

Supplementary Data:

Design and synthesis of new hydantoin acetanilide derivatives as anti-NSCLC targeting EGFR^{L858R/T790M} mutations

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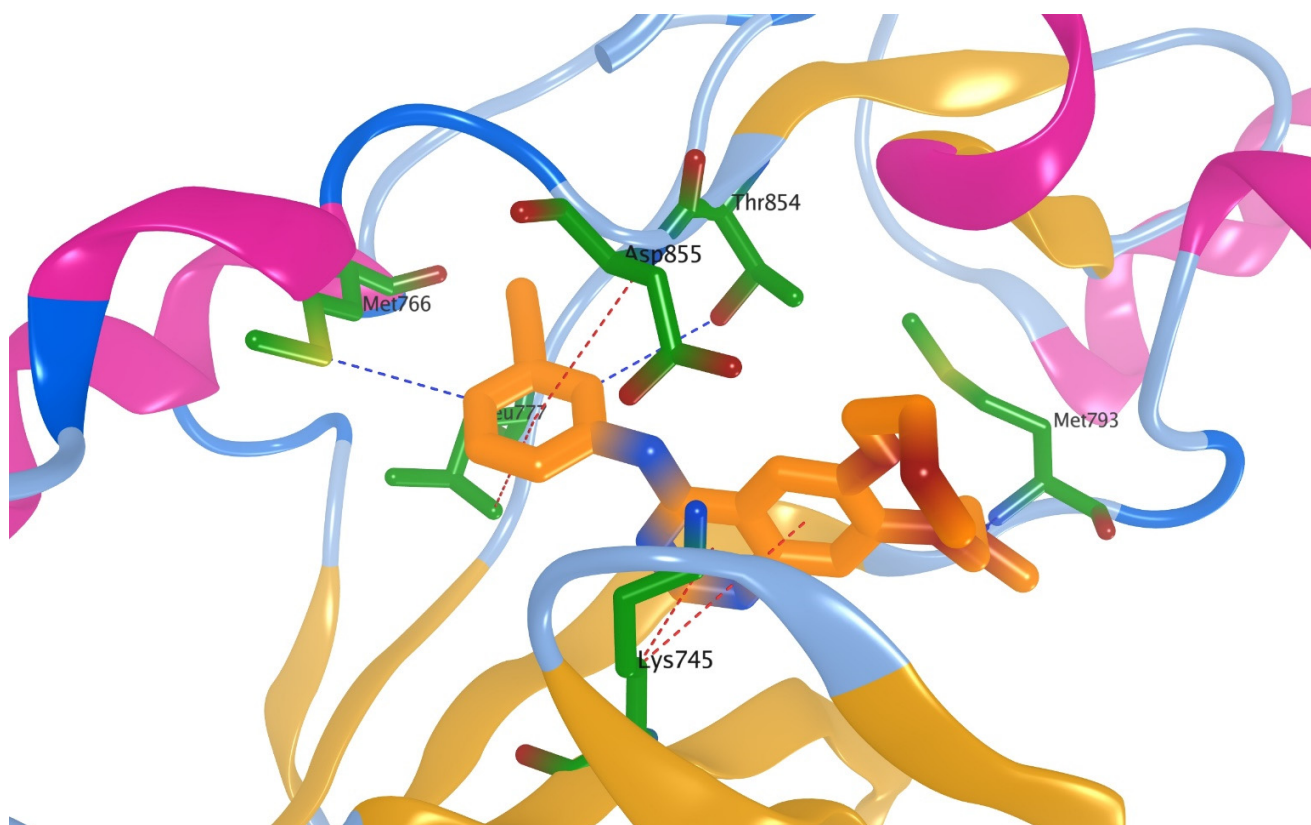


Figure S1. 3D representation of erlotinib within EGFR active site

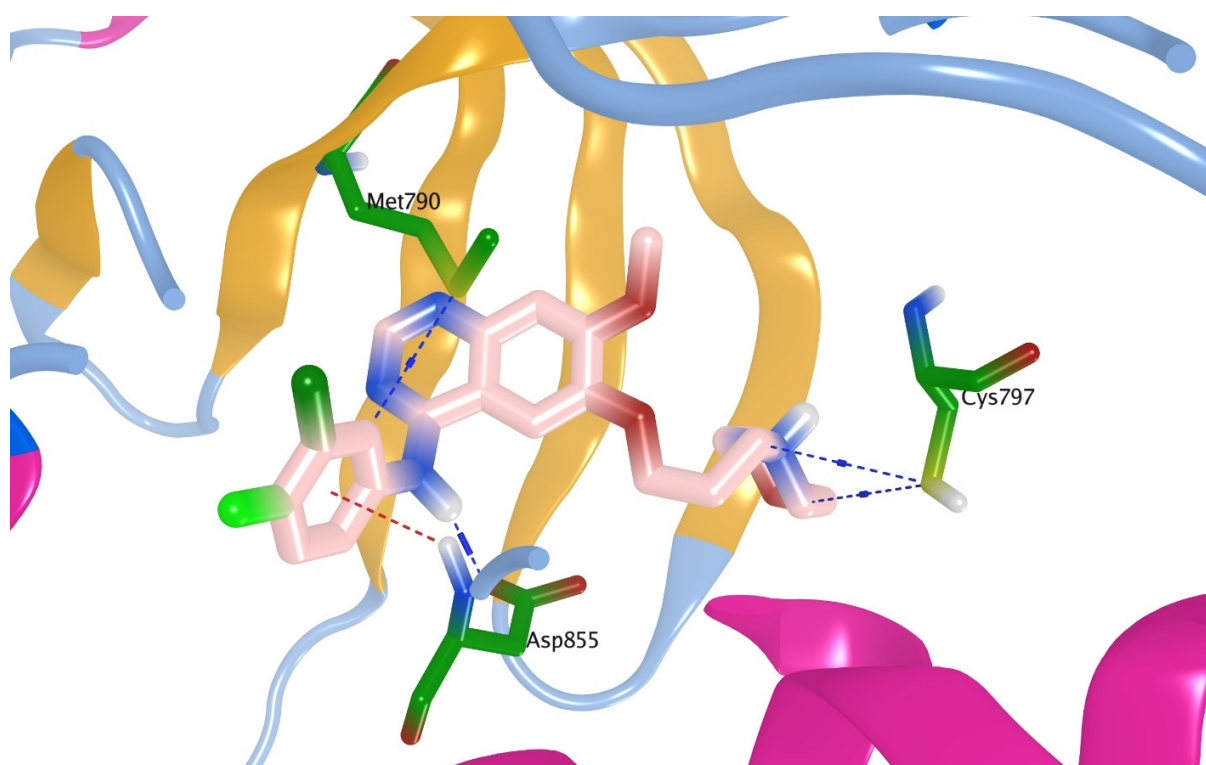


Figure S2. 3D representation of gefitinib within EGFR active site

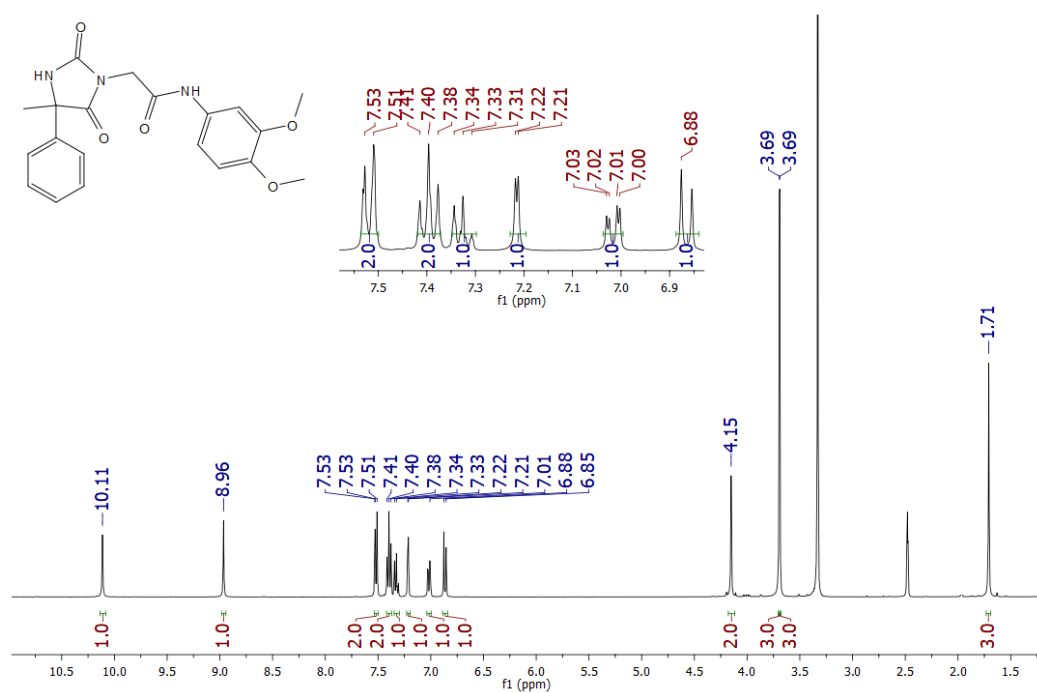


Figure S3. ¹H-NMR spectrum of compound **5a** in DMSO-*d*₆ at 400MHz.

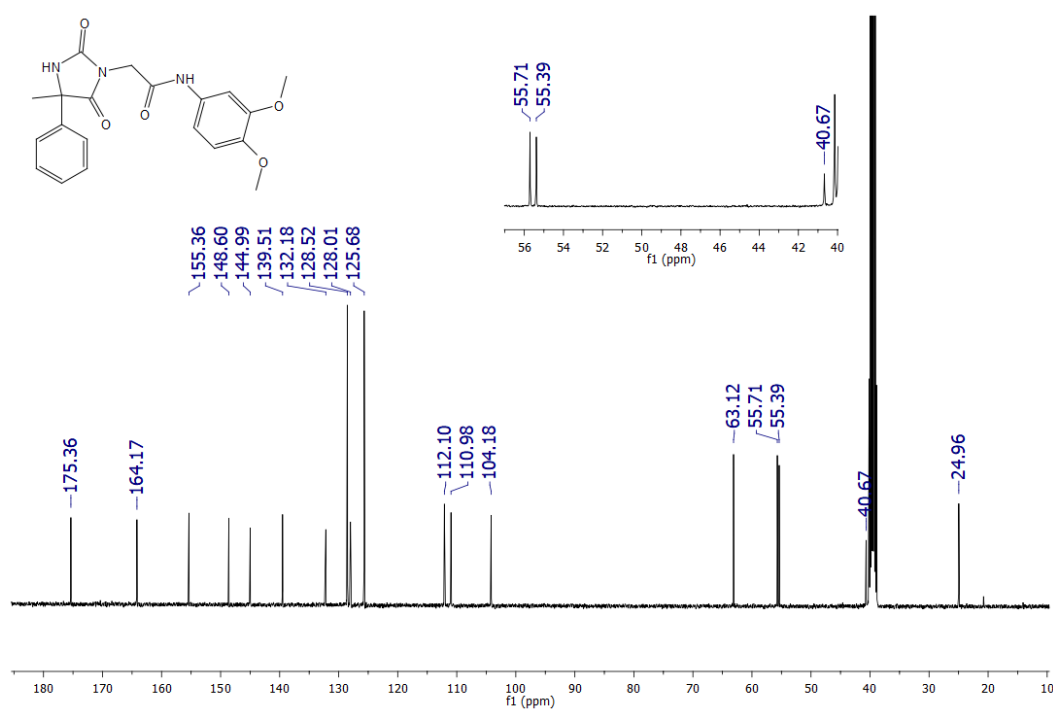


Figure S4. ¹³C-NMR spectrum of compound **5a** in DMSO-*d*₆ at 100MHz.

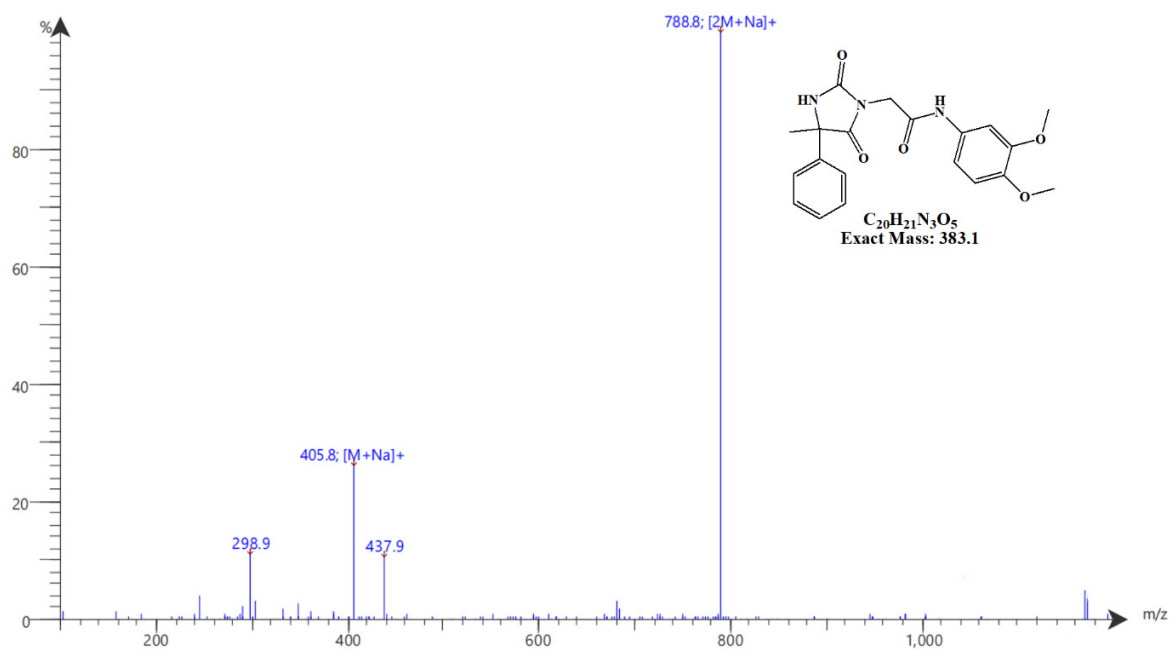


Figure S5. ESI mass spectrum of compound **5a**.

