

Supporting Information for

***Mycobacterium tuberculosis* inhibitors based on arylated quinoline carboxylic acid backbones with anti-*Mtb* gyrase activity**

**Mark Tristan J. Quimque, Adrian D. Go, Justin Allen K. Lim, Warren S. Vidar,
and Allan Patrick G. Macabeo***

¹The Graduate School, University of Santo Tomas, España Blvd., Manila 1015 Philippines

²Laboratory for Organic Reactivity, Discovery and Synthesis (Rm. 410) Research Center for the Natural and Applied Sciences University of Santo Tomas Espana Blvd., Manila 1015, Philippines

³Chemistry Department, College of Science and Mathematics, Mindanao State University – Iligan Institute of Technology, Tibanga, Iligan City, Philippines

*Corresponding author: A. P. G. Macabeo (agmacabeo@ust.edu.ph)

TABLE OF CONTENTS

Figure S1. 600 MHz ^1H NMR spectrum of 1d (DMSO- d_6).....	4
Figure S2. 151 MHz ^{13}C NMR spectrum of 1d (DMSO- d_6).....	4
Figure S3. 600 MHz ^{13}H NMR spectrum of 1o (DMSO- d_6).....	5
Figure S4. 151 MHz ^{13}C NMR spectrum of 1o (DMSO- d_6).....	5
Figure S5. 600 MHz ^1H NMR spectrum of 1p (MeOH- d_4)	6
Figure S6. 151 MHz ^{13}C NMR spectrum of 1p (MeOH- d_4)	6
Figure S7. 600 MHz ^1H NMR spectrum of 6b (DMSO- d_6).....	7
Figure S8. 151 MHz ^{13}C NMR spectrum of 6b (DMSO- d_6).....	7
Figure S9. 600 MHz ^{13}C NMR spectrum of 6c (DMSO- d_6).....	8
Figure S10. 151 MHz ^{13}C NMR spectrum of 6c (DMSO- d_6)	8
Figure S11. 600 MHz ^1H NMR spectrum of 6d (DMSO- d_6).....	9
Figure S12. 151 MHz ^{13}C NMR spectrum of 6d (DMSO- d_6).....	9
Figure S13. 600 MHz ^{13}C NMR spectrum of 6g (DMSO- d_6).....	10
Figure S14. 151 MHz ^{13}C NMR spectrum of 6g (DMSO- d_6).....	10
Figure S15. 600 MHz ^1H NMR spectrum of 6h (DMSO- d_6).....	11
Figure S16. 151 MHz ^{13}C NMR spectrum of 6h (DMSO- d_6).....	11
Figure S17. 600 MHz ^1H NMR spectrum of 6i (DMSO- d_6).....	12
Figure S18. 151 MHz ^{13}C NMR spectrum of 6i (DMSO- d_6).....	12
Figure S19. 600 MHz ^1H NMR spectrum of 6j (DMSO- d_6).....	13
Figure S20. 151 MHz ^{13}C NMR spectrum of 6j (DMSO- d_6).....	13
Figure S21. 600 MHz ^1H NMR spectrum of 6k (DMSO- d_6).....	14
Figure S22. 151 MHz ^{13}C NMR spectrum of 6k (DMSO- d_6).....	14
Figure S23. 600 MHz ^1H NMR spectrum of 6l (DMSO- d_6).....	15
Figure S24. 151 MHz ^{13}C NMR spectrum of 6l (DMSO- d_6).....	15
Figure S25. 600 MHz ^1H NMR spectrum of 6n (DMSO- d_6).....	16
Figure S26. 151 MHz ^{13}C NMR spectrum of 6n (DMSO- d_6).....	16
Figure S27. 600 MHz ^1H NMR spectrum of 6p (DMSO- d_6).....	17
Figure S28. 151 MHz ^{13}C NMR spectrum of 6p (DMSO- d_6).....	17
Figure S29. 600 MHz ^1H NMR spectrum of 6q (DMSO- d_6).....	18
Figure S30. 151 MHz ^{13}C NMR spectrum of 6q (DMSO- d_6).....	18
Figure S31. 600 MHz ^1H NMR spectrum of 6r (DMSO- d_6)	19

Figure S32. 151 MHz ^{13}C NMR spectrum of 6r (DMSO- d_6)	19
Figure S33. 600 MHz ^1H NMR spectrum of 7b (DMSO- d_6).....	20
Figure S34. 151 MHz ^{13}C NMR spectrum of 7b (DMSO- d_6).....	20
Figure S35. 600 MHz ^1H NMR spectrum of 7c (MeOH- d_4).....	21
Figure S36. 151 MHz ^{13}C NMR spectrum of 7c (MeOH- d_4).....	21
Figure S37. 600 MHz ^1H NMR spectrum of 7d (MeOH- d_4)	22
Figure S38. 151 MHz ^{13}C NMR spectrum of 7d (MeOH- d_4)	22
Figure S39. 600 MHz ^1H NMR spectrum of 7g (DMSO- d_6)	23
Figure S40. 151 MHz ^{13}C NMR spectrum of 7g (DMSO- d_6)	23
Figure S41. 600 MHz ^1H NMR spectrum of 7h (MeOH- d_4)	24
Figure S42. 151 MHz ^{13}C NMR spectrum of 7h (MeOH- d_4)	24
Figure S43. 600 MHz ^1H NMR spectrum of 7i (DMSO- d_6).....	25
Figure S44. 151 MHz ^{13}C NMR spectrum of 7i (DMSO- d_6).....	25
Figure S45. 600 MHz ^1H NMR spectrum of 7j (DMSO- d_6).....	26
Figure S46. 151 MHz ^{13}C NMR spectrum of 7j (DMSO- d_6).....	26
Figure S47. 600 MHz ^1H NMR spectrum of 7k (DMSO- d_6).....	27
Figure S48. 151 MHz ^{13}C NMR spectrum of 7k (DMSO- d_6).....	27
Figure S49. 600 MHz ^1H NMR spectrum of 7l (DMSO- d_6)	28
Figure S50. 151 MHz ^{13}C NMR spectrum of 7l (DMSO- d_6)	28
Figure S51. 600 MHz ^1H NMR spectrum of 7m (DMSO- d_6)	29
Figure S52. 151 MHz ^{13}C NMR spectrum of 7m (MeOH- d_4)	29
Figure S53. 600 MHz ^1H NMR spectrum of 7n (MeOH- d_4)	30
Figure S54. 151 MHz ^{13}C NMR spectrum of 7n (MeOH- d_4)	30
Figure S55. Agarose gel electrophoresis result showing inhibition of QCA 7i and 7m against <i>Mtb</i> DNA gyrase; (-) negative control without gyrase; (+) positive control with gyrase.....	32

