Click Chemistry of Phenyl 1,2,3-Triazole–2-Pyridylpiperazine Hybrids: Synthesis, Targeted Anticancer Activity, Molecular Modeling and Computational Studies

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Compound 13

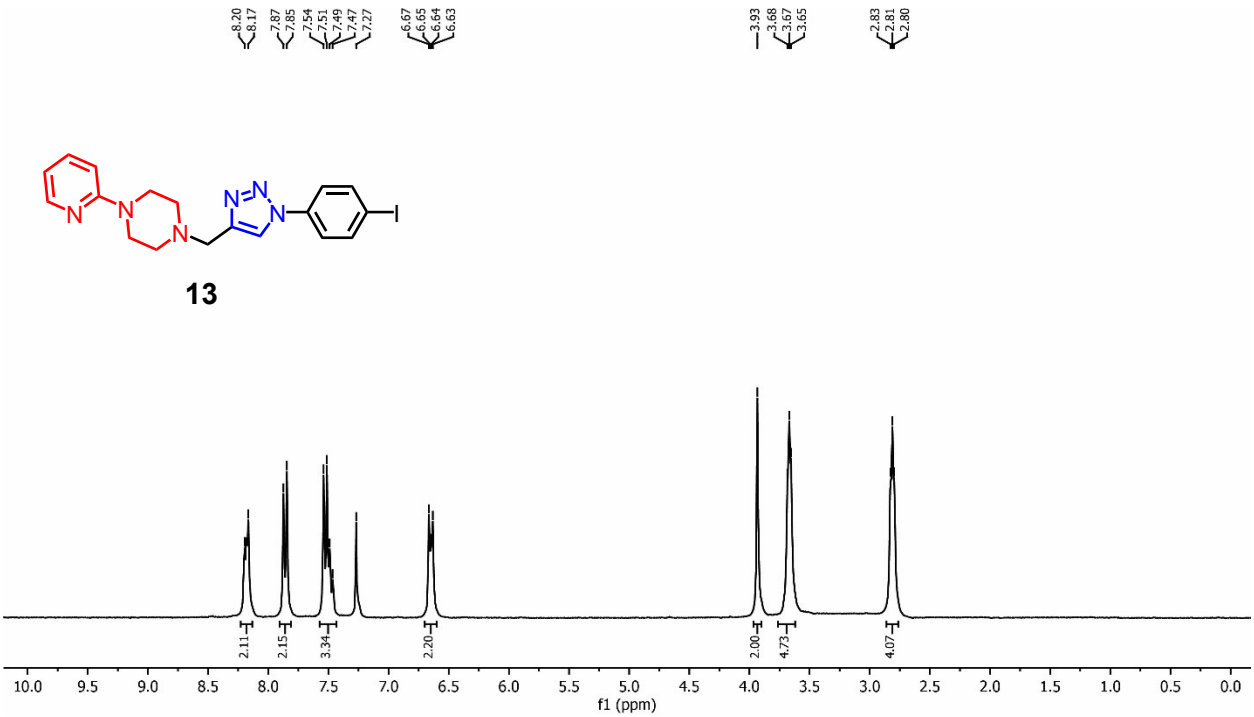


Figure S1. ^{1}H NMR spectrum of compound **13** (400 MHz, $CDCl_3$, 25 °C)

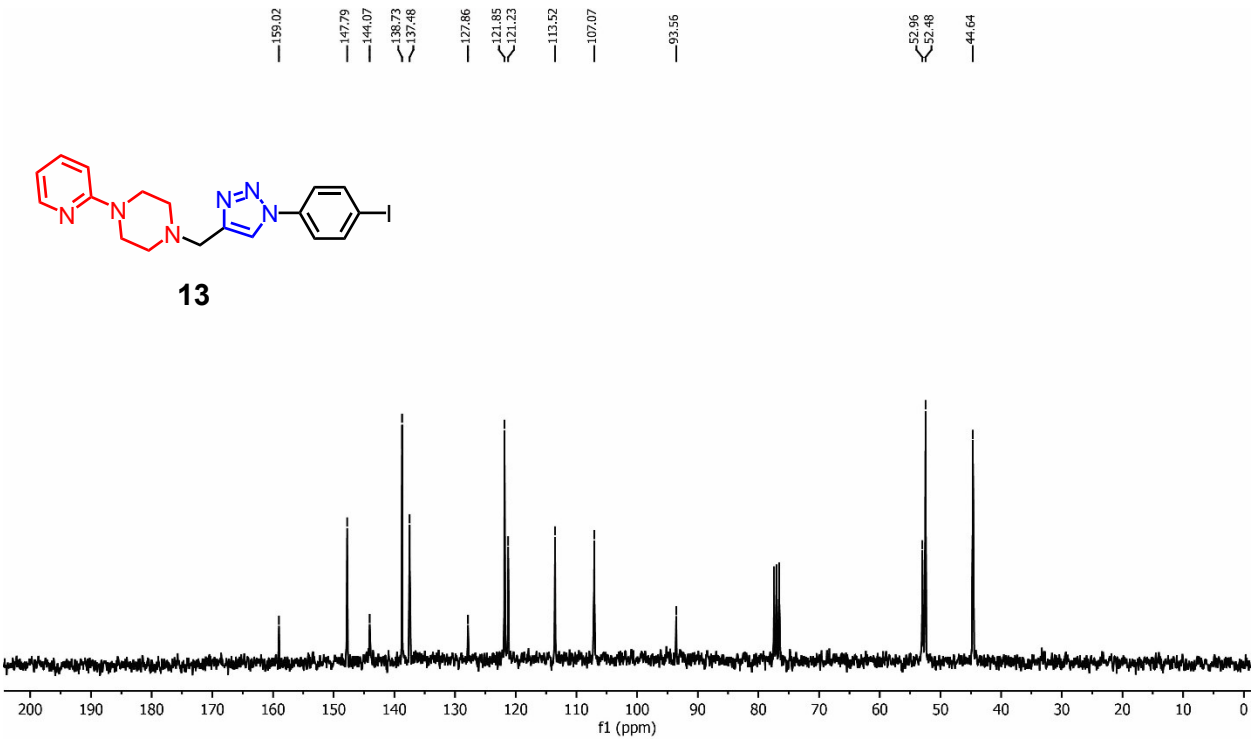


Figure S2. ^{13}C NMR spectrum of compound **13** (100 MHz, $CDCl_3$, 25 °C)

Compound 14

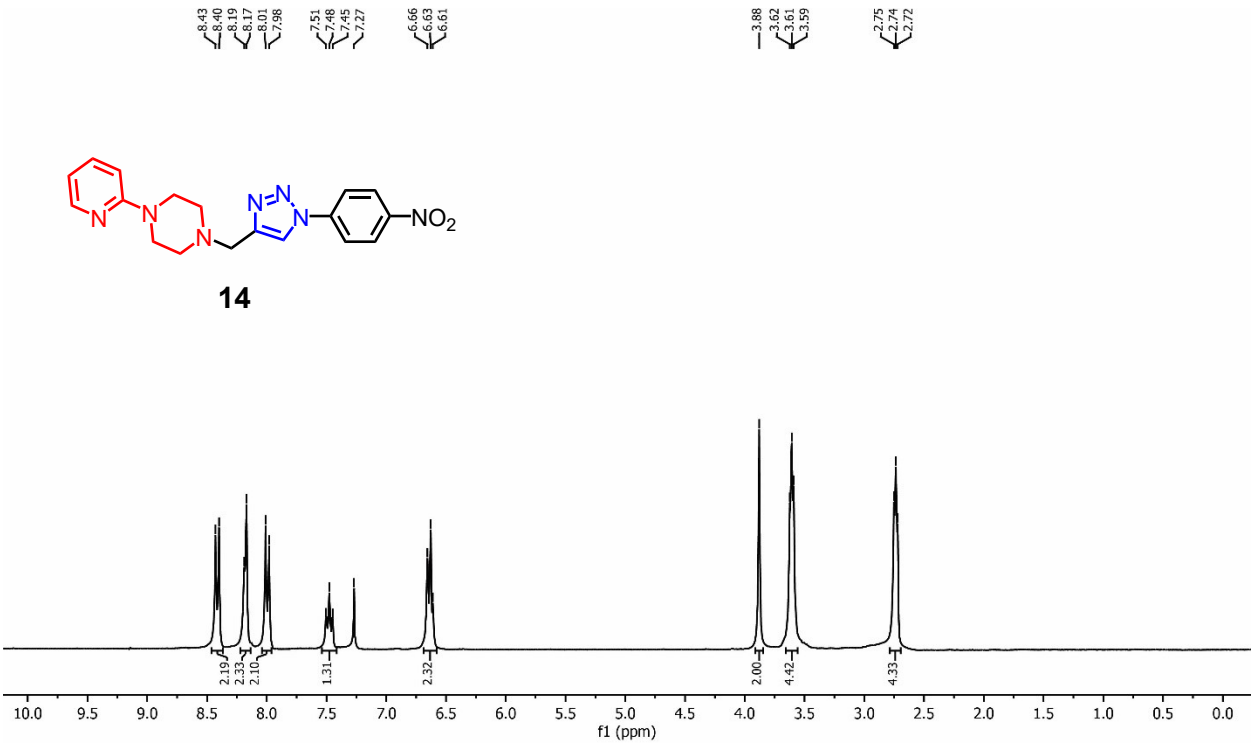


Figure S3. ^{1}H NMR spectrum of compound **14** (400 MHz, $CDCl_3$, 25 °C)

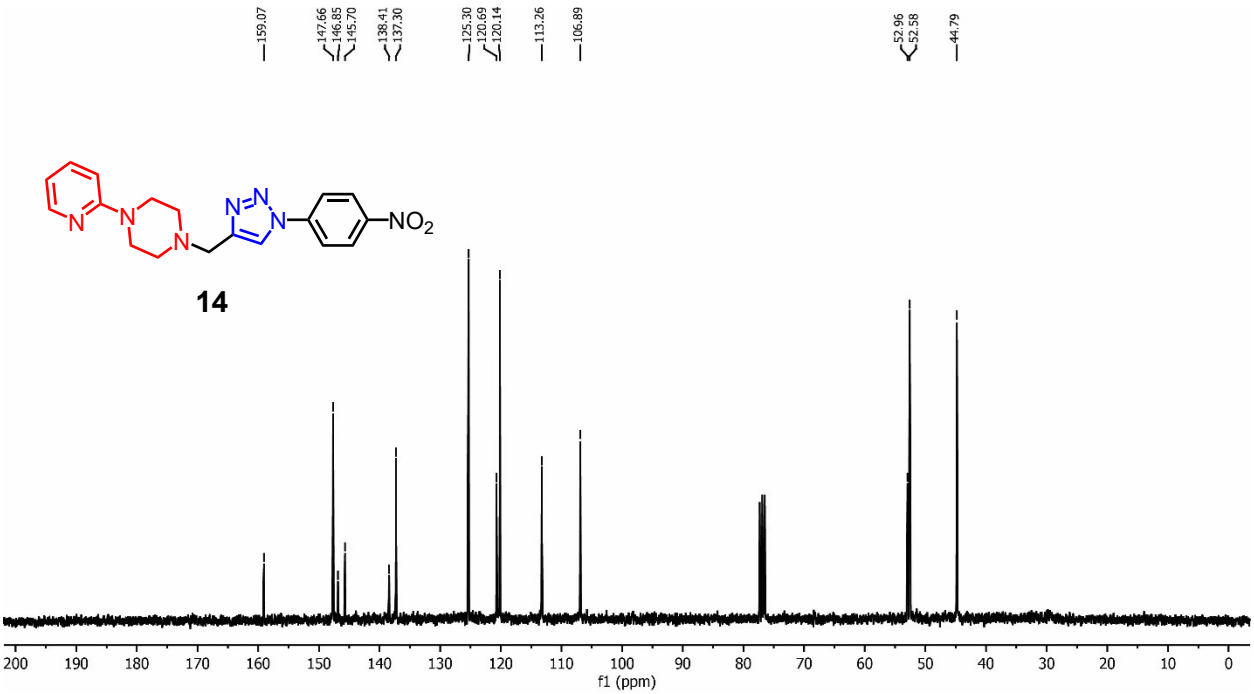


Figure S4. ^{13}C NMR spectrum of compound **14** (100 MHz, $CDCl_3$, 25 °C)