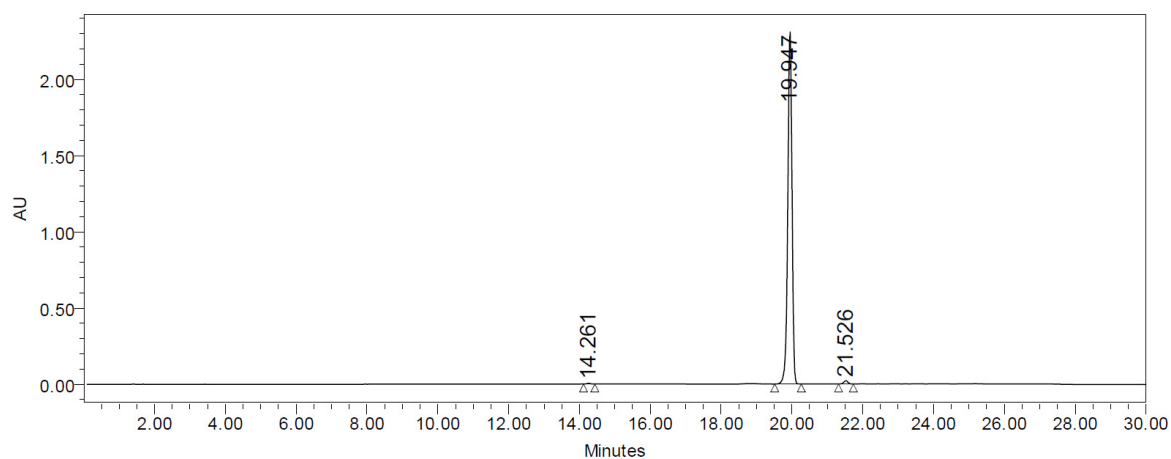


Figure S6. HPLC analysis for compound **5a**, retention time (19.947 min)

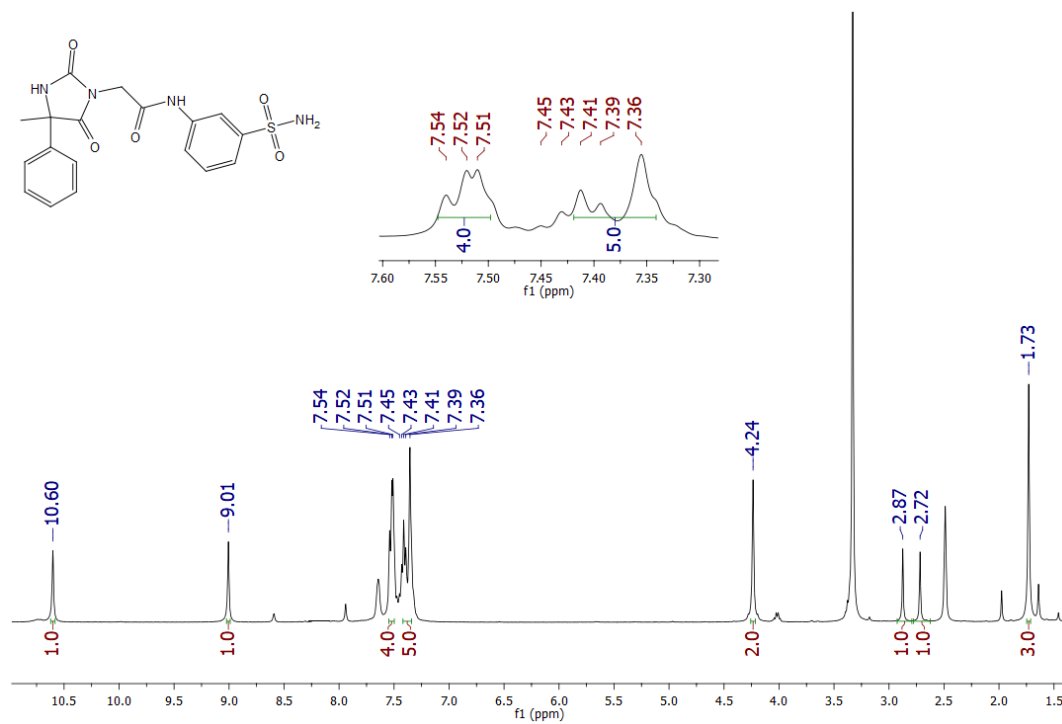


Figure S7. ¹H-NMR spectrum of compound **5b** in DMSO-*d*₆ at 400MHz.

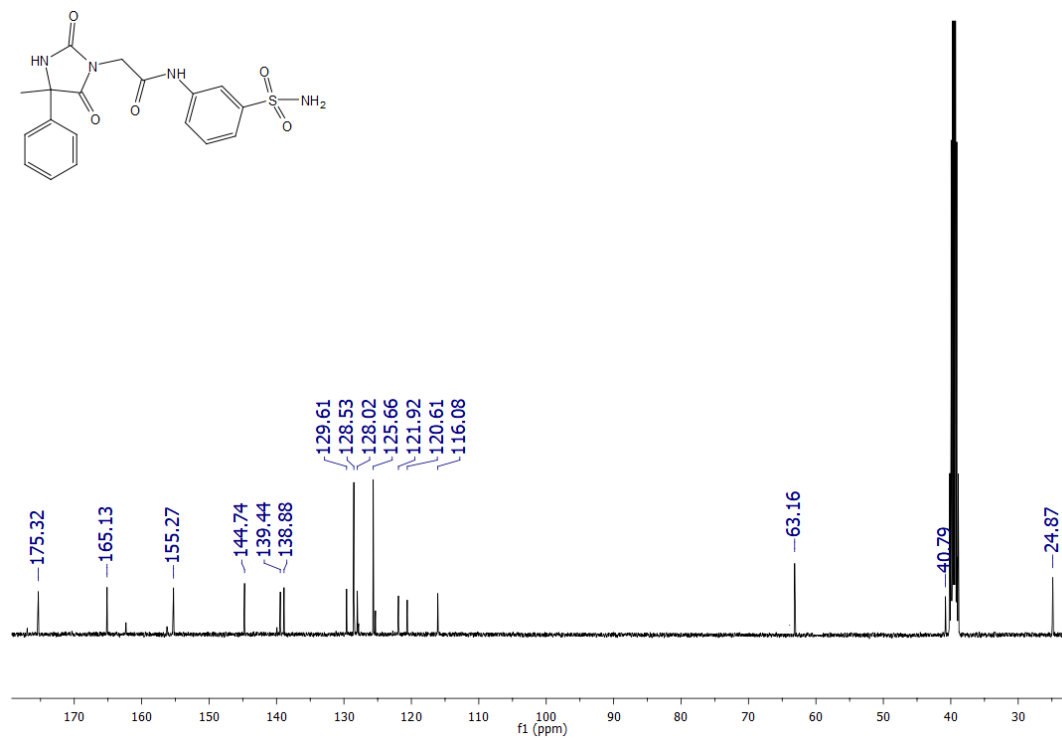


Figure S8. ¹³C-NMR spectrum of compound **5b** in DMSO-*d*₆ at 100MHz.

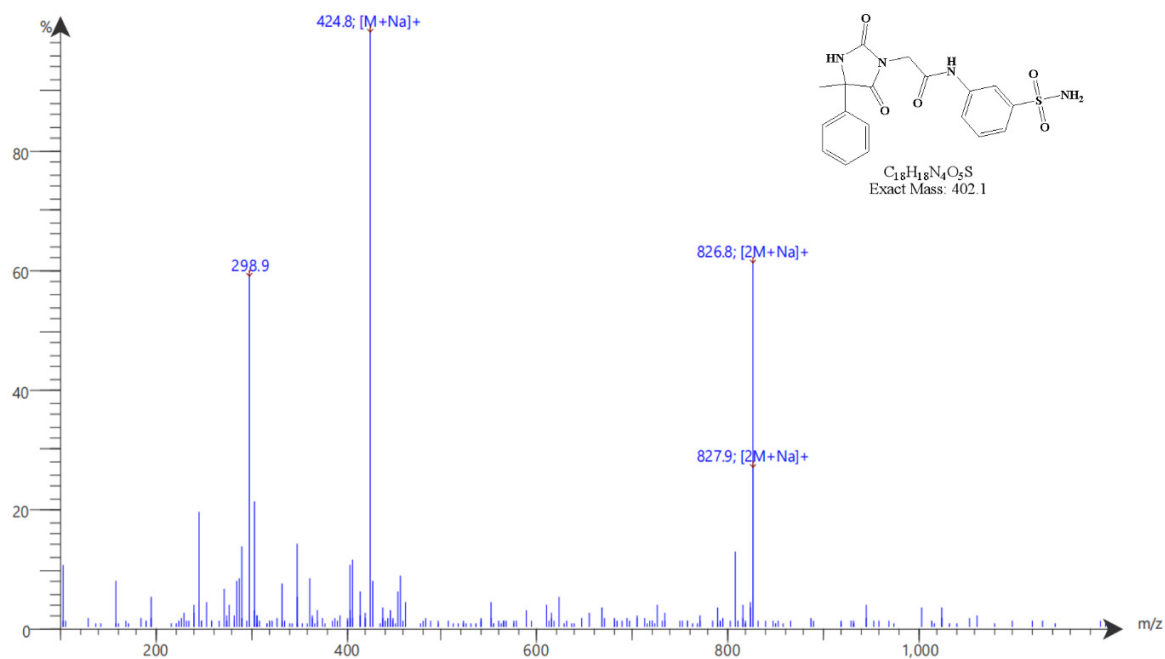


Figure S9. ESI mass spectrum of compound **5b**.

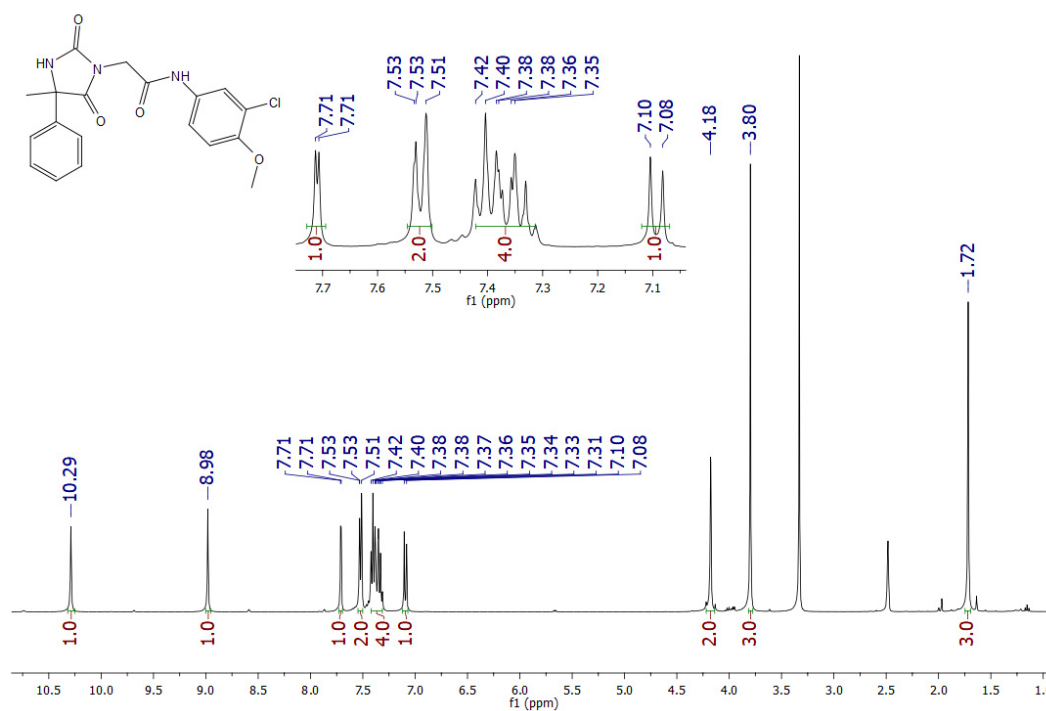


Figure S10. 1H -NMR spectrum of compound **5c** in $DMSO-d_6$ at 400MHz.

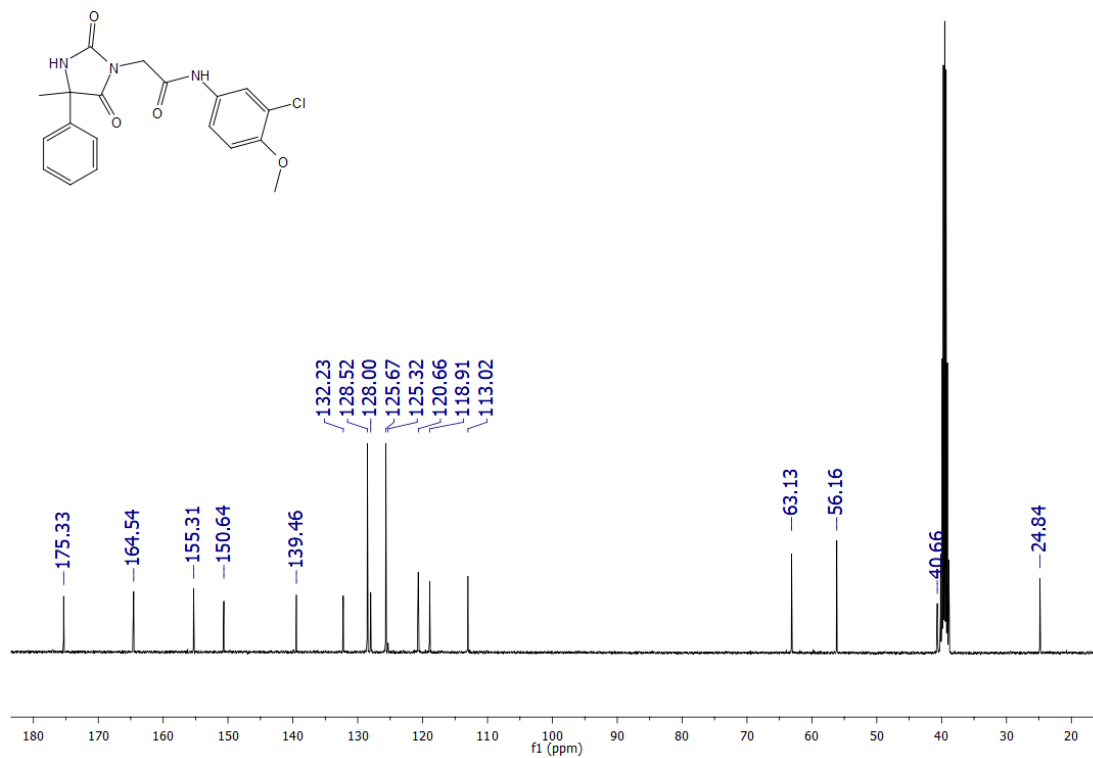


Figure S11. ¹³C-NMR spectrum of compound **5c** in DMSO-*d*₆ at 100MHz.

