

Supplementary Information

Synthesis of New C-3 Substituted Kynurenic Acid Derivatives

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3-(((2-Morpholinoethyl)amino)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (2)

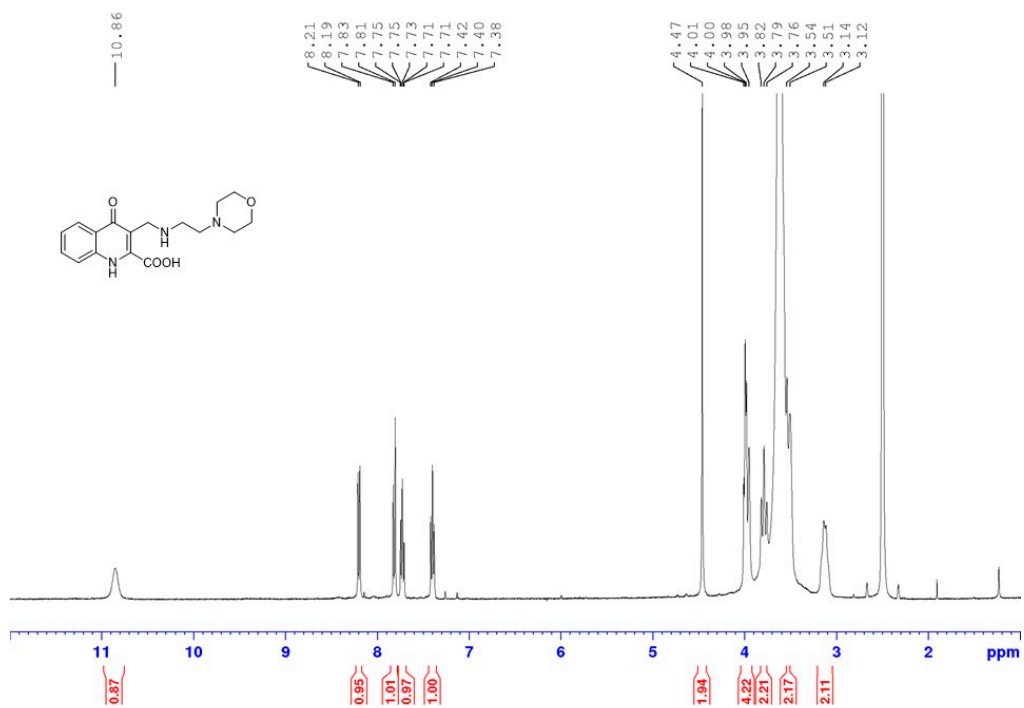


Figure S1. ¹H-NMR spectrum of 2

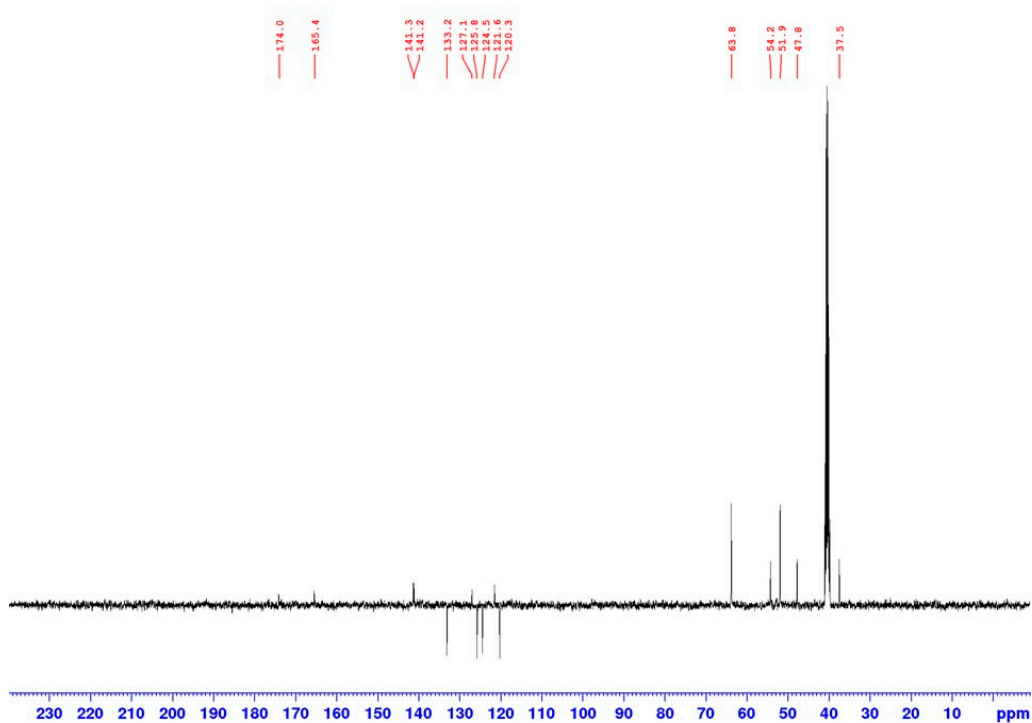


Figure S2. ¹³C-NMR spectrum of 2

3-(((2-(Dimethylamino)ethyl)amino)(phenyl)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (**3**)

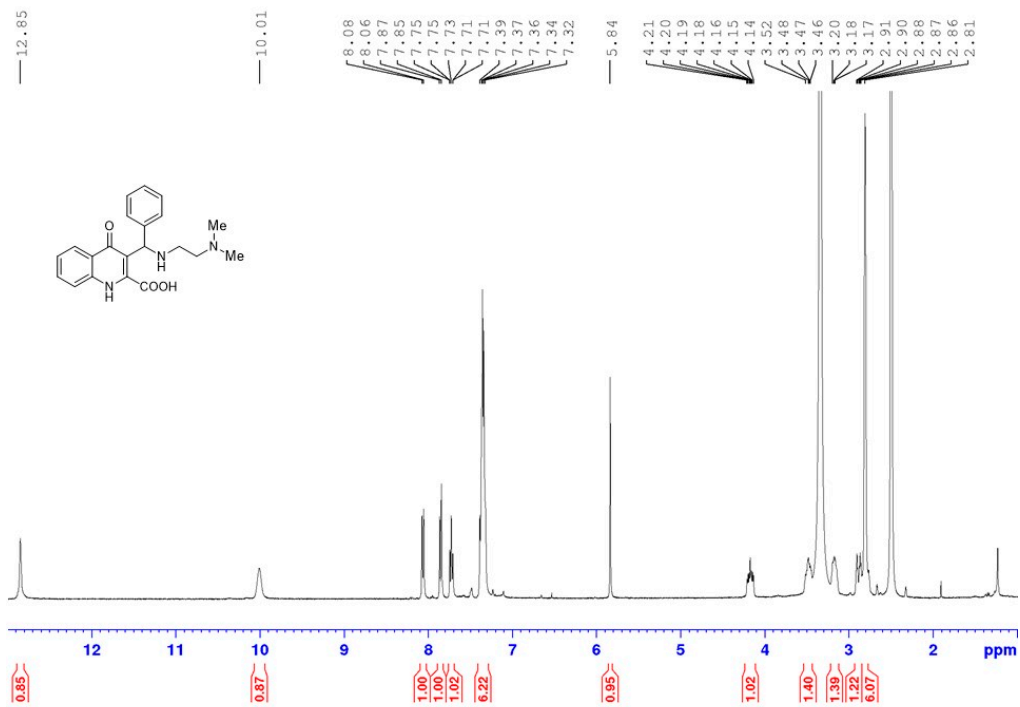


Figure S3. ¹H-NMR spectrum of **3**

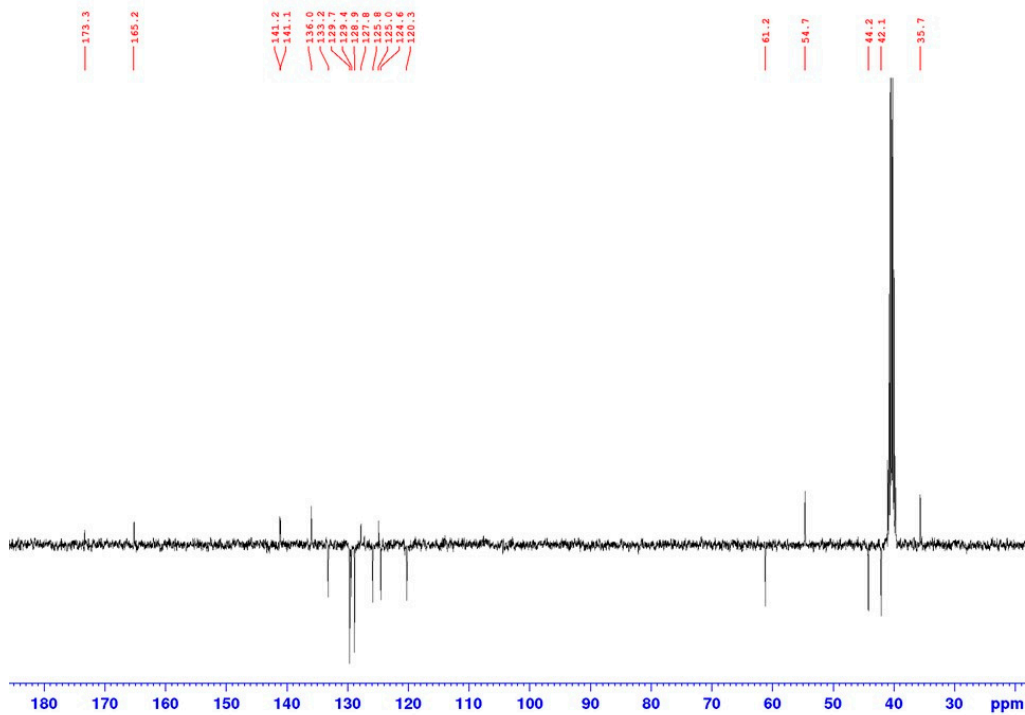


Figure S4. ¹³C-NMR spectrum of **3**

3-((Dimethylamino)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (4a)

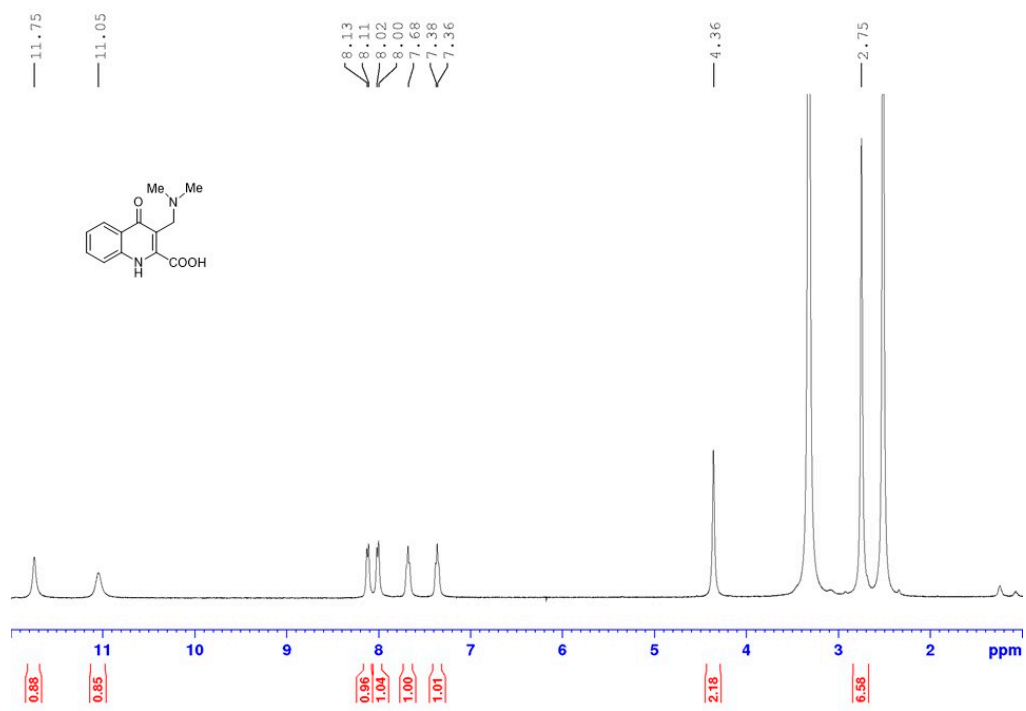


Figure S5. ¹H-NMR spectrum of 4a

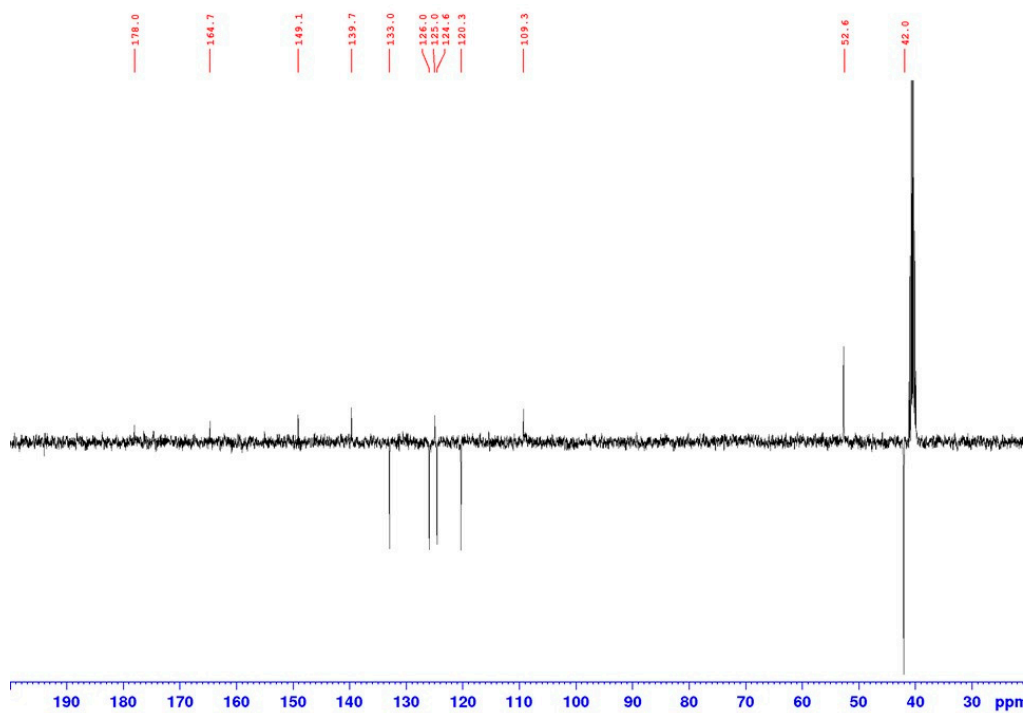


Figure S6. ¹³C-NMR spectrum of 4a

3-((Benzyl(methyl)amino)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (**4b**)

