

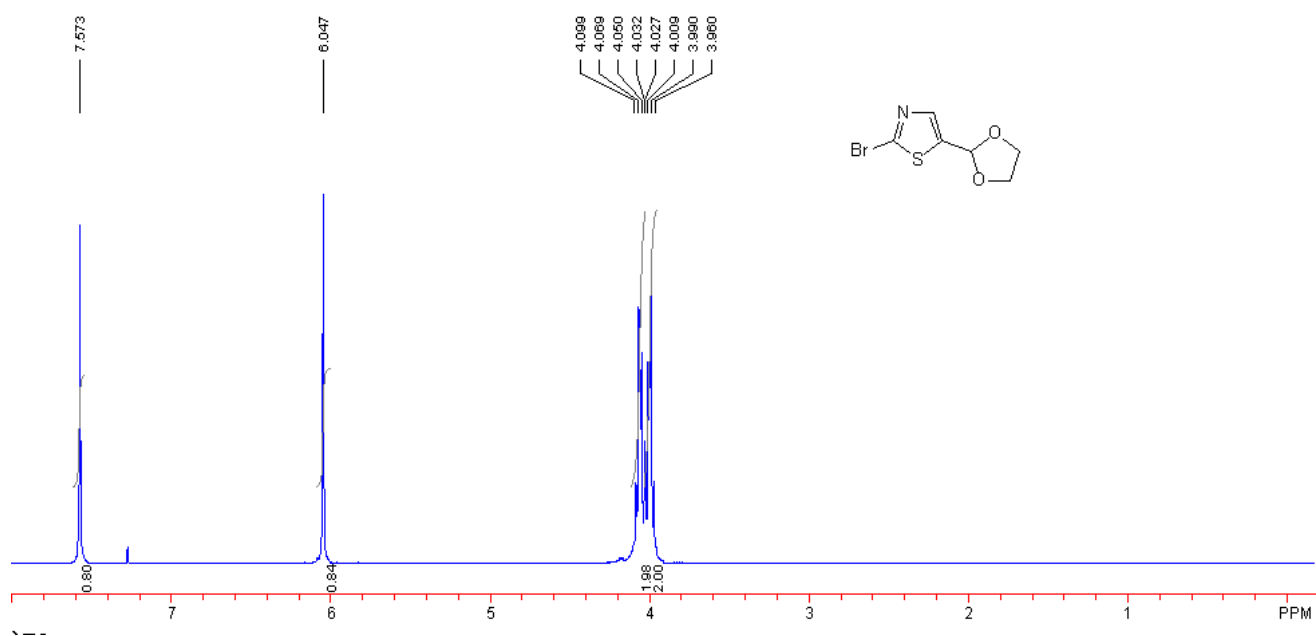
ELECTRONIC SUPPLEMENTARY INFORMATION

Functionalized 1,3-thiazoles by combined halogen dance

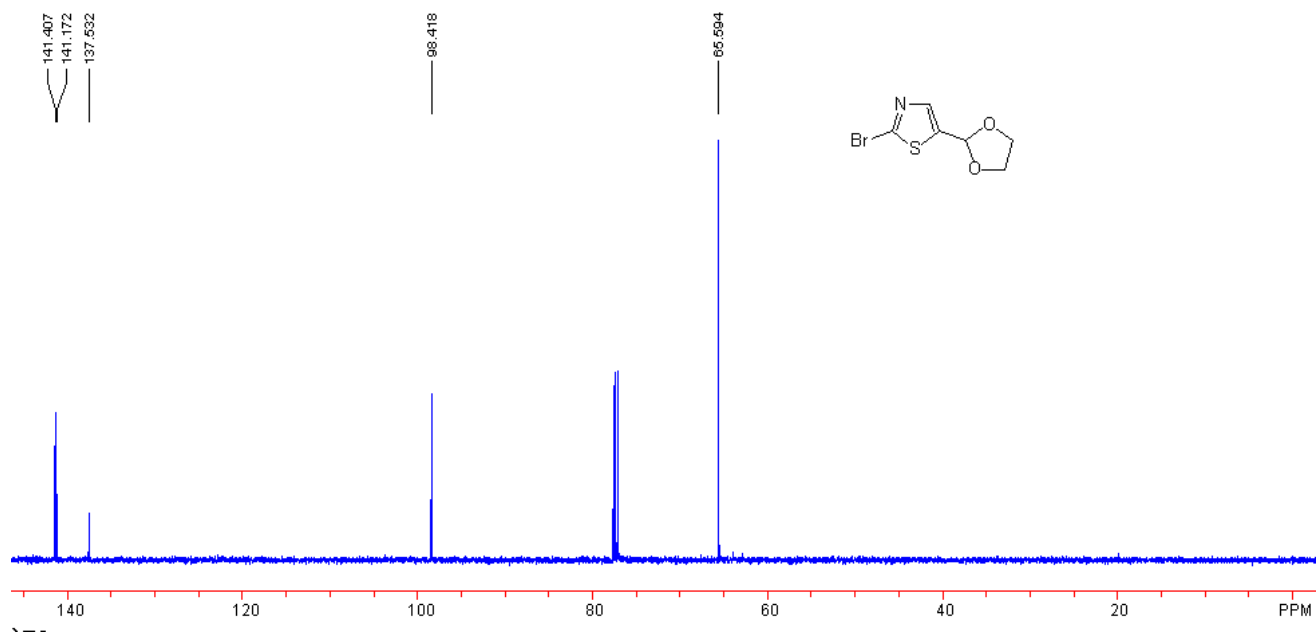
Vitalii O. Sinenko, Oleksandr V. Los, Lyudmyla M. Potikha and Volodymyr S. Brovarets*

Figure S1. Compound 2

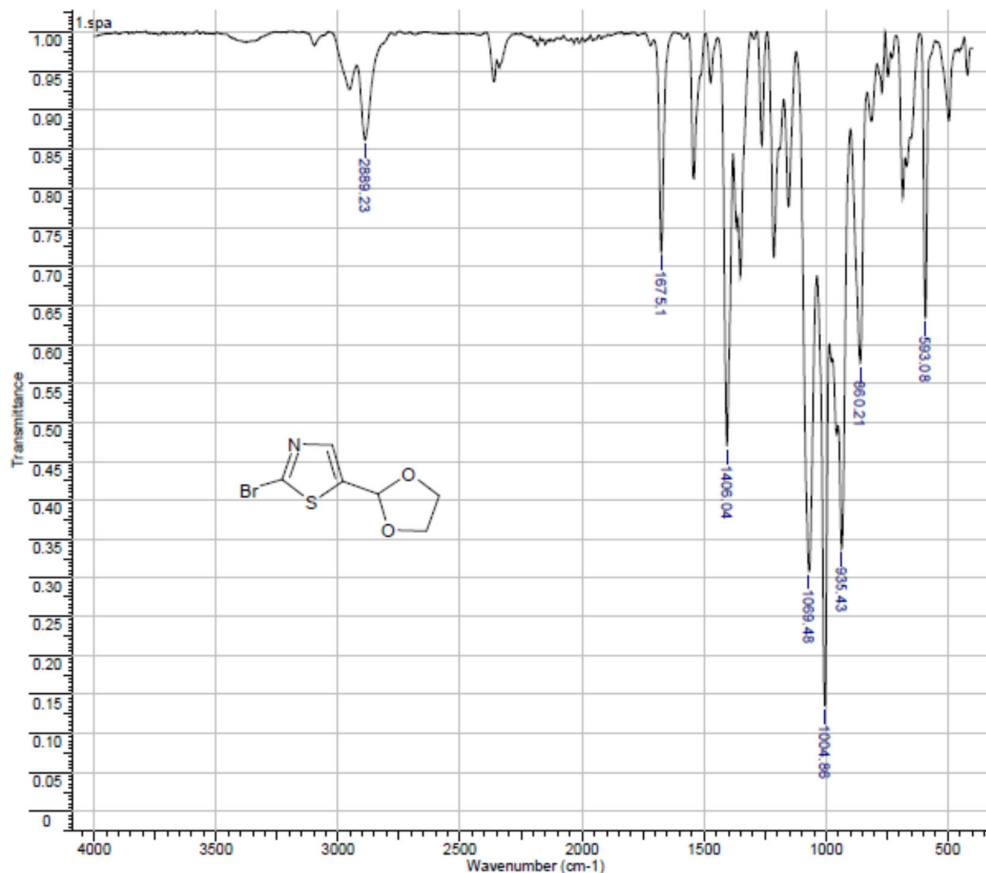
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



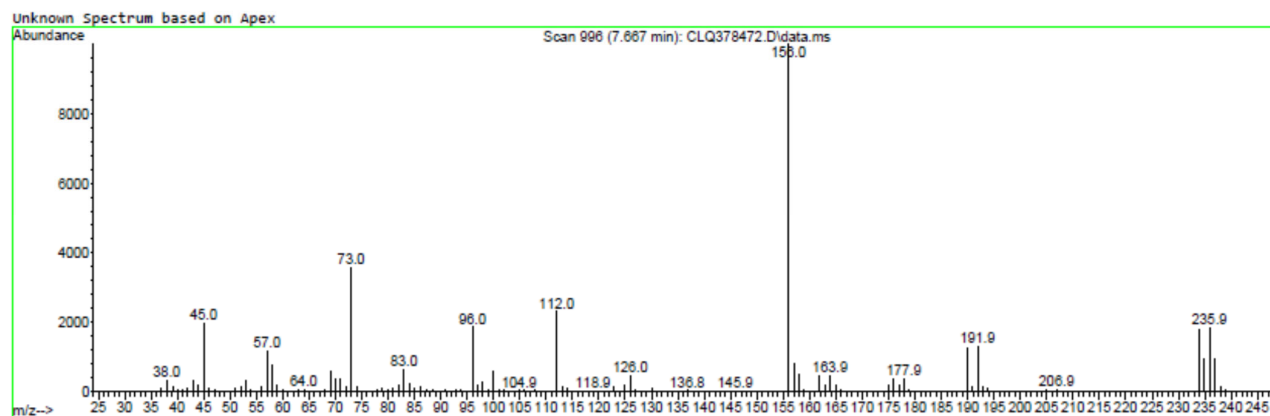
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) ATR-IR spectrum



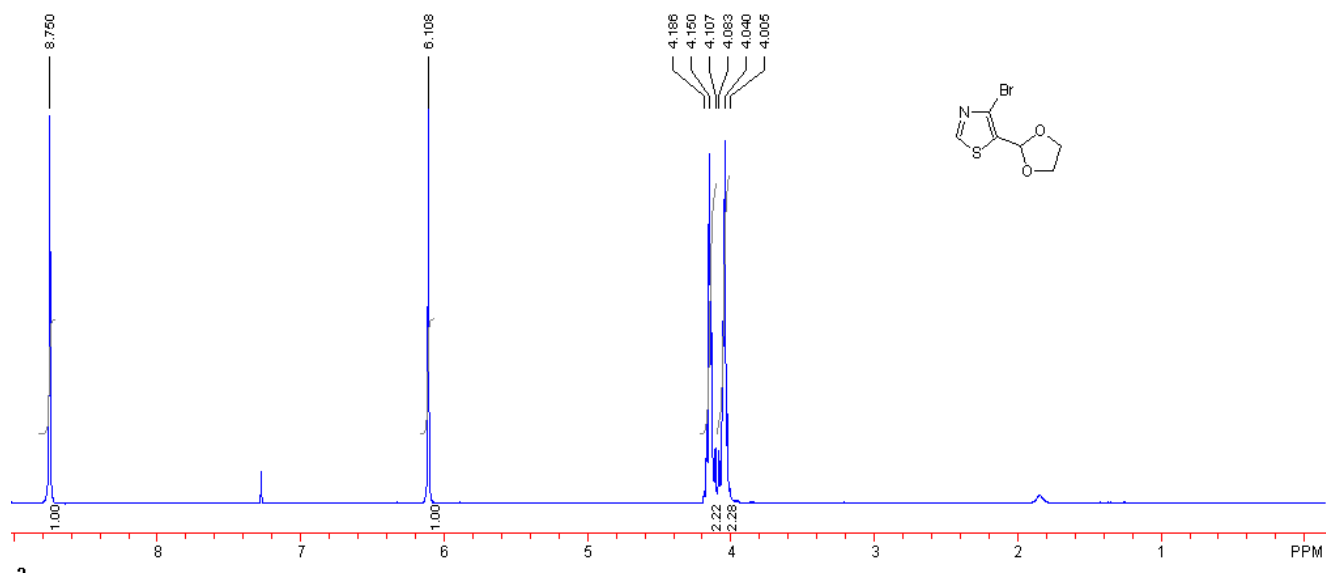
(D) GC/MS spectrum of compound 2



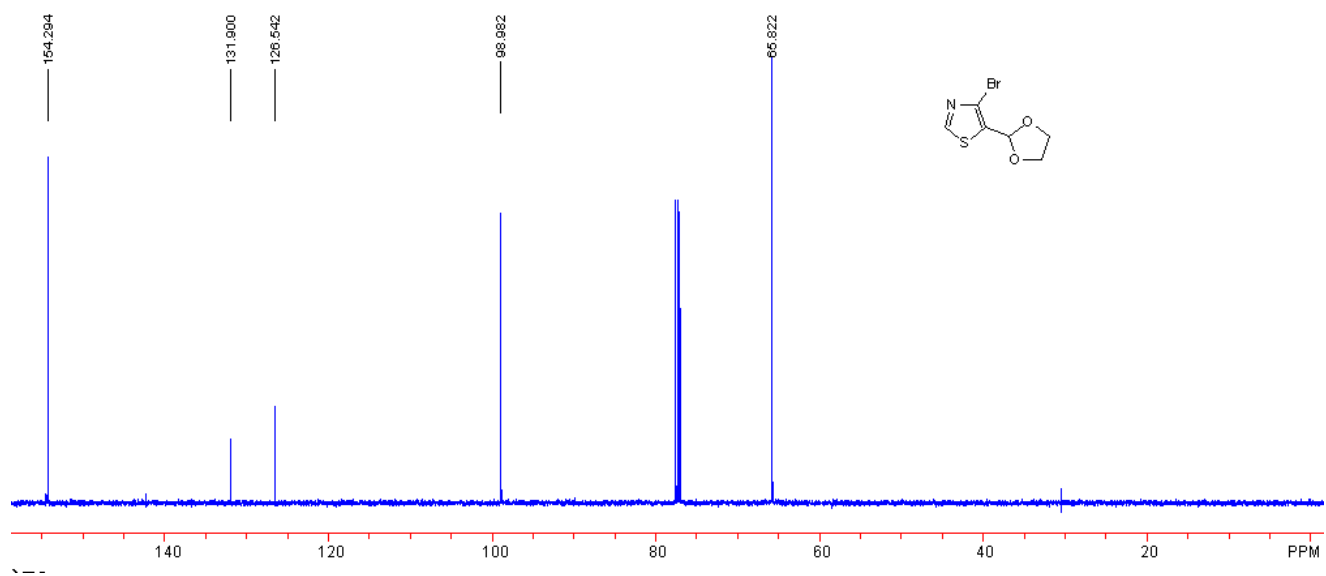
RT = 7.668 min

Figure S2. Compound 3

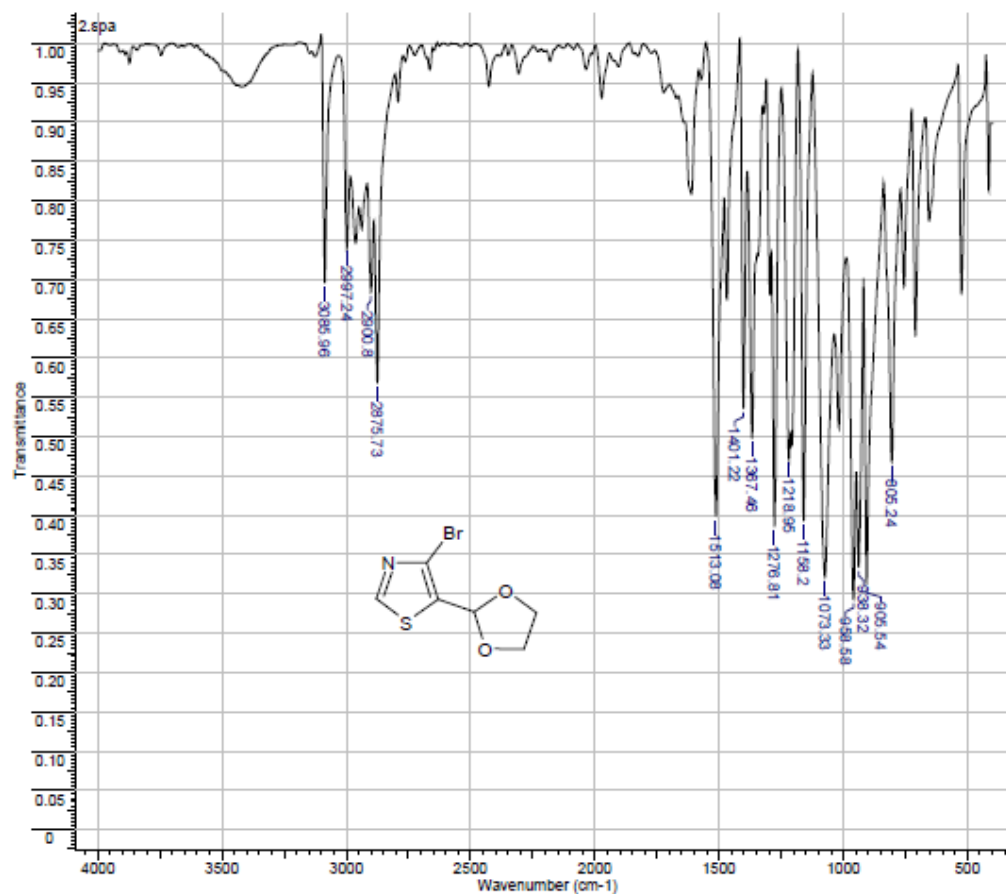
(A) ^1H -NMR spectrum (CDCl_3)



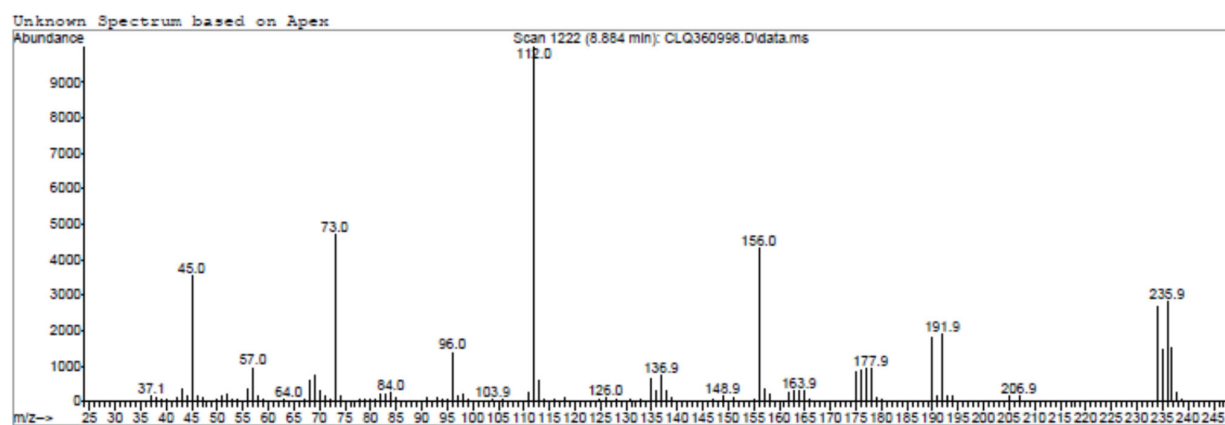
(B) ^{13}C -NMR spectrum (CDCl_3)



(C) IR spectrum (KBr)



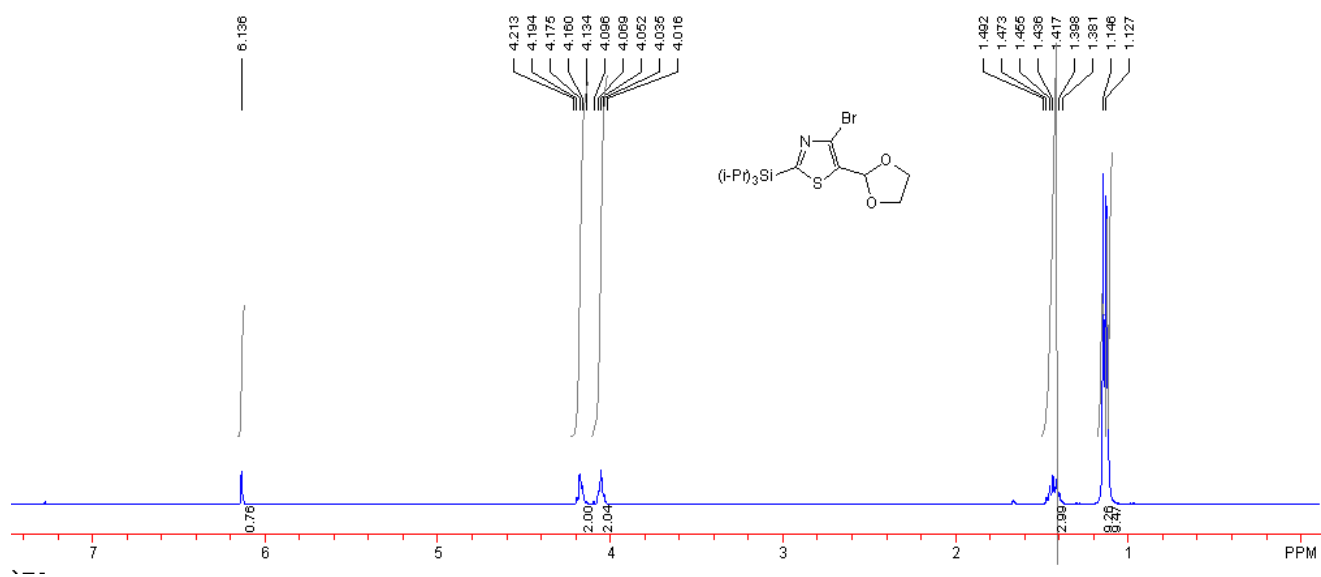
(D) GC/MS spectrum of compound 3



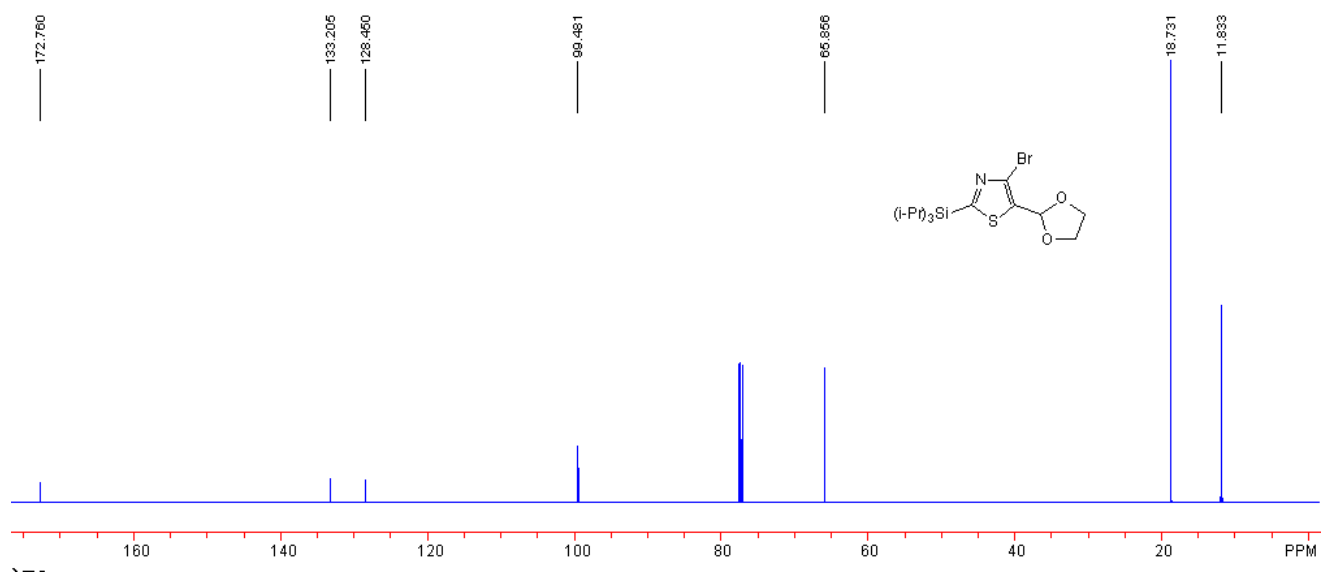
RT = 8.886 min

Figure S3. Compound 4

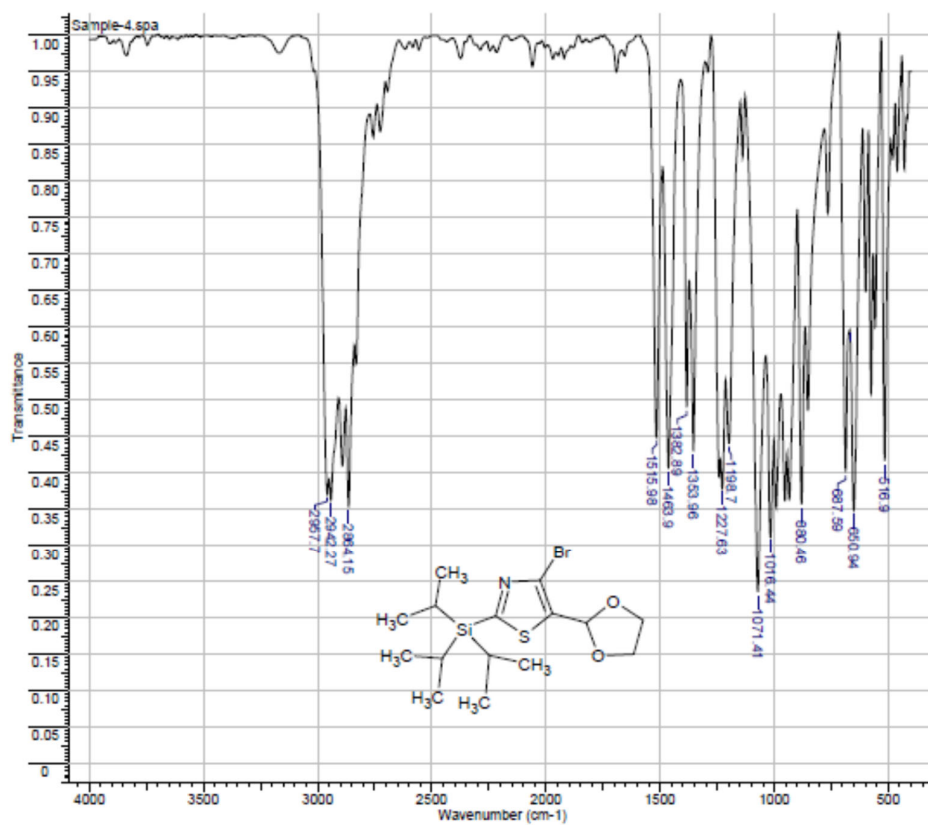
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



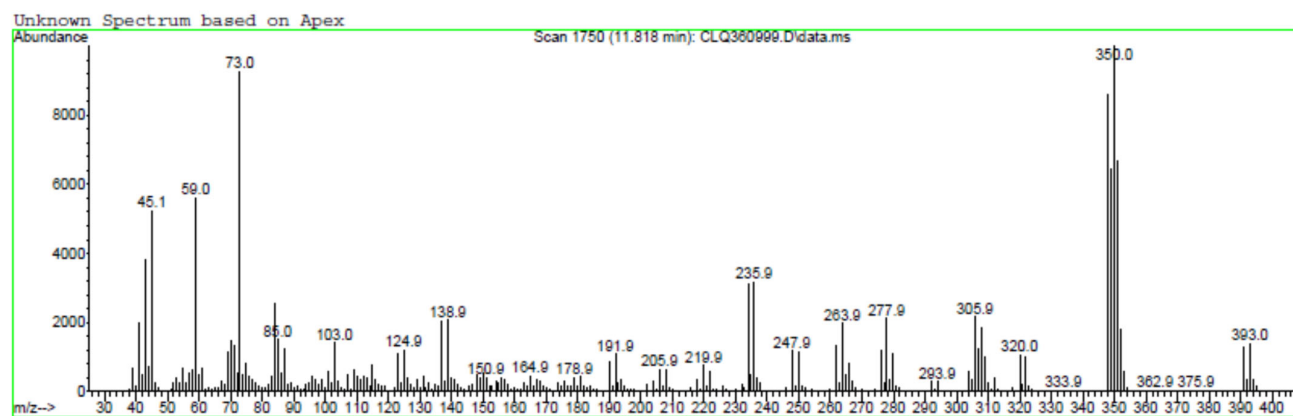
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



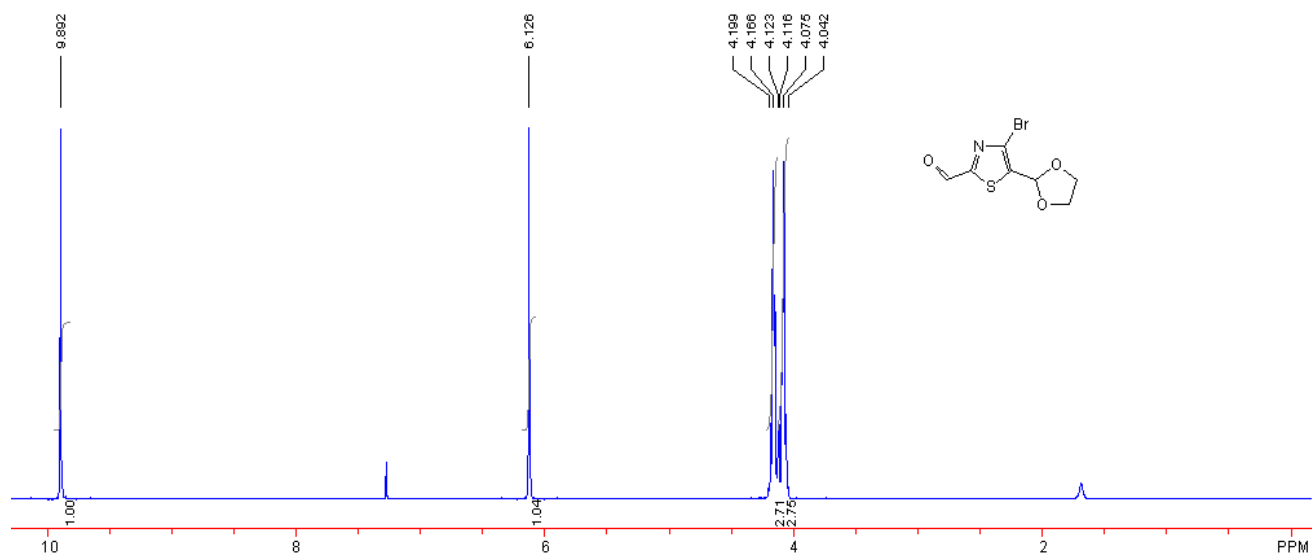
(D) GC/MS spectrum of compound 4



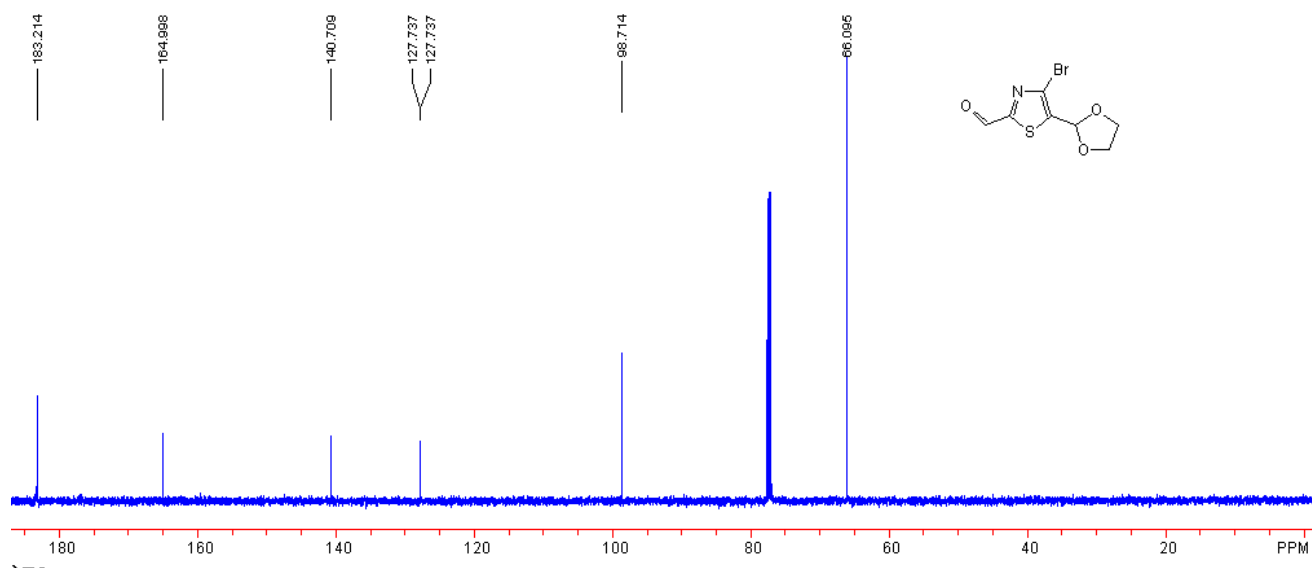
RT = 11.819 min

Figure S4. Compound 5

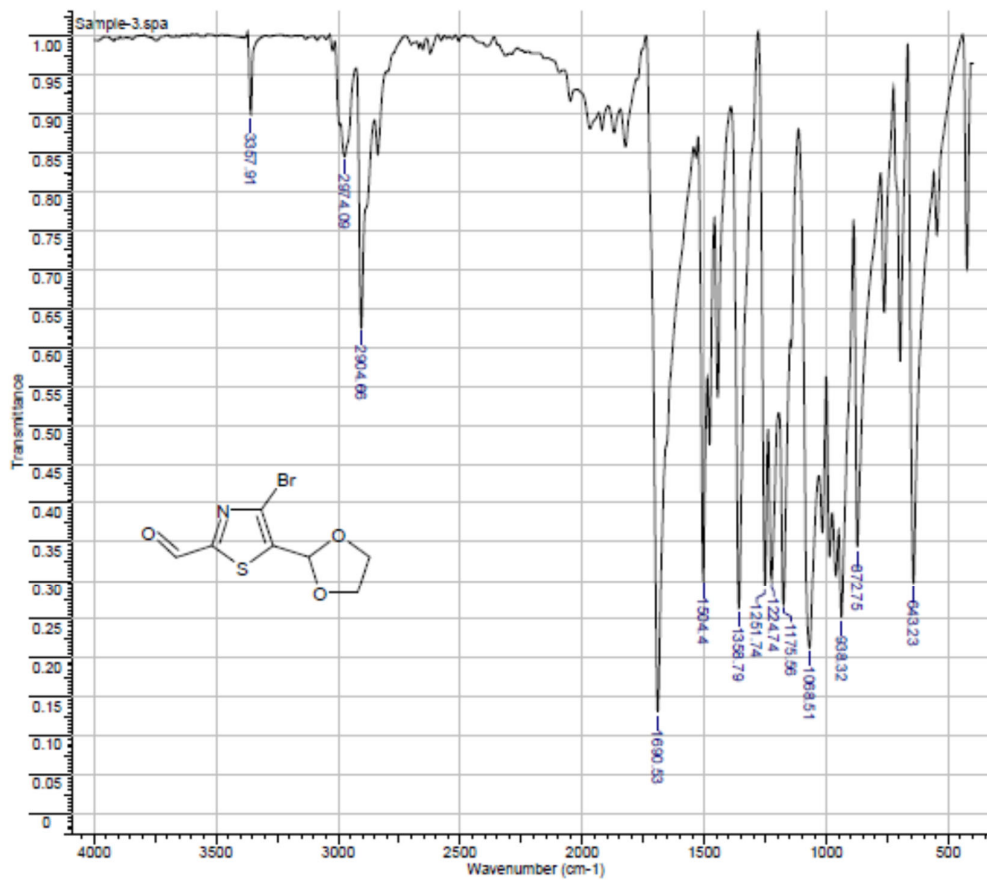
(A) ^1H -NMR spectrum (CDCl_3)



