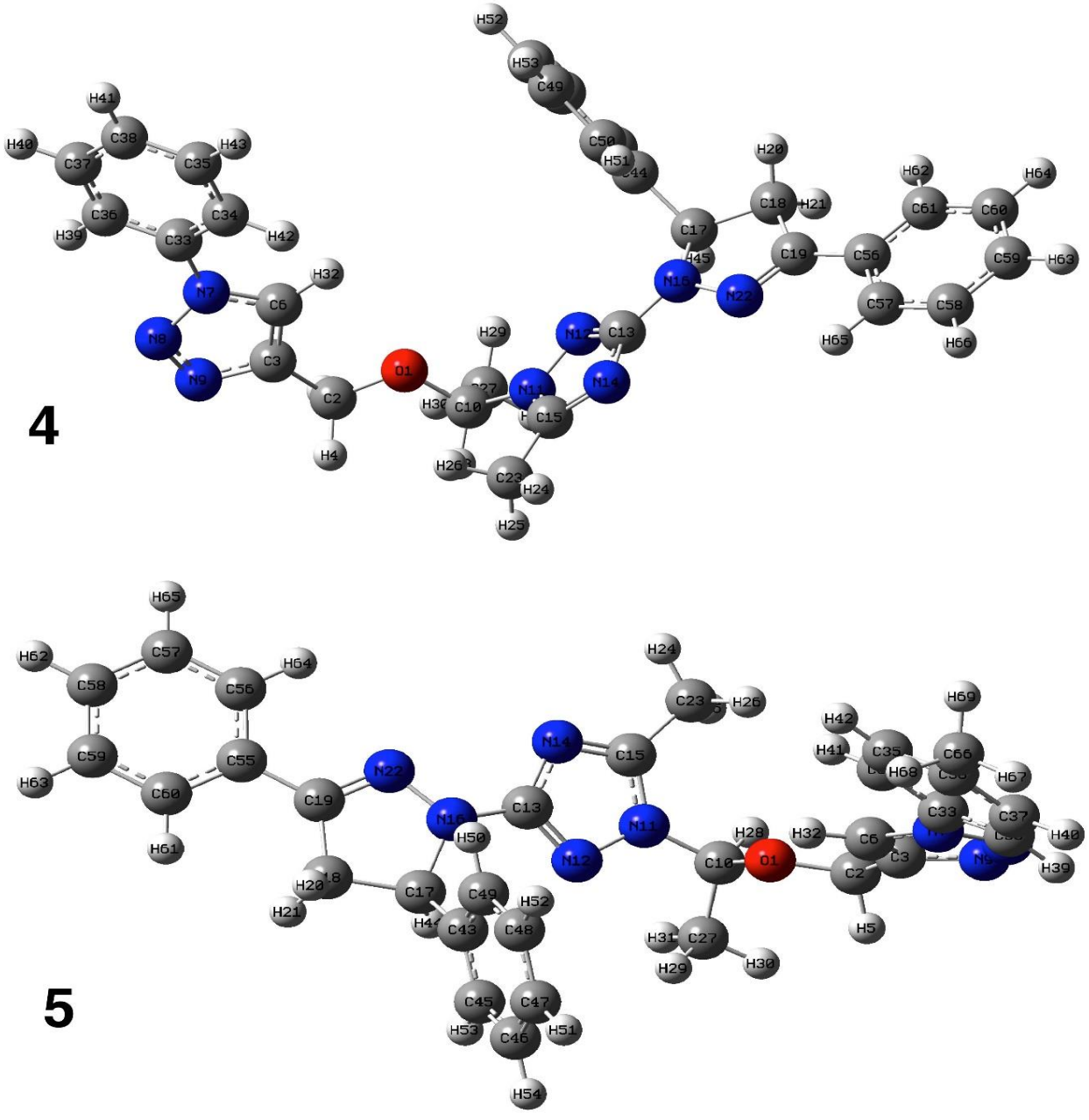
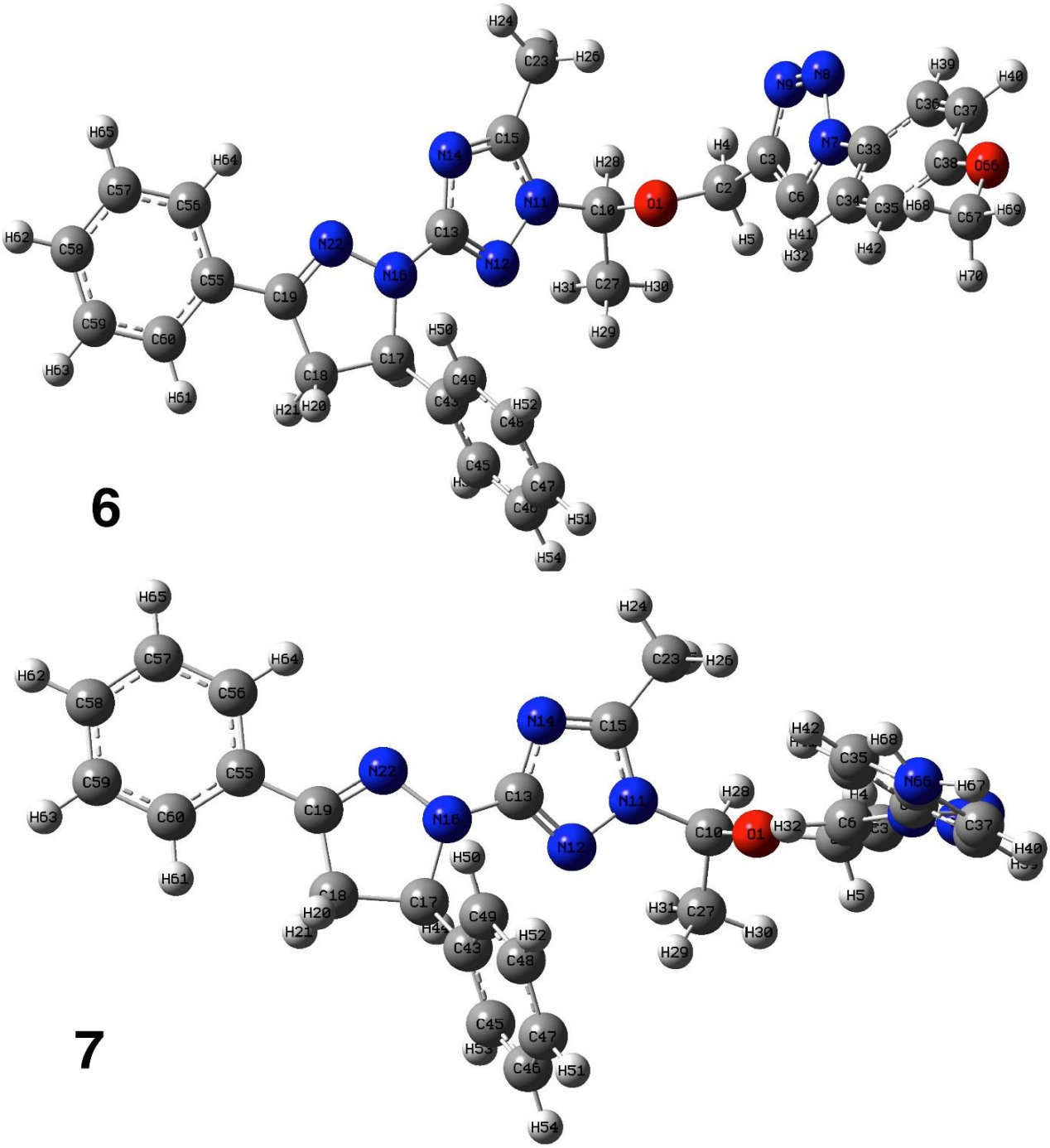
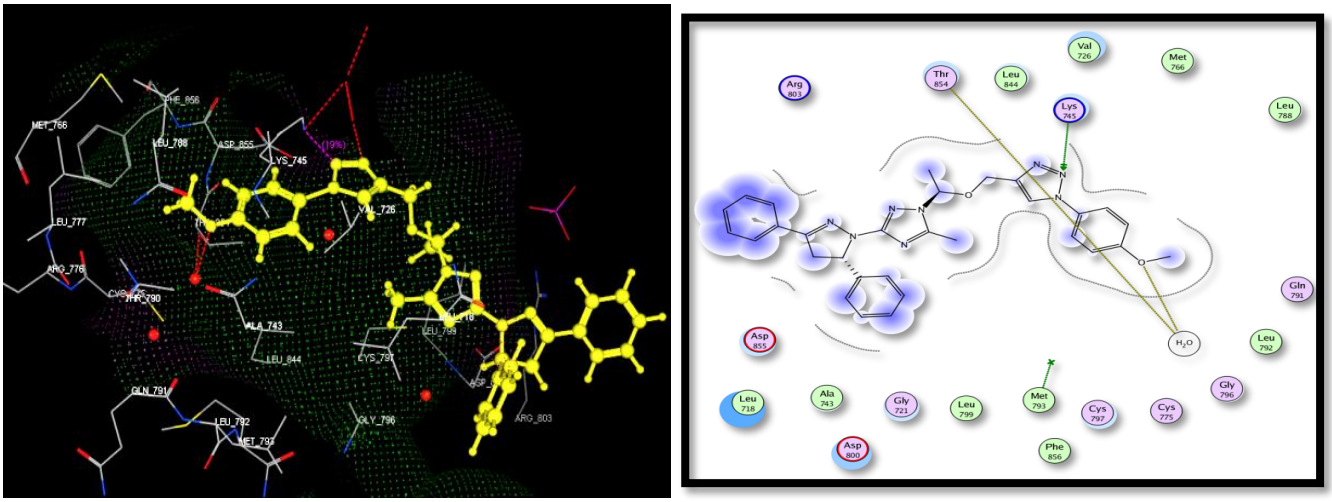