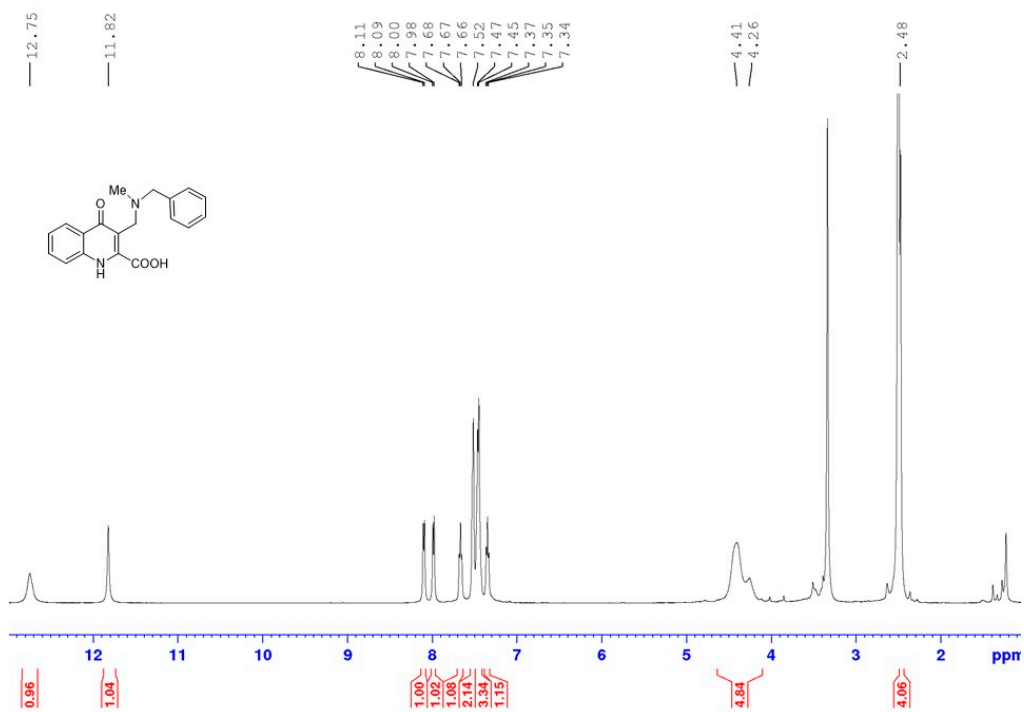


Figure S7. ¹H-NMR spectrum of **4b**

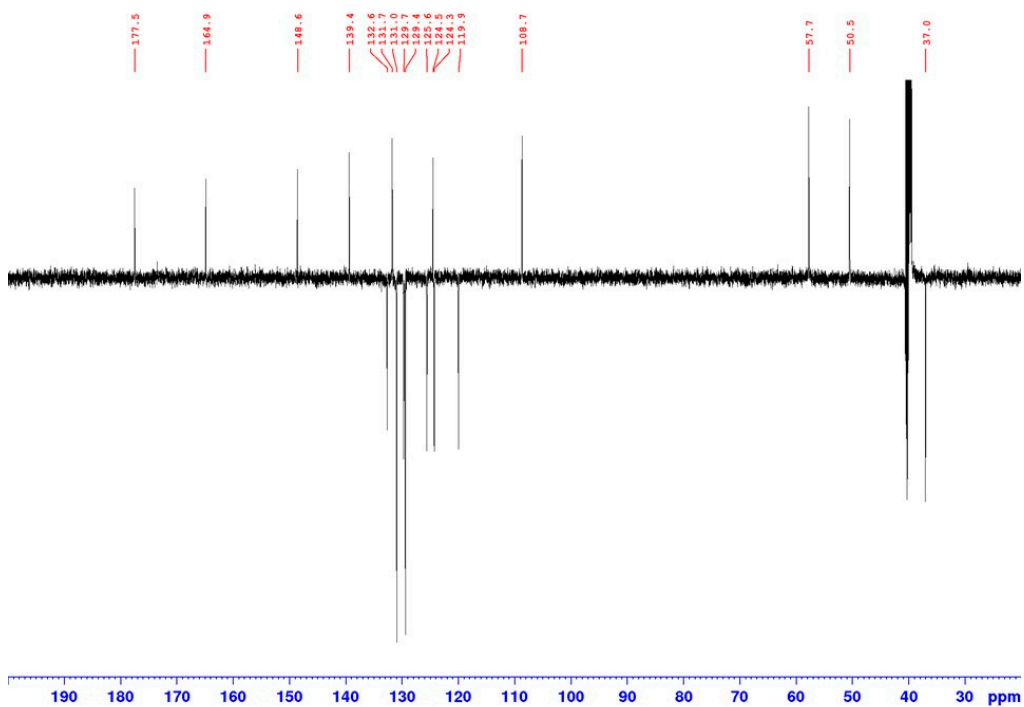


Figure S8. ¹³C-NMR spectrum of **4b**

4-Oxo-3-(piperidin-1-ylmethyl)-1,4-dihydroquinoline-2-carboxylic acid (**5b**)

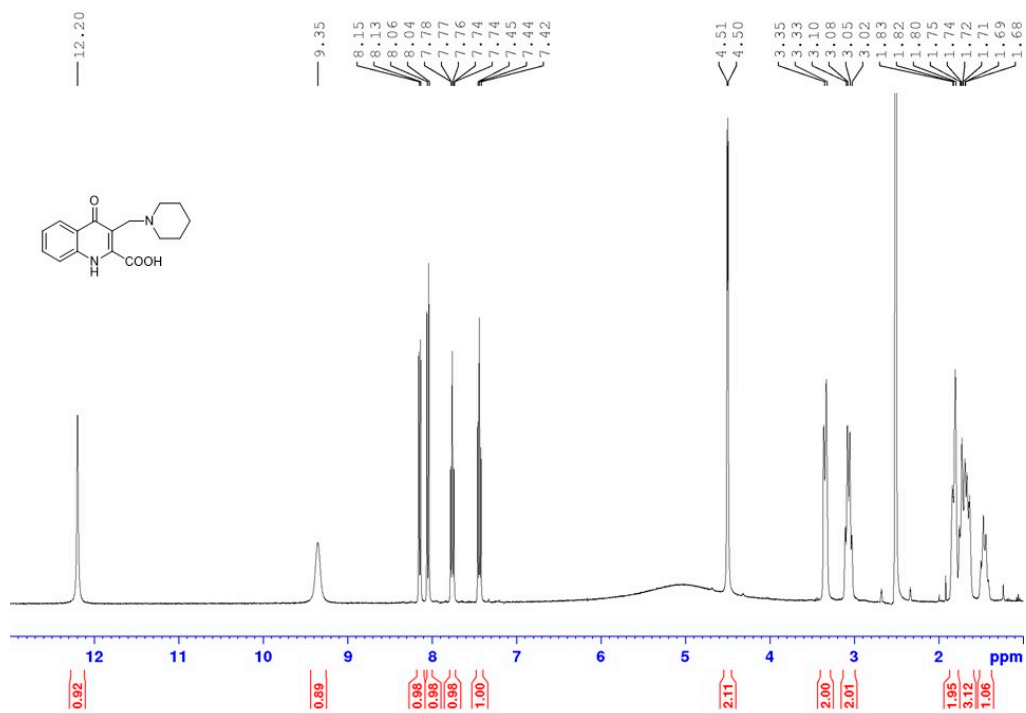


Figure S9. ¹H-NMR spectrum of **5b**

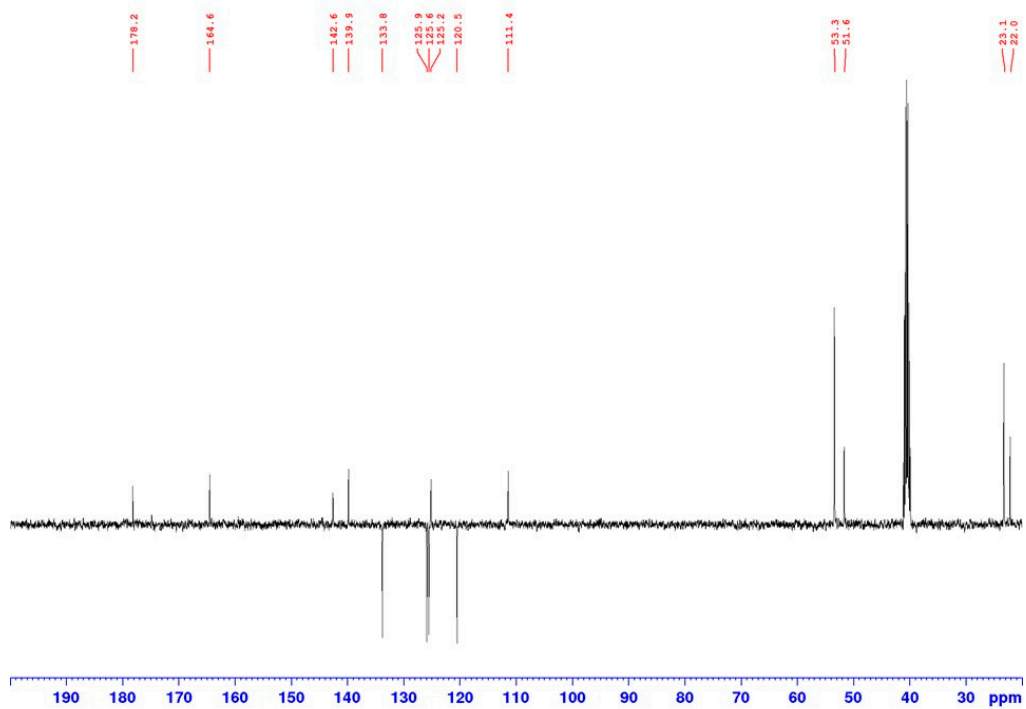


Figure S10. ¹³C-NMR spectrum of **5b**

3-((4-Methylpiperazin-1-yl)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (5c)

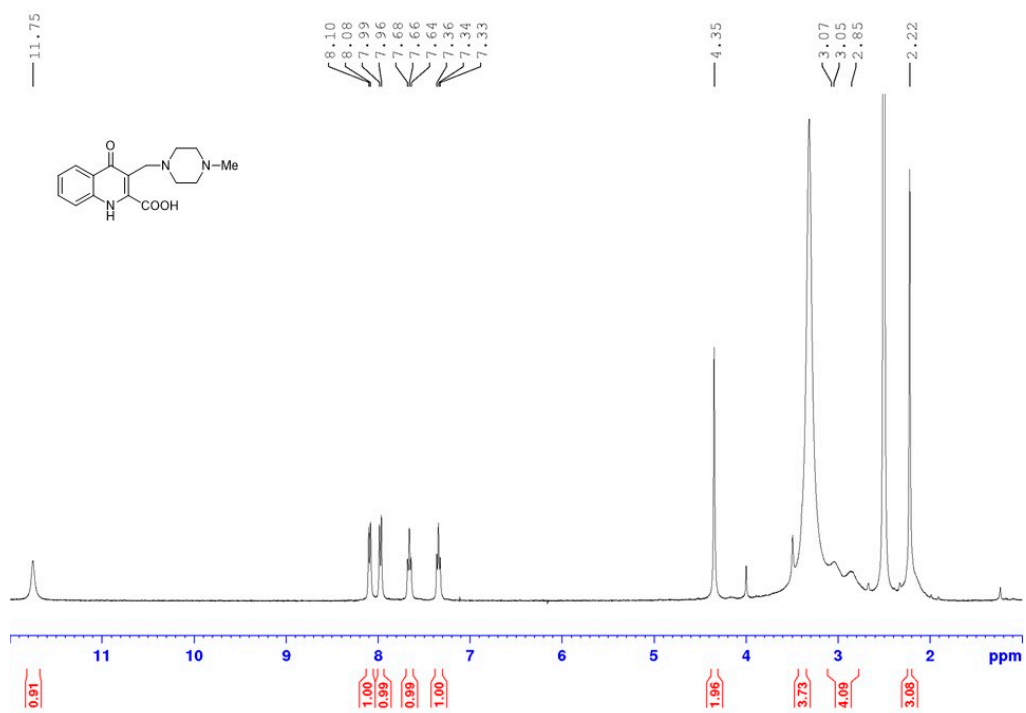


Figure S11. ¹H-NMR spectrum of 5c

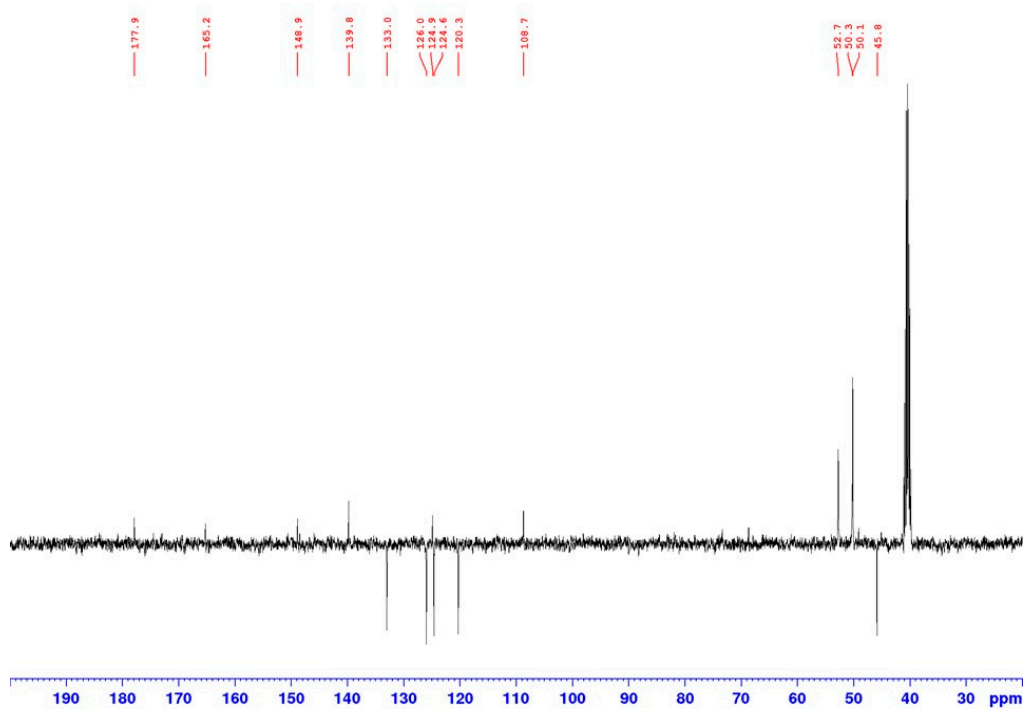


Figure S12. ¹³C-NMR spectrum of 5c

3-((3,4-Dihydroisoquinolin-2(1H)-yl)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (6a)

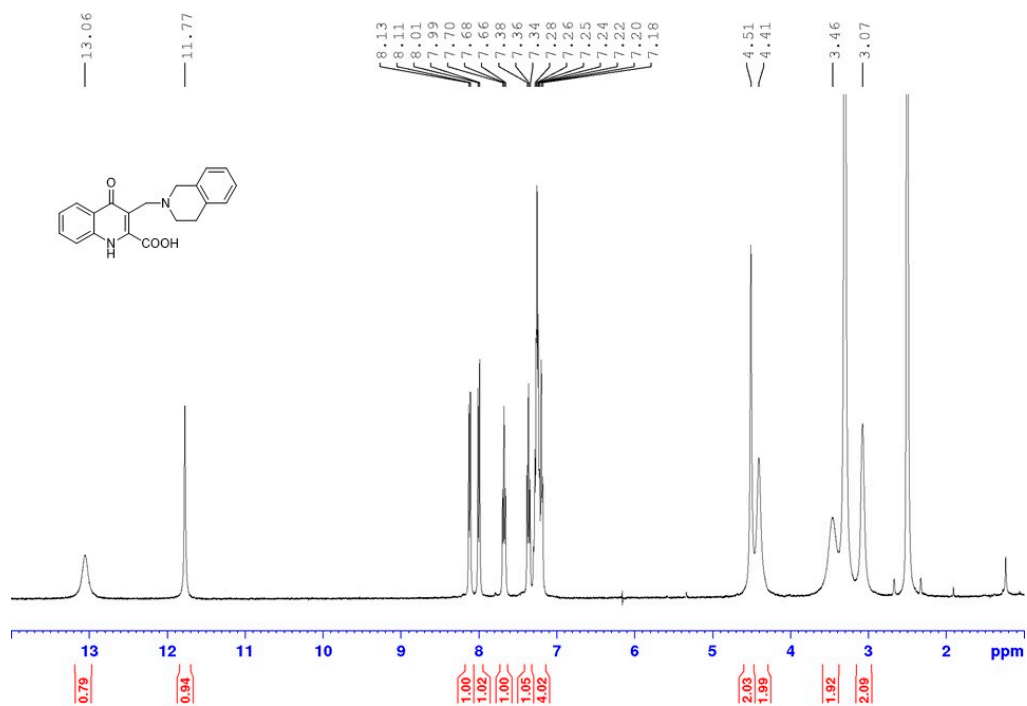


Figure S13. ¹H-NMR spectrum of 6a

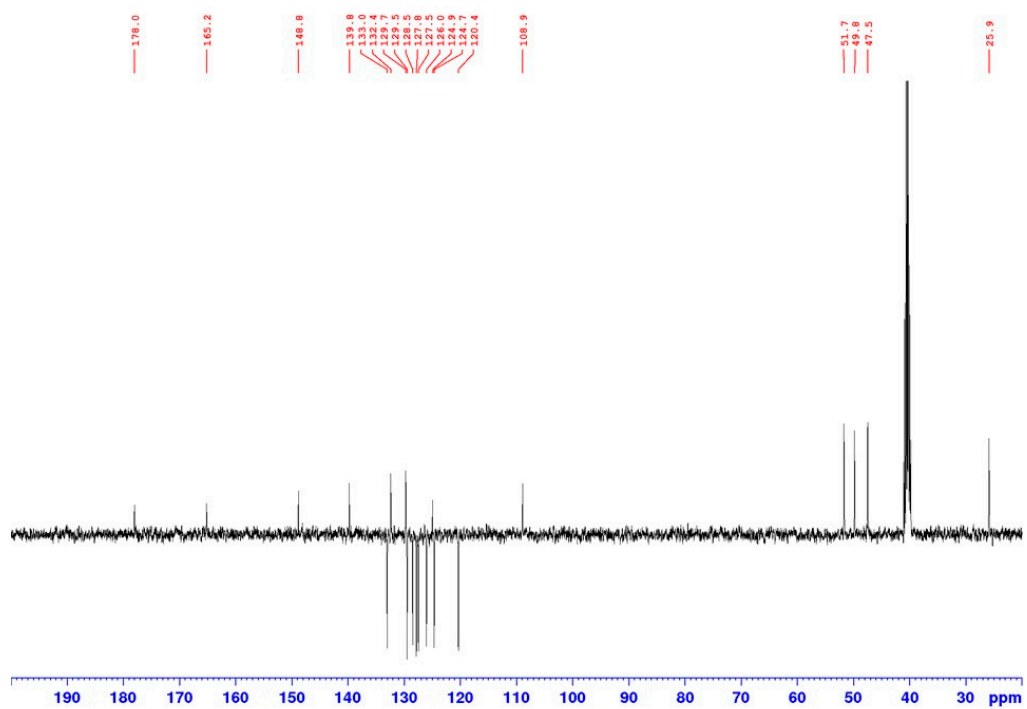


Figure S14. ¹³C-NMR spectrum of 6a

3-((6,7-Dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (6b)