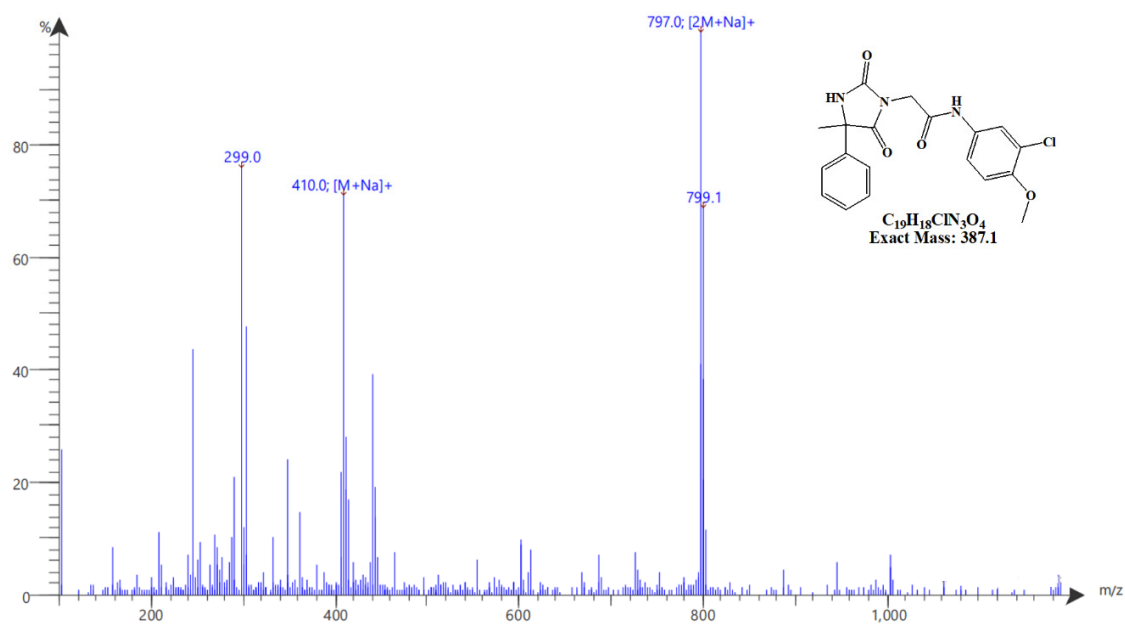


Figure S12. ESI mass spectrum of compound **5c**.

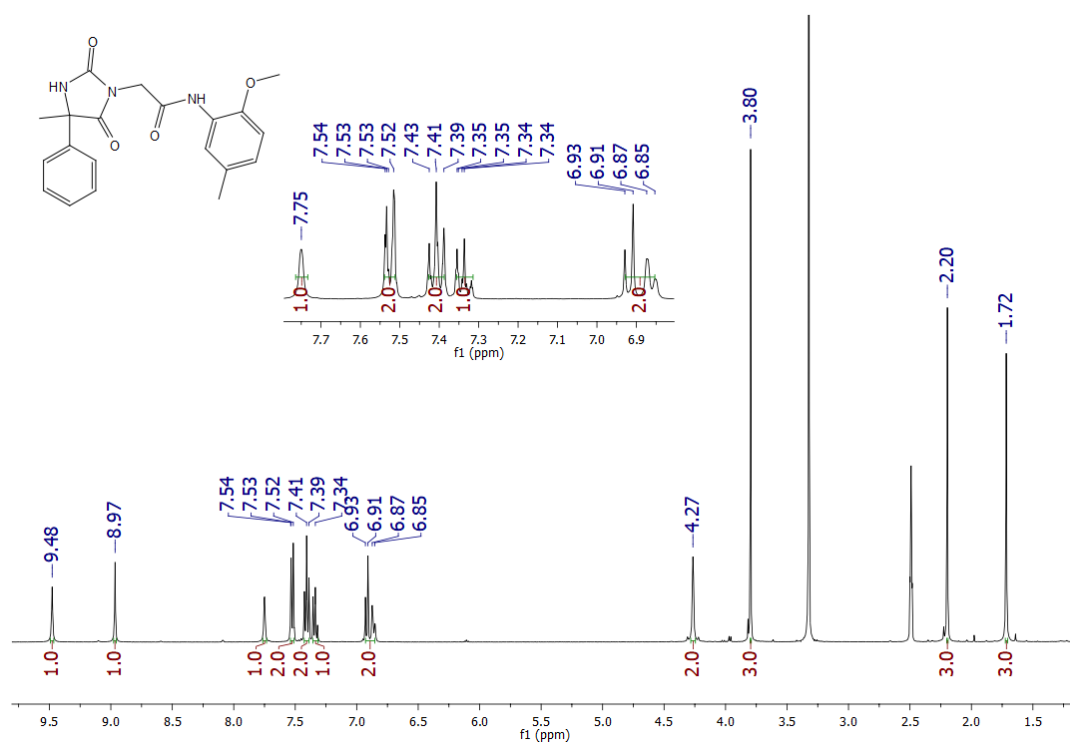


Figure S13. ¹H-NMR spectrum of compound **5d** in DMSO-*d*₆ at 400MHz.

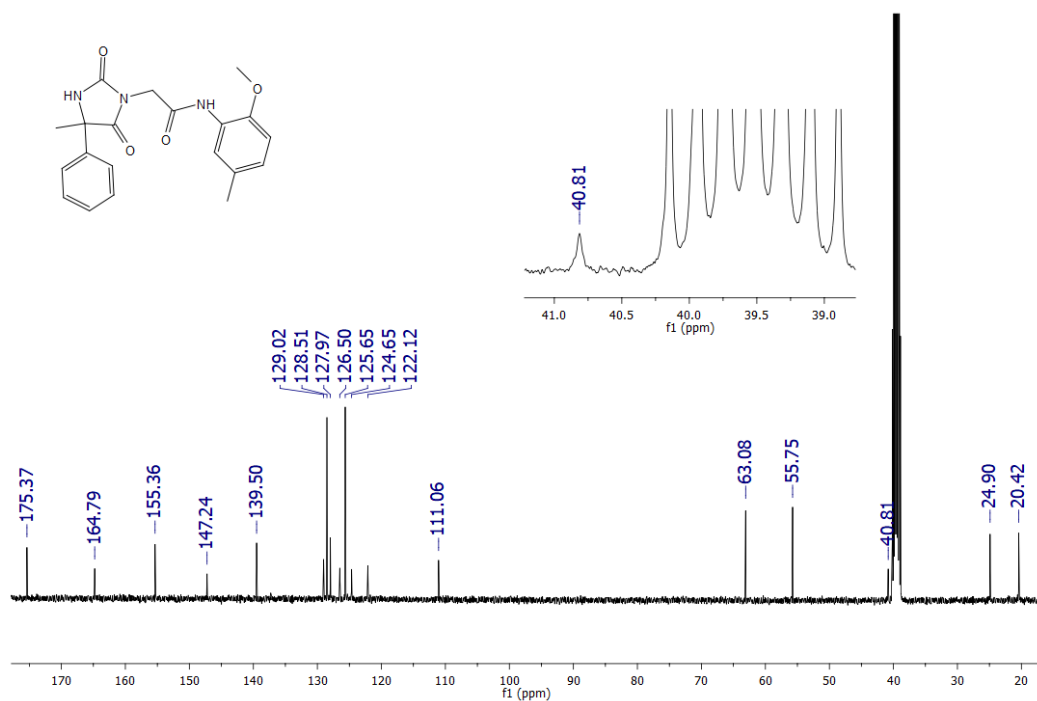


Figure S14. ¹³C-NMR spectrum of compound **5d** in DMSO-*d*₆ at 100MHz.

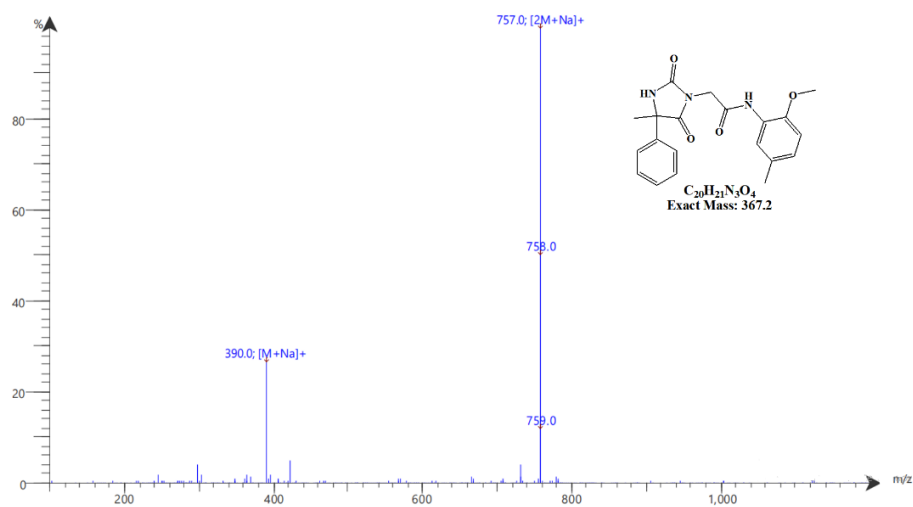


Figure S15. ESI mass spectrum of compound **5d**.

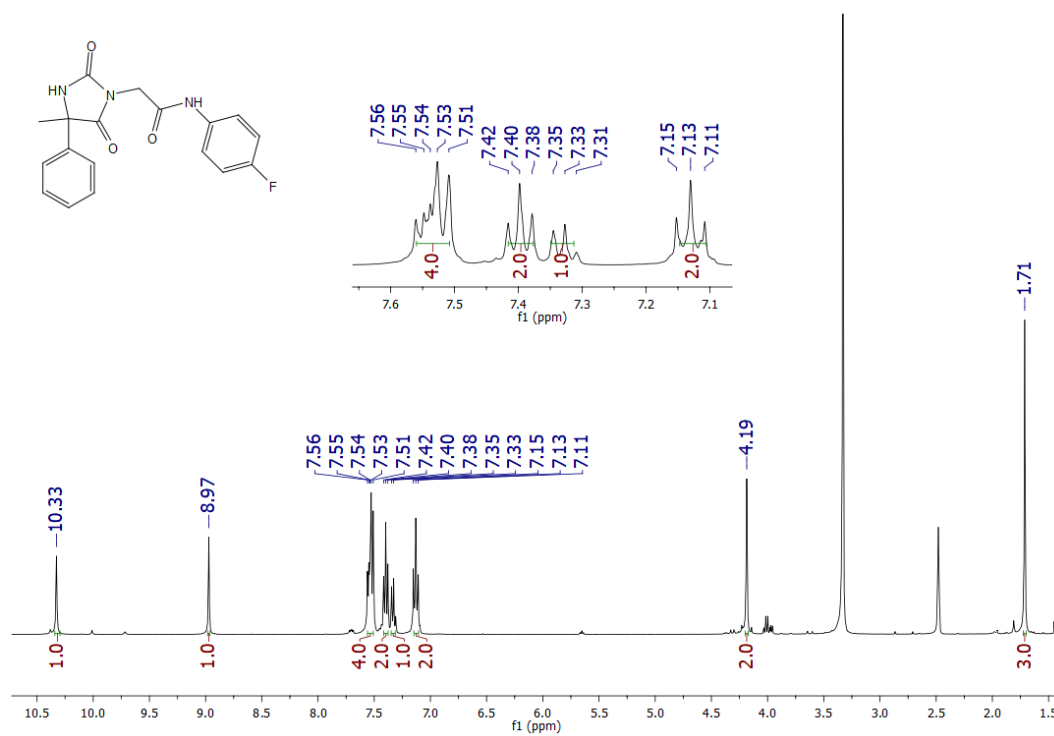


Figure S16. 1H -NMR spectrum of compound **5e** in $DMSO-d_6$ at 400MHz.

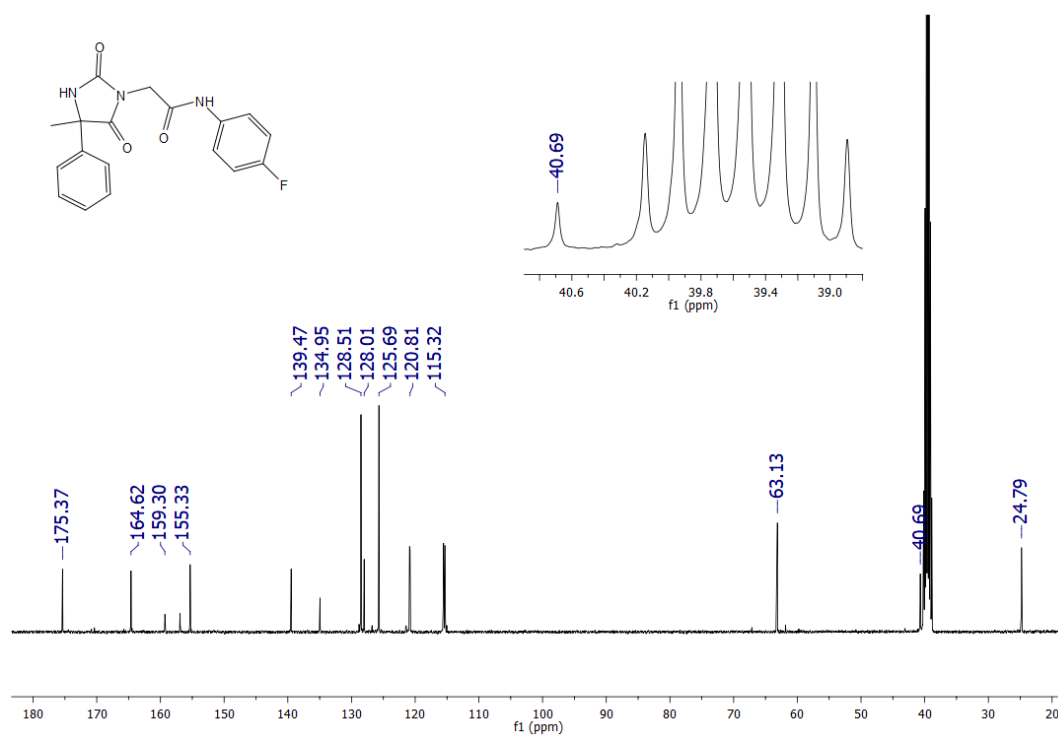


Figure S17. ¹³C-NMR spectrum of compound **5e** in DMSO-*d*₆ at 100MHz.