Compound 15

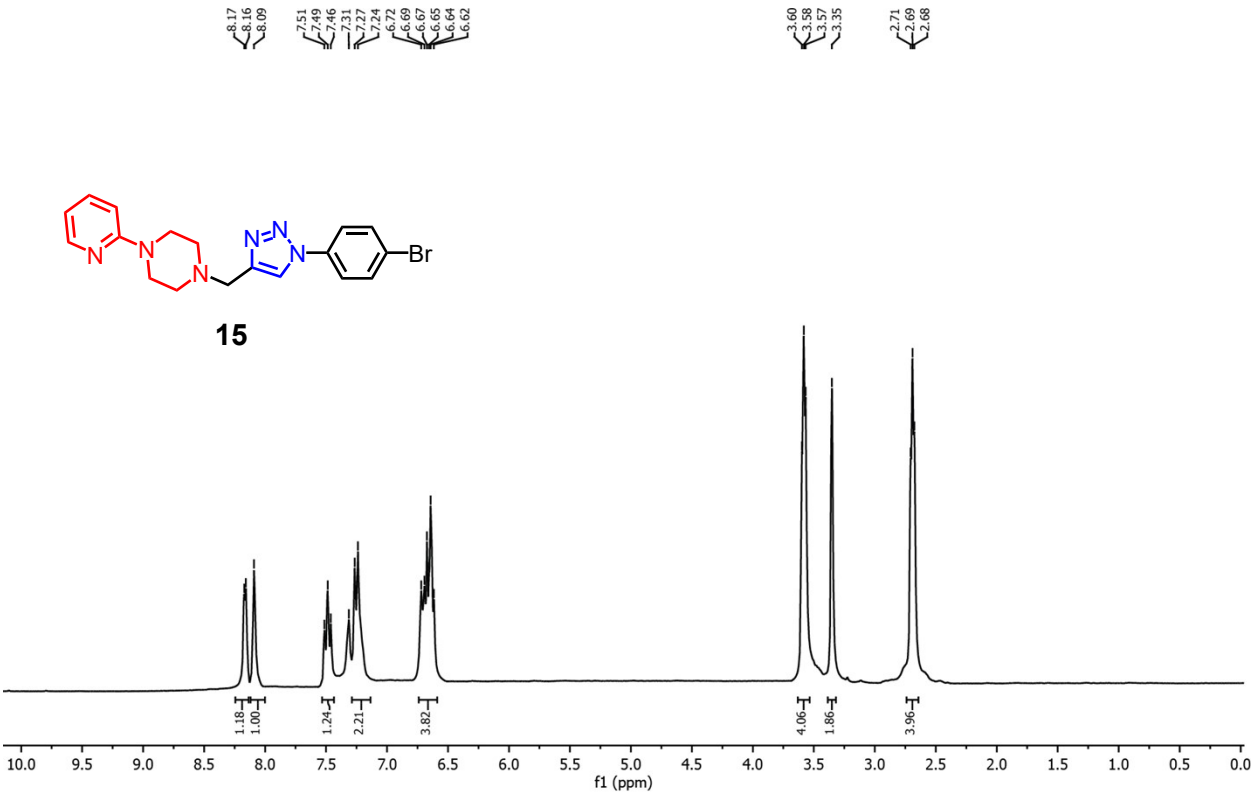


Figure S5. ^{1}H NMR spectrum of compound **15** (400 MHz, $CDCl_3$, 25 °C)

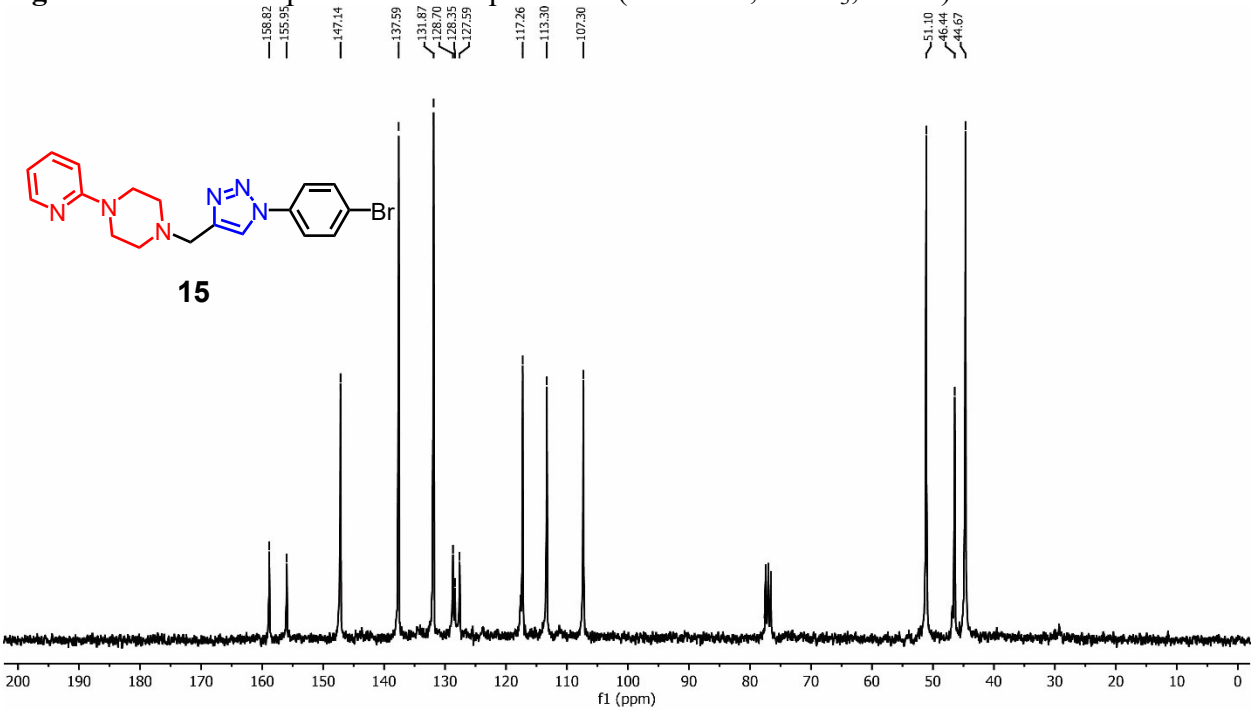


Figure S6. ^{13}C NMR spectrum of compound **15** (100 MHz, $CDCl_3$, 25 °C)

Compound 16

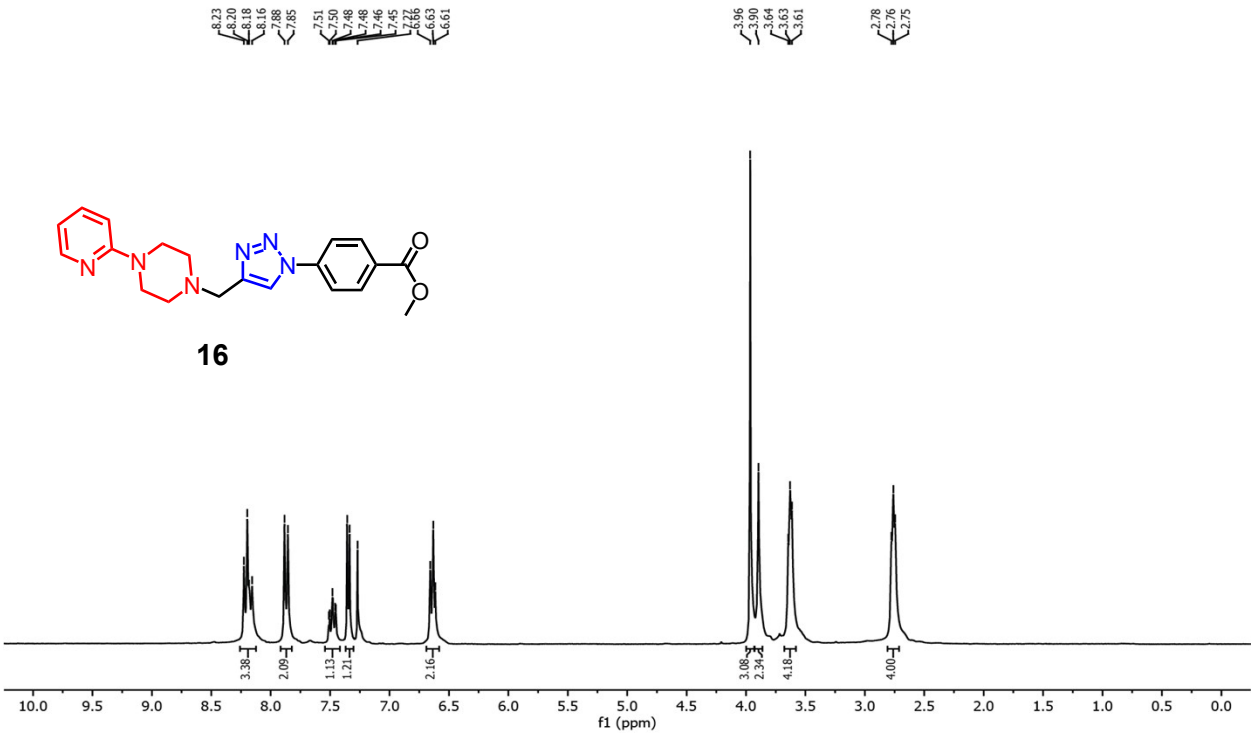


Figure S7. ^{1}H NMR spectrum of compound **16** (400 MHz, $CDCl_3$, 25 °C)