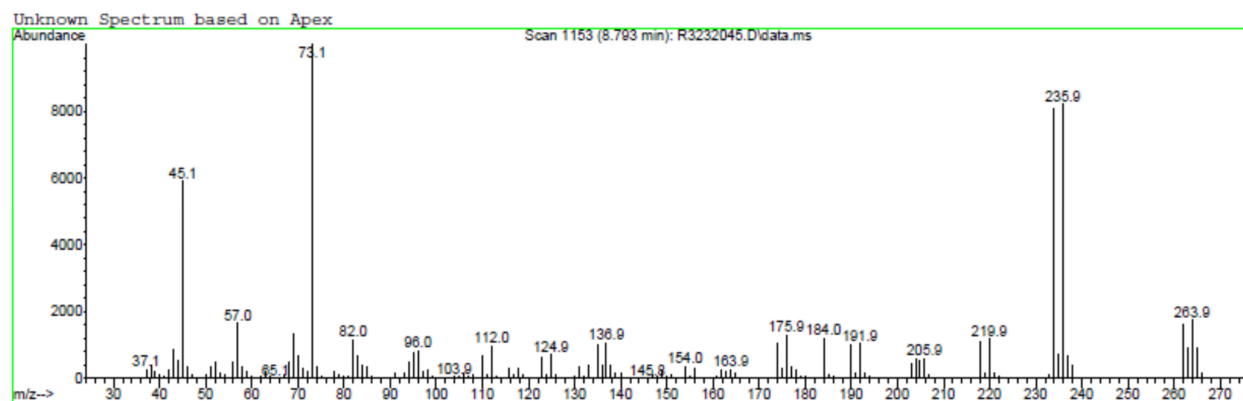
(B) ^{13}C -NMR spectrum (CDCl_3)



(C) IR spectrum (KBr)



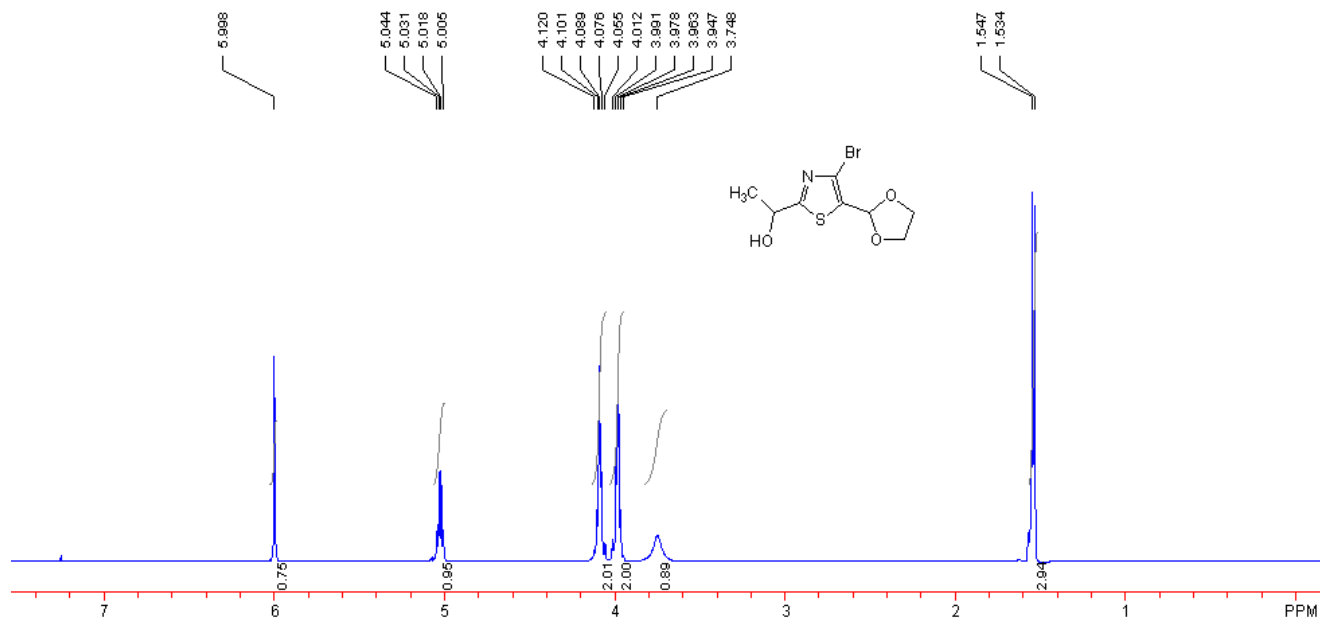
(D) GC/MS spectrum of compound 5



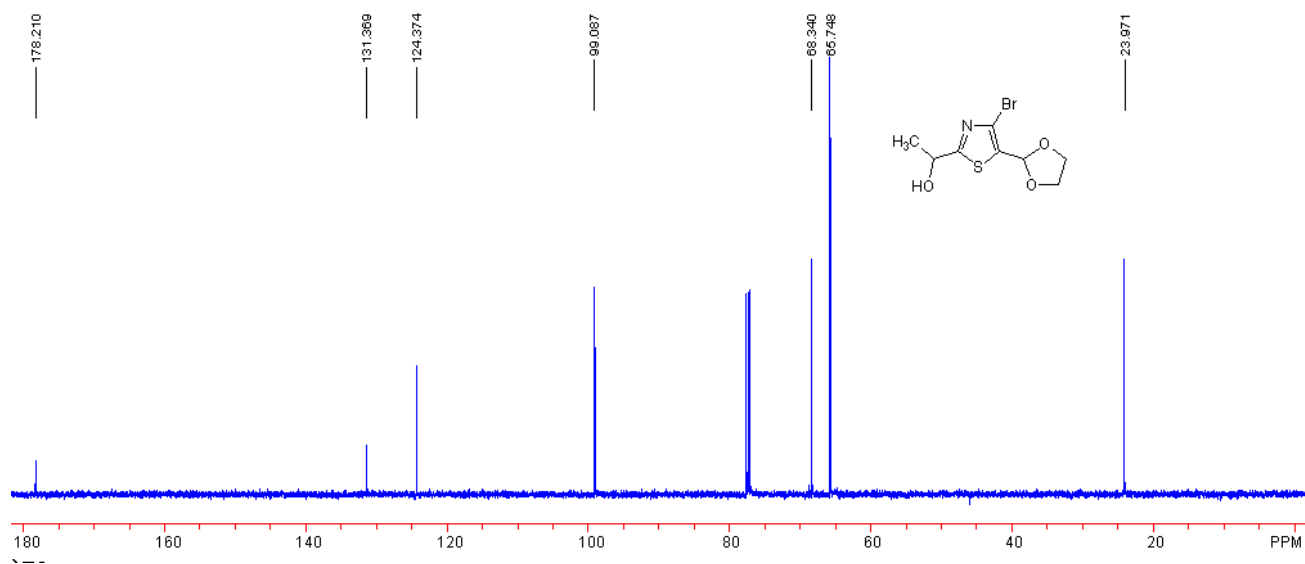
RT = 8.796 min

Figure S5. Compound 6

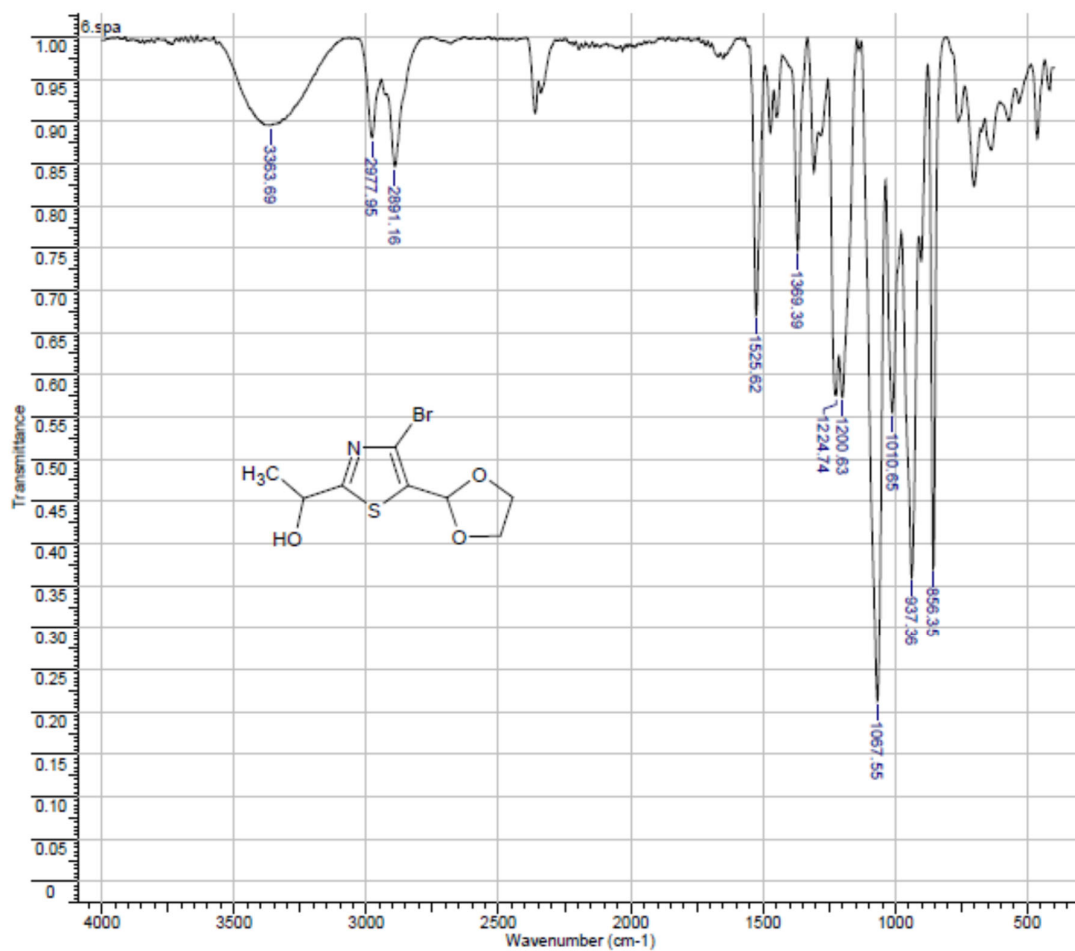
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



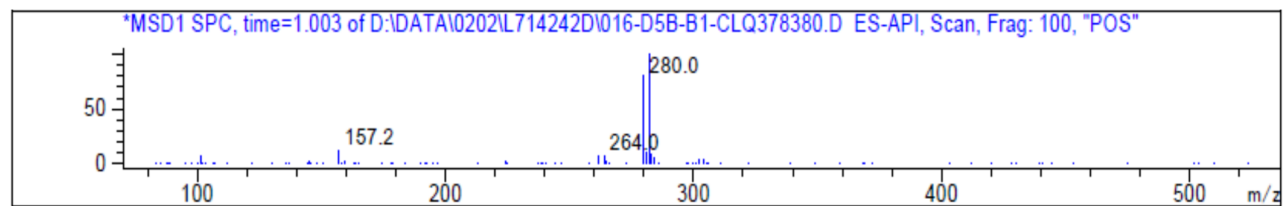
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) ATR-IR spectrum



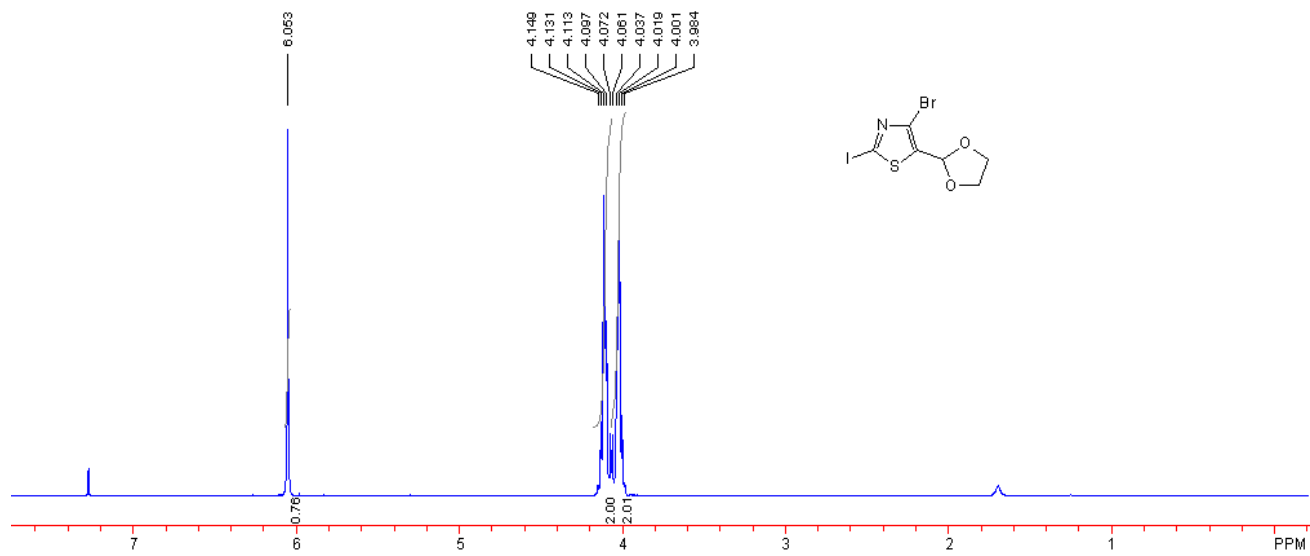
(D) LC/MS spectrum of compound 6



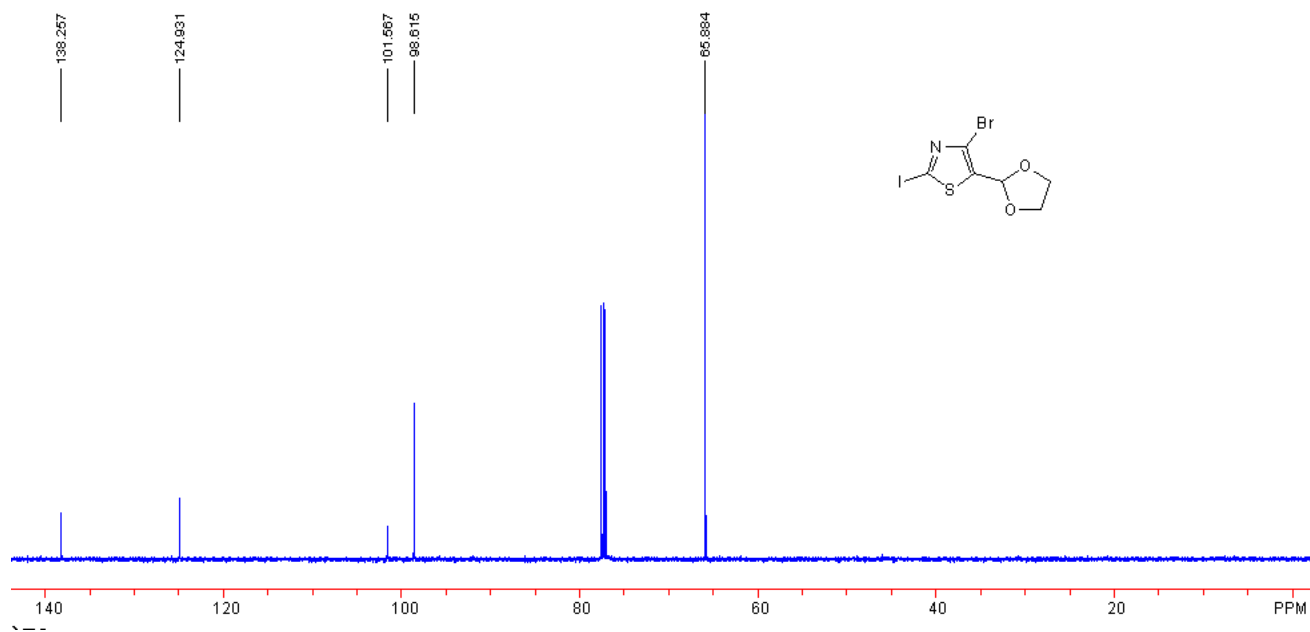
RT = 1.005 min

Figure S6. Compound 7

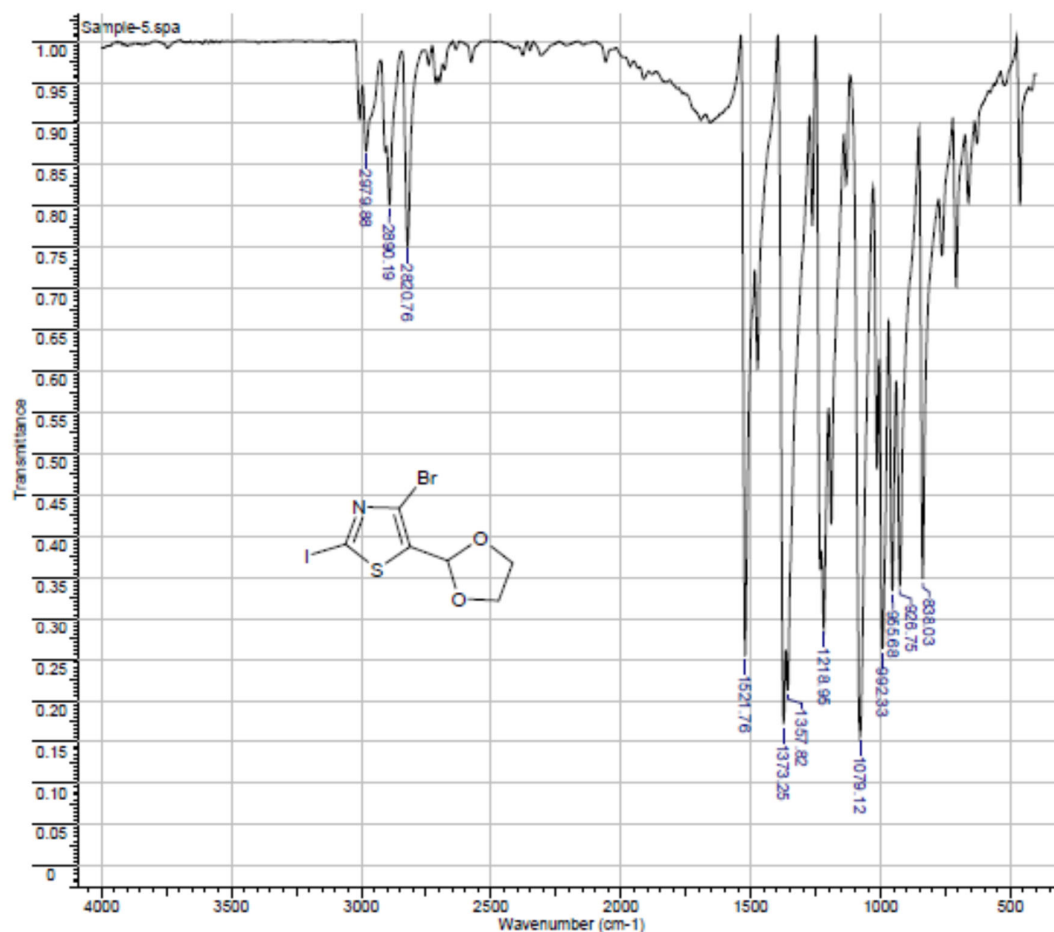
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



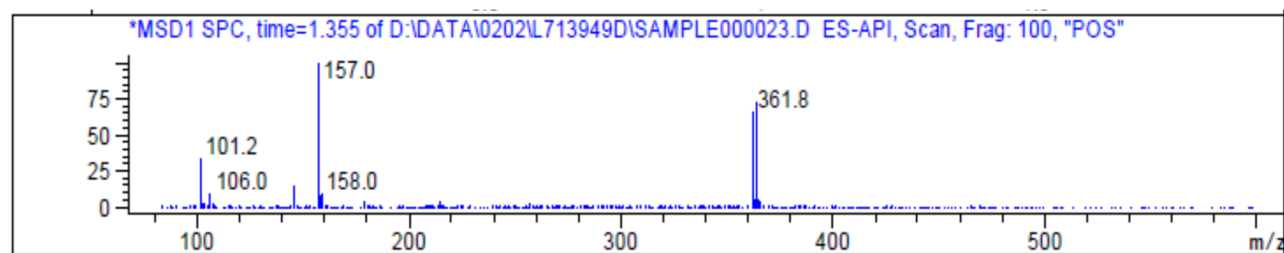
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



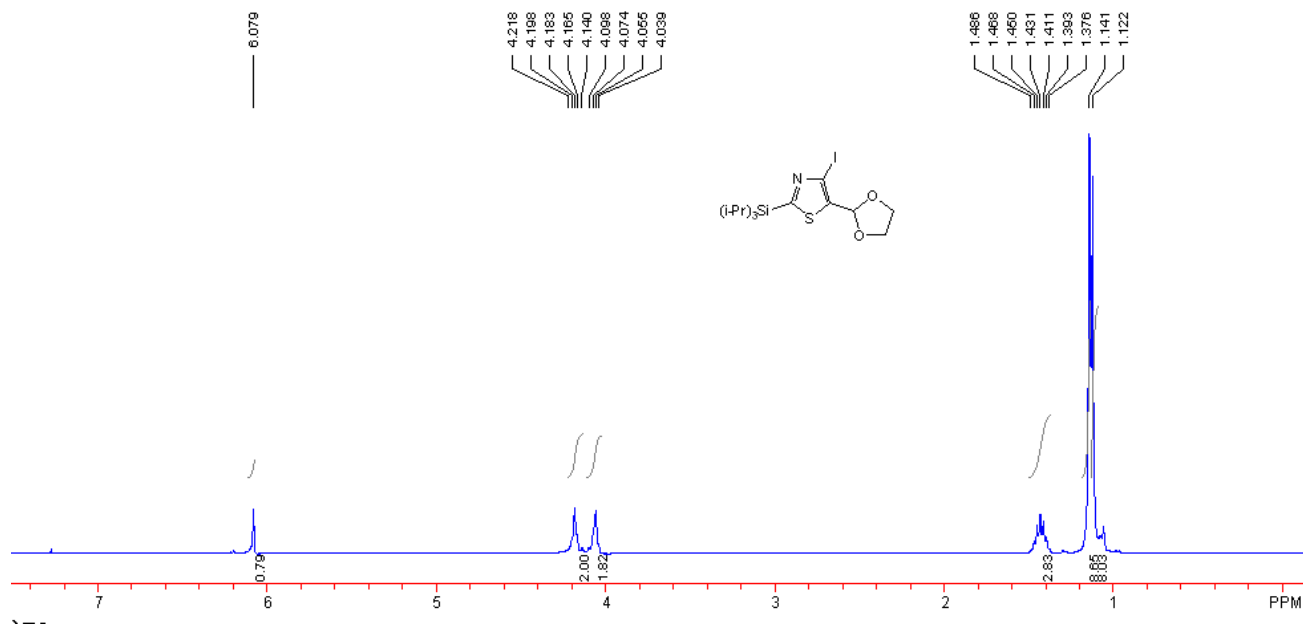
(D) LC/MS spectrum of compound 7



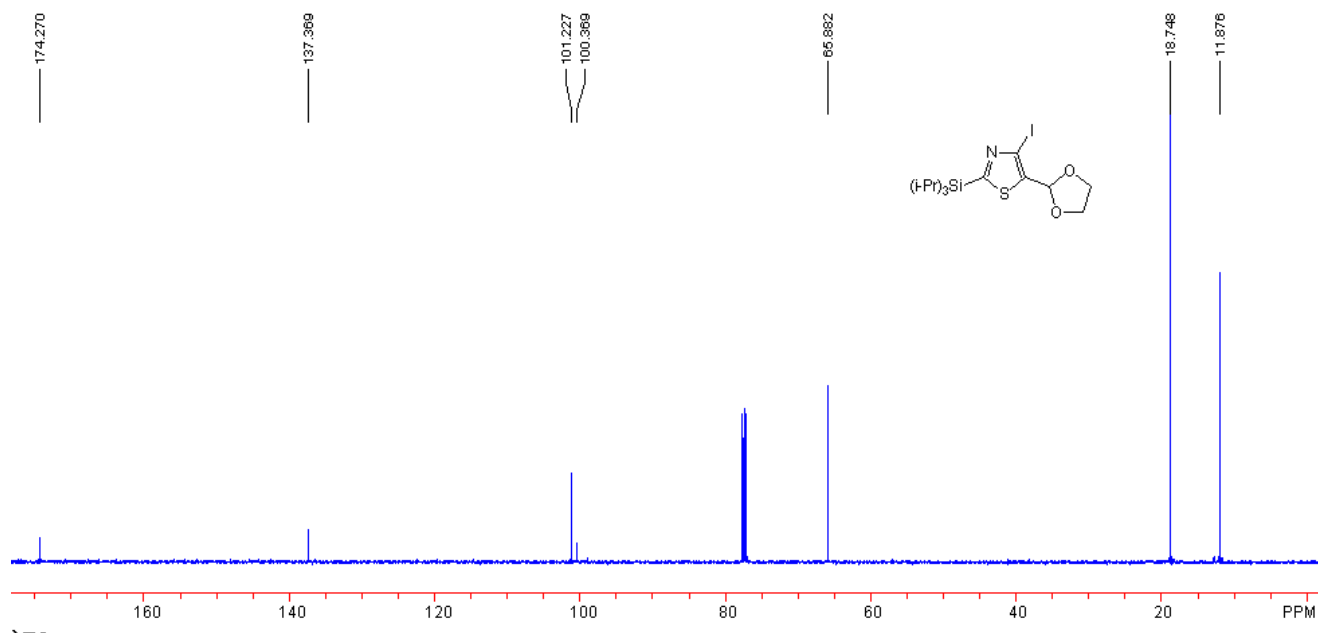
RT = 1.358 min

Figure S7. Compound 8

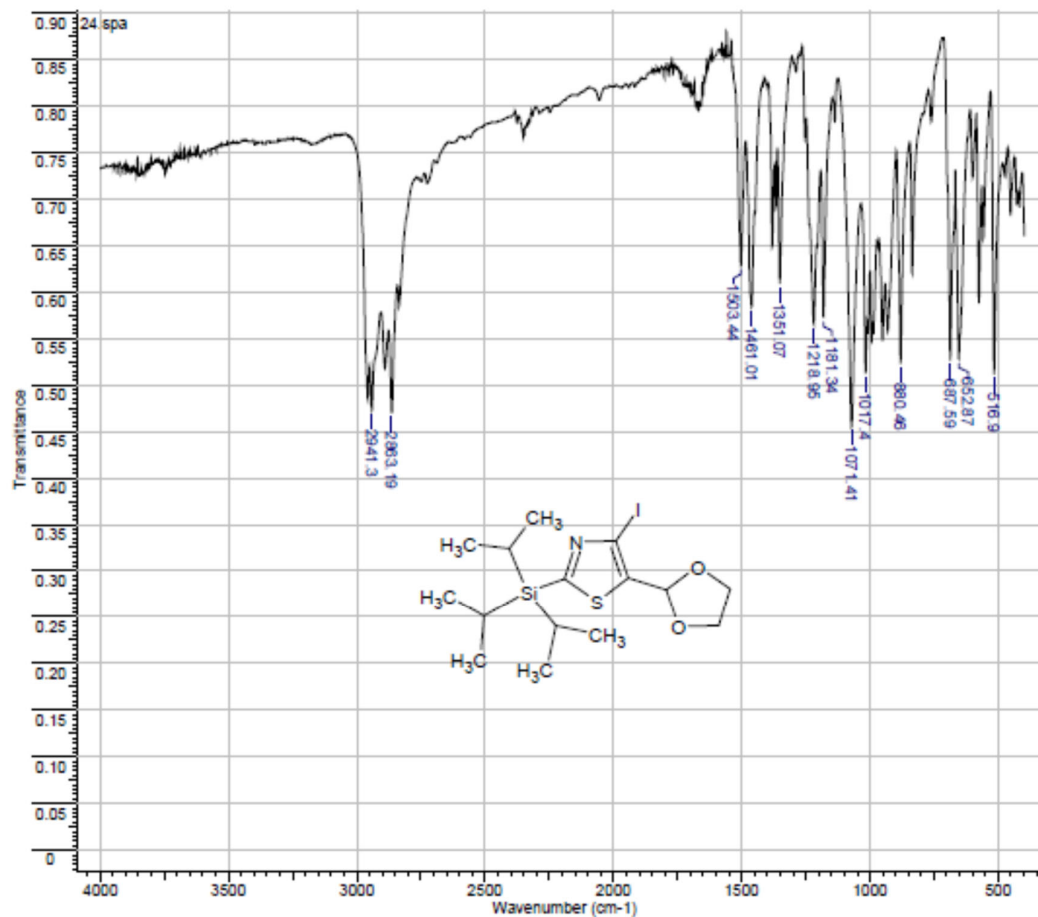
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



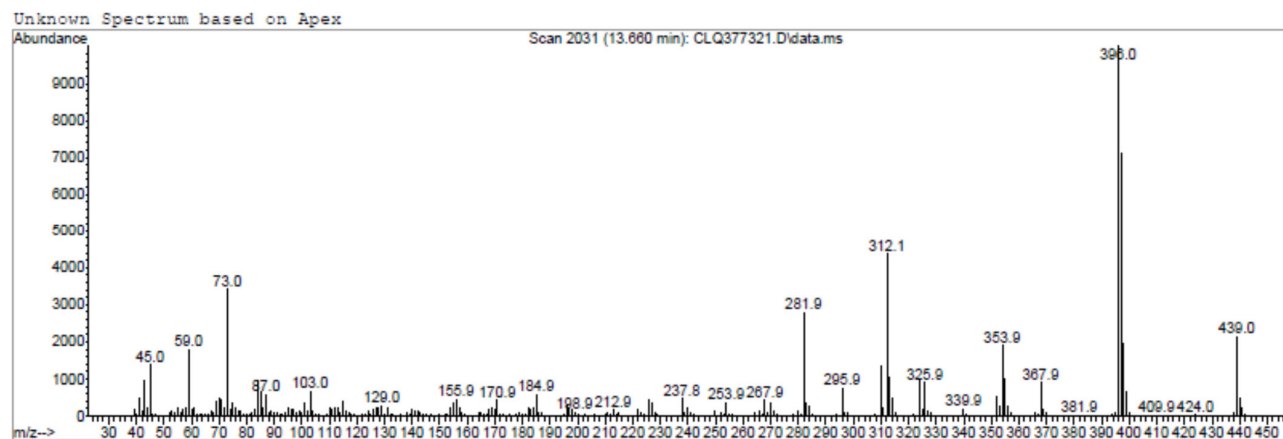
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