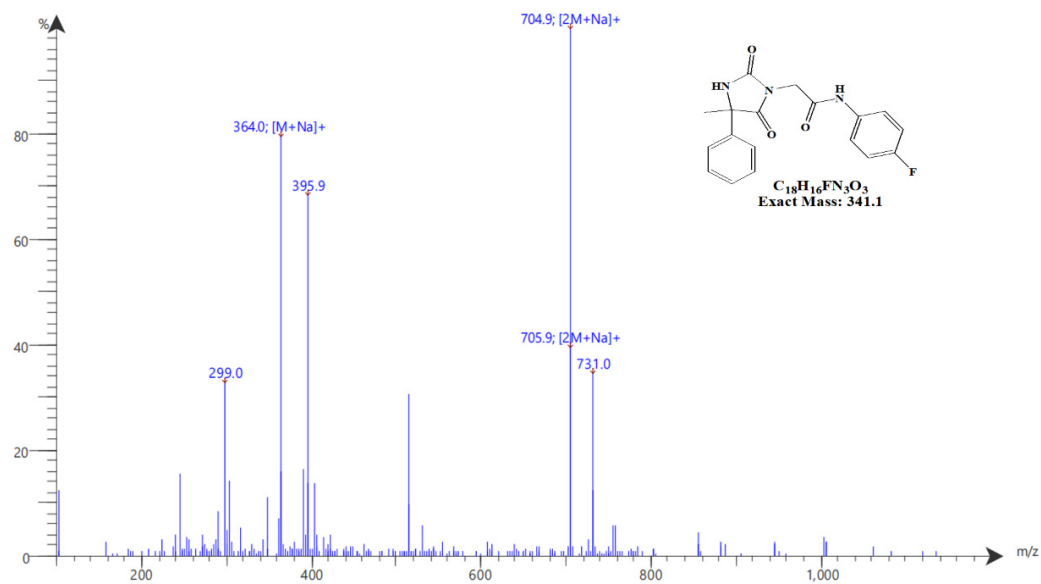


Figure S18. ESI mass spectrum of compound **5e**.

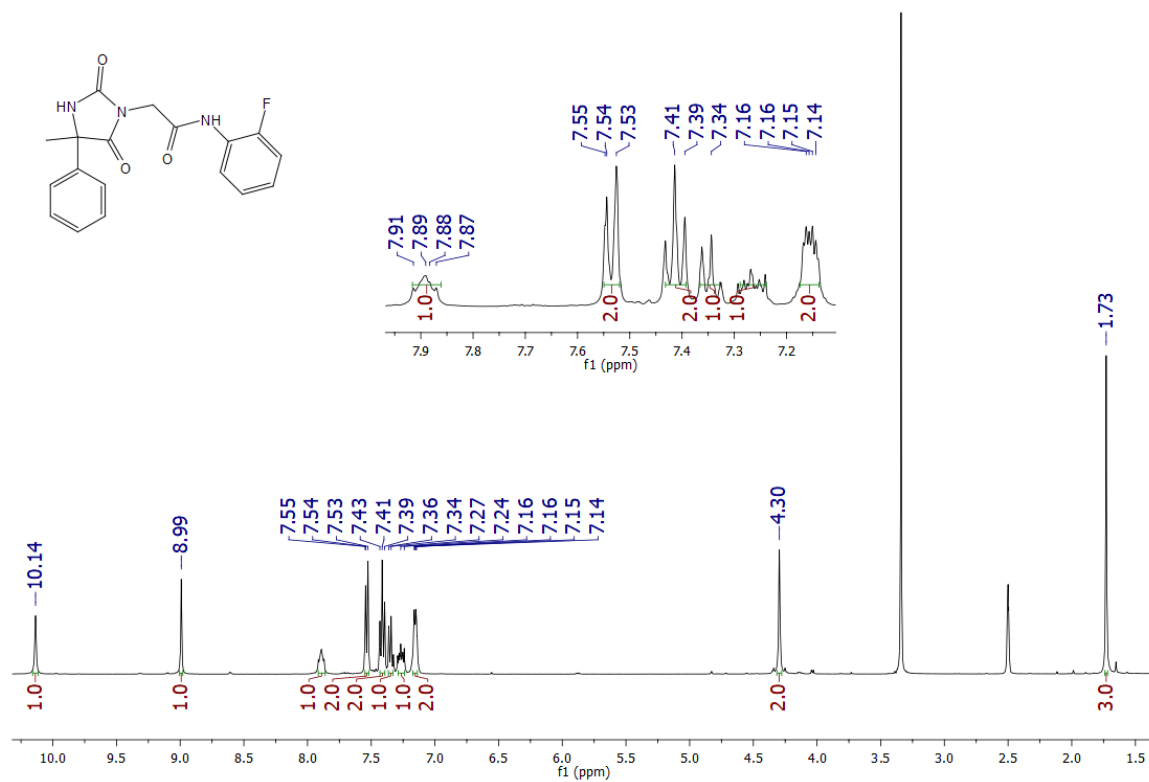


Figure S19. ¹H-NMR spectrum of compound **5f** in DMSO-*d*₆ at 400MHz.

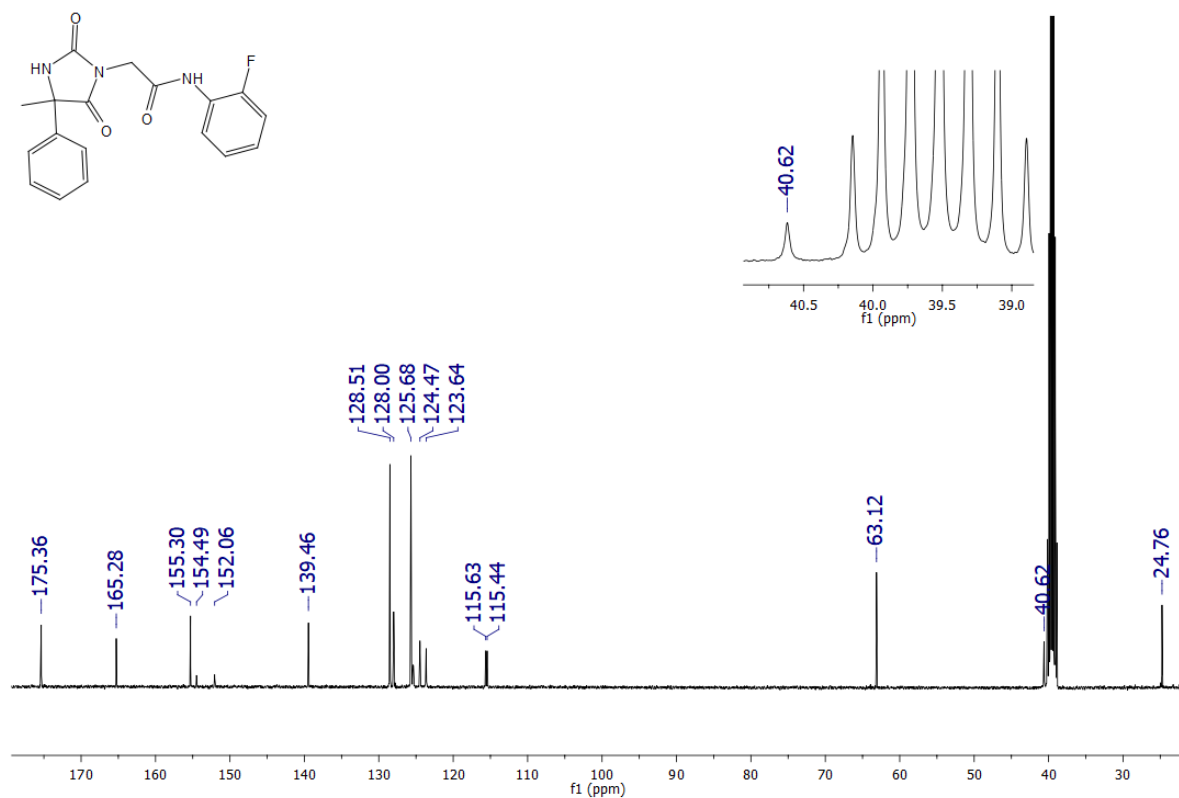


Figure S20. ¹³C-NMR spectrum of compound **5f** in DMSO-*d*₆ at 100MHz.

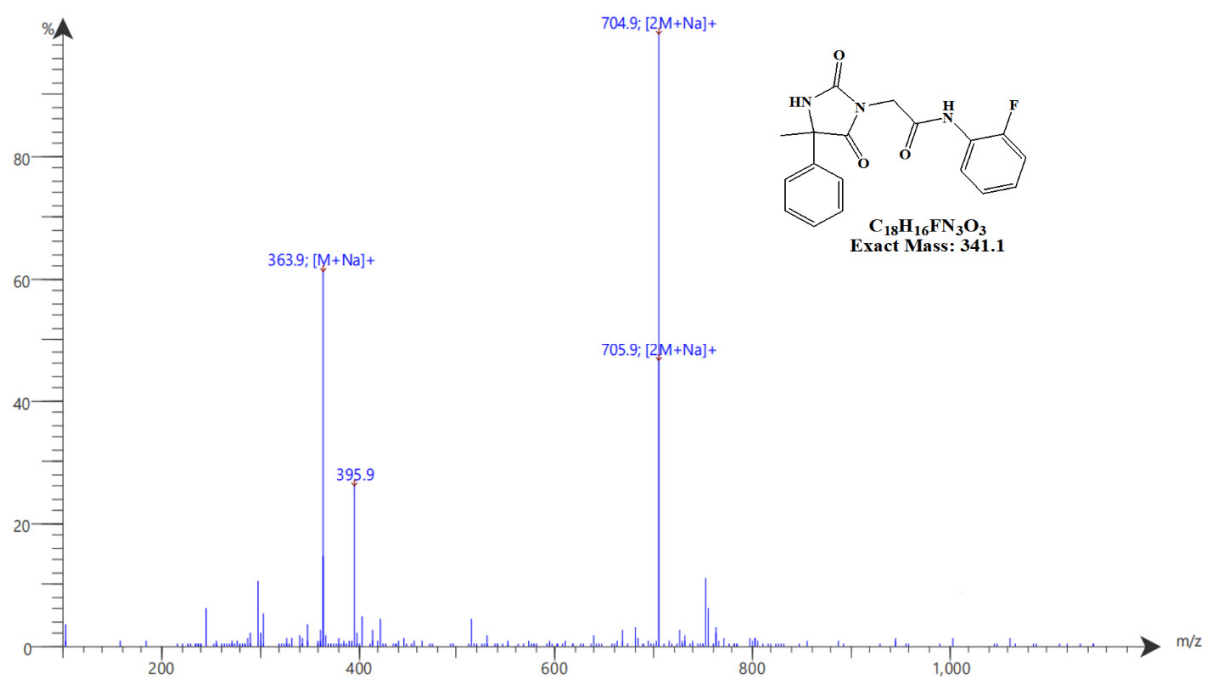


Figure S21. ESI mass spectrum of compound **5f**.

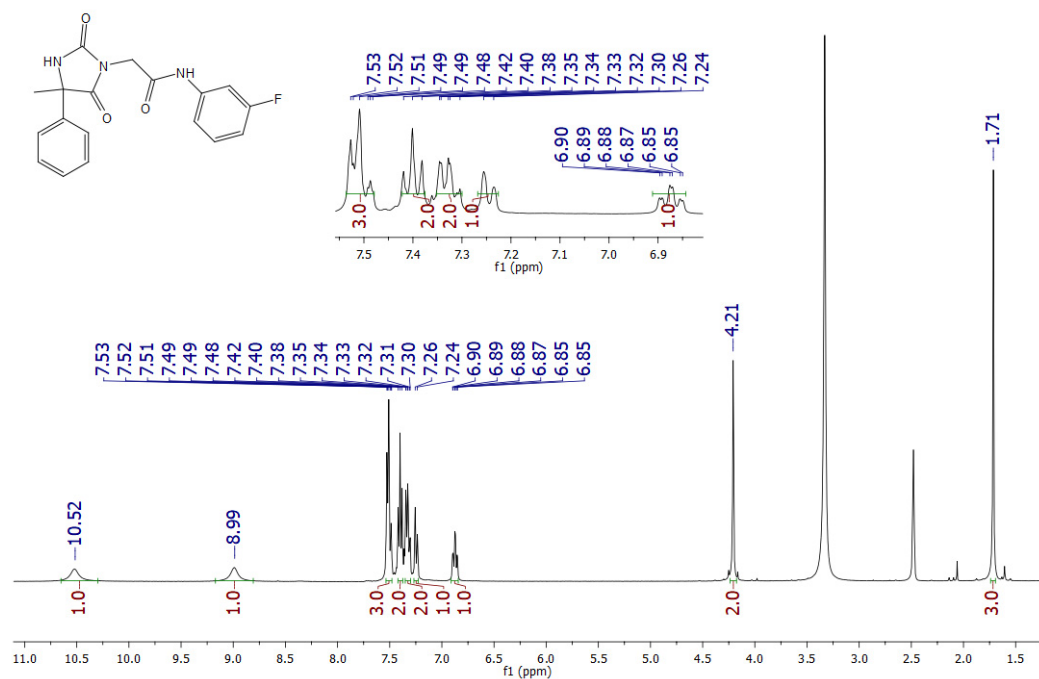


Figure S22. ¹H-NMR spectrum of compound **5g** in DMSO-*d*₆ at 400MHz.