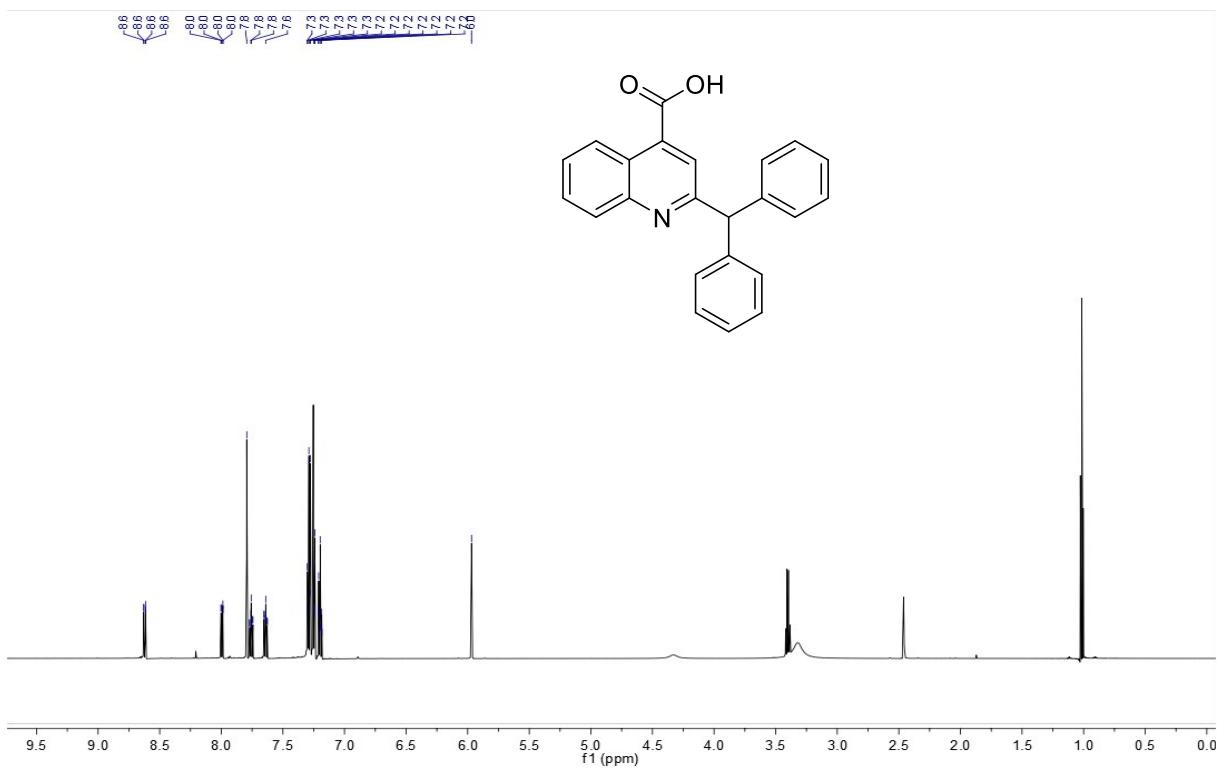


Figure S1. 600 MHz ^1H NMR spectrum of **1d** (DMSO- d_6)

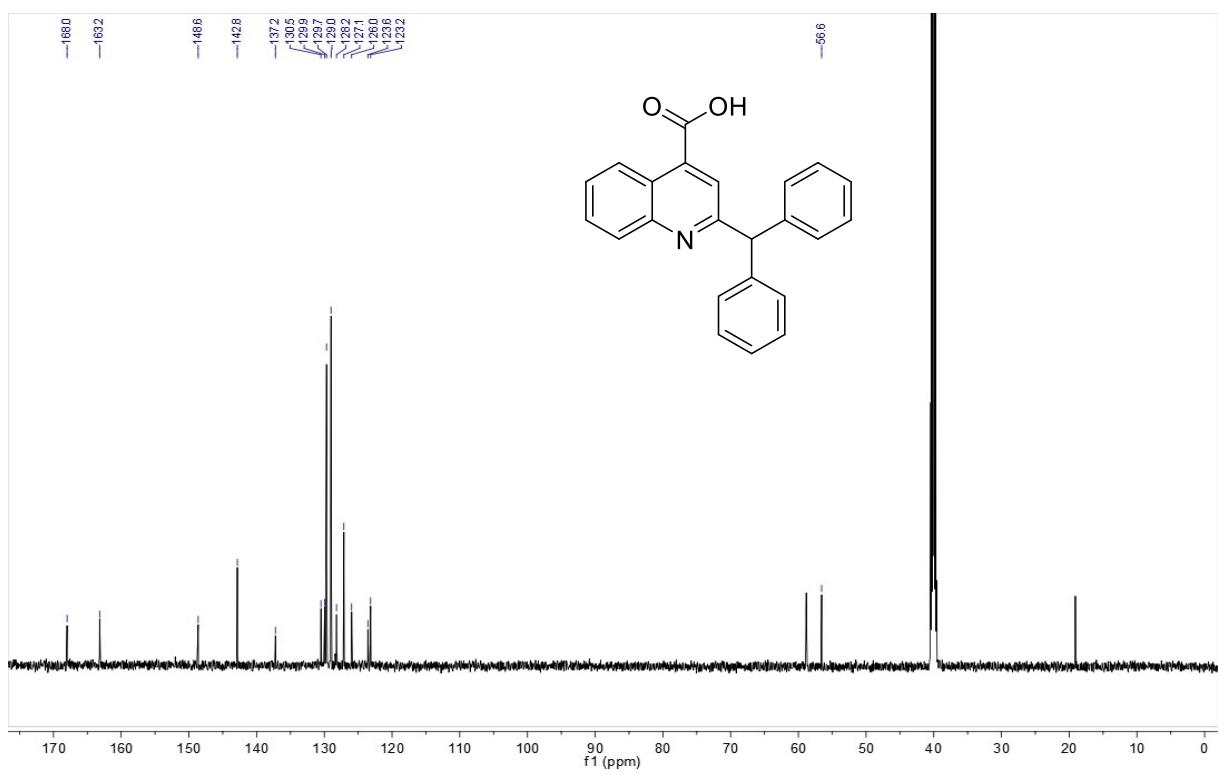


Figure S2. 151 MHz ^{13}C NMR spectrum of **1d** ($\text{DMSO}-d_6$)

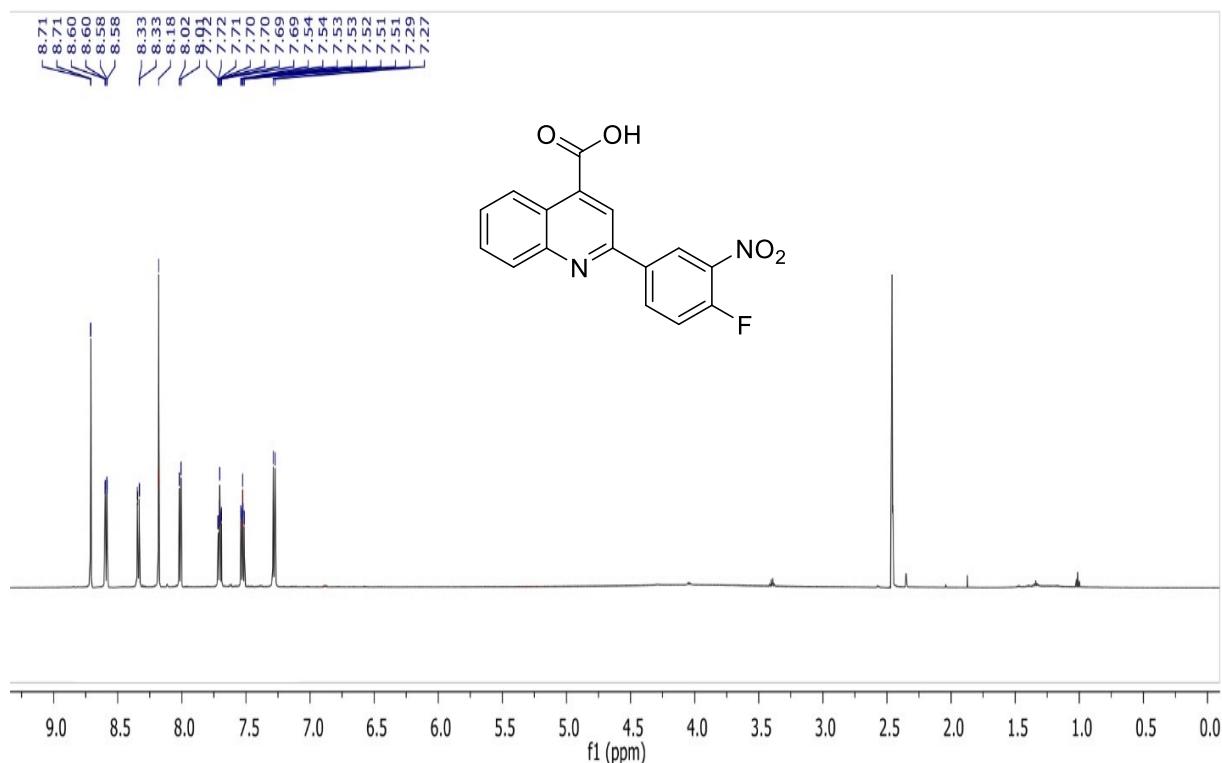


Figure S3. 600 MHz ^{13}H NMR spectrum of **1o** (DMSO- d_6)

