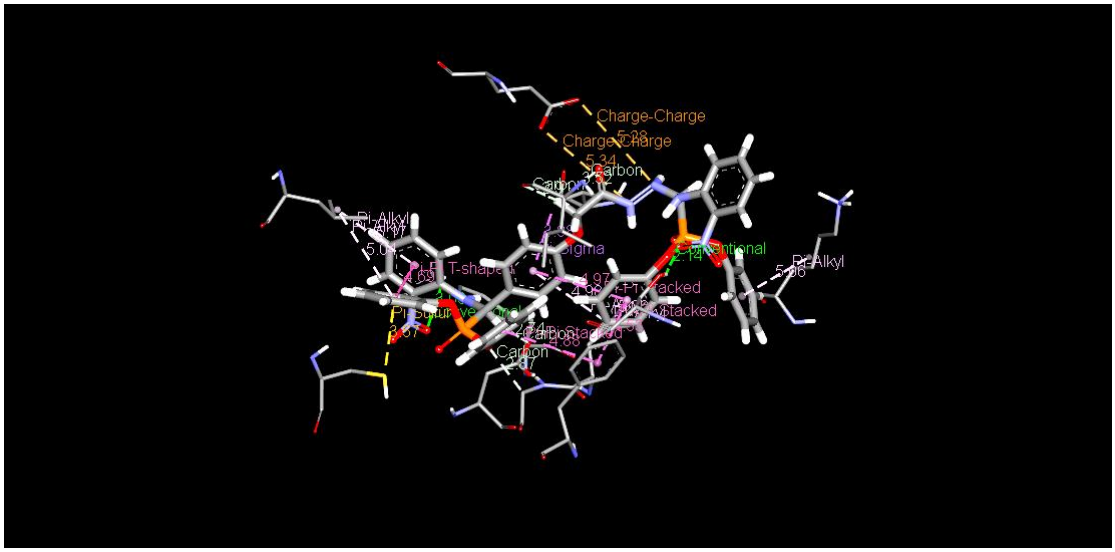
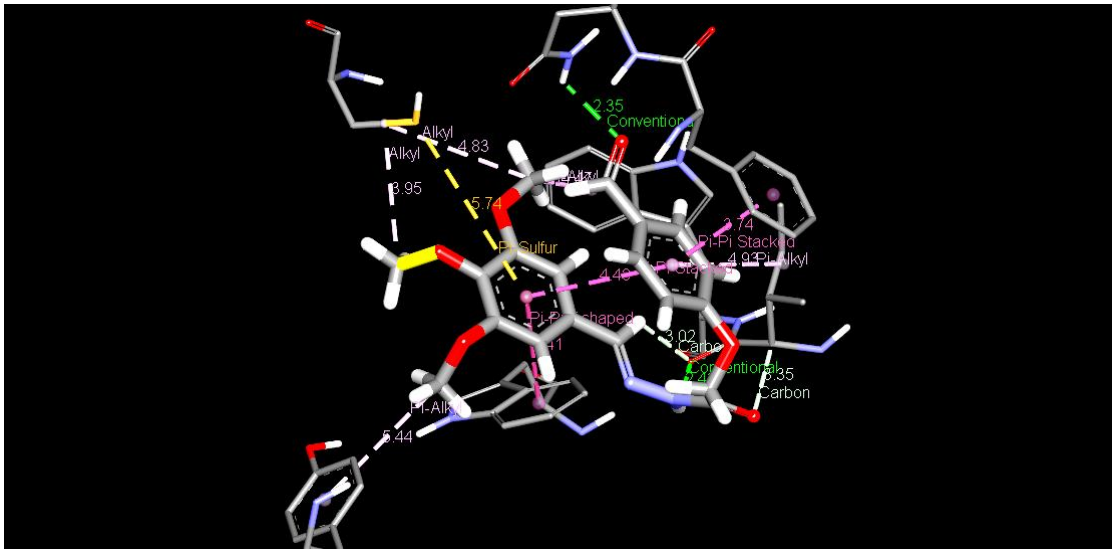
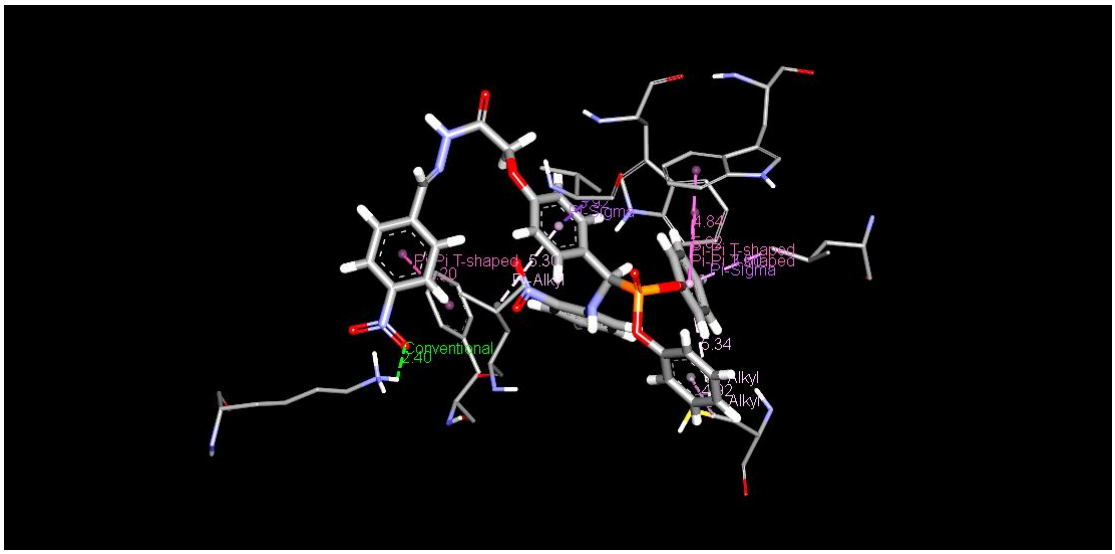
Supplementary materials