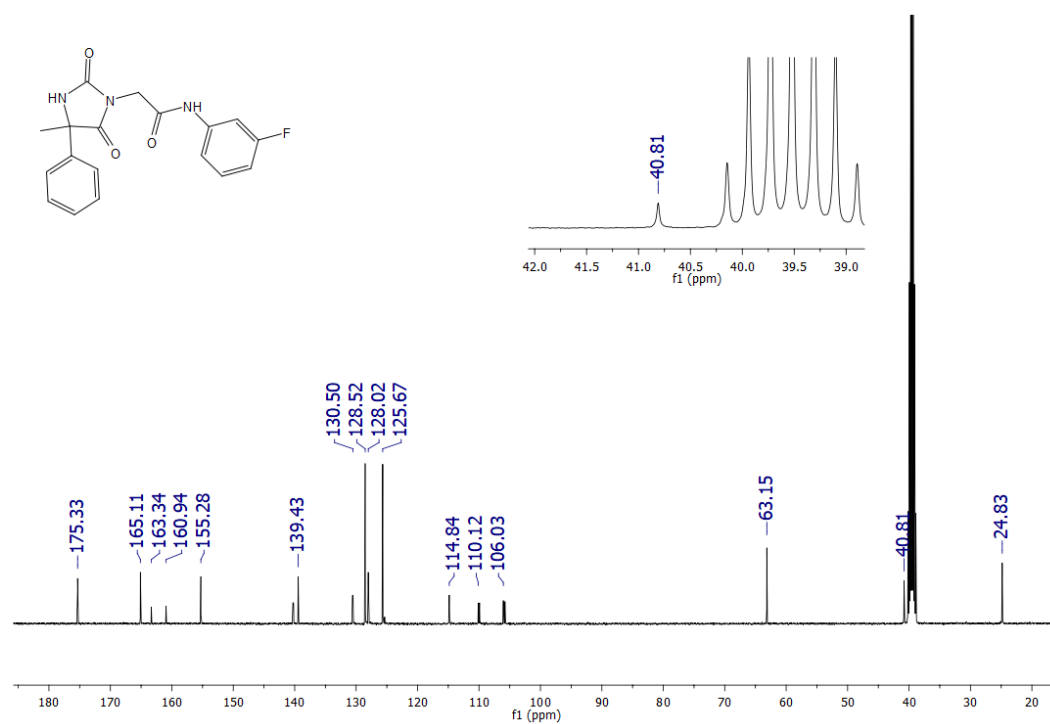


Figure S23. ¹³C-NMR spectrum of compound **5g** in DMSO-*d*₆ at 100MHz.

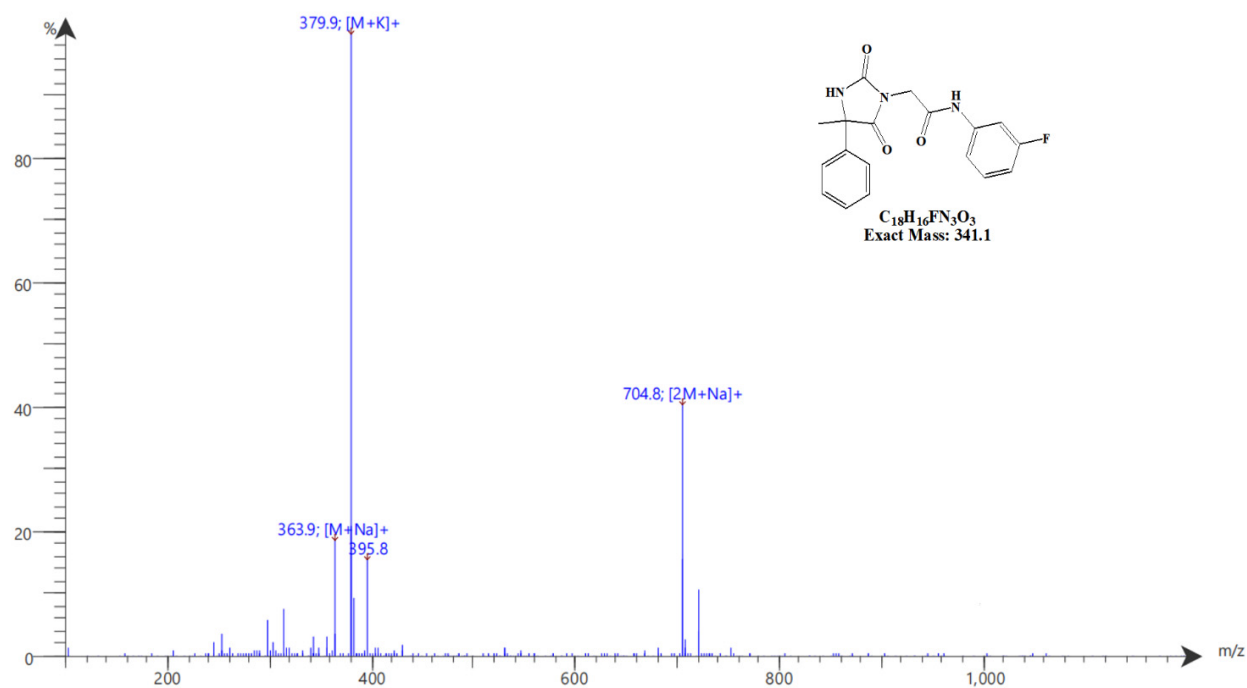


Figure S24. ESI mass spectrum of compound **5g**.

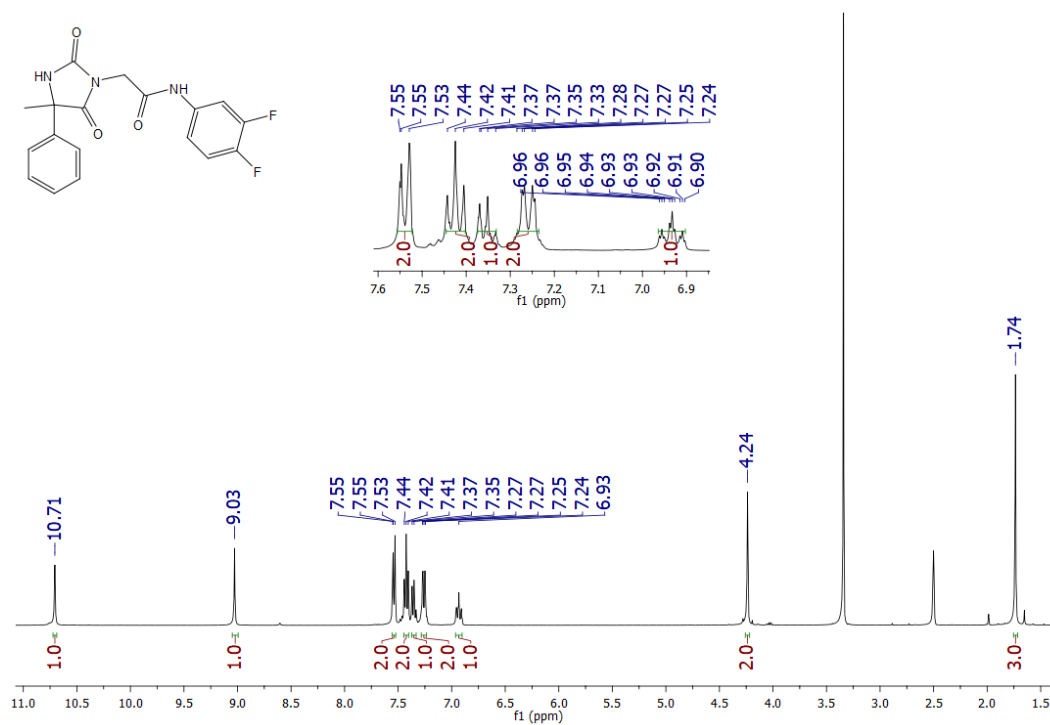


Figure S25. 1H -NMR spectrum of compound **5h** in $DMSO-d_6$ at 400MHz.

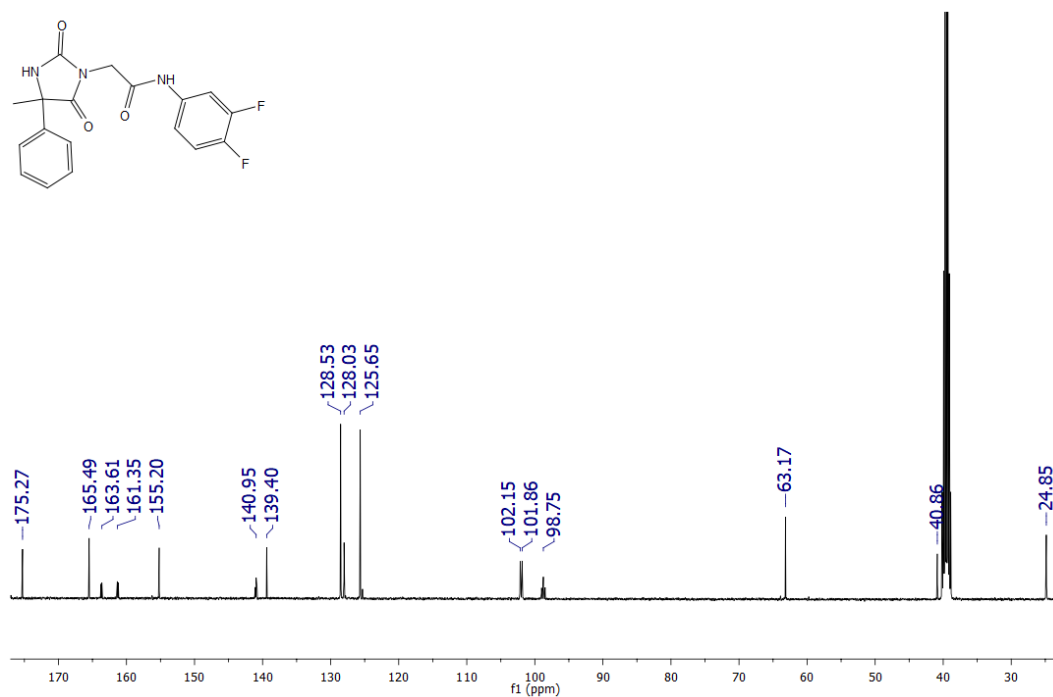


Figure S26. ¹³C-NMR spectrum of compound **5h** in DMSO-*d*₆ at 100MHz.

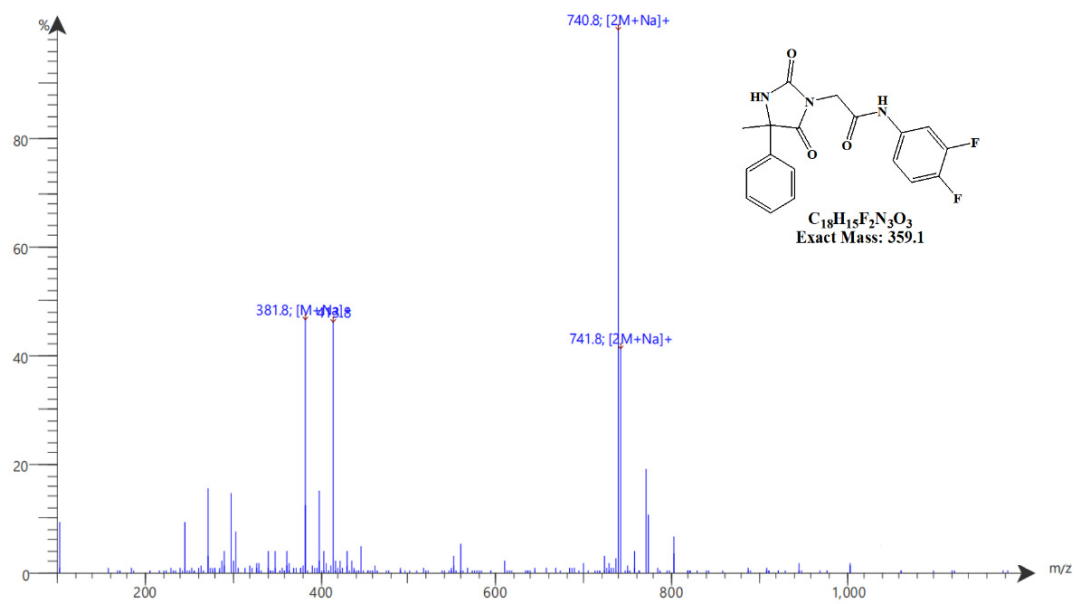


Figure S27. ESI mass spectrum of compound **5h**.

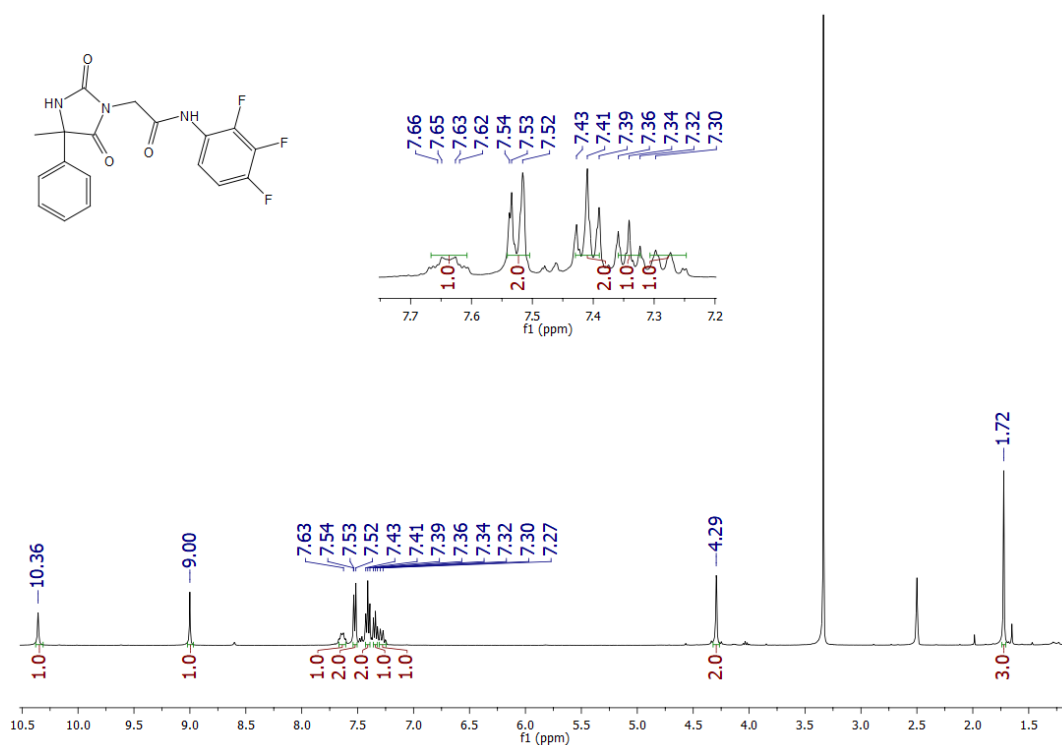


Figure S28. ¹H-NMR spectrum of compound **5i** in DMSO-*d*₆ at 400MHz.