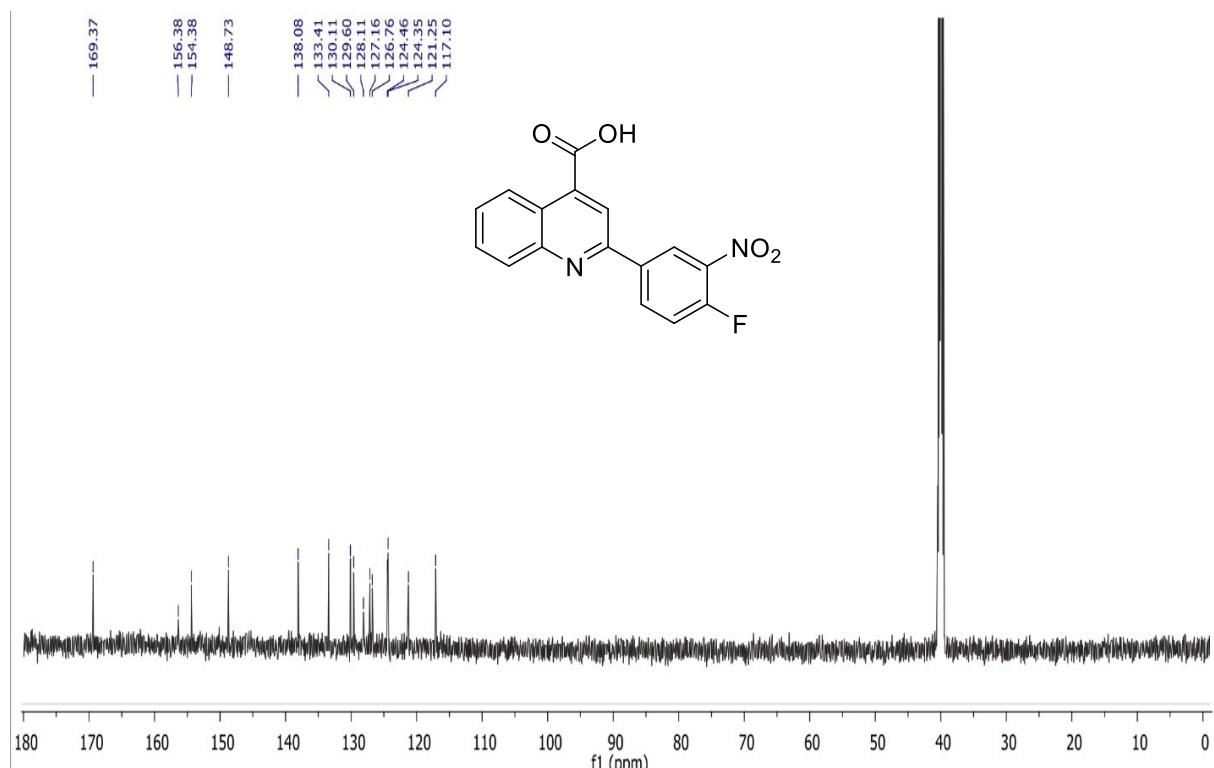


Figure S4. 151 MHz ^{13}C NMR spectrum of **1o** (DMSO- d_6)

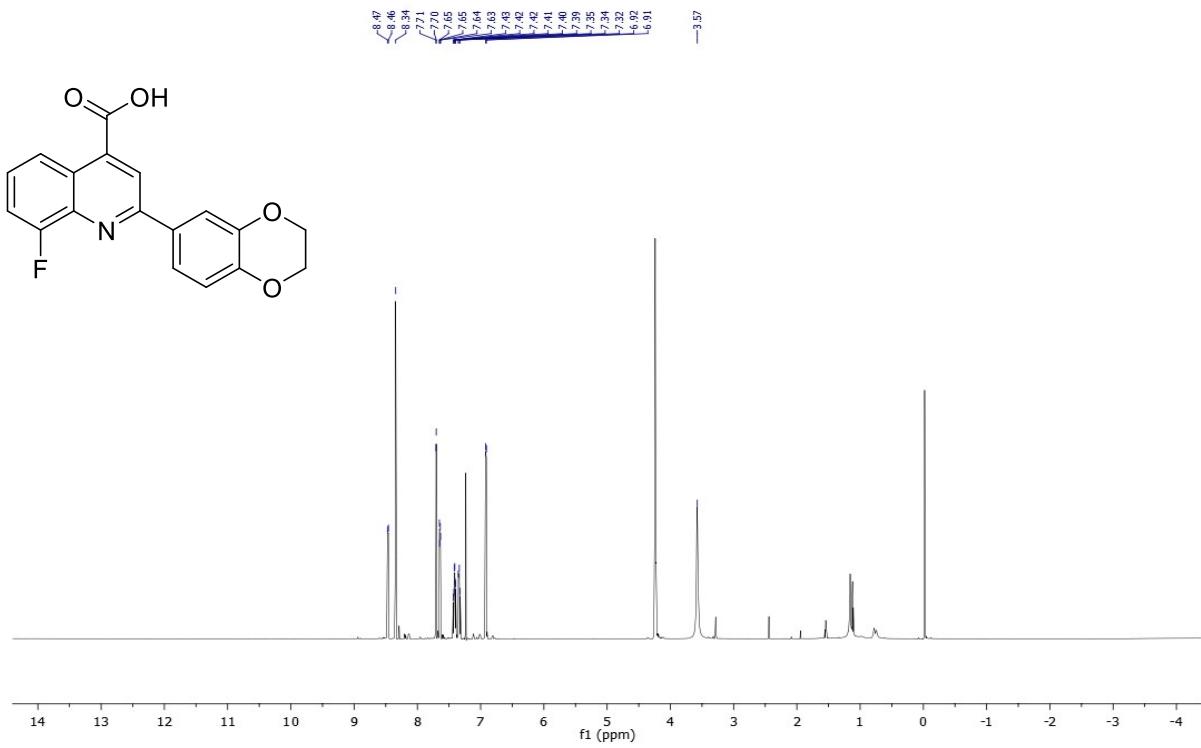


Figure S5. 600 MHz ^1H NMR spectrum of **1p** ($\text{MeOH}-d_4$)

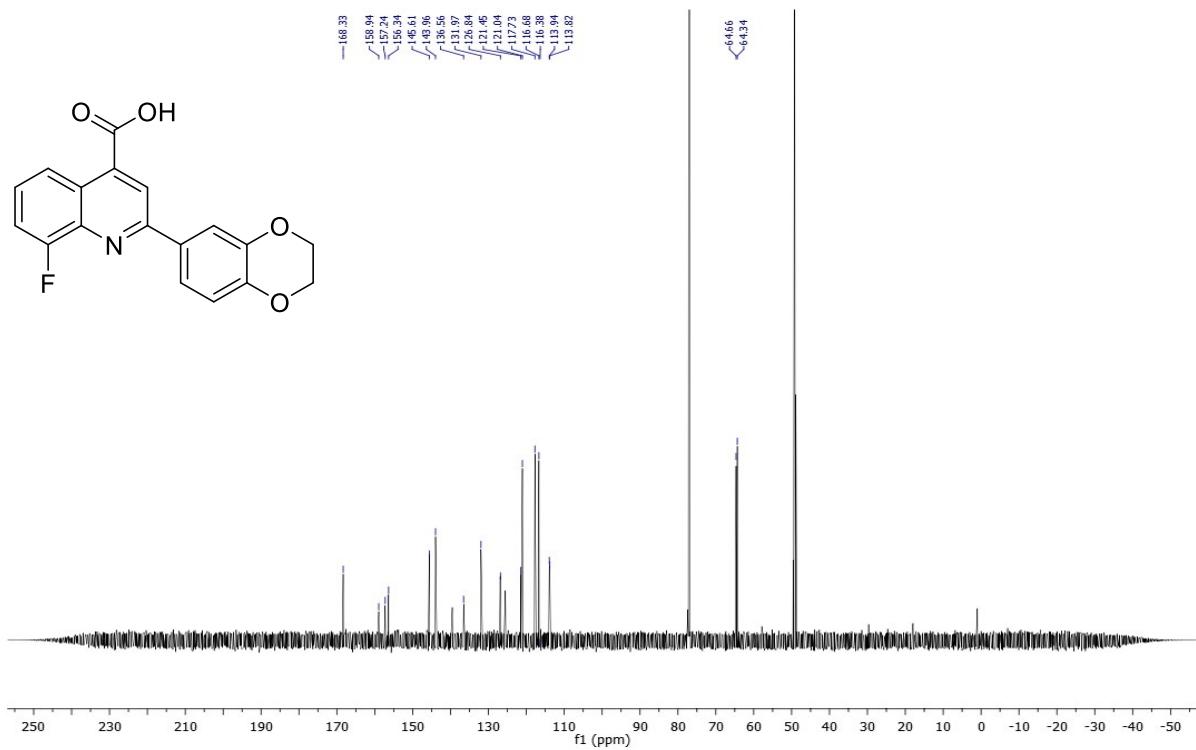


Figure S6. 151 MHz ^{13}C NMR spectrum of **1p** ($\text{MeOH-}d_4$)