Figure S2: optimized structure of **6** and **7** derivatives at B3LYP/6-311++G(d,p) level of theory in the gas phase.

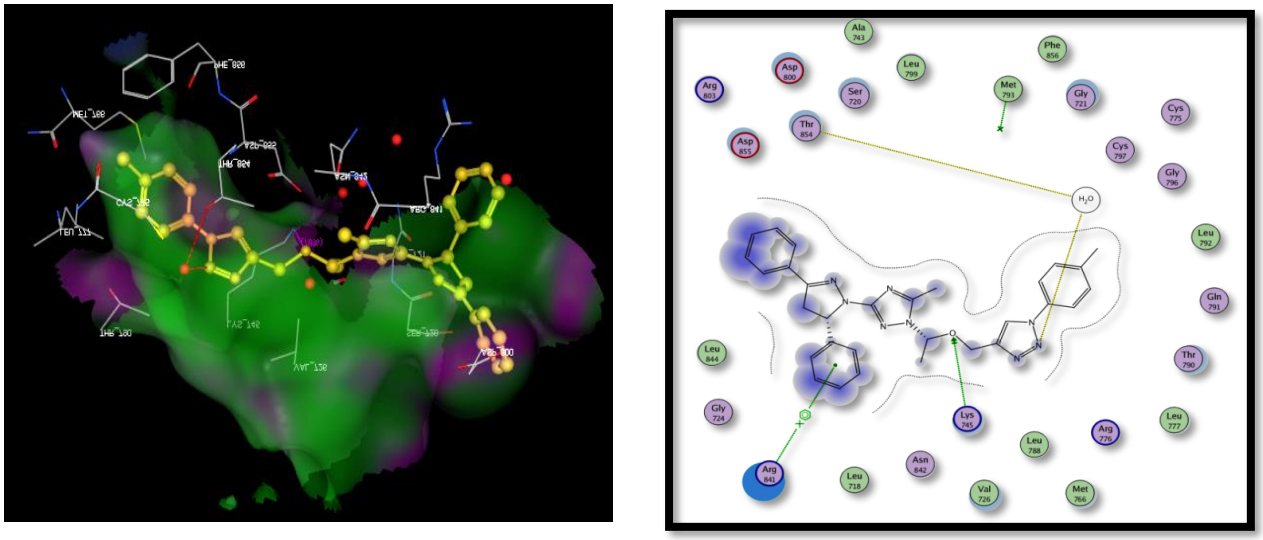


II- **Molecular docking data**



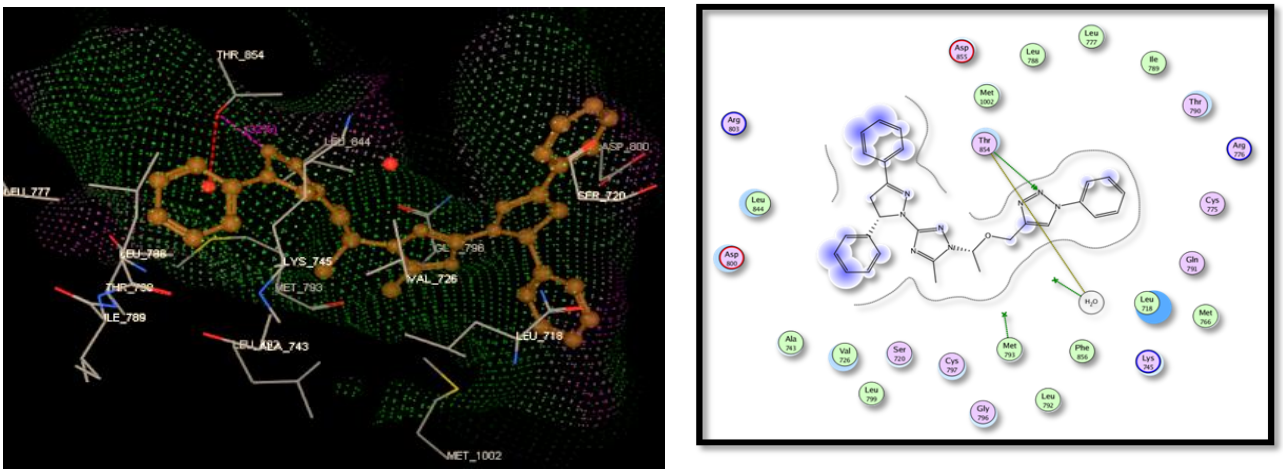
(A) **(B)**

Figure S3. Docking of compound **6** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



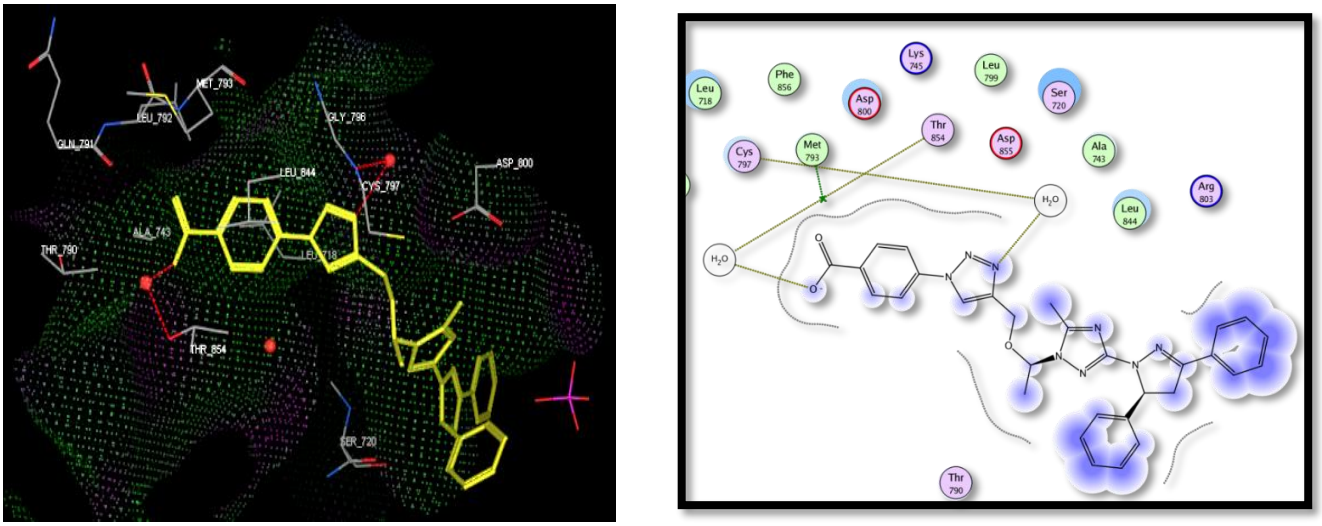
(A) (B)