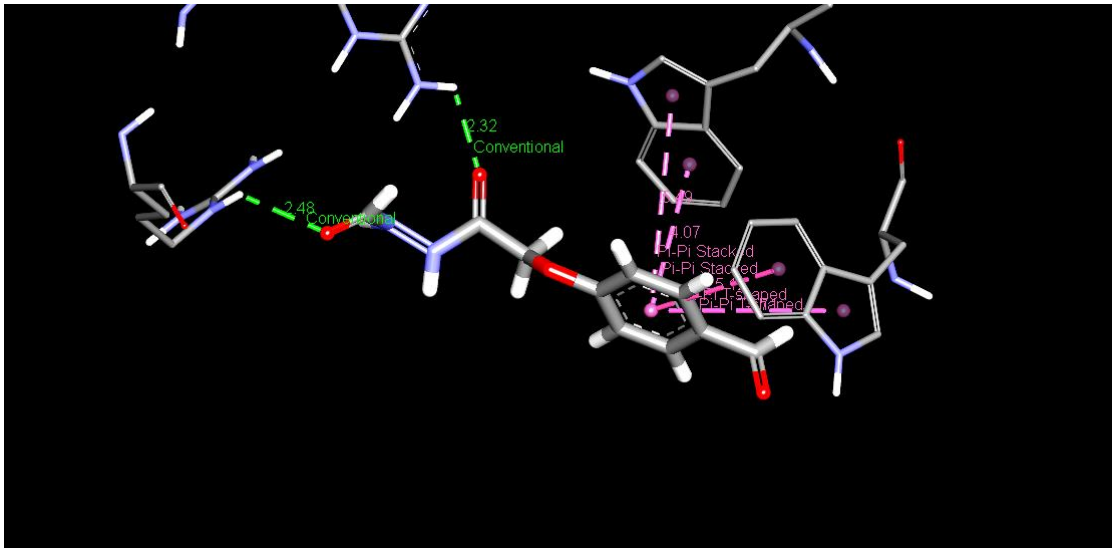
Compound **7b**



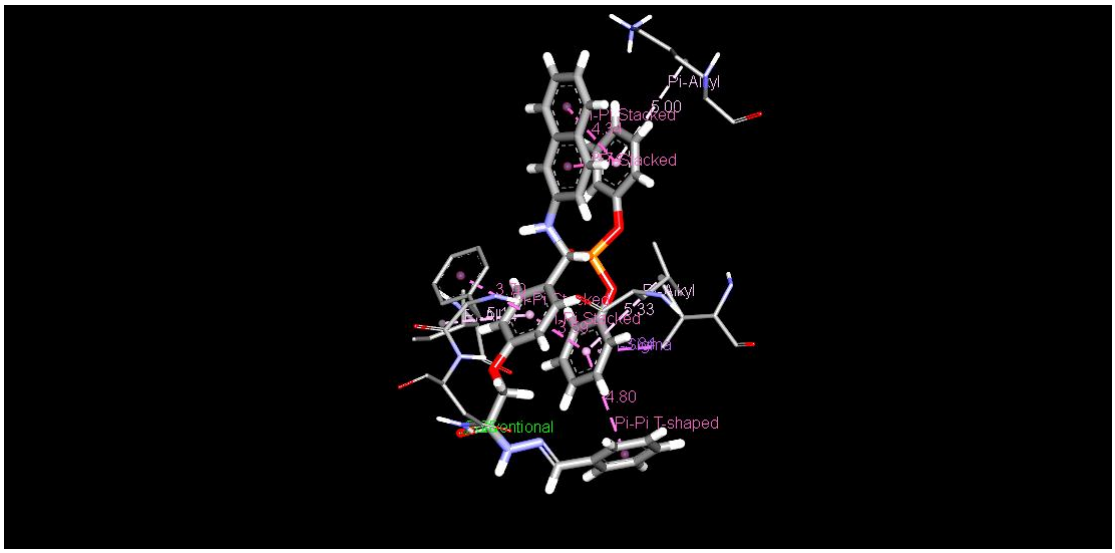
Compound **4c**



Compound **5k**

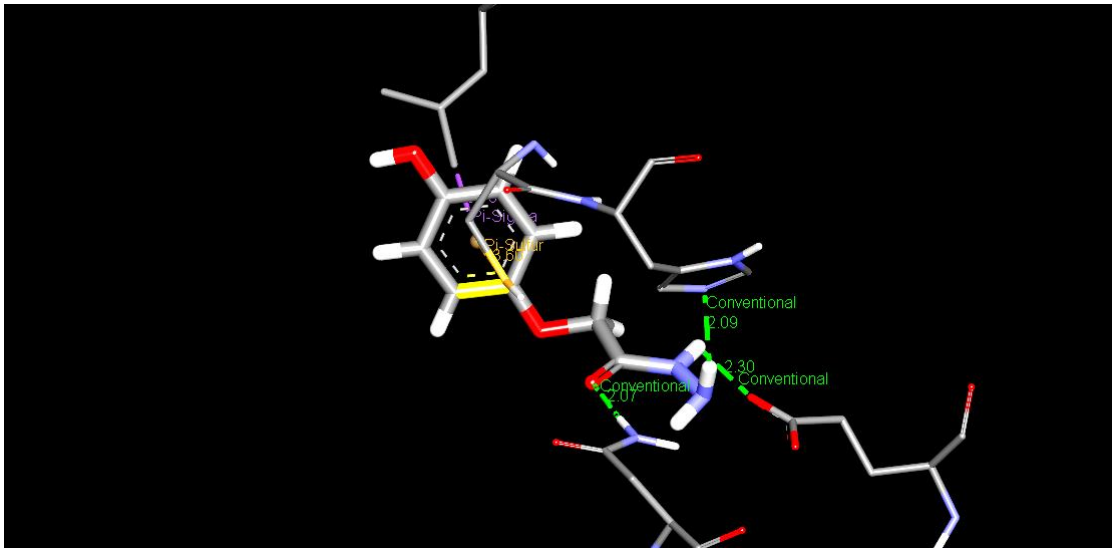


Compound **6**

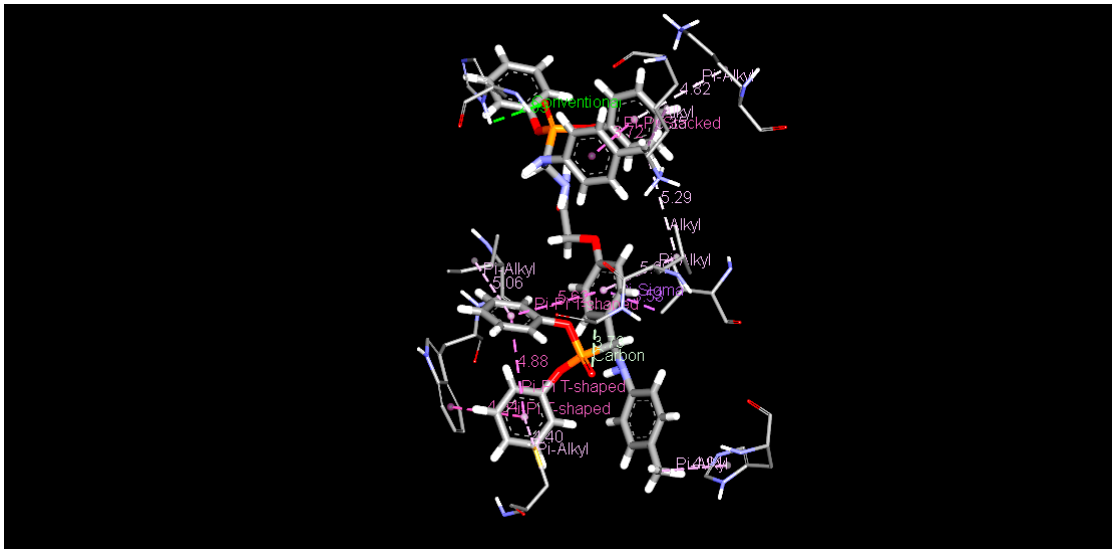


Compound **5a**

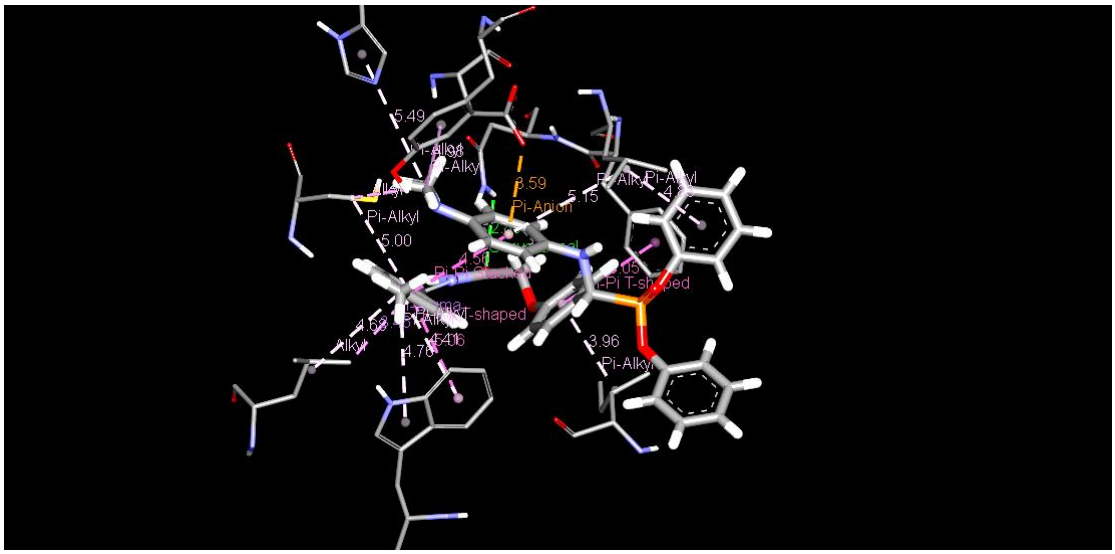
Figure S1. Show the 3D interactions between (1AN5) and the studied compounds (**7b**, **4c**, **5k**, **6**, and **5a**, respectively).



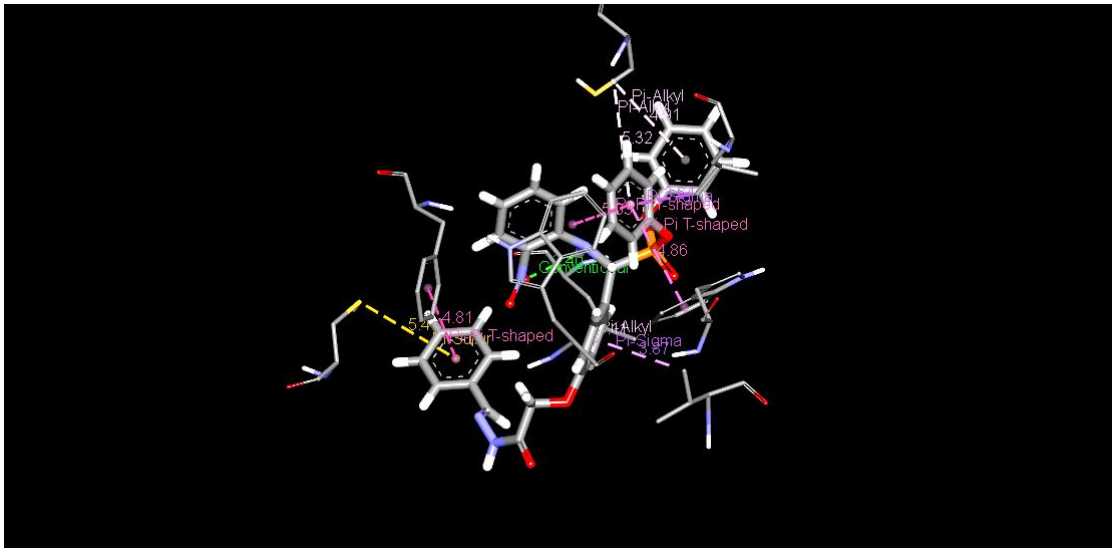
Compound **3**



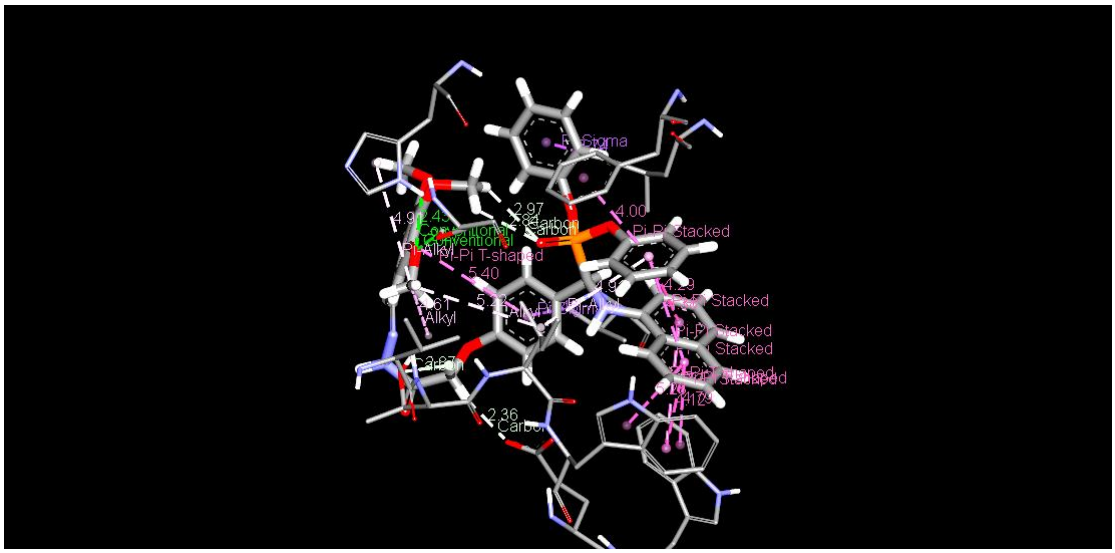
Compound **7c**



Compound **5f**

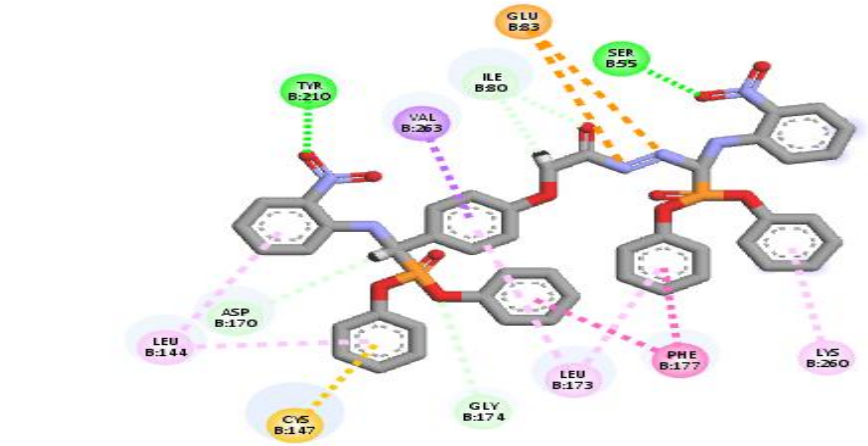


Compound **5b**



Compound **5g**

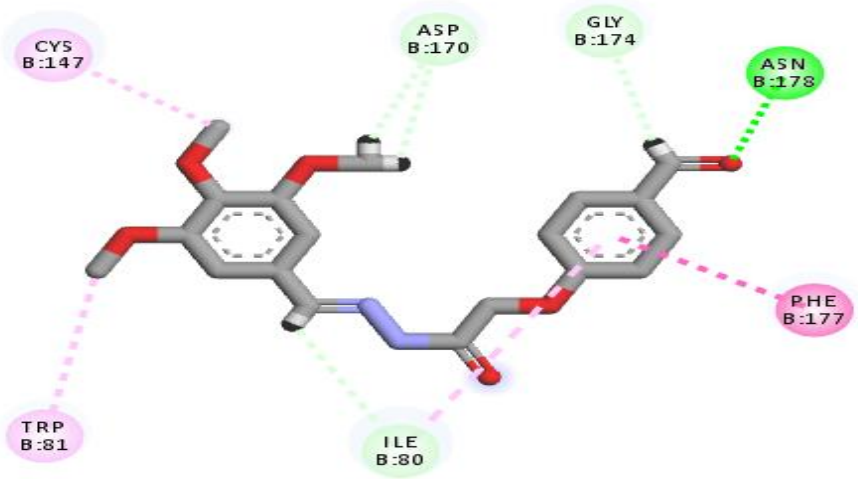
Figure S2. Show the 3D interactions between (1AN5) and the studied compounds (**3**, **7c**, **5f**, **5b**, and **5g**, respectively).