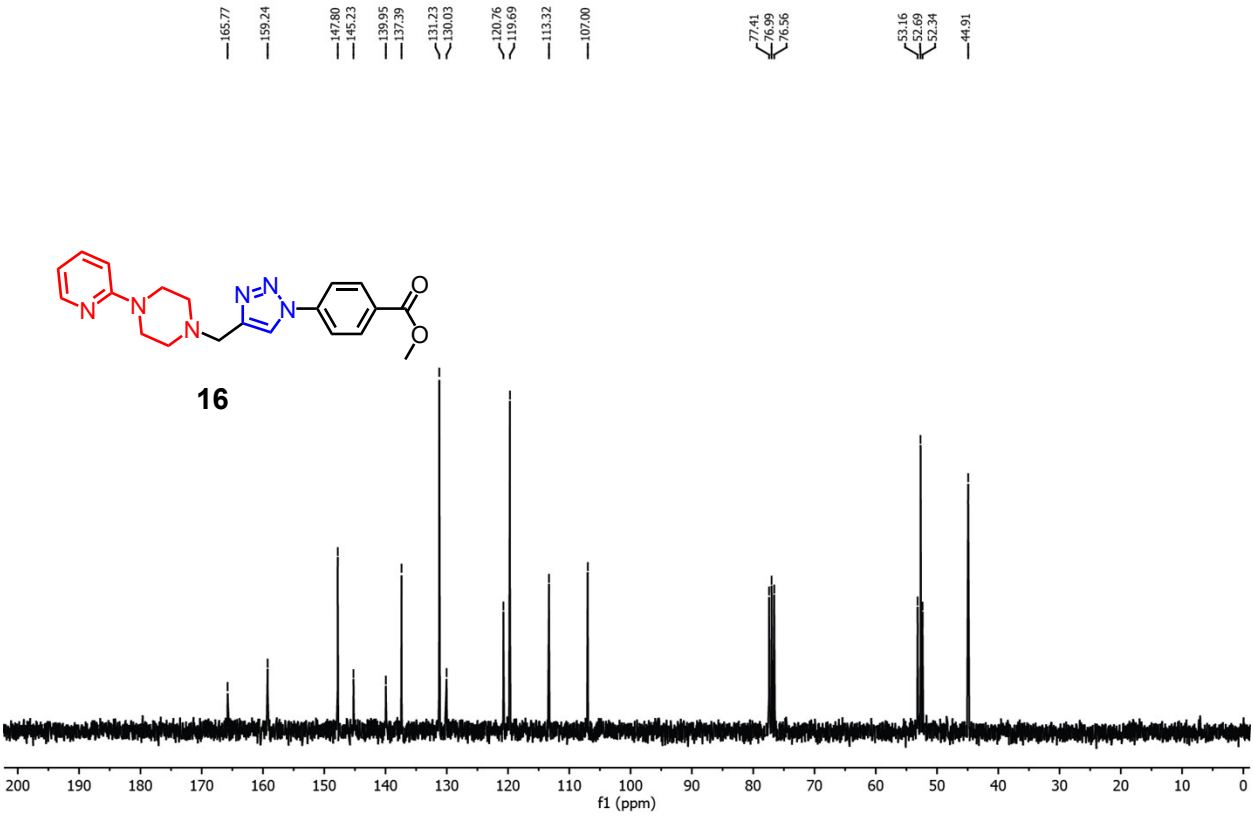


Figure S8. ^{13}C NMR spectrum of compound **16** (100 MHz, $CDCl_3$, 25 °C)

Compound 17

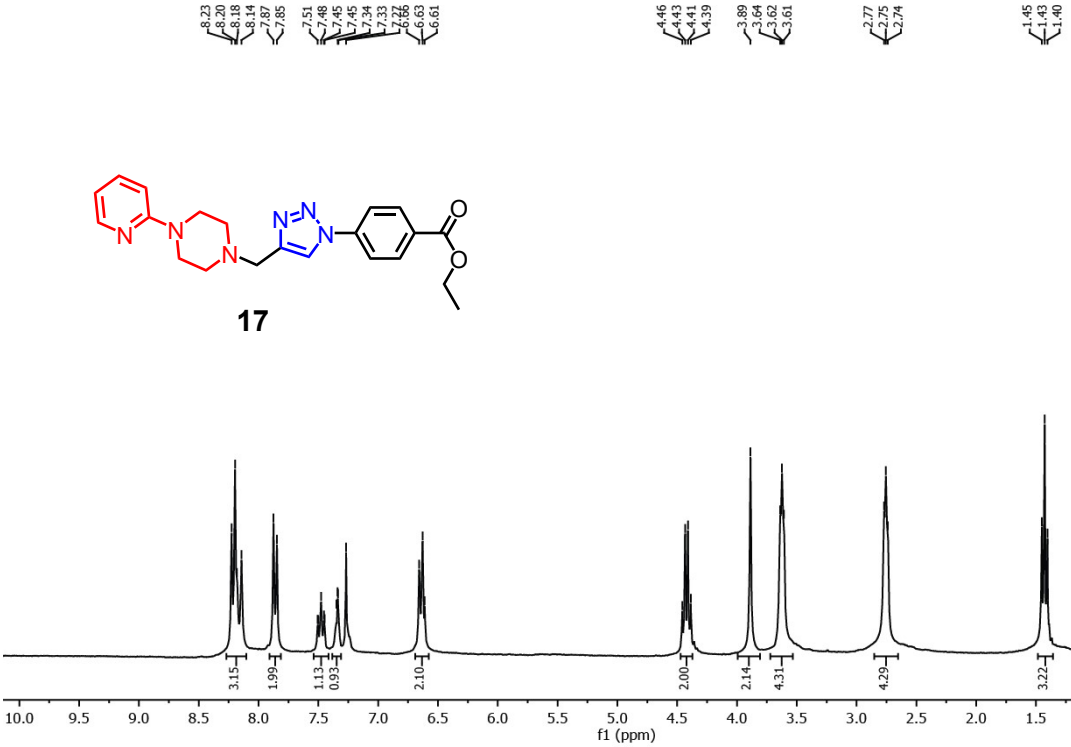


Figure S9. ^{1}H NMR spectrum of compound **17** (400 MHz, $CDCl_3$, 25 °C)

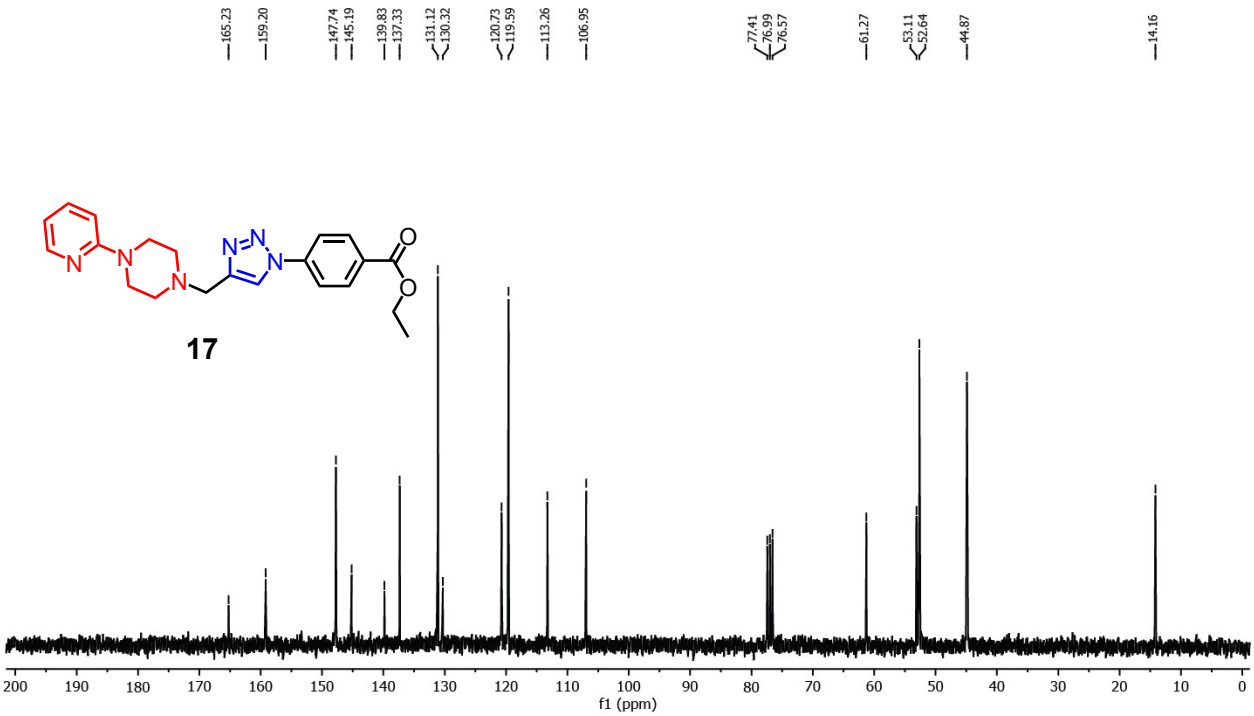


Figure S10. ^{13}C NMR spectrum of compound **17** (100 MHz, $CDCl_3$, 25 °C)

Compound 18

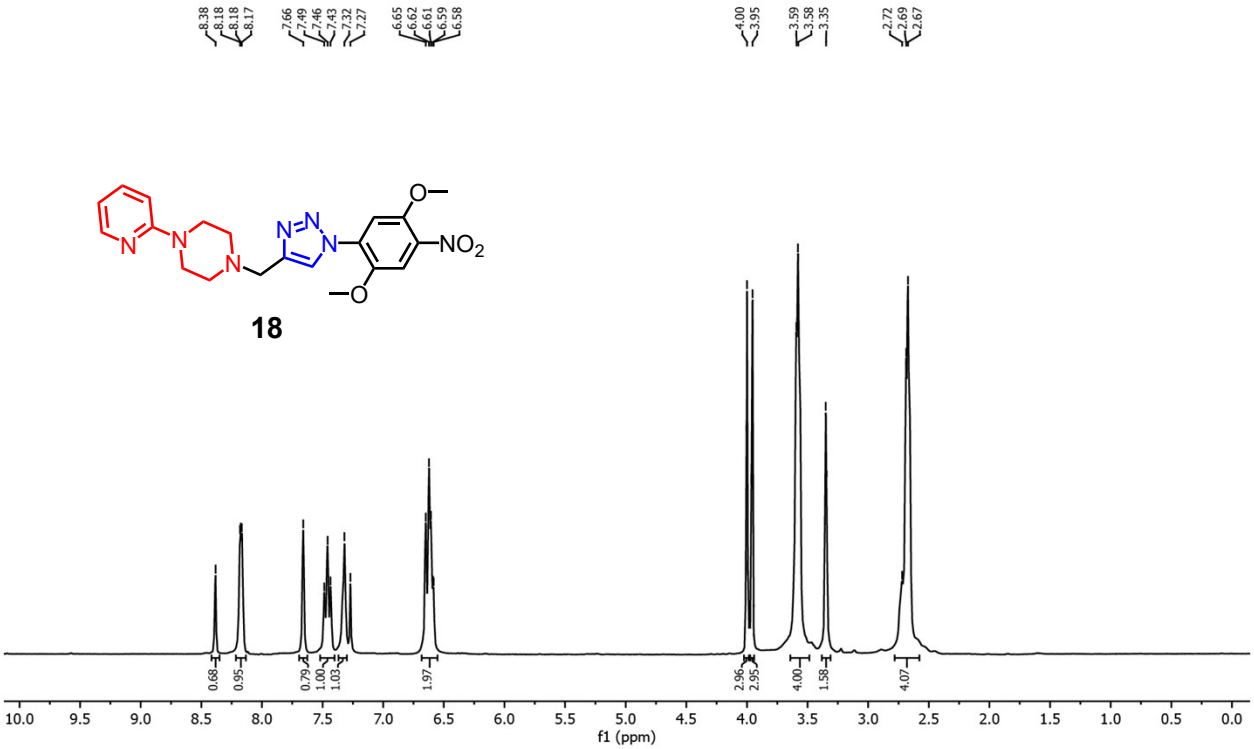


Figure S11. ^{1}H NMR spectrum of compound **18** (400 MHz, $CDCl_3$, 25 °C)