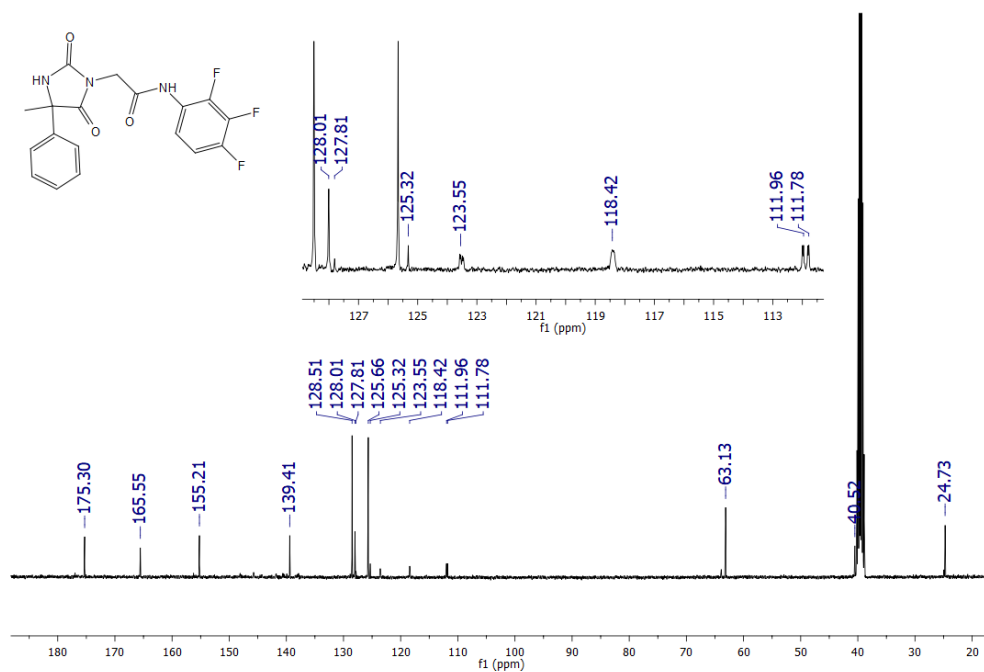


Figure S29. ¹³C-NMR spectrum of compound **5i** in DMSO-*d*₆ at 100MHz.

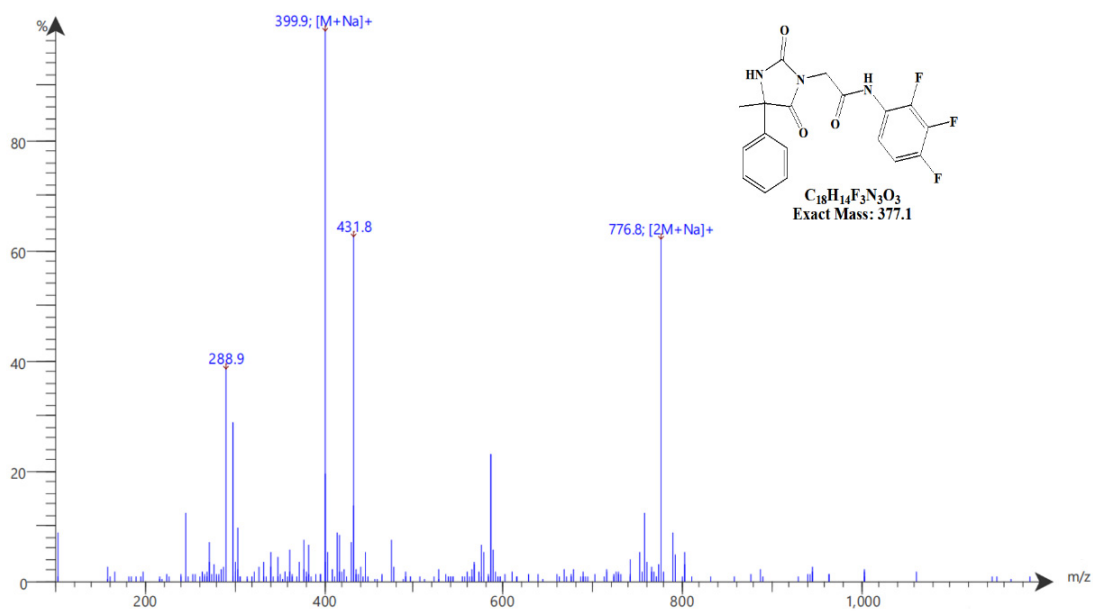


Figure S30. ESI mass spectrum of compound **5i**.

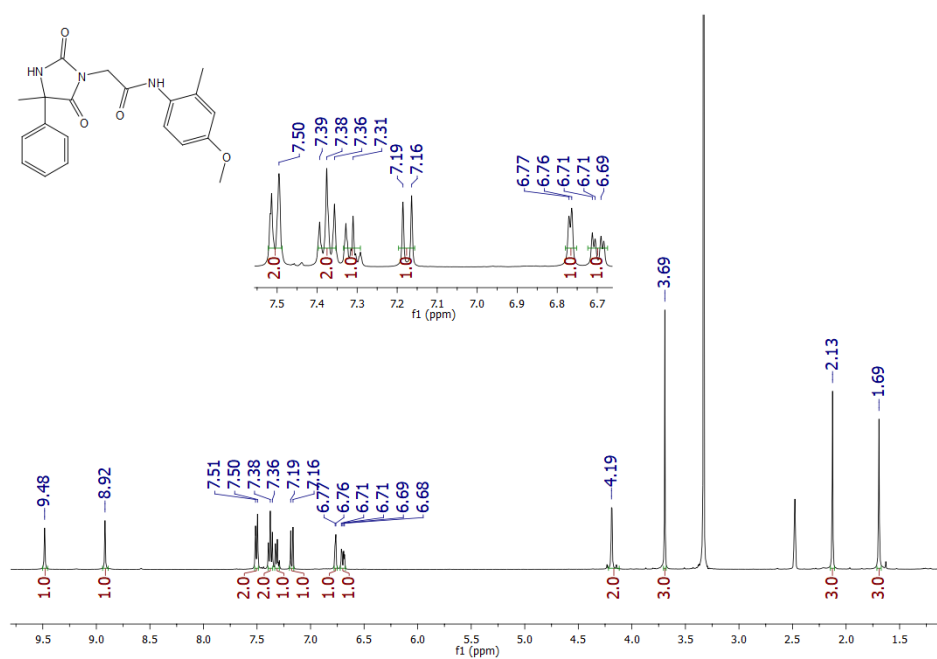


Figure S31. 1H -NMR spectrum of compound **5j** in $DMSO-d_6$ at 400 MHz.

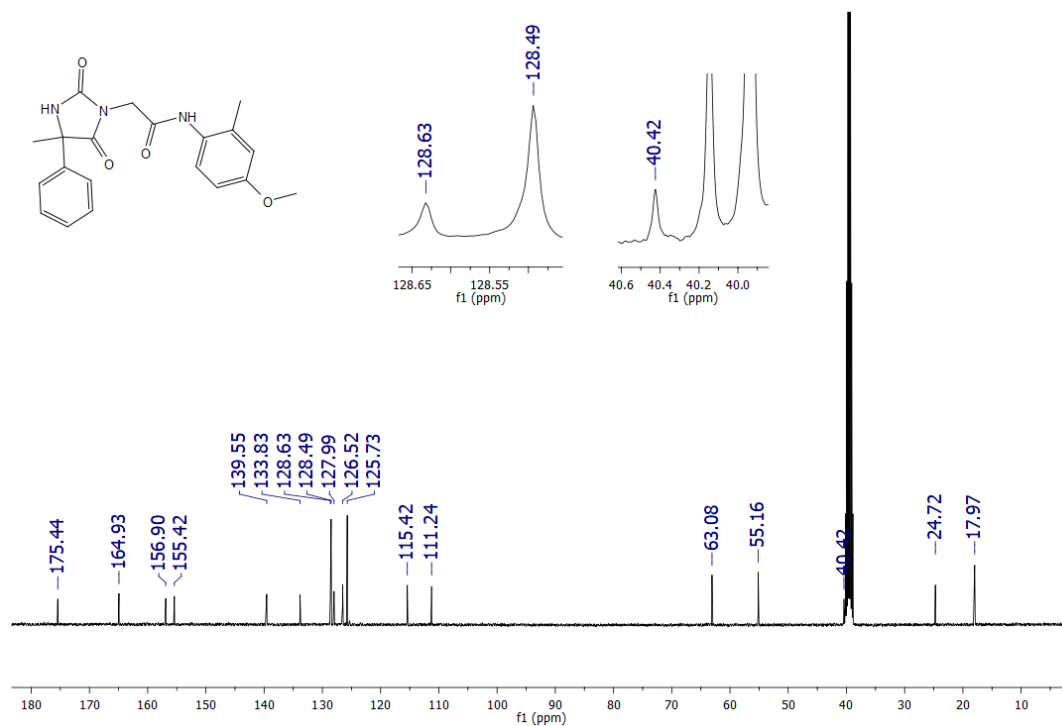


Figure S32. ^{13}C -NMR spectrum of compound **5j** in $\text{DMSO-}d_6$ at 100MHz.

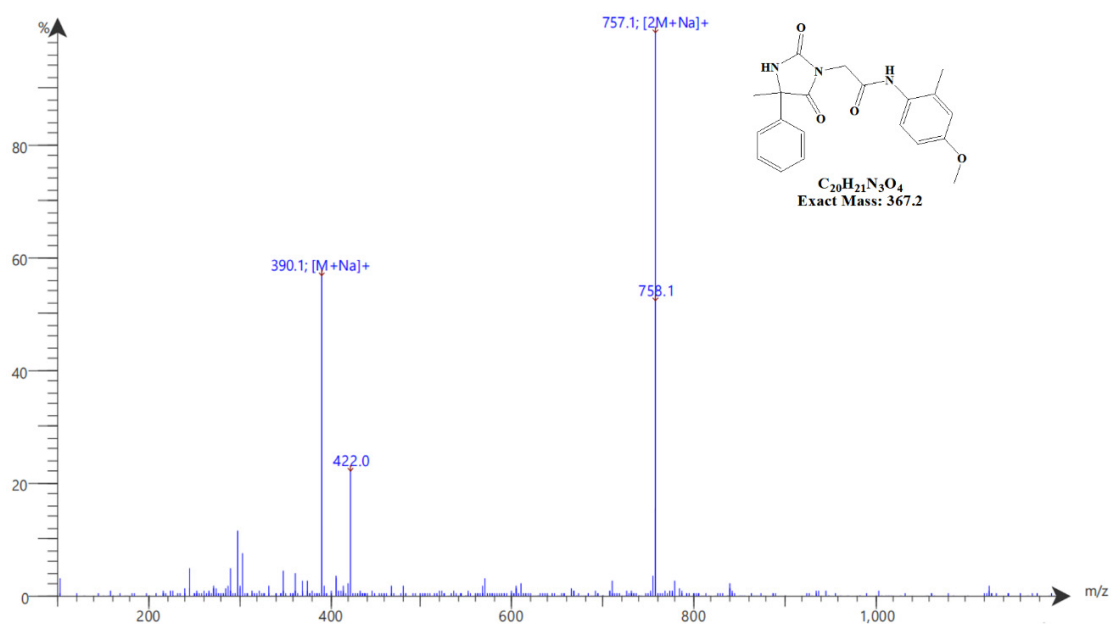


Figure S33. ESI mass spectrum of compound **5j**.

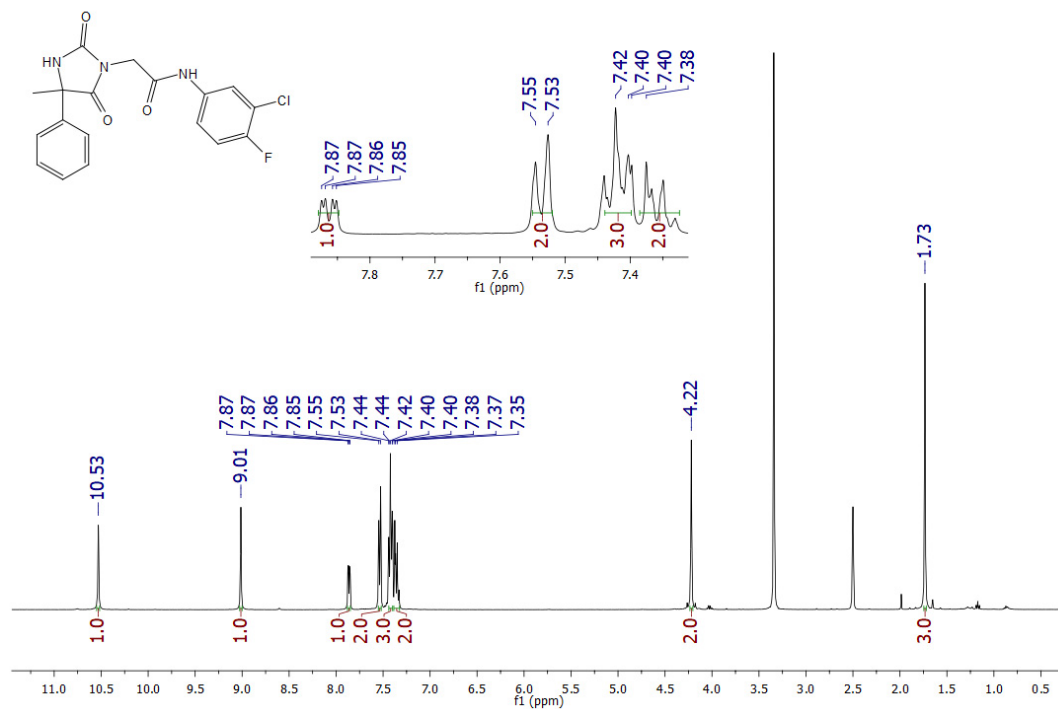


Figure S34. ¹H-NMR spectrum of compound **5k** in DMSO-*d*₆ at 400MHz.