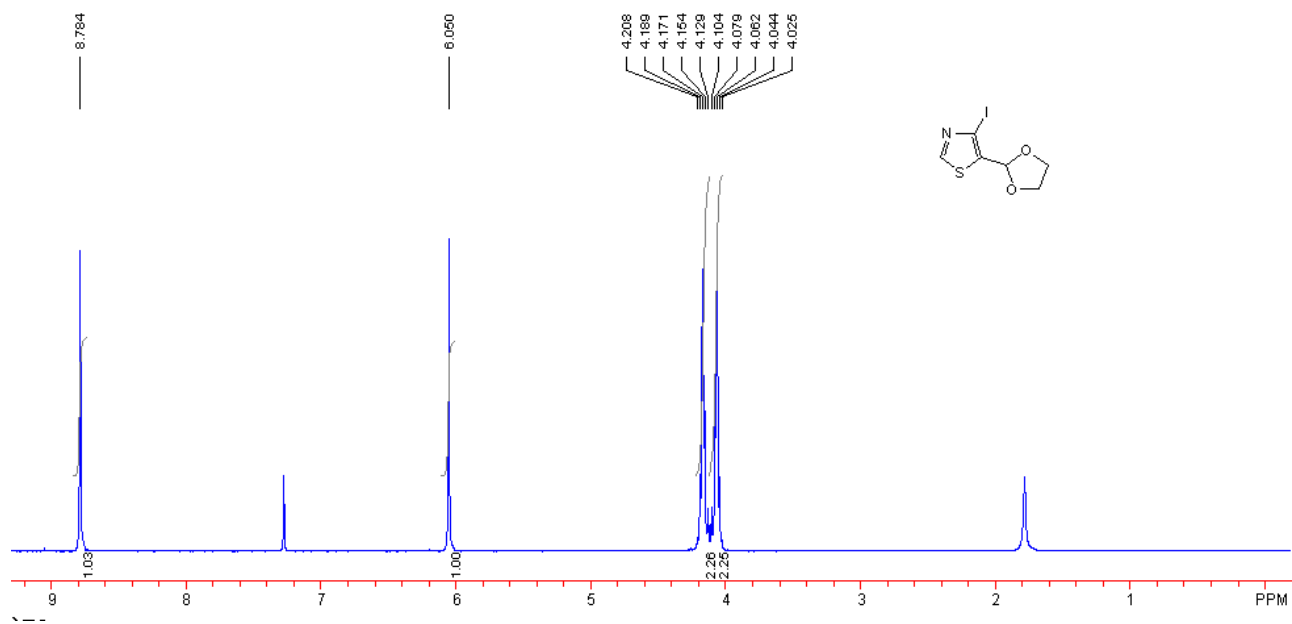
(D) GC/MS spectrum of compound 8



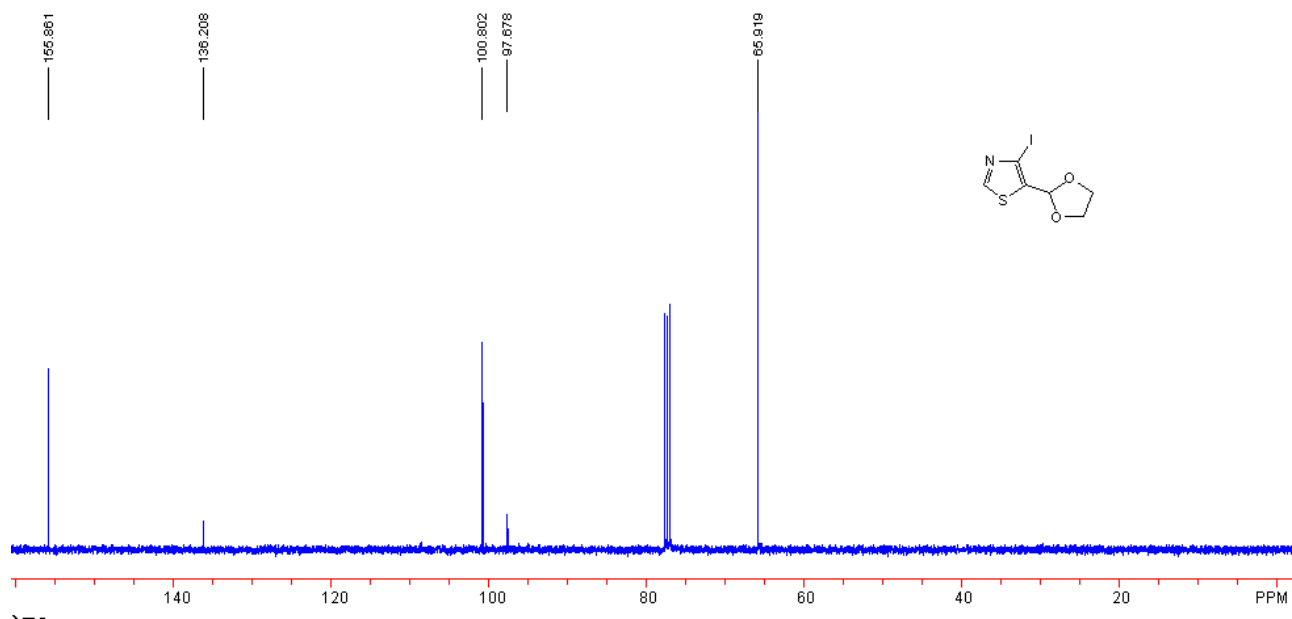
RT = 13.658 min

Figure S8. Compound 9

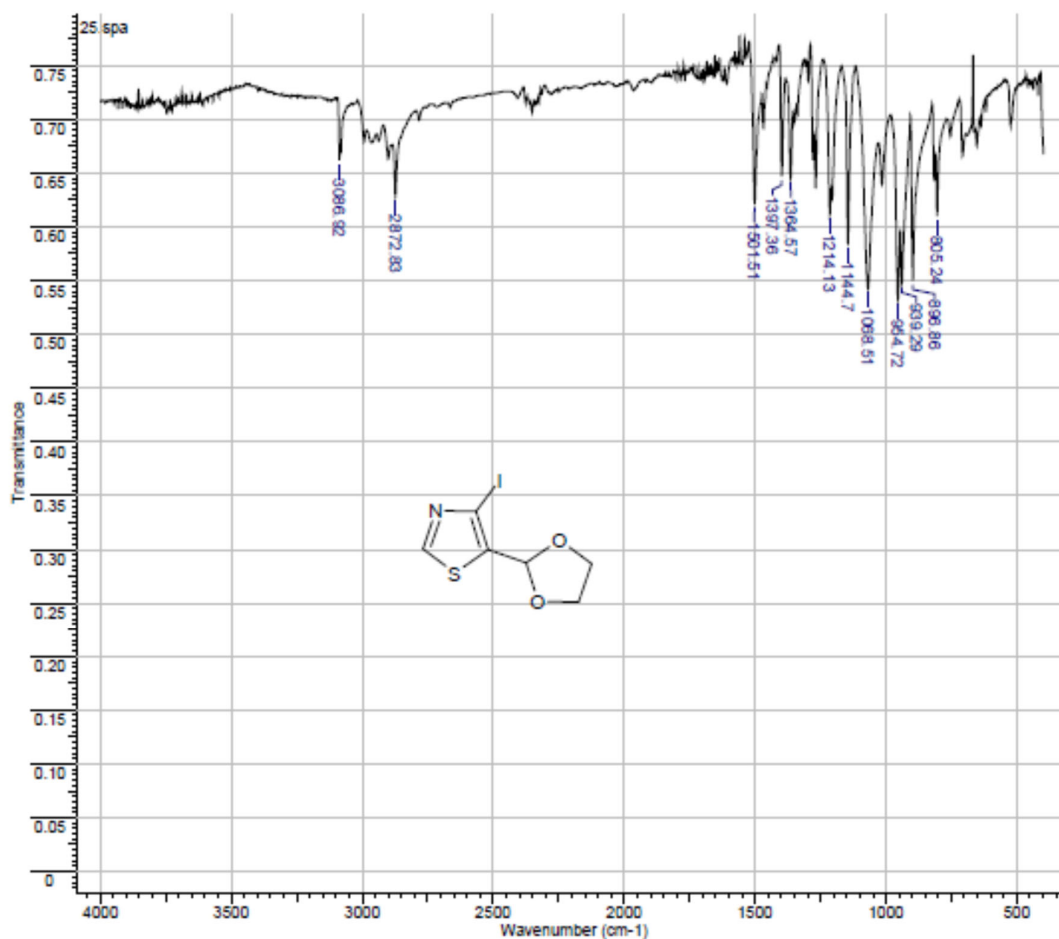
(A) ^1H -NMR spectrum (CDCl_3)



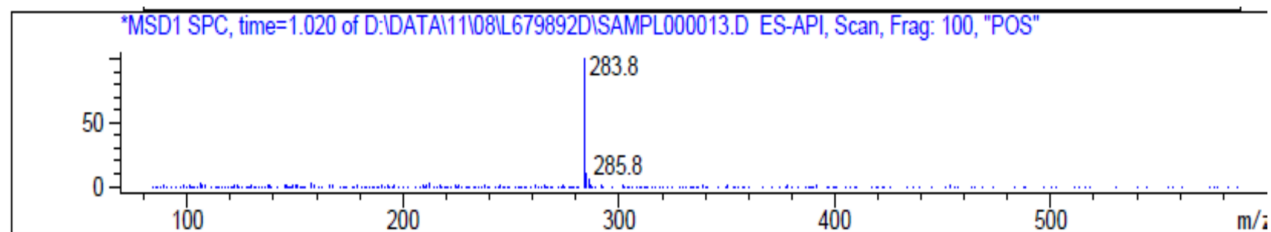
(B) ^{13}C -NMR spectrum (CDCl_3)



(C) IR spectrum (KBr)



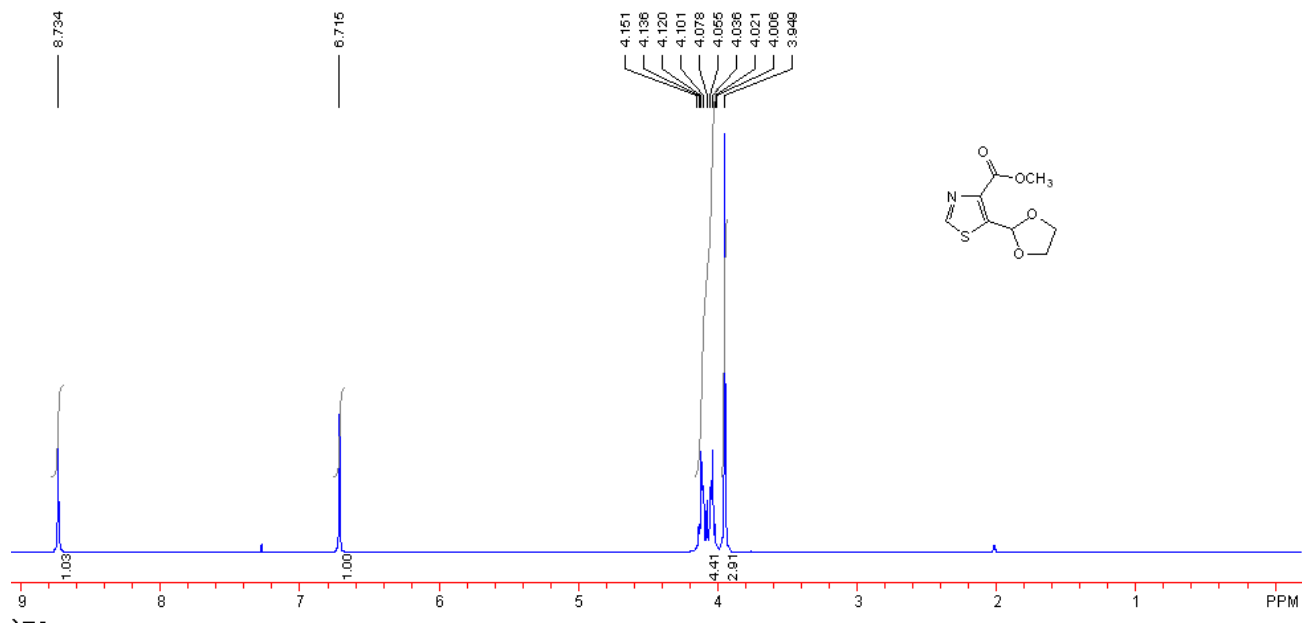
(D) LC/MS spectrum of compound 9



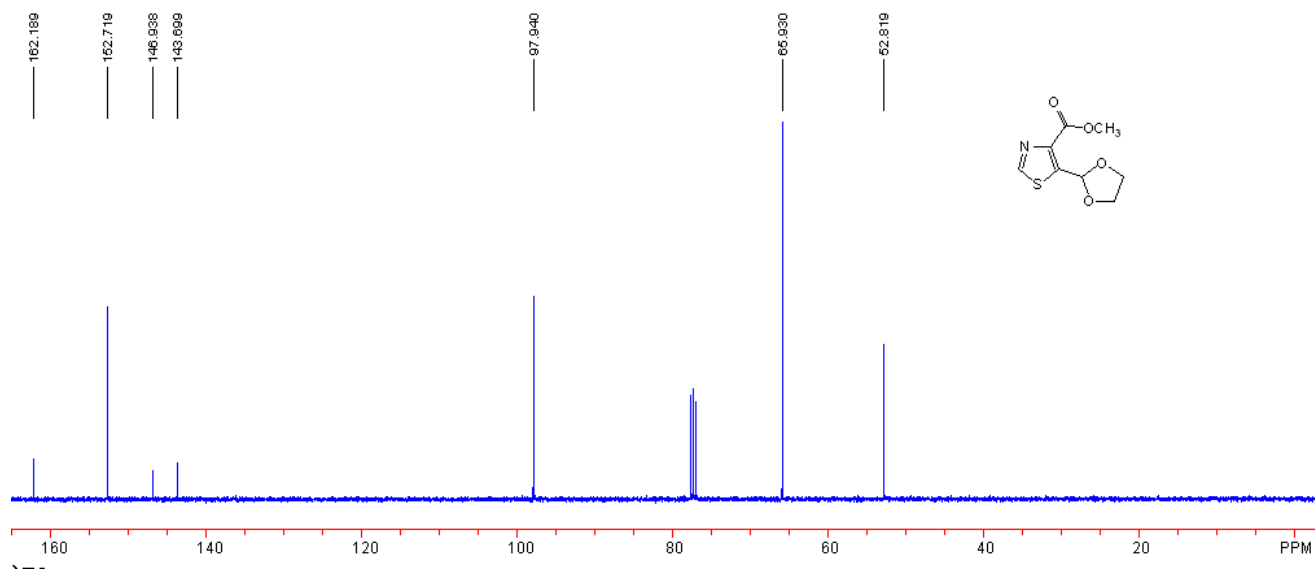
RT = 1.021 min

Figure S9. Compound 10

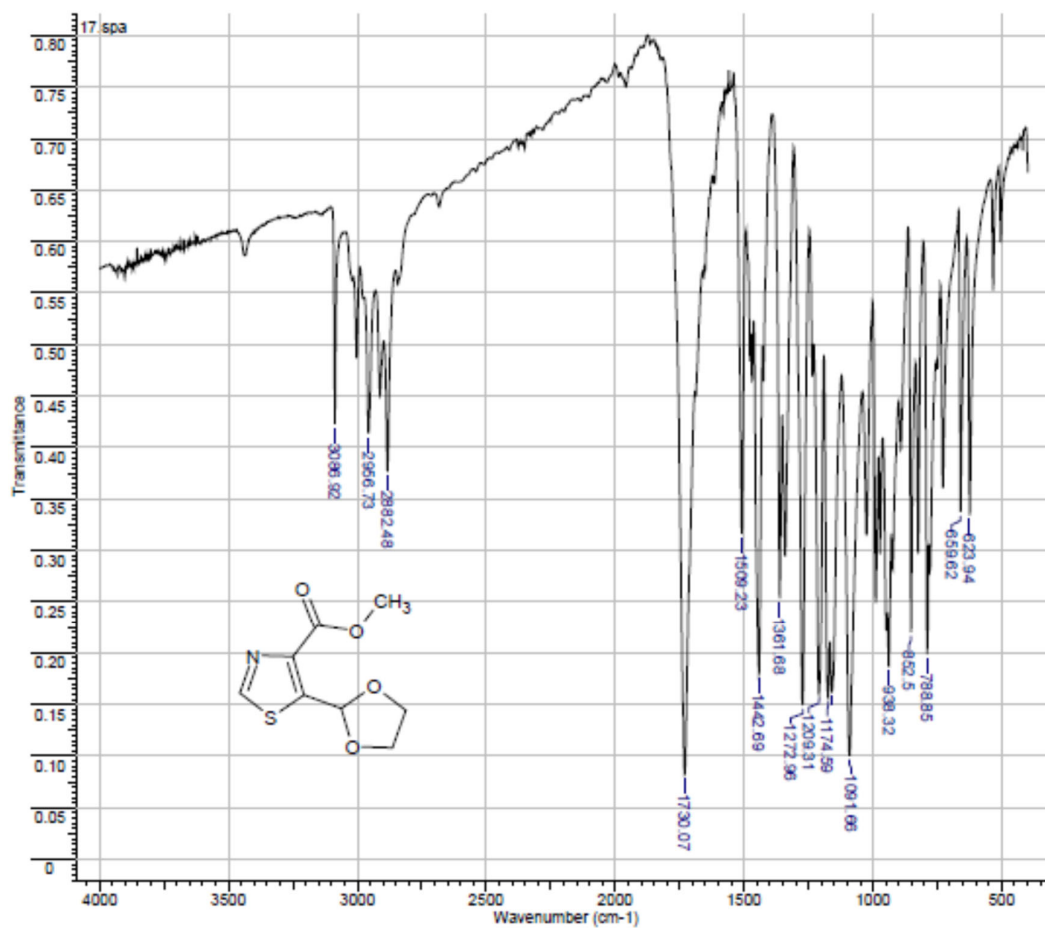
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



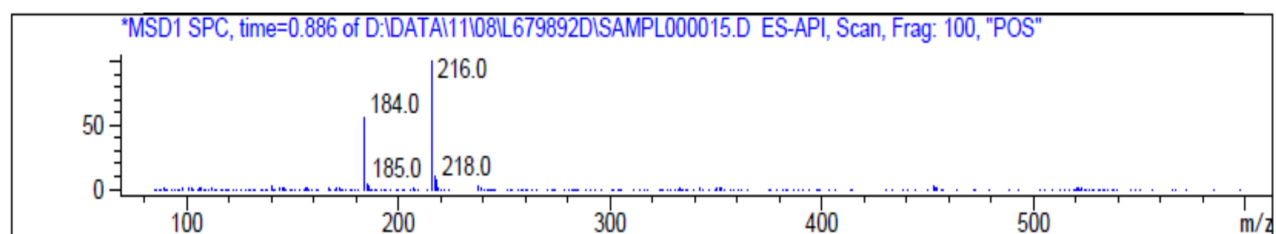
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



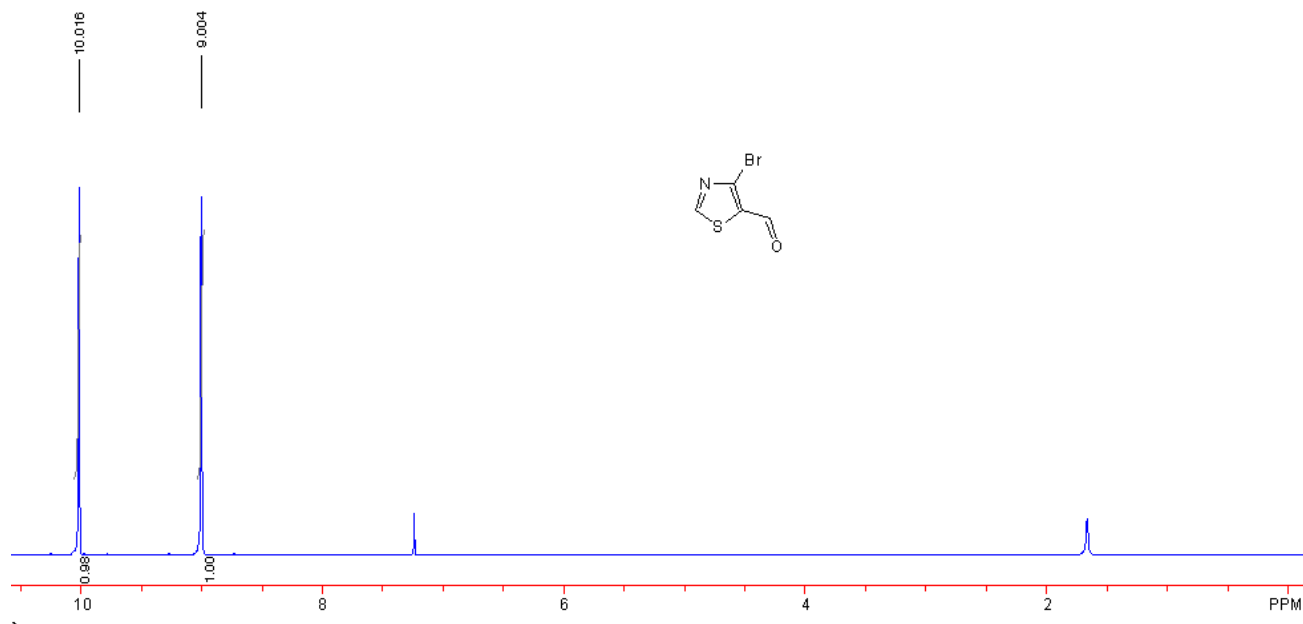
(D) LC/MS spectrum of compound 10



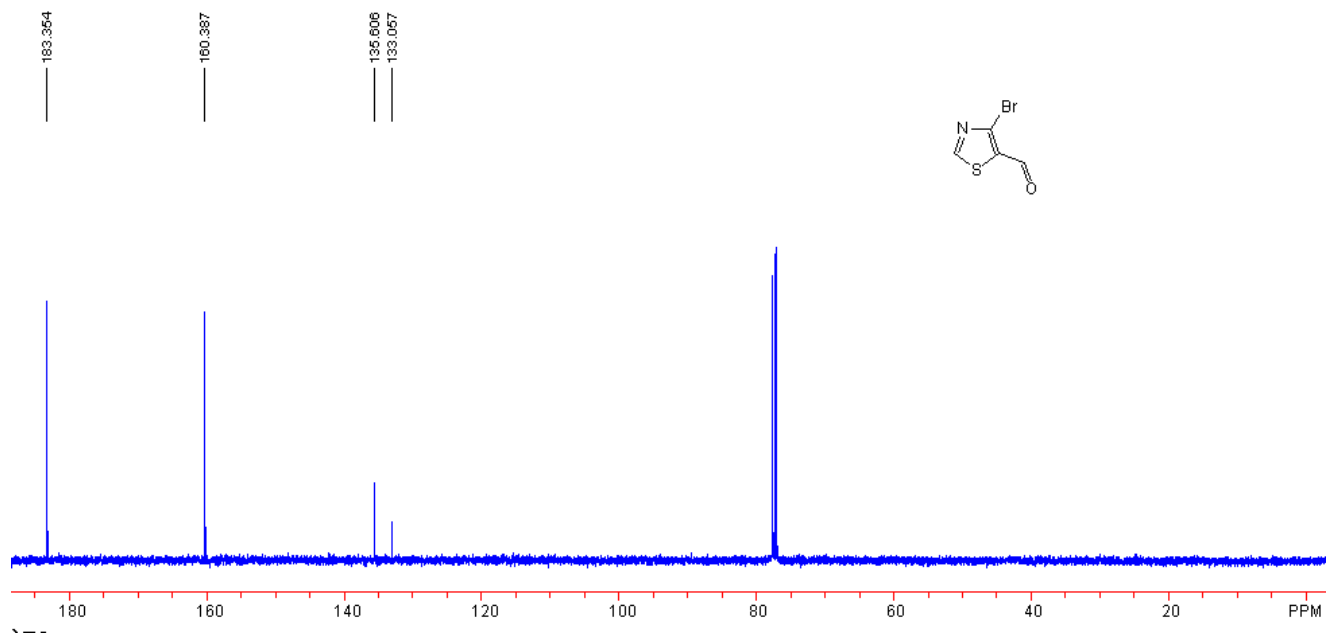
RT = 0.885 min

Figure S10. Compound 11

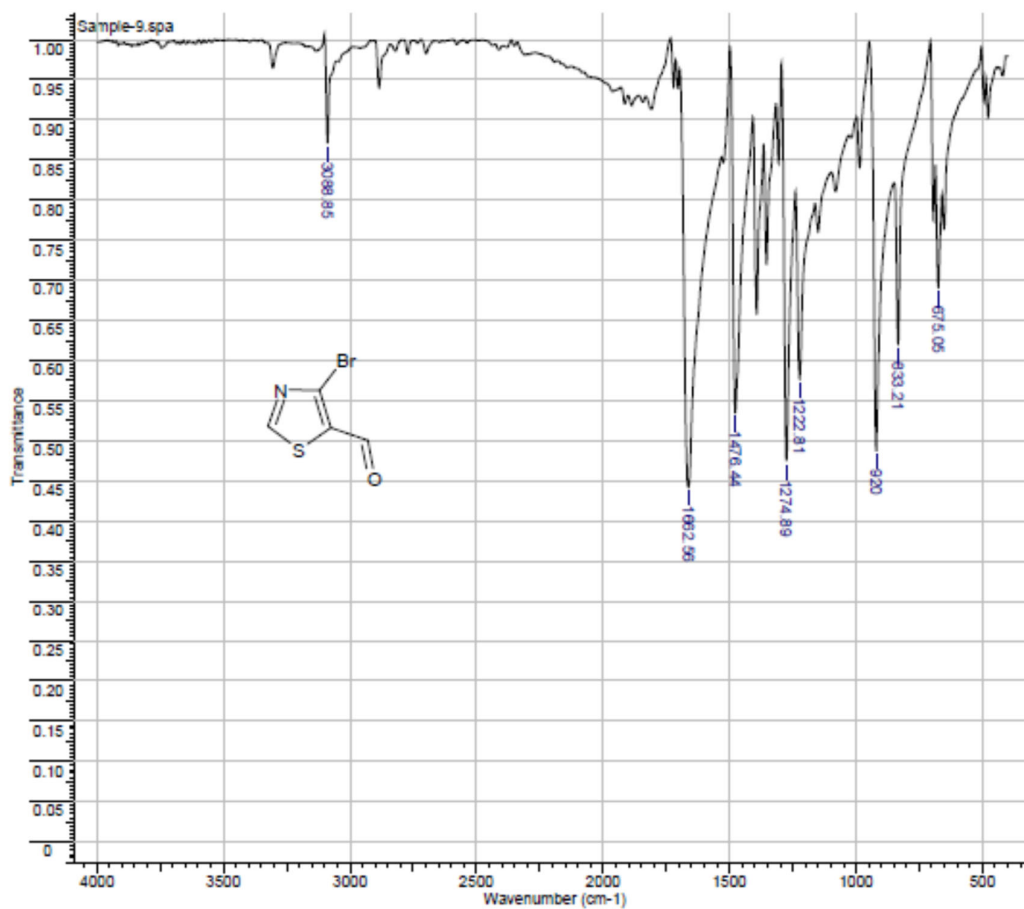
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



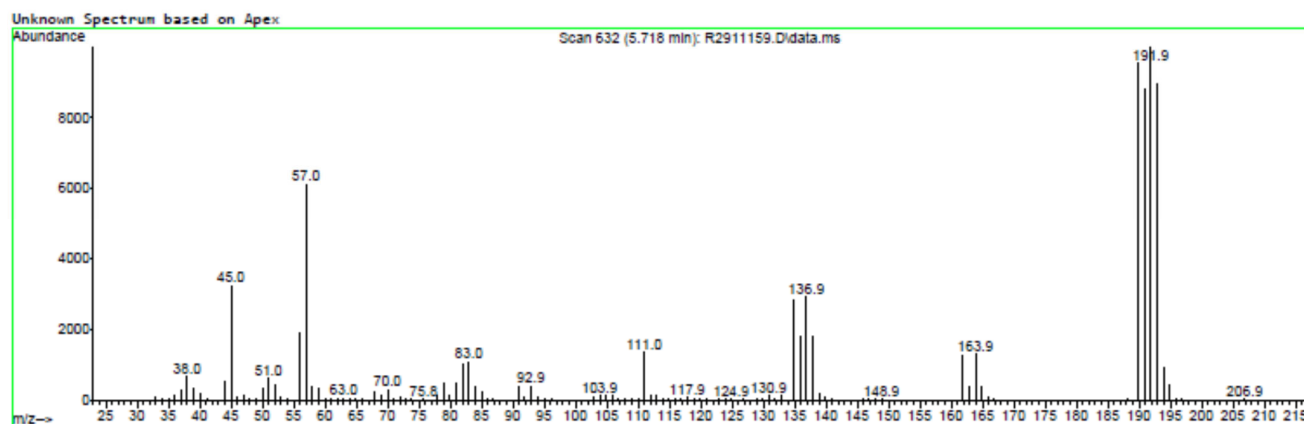
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