Interactions

- Attractive Charge
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked
- Pi-Alkyl

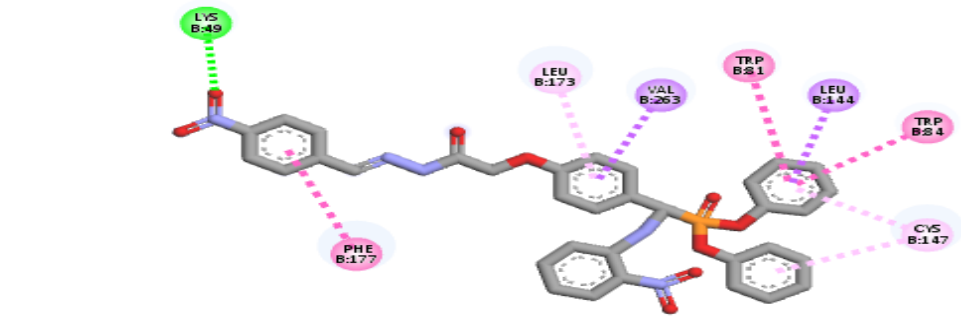
Compound **7b**



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl

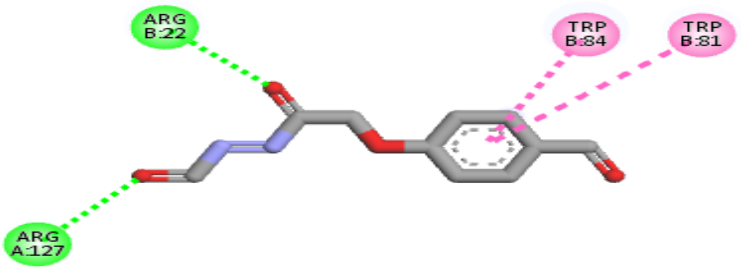
Compound **4c**



Interactions

Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi T-shaped
Pi-Alkyl

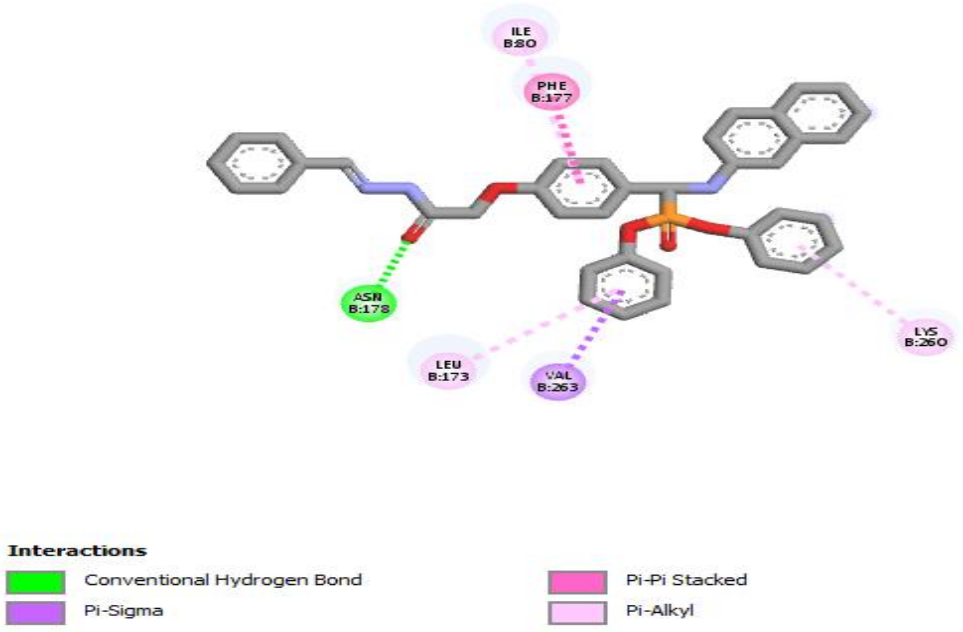
Compound **5k**



Interactions

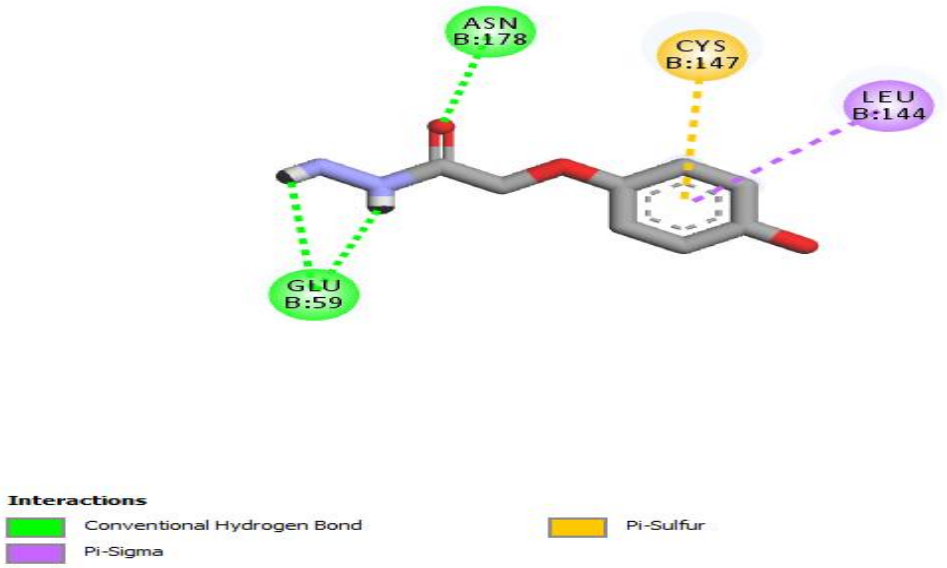
Conventional Hydrogen Bond
Pi-Pi Stacked
Pi-Pi T-shaped

Compound **6**

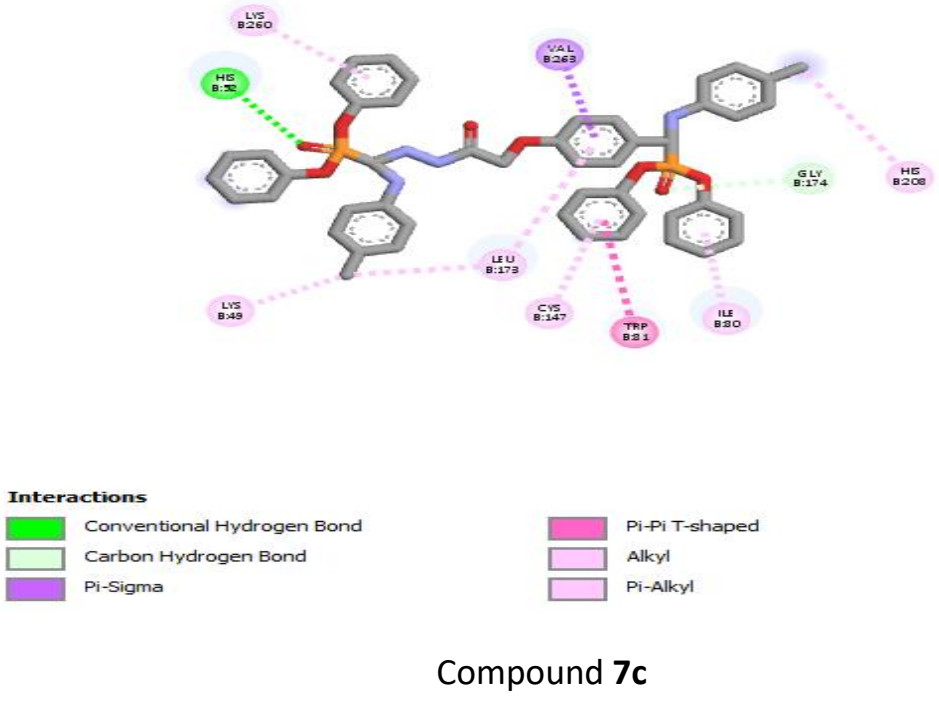


Compound **5a**

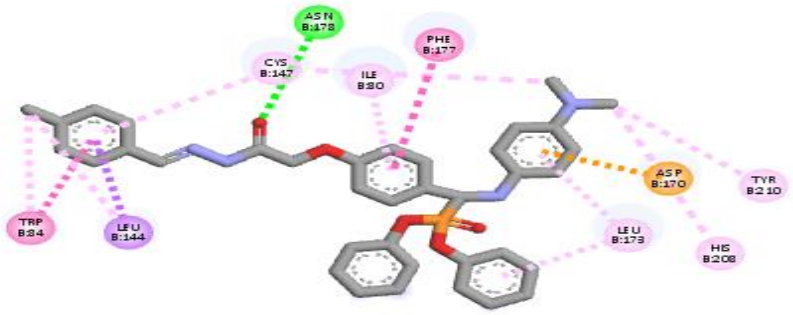
Figure S3. Show the 2D interactions between (1AN5) and the studied compounds (**7b**, **4c**, **5k**, **6**, and **5a**, respectively).



Compound **3**


LYS B:260
VAL B:263
HIS B:32
GLY B:174
HIS B:208
LEU B:173
LYS B:49
CYS B:147
TRP B:31
ILE B:30
Interactions
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

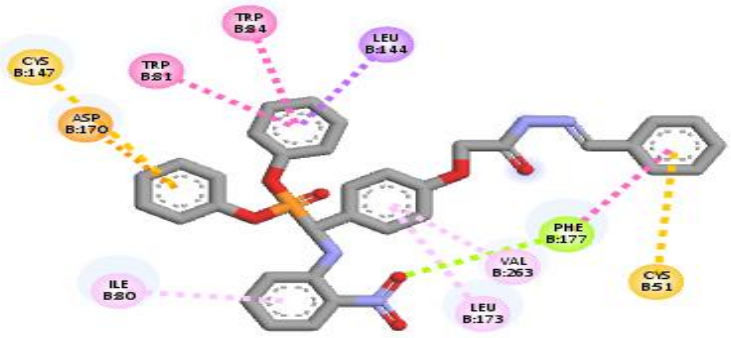
Compound **7c**



Interactions

- Conventional Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl

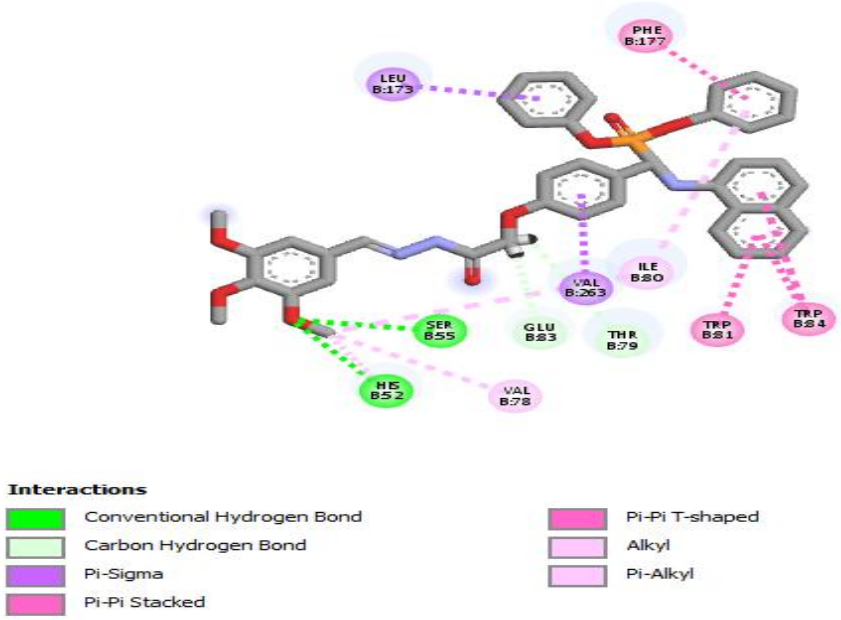
Compound **5f**



Interactions

- Pi-Anion
- Pi-Sigma
- Pi-Sulfur
- Pi-Lone Pair
- Pi-Pi T-shaped
- Pi-Alkyl

Compound **5b**



Compound **5g**

Figure S4. Show the 2D interactions between (1AN5) and the studied compounds (**3**, **7c**, **5f**, **5b**, and **5g**, respectively).