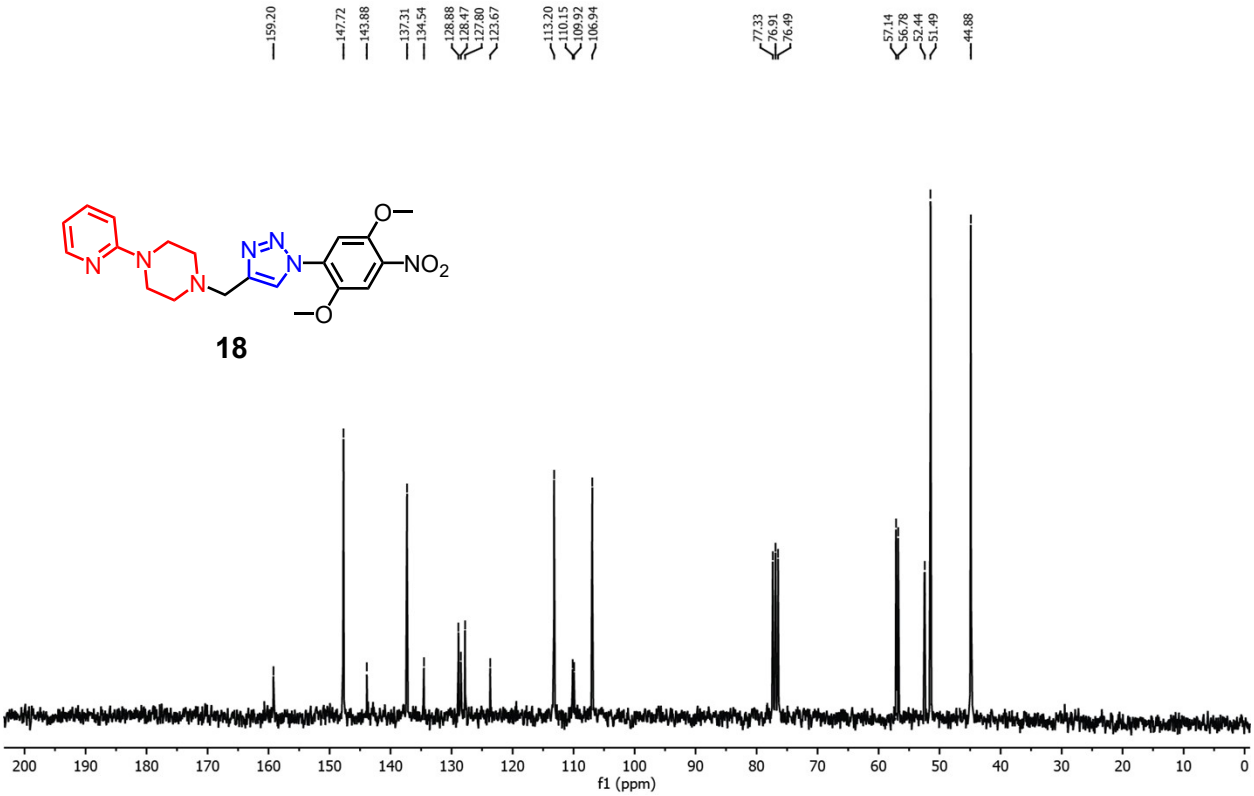


Figure S12. ^{13}C NMR spectrum of compound **18** (100 MHz, $CDCl_3$, 25 °C)

Compound 19

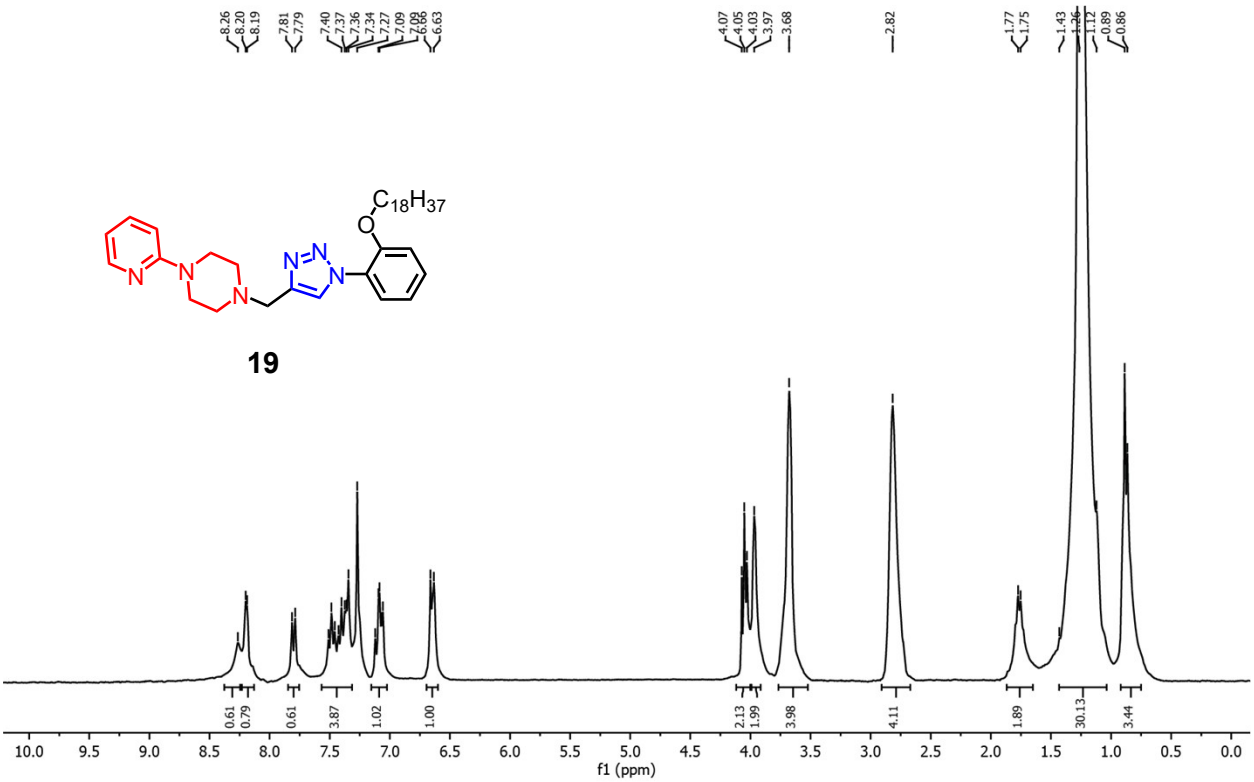


Figure S13. ^{1}H NMR spectrum of compound **19** (400 MHz, $CDCl_3$, 25 °C)

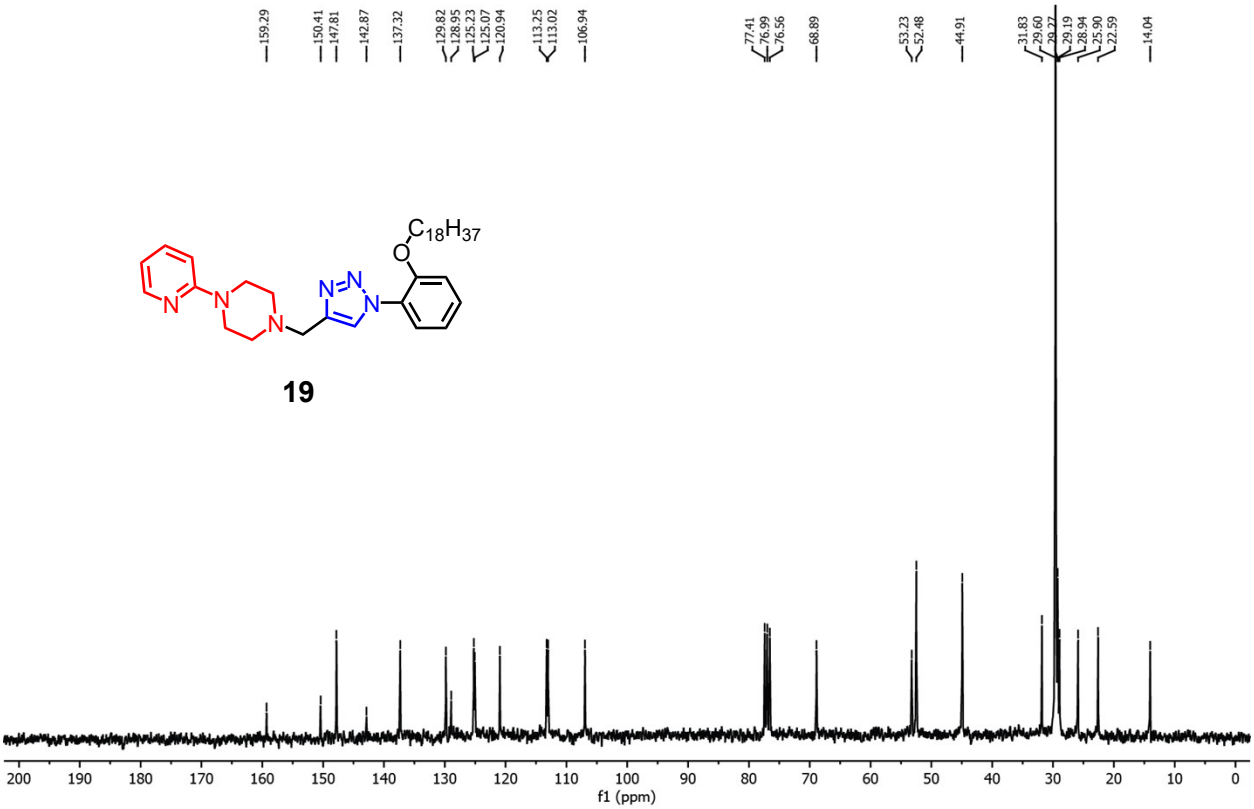


Figure S14. ^{13}C NMR spectrum of compound **19** (100 MHz, $CDCl_3$, 25 °C)