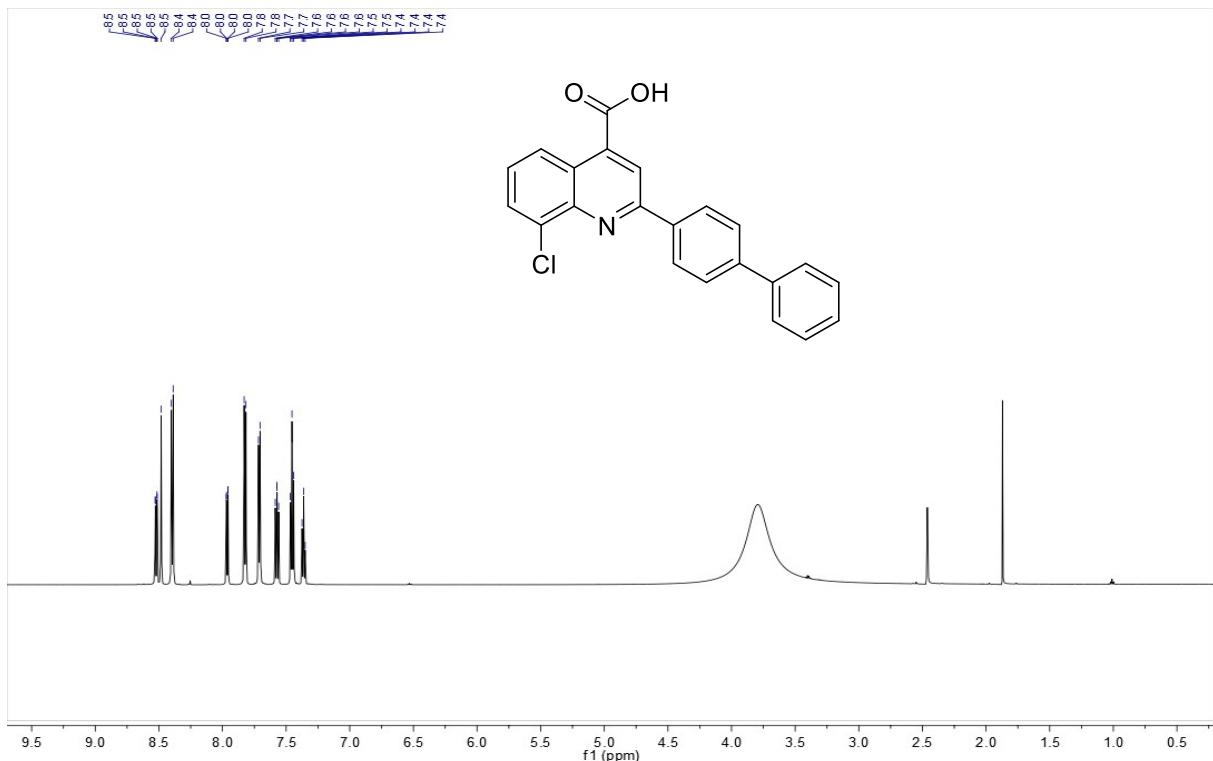


Figure S7. 600 MHz ^1H NMR spectrum of **6b** (DMSO- d_6)

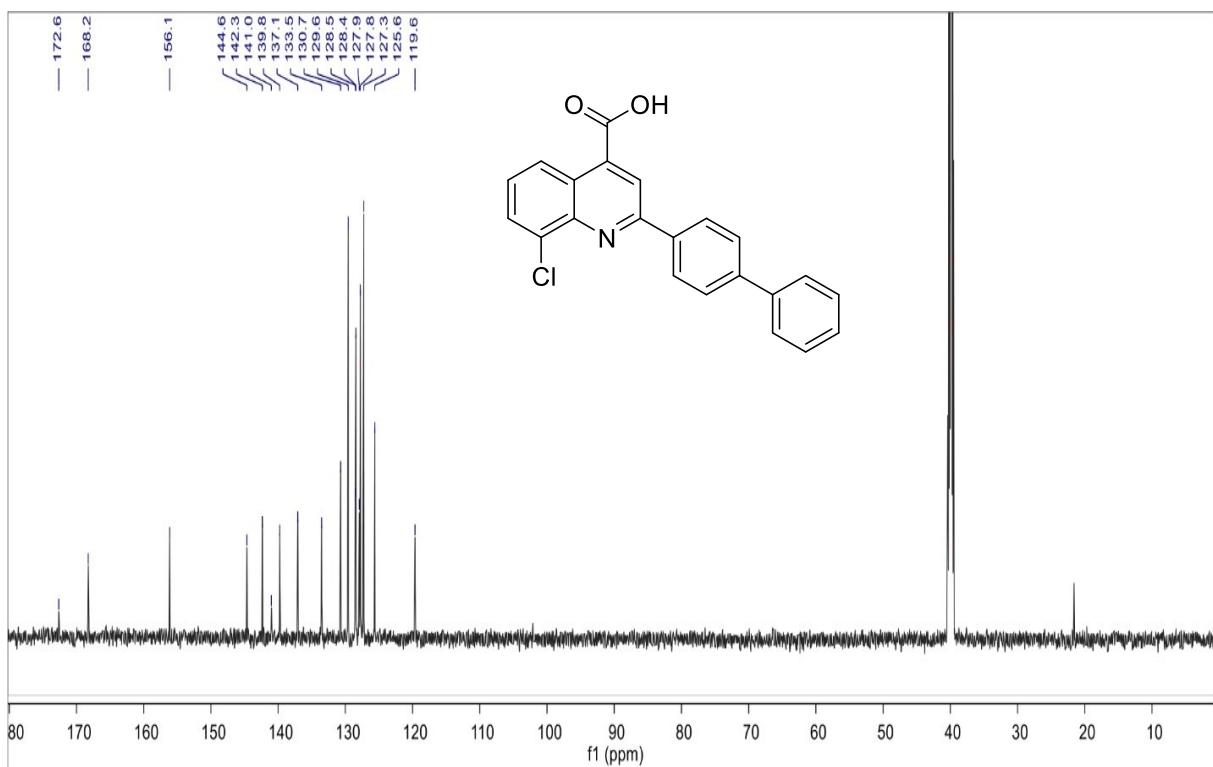


Figure S8. 151 MHz ^{13}C NMR spectrum of **6b** (DMSO- d_6)

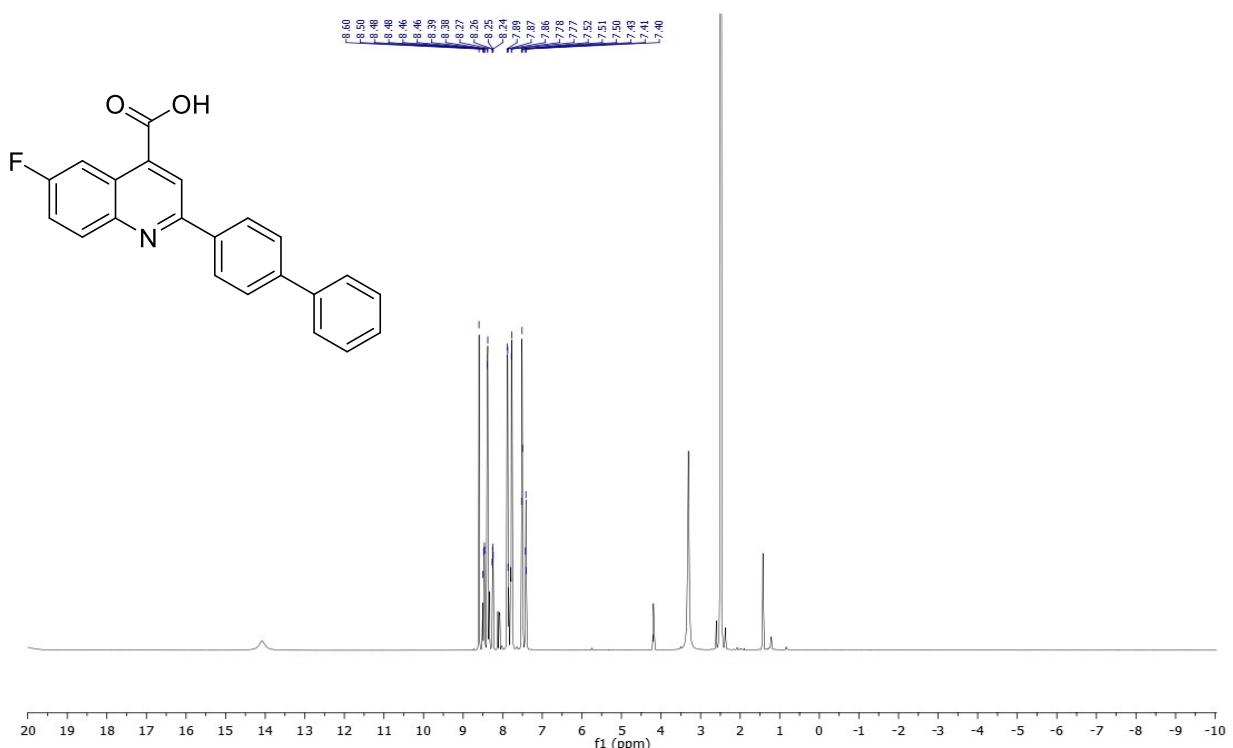


Figure S9. 600 MHz ^{13}C NMR spectrum of **6c** (DMSO- d_6)