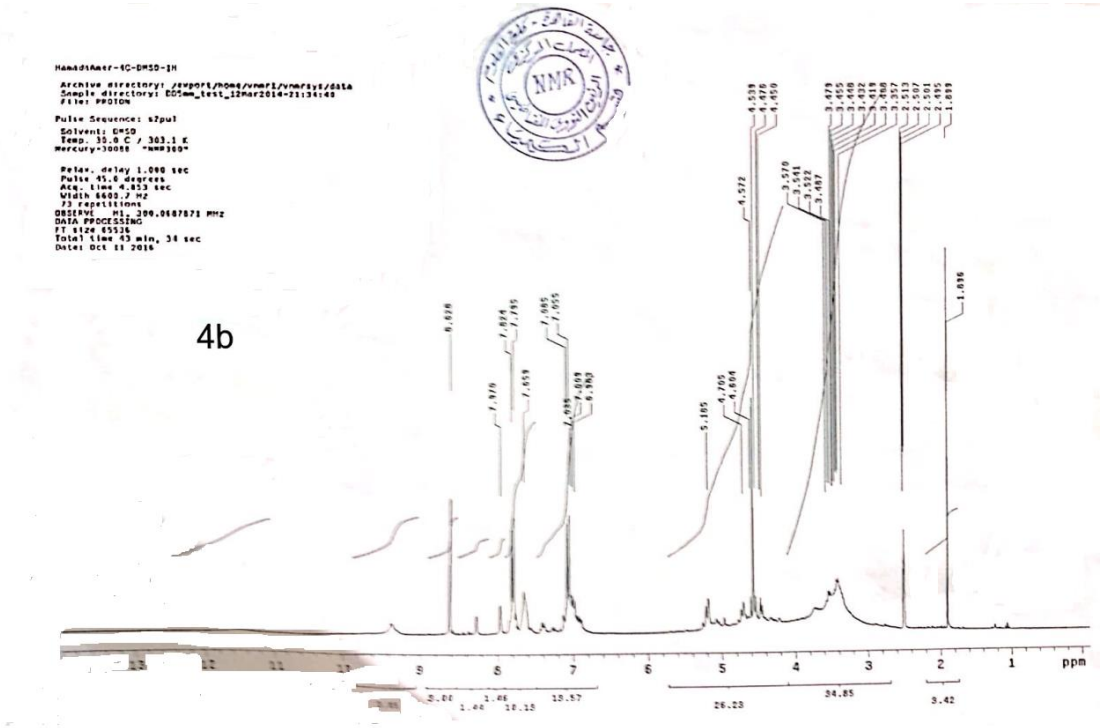


Figure S5. ^{1}H NMR spectrum of compound **4b**

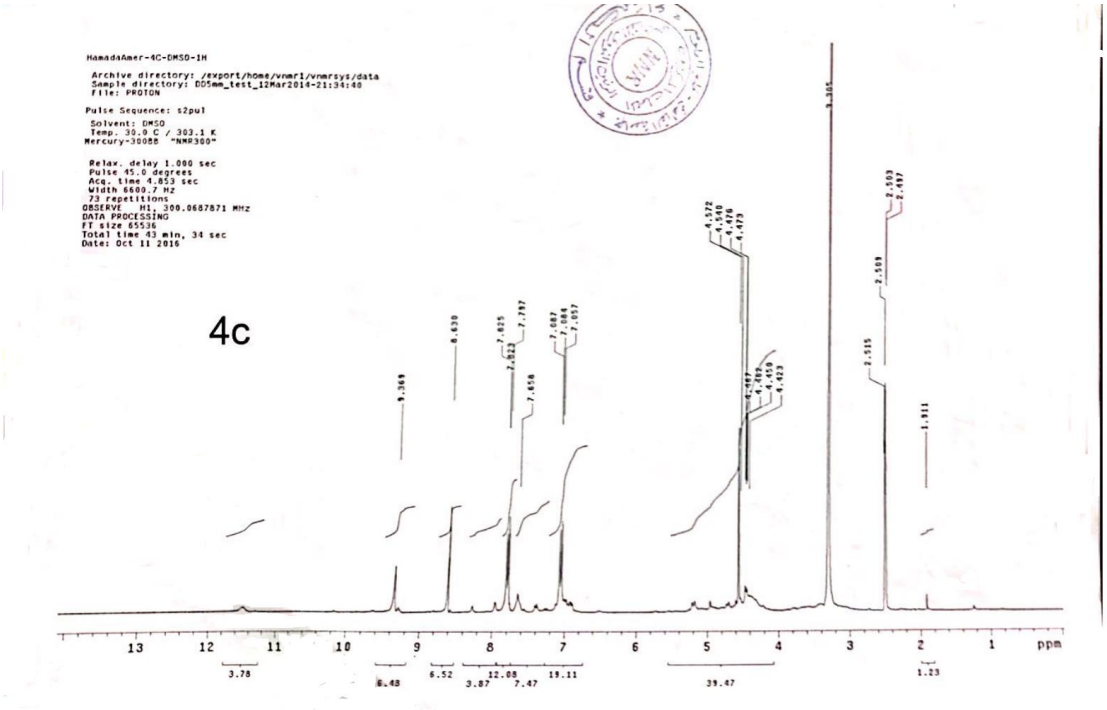


Figure S6. ^{1}H NMR spectrum of compound **4c**

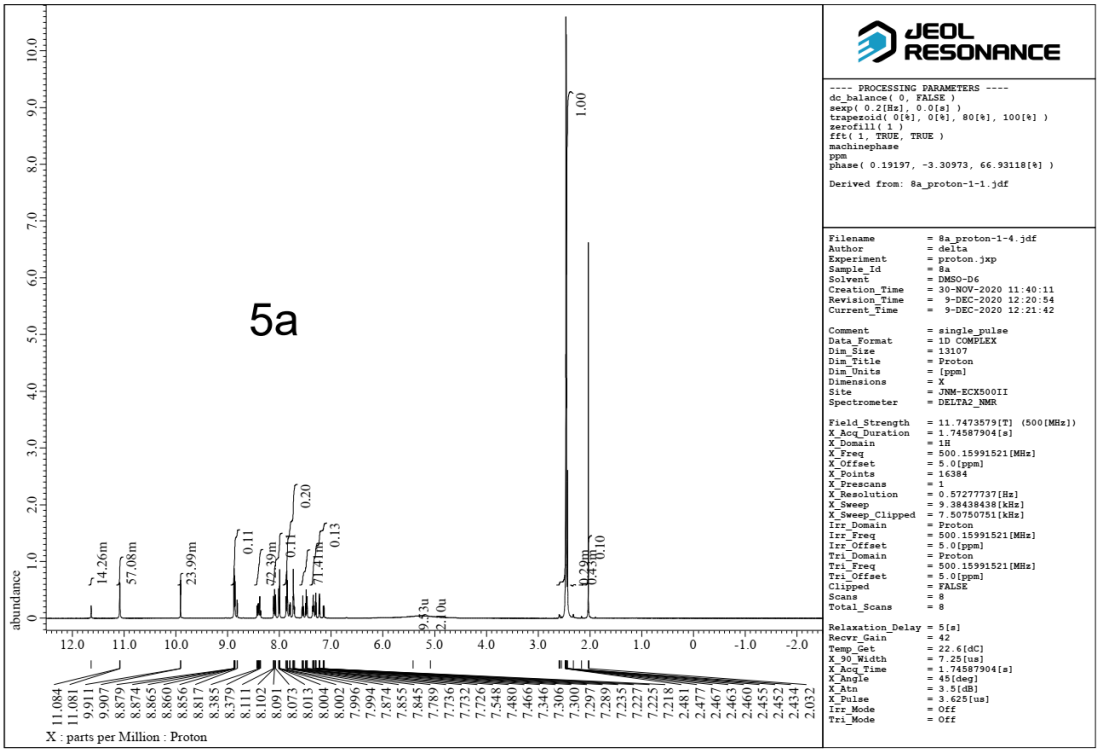


Figure S7. ^{1}H NMR spectrum of compound **5a**

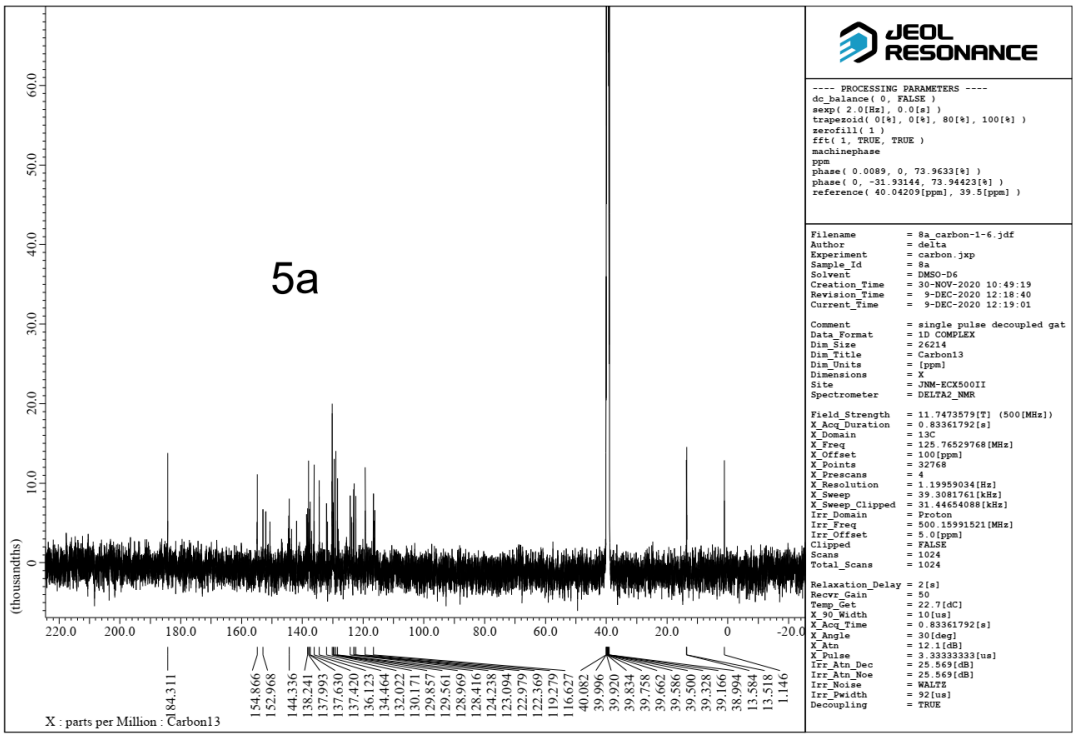


Figure S8. ^{13}C NMR spectrum of compound **5a**

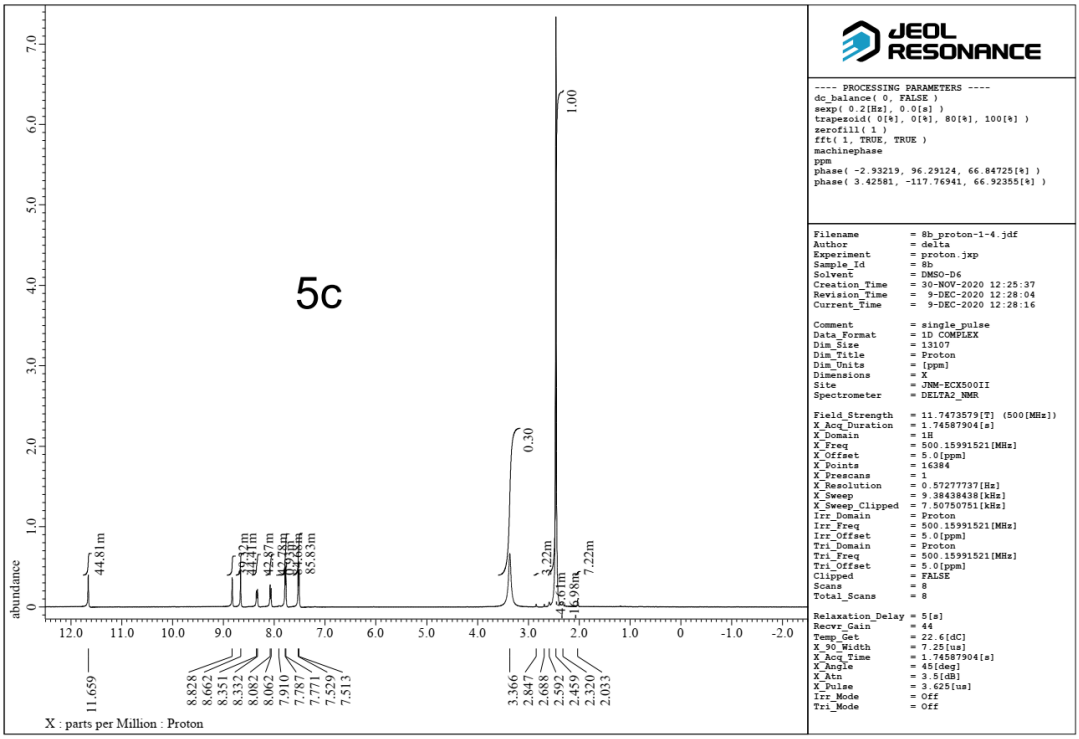


Figure S9. ^{1}H NMR spectrum of compound **5c**

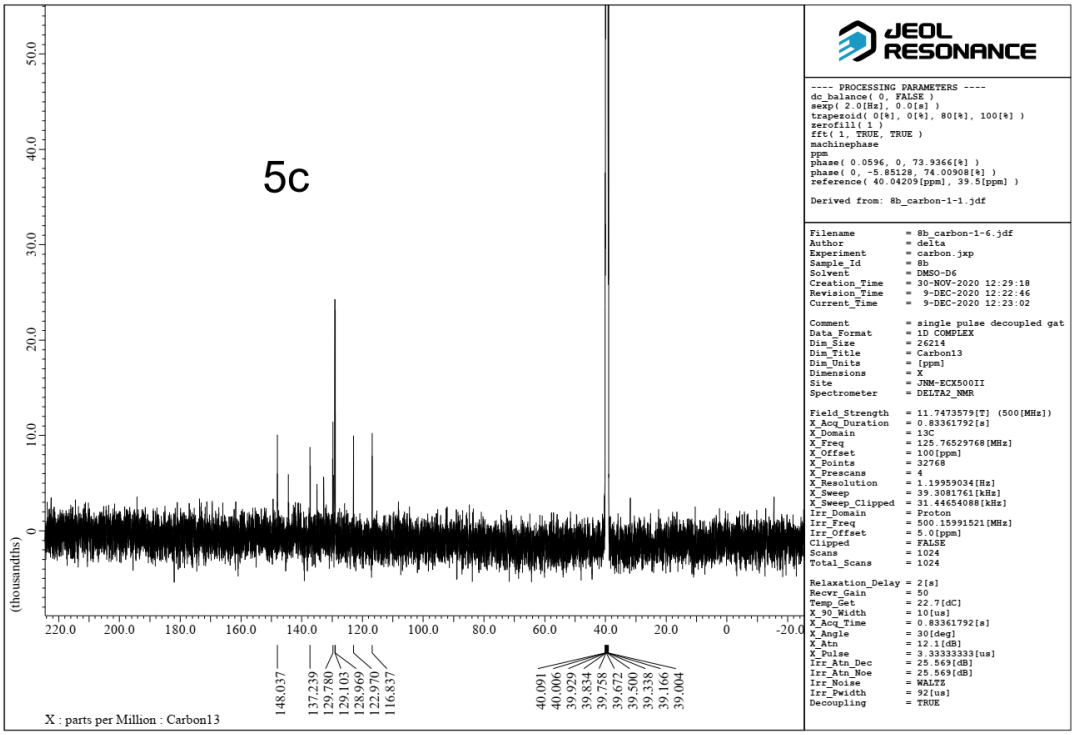


Figure S10. ^{13}C NMR spectrum of compound **5c**

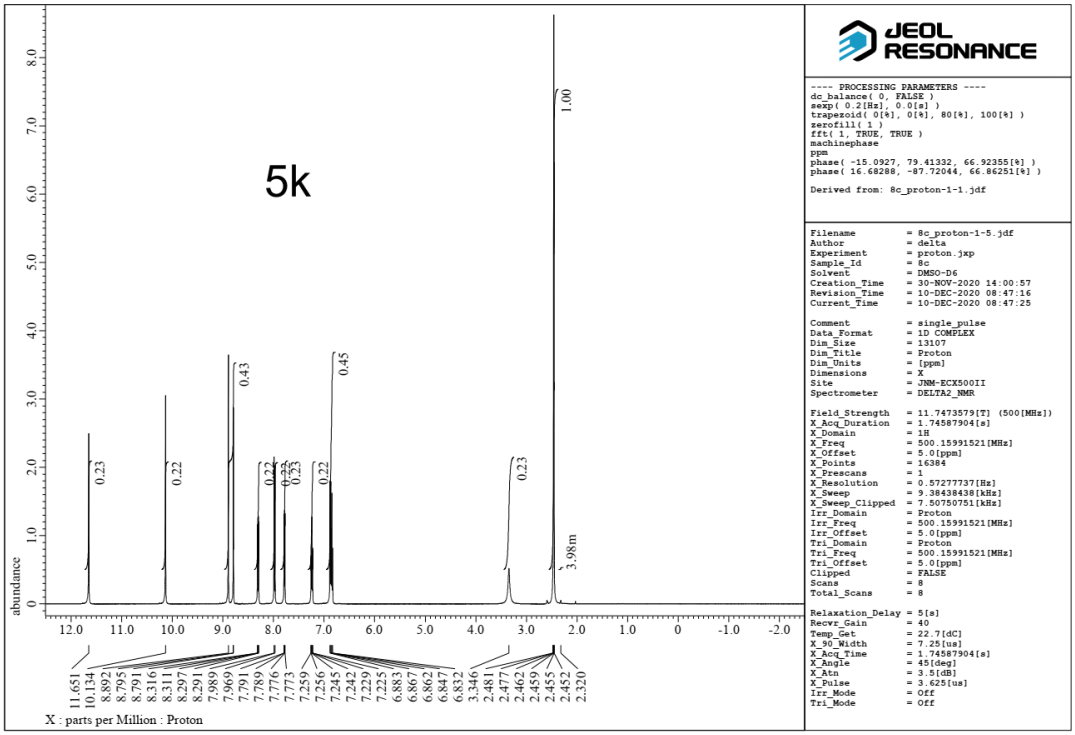


Figure S11. ^{1}H NMR spectrum of compound **5k**

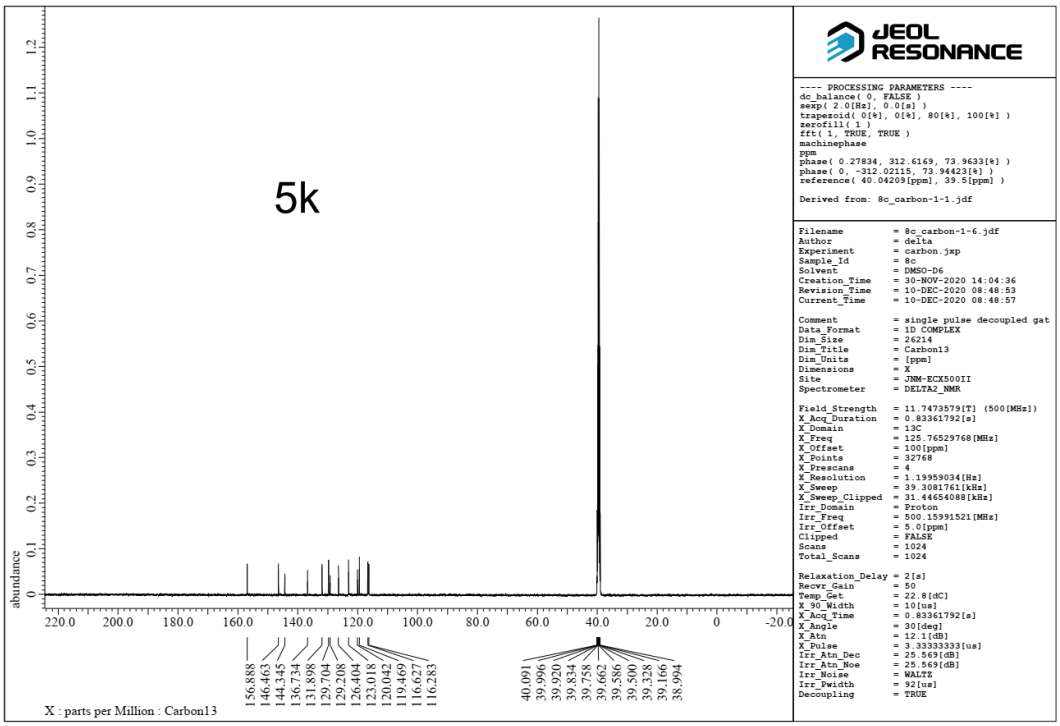