Compound 20

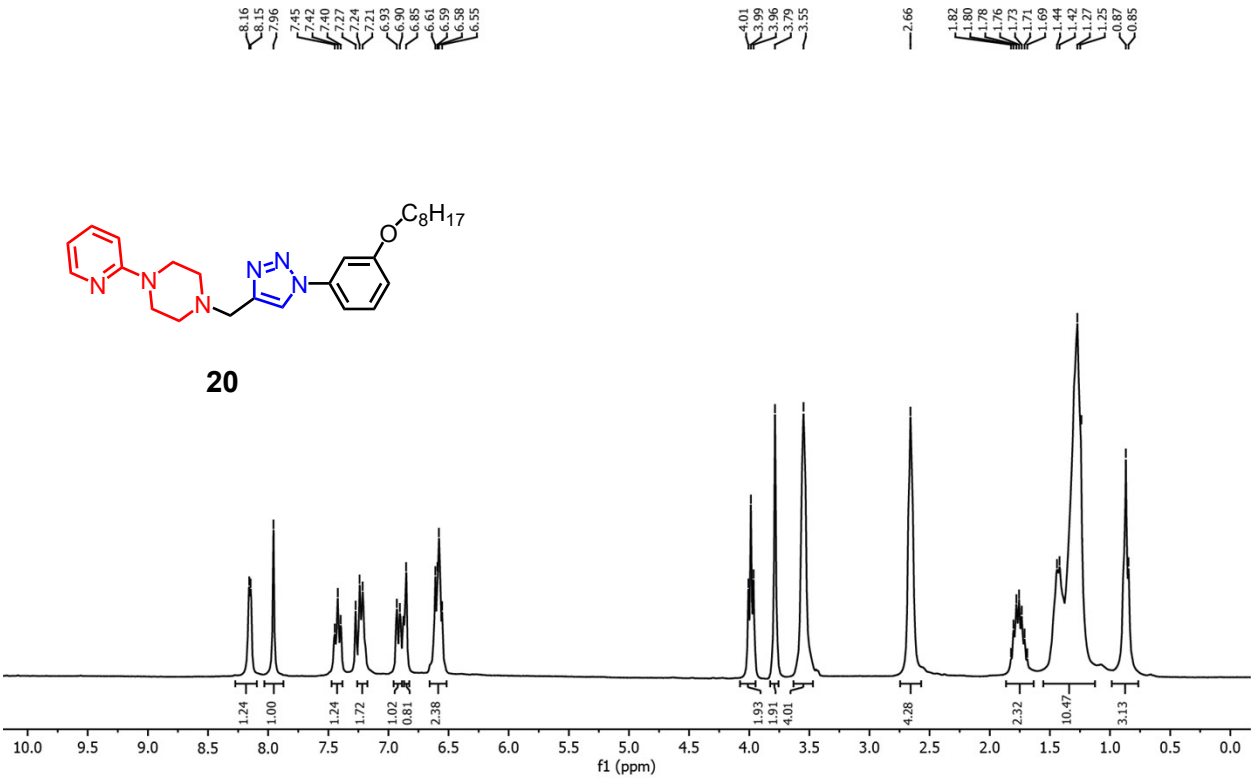


Figure S15. ^{1}H NMR spectrum of compound **20** (400 MHz, $CDCl_3$, 25 °C)

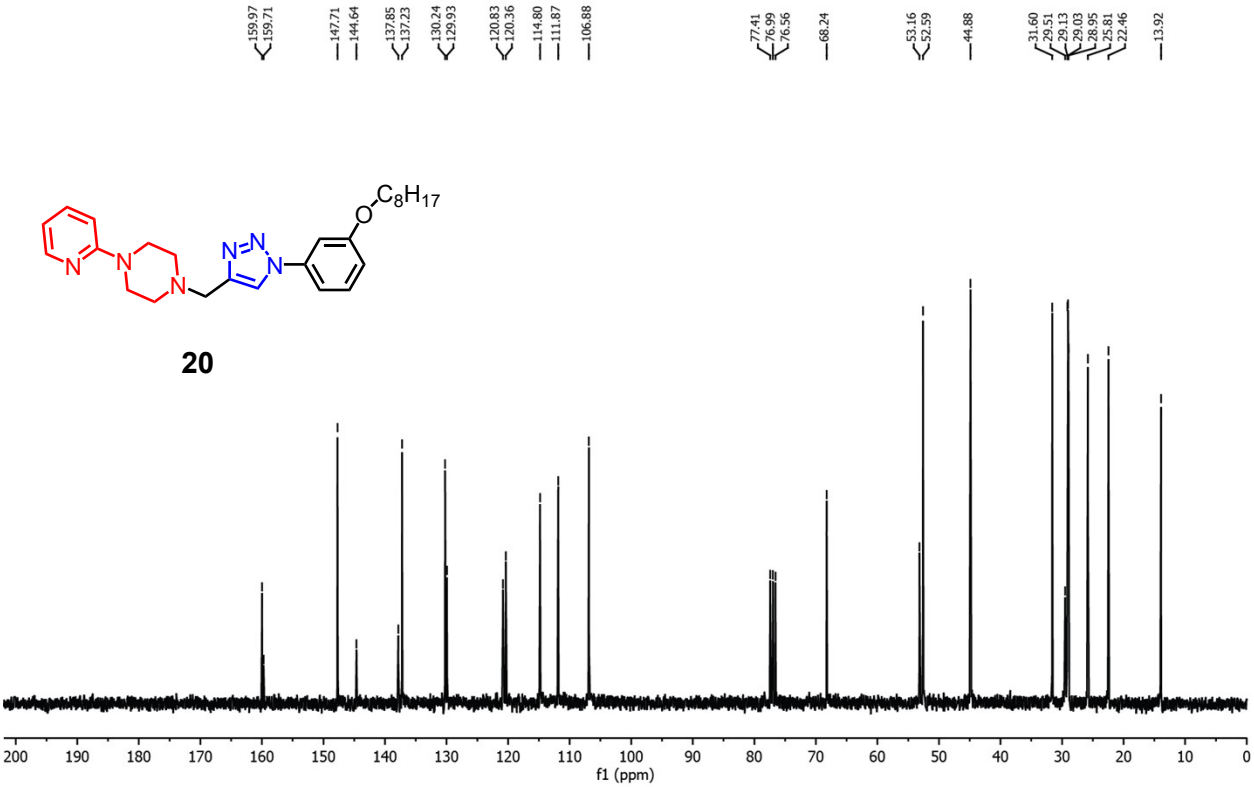


Figure S16. ^{13}C NMR spectrum of compound **20** (100 MHz, $CDCl_3$, 25 °C)

Compound 21

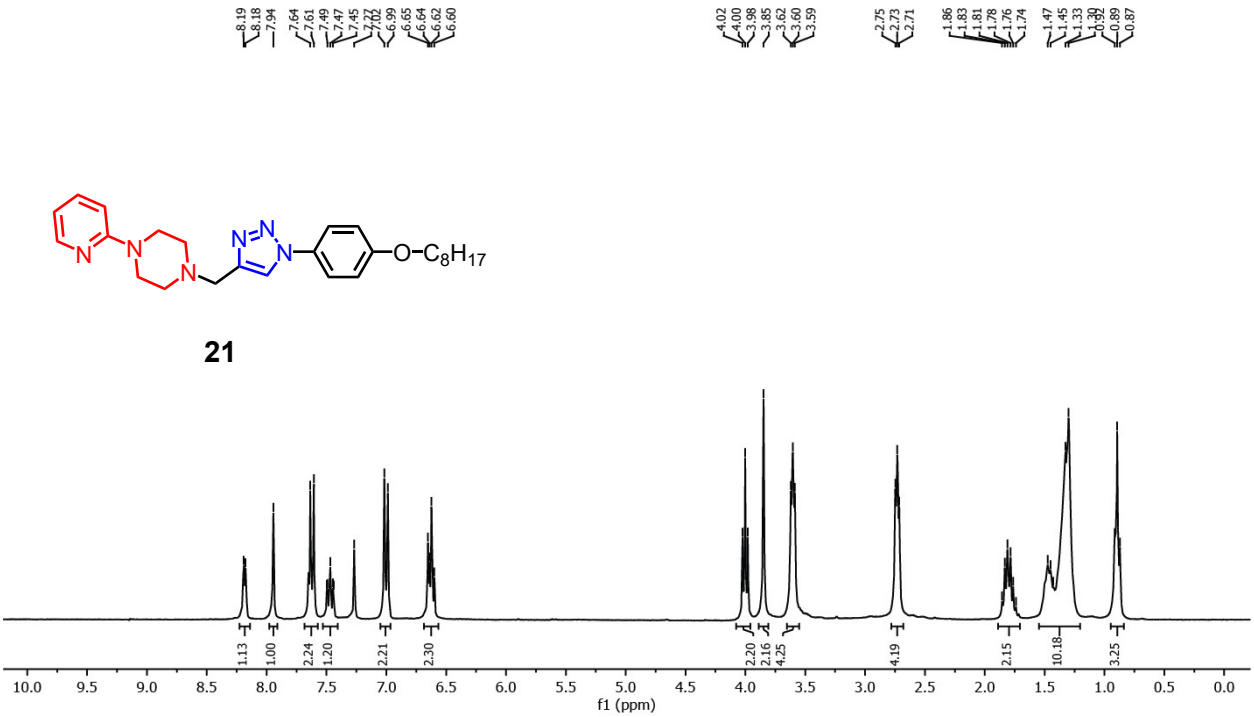


Figure S17. ^{1}H NMR spectrum of compound **21** (400 MHz, $CDCl_3$, 25 °C)

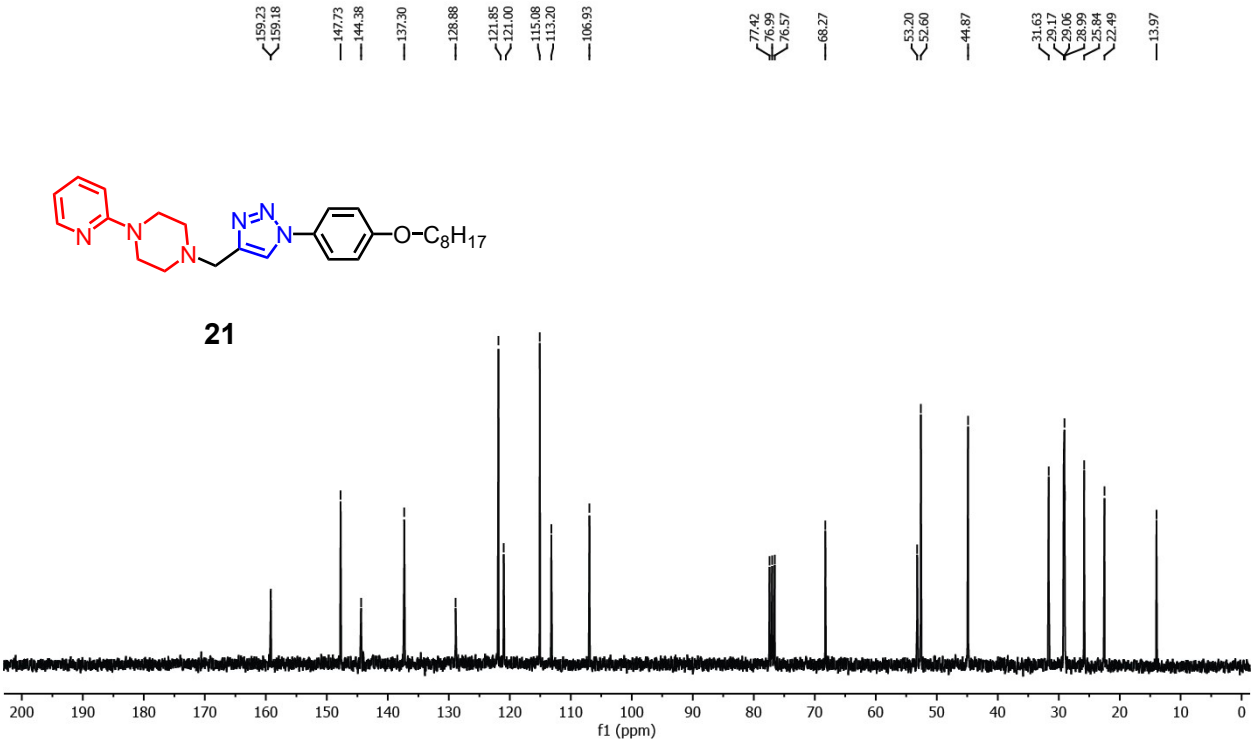


Figure S18. ^{13}C NMR spectrum of compound **21** (100 MHz, $CDCl_3$, 25 °C)