Figure S4. Docking of compound **5** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



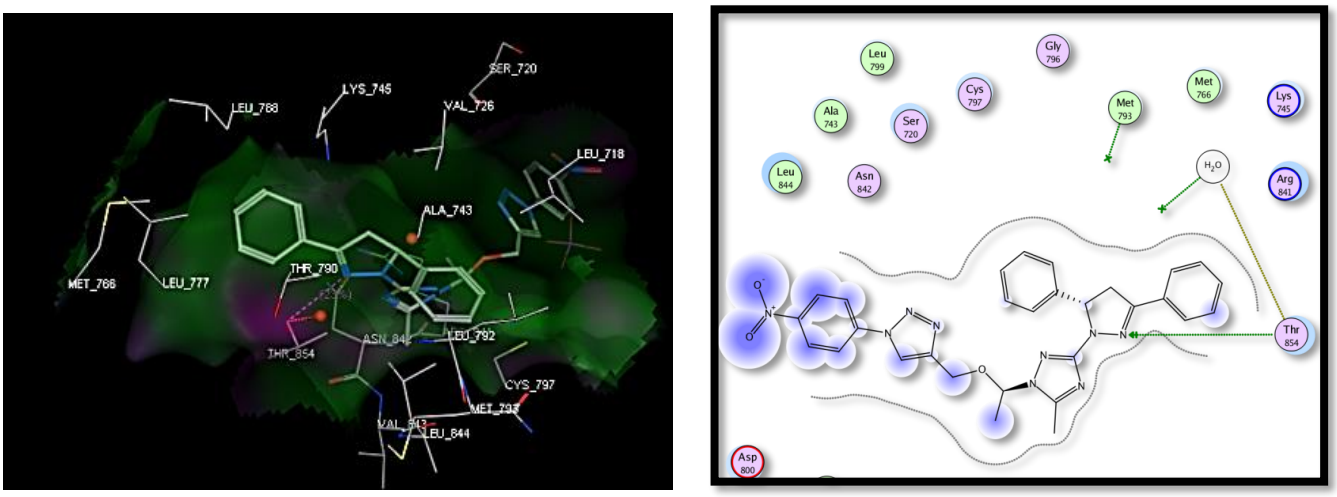
(A) (B)

Figure S5. Docking of compound **4** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



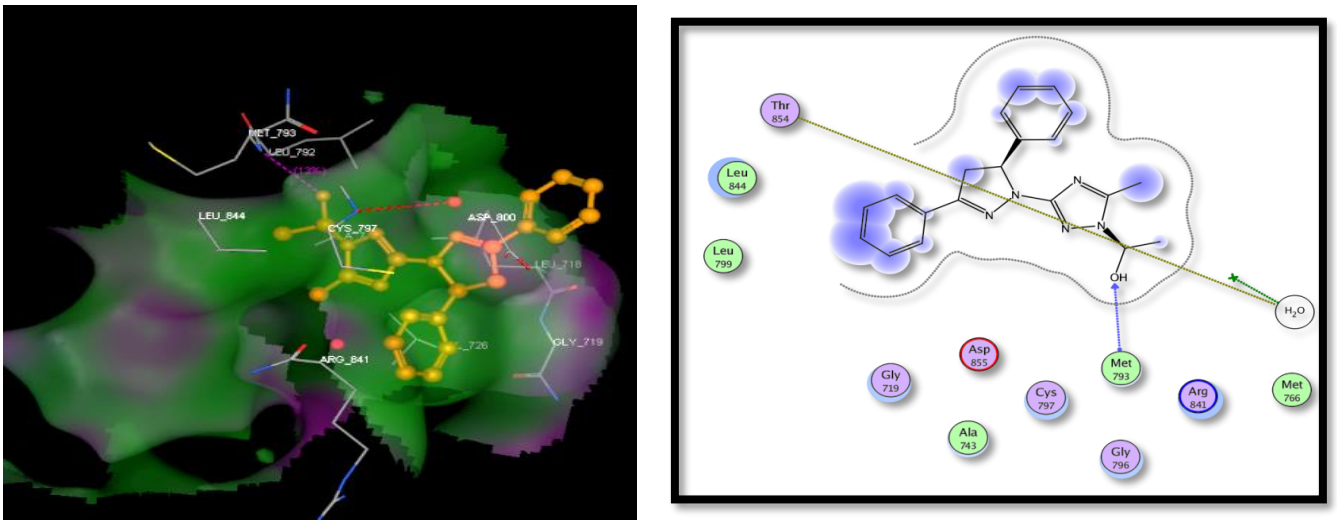
(A) (B)

Figure S6. Docking of compound **8** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



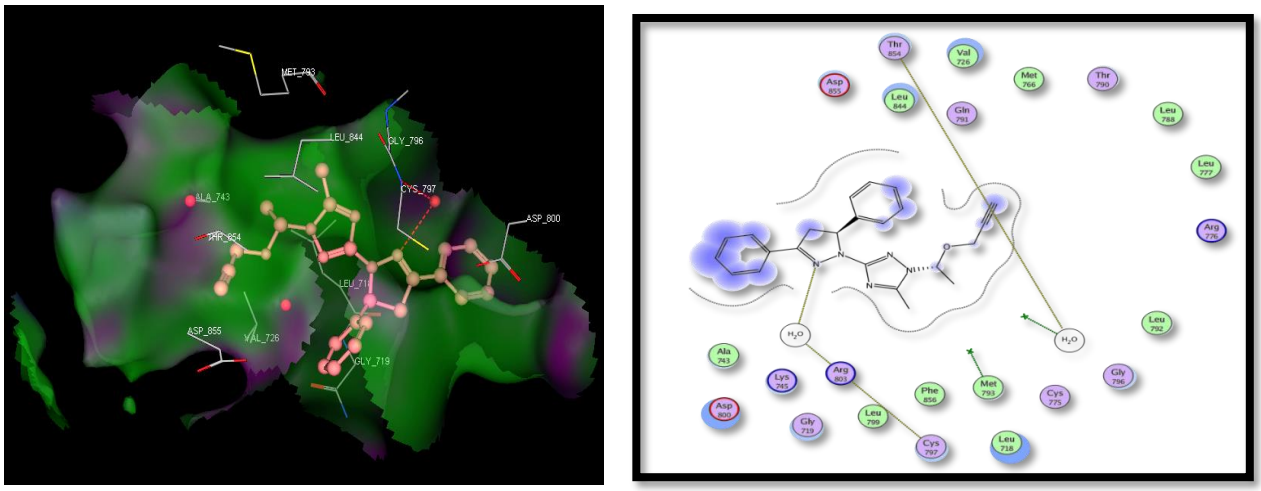
(A) (B)

Figure S7. Docking of compound **9** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



(A) (B)

Figure S8. Docking of compound **2** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.



(A) (B)

Figure S9. Docking of compound **3** within ATP bind site of EGFR. A) 3D biding mode. B) 2D binding mode.