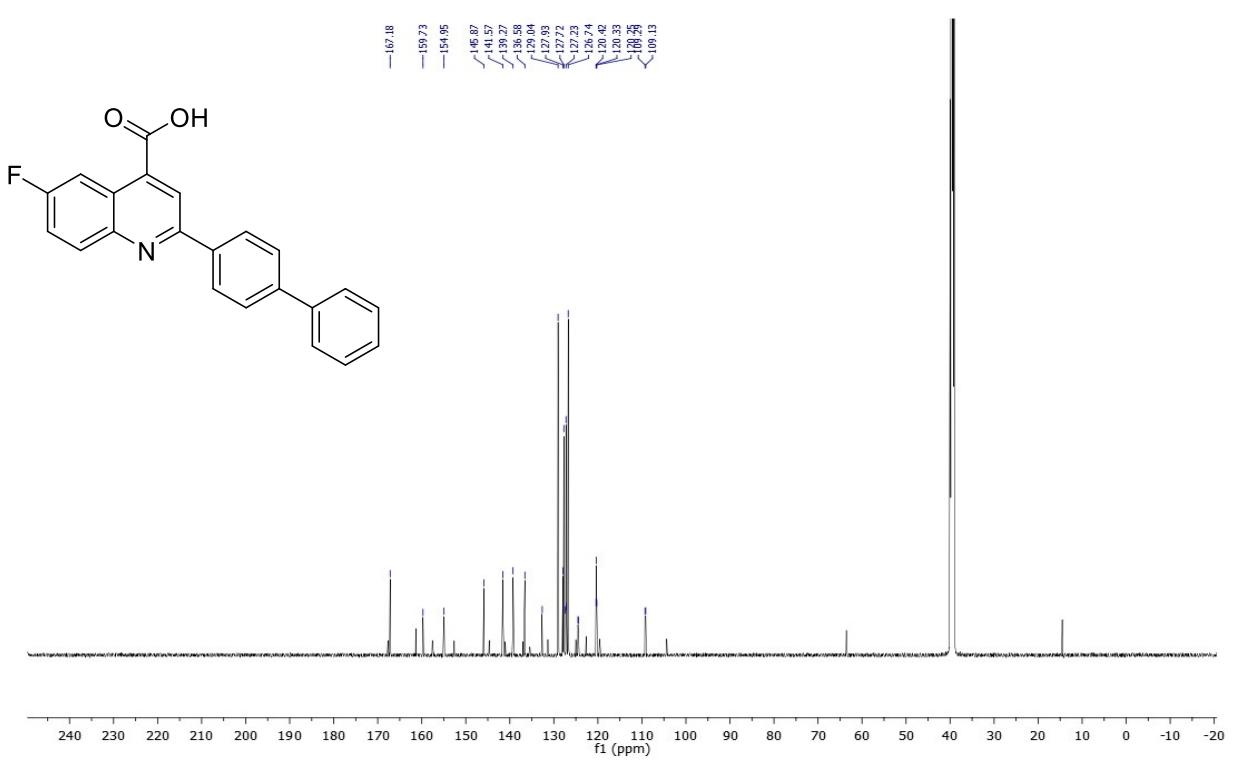


Figure S10. 151 MHz ^{13}C NMR spectrum of **6c** (DMSO- d_6)

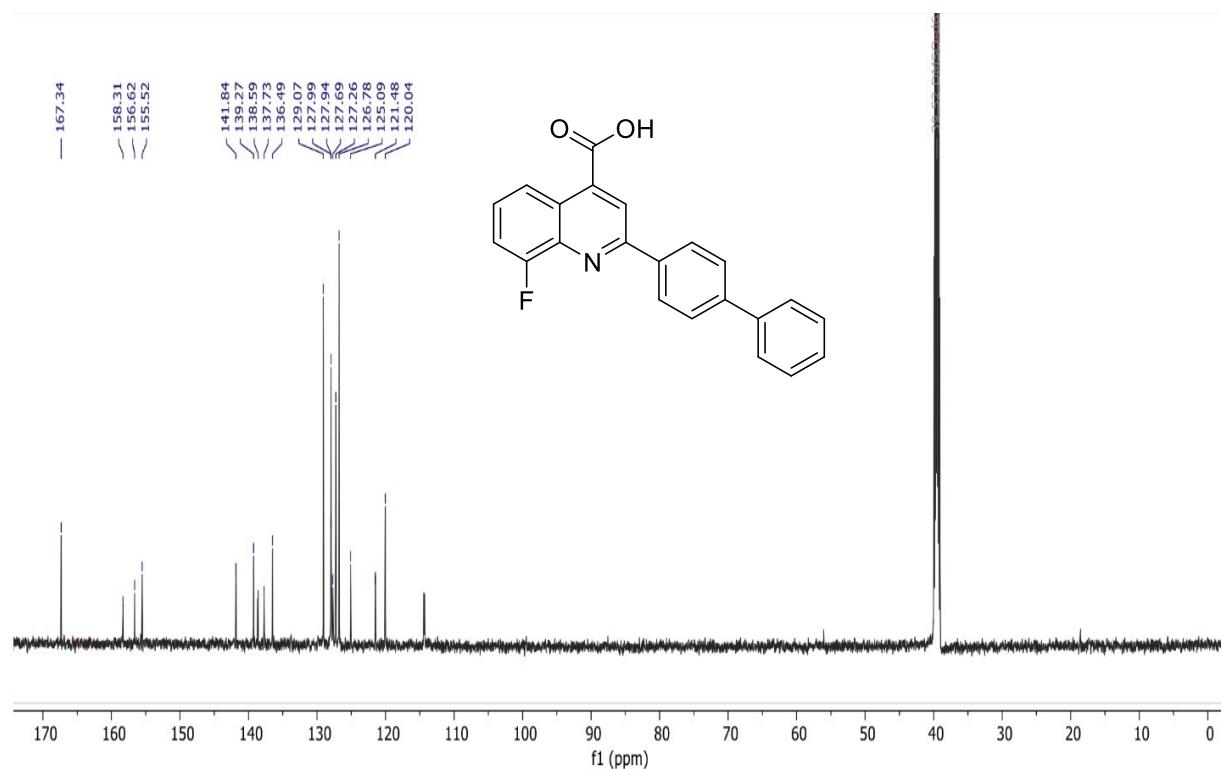
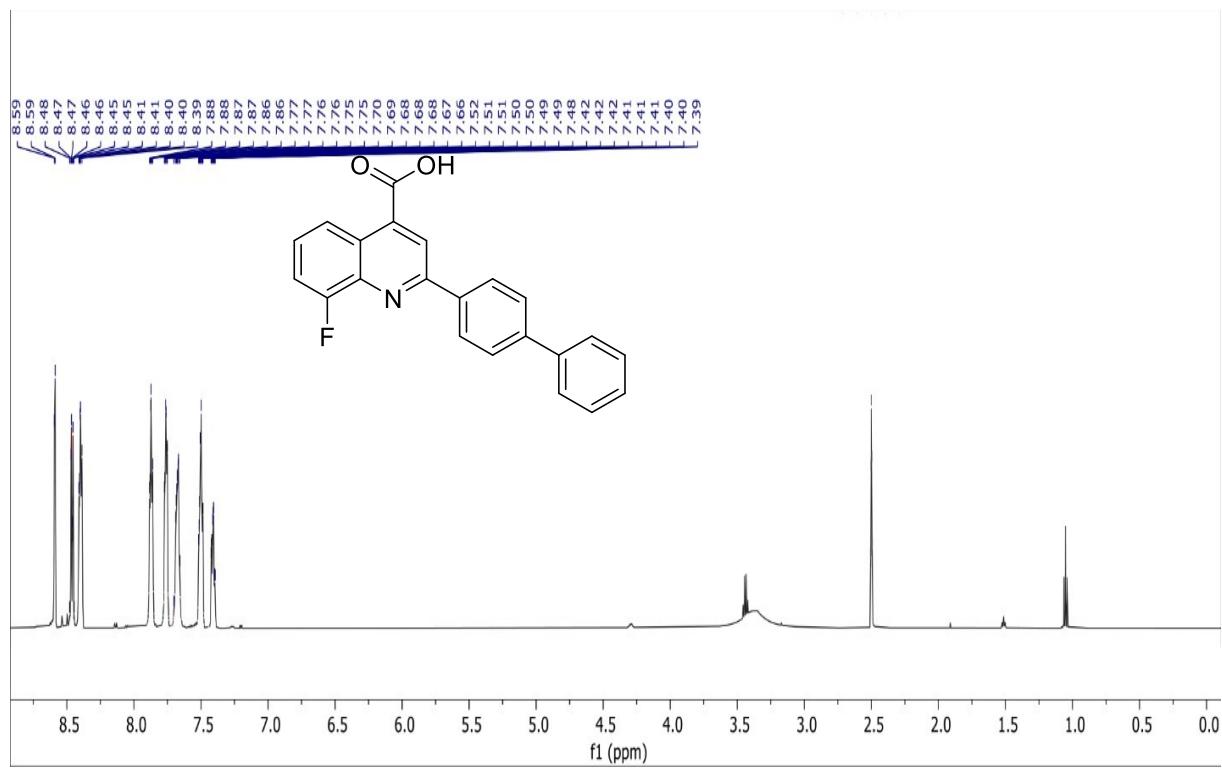