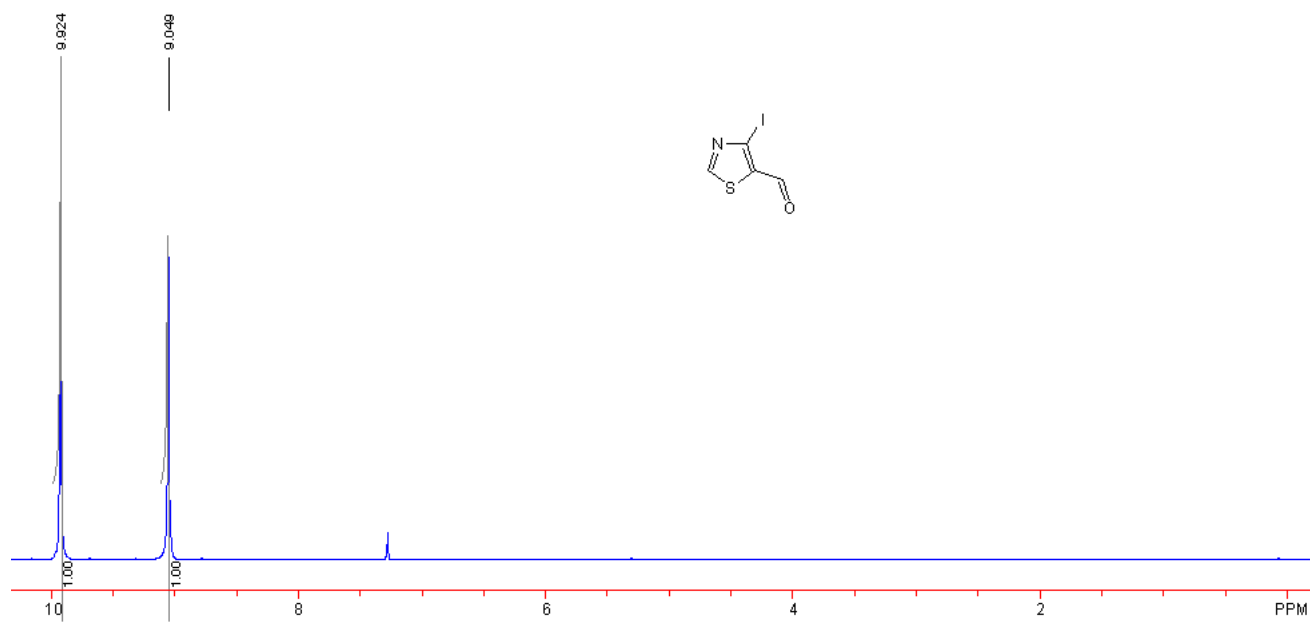
(D) GC/MS spectrum of compound 11



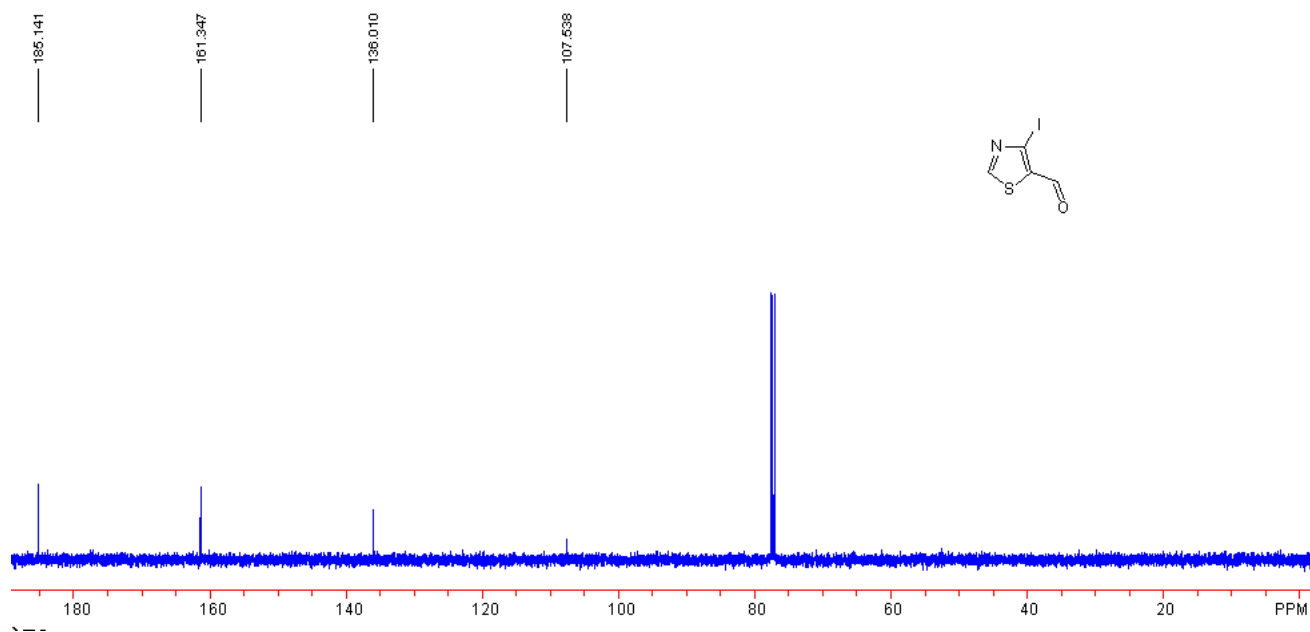
RT = 5.721 min

Figure S11. Compound 12

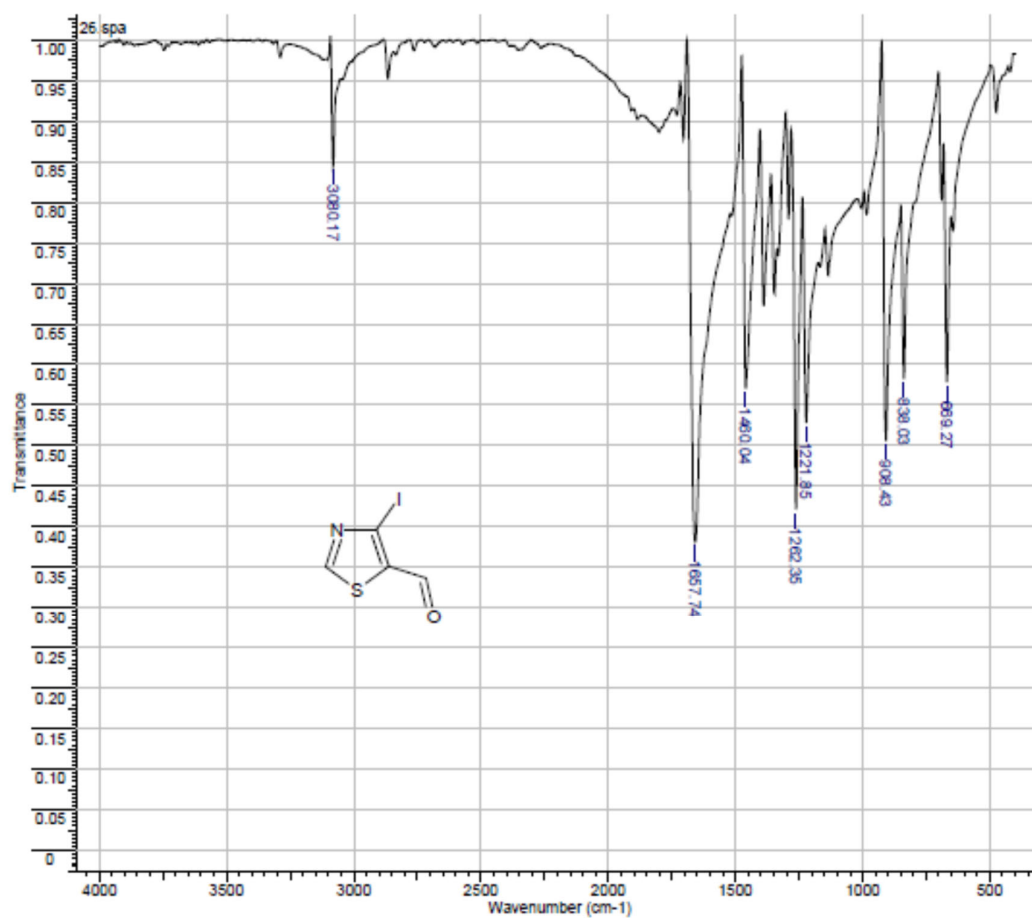
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



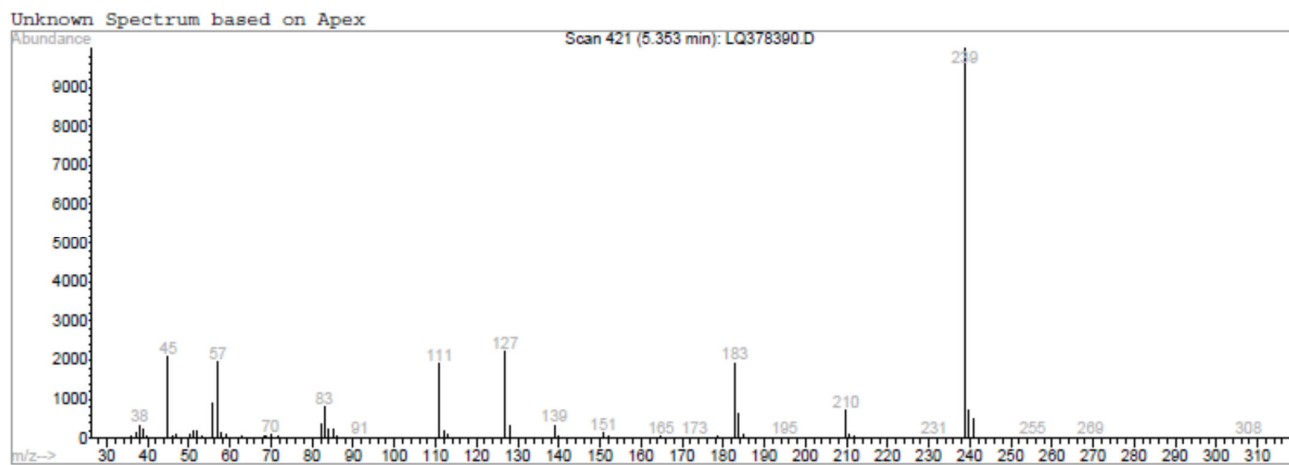
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



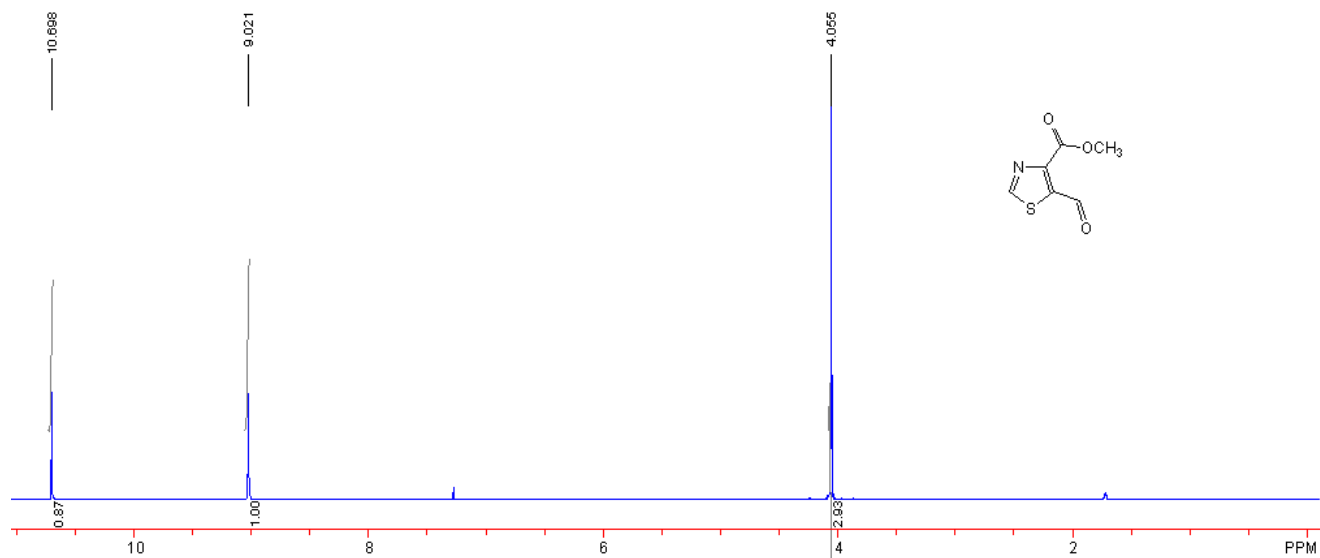
(D) GC/MS spectrum of compound 12



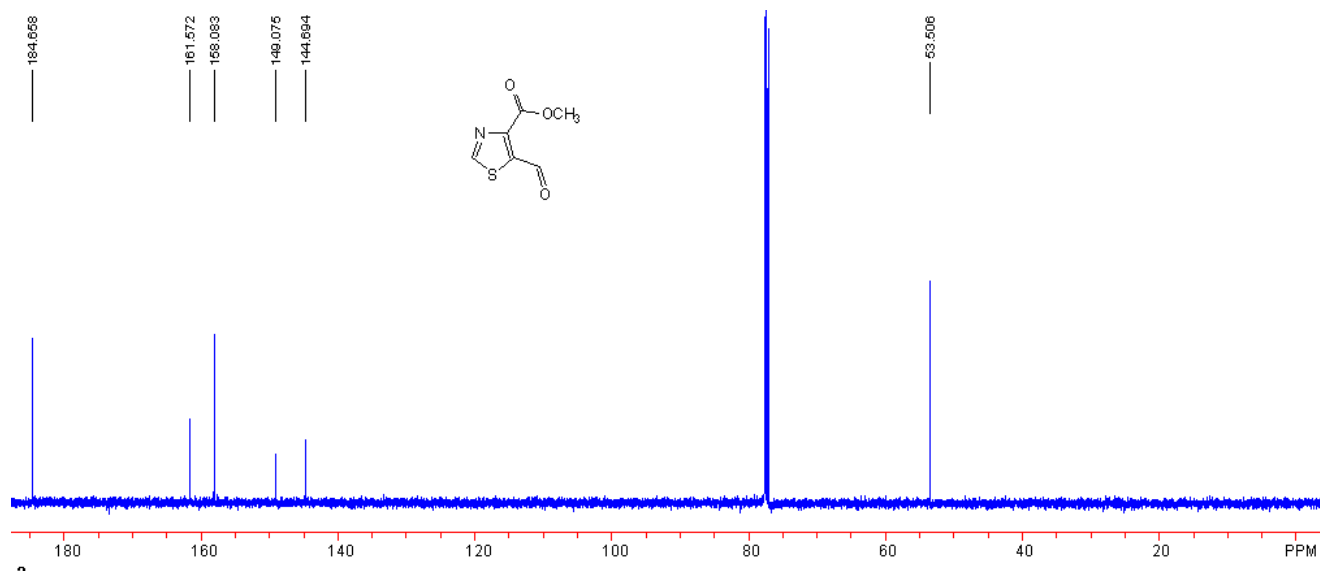
RT = 5.35 min

Figure S12. Compound 13

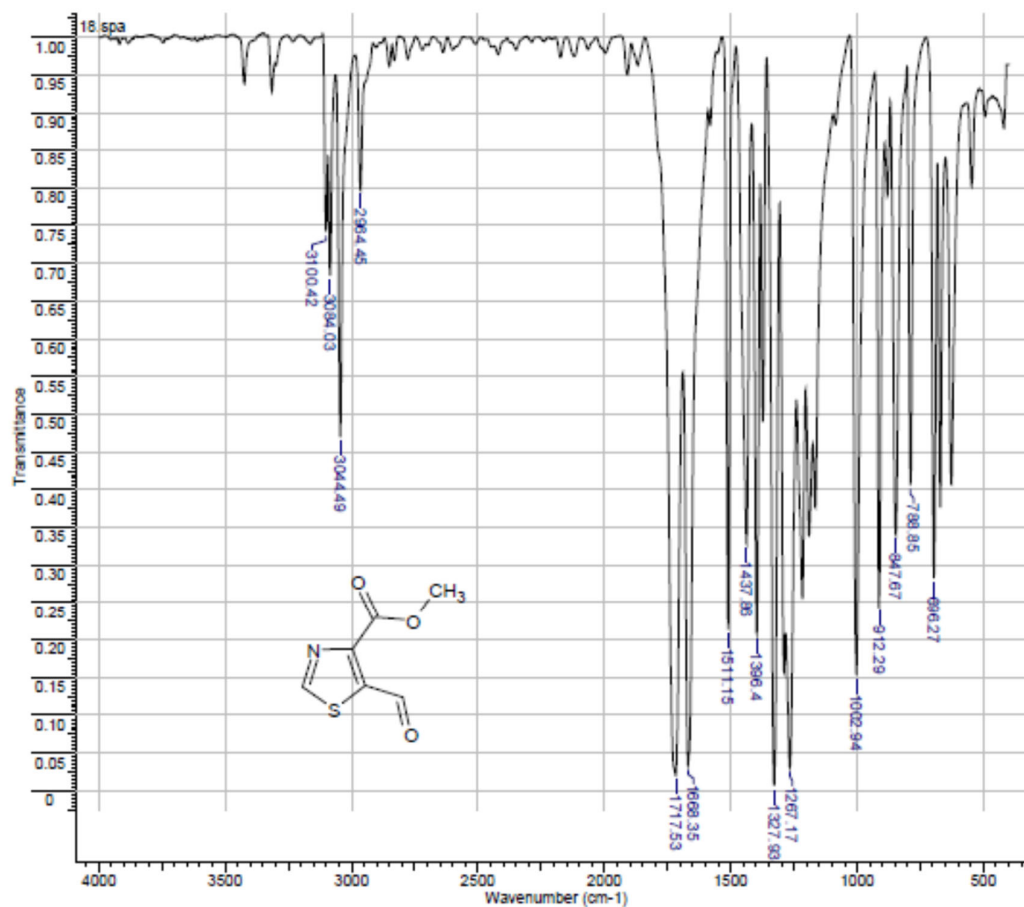
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



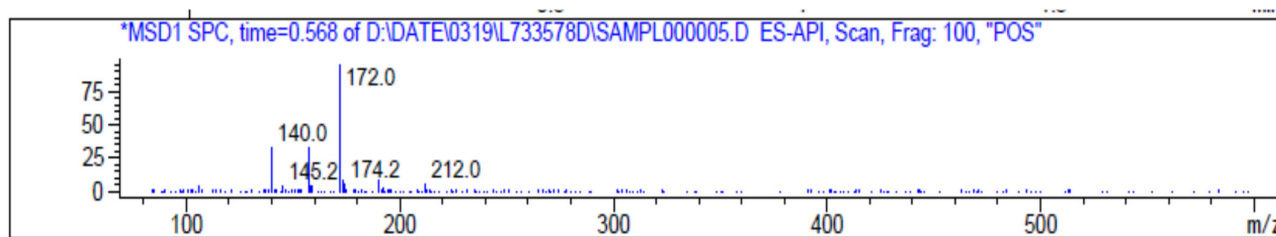
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



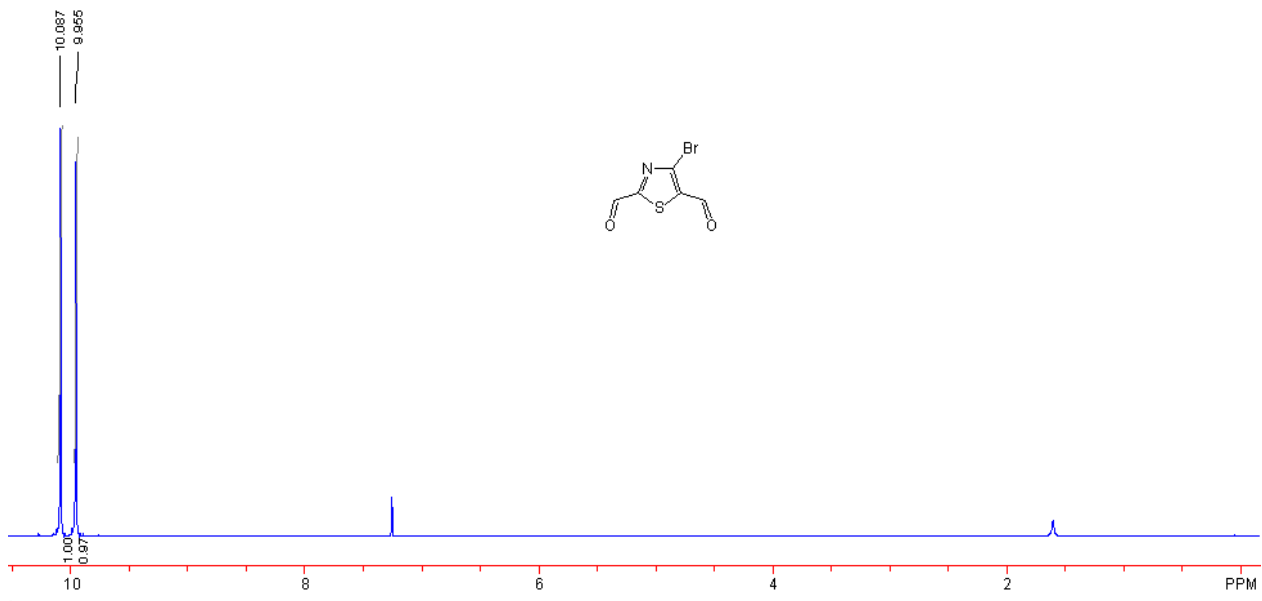
(D) LC/MS spectrum of compound 13



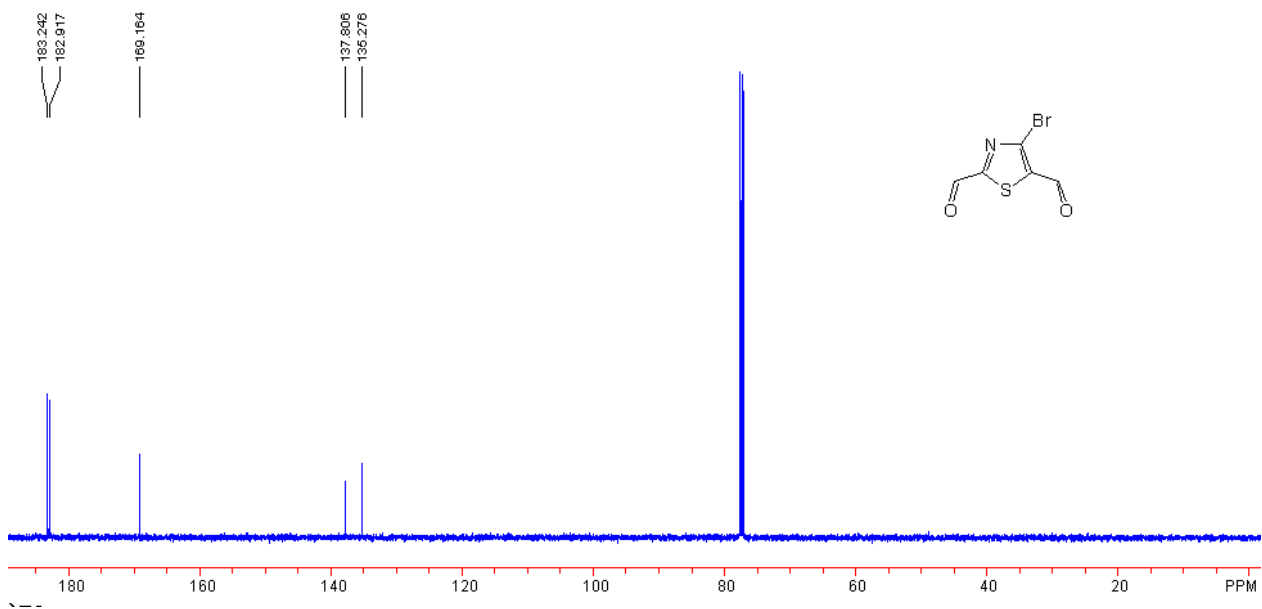
RT = 0.568 min

Figure S13. Compound 14

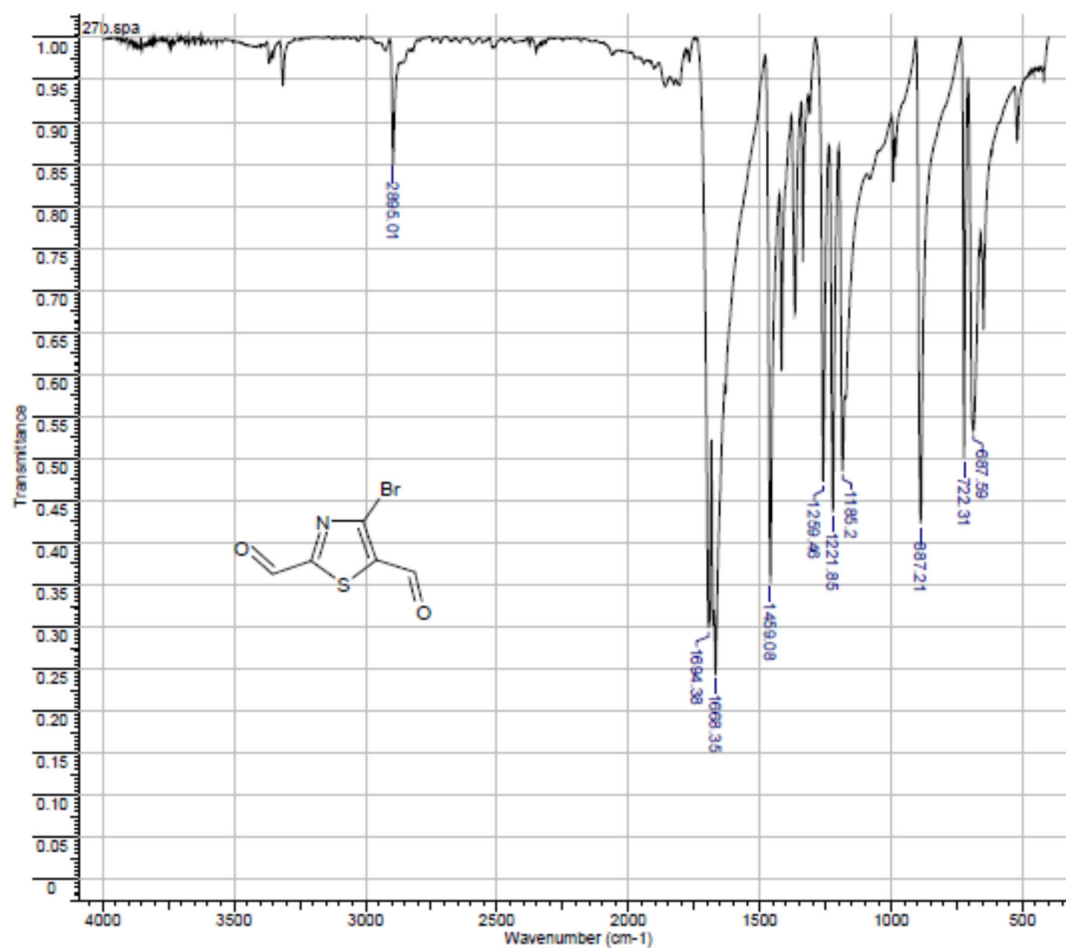
(A) ^1H -NMR spectrum (CDCl_3)



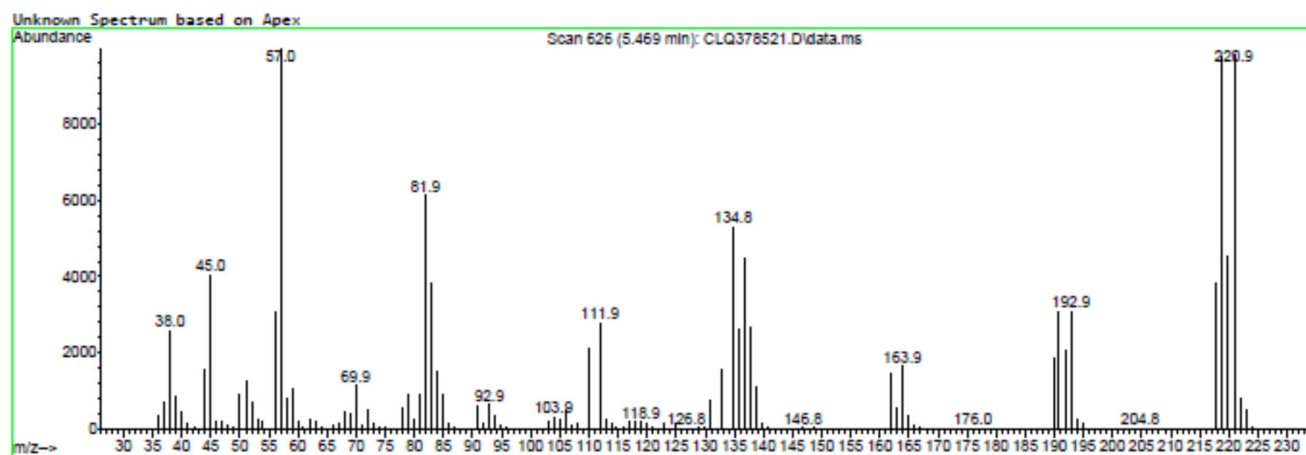
(B) ^{13}C -NMR spectrum (CDCl_3)



(C) IR spectrum (KBr)



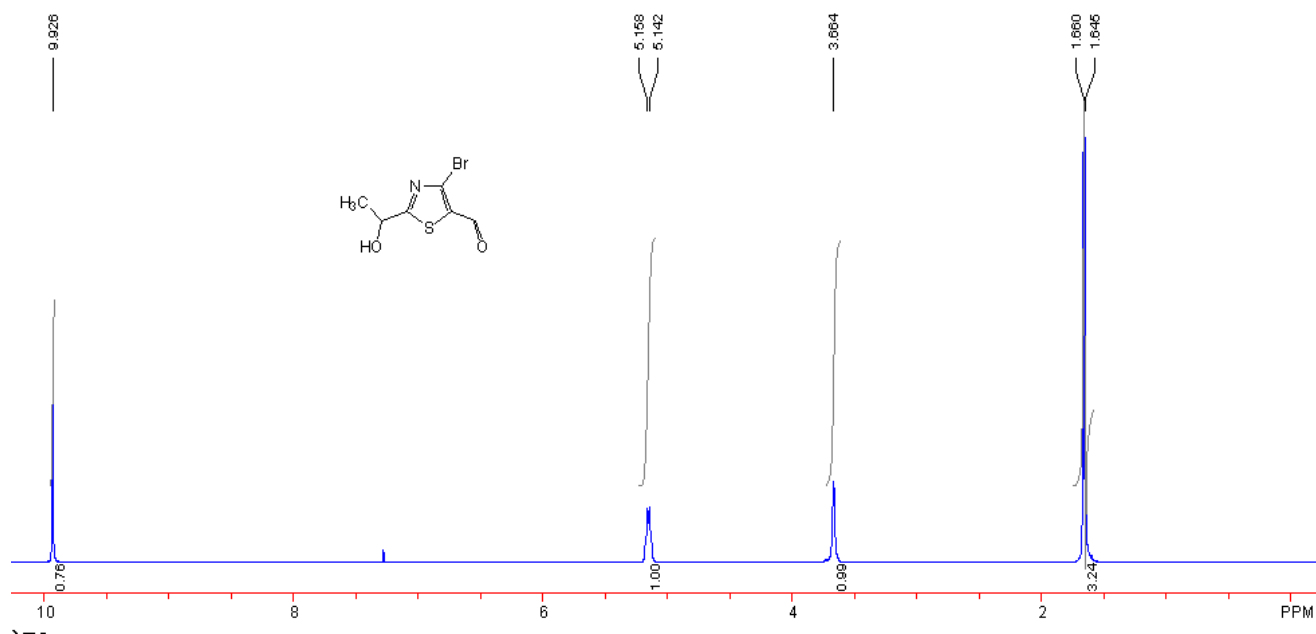
(D) GC/MS spectrum of compound 14



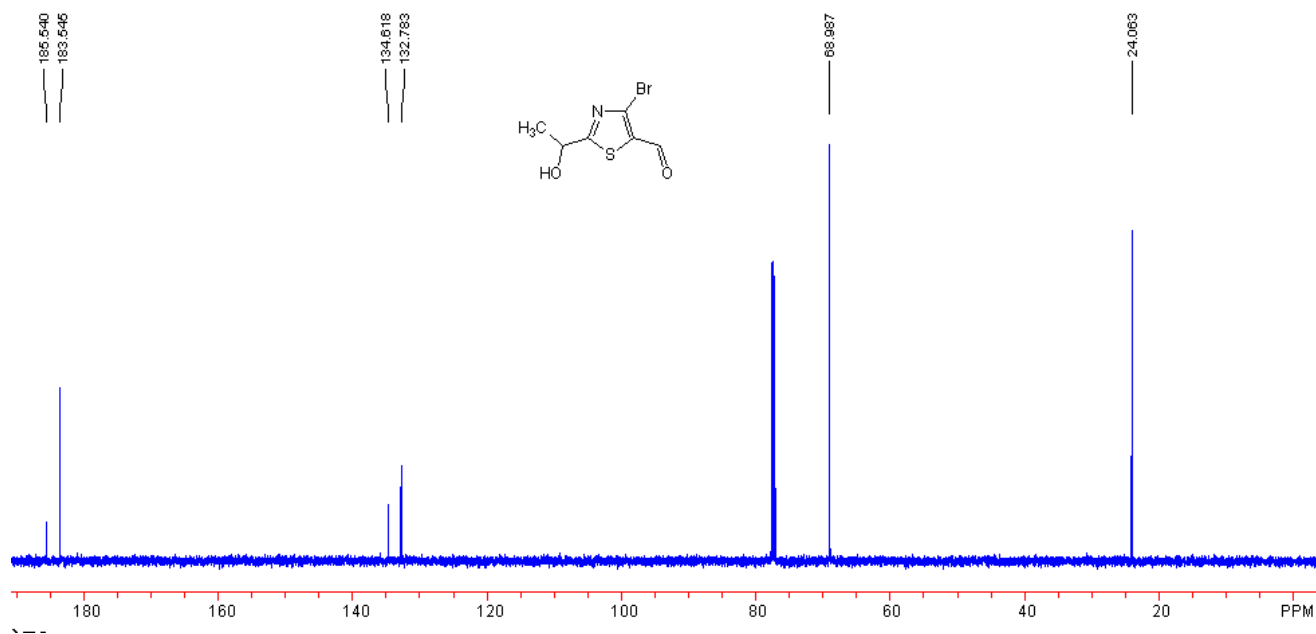
RT = 5.470 min

Figure S14. Compound 15

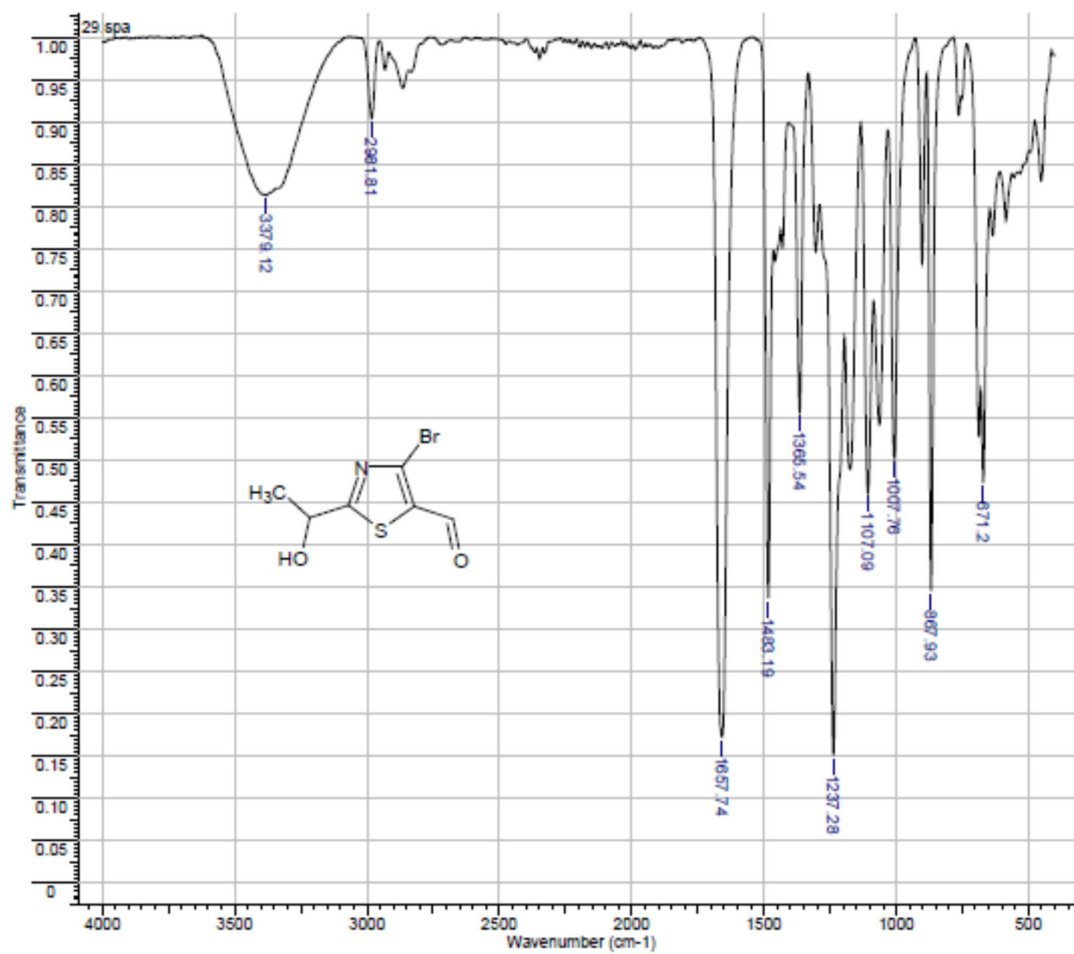
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