Figure S12. ^{13}C NMR spectrum of compound **5k**

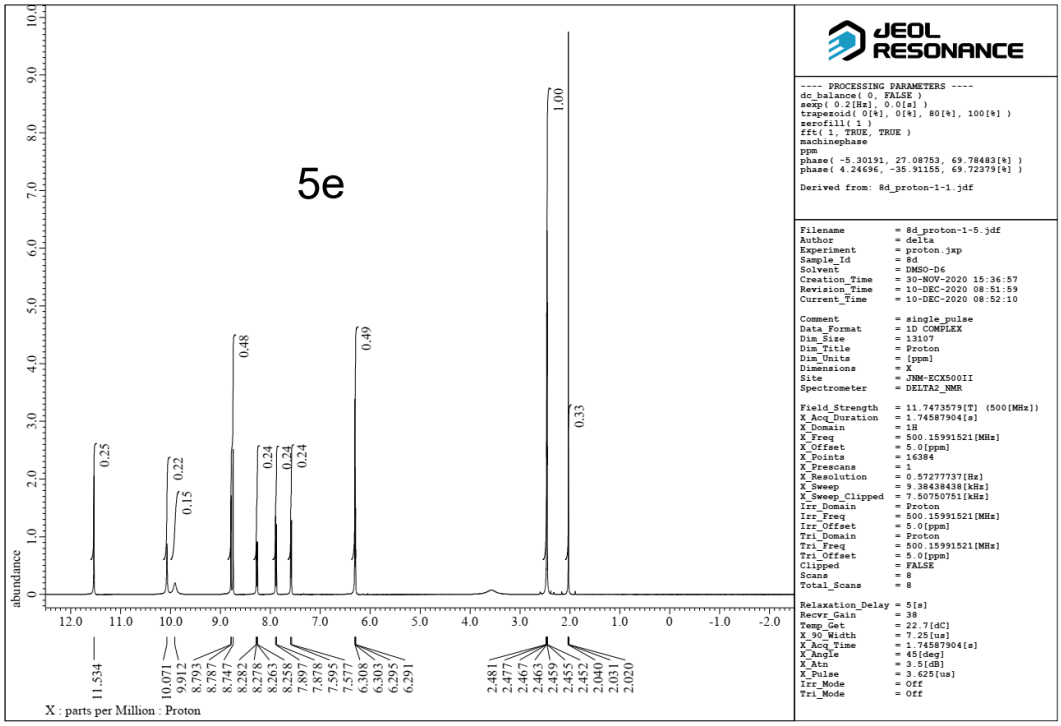


Figure S13. ^{1}H NMR spectrum of compound **5e**

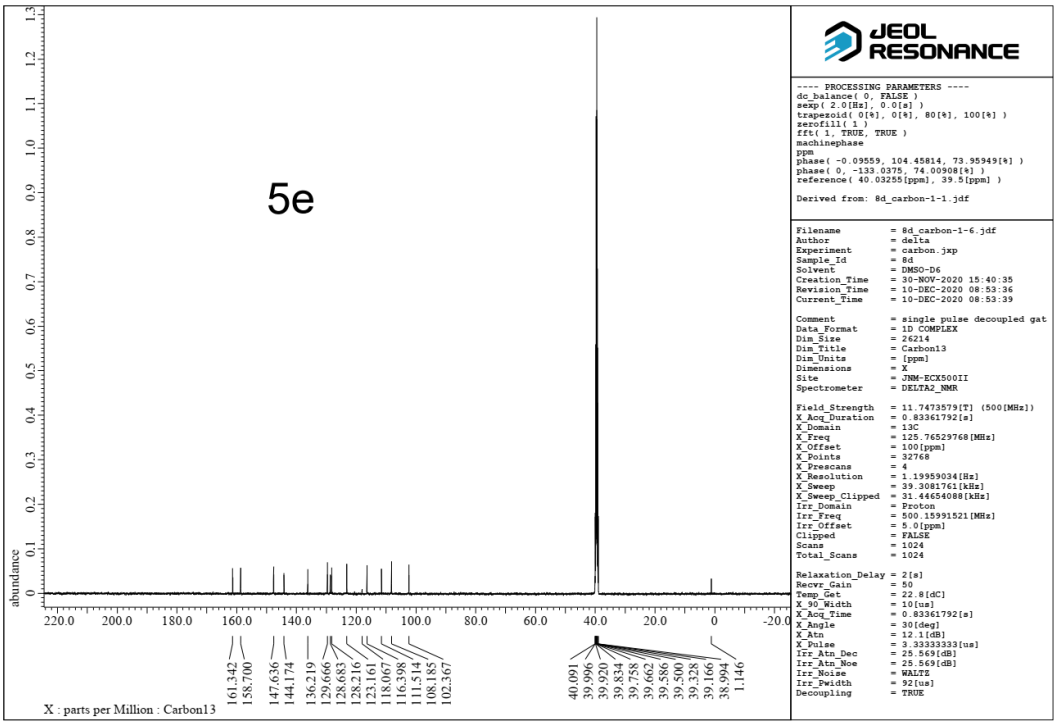


Figure S14. ^{13}C NMR spectrum of compound **5e**

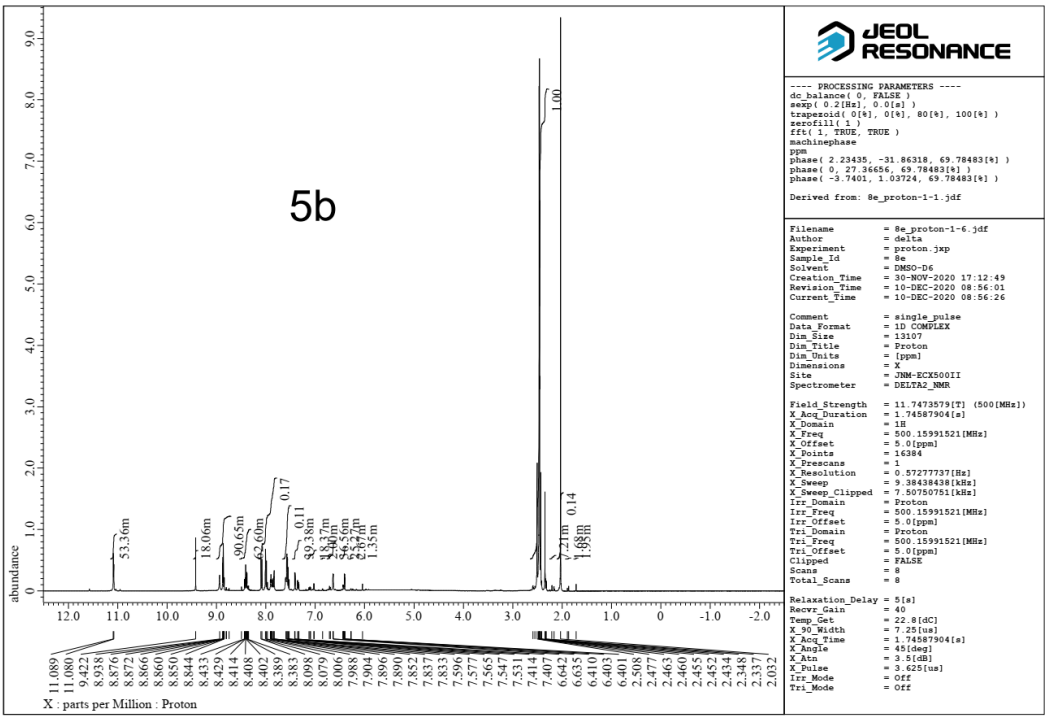


Figure S15. ^{1}H NMR spectrum of compound **5b**

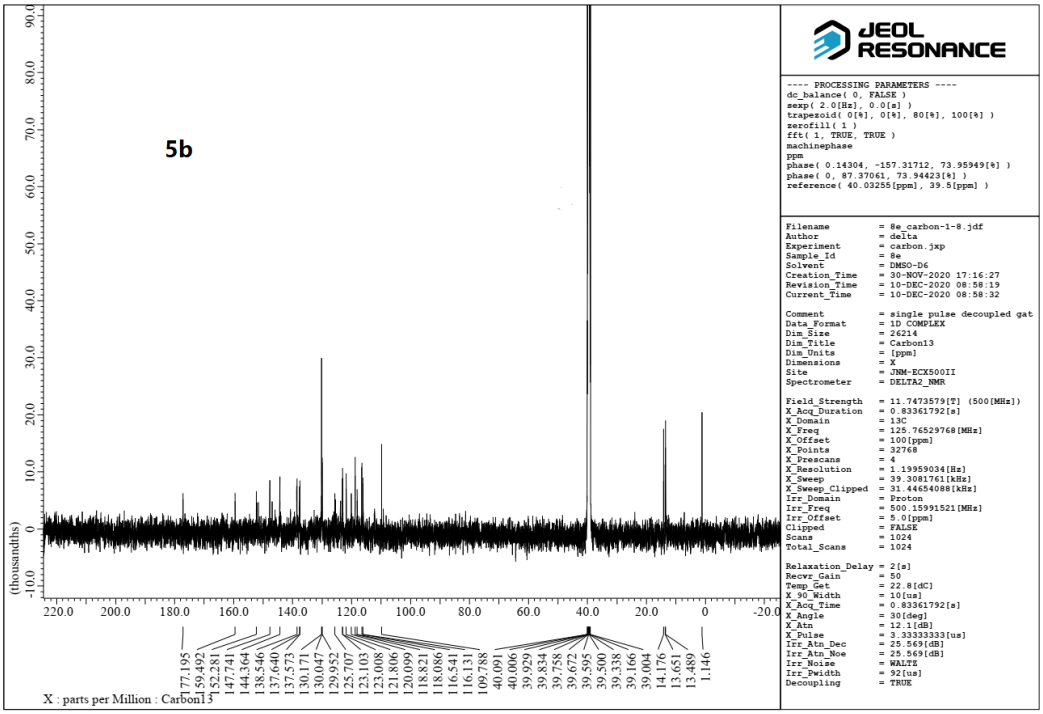


Figure S16. ^{13}C NMR spectrum of compound **5b**

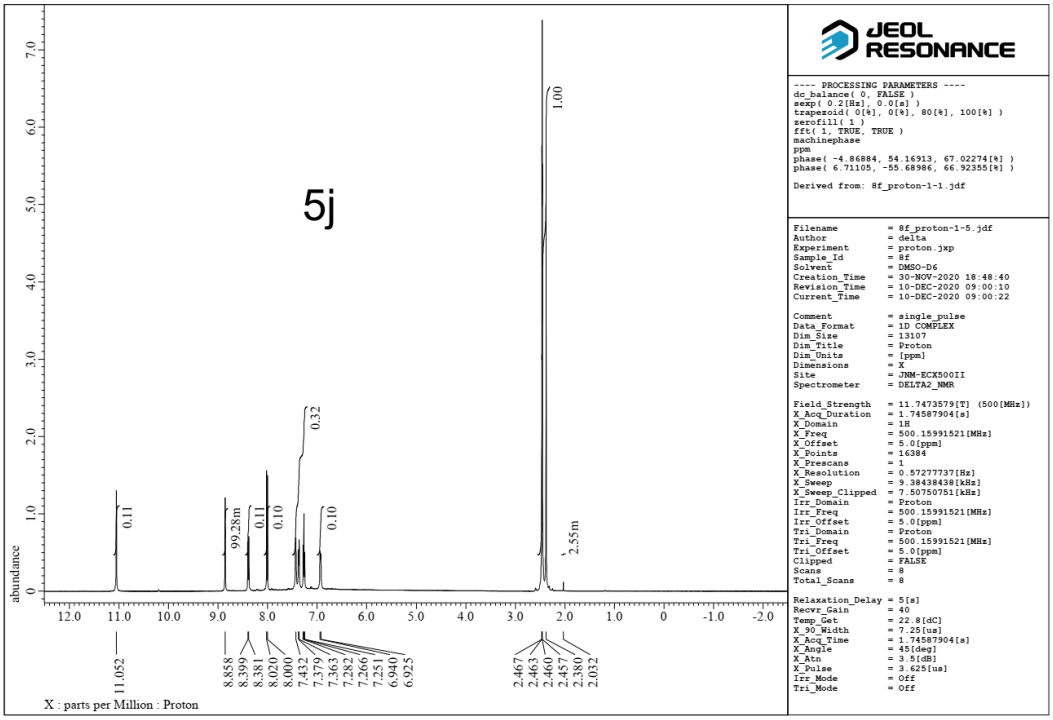


Figure S17. ^{1}H NMR spectrum of compound **5j**

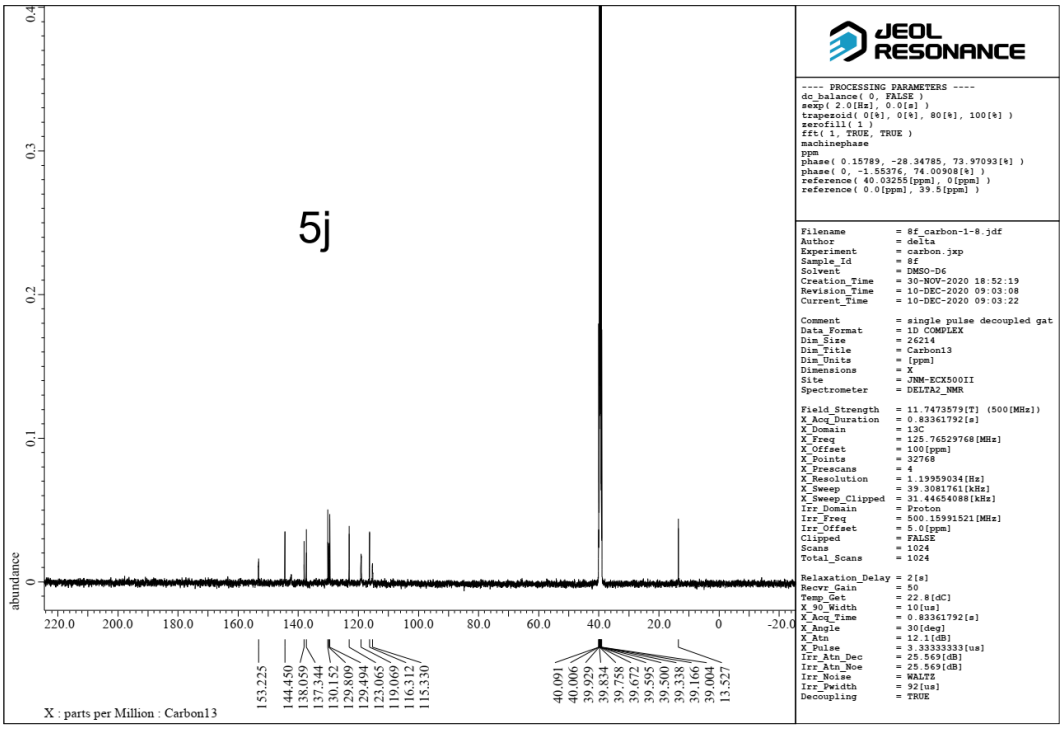


Figure S18. ^{13}C NMR spectrum of compound **5j**

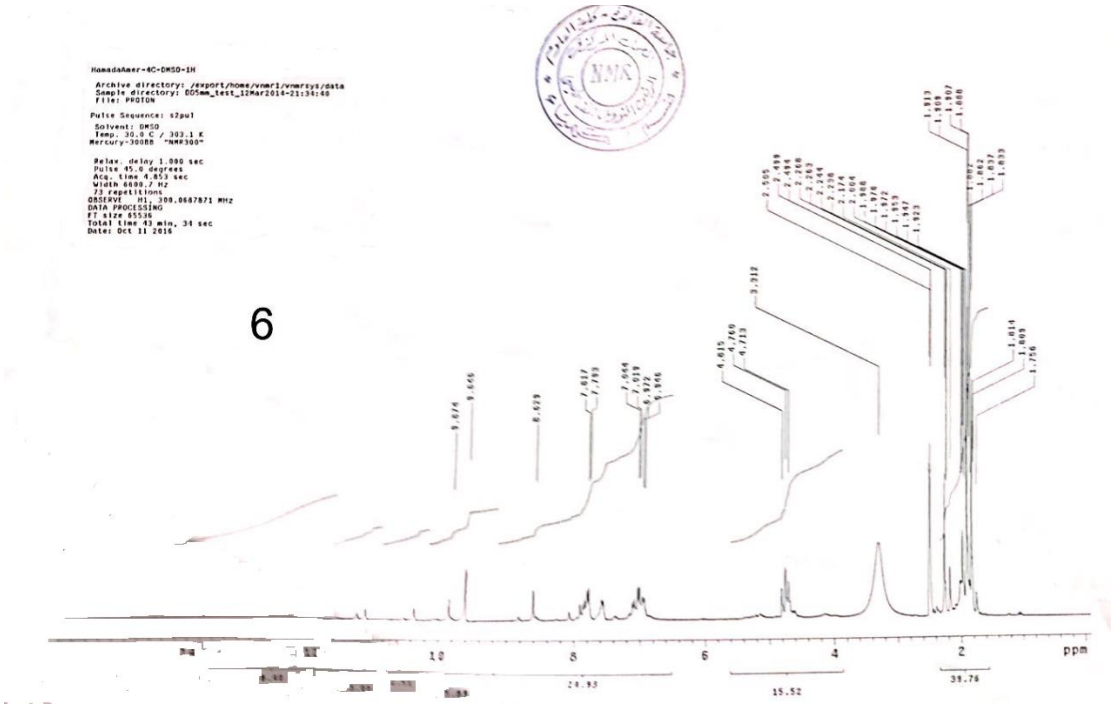


Figure S19. ^{1}H NMR spectrum of compound **6**