Figure S12. 151 MHz ^{13}C NMR spectrum of **6d** (DMSO- d_6)

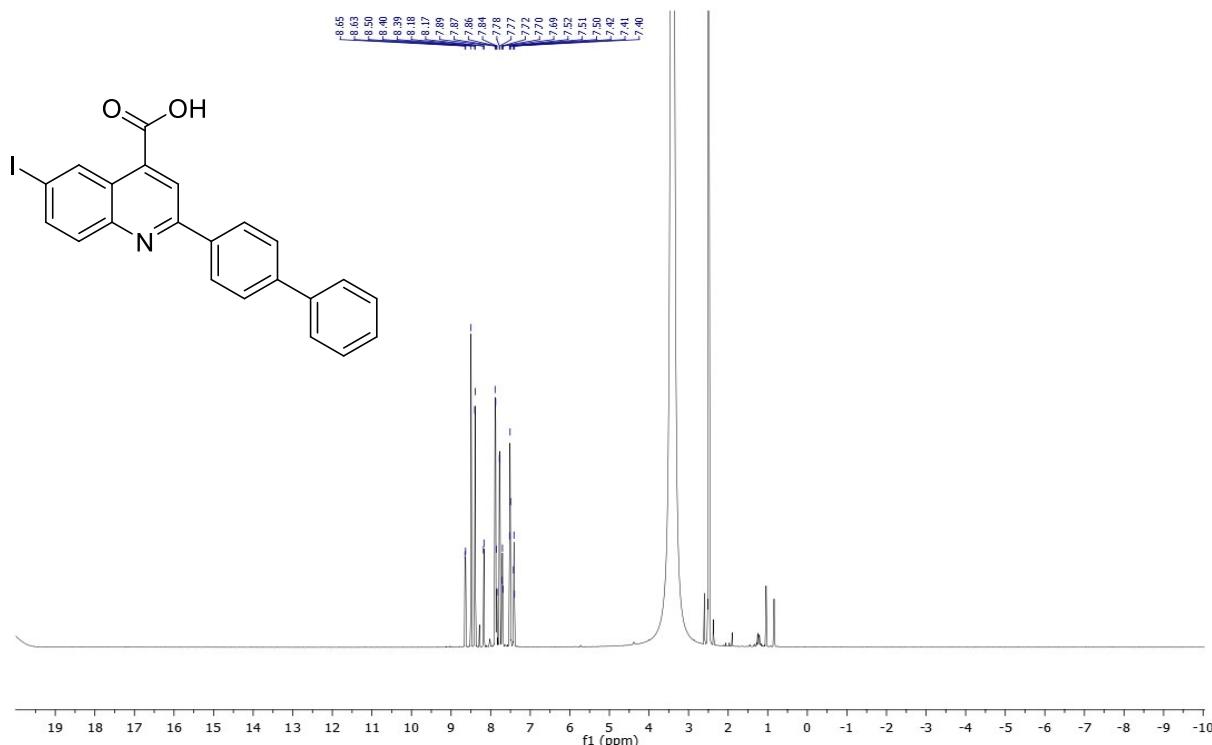


Figure S13. 600 MHz ^{13}C NMR spectrum of **6g** (DMSO- d_6)

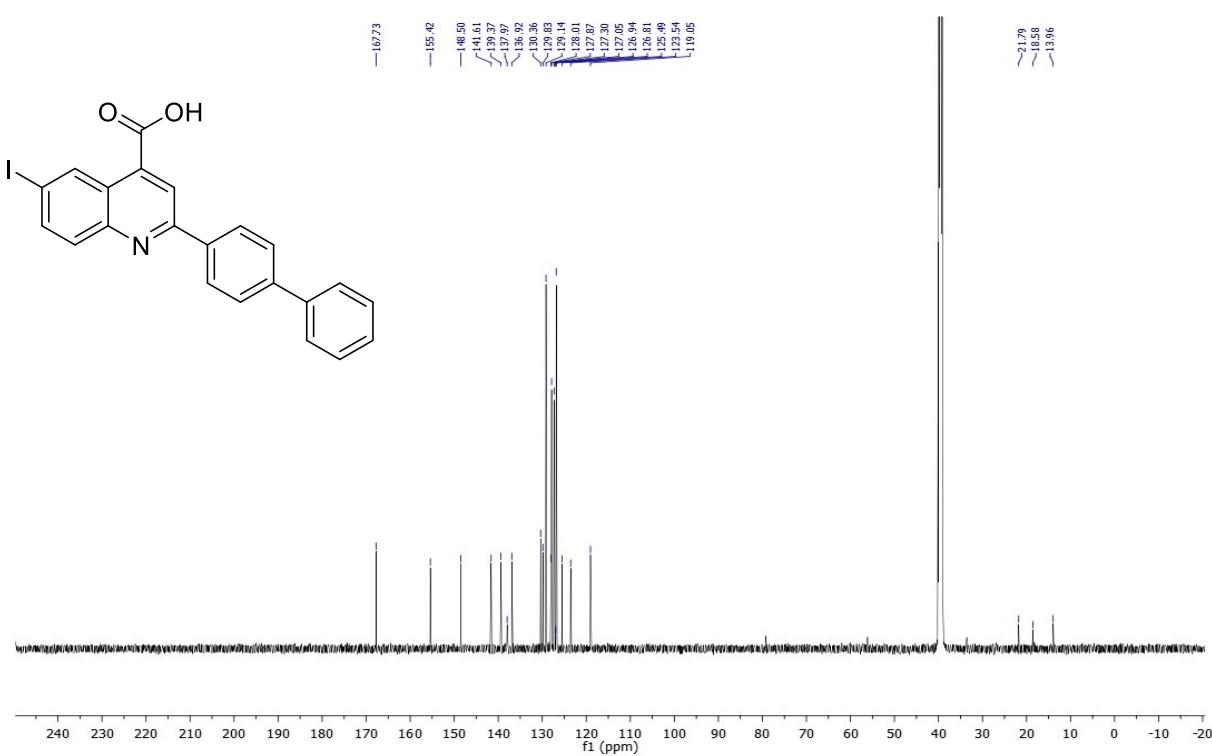


Figure S14. 151 MHz ^{13}C NMR spectrum of **6g** (DMSO- d_6)