Compound 22

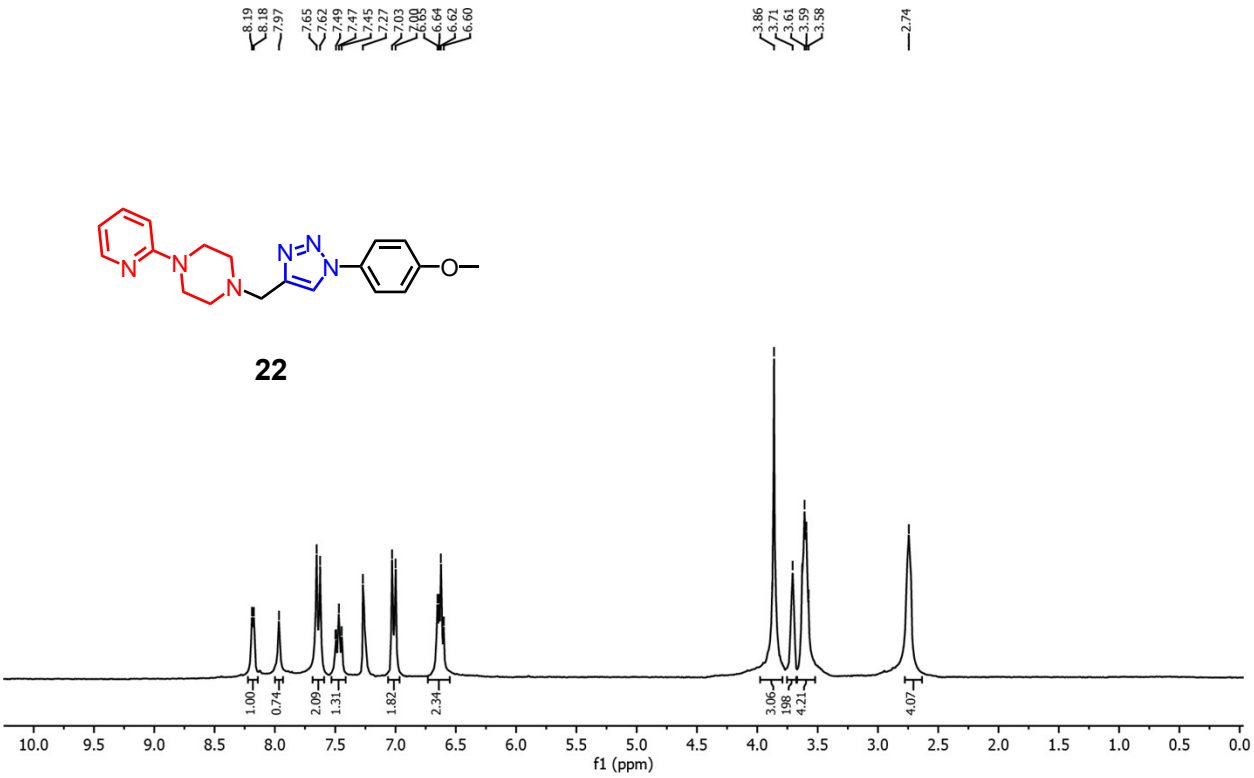


Figure S19. ^{1}H NMR spectrum of compound **22** (400 MHz, $CDCl_3$, 25 °C)

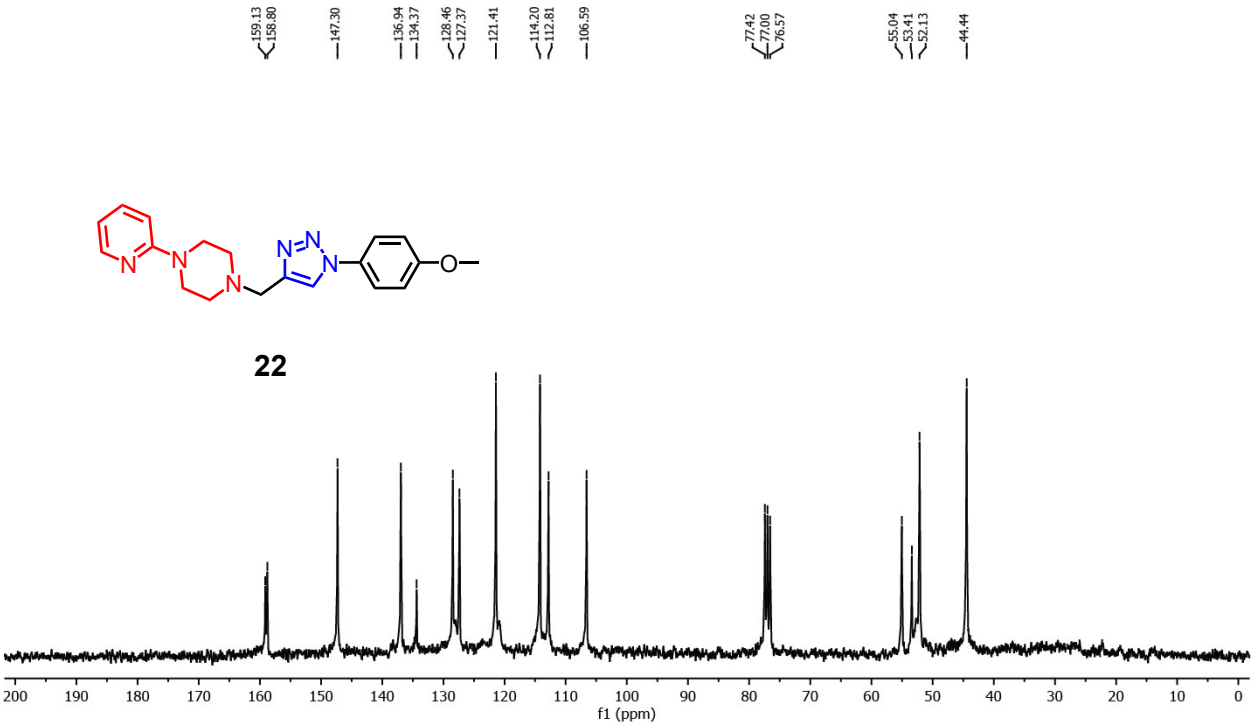


Figure S20. ^{13}C NMR spectrum of compound **22** (100 MHz, $CDCl_3$, 25 °C)

Compound 23

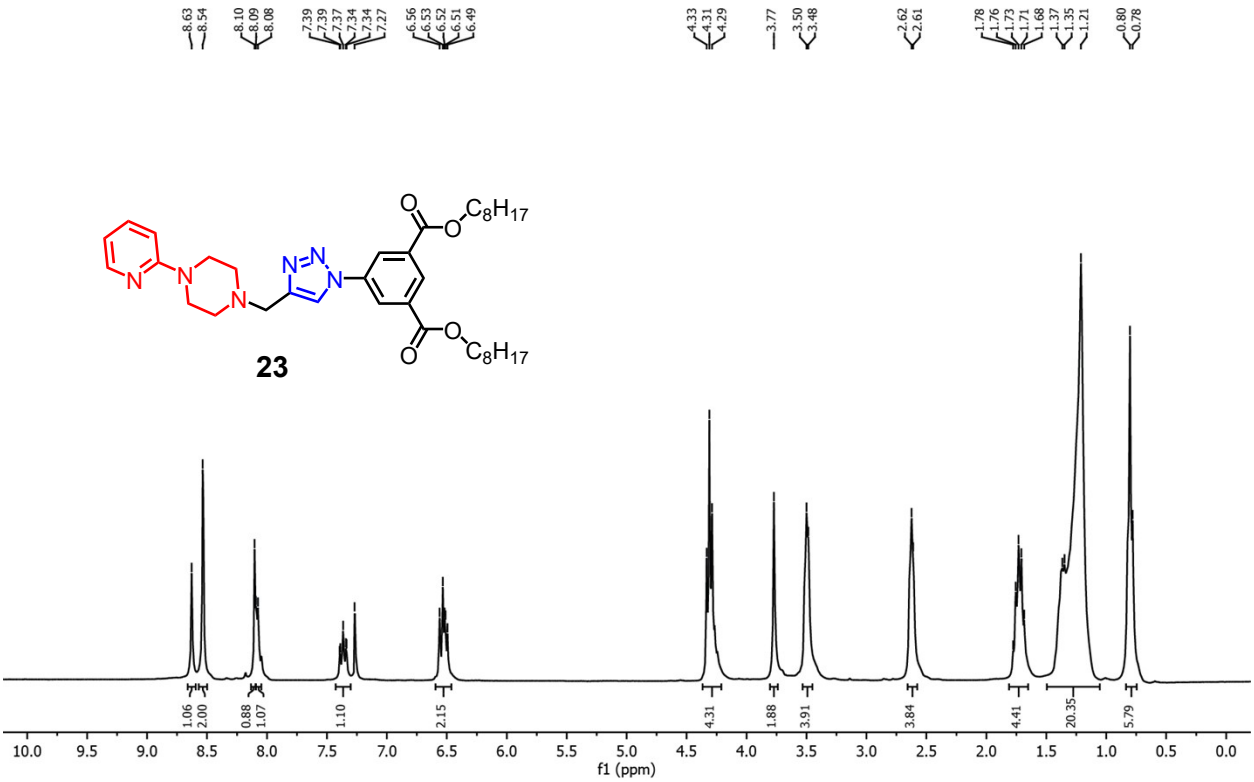


Figure S21. ^{1}H NMR spectrum of compound **23** (400 MHz, $CDCl_3$, 25 °C)