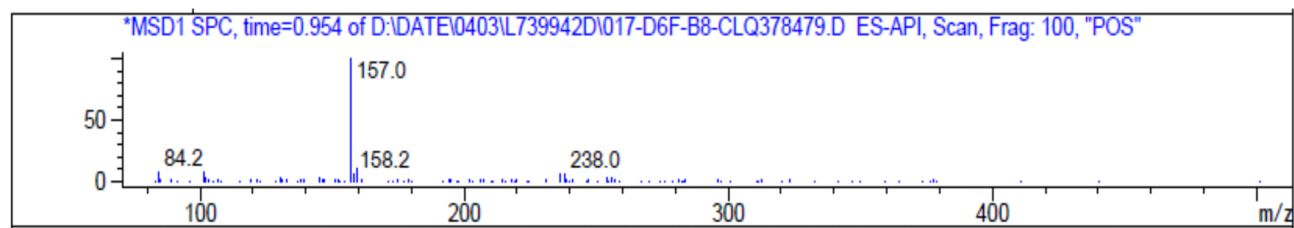
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) ATR-IR spectrum



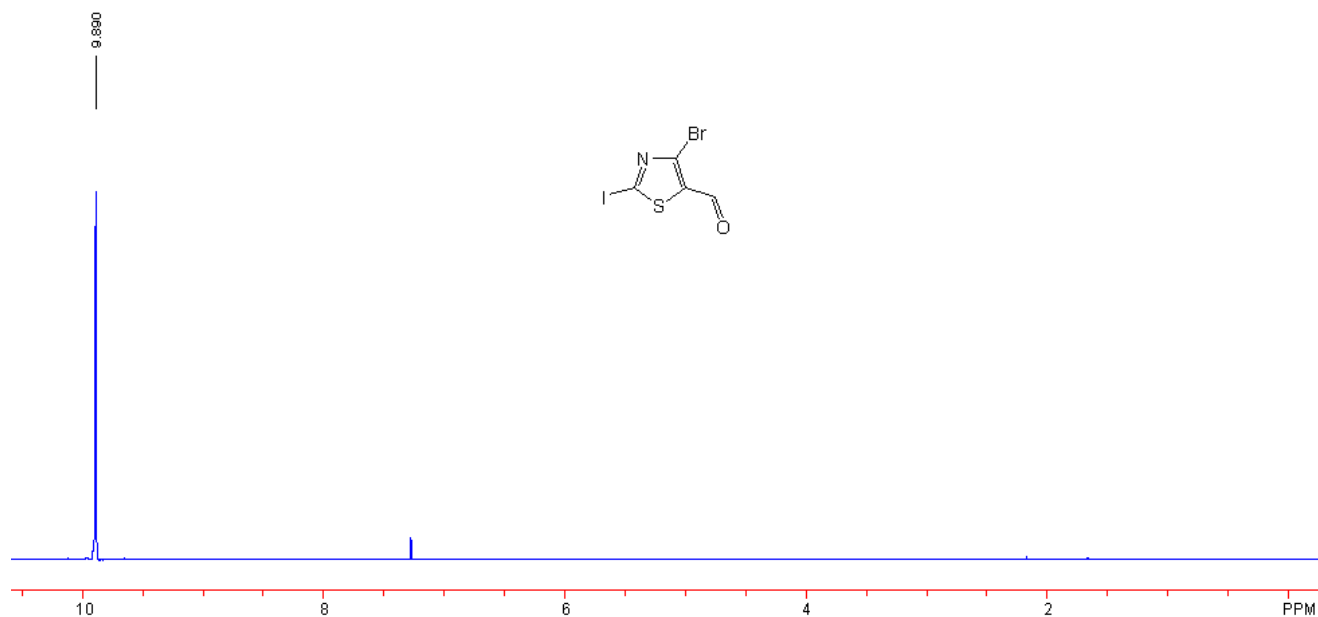
(D) LC/MS spectrum of compound 15



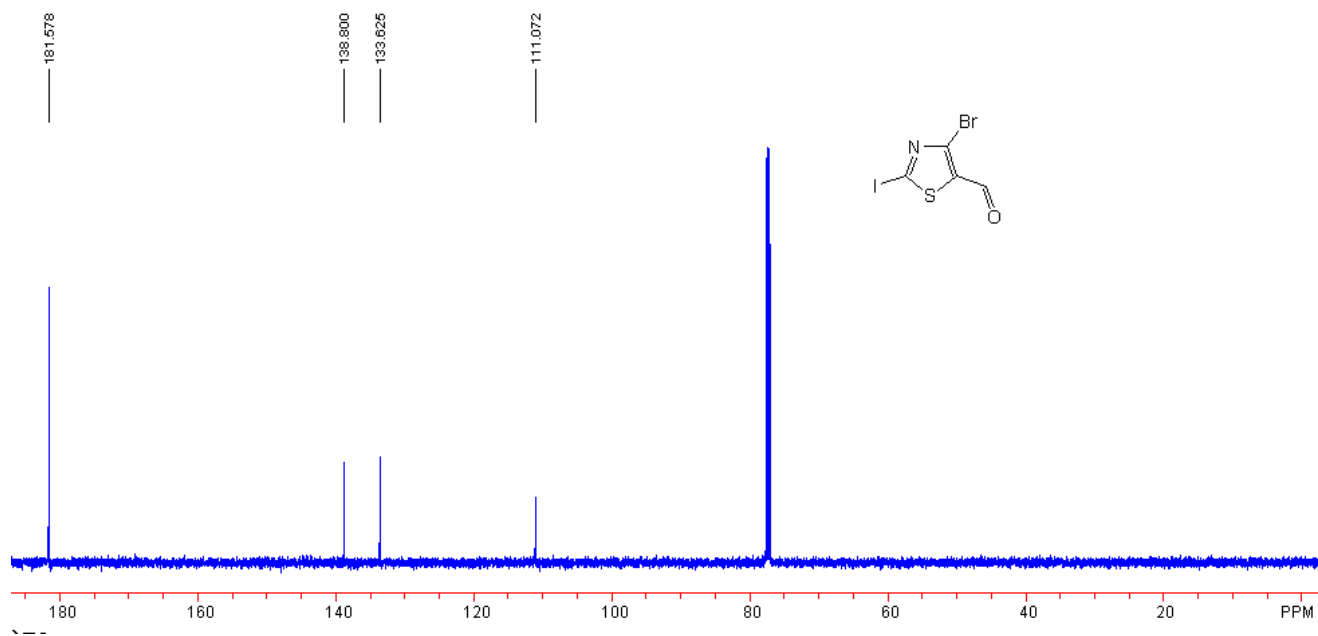
RT = 0.958 min

Figure S15. Compound 16

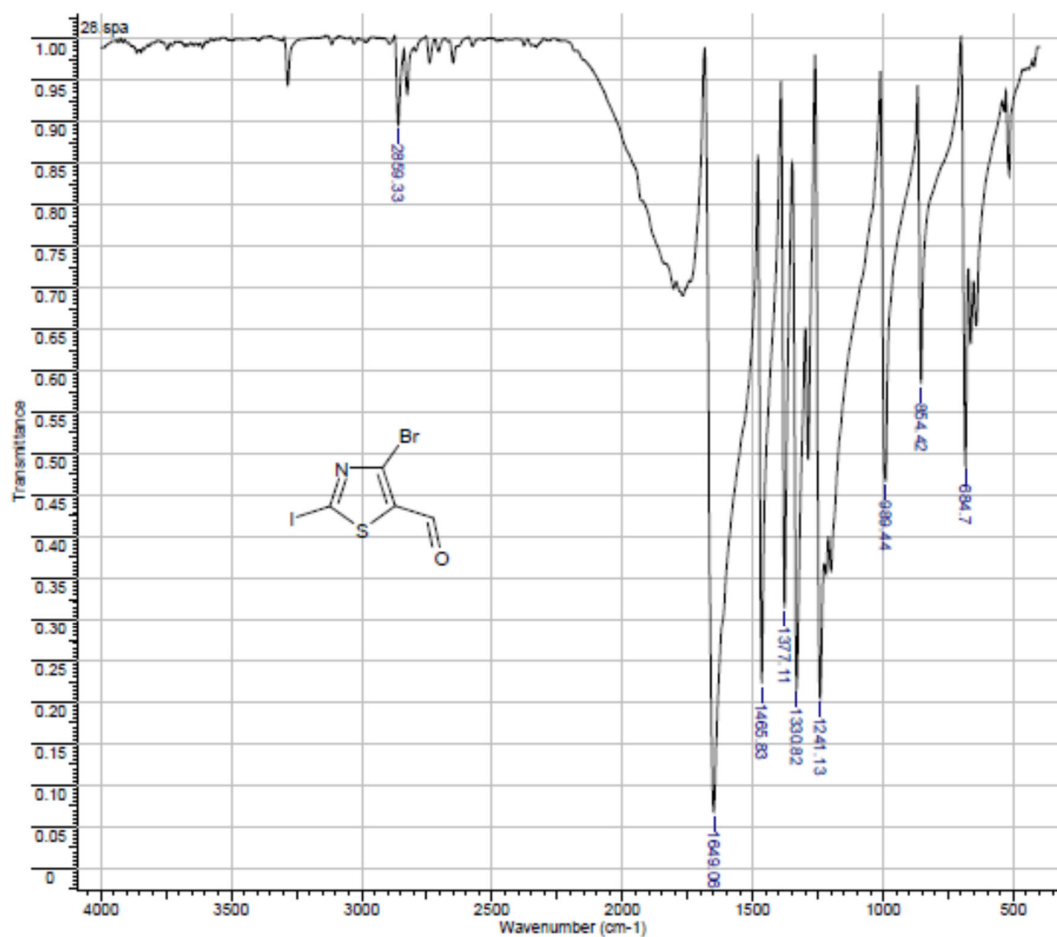
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



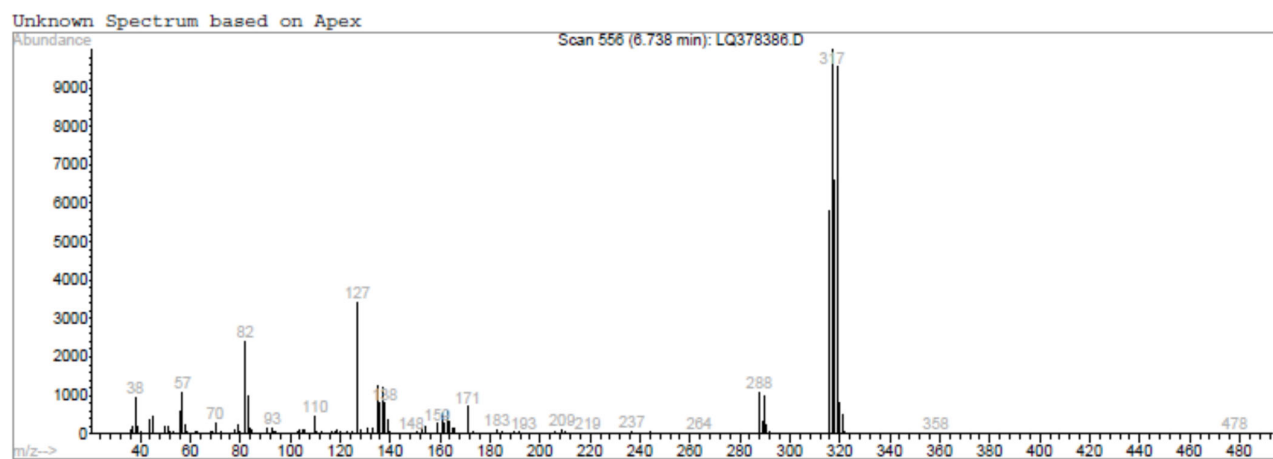
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)



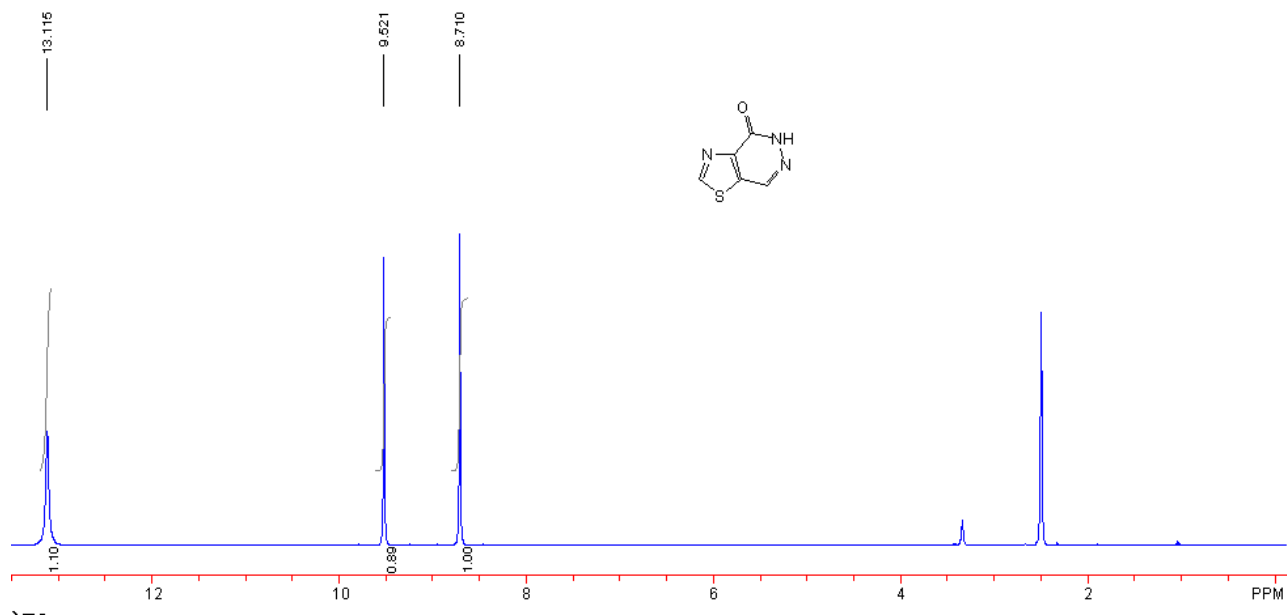
(D) GC/MS spectrum of compound 16



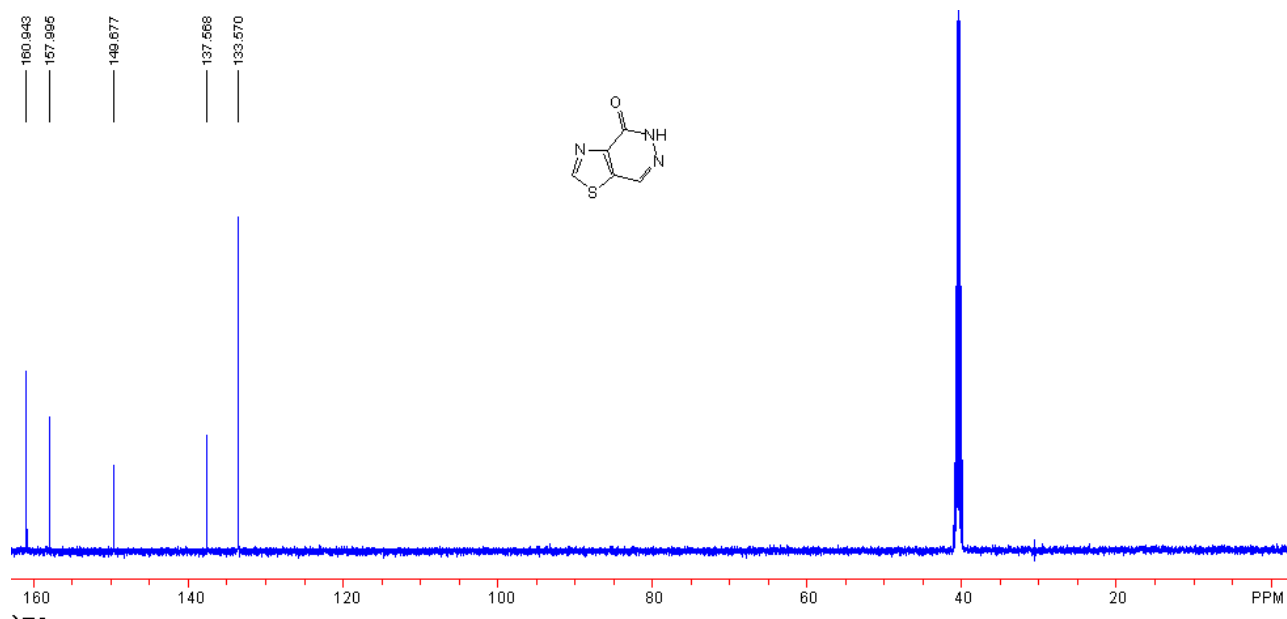
RT = 6.74 min

Figure S16. Compound 17

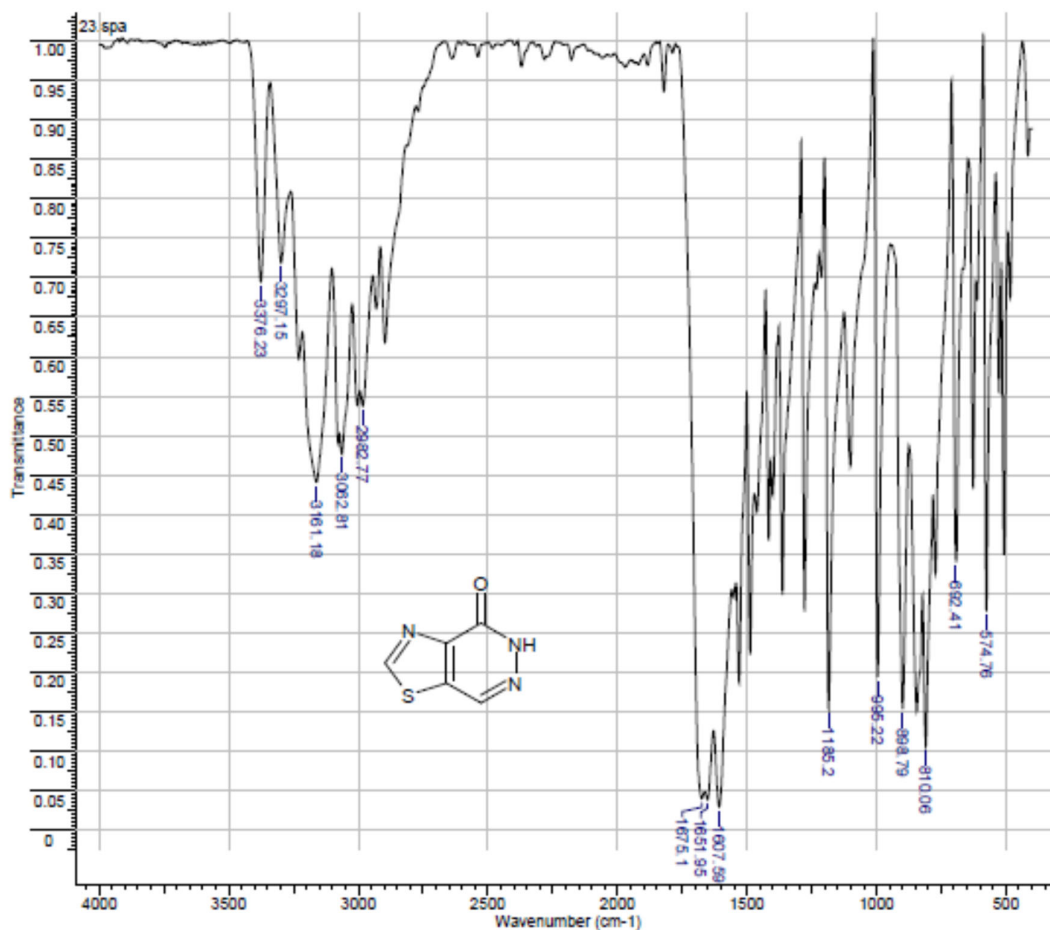
(A) ^1H -NMR spectrum (DMSO- d_6)



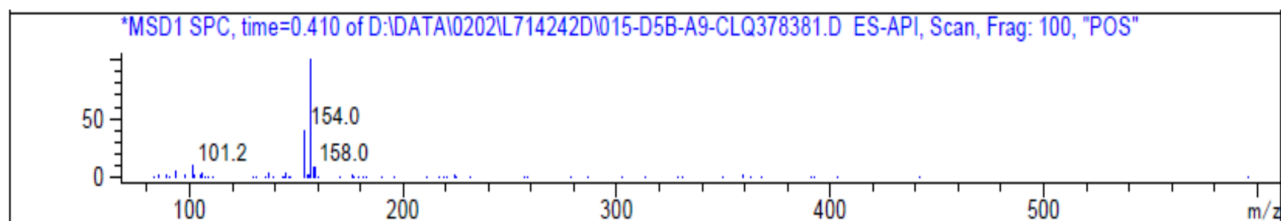
(B) ^{13}C -NMR spectrum (DMSO- d_6)



(C) IR spectrum (KBr)



(D) LC/MS spectrum of compound 17



RT = 0.408 min

Figure S17. Compound 18. IR spectrum (KBr)

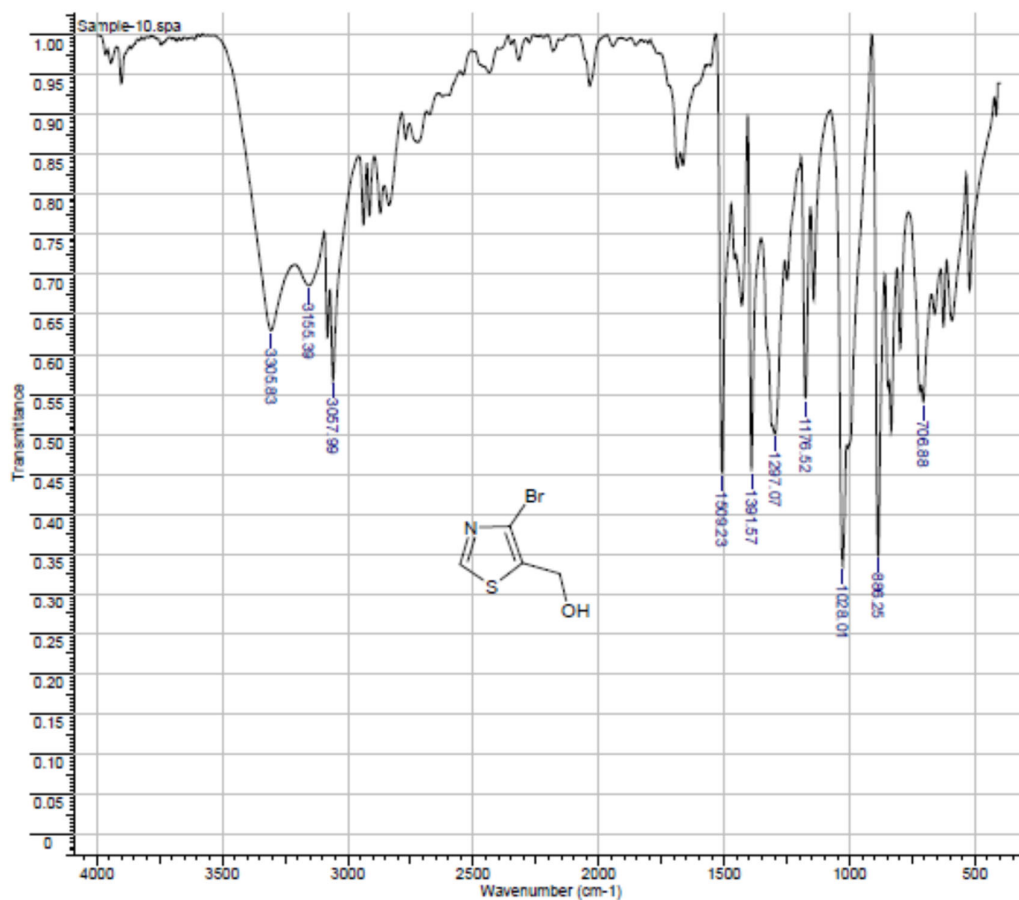
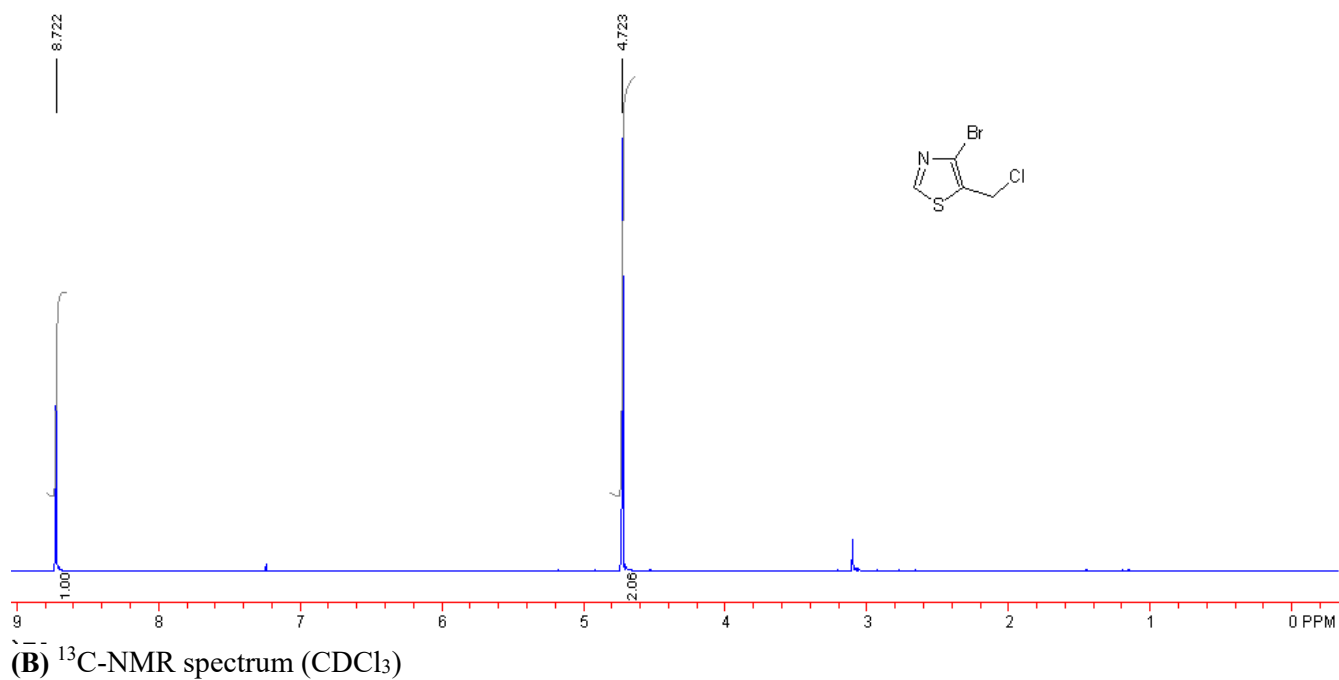
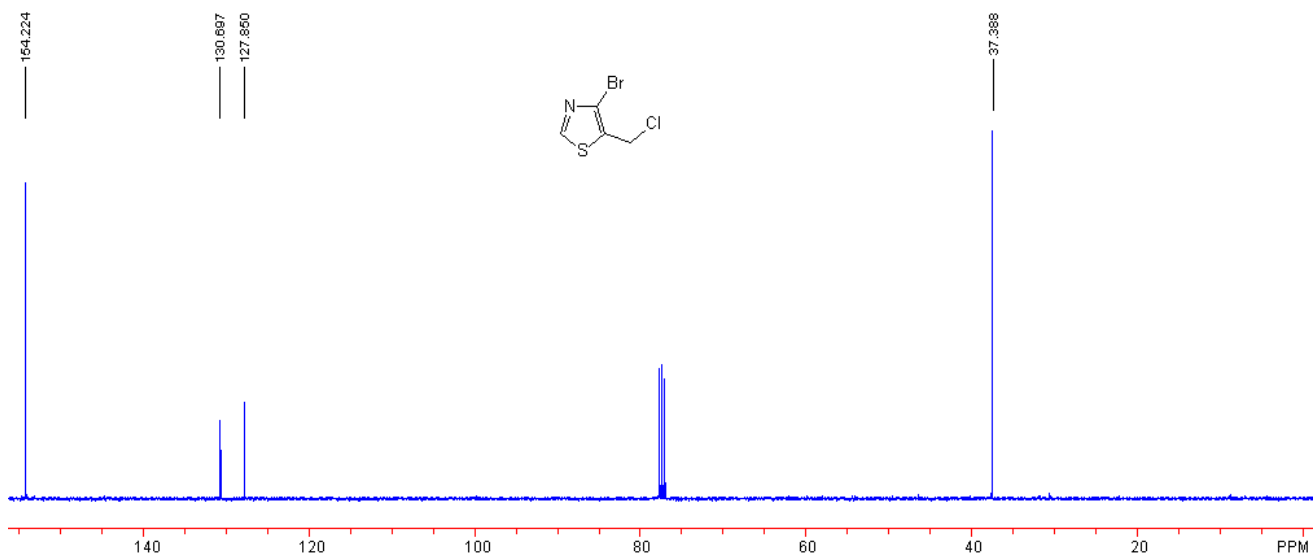
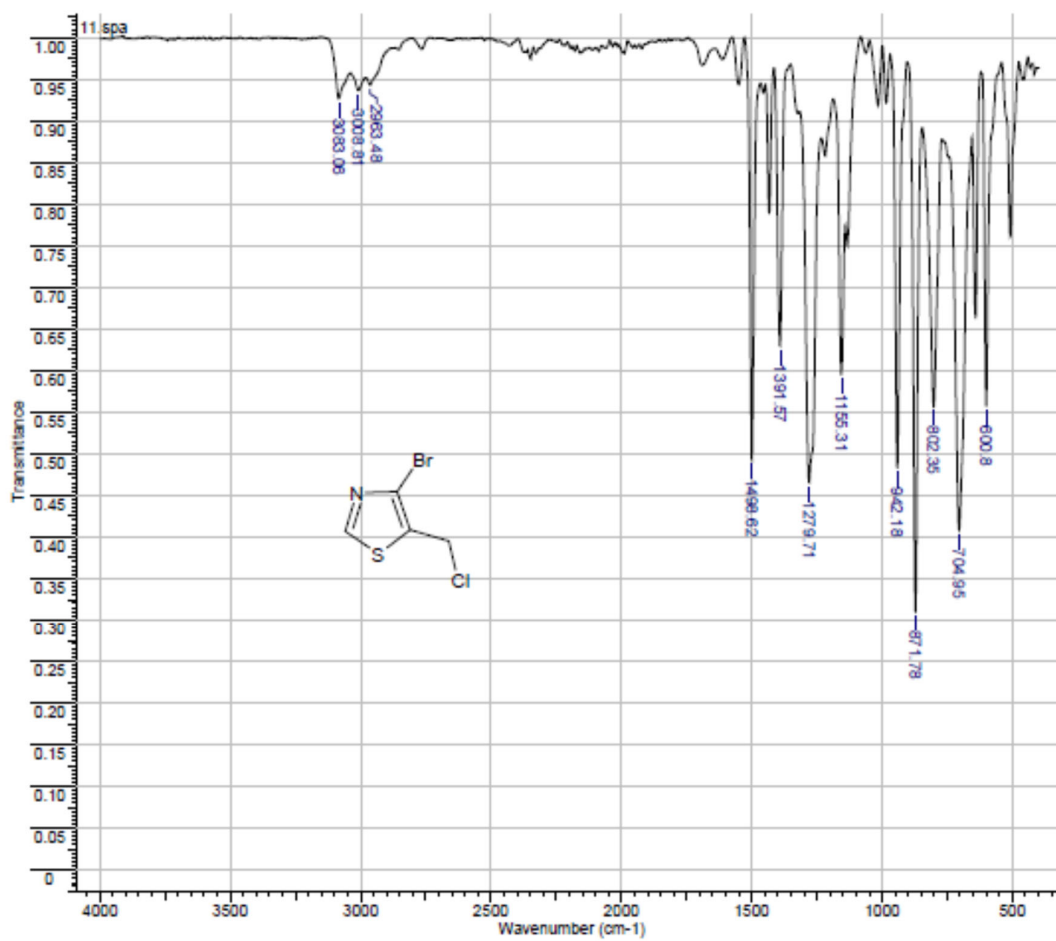