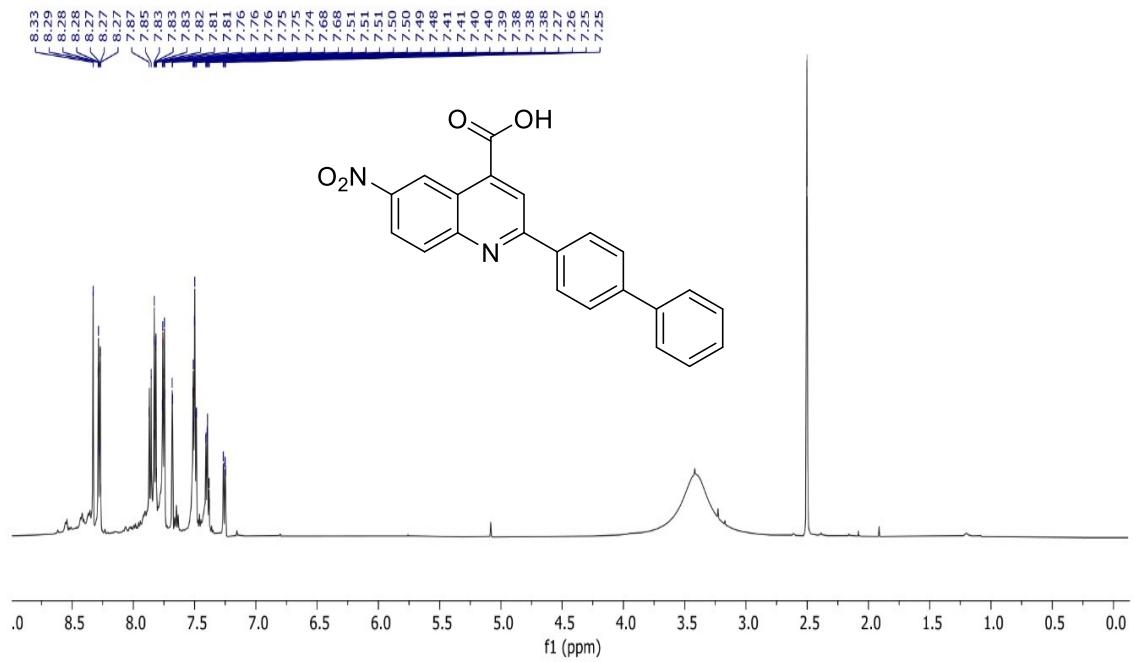


Figure S15. 600 MHz ^1H NMR spectrum of **6h** (DMSO- d_6)

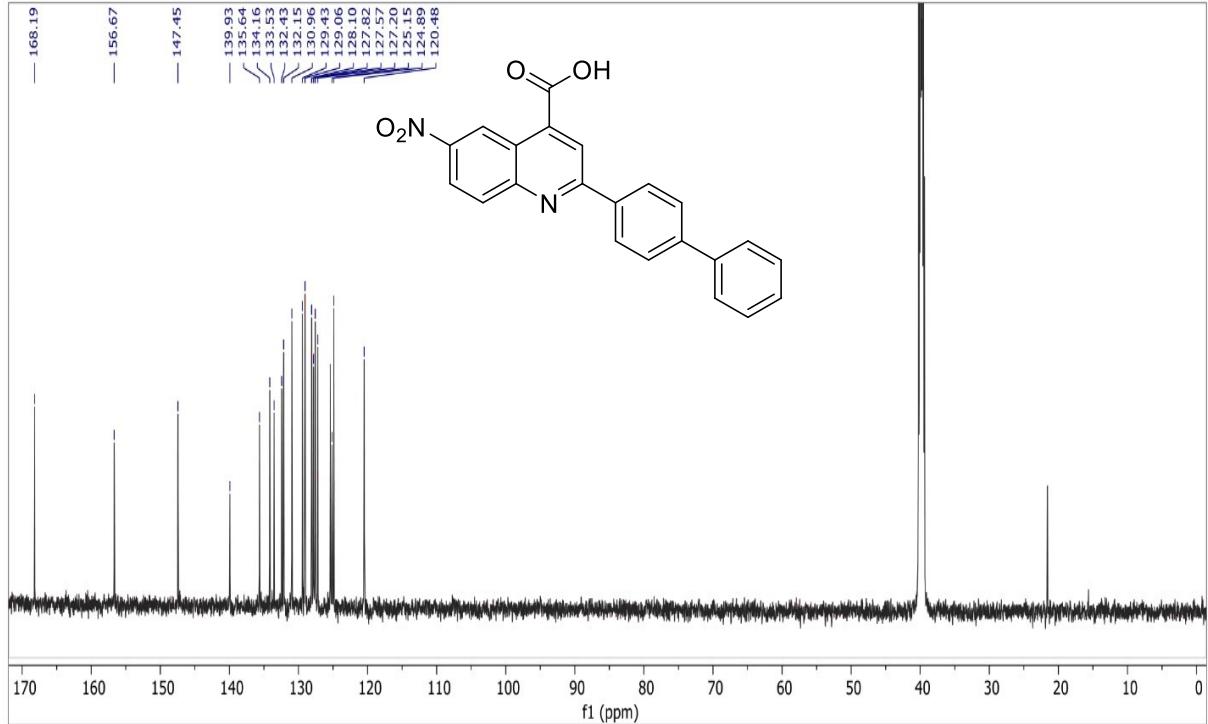


Figure S16. 151 MHz ^{13}C NMR spectrum of **6h** (DMSO- d_6)

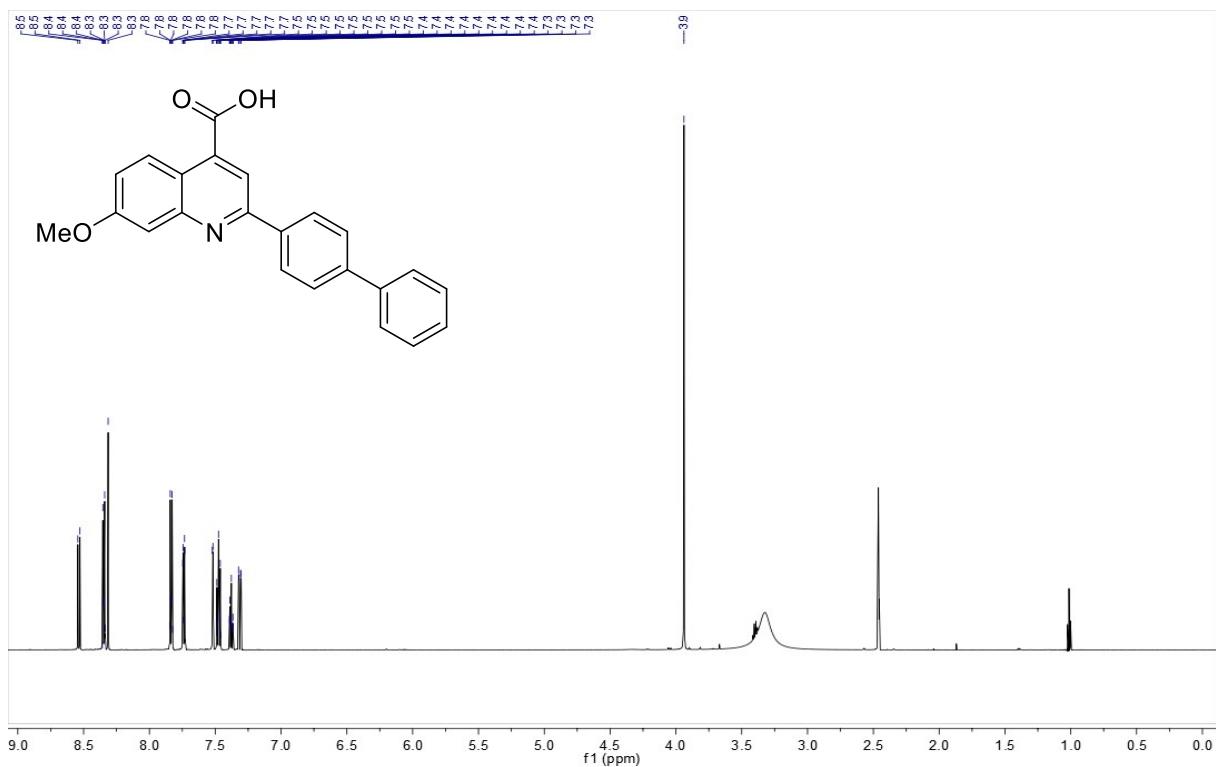


Figure S17. 600 MHz ¹H NMR spectrum of **6i** (DMSO-*d*₆)