III. Spectra of synthesized compounds

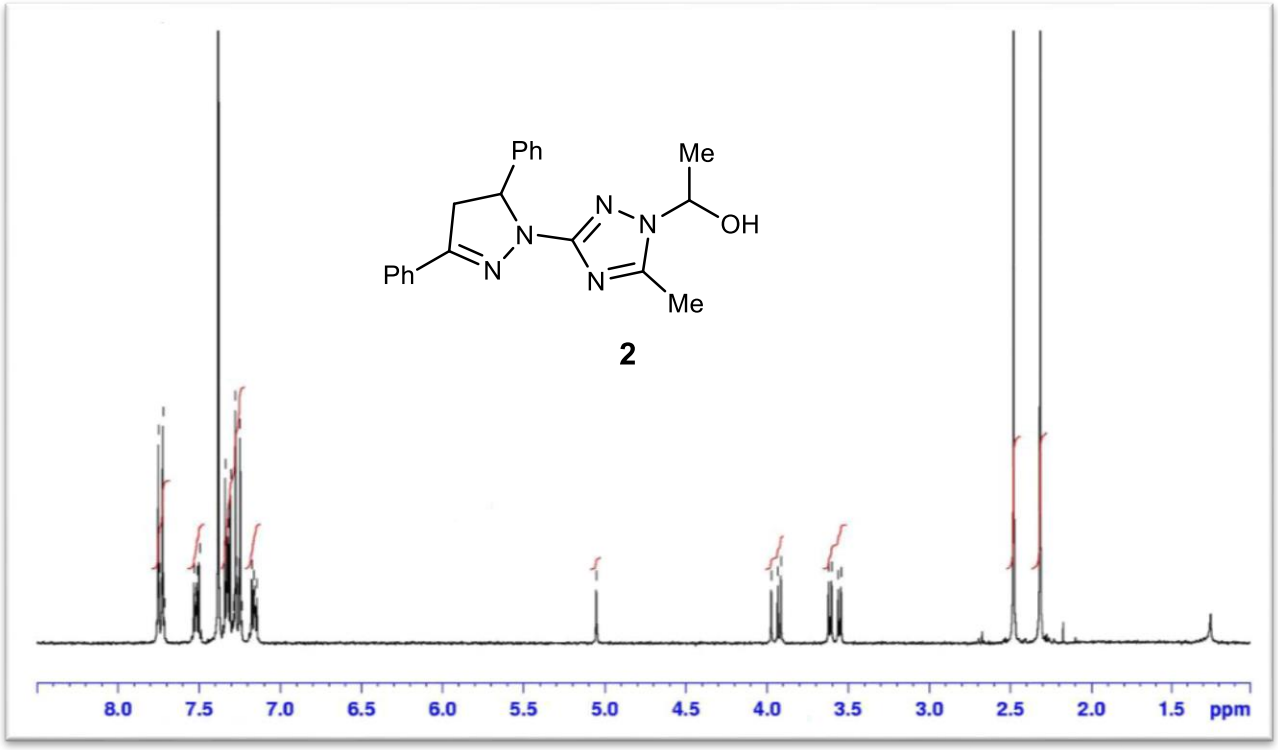
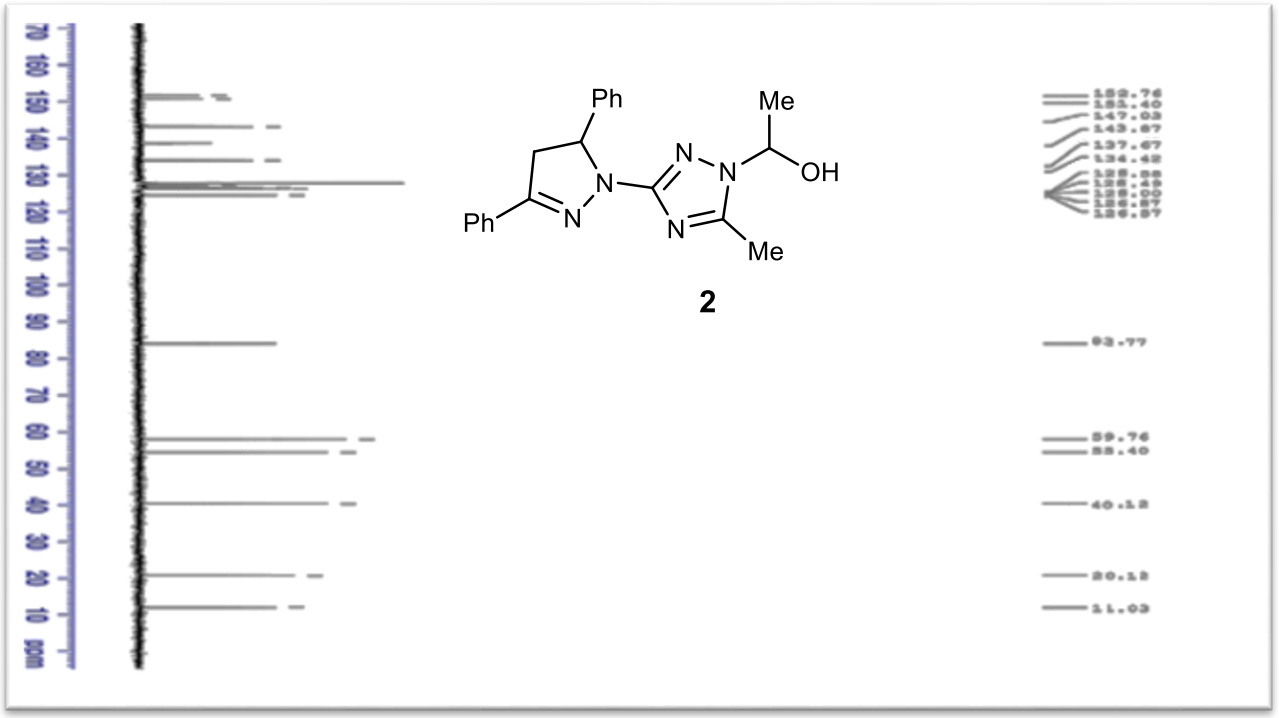