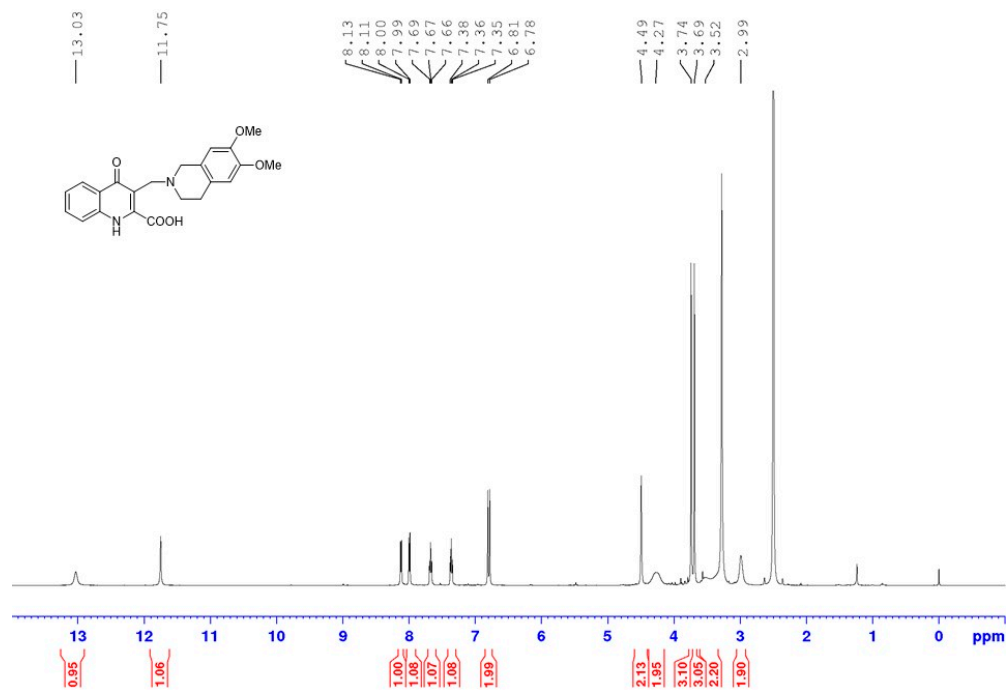


Figure S15. ¹H-NMR spectrum of **6b**

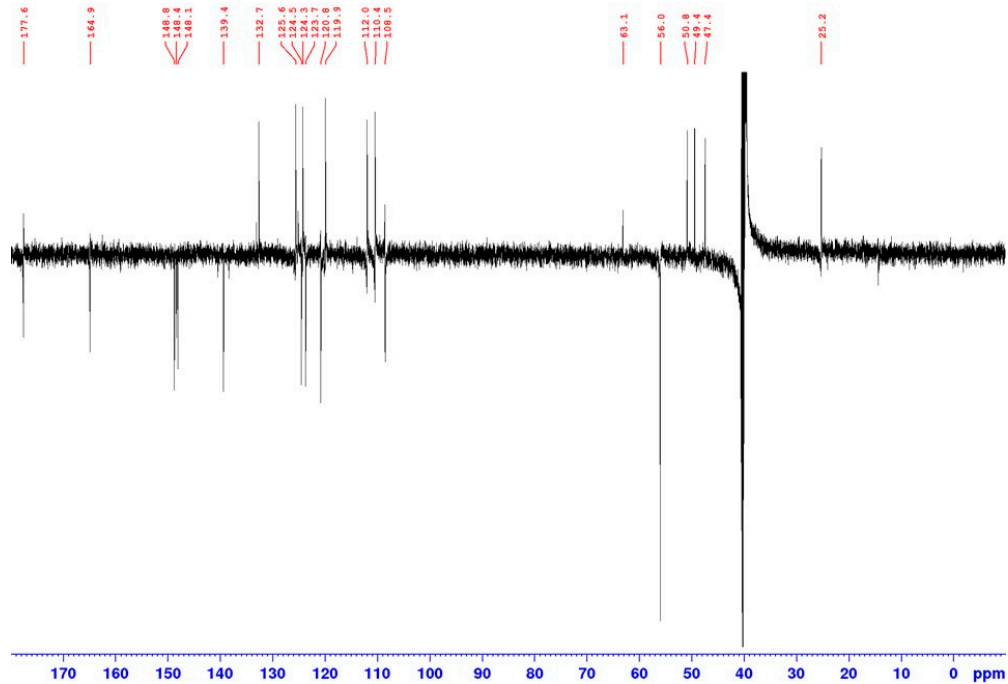


Figure S16. ¹³C-NMR spectrum of **6b**

Ethyl 5-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (7)

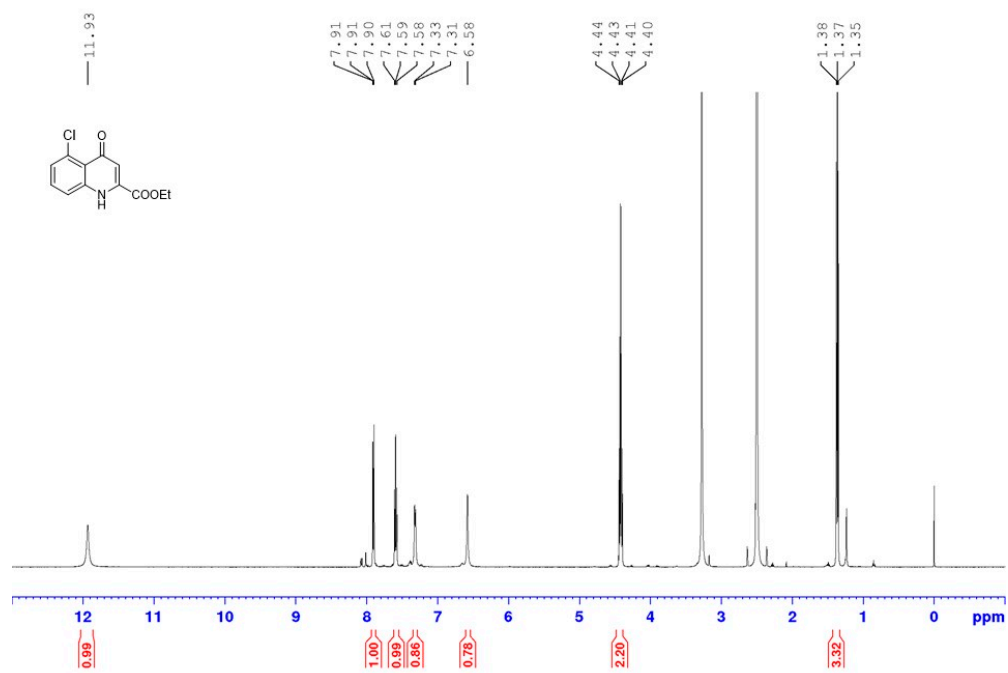


Figure S17. ¹H-NMR spectrum of 7

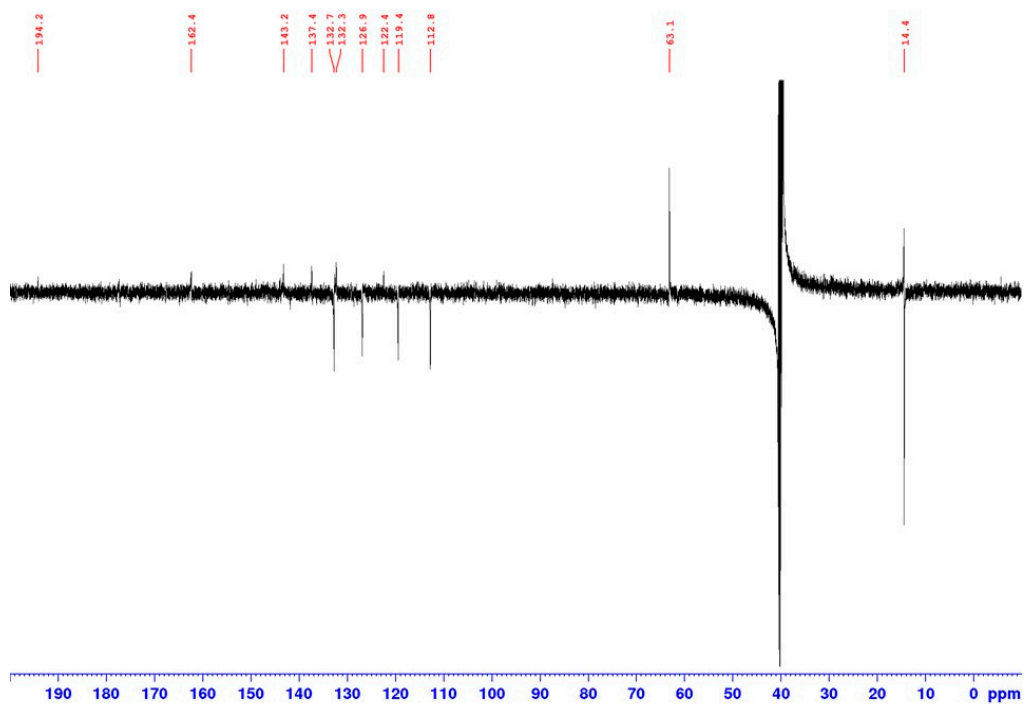


Figure S18. ¹³C-NMR spectrum of 7

Ethyl 4-oxo-6-phenyl-1,4-dihydroquinoline-2-carboxylate (8)

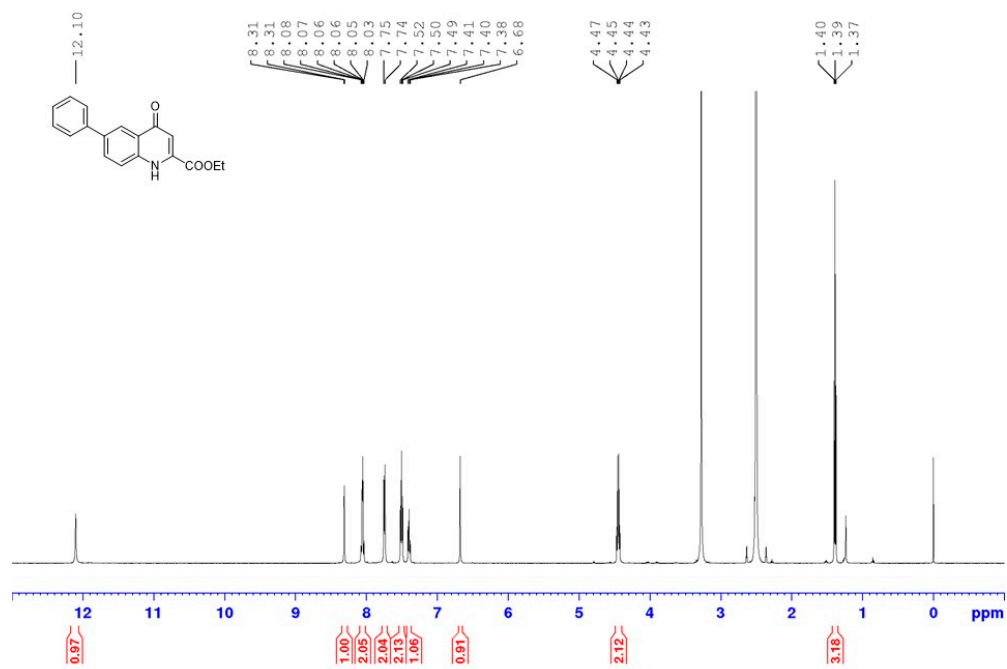


Figure S19. ¹H-NMR spectrum of 8

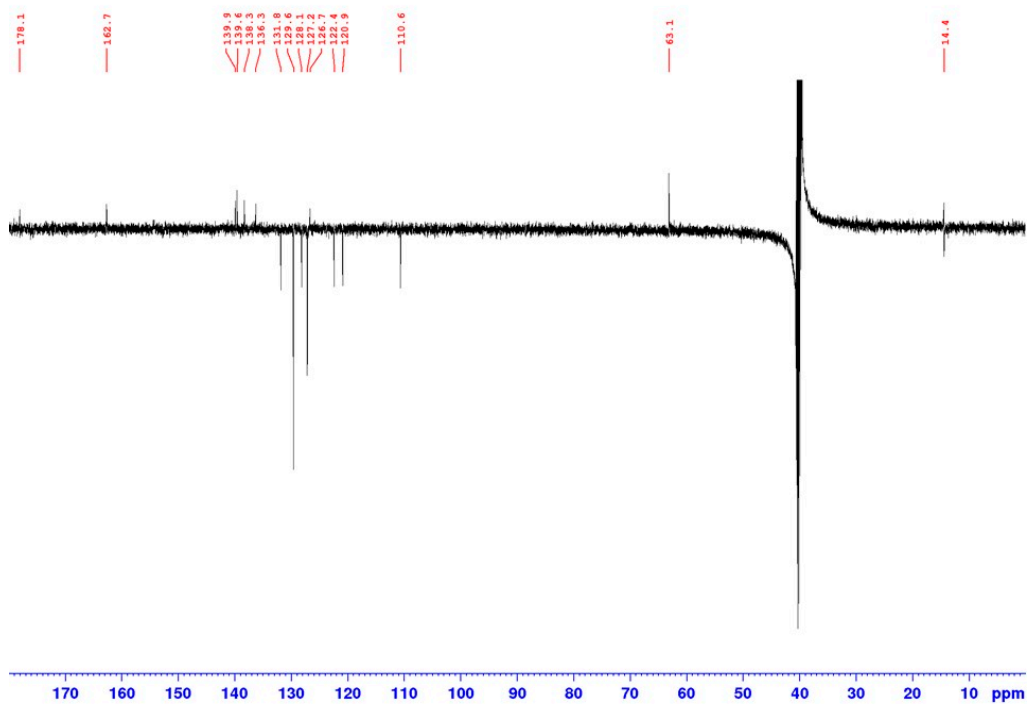


Figure S20. ¹³C-NMR spectrum of 8

Ethyl 7-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (9)