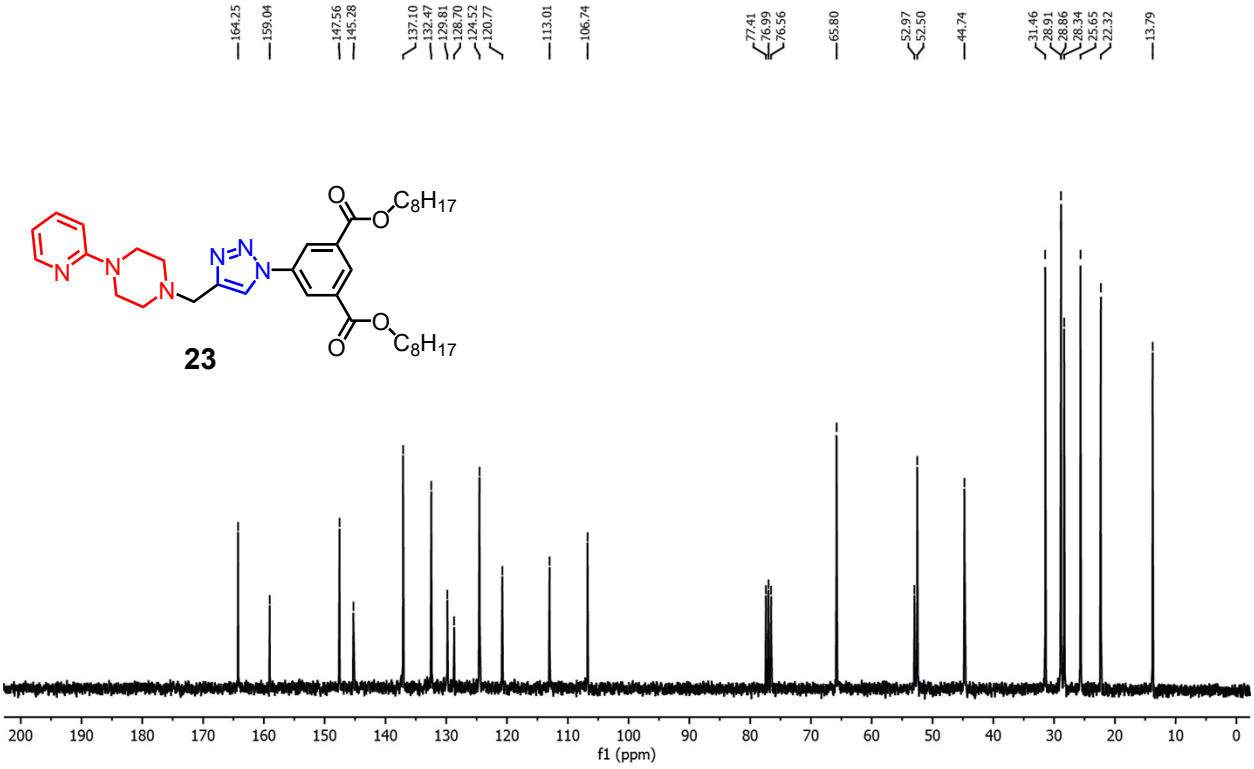
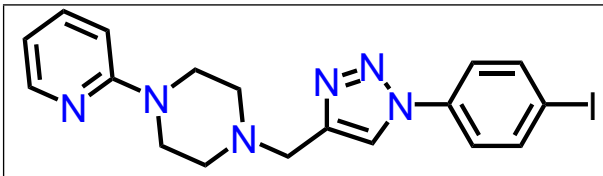
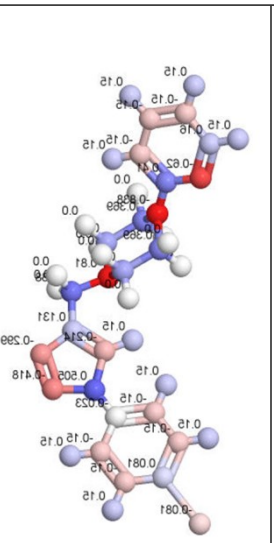
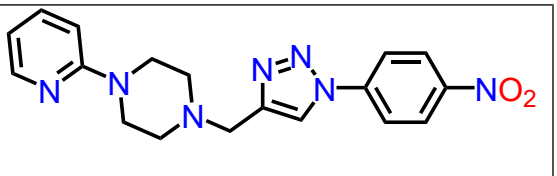


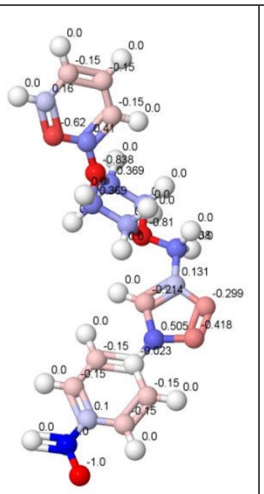
Figure S22. ^{13}C NMR spectrum of compound **23** (100 MHz, $CDCl_3$, 25 °

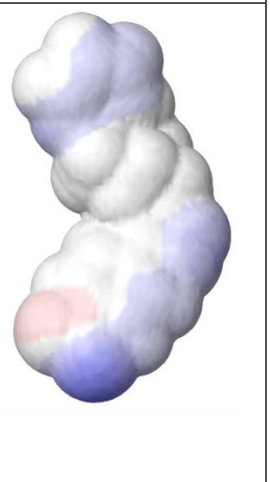




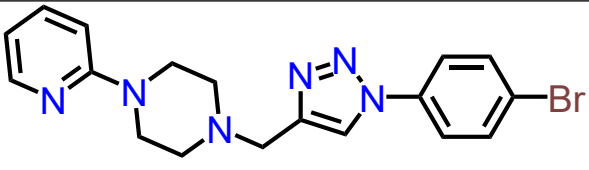
Compound 13

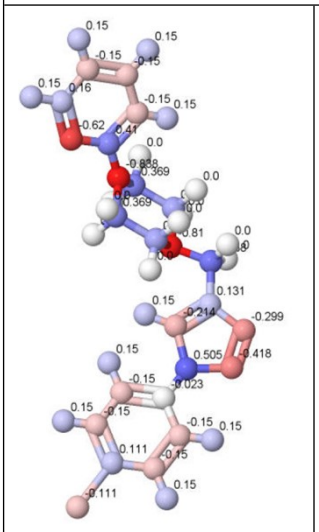


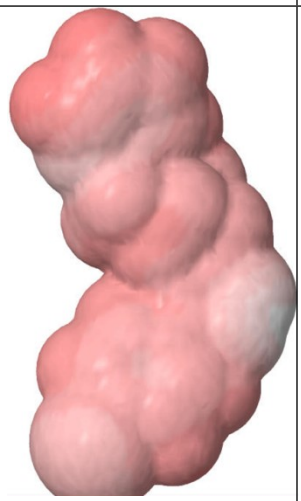




Compound 14







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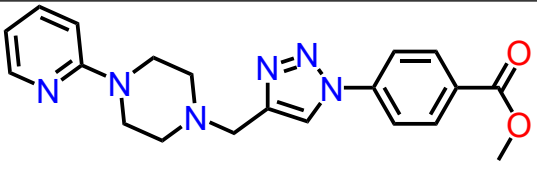
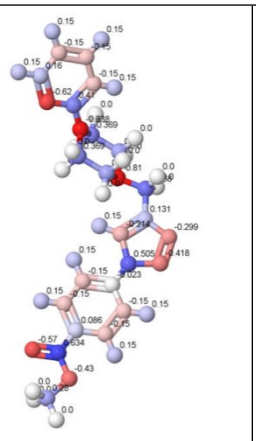
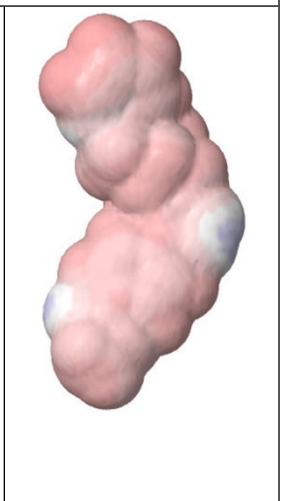
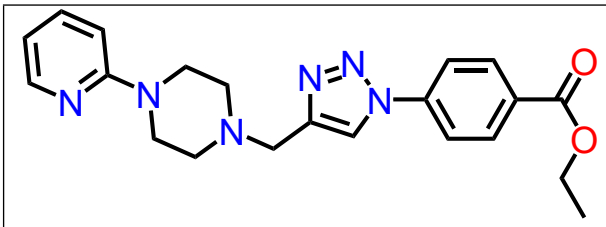
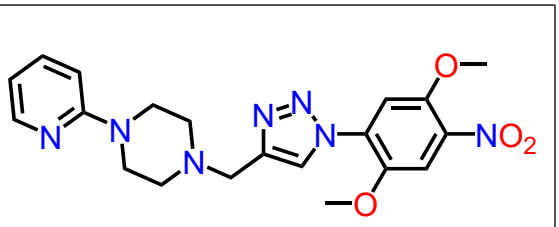