Figure S10. [1]H NMR of compound 2



^{13}C NMR of compound 2

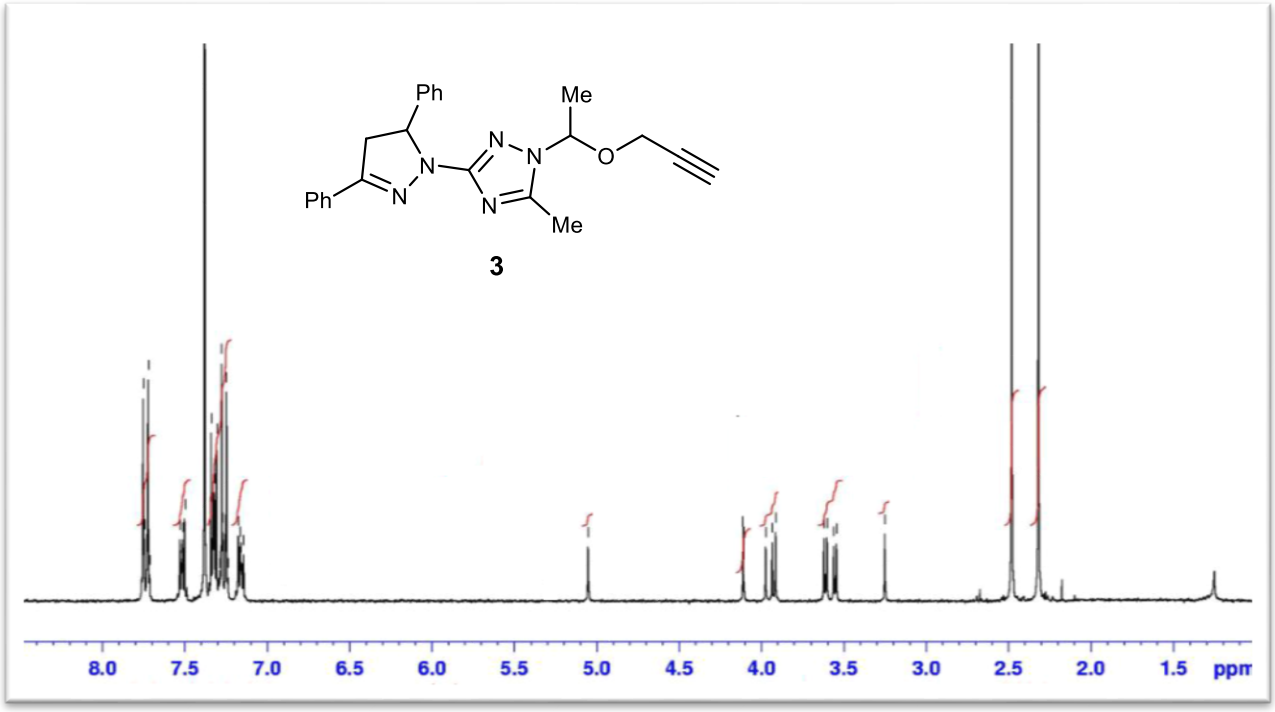


Figure S11. ^{1}H NMR of compound 3

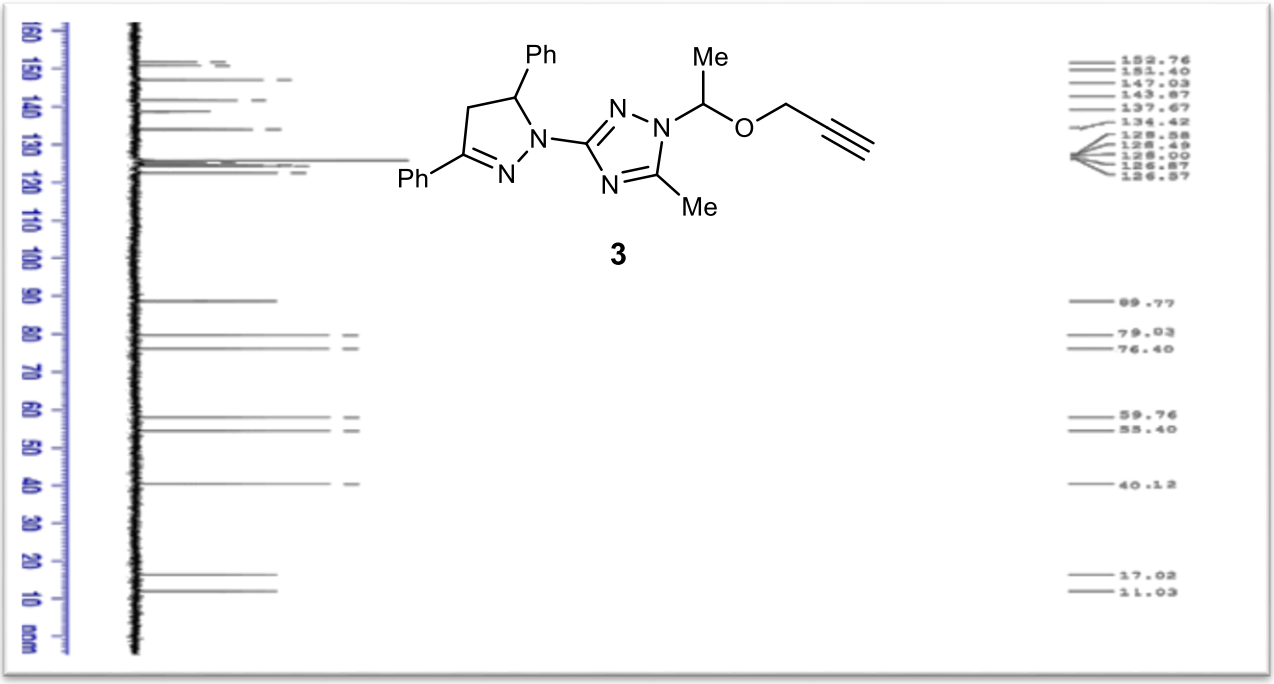


Figure S12. ^{13}C NMR of compound 3

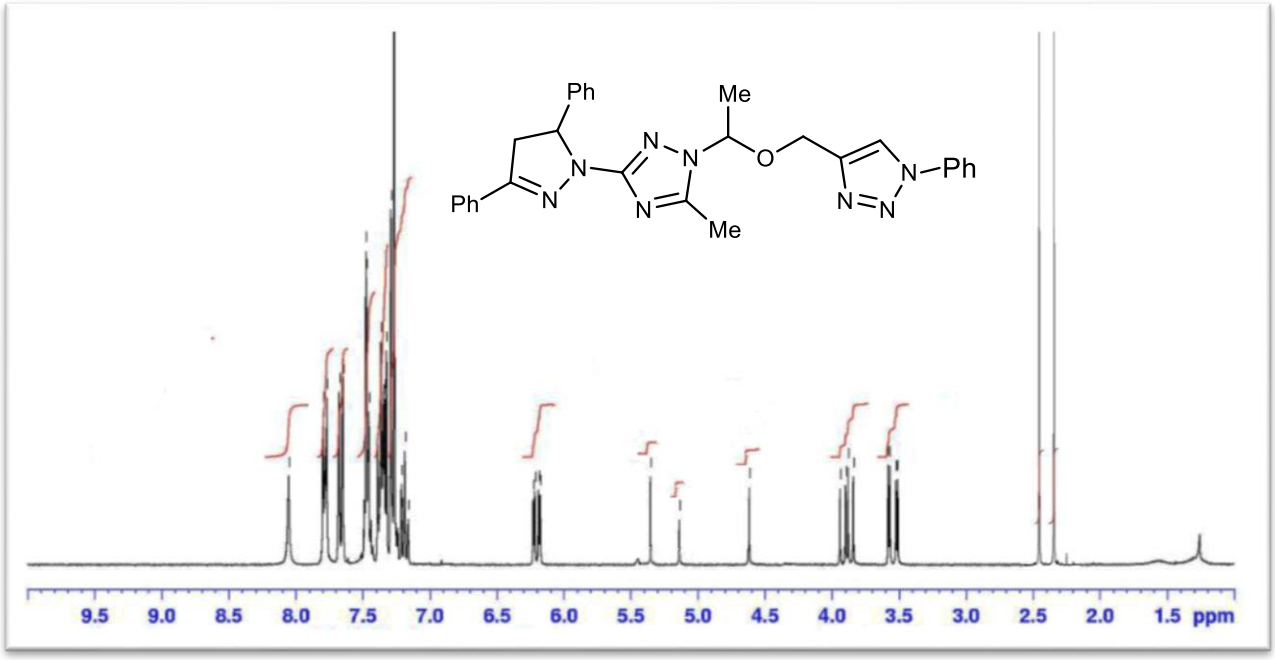