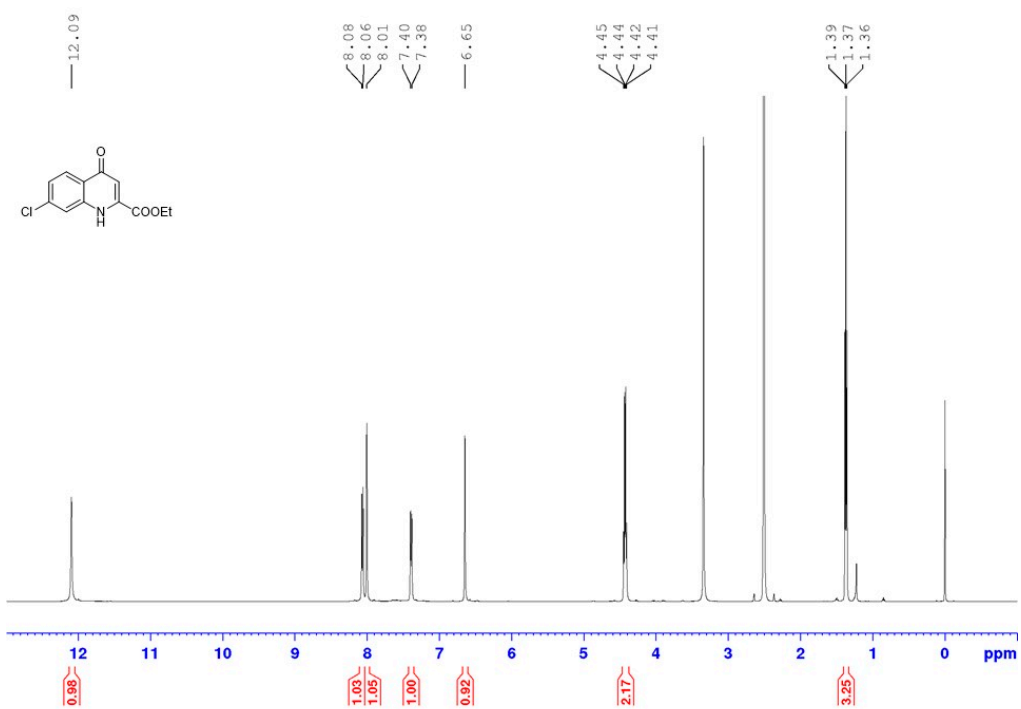


Figure S21. ¹H-NMR spectrum of 9

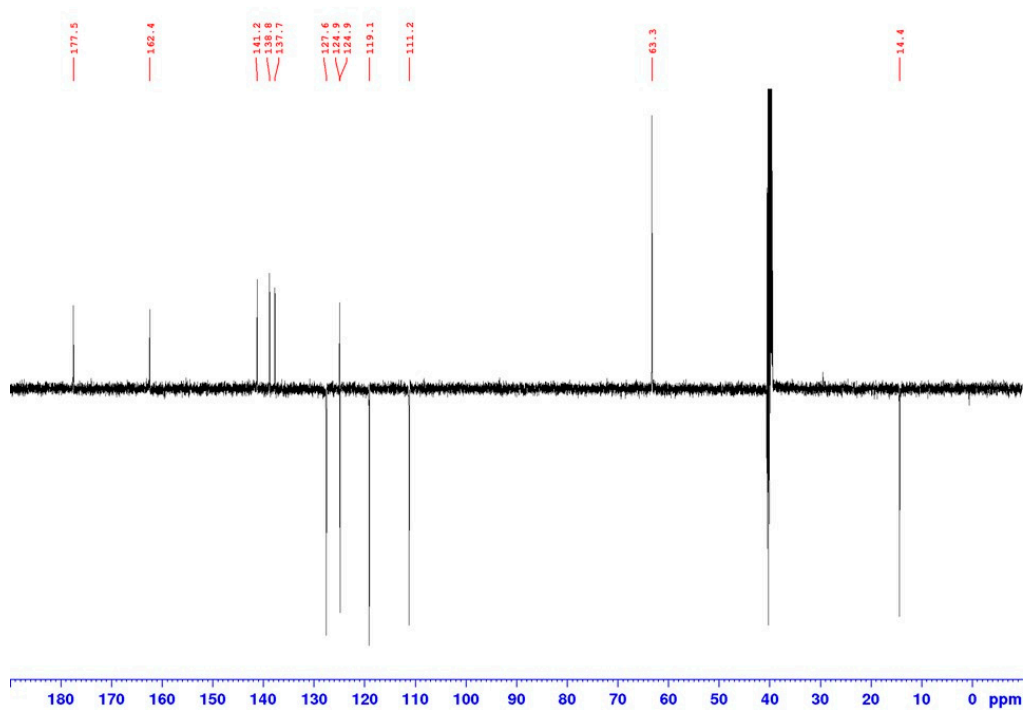


Figure S22. ¹³C-NMR spectrum of 9

Ethyl 4-oxo-8-methyl-1,4-dihydroquinoline-2-carboxylate (10)

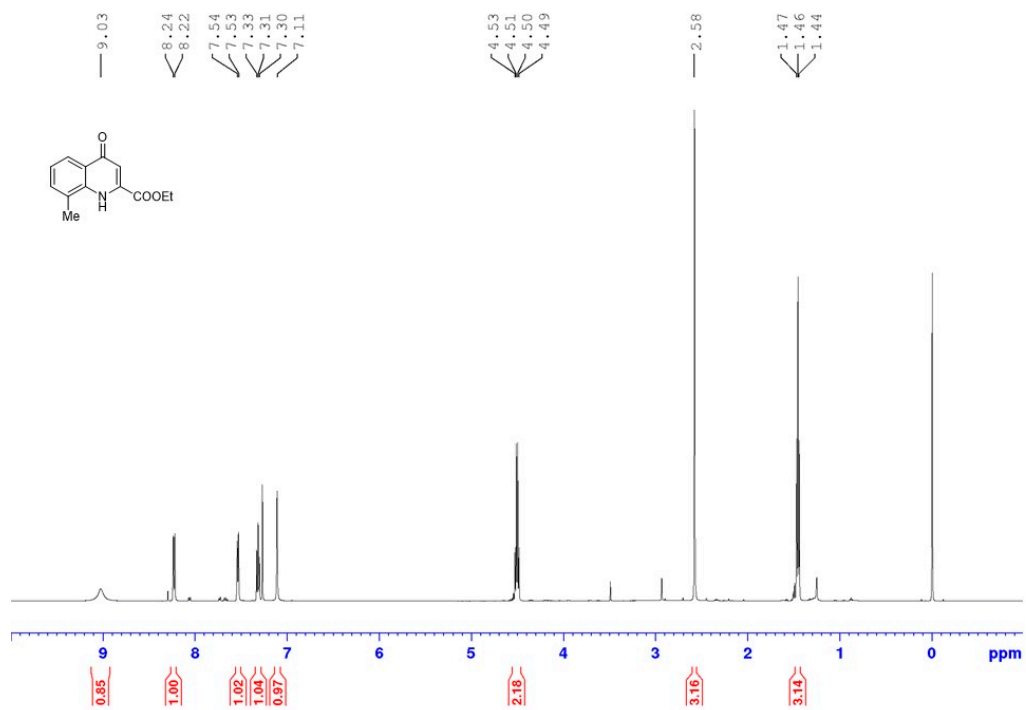


Figure S23. ¹H-NMR spectrum of 10

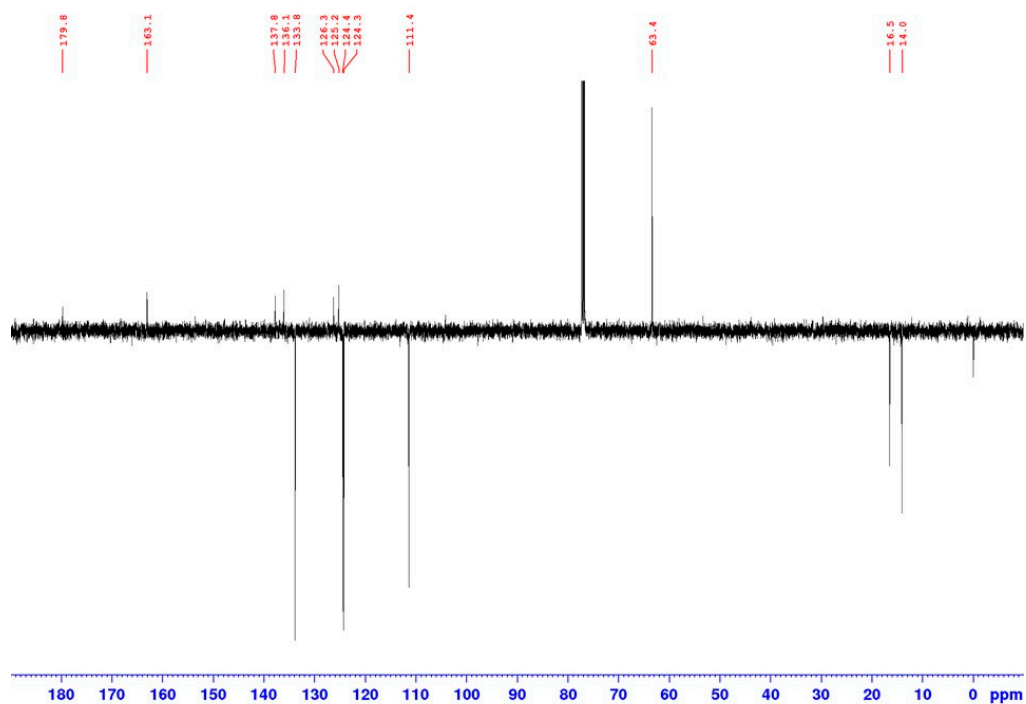


Figure S24. ¹³C-NMR spectrum of 10

5-Chloro-3-(morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (**11**)

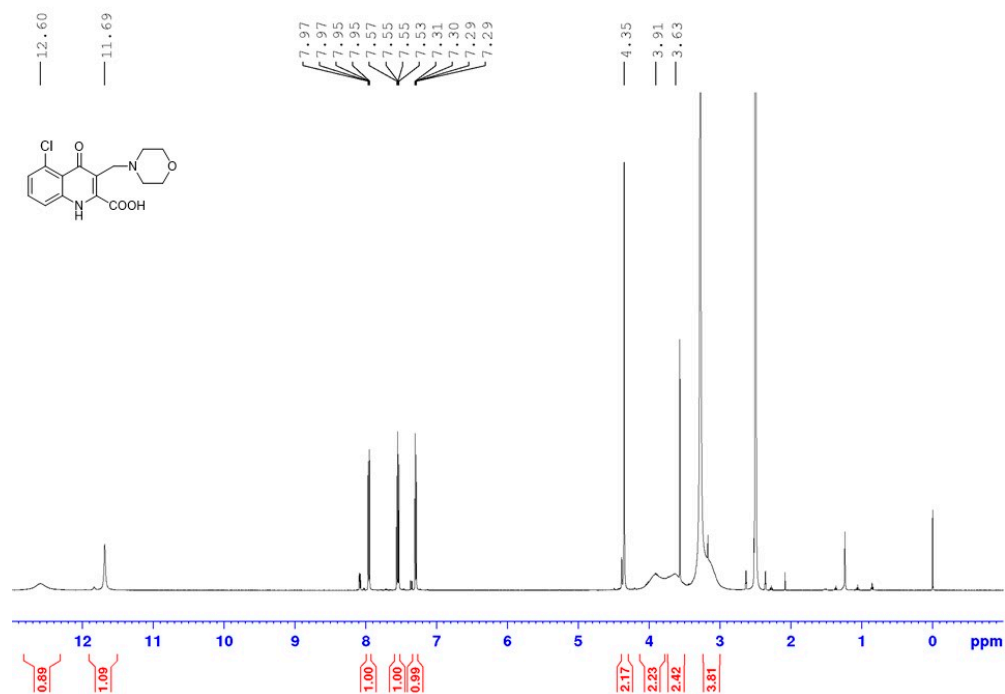


Figure S25. ¹H-NMR spectrum of **11**

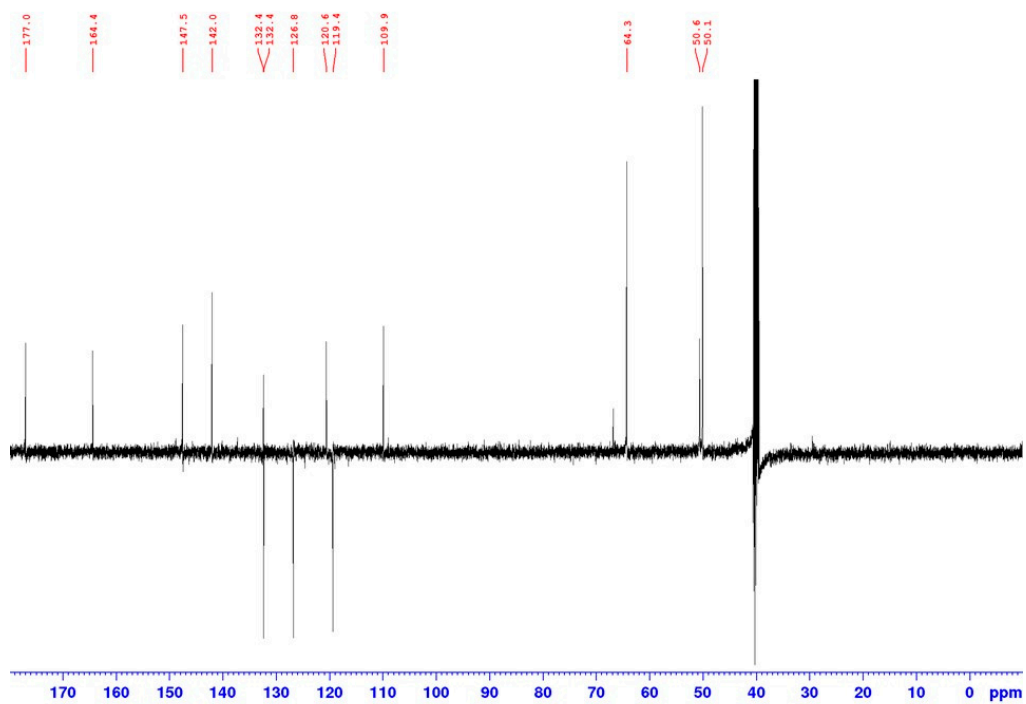


Figure S26. ¹³C-NMR spectrum of **11**

3-(Morpholinomethyl)-4-oxo-6-phenyl-1,4-dihydroquinoline-2-carboxylic acid (**12**)