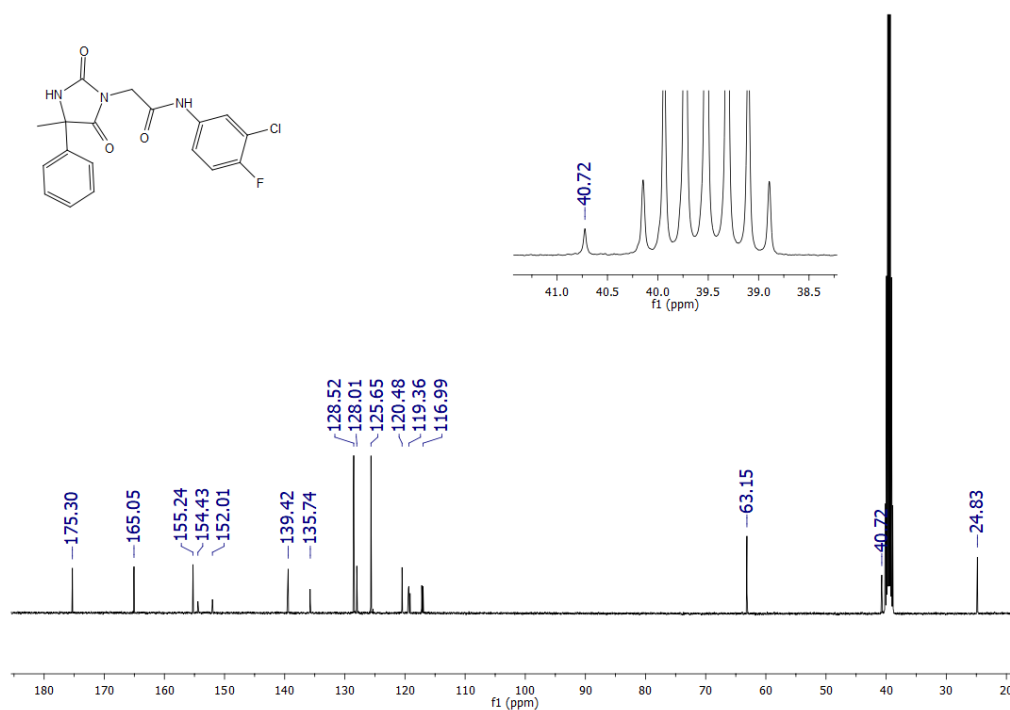


Figure S35. ¹³C-NMR spectrum of compound **5k** in DMSO-*d*₆ at 100MHz.

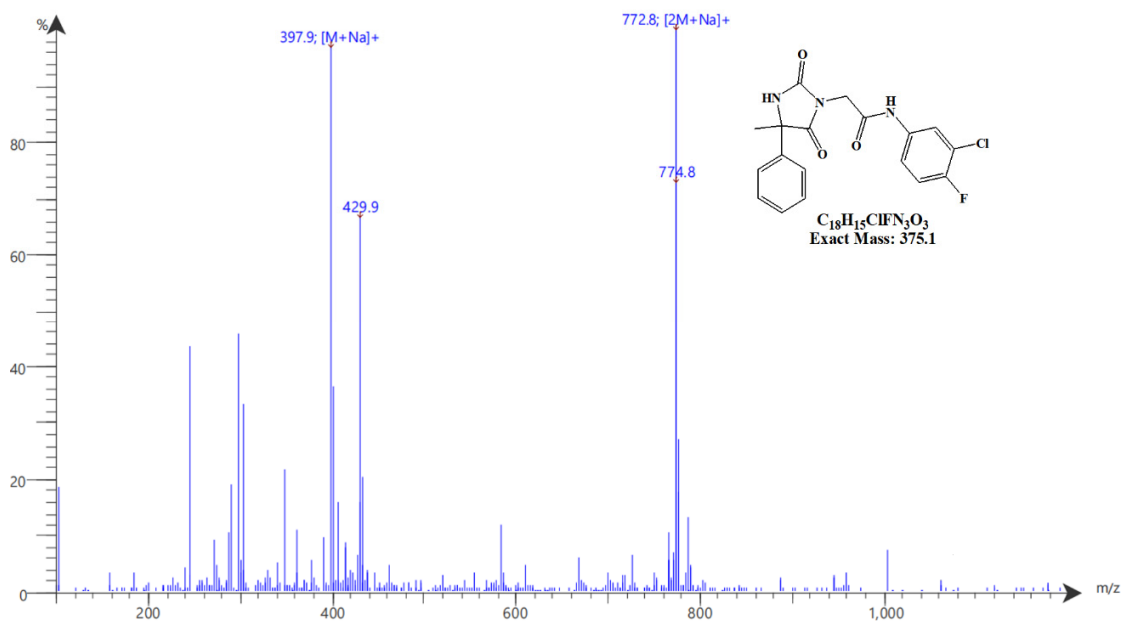


Figure S36. ESI mass spectrum of compound **5k**.

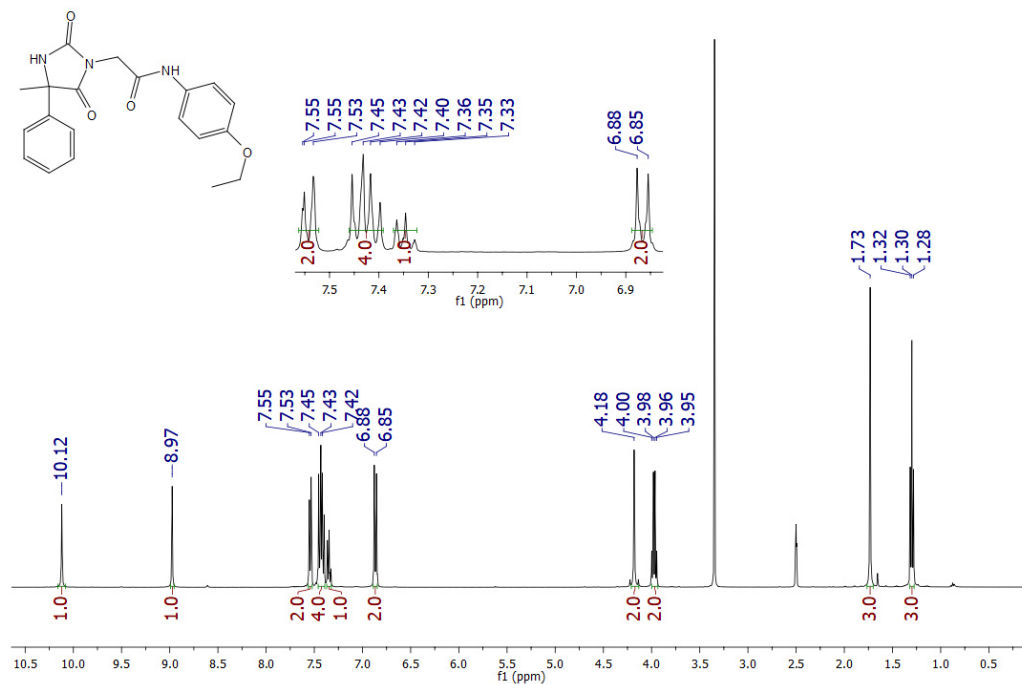


Figure S37. 1H -NMR spectrum of compound **5l** in $DMSO-d_6$ at 400 MHz.

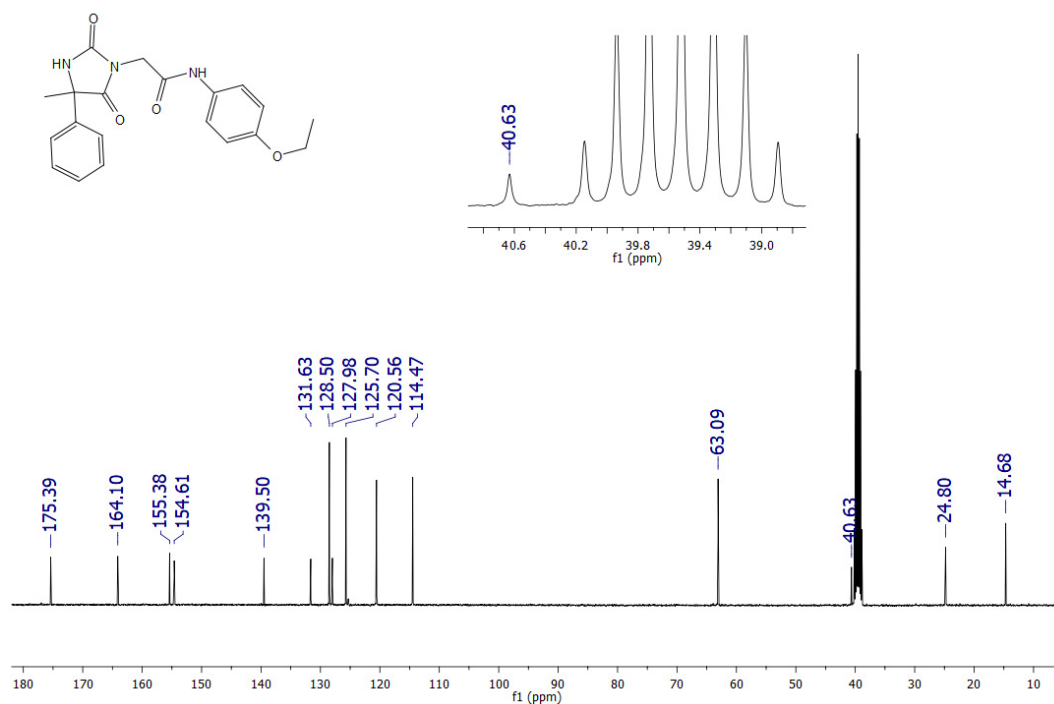


Figure S38. ¹³C-NMR spectrum of compound **5I** in DMSO-*d*₆ at 100MHz.

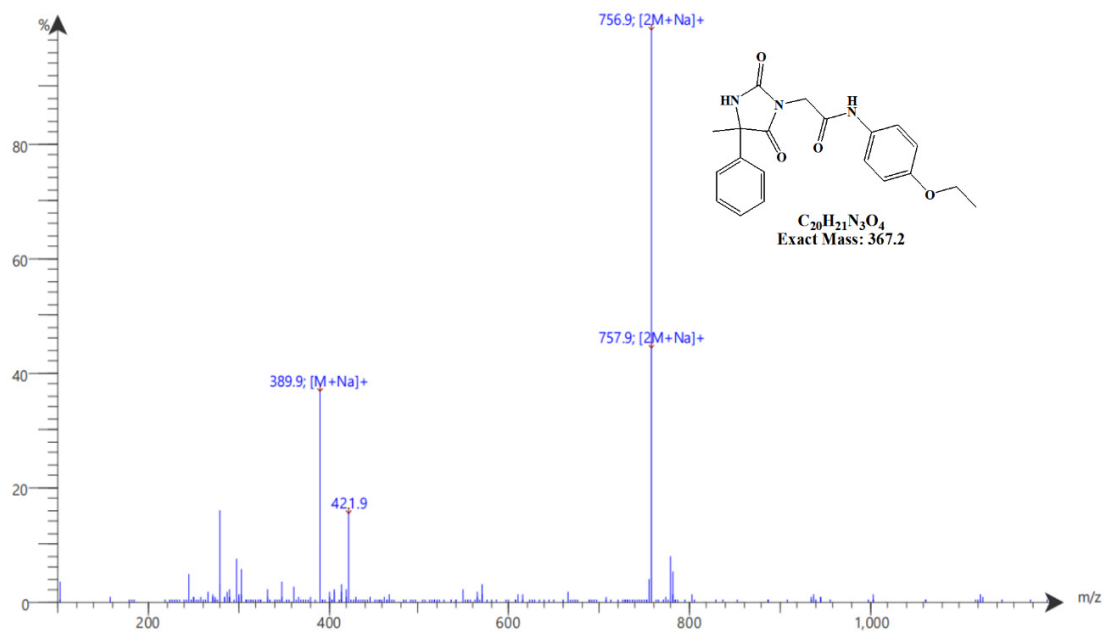


Figure S39. ESI mass spectrum of compound **5I**.

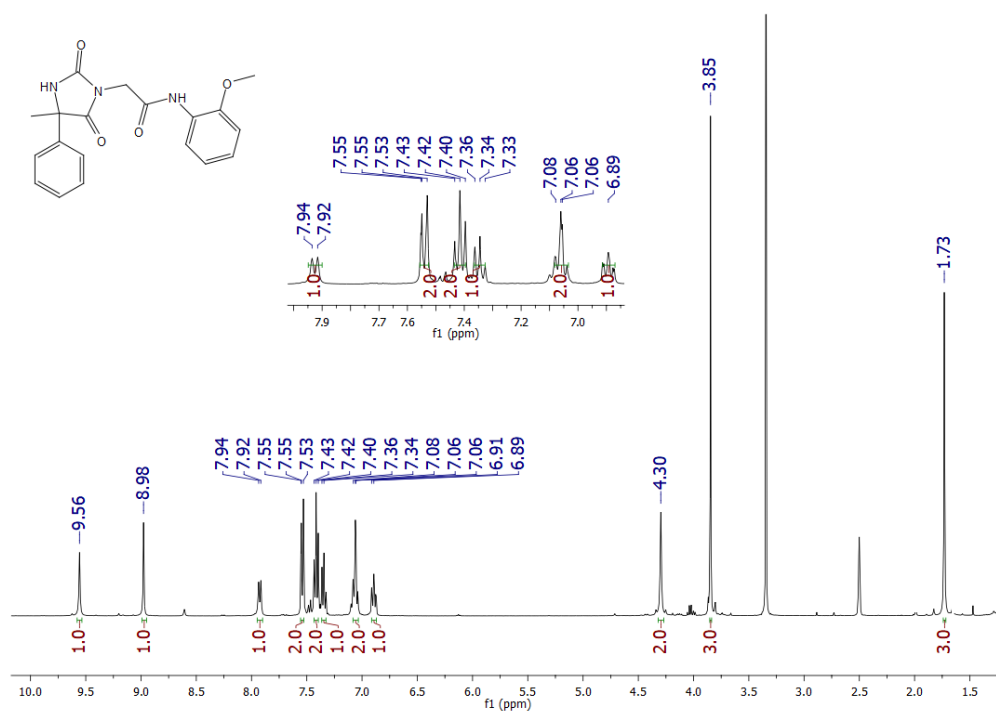


Figure S40. ¹H-NMR spectrum of compound **5m** in DMSO-*d*₆ at 400MHz.