Figure S13. 1H NMR of compound 4

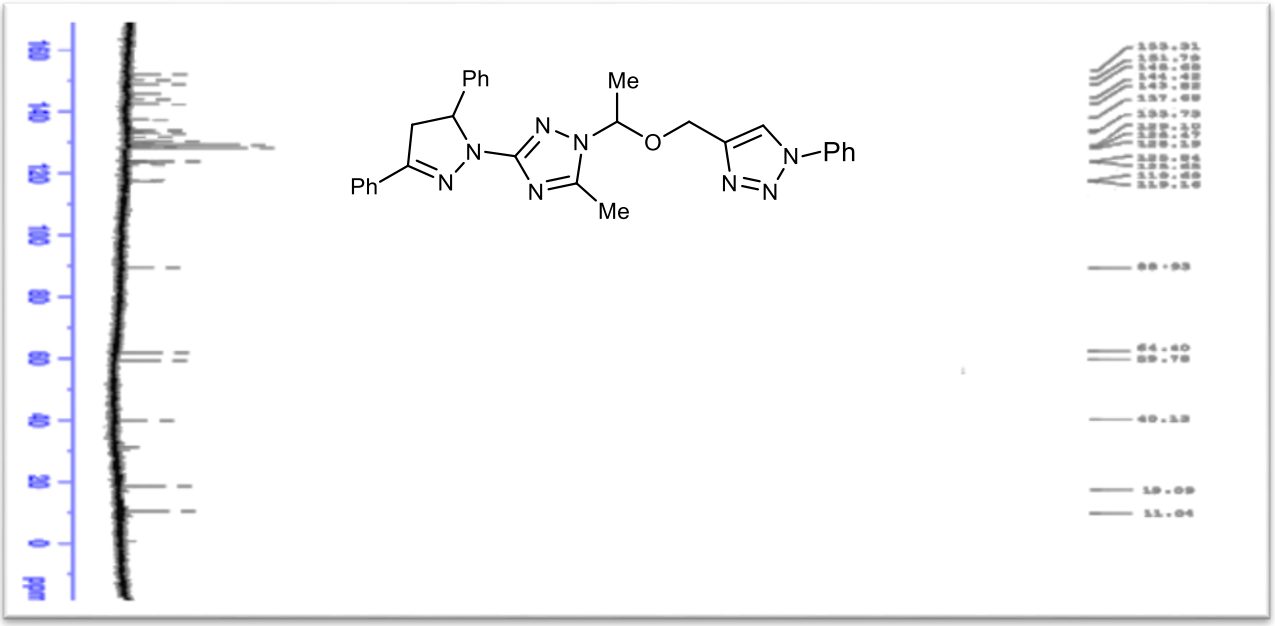


Figure S14. ^{13}C NMR of compound 4

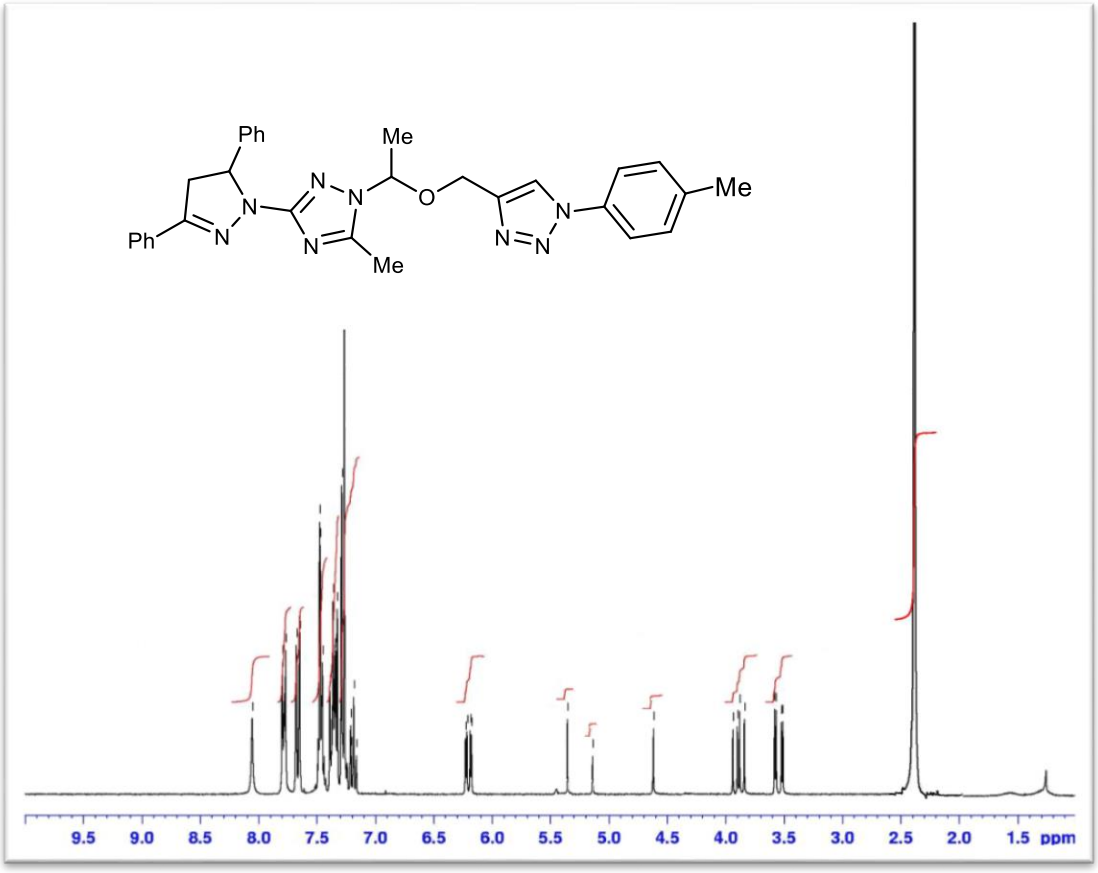


Figure S15. ^{1}H NMR of compound 5

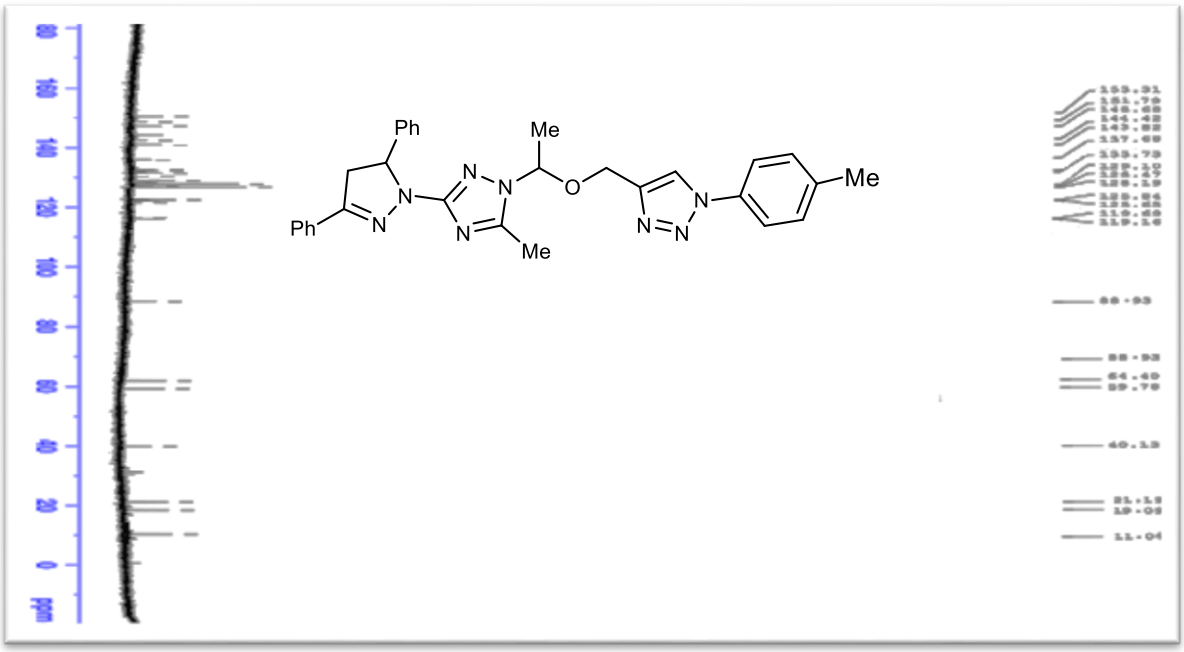