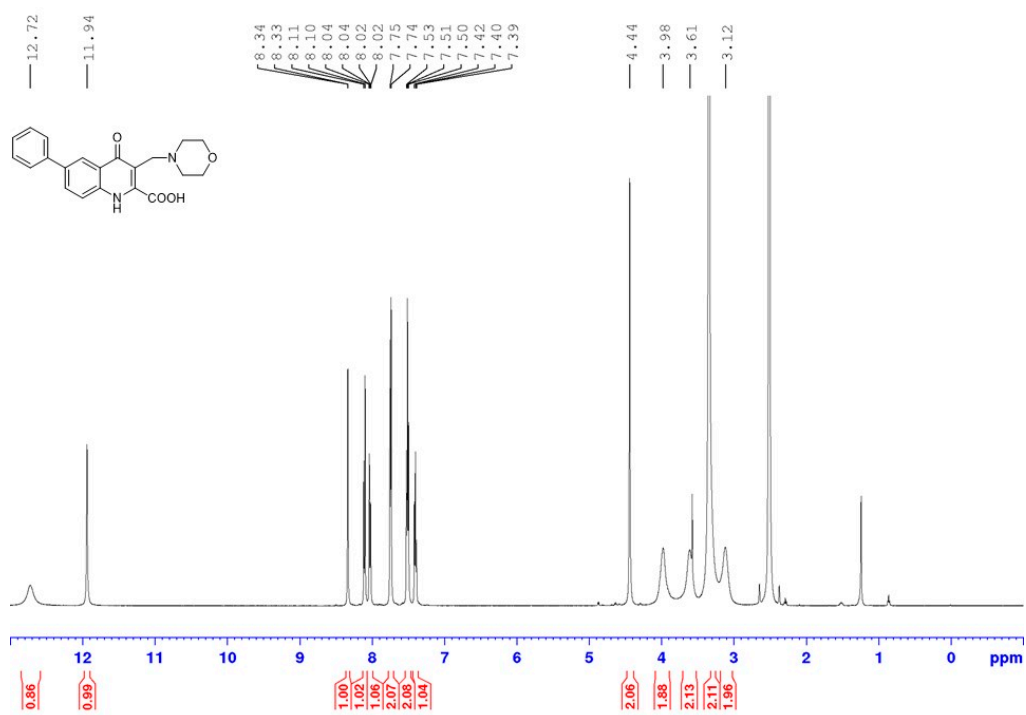


Figure S27. ¹H-NMR spectrum of **12**

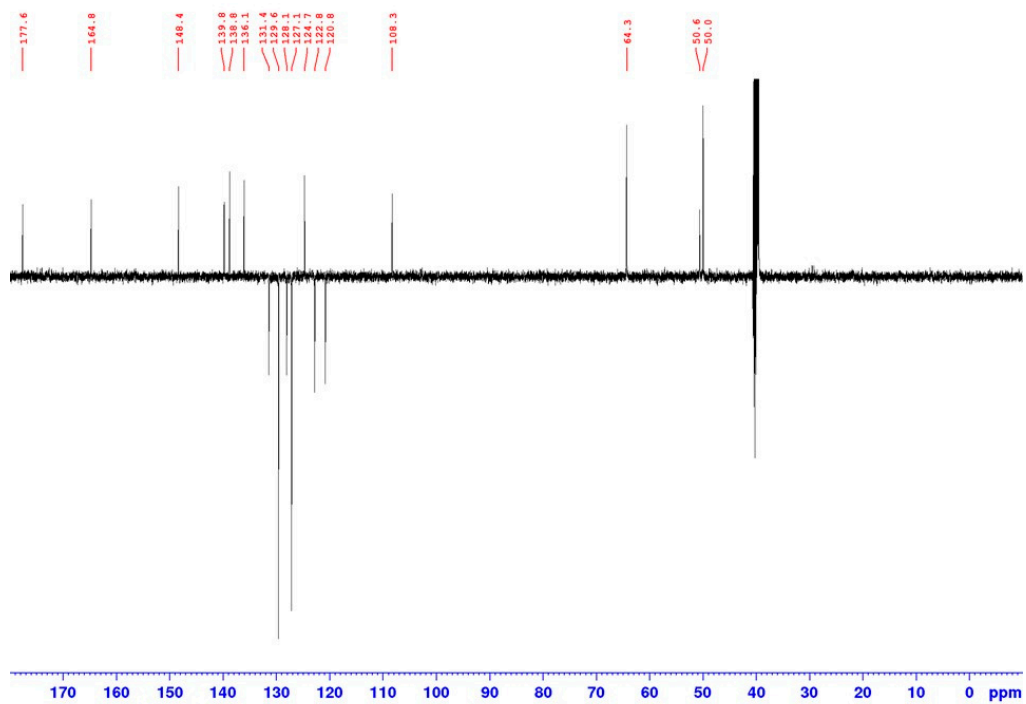


Figure S28. ¹³C-NMR spectrum of **12**

7-Chloro-3-(morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (13)

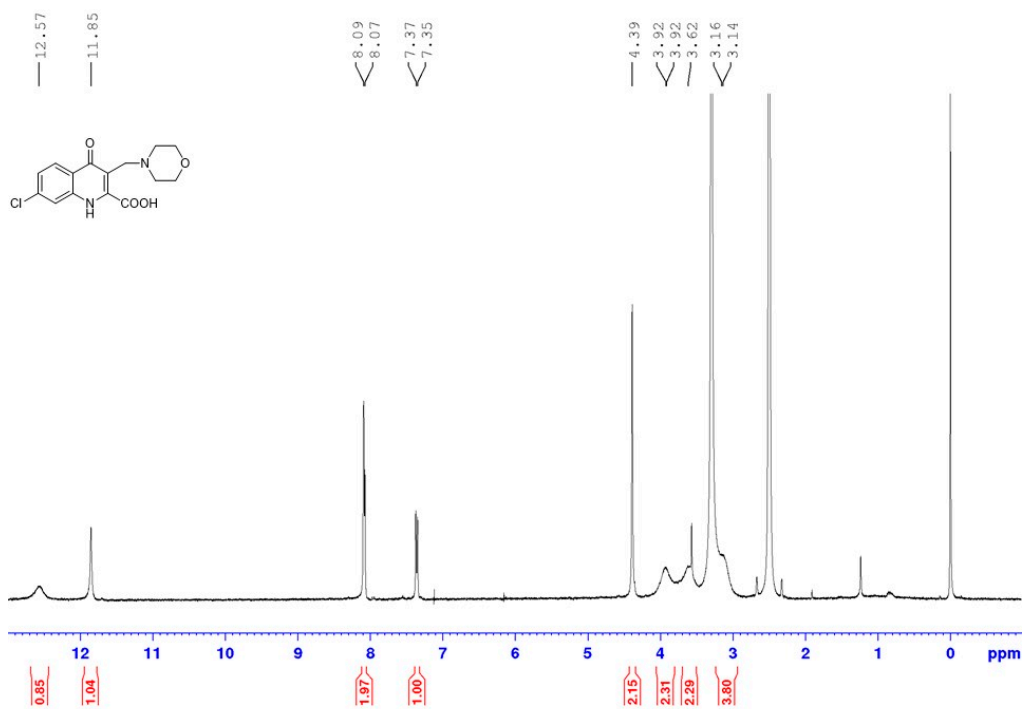


Figure S29. ¹H-NMR spectrum of 13

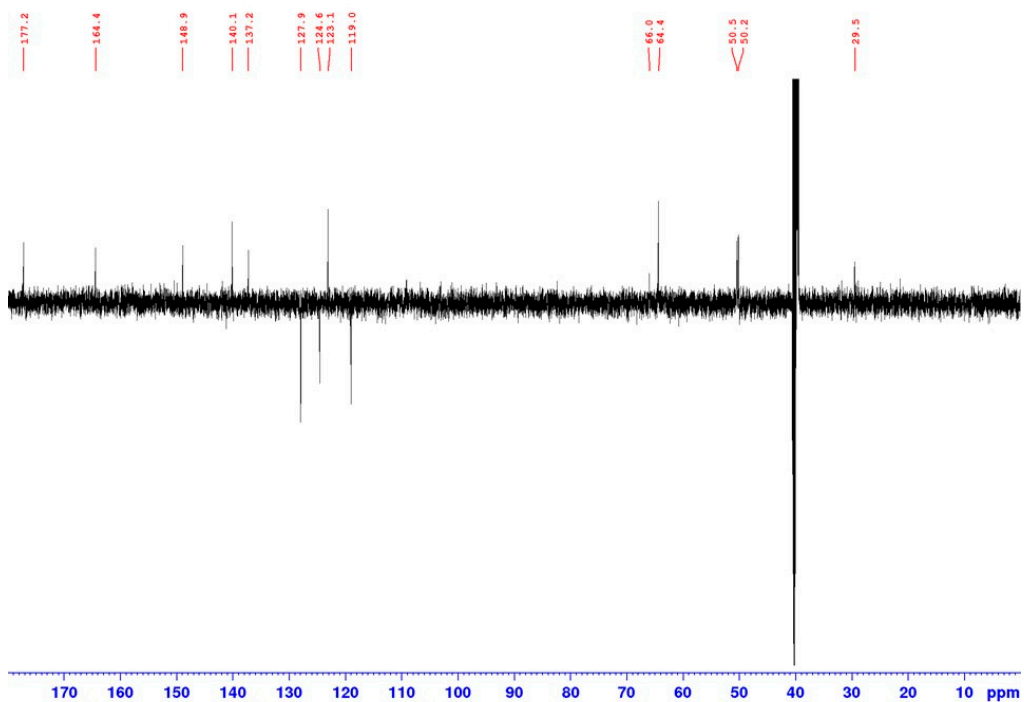


Figure S30. ¹³C-NMR spectrum of 13

8-Methyl-3-(morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxylic acid (**14**)

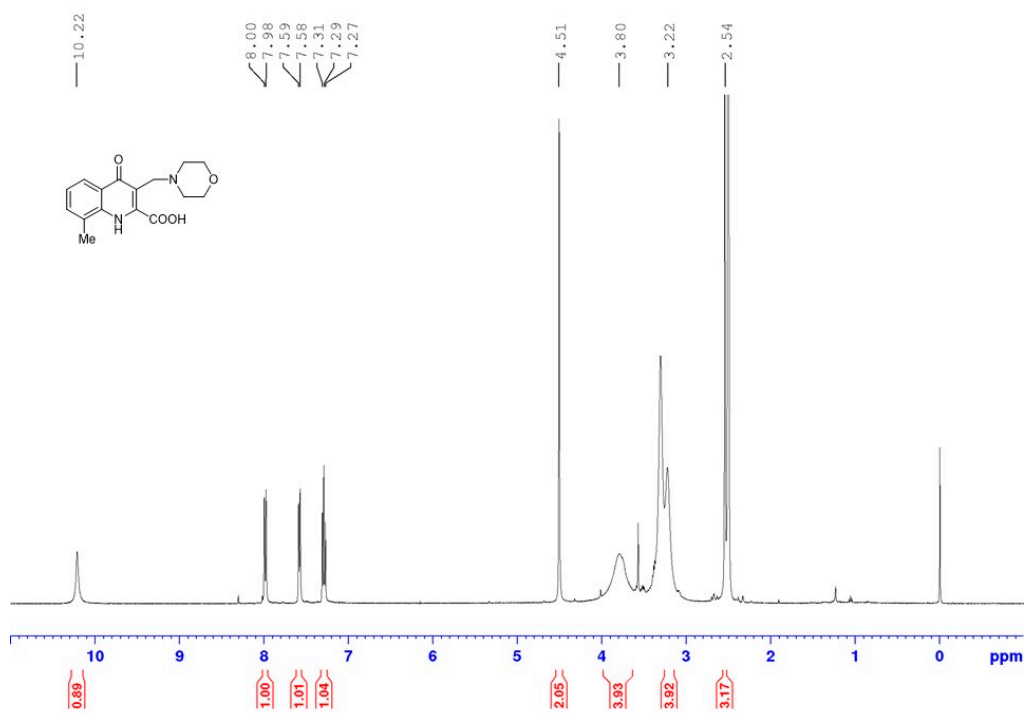


Figure S31. ¹H-NMR spectrum of **14**

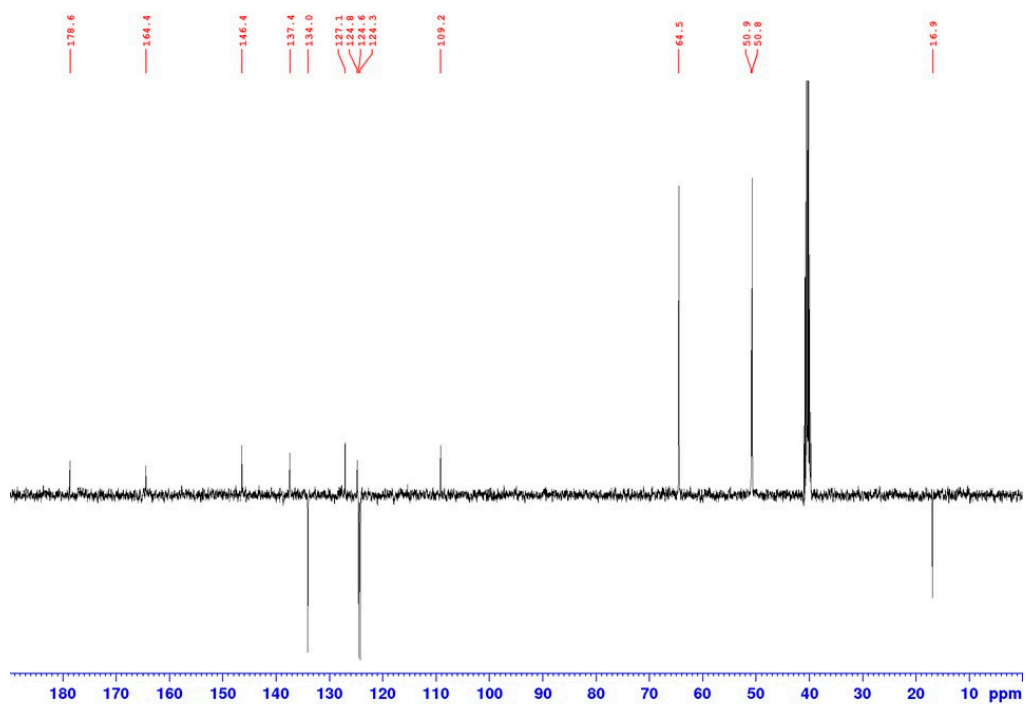


Figure S32. ¹³C-NMR spectrum of **14**

***N*-2-(Dimethylamino)ethyl-4-oxo-3-(pyrrolidin-1-ylmethyl)-1,4-dihydroquinoline-2-carboxamide (18a)**

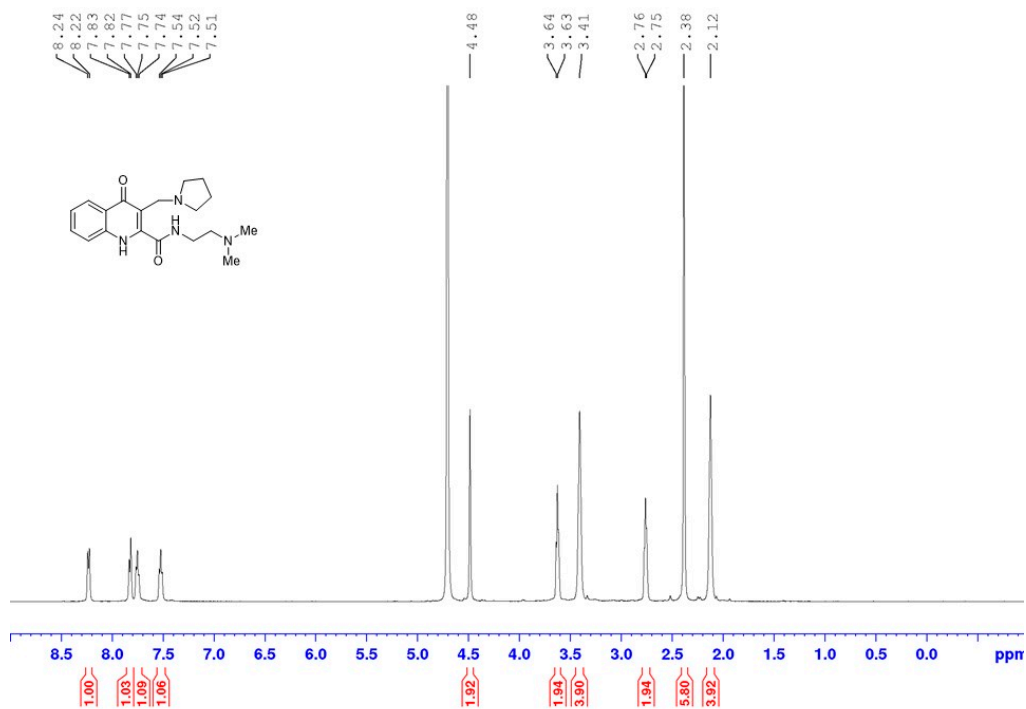


Figure S33. ¹H-NMR spectrum of **18a**

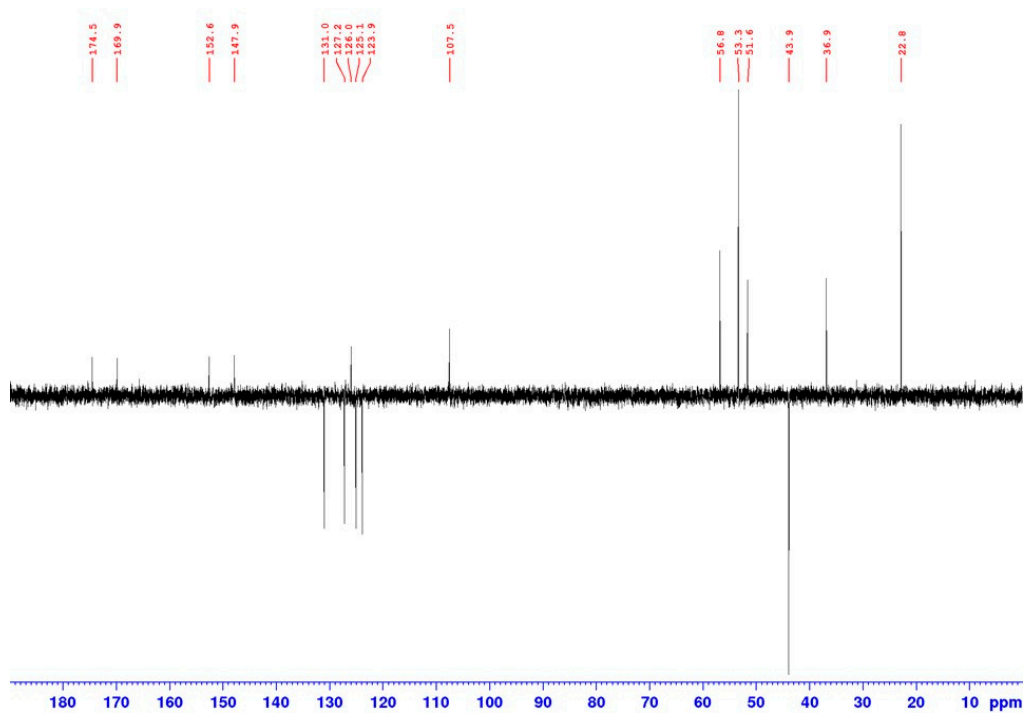


Figure S34. ¹³C-NMR spectrum of **18a**

N-(2-(Dimethylamino)ethyl)-4-oxo-3-(piperidin-1-ylmethyl)-1,4-dihydroquinoline-2-carboxamide (18b)