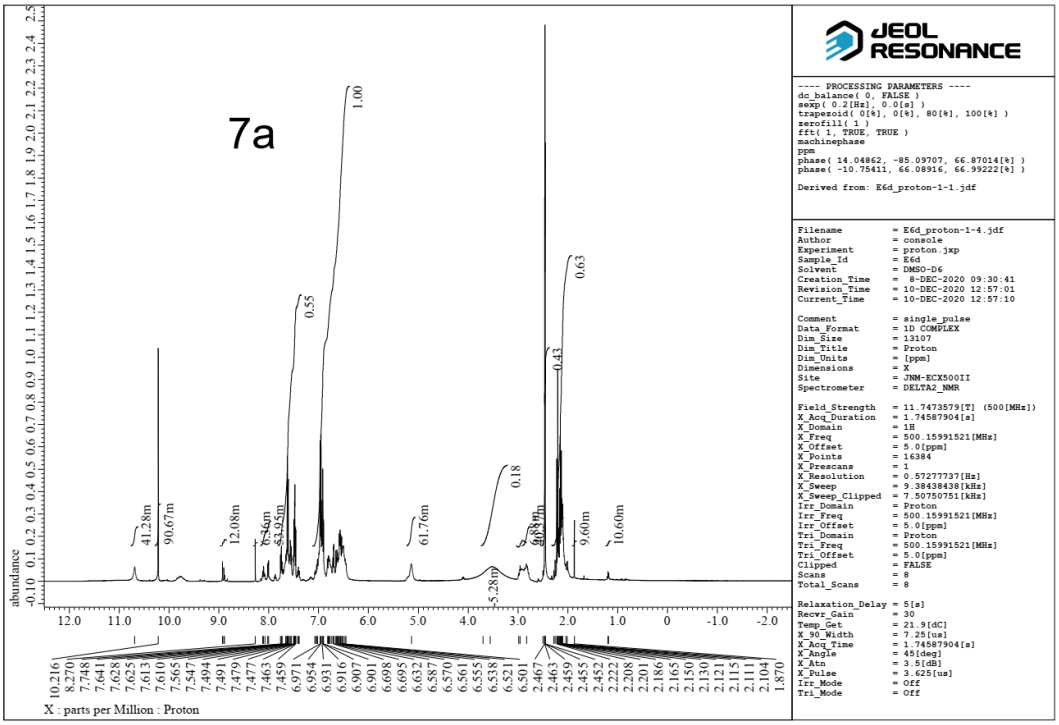


Figure S20. ^{1}H NMR spectrum of compound **7a**

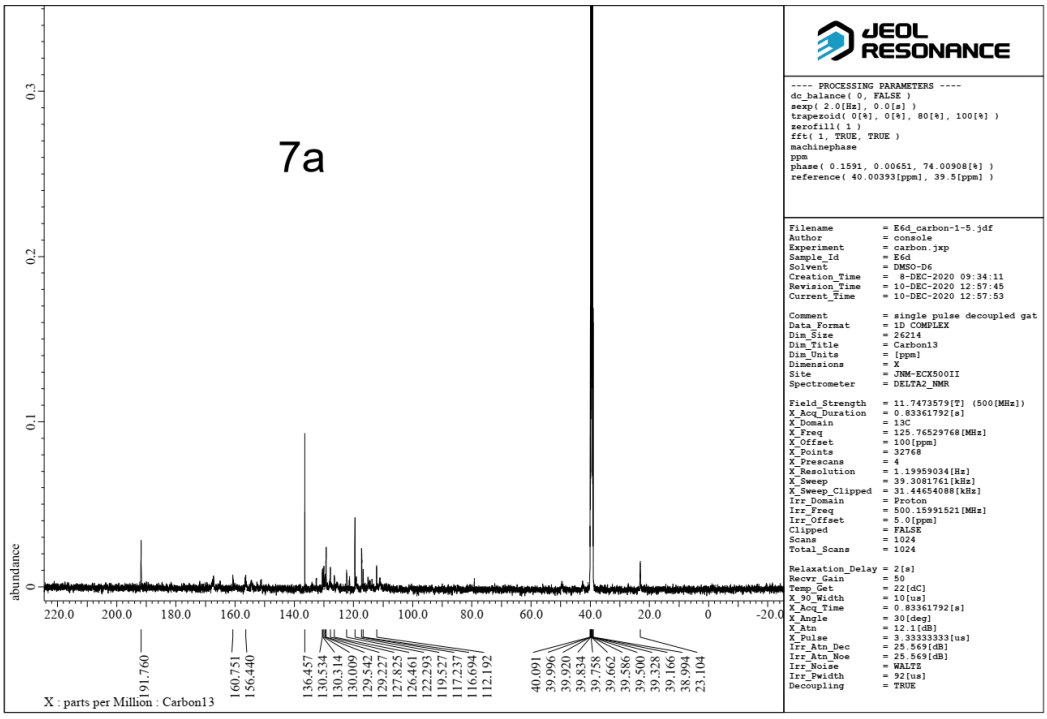


Figure S21. ^{13}C NMR spectrum of compound **7a**

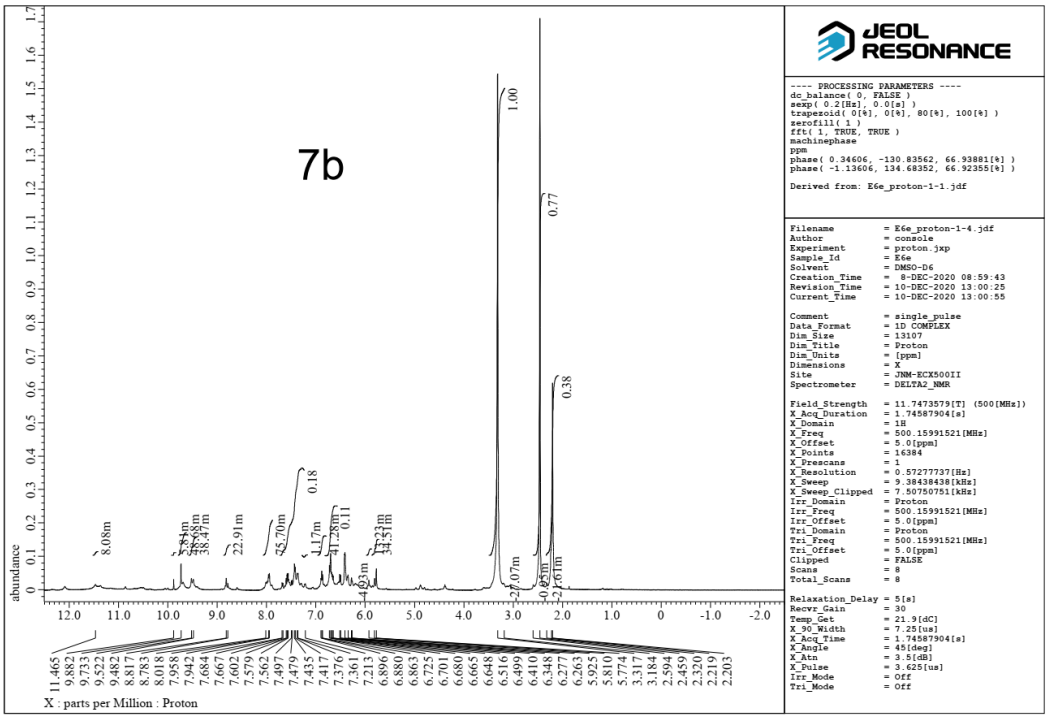


Figure S22. ^{1}H NMR spectrum of compound **7b**

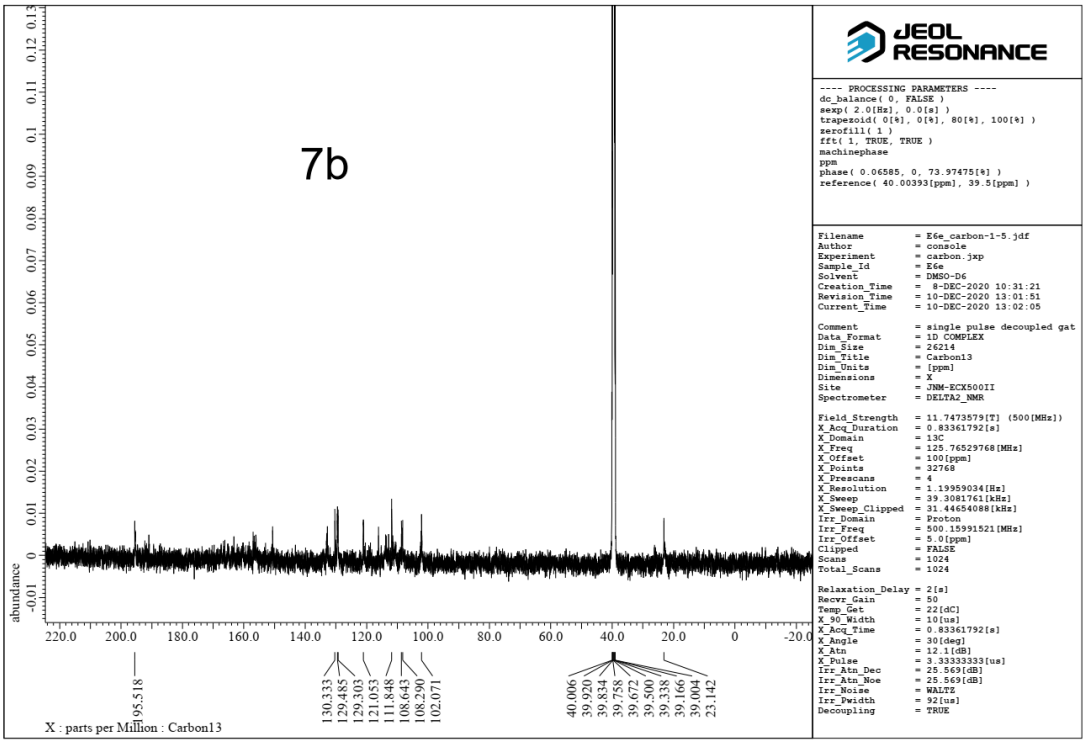


Figure S23. ^{13}C NMR spectrum of compound **7b**

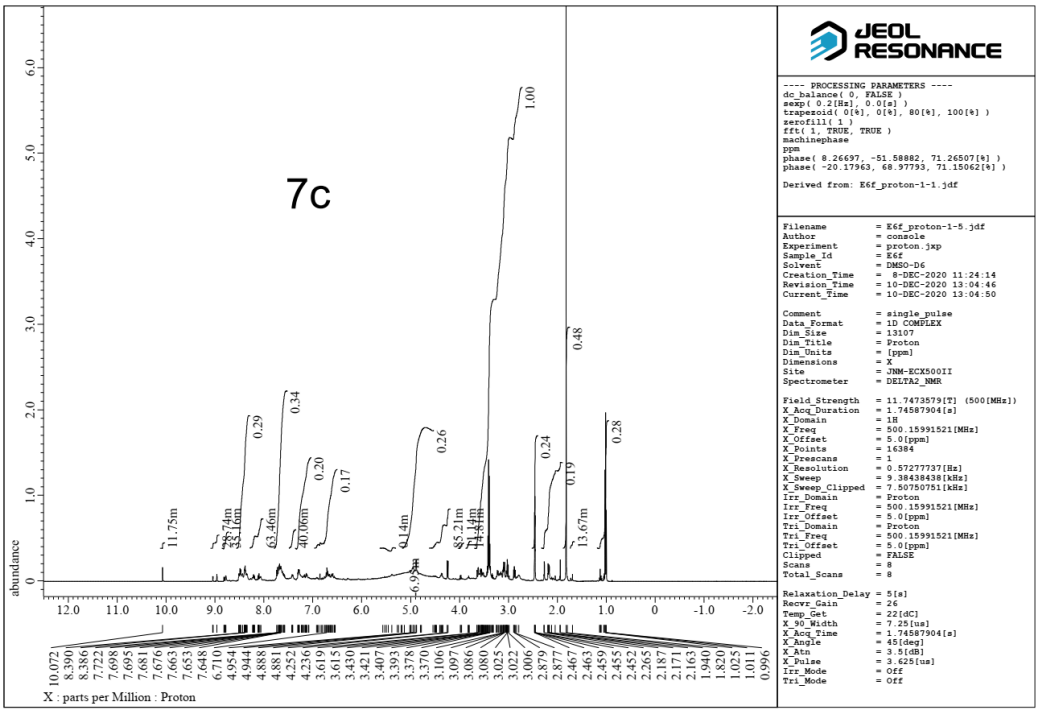


Figure S24. ^{1}H NMR spectrum of compound **7c**

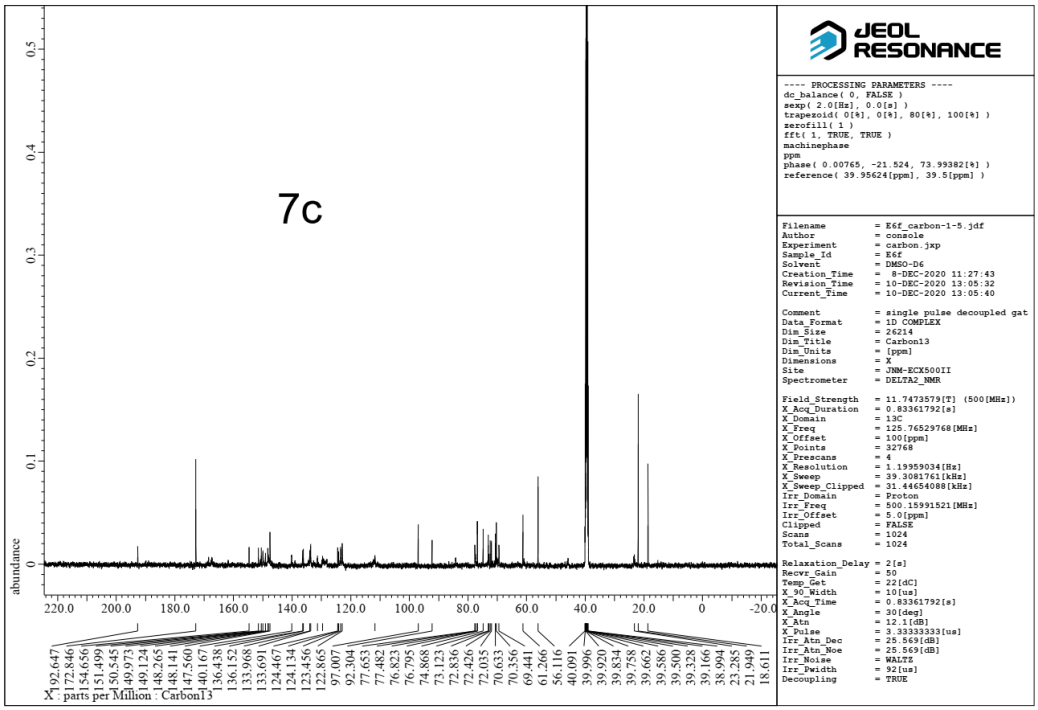
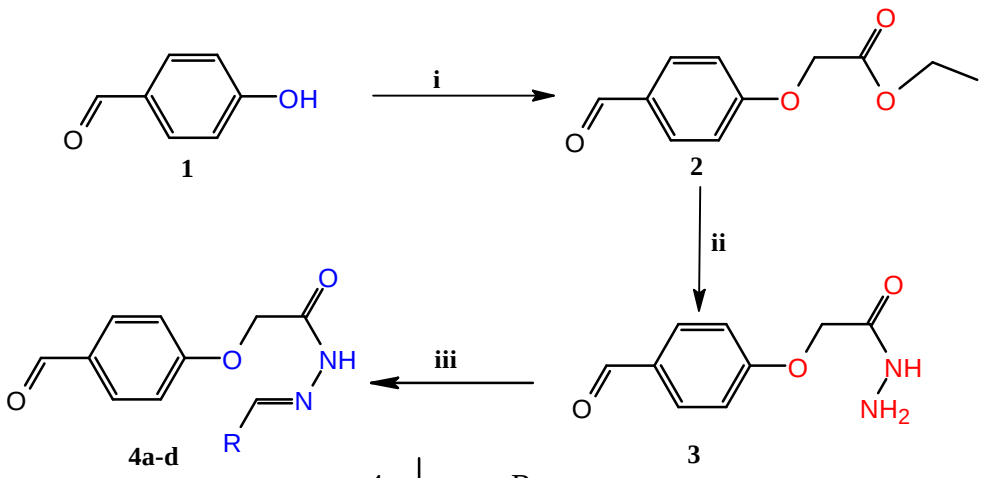


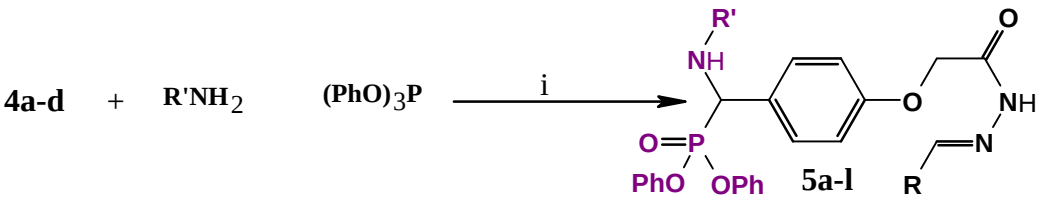
Figure S25. ^{13}C NMR spectrum of compound **7c**



4	R
a	phenyl