Figure S16. ^{13}C NMR of compound 5

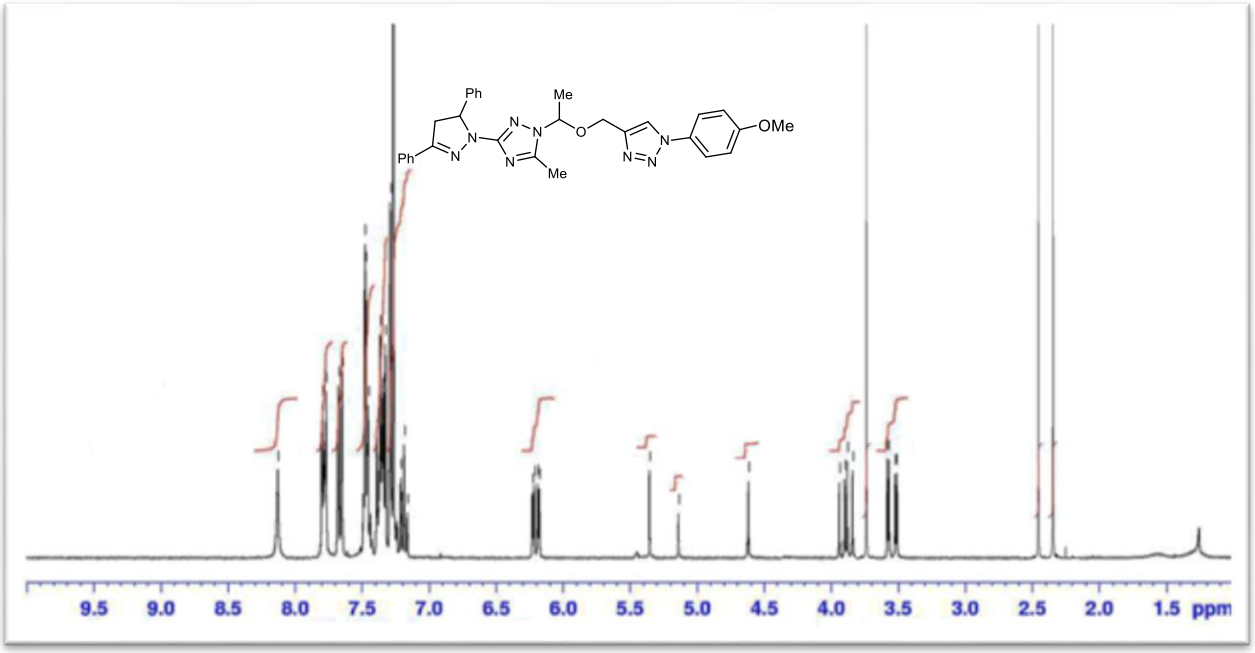


Figure S17. ^{1}H NMR of compound 6

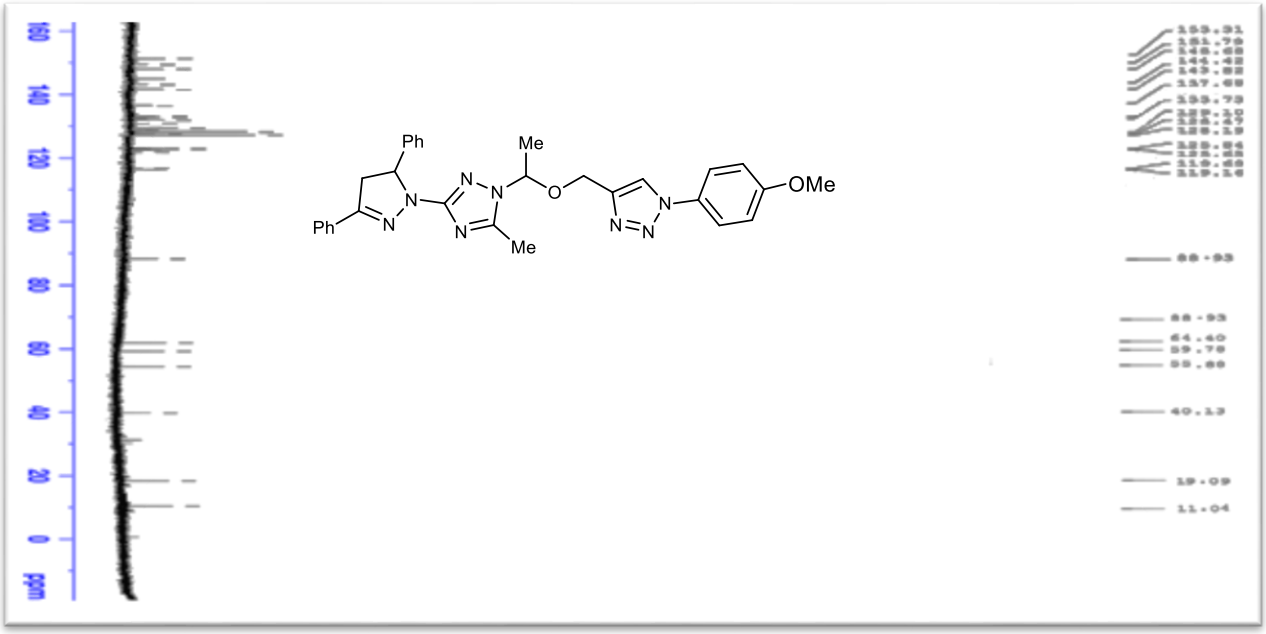


Figure S18. ^{13}C NMR of compound 6

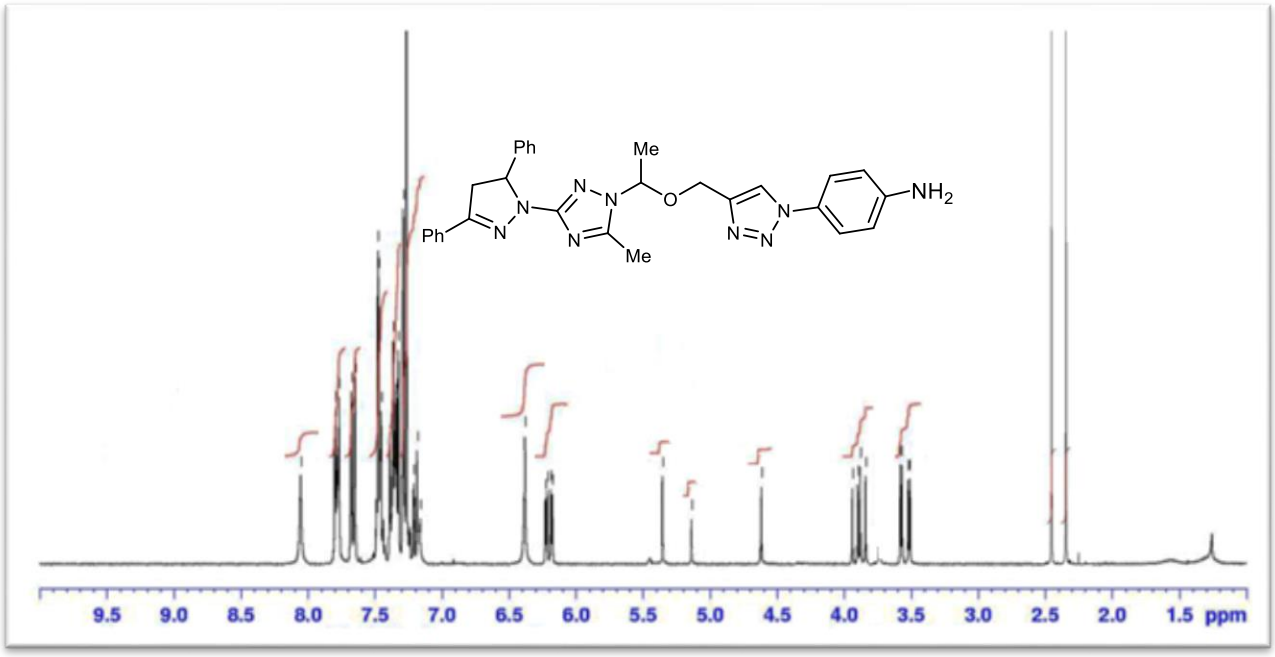


Figure S19. ^{1}H NMR of compound 7