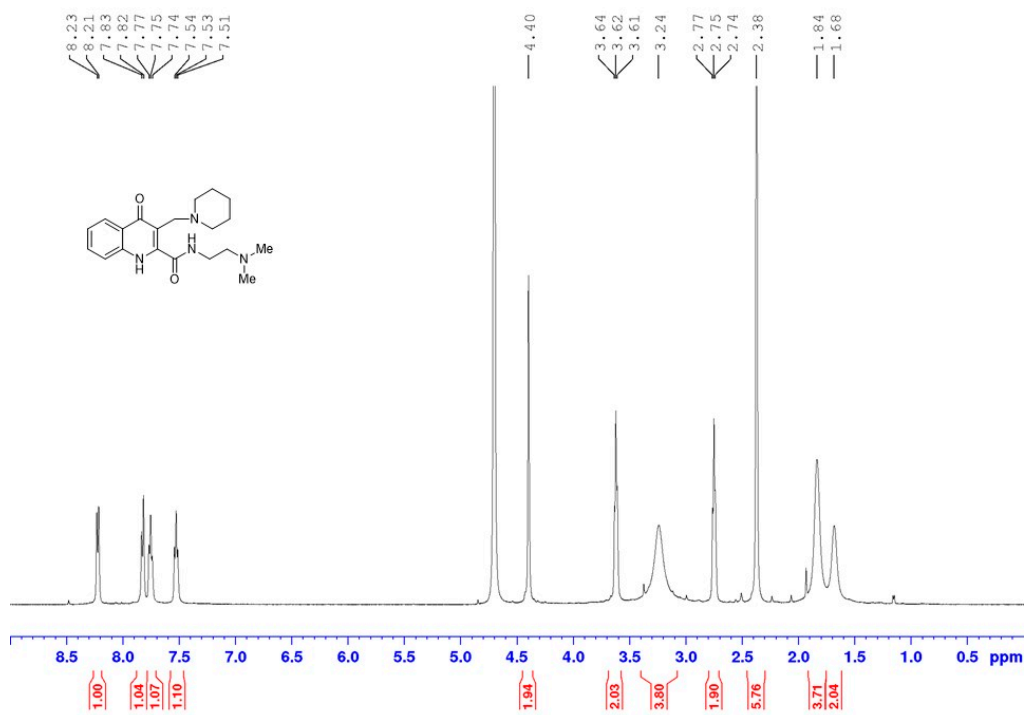


Figure S35. ¹H-NMR spectrum of **18b**

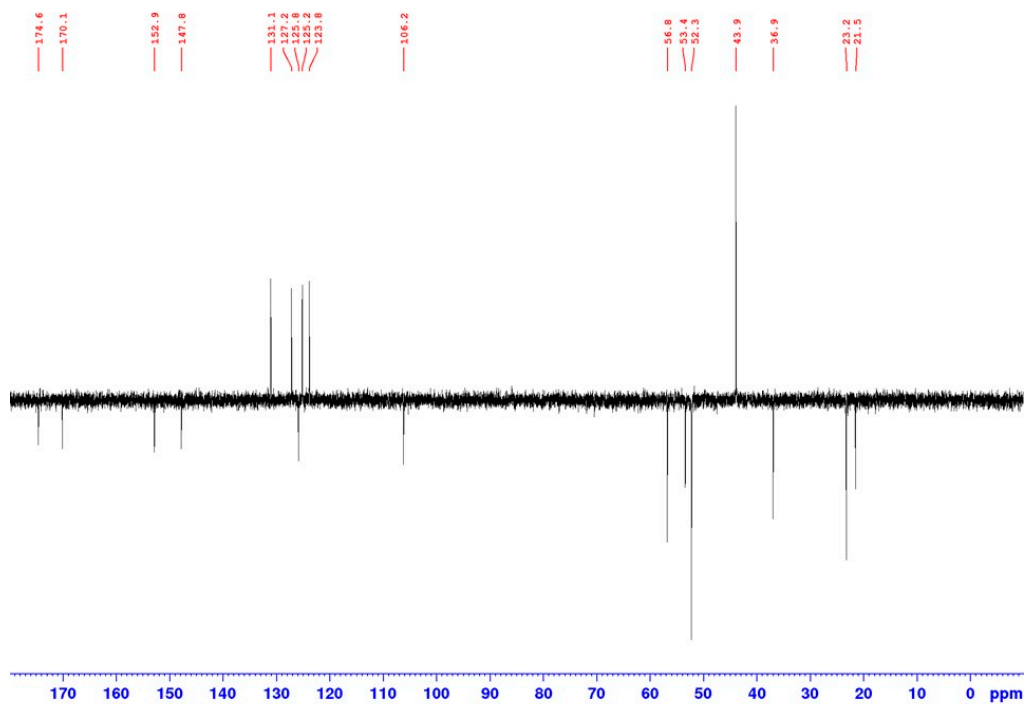


Figure S36. ¹³C-NMR spectrum of **18b**

N-(2-(Dimethylamino)ethyl)-3-(morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxamide (18c)

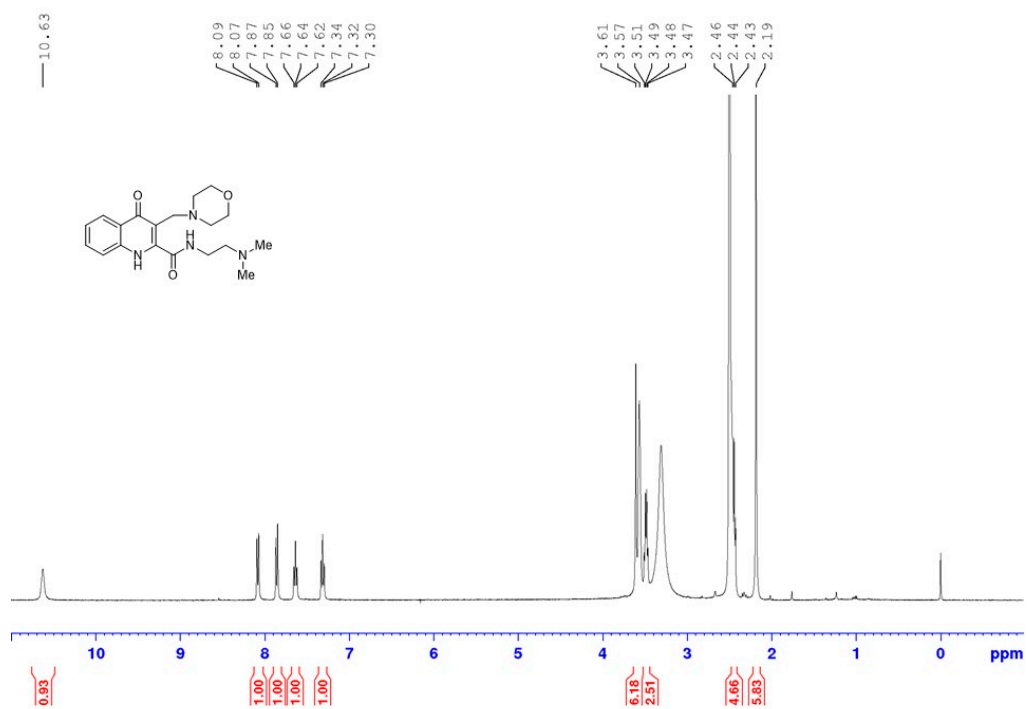


Figure S37. ¹H-NMR spectrum of 18c

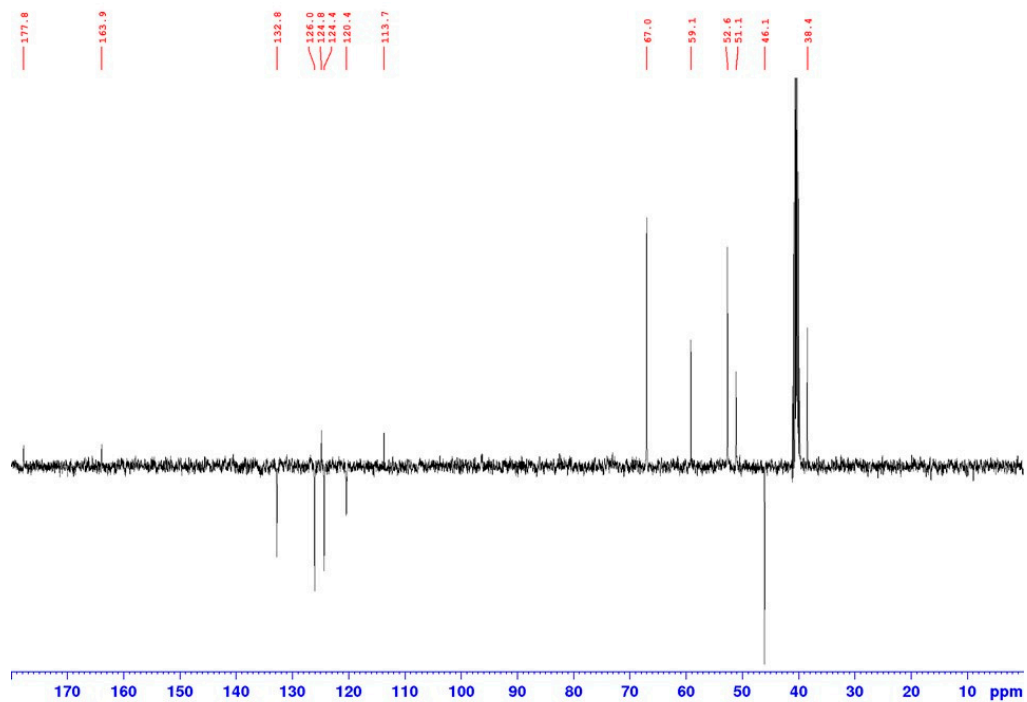


Figure S38. ¹³C-NMR spectrum of 18c

4-oxo-*N*-(2-(pyrrolidin-1-yl)ethyl)-3-(pyrrolidin-1-ylmethyl)-1,4-dihydroquinoline-2-carboxamide (19a)