b	4-*N*,*N*-dimethylphenyl
c	3,4,5-trimethoxyphenyl
d	4-nitrophenyl

Scheme 1. Reagents conditions: (i) Ethylchloroacetate, K_2CO_3, acetone, reflux, 12h, 87%; (ii) $NH_2NH_2.H_2O$, EtOH, reflux, 5h, 90%; (iii) RCHO, EtOH, AcOH, reflux, 15h, for **4a**: 87%; for **4b**: 88%; for **4c**: 90%; for **4d**: 90%.

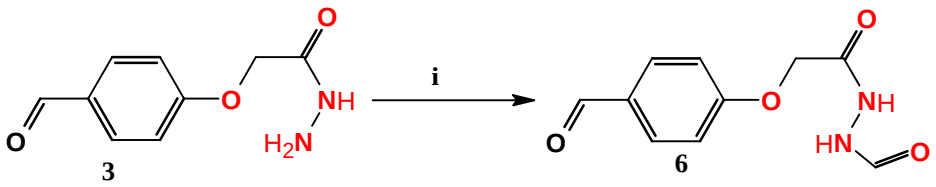
Synthesis of arylidene derivatives **4a-d**



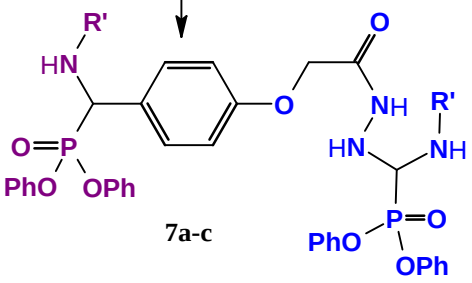
5	R	R'
a	phenyl	1-naphthyl
b	phenyl	2-nitrophenyl
c	phenyl	4-methylphenyl
d	4-(dimethylamino)phenyl	1-naphthyl
e	4-(dimethylamino)phenyl	2-nitrophenyl
f	4-(dimethylamino)phenyl	4-methylphenyl
g	3,4,5-trimethoxyphenyl	1-naphthyl
h	3,4,5-trimethoxyphenyl	2-nitrophenyl
i	3,4,5-trimethoxyphenyl	4-methylphenyl
j	4-nitropheneyl	1-naphthyl
k	4-nitropheneyl	2-nitrophenyl
l	4-nitropheneyl	4-methylphenyl

Scheme 2. Reagents conditions: (i) $HClO_4$, MeCN, r.t, 20h, for **5a**: 75%; for **5b**: 75%; for **5c**: 77%; for **5d**: 82%; for **5e**: 80%; for **5f**: 80%; for **5g**: 85%; for **5h**: 85%; for **5i**: 80%; for **5j**: 86%; for **5k**: 88%; for **5l**: 92%.

Synthesis of α-aminophosphonates **5a- l**



7	R'
a	1-naphthyl
b	2-nitrophenyl
c	4-methylphenyl



Scheme 3. Reagents conditions: (i) HCOOH, reflux, 14h, 90%; (ii) $R'NH_2$, $(PhO)_3P$,$HClO_4$,MeCN, 24h, for **7a**: 85%; for **7b**: 87%; for **7c**: 88%.

Synthesis of phosphonates **7a-c**