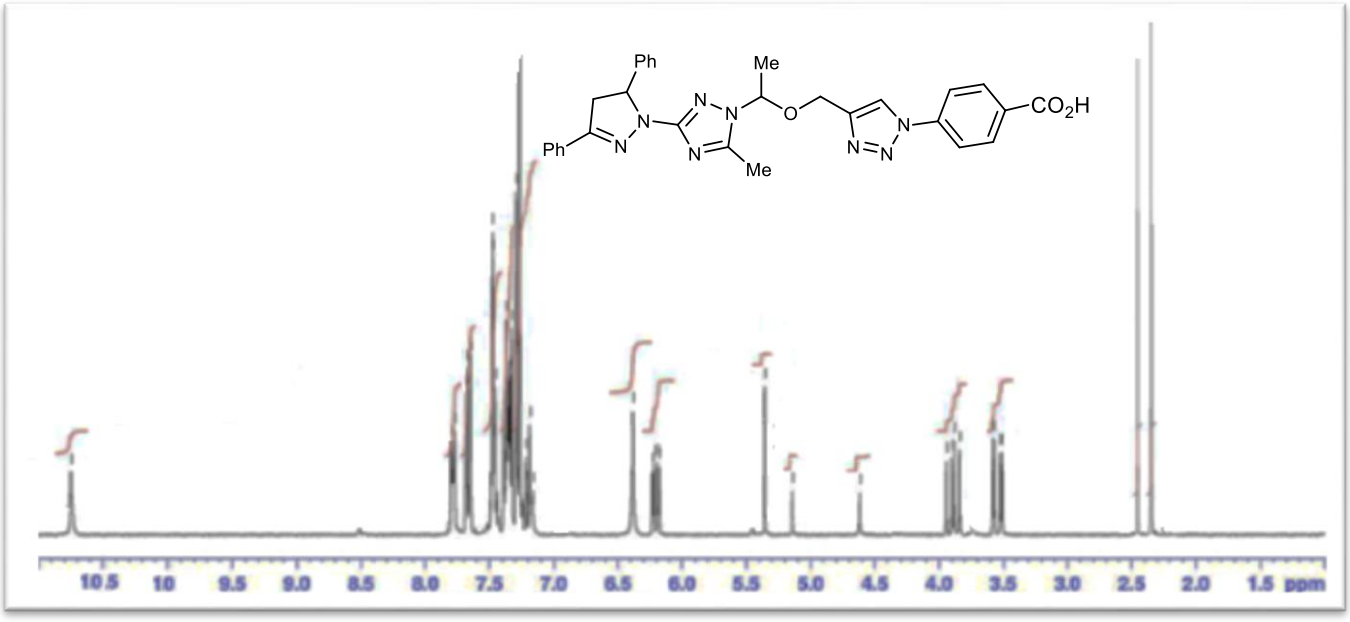


Figure S20. ^{1}H NMR of compound 8

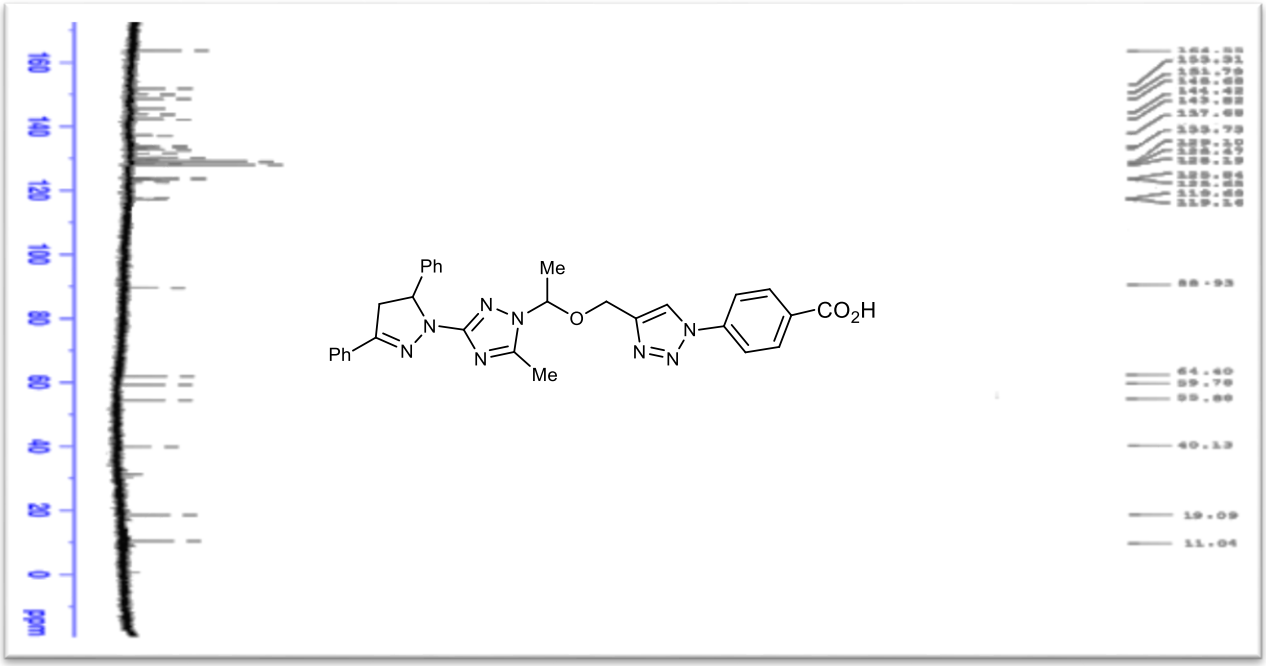


Figure S21. ^{13}C NMR of compound 8

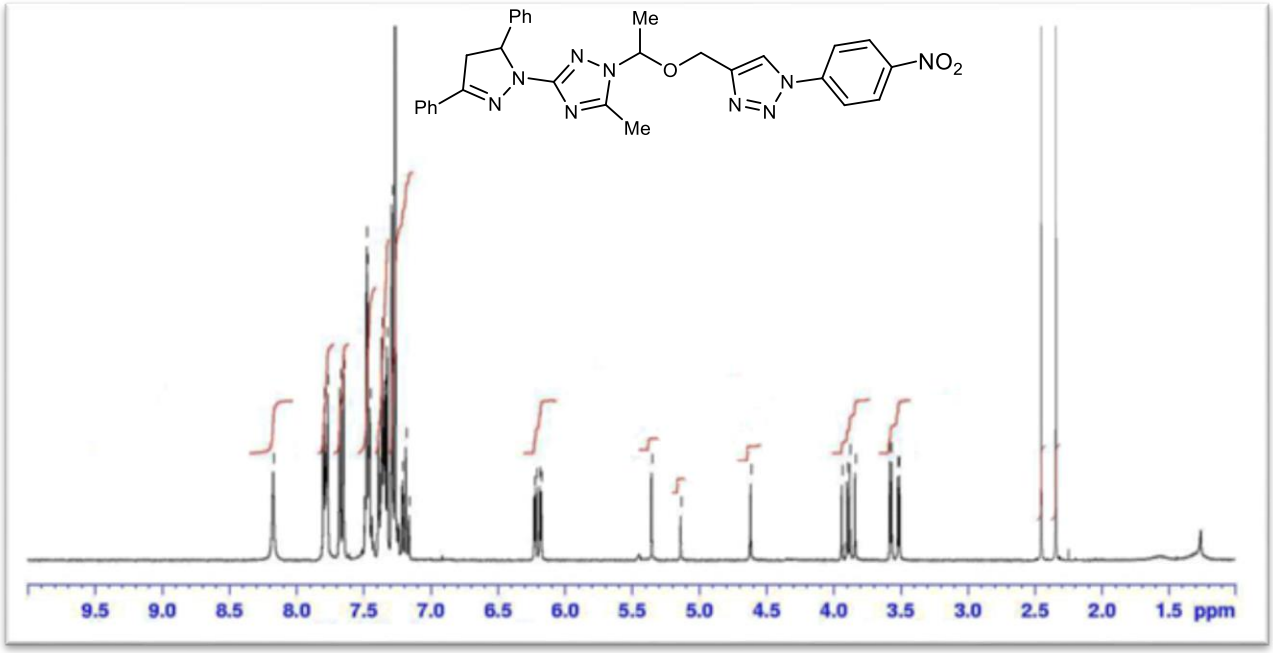


Figure S22. ^{1}H NMR of compound 9