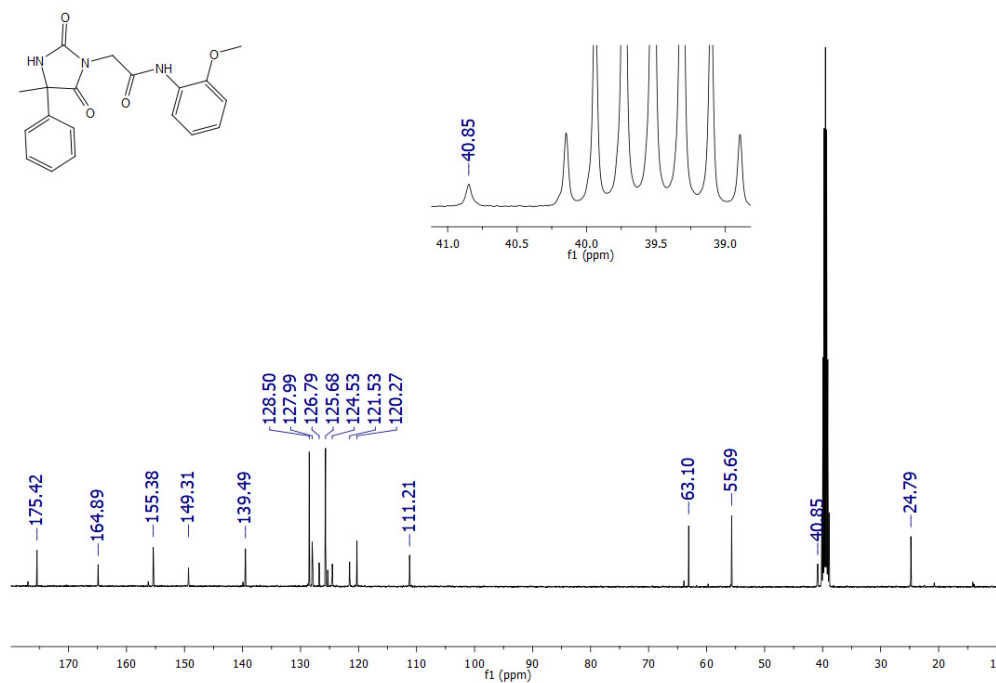


Figure S41. ¹³C-NMR spectrum of compound **5m** in DMSO-*d*₆ at 100MHz.

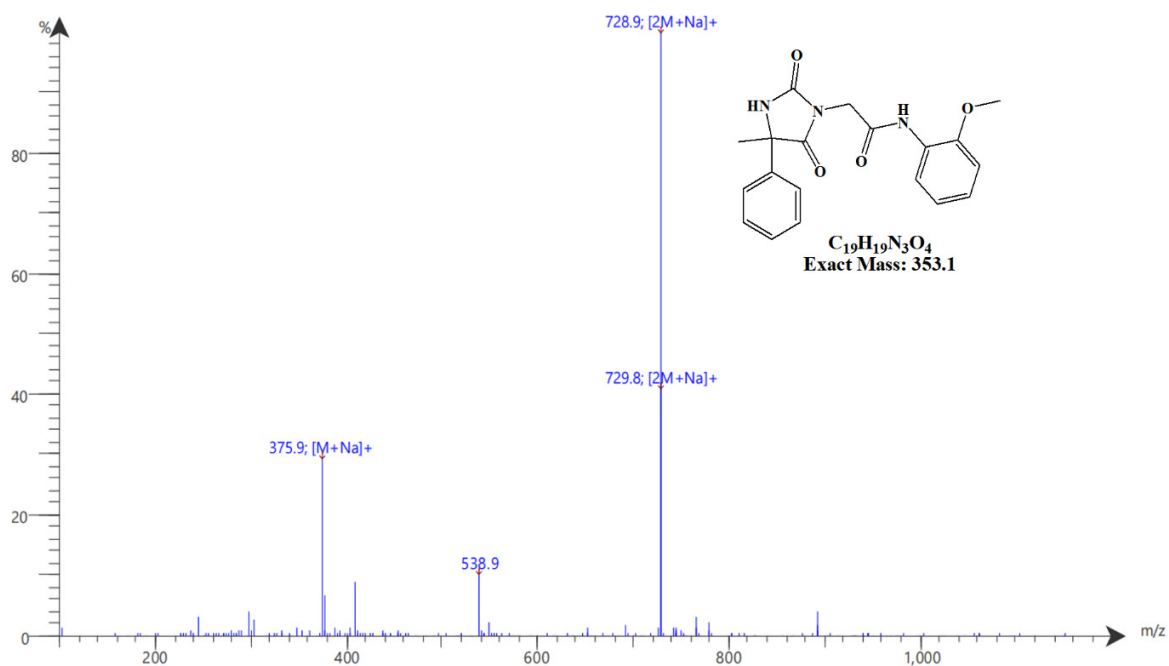


Figure S42. ESI mass spectrum of compound **5m**.

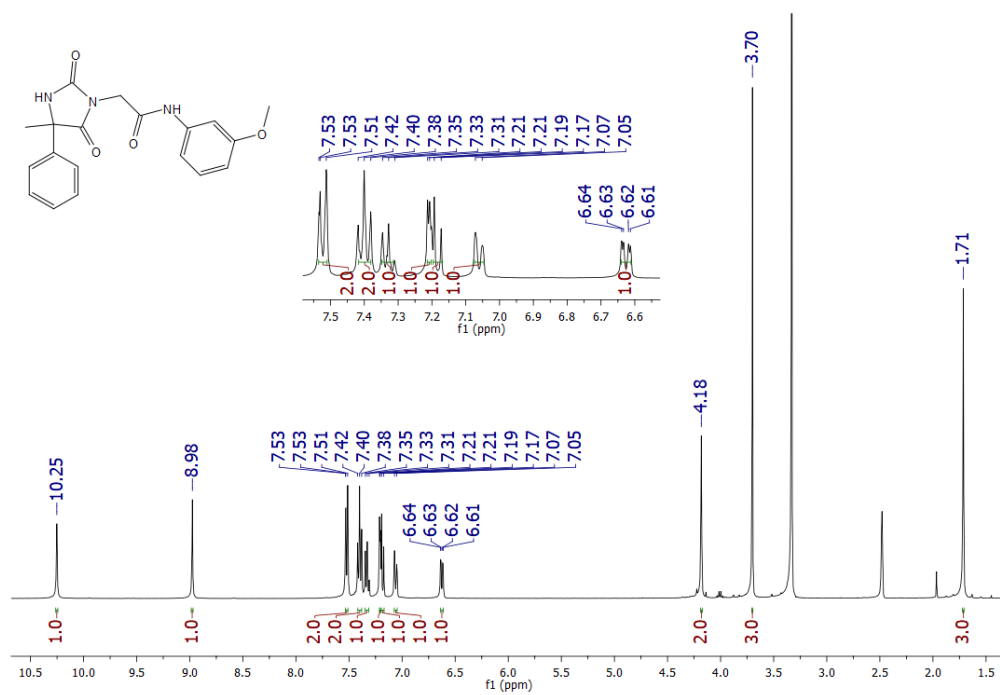


Figure S43. 1H -NMR spectrum of compound **5n** in $DMSO-d_6$ at 400MHz.

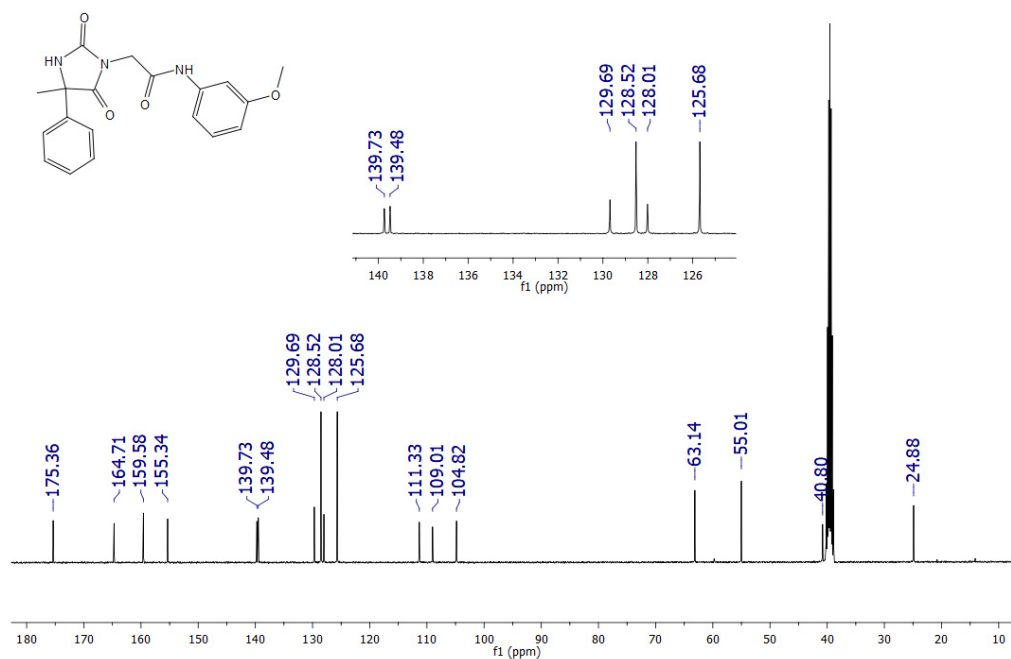


Figure S44. ¹³C-NMR spectrum of compound **5n** in DMSO-*d*₆ at 100MHz.

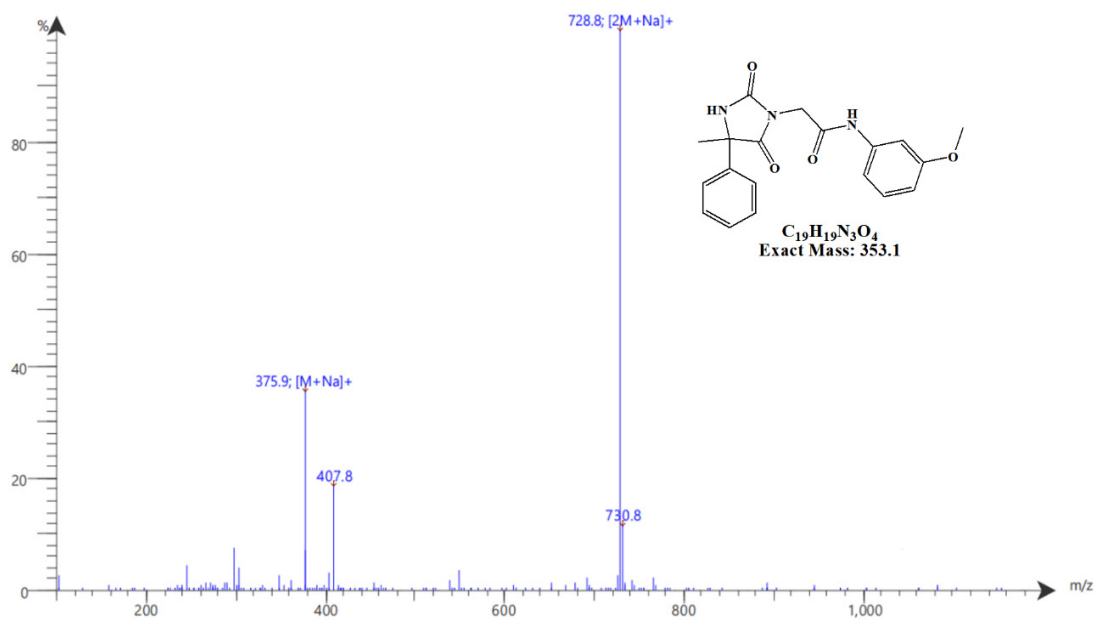


Figure S45. ESI mass spectrum of compound **5n**.

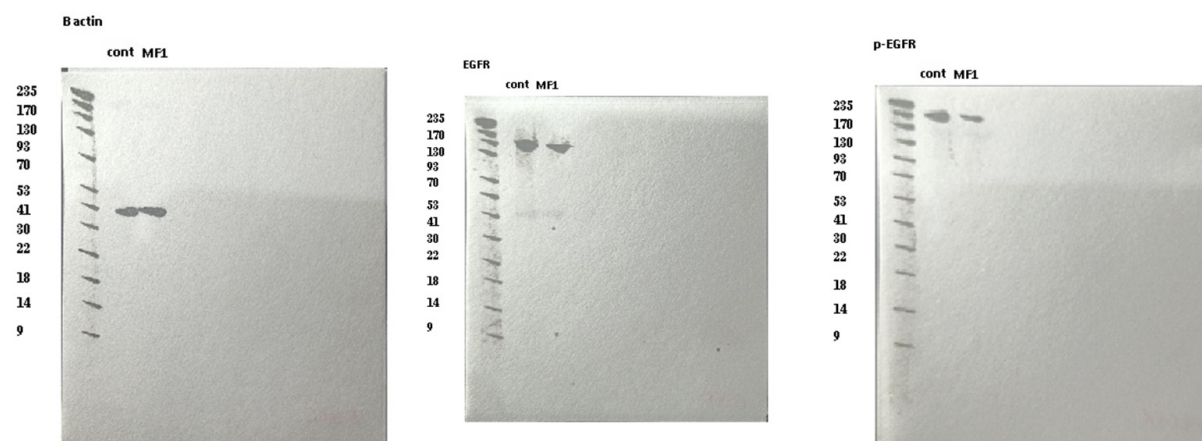


Figure S46. Western blotting analysis measuring the expression of **5a** on EGFR.