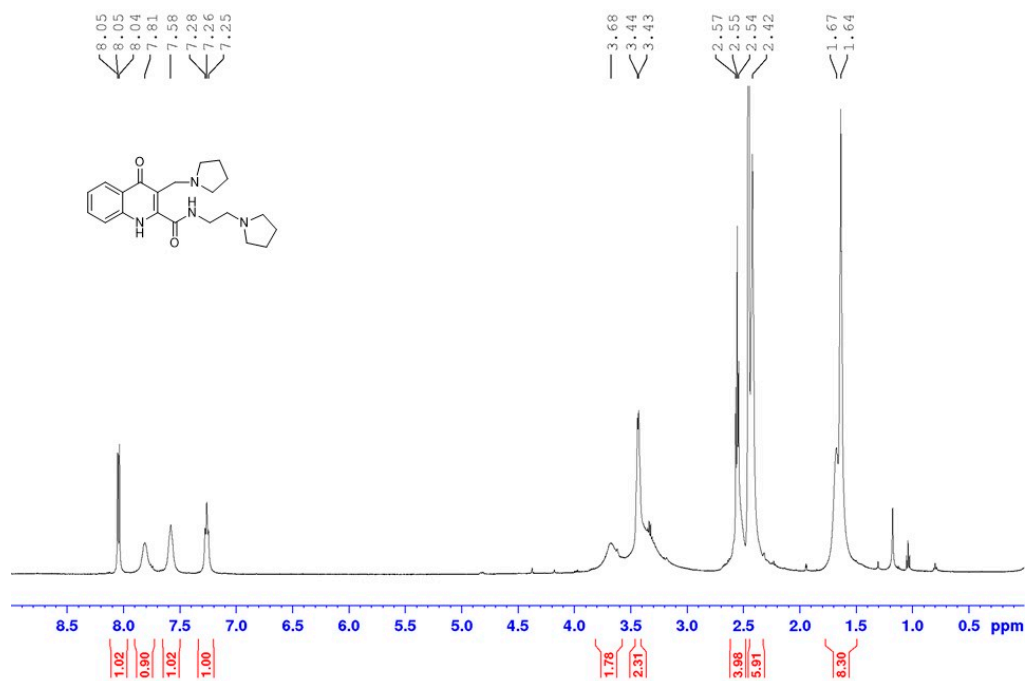


Figure S39. ¹H-NMR spectrum of 19a

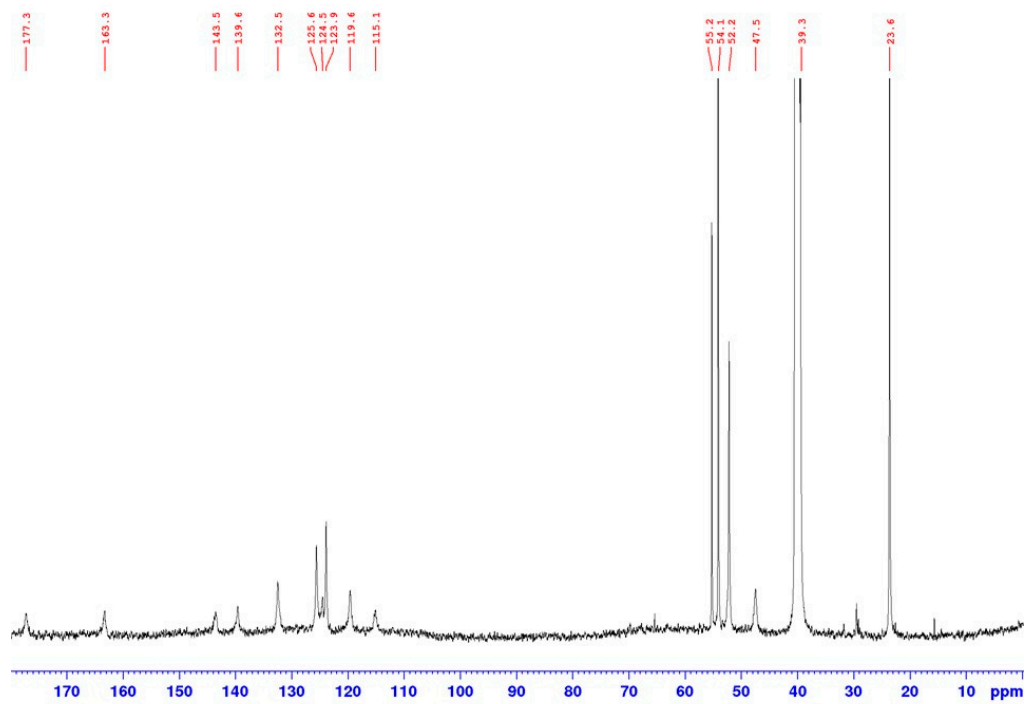


Figure S40. ¹³C-NMR spectrum of 19a

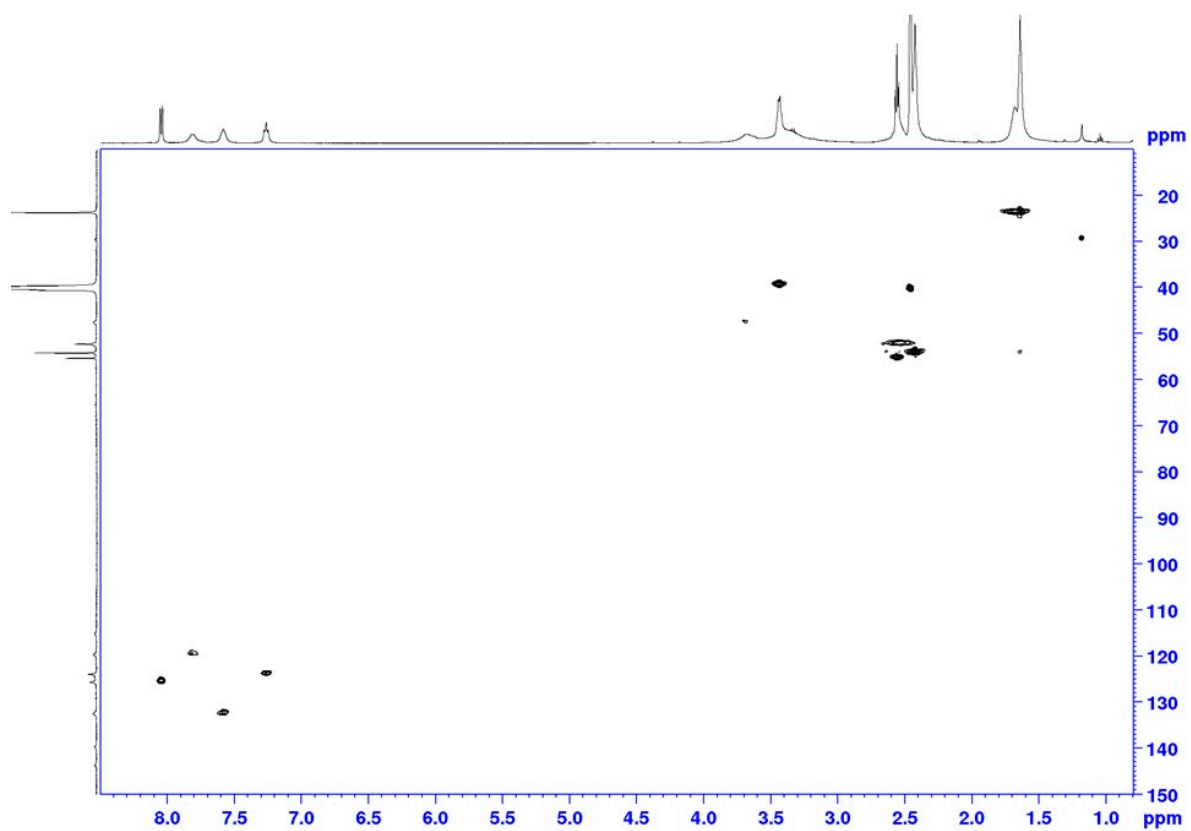


Figure S41. HSQC-NMR spectrum of **19a**

4-oxo-N-(2-(pyrrolidin-1-yl)ethyl)-3-(pyrrolidin-1-ylmethyl)-1,4-dihydroquinoline-2-carboxamide (19b)

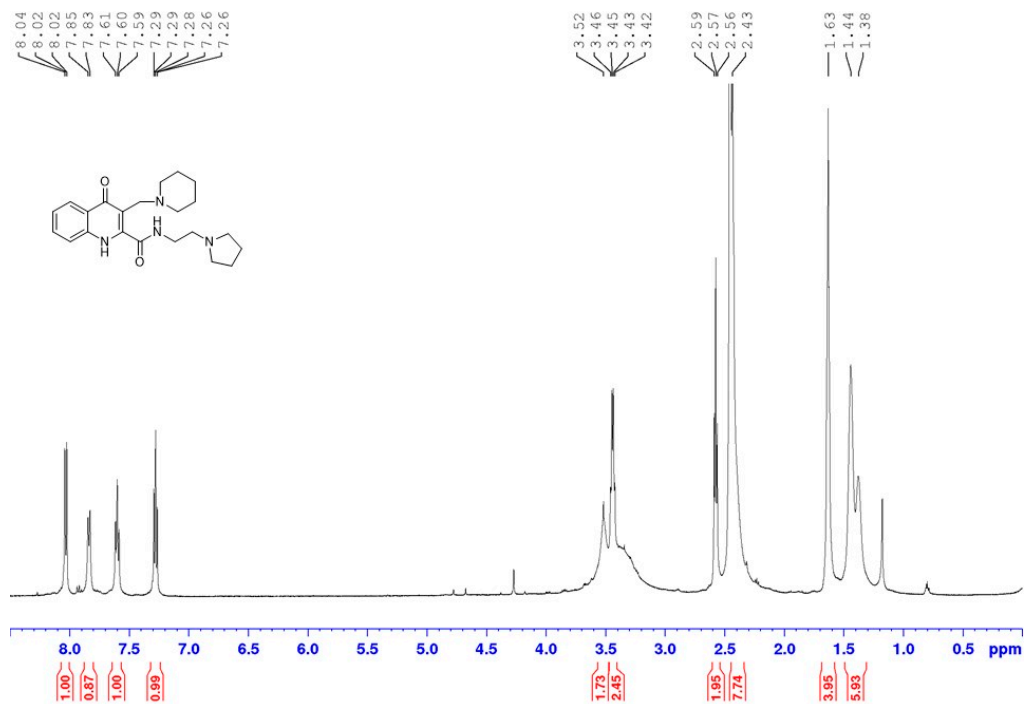


Figure S42. ¹H-NMR spectrum of **19b**

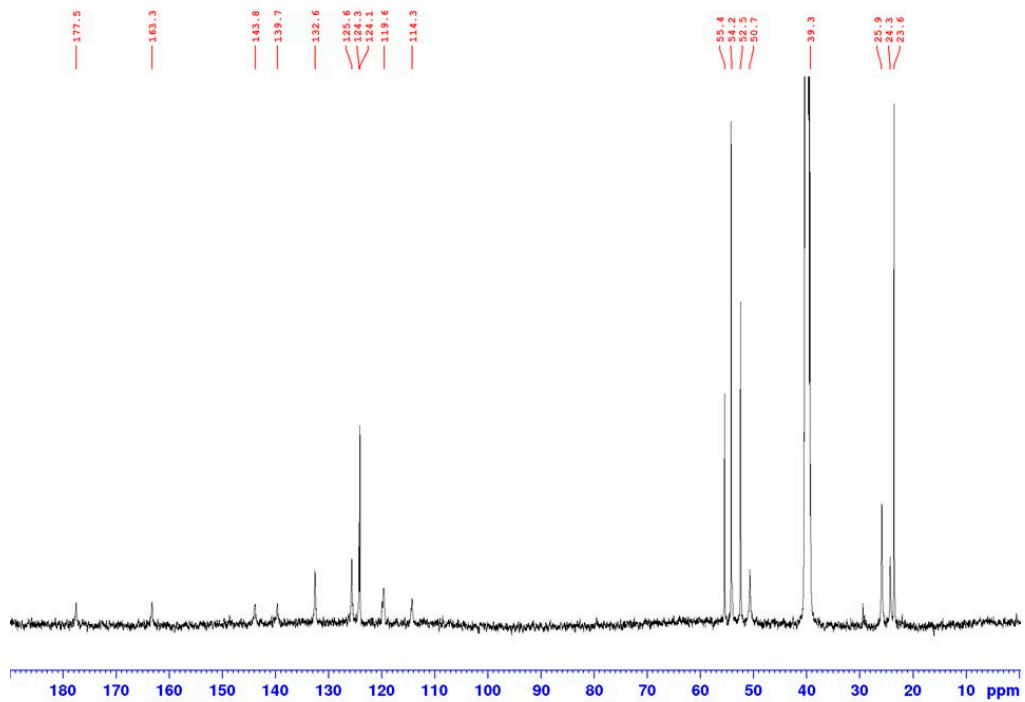


Figure S43. ¹³C-NMR spectrum of **19b**

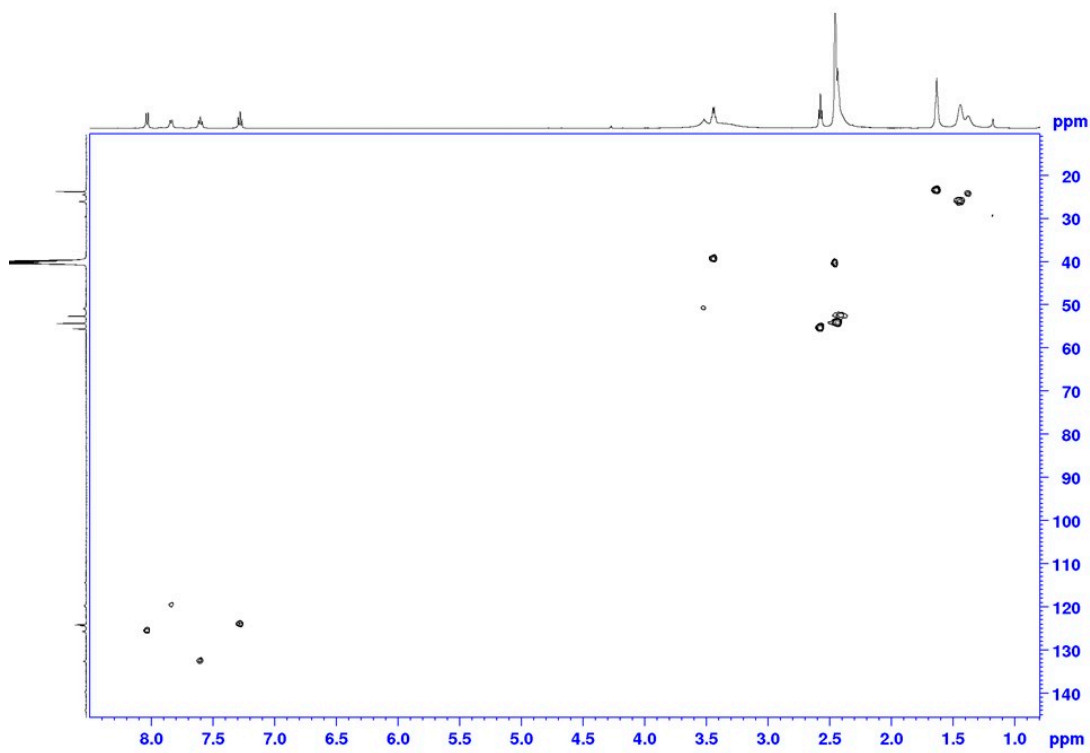


Figure S44. HSQC-NMR spectrum of **19b**

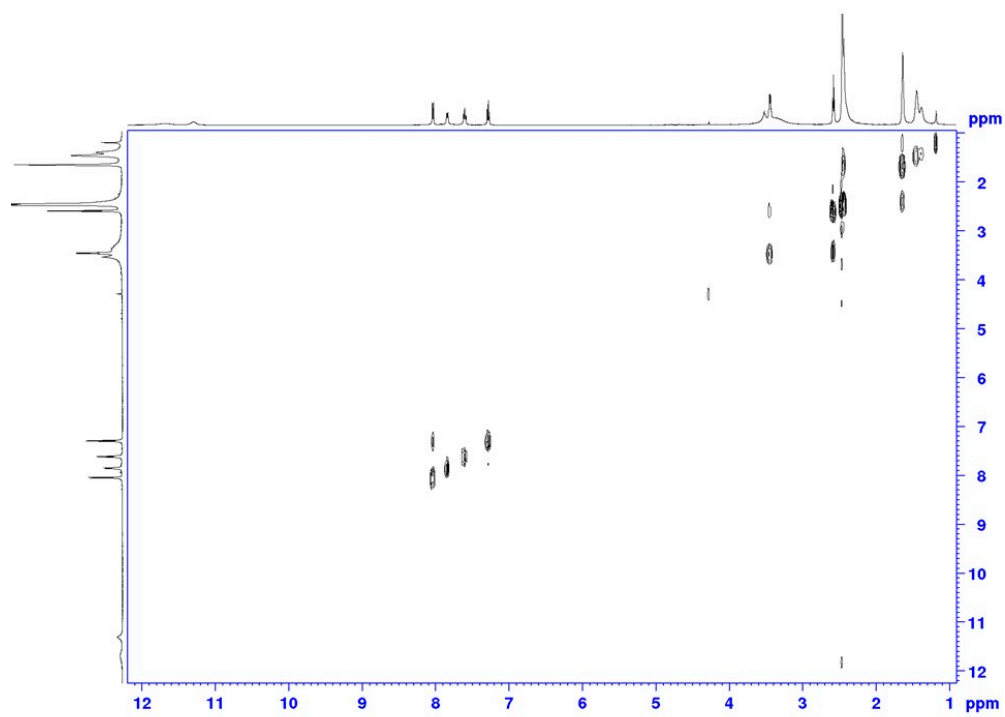


Figure S45. COSY-NMR spectrum of **19b**

4-Oxo-3-(morpholinomethyl)-N-(2-(pyrrolidin-1-yl)ethyl)-1,4-dihydroquinoline-2-carboxamide (19c)

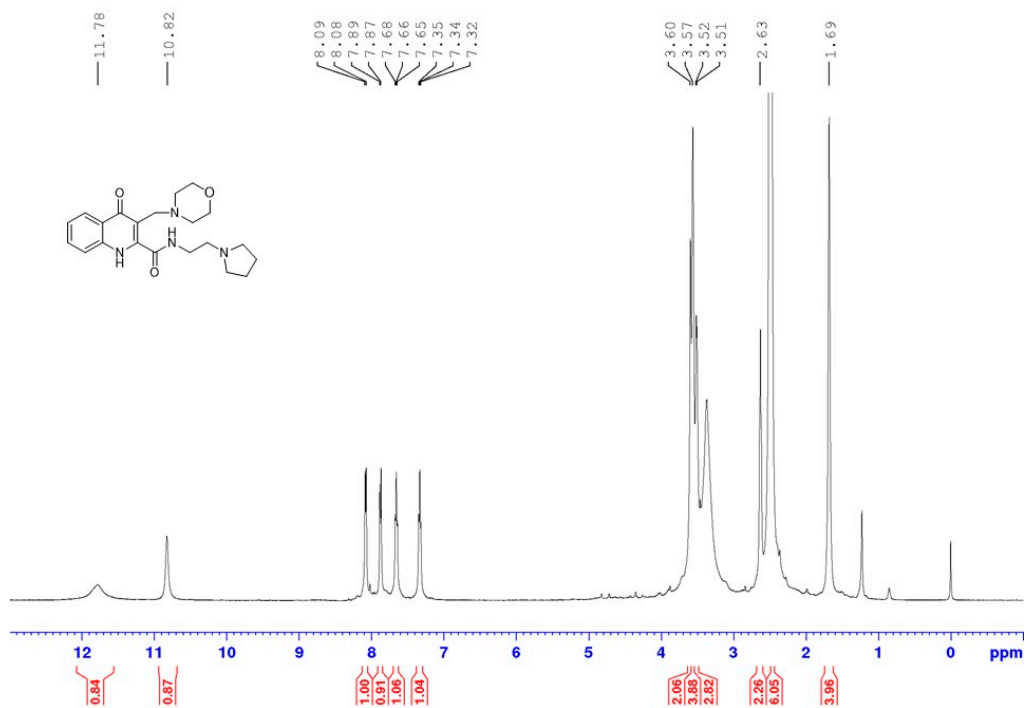


Figure S46. ¹H-NMR spectrum of 19c

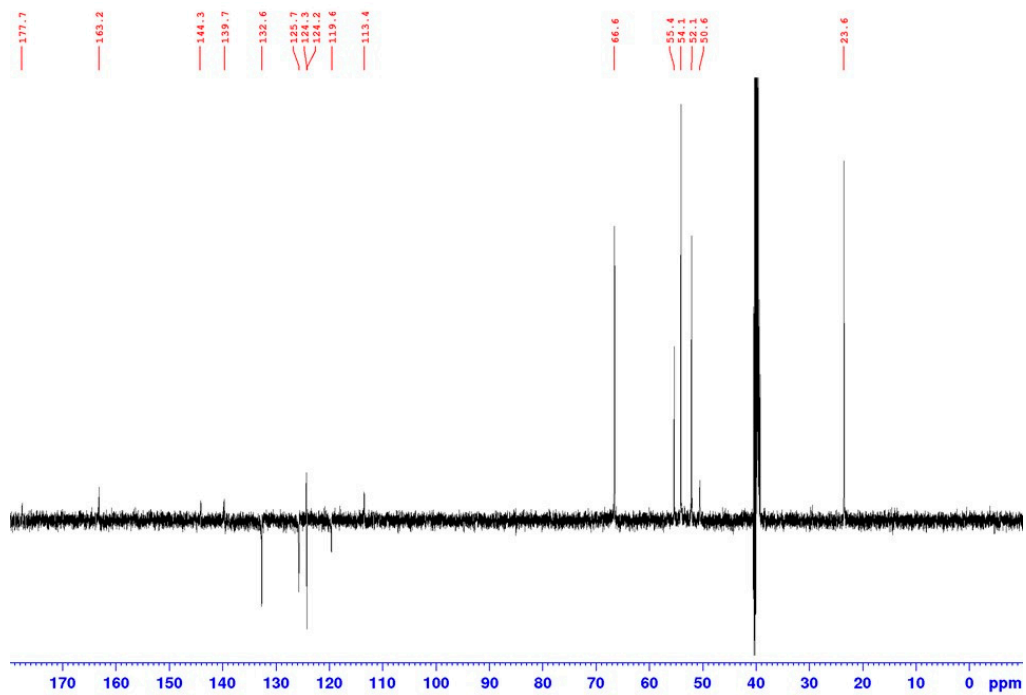


Figure S47. ¹³C-NMR spectrum of 19c

4-oxo-1,4-dihydroquinoline-2-carboxamide (20)