Figure S18. Compound 19
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)

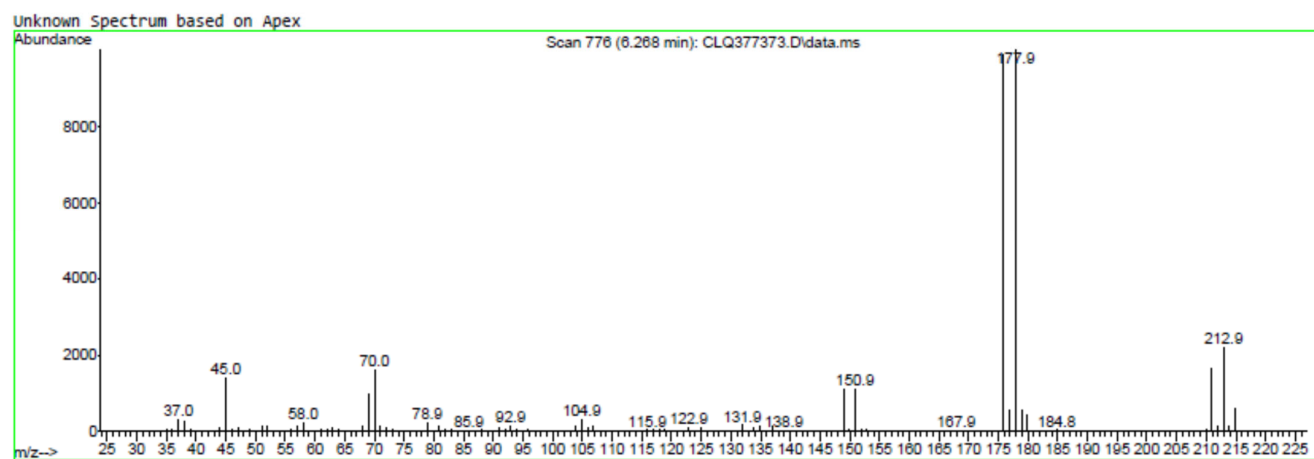




(C) ATR-IR spectrum



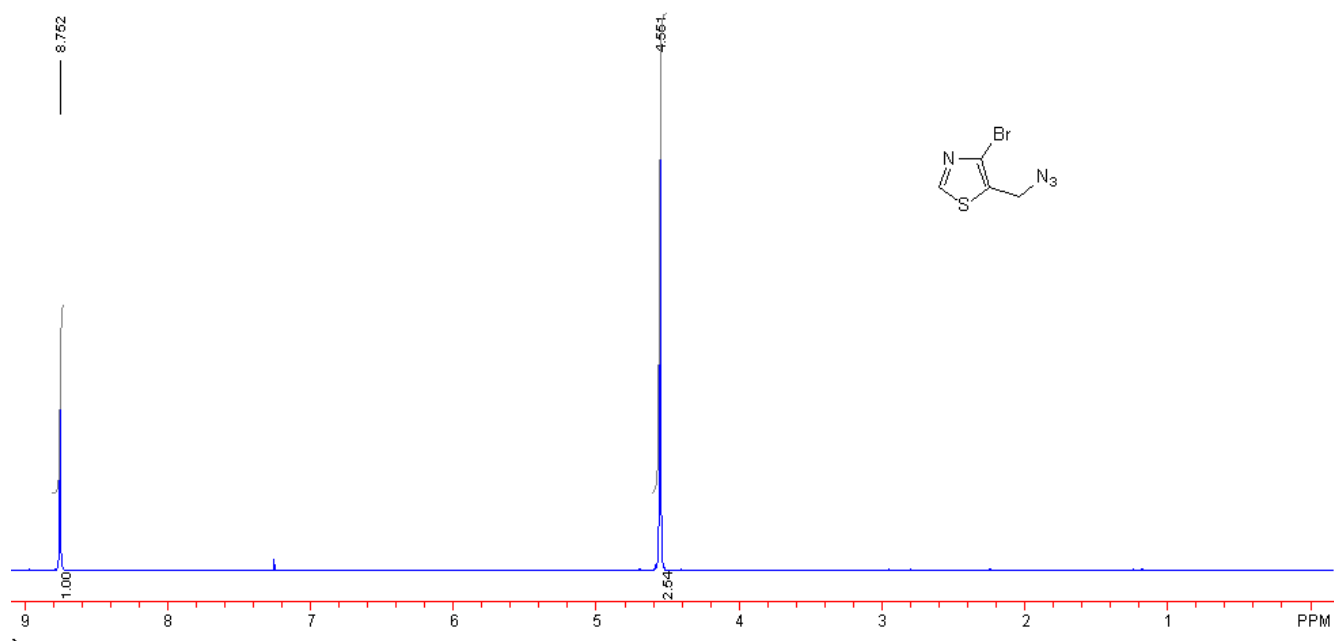
(D) GC/MS spectrum of compound 19



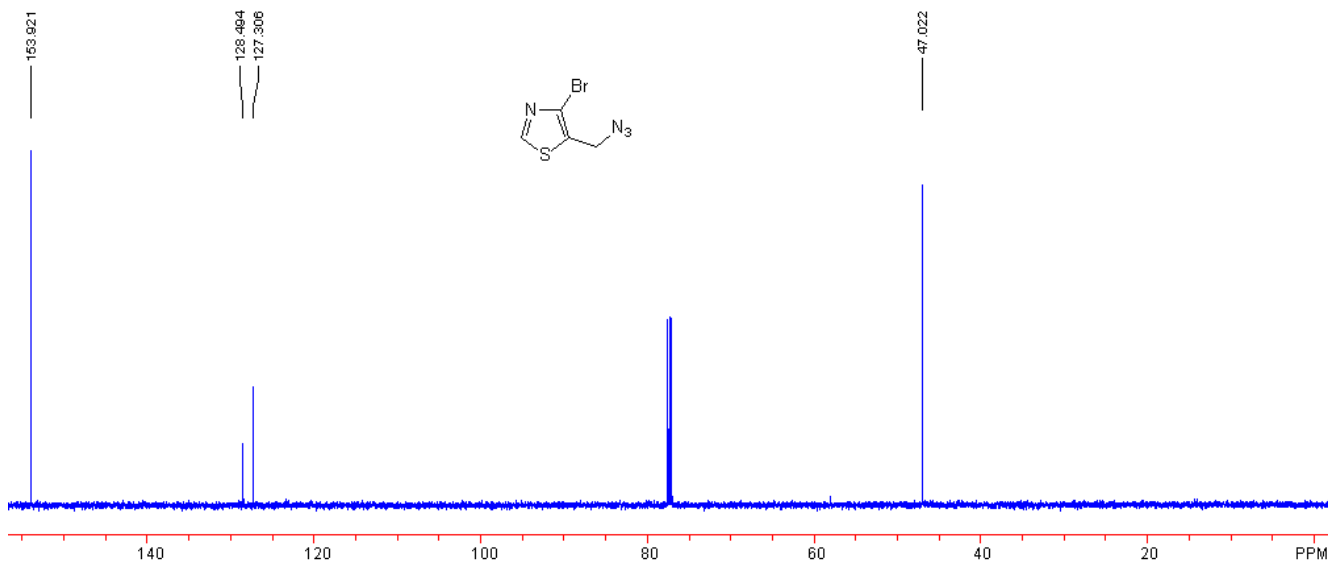
RT = 6.267 min

Figure S19. Compound 20

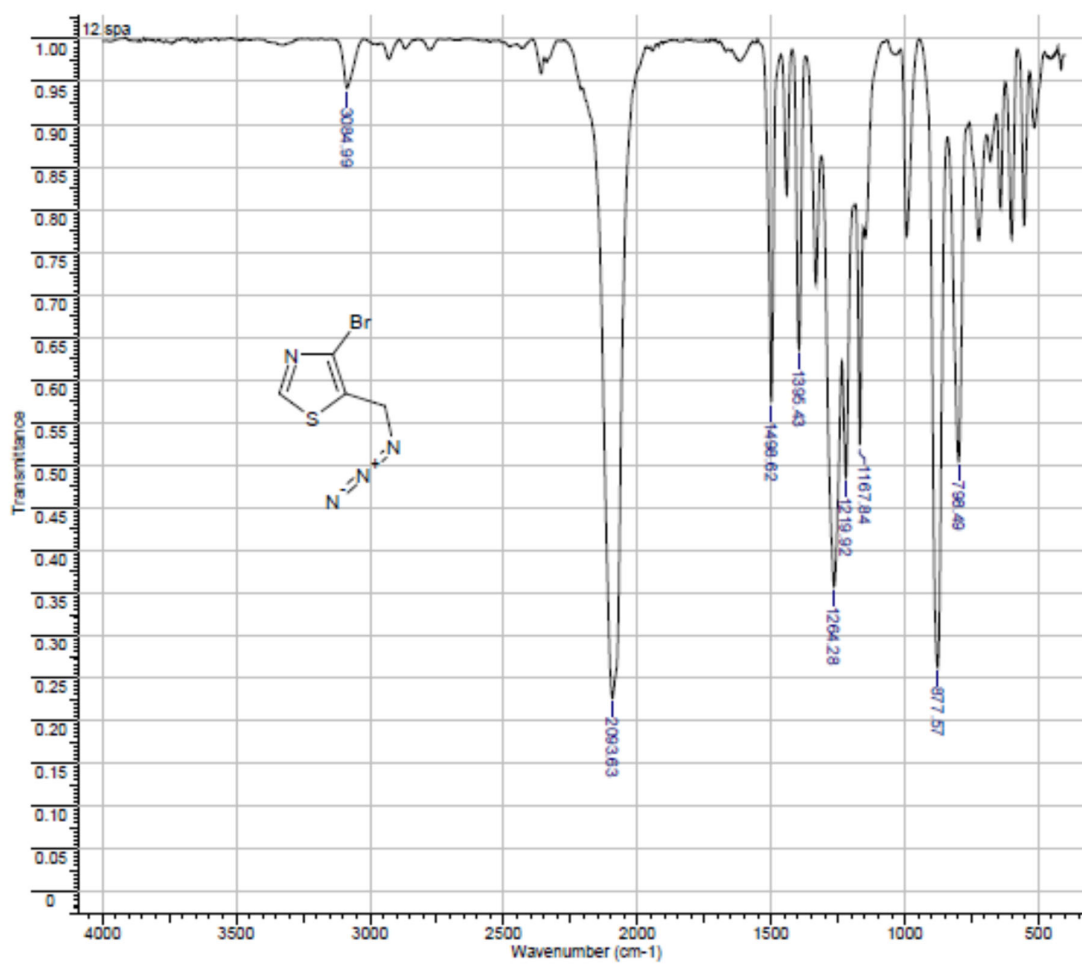
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



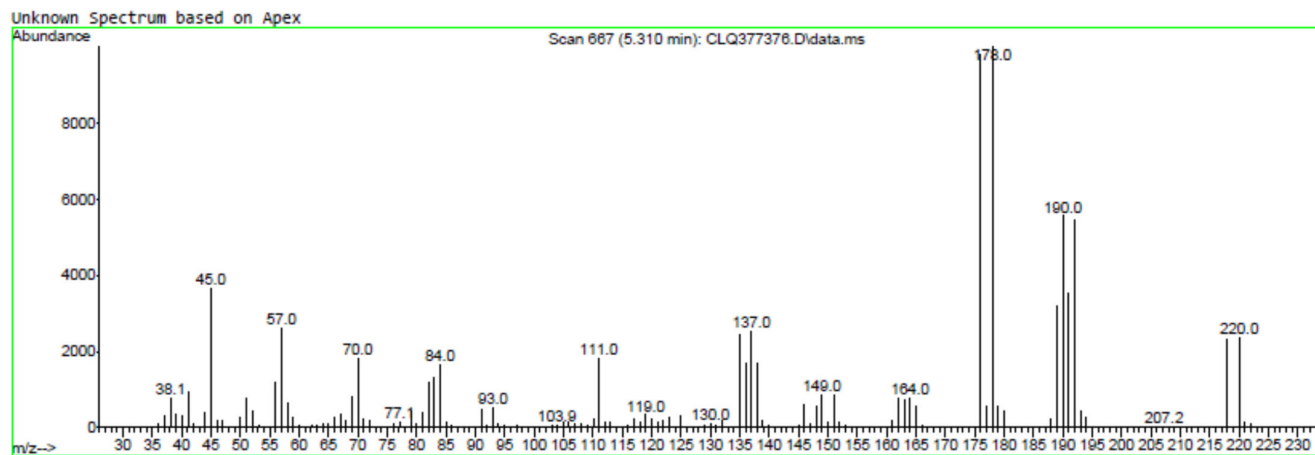
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) ATR-IR spectrum

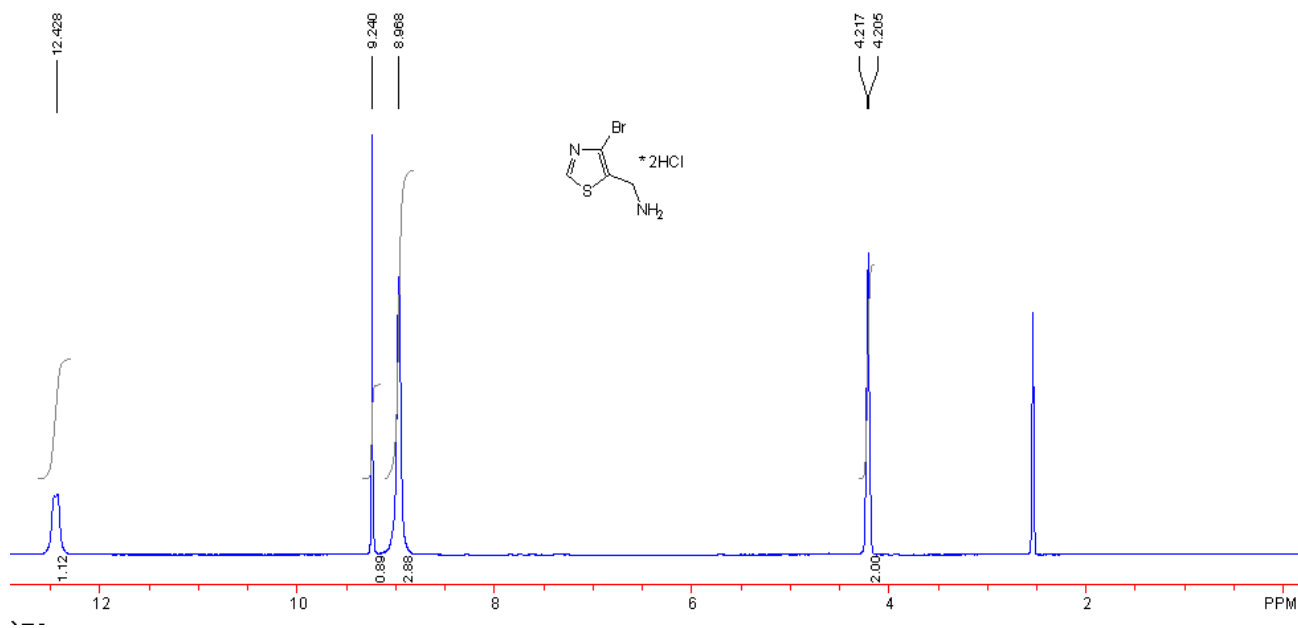


(D) GC/MS spectrum of compound 20

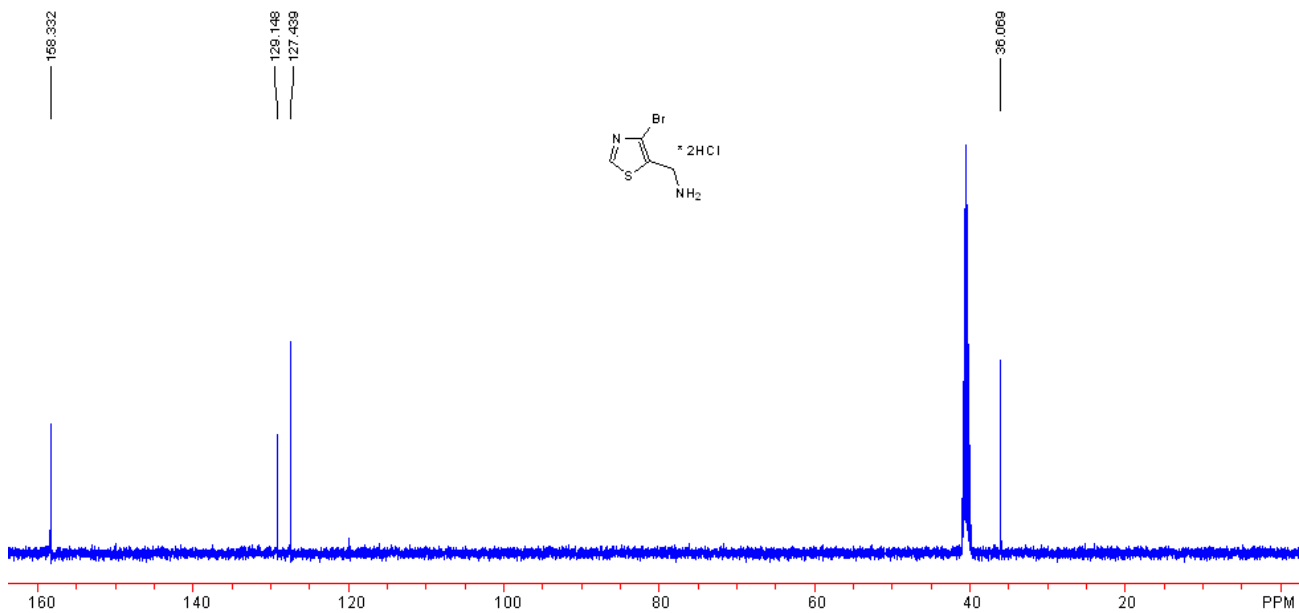


RT = 5.311 min

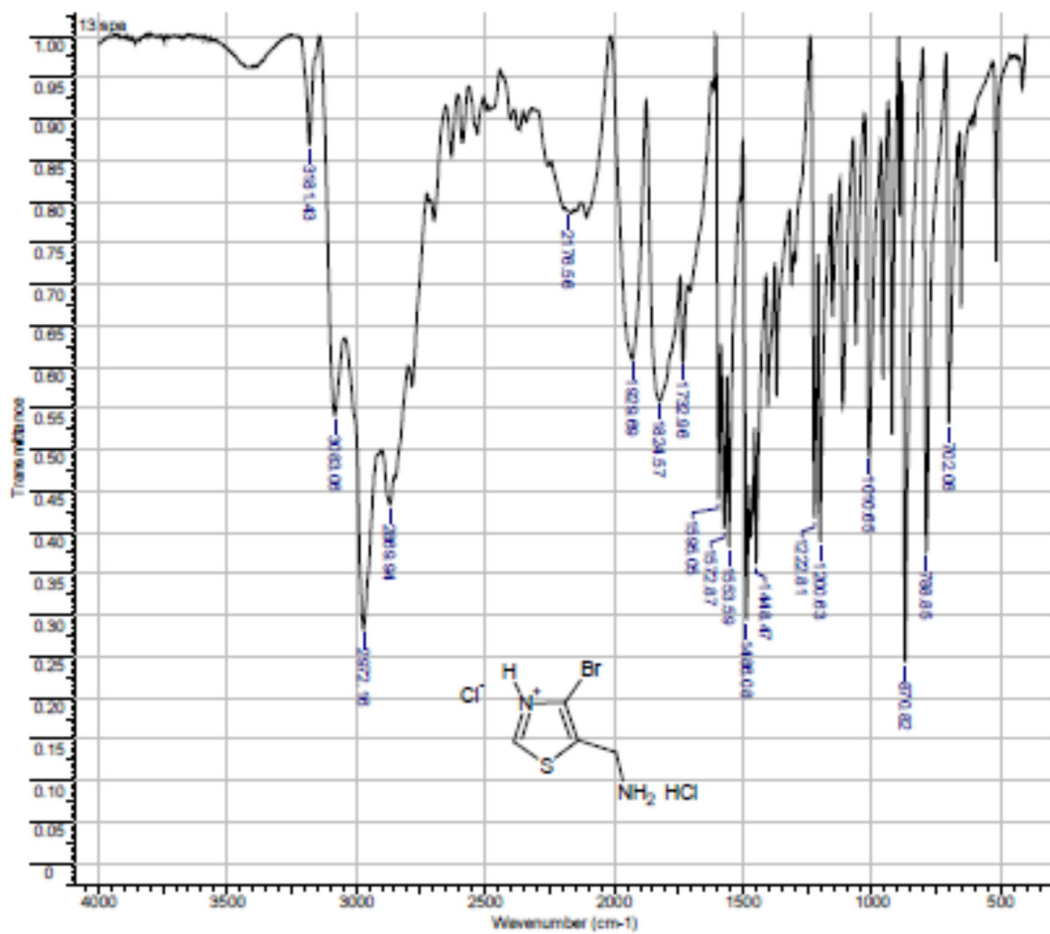
Figure S20. Compound 21
(A) $^1\text{H-NMR}$ spectrum (DMSO- d_6)



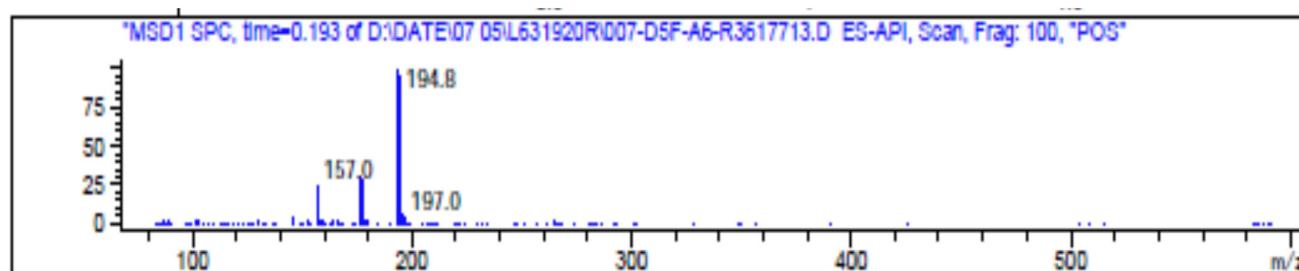
(B) $^{13}\text{C-NMR}$ spectrum (DMSO- d_6)



(C) IR spectrum (KBr)

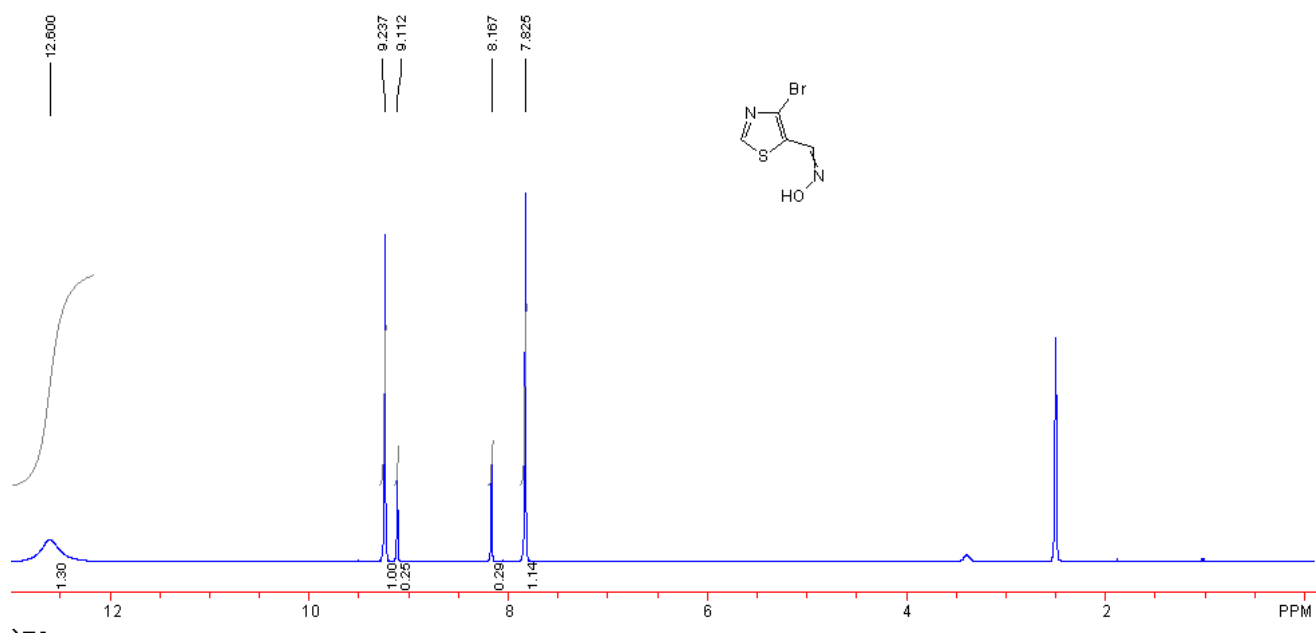


(D) LC/MS spectrum of compound 21

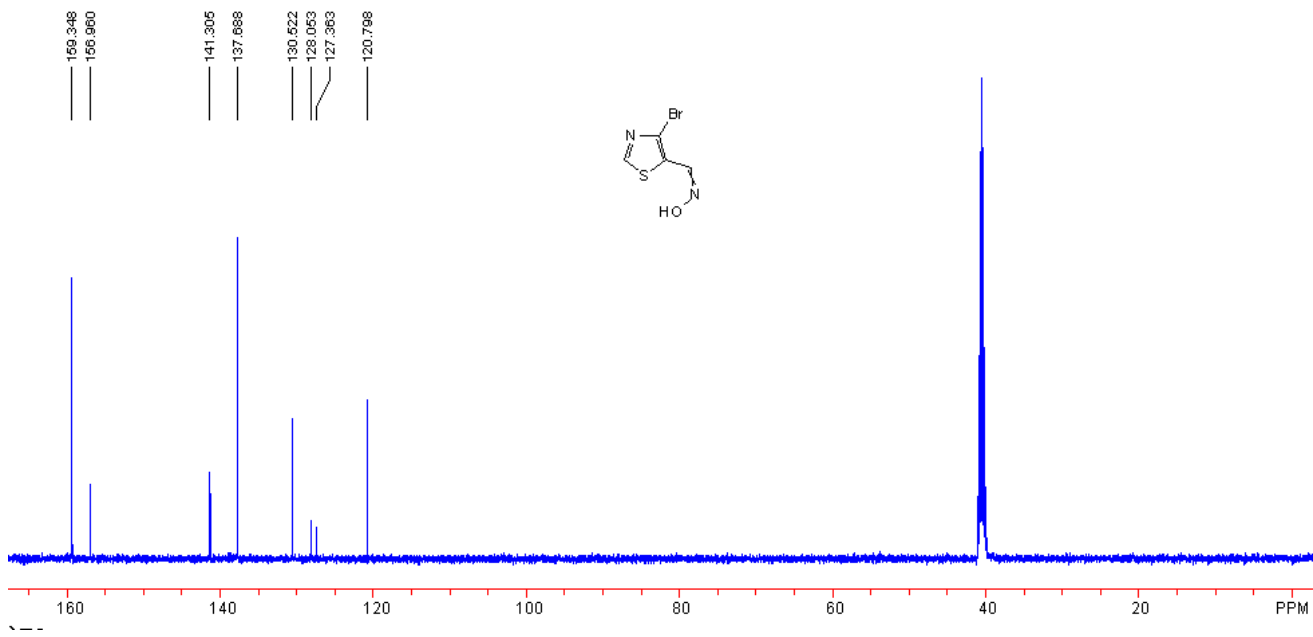


RT = 0.191 min

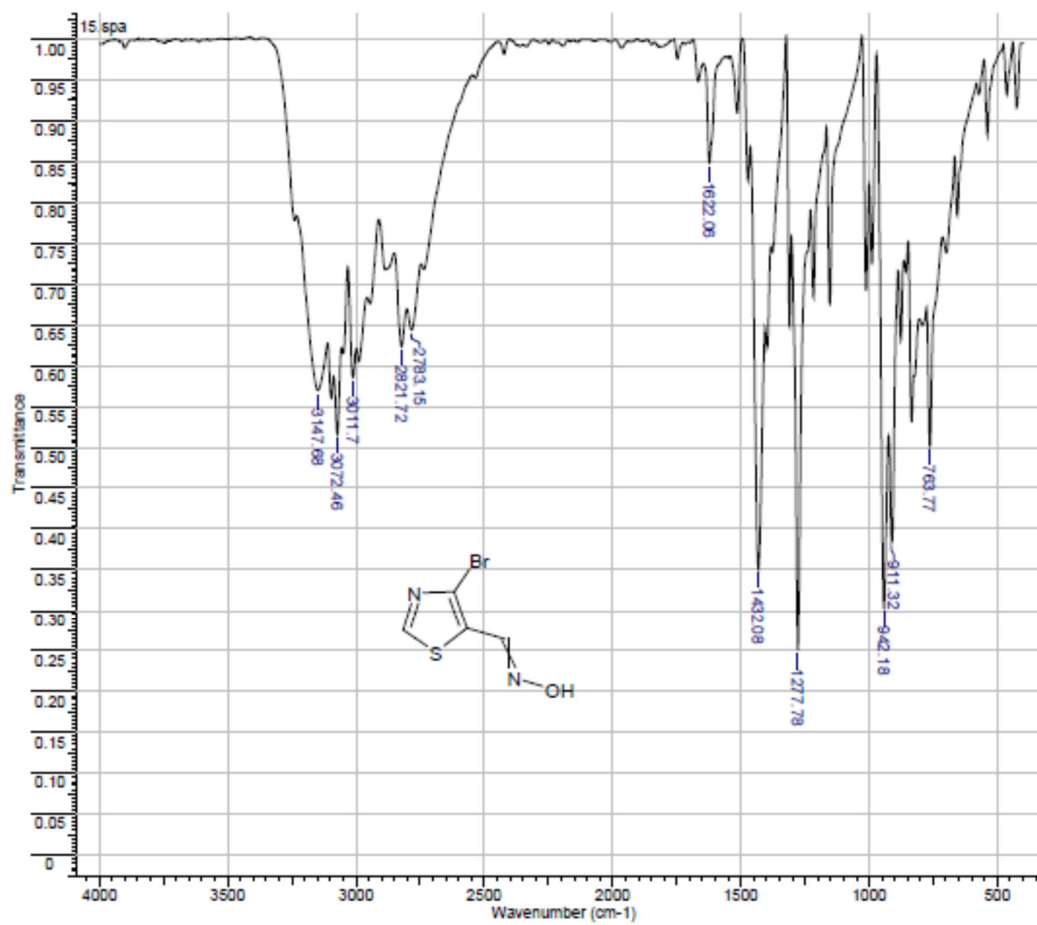
Figure S21. Compound 22
(A) $^1\text{H-NMR}$ spectrum (DMSO- d_6)



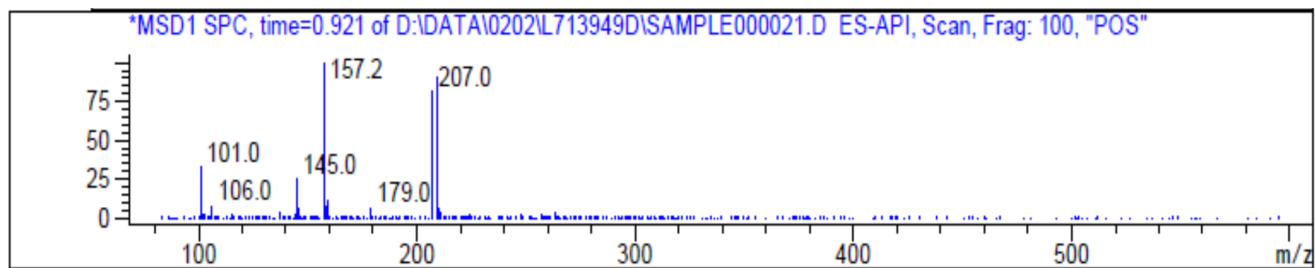
(B) $^{13}\text{C-NMR}$ spectrum (DMSO- d_6)



(C) IR spectrum (KBr)