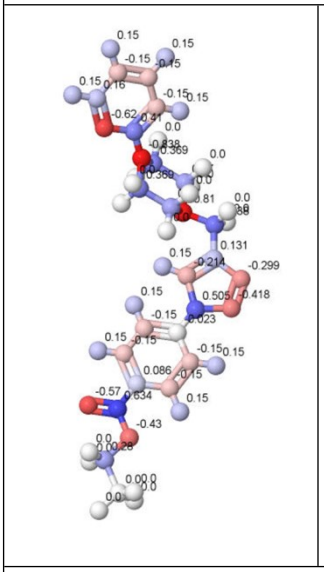


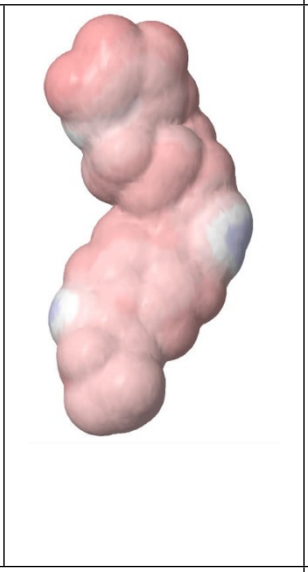


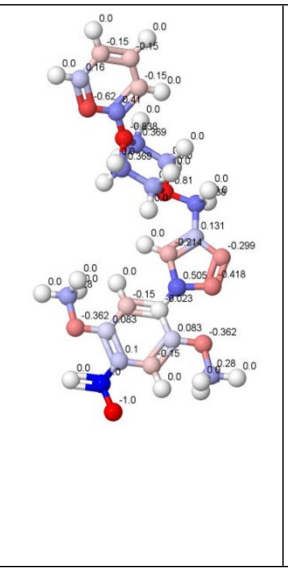
Compound 16

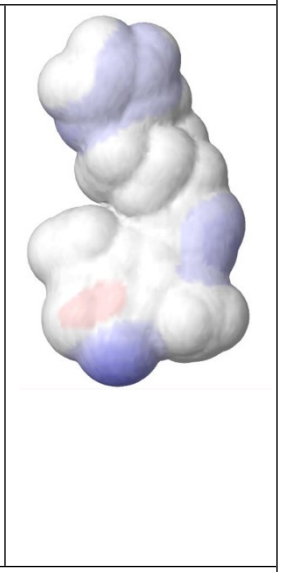






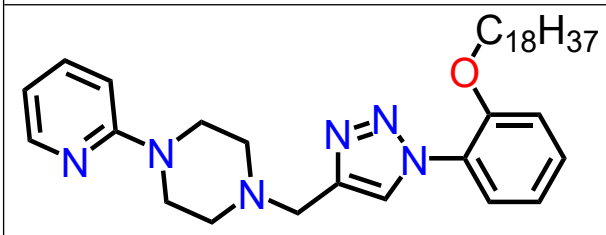


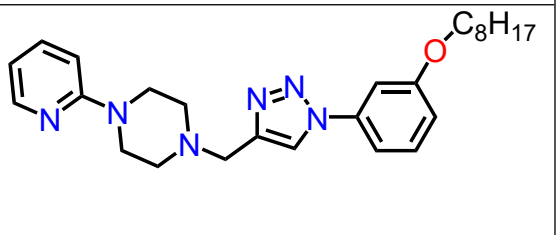


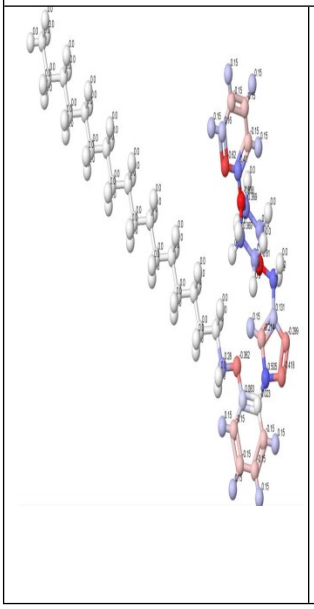


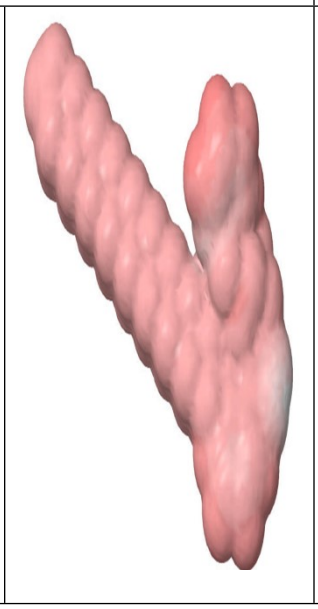
Compound 17

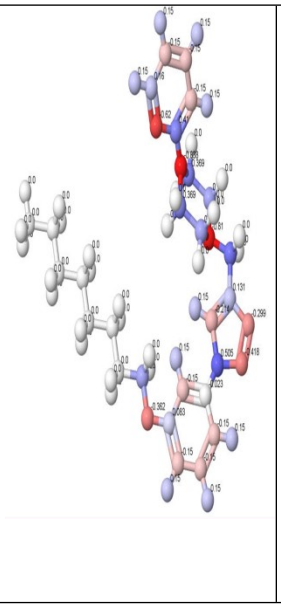
Compound 18

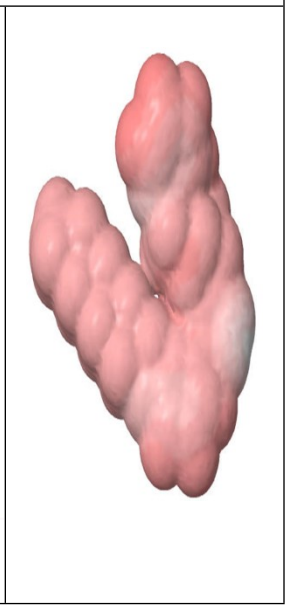


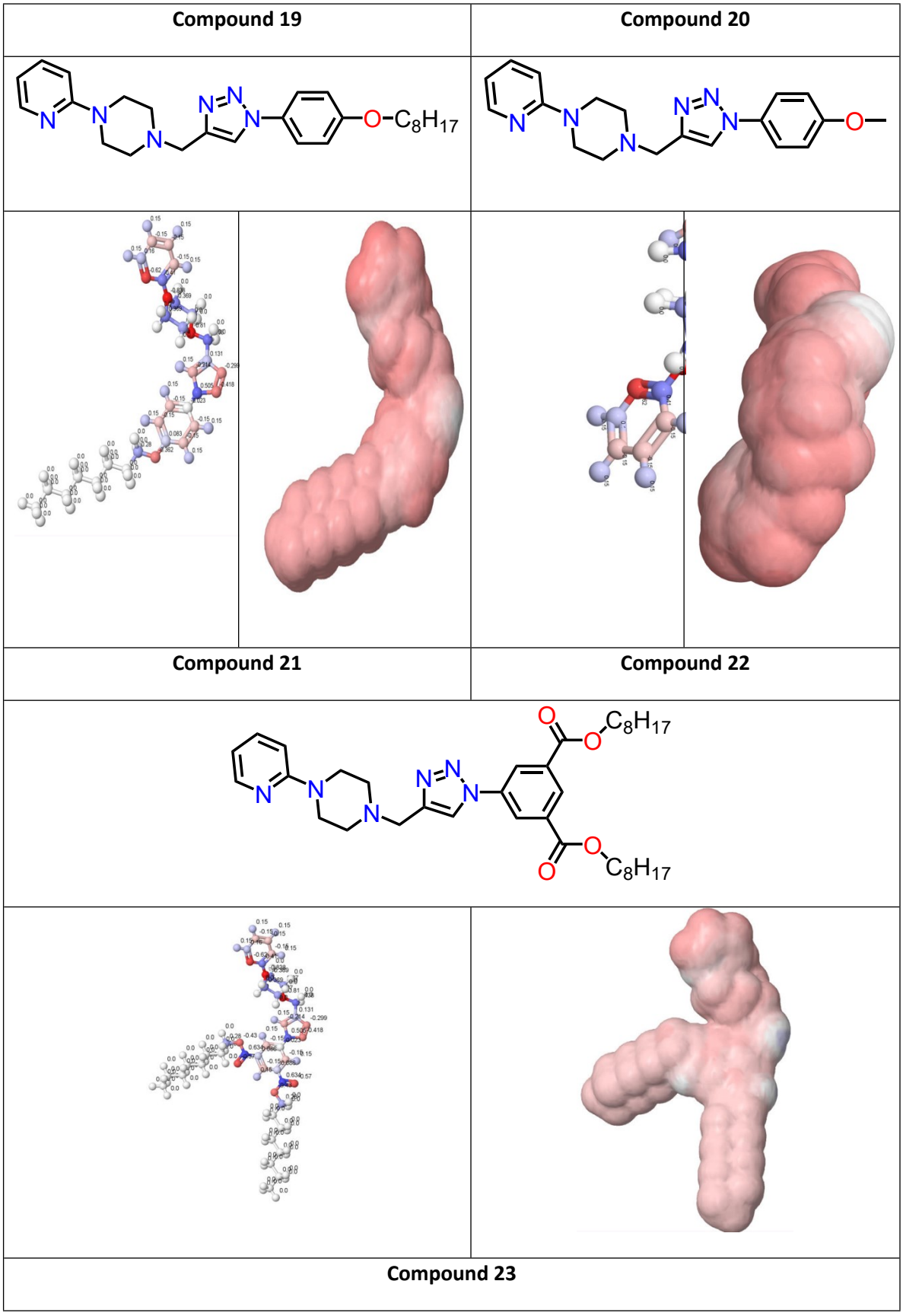












Figuer 23s : Atomic charge calculation for compounds **13-23**.

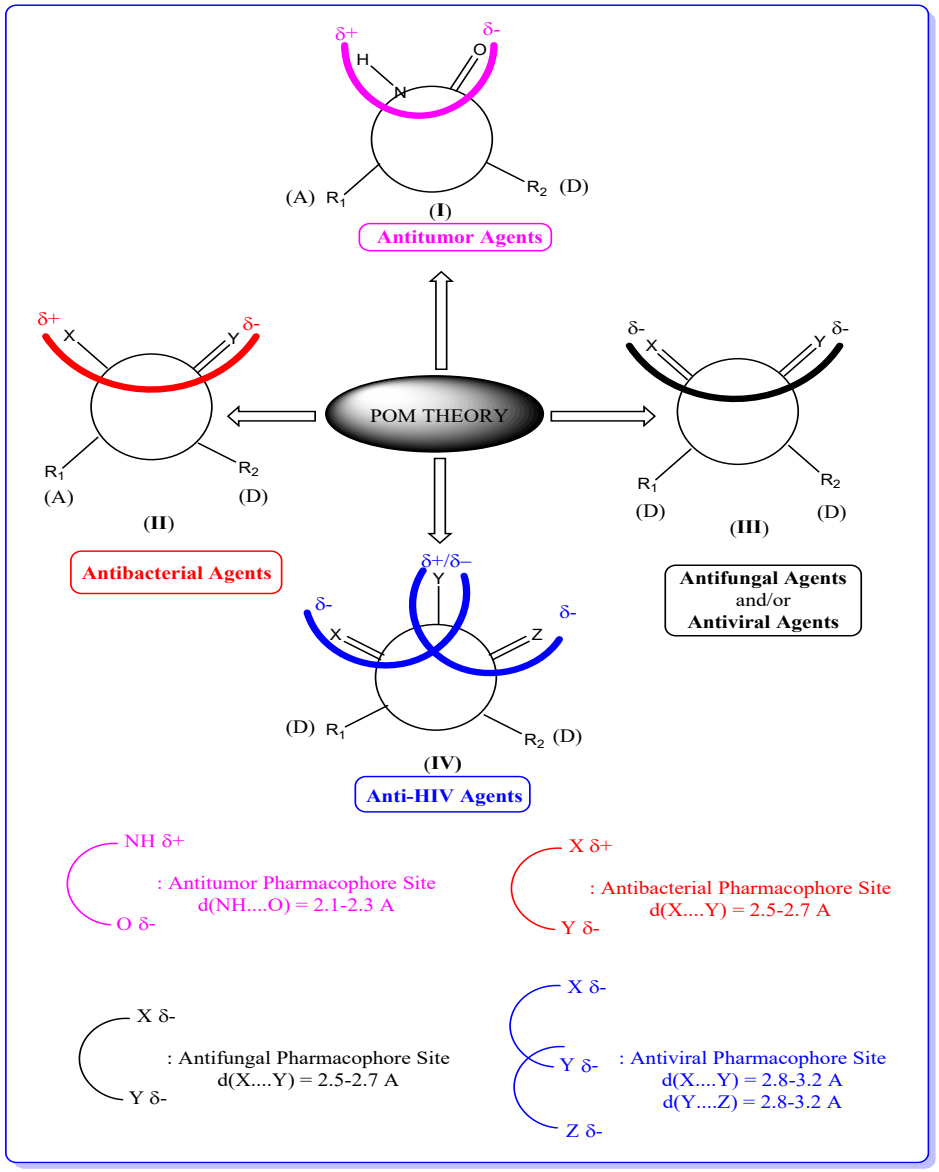


Figure 24s:. The Concept and Applications of POM Theory in the identification and optimization of pharmacophore sites of various classes of drugs, was developed by Prof. T. Ben Hadda (Principal Inventor of POM Theory) in collaboration with NCI and TAACF of theUSA.