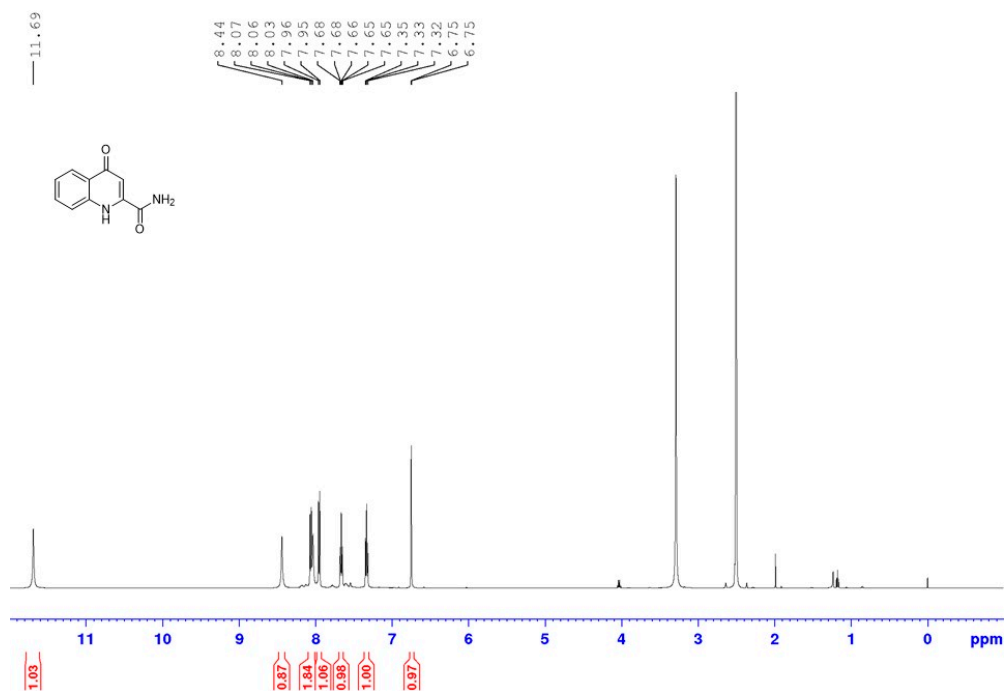


Figure S48. ¹H-NMR spectrum of 20

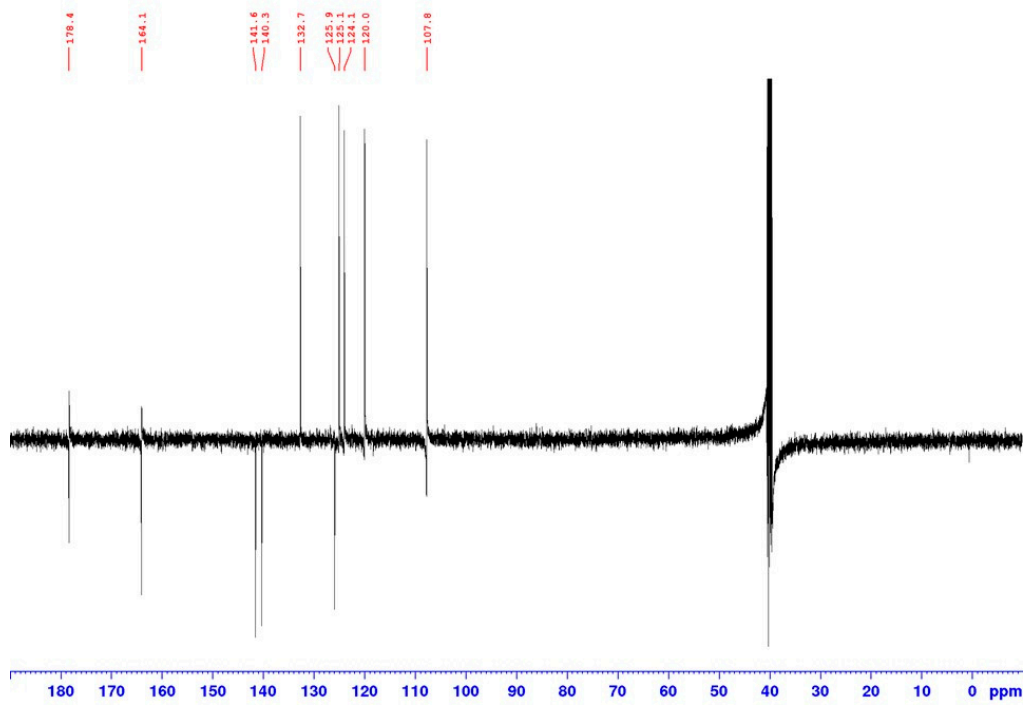


Figure S49. ¹³C-NMR spectrum of 20

3-(Morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxamide (21)

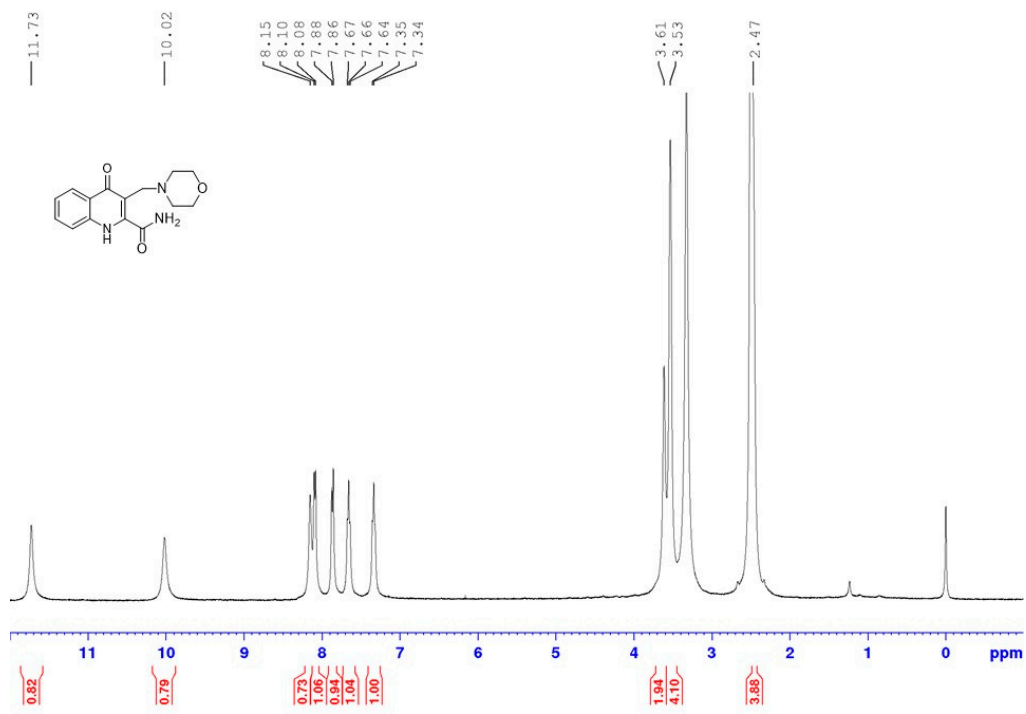


Figure S50. ¹H-NMR spectrum of 21

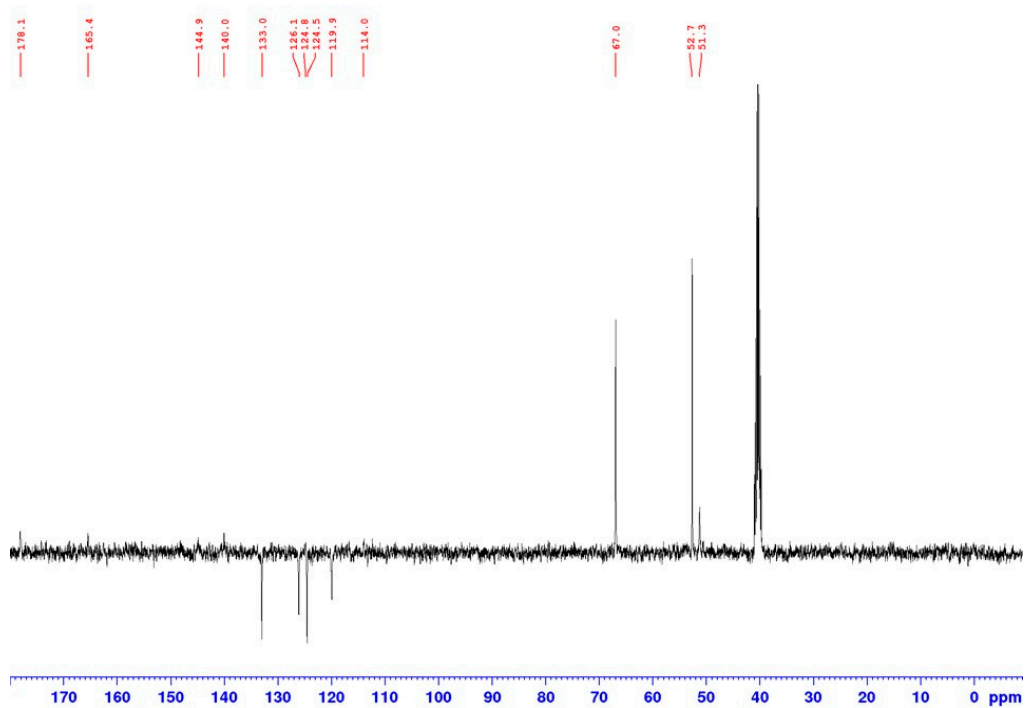


Figure S51. ¹³C-NMR spectrum of 21

Methyl 3-(morpholinomethyl)-4-oxo-1,4-dihydroquinoline-2-carboxylate (22)

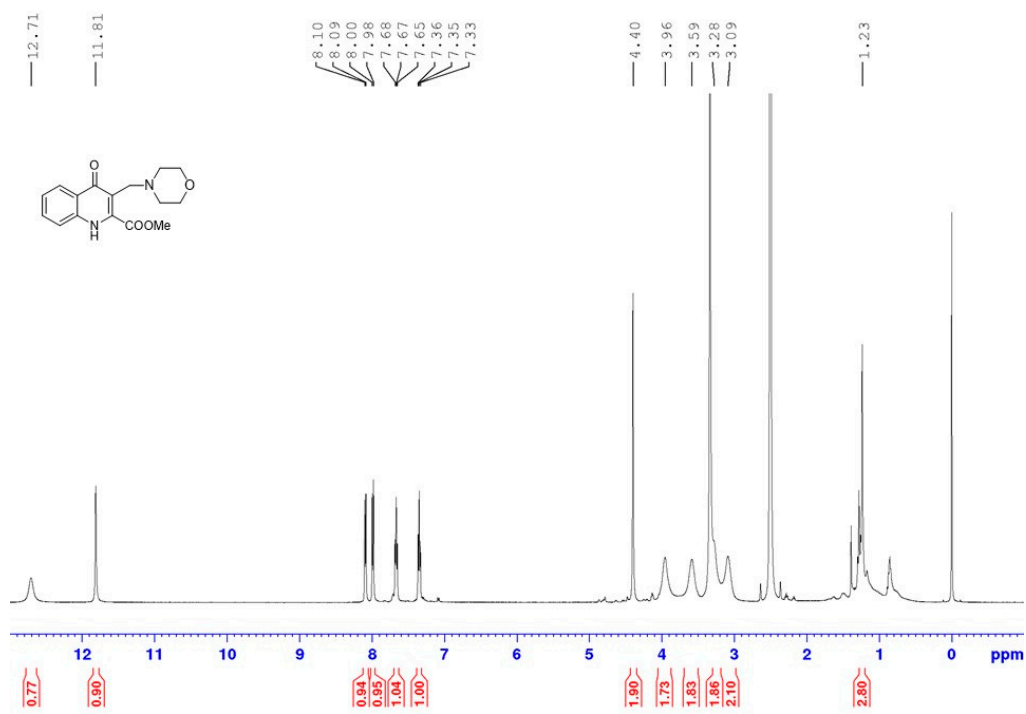


Figure S52. ¹H-NMR spectrum of 22

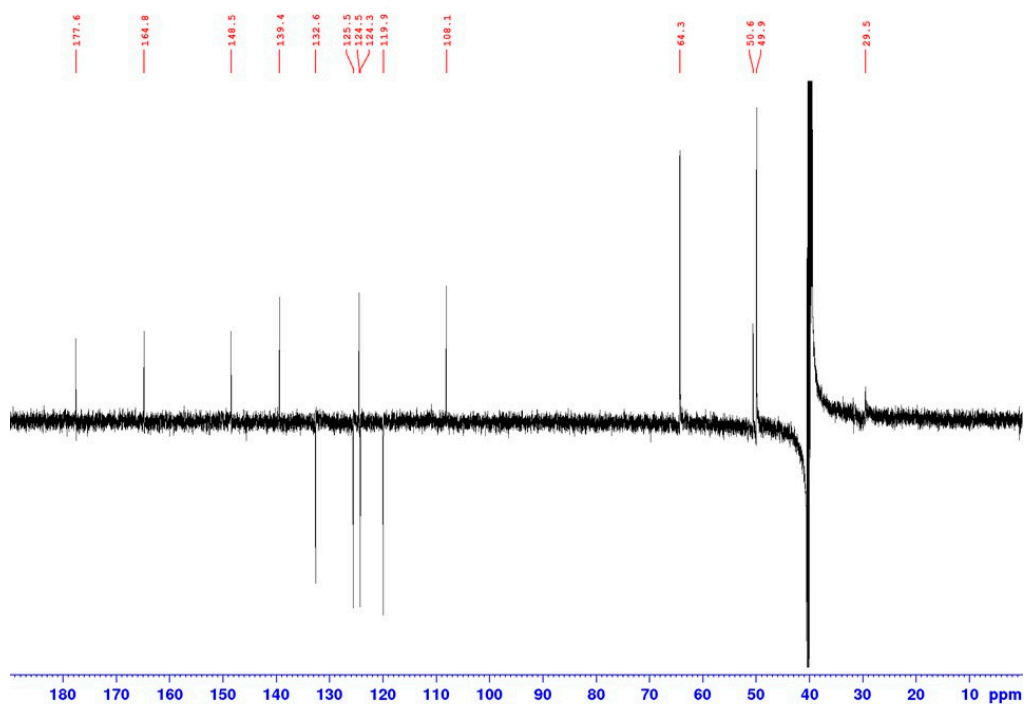


Figure S53. ¹³C-NMR spectrum of 22