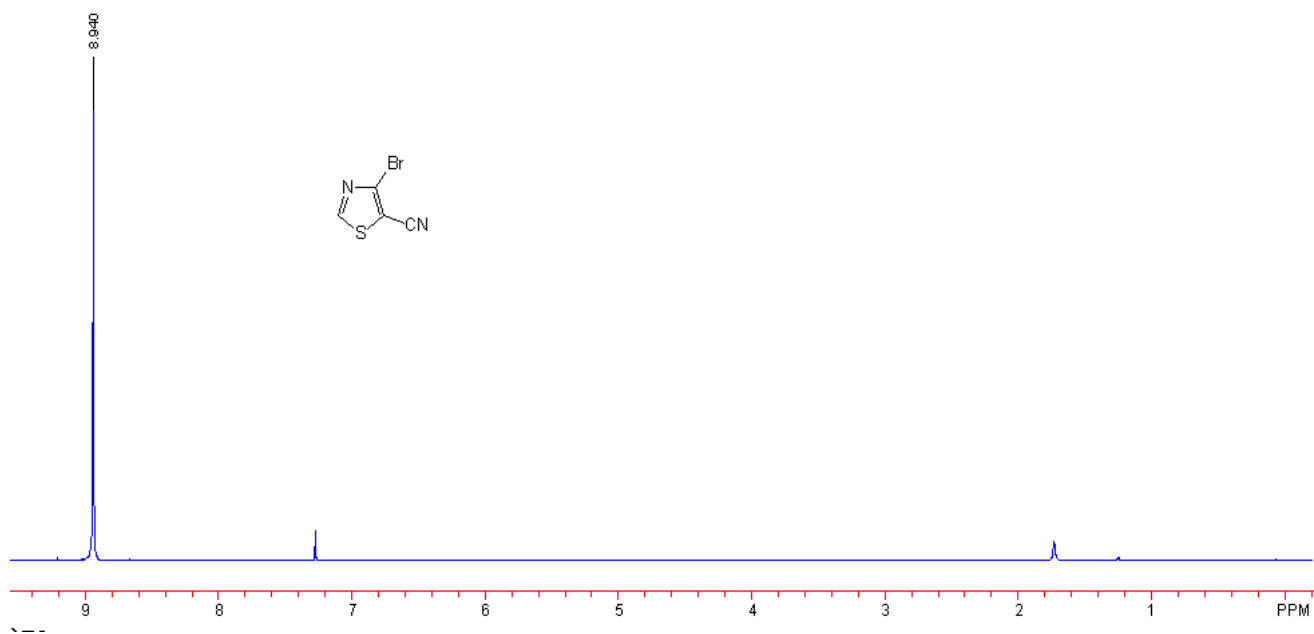
(D) LC/MS spectrum of compound 22



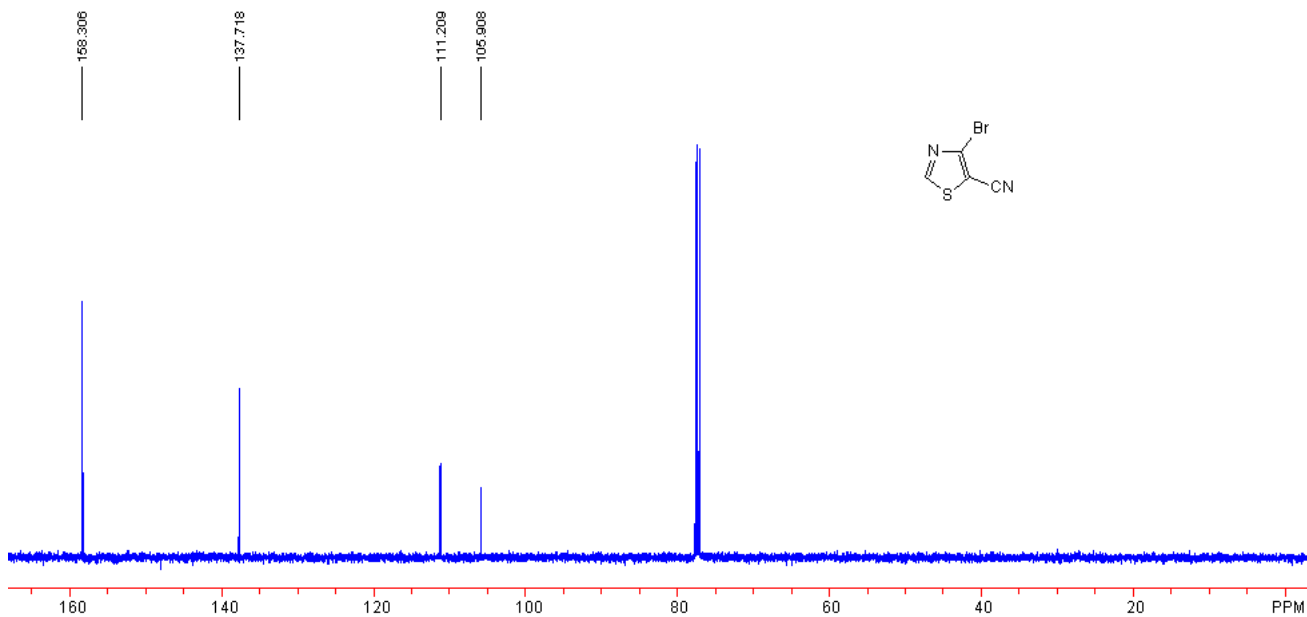
RT = 0.917 min

Figure S22. Compound 23

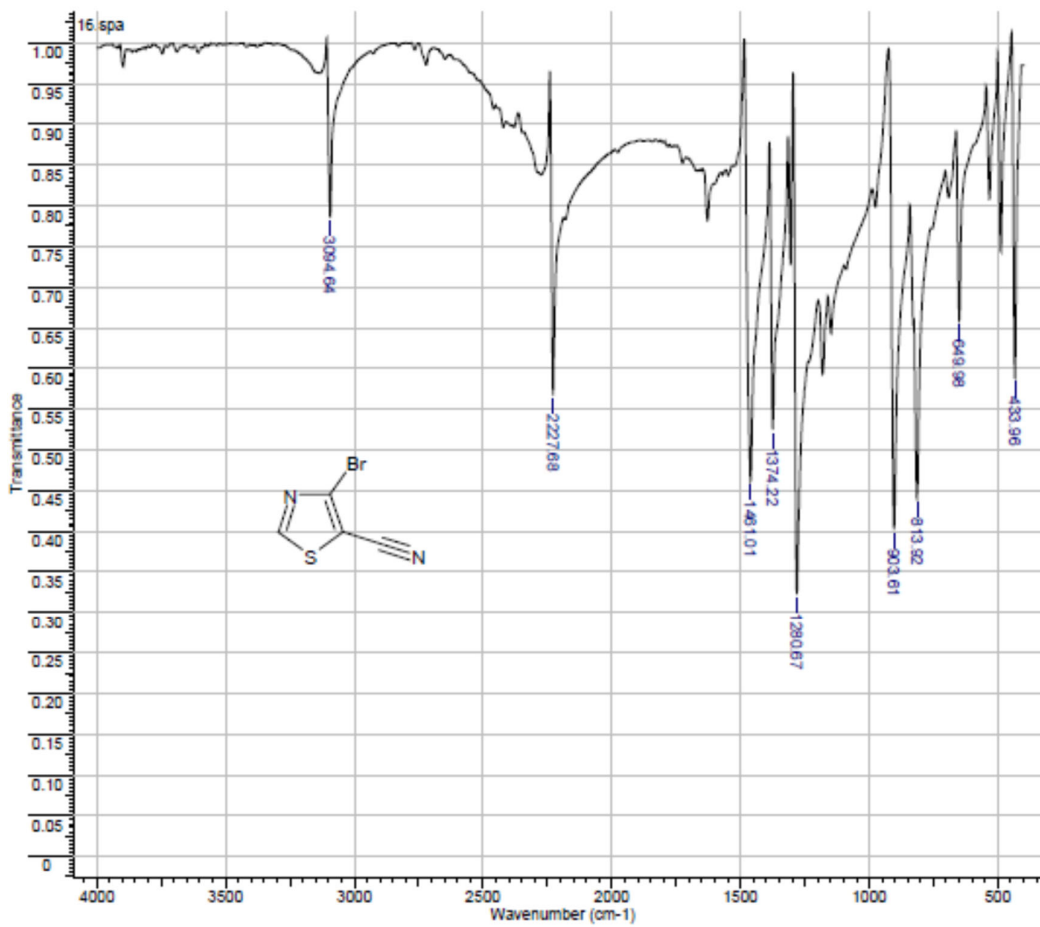
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



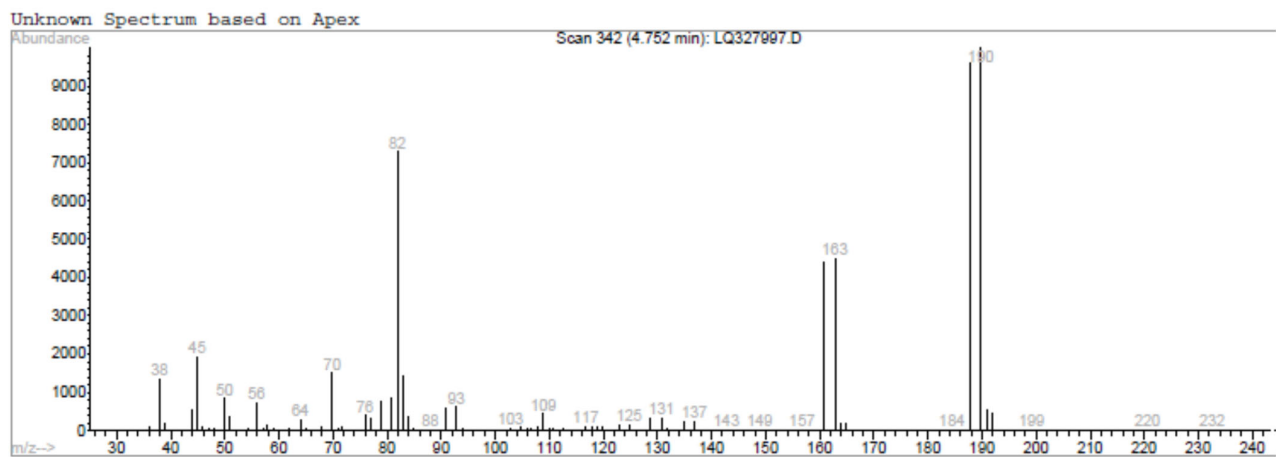
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



(C) IR spectrum (KBr)

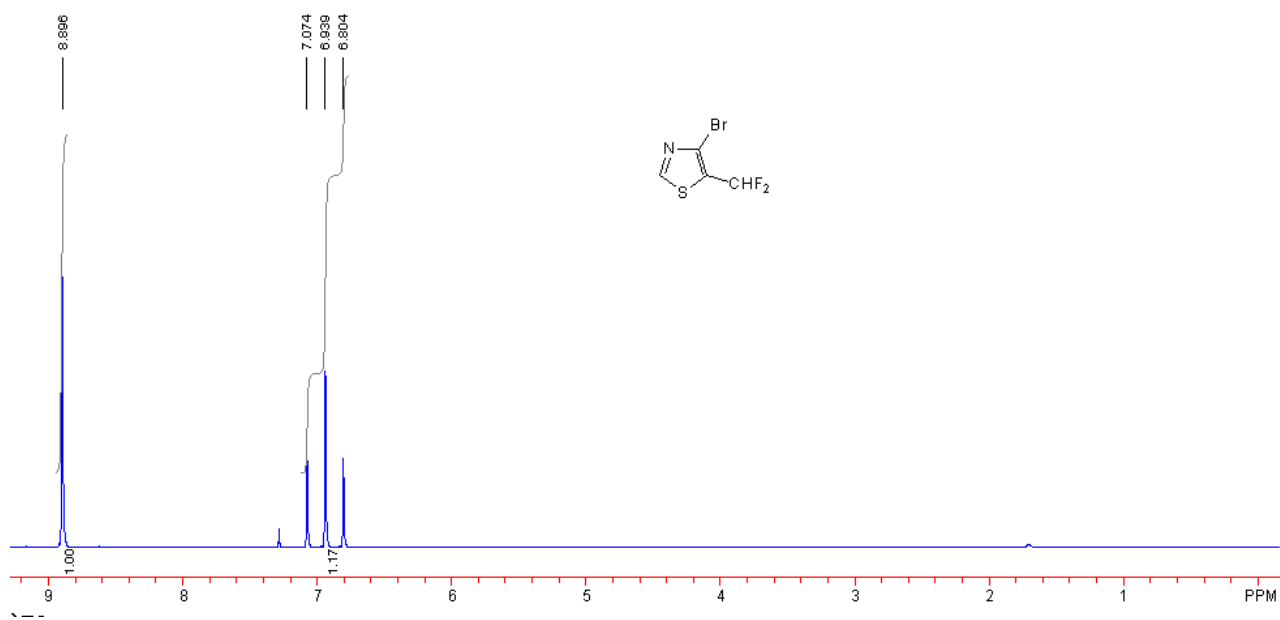


(D) GC/MS spectrum of compound 23

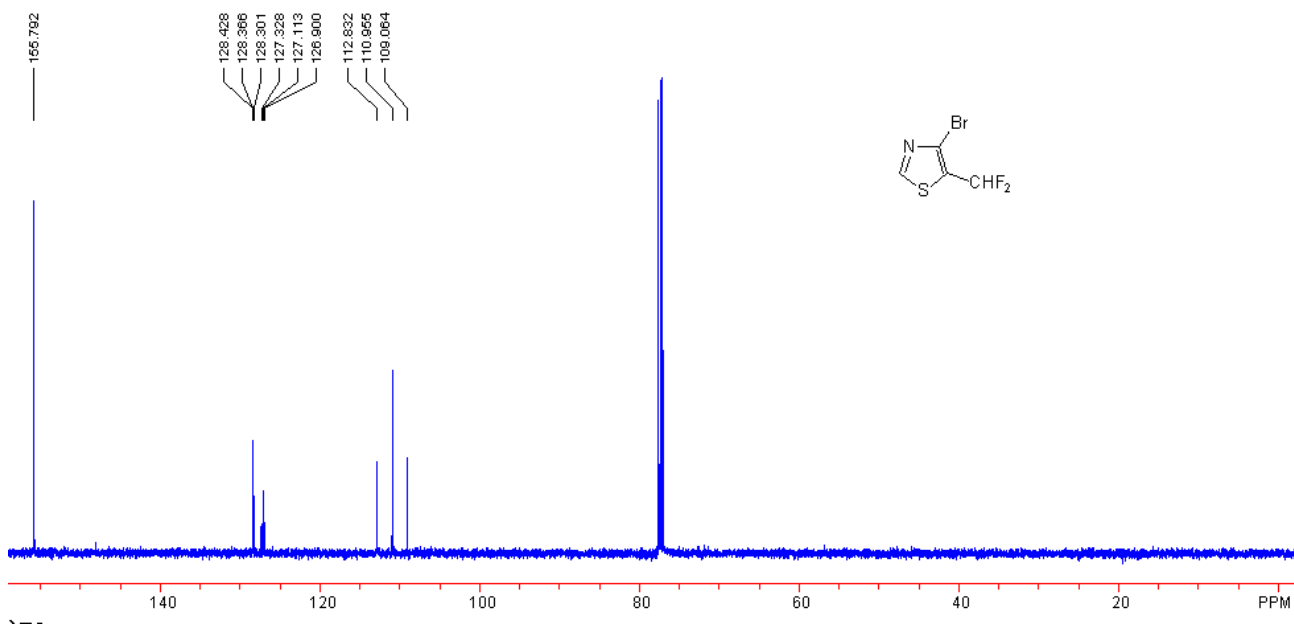


RT = 4.75 min

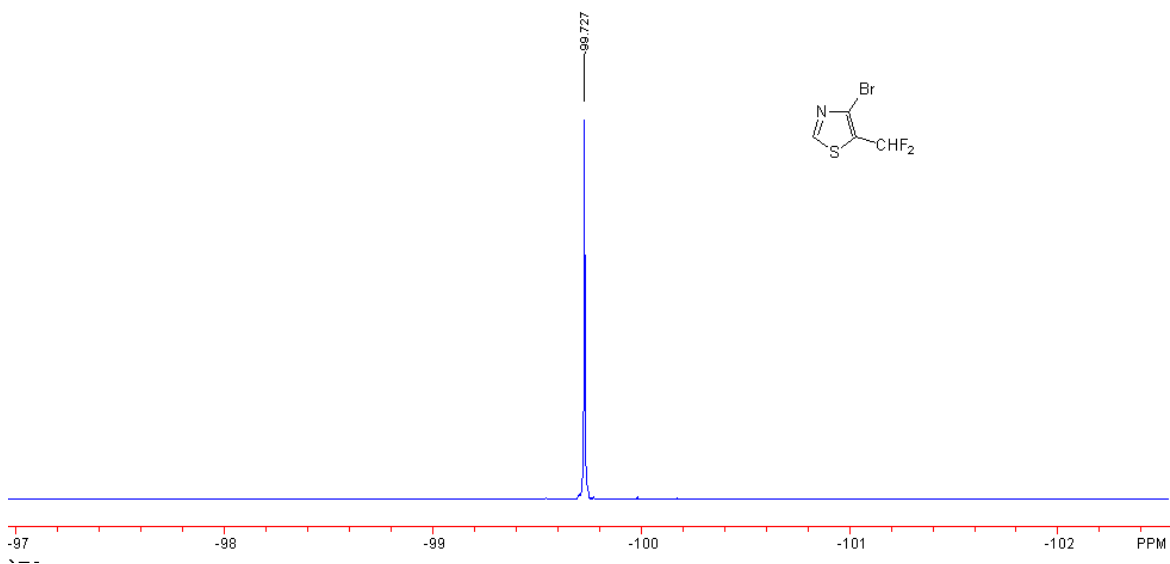
Figure S23. Compound 24
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



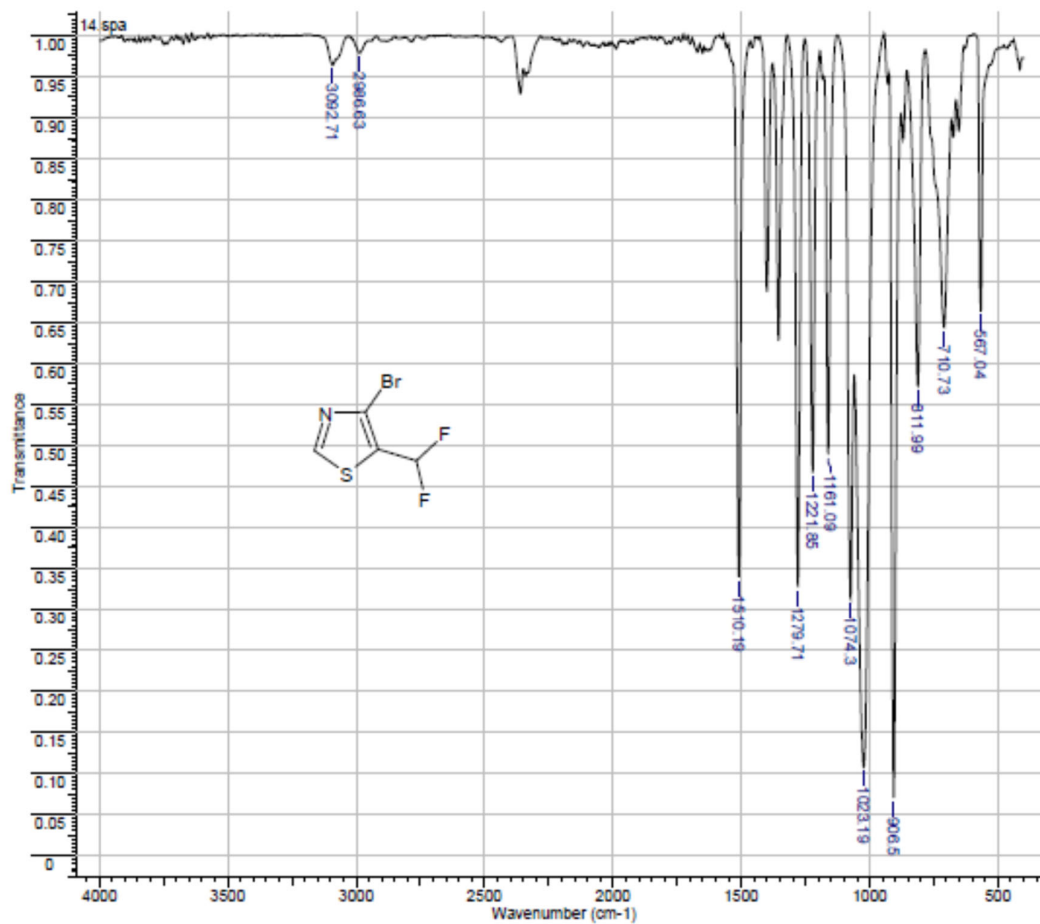
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



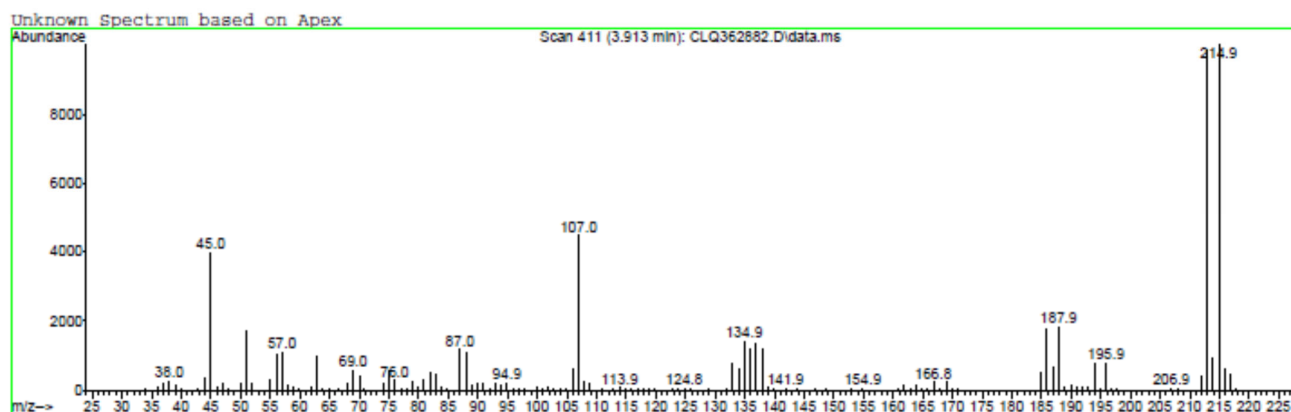
(C) ¹⁹F-NMR spectrum (CDCl₃)



(D) ATR-IR spectrum



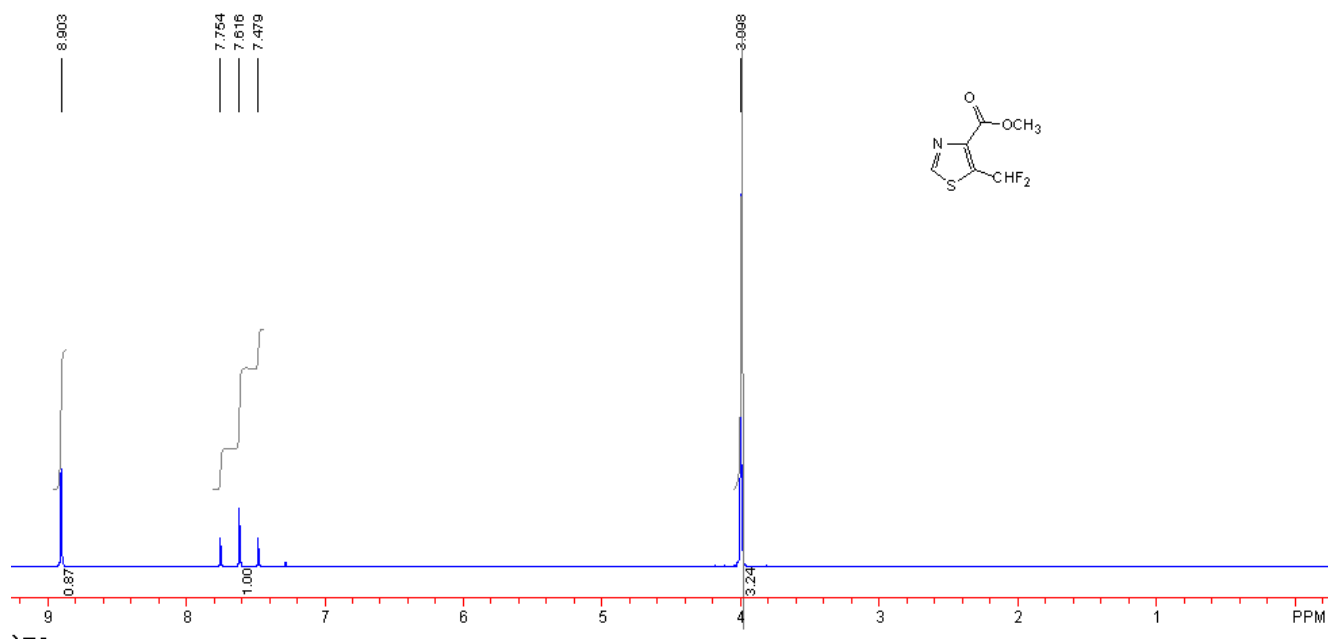
(E) LC/MS spectrum of compound 24



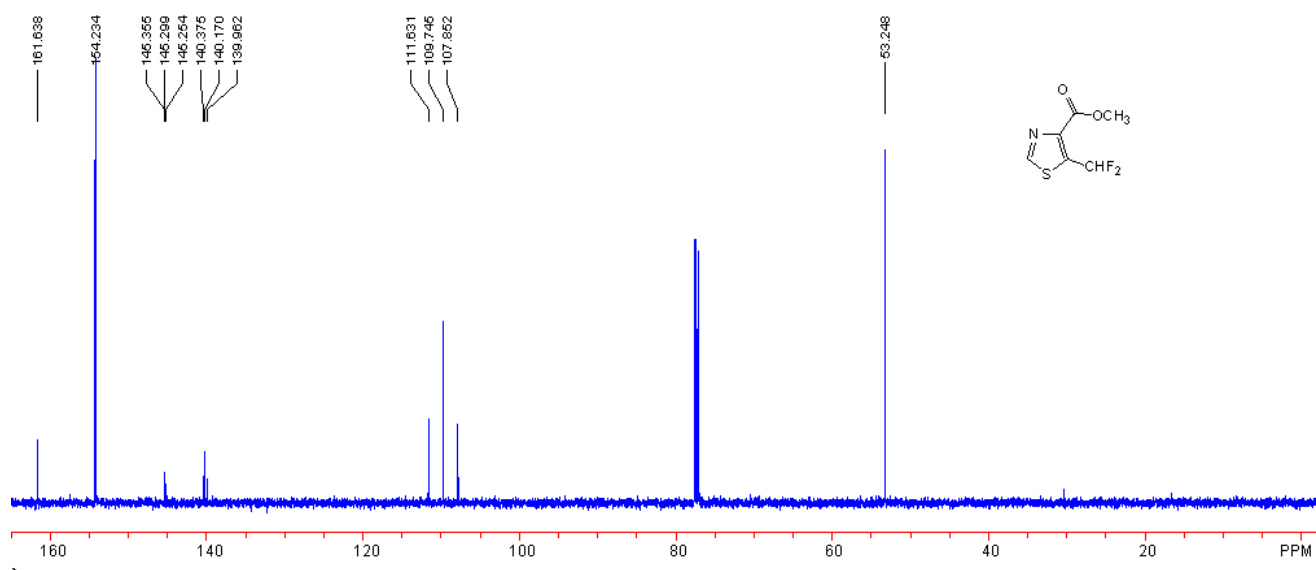
RT = 3.915 min

Figure S24. Compound 25

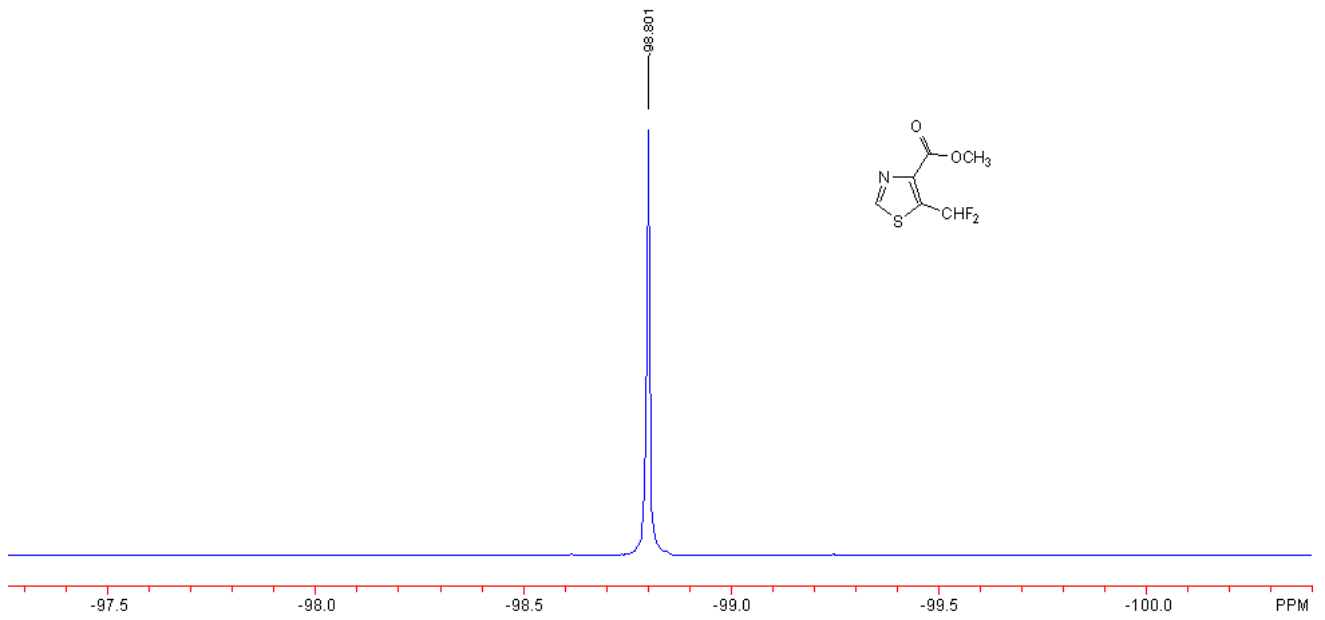
(A) $^1\text{H-NMR}$ spectrum (CDCl_3)



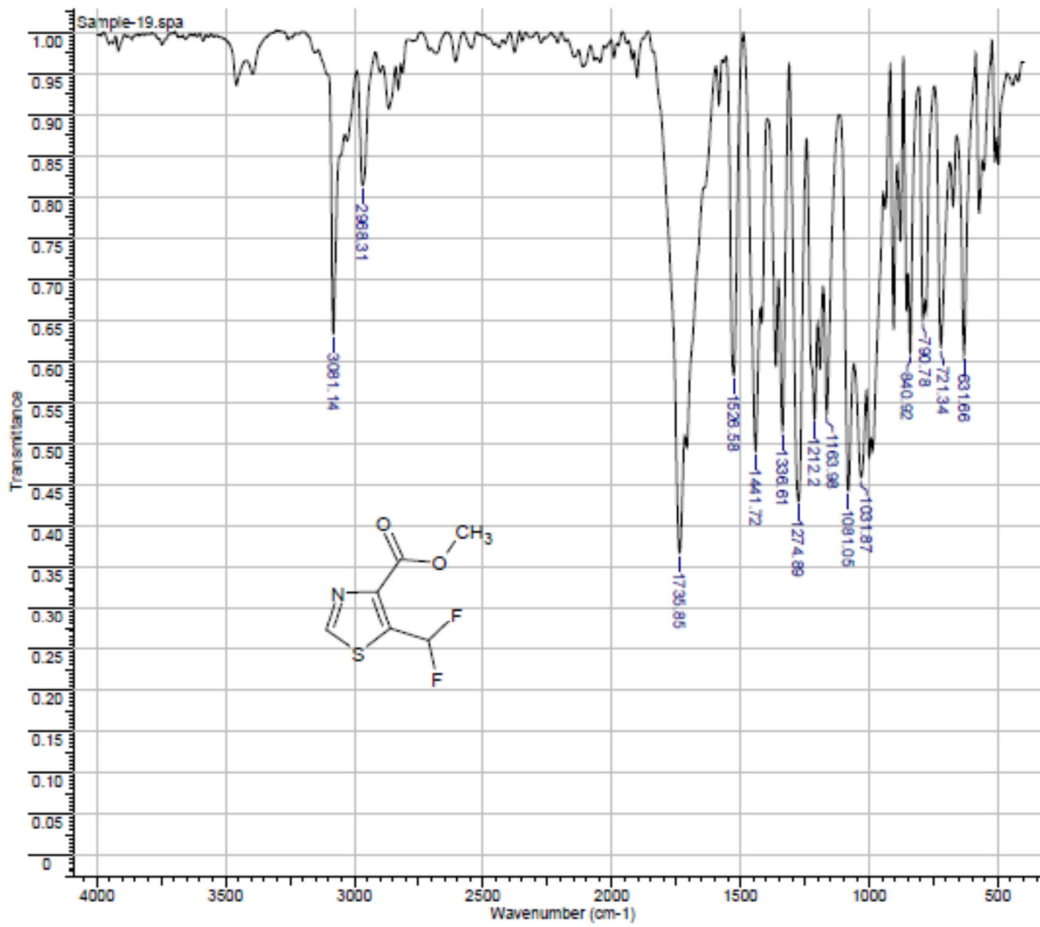
(B) $^{13}\text{C-NMR}$ spectrum (CDCl_3)



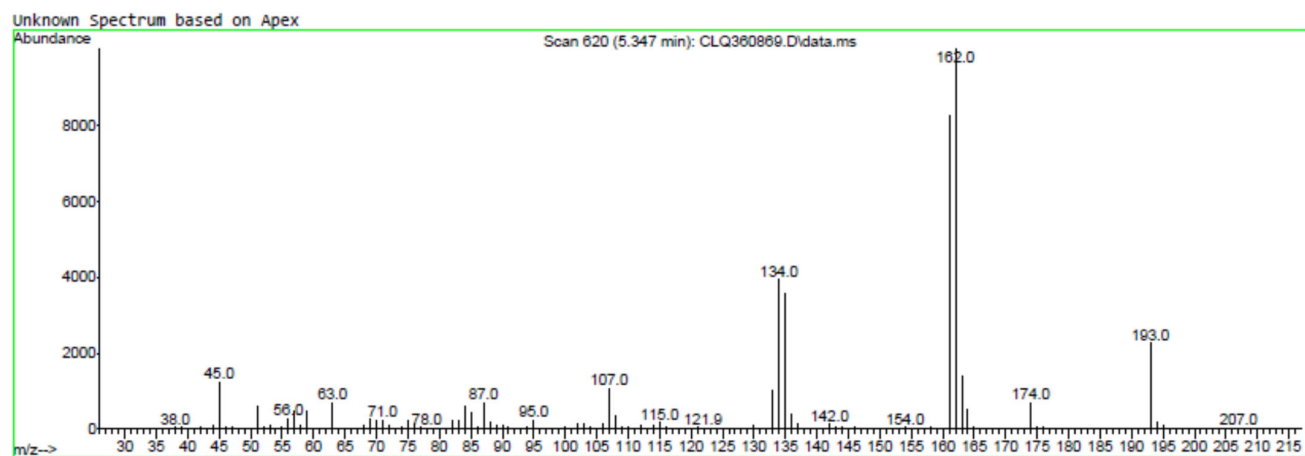
(C) $^{19}\text{F-NMR}$ spectrum (CDCl_3)



(D) IR spectrum (KBr)

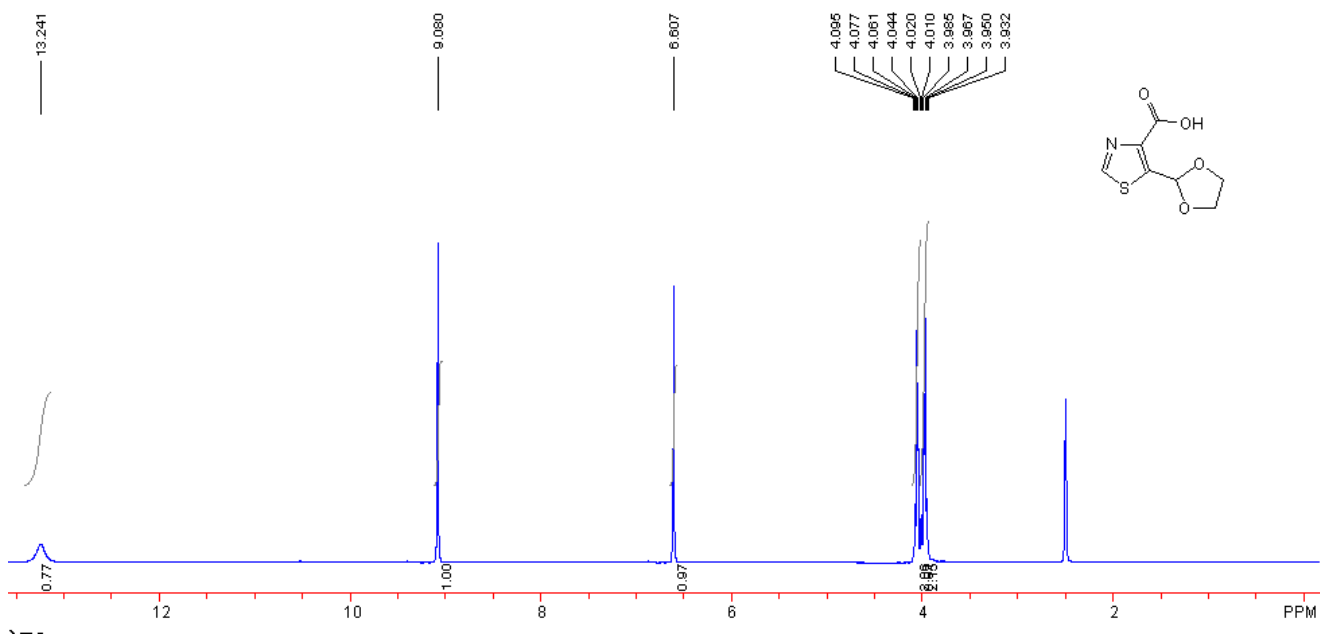


(E) GC/MS spectrum of compound 25

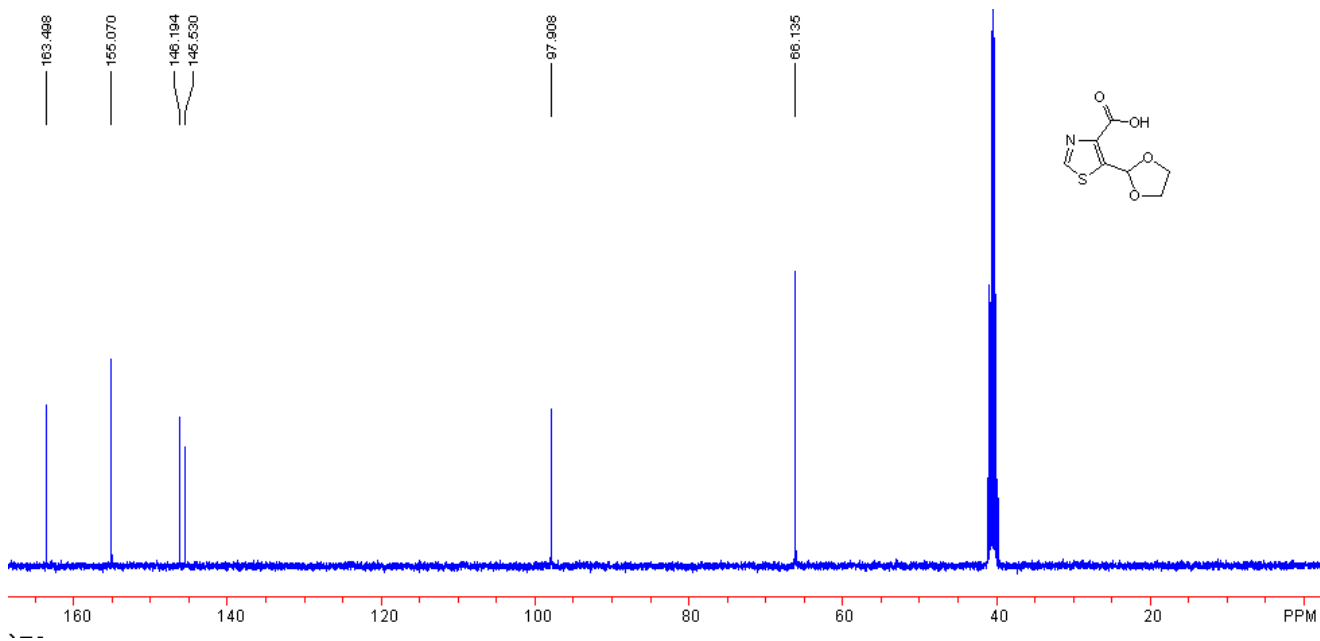


RT = 5.347 min

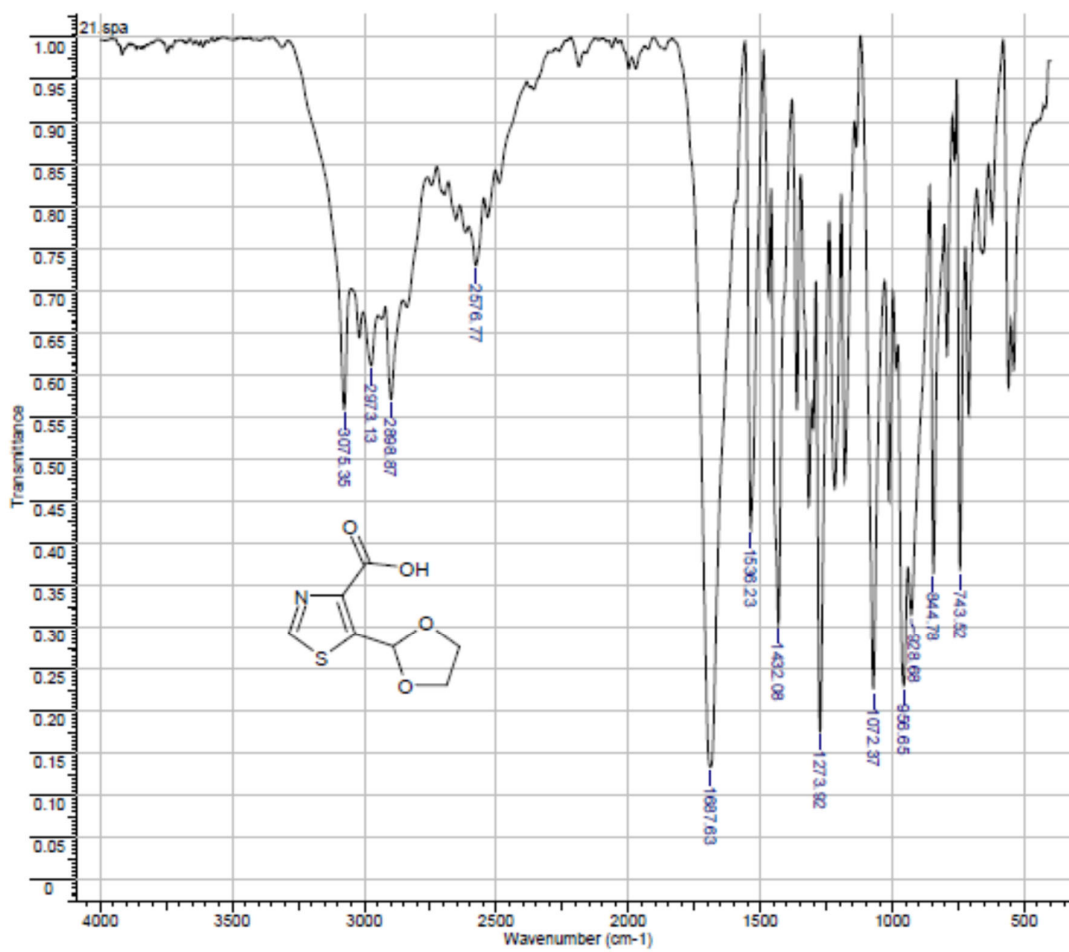
Figure S25. Compound 26
(A) $^1\text{H-NMR}$ spectrum (DMSO- d_6)



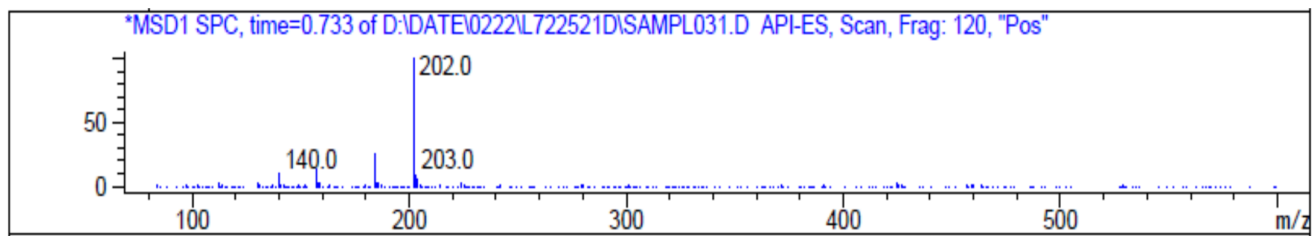
(B) $^{13}\text{C-NMR}$ spectrum (DMSO- d_6)



(C) IR spectrum (KBr)

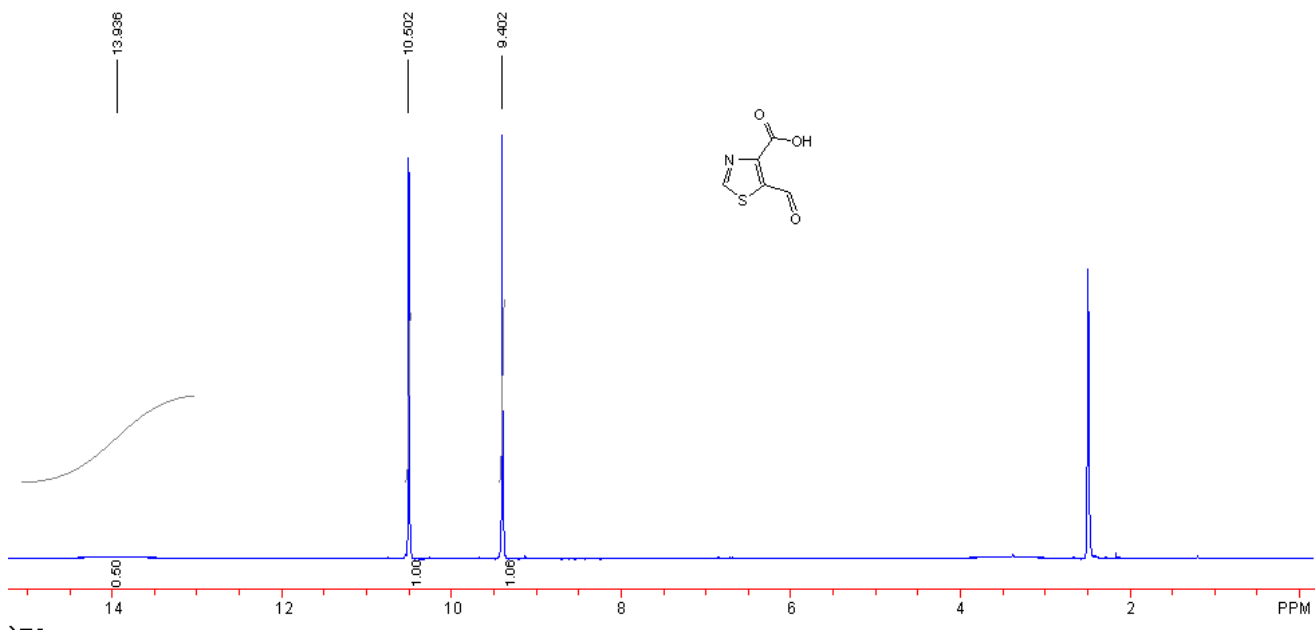


(D) LC/MS spectrum of compound 26

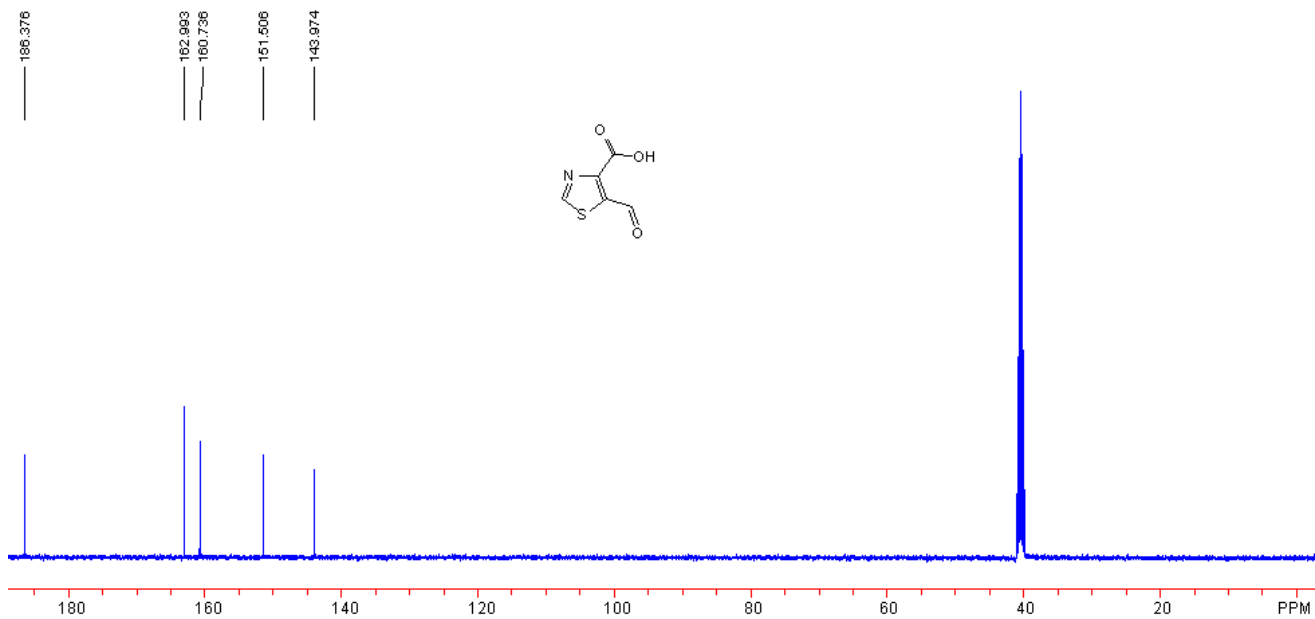


RT = 0.734 min

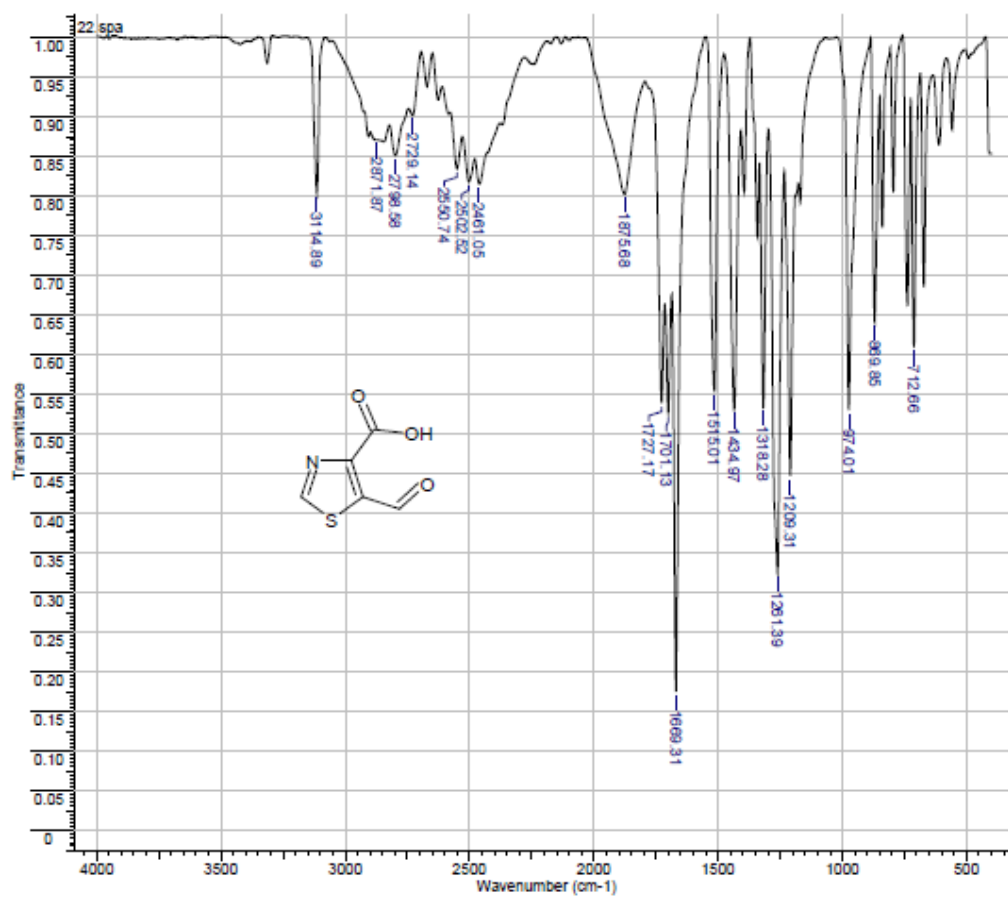
Figure S26. Compound 27
(A) $^1\text{H-NMR}$ spectrum (DMSO- d_6)



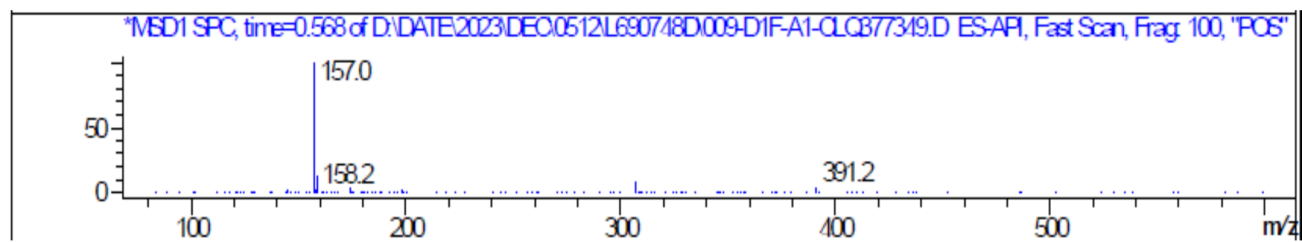
(B) $^{13}\text{C-NMR}$ spectrum (DMSO- d_6)



(C) IR spectrum (KBr)

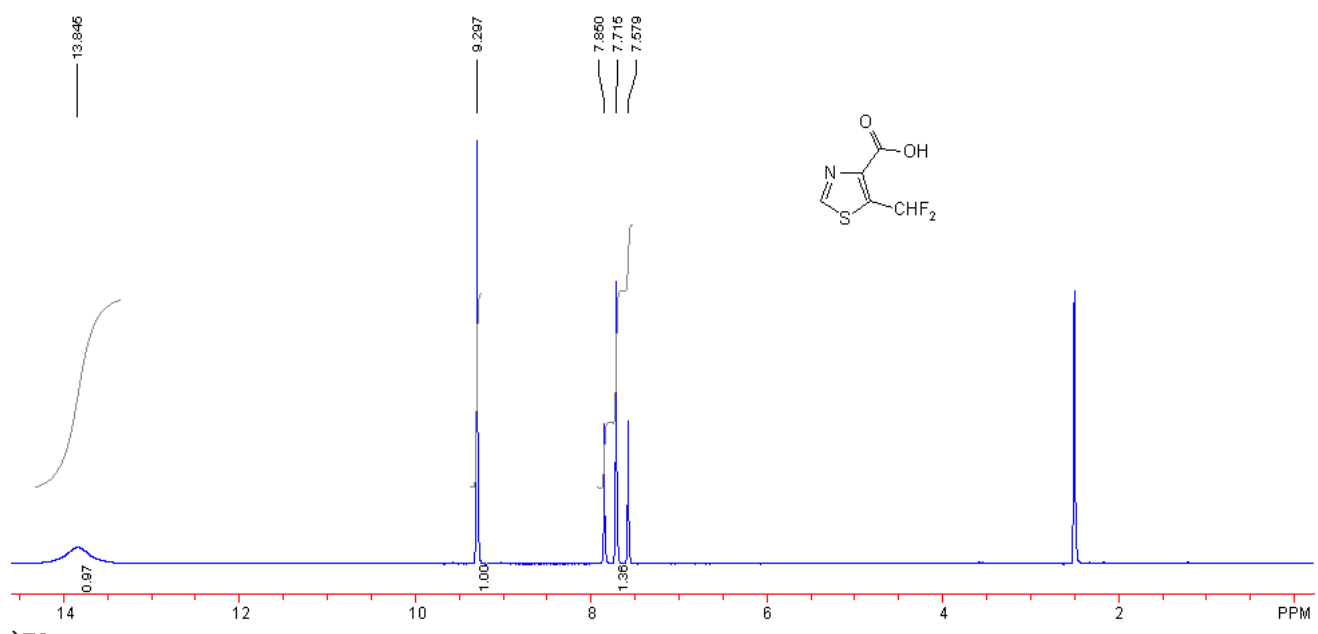


(D) LC/MS spectrum of compound 27

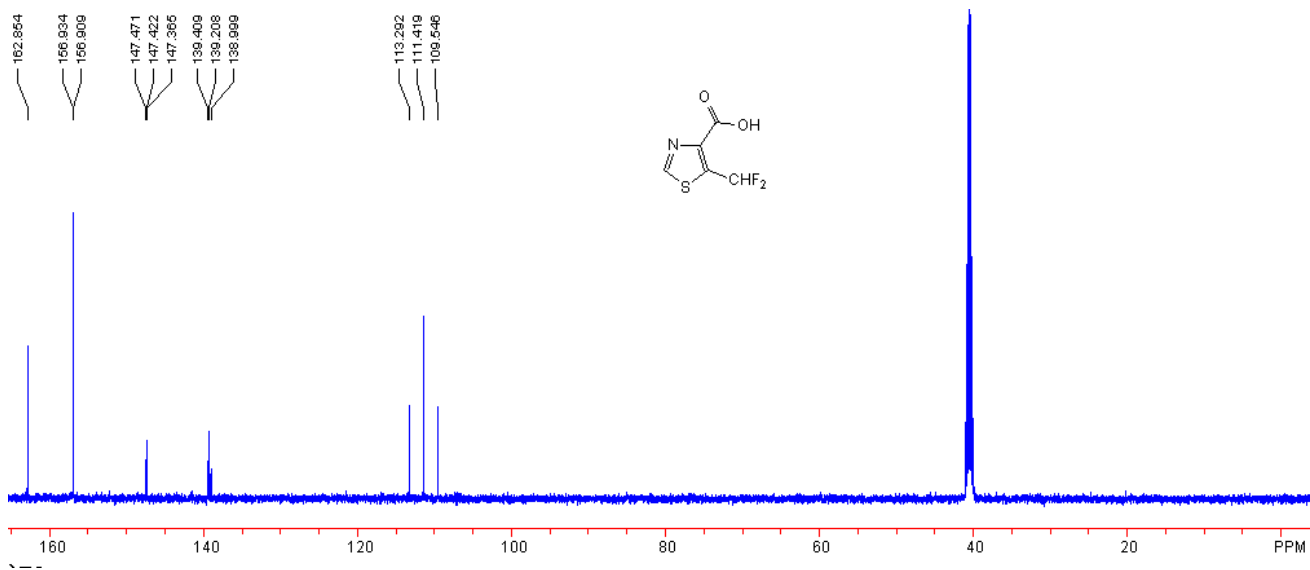


RT = 0.565 min

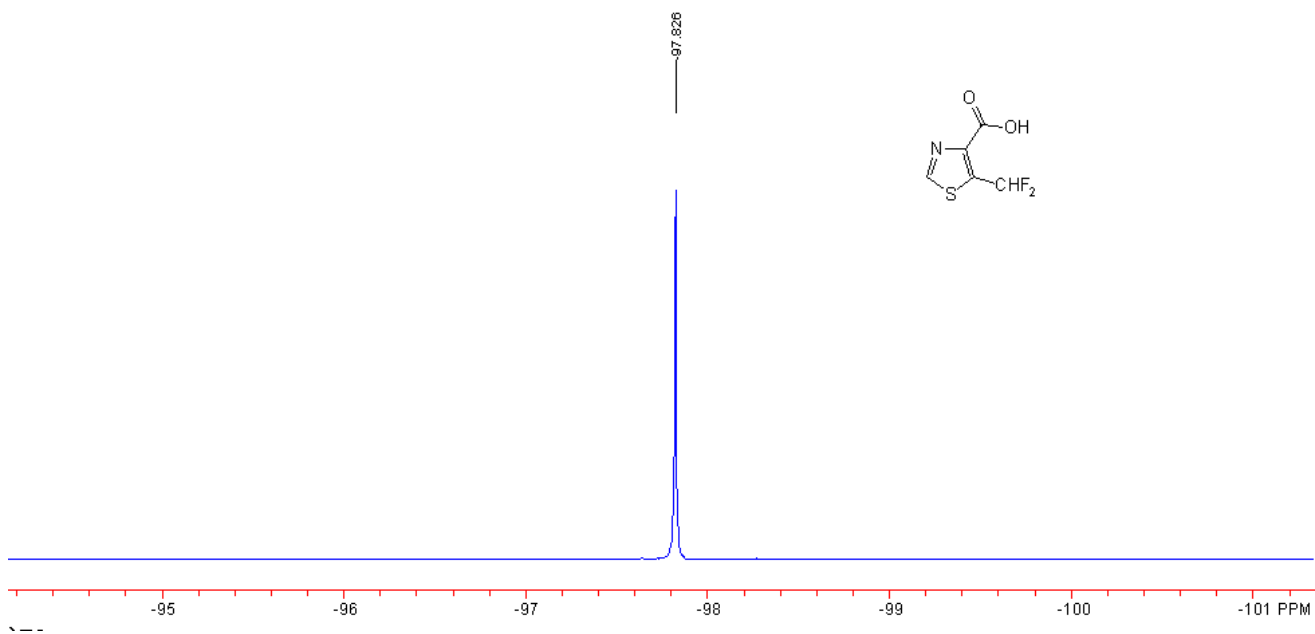
Figure S27. Compound 28
(A) $^1\text{H-NMR}$ spectrum (DMSO- d_6)



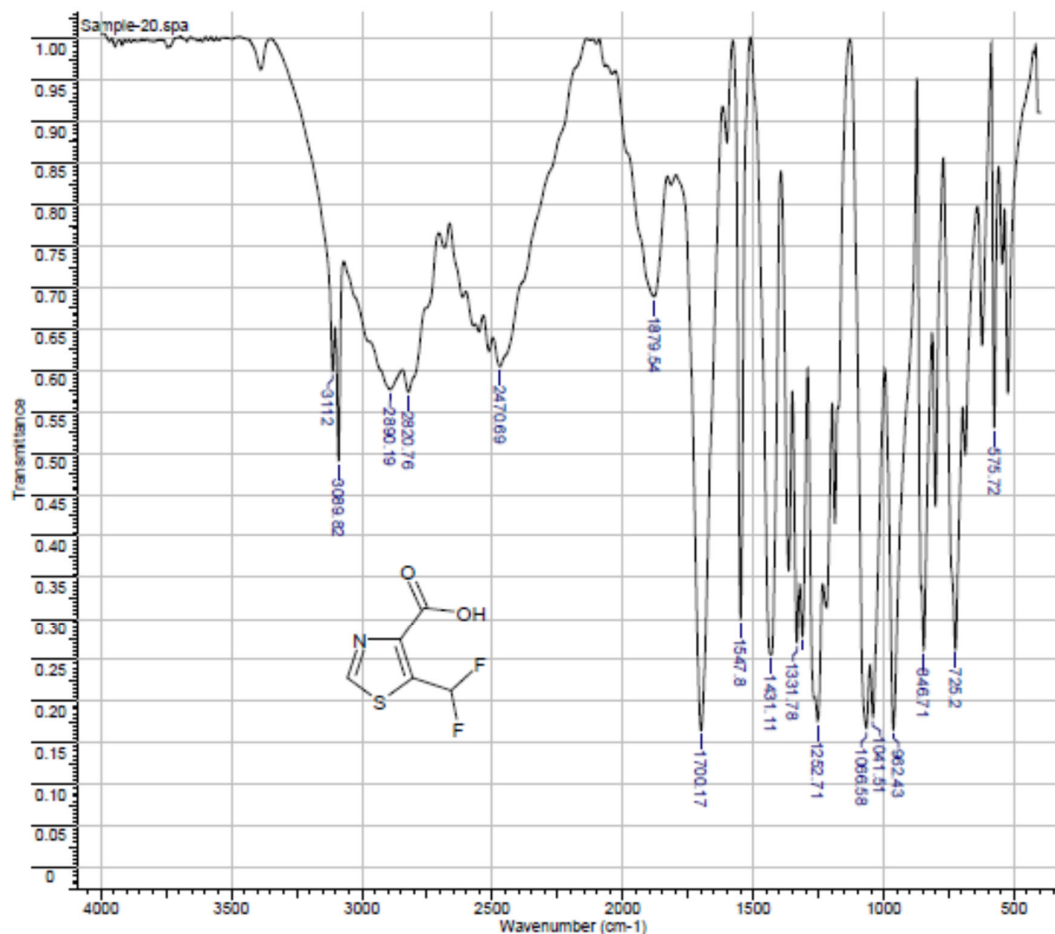
(B) $^{13}\text{C-NMR}$ spectrum (DMSO- d_6)



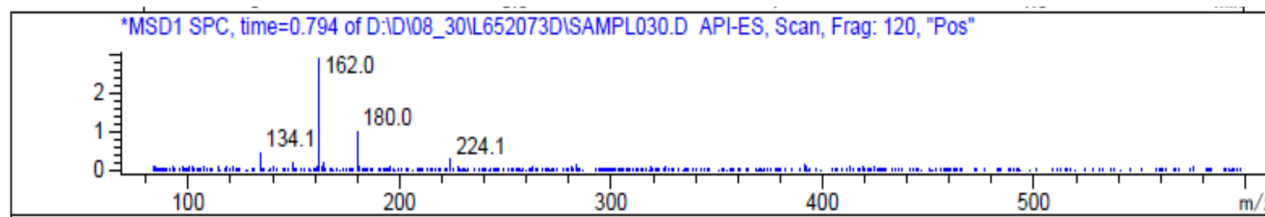
(C) ¹⁹F-NMR spectrum (DMSO-d₆)



(D) IR spectrum (KBr)



(E) LC/MS spectrum of compound 28



RT = 0.802 min