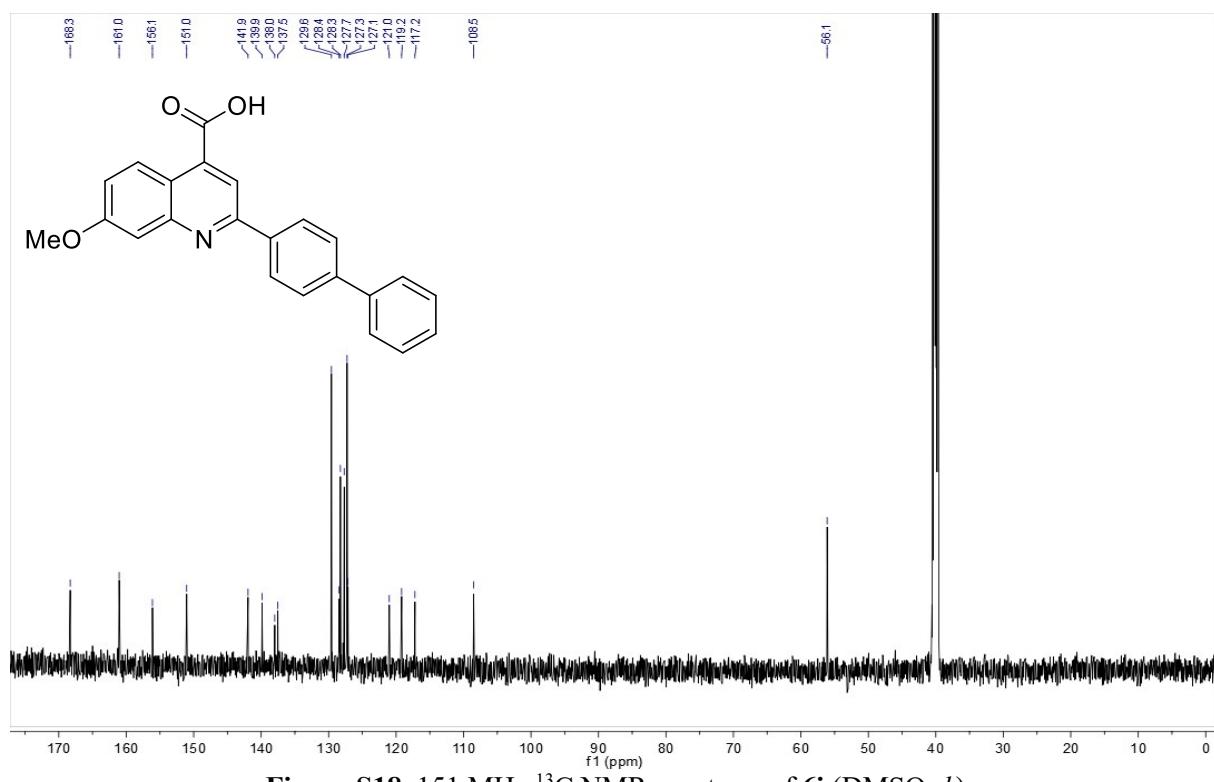


Figure S18. 151 MHz ¹³C NMR spectrum of **6i** (DMSO-*d*₆)

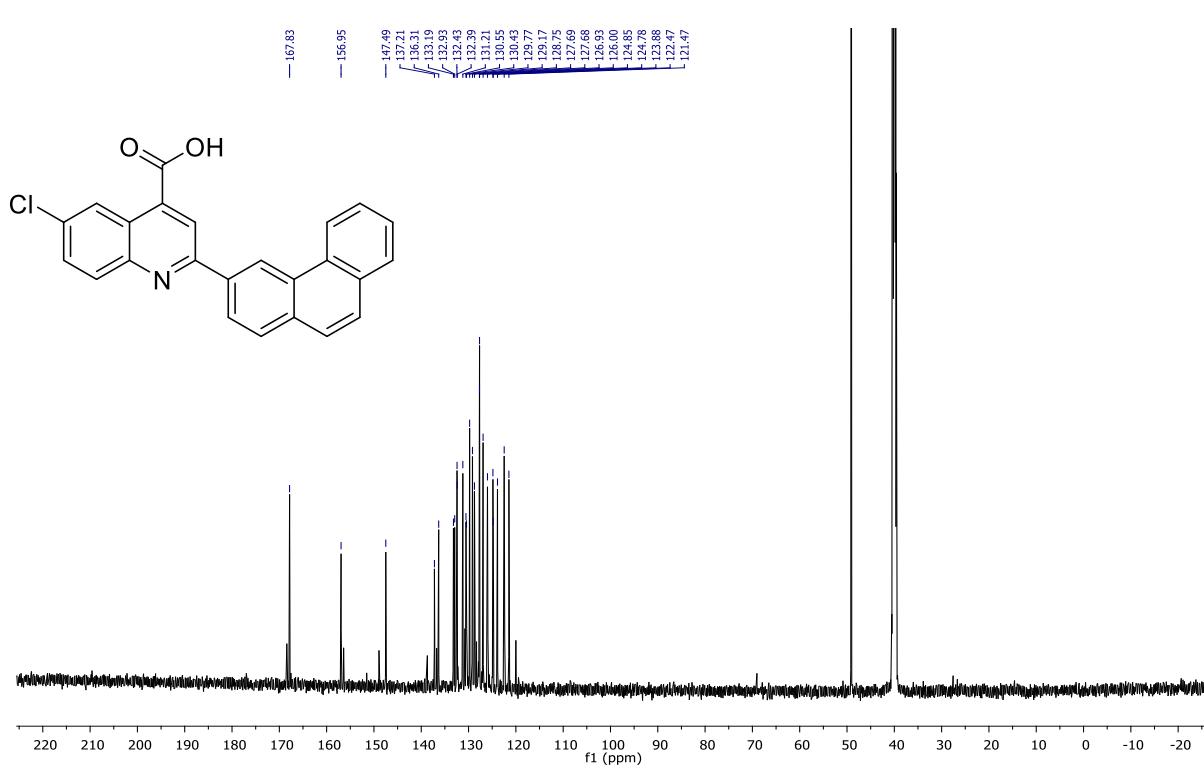
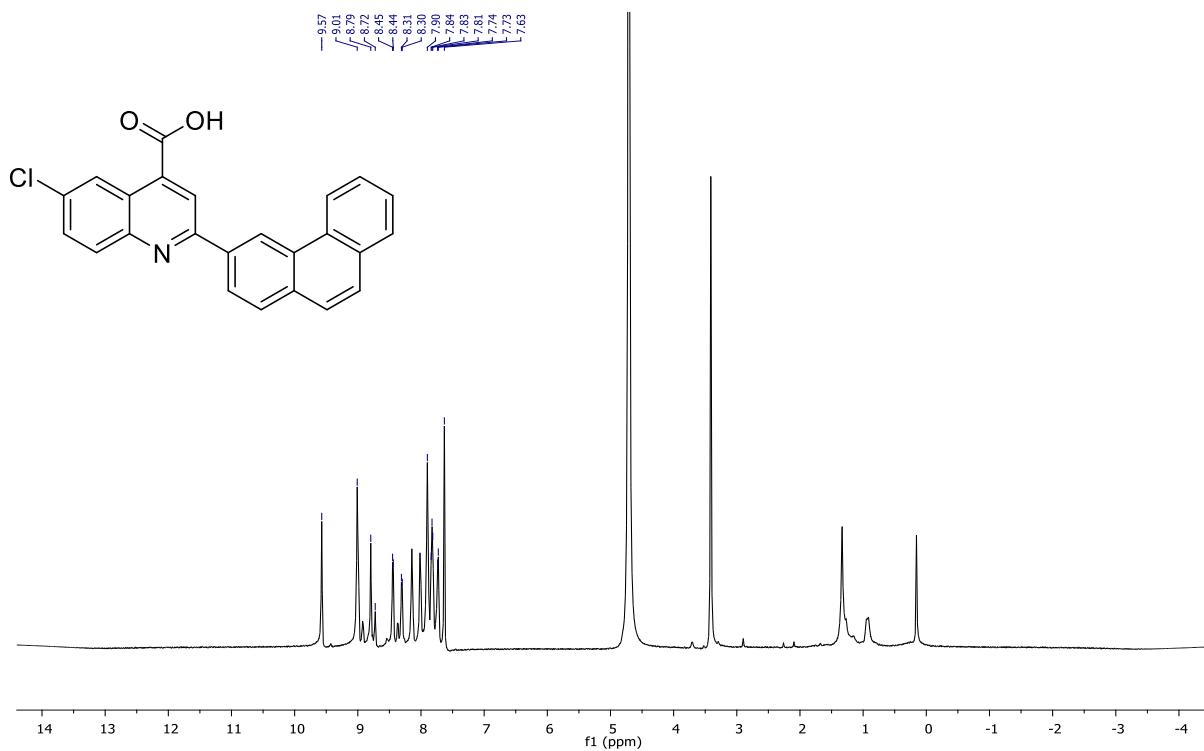


Figure S20. 151 MHz ^{13}C NMR spectrum of **6j** (DMSO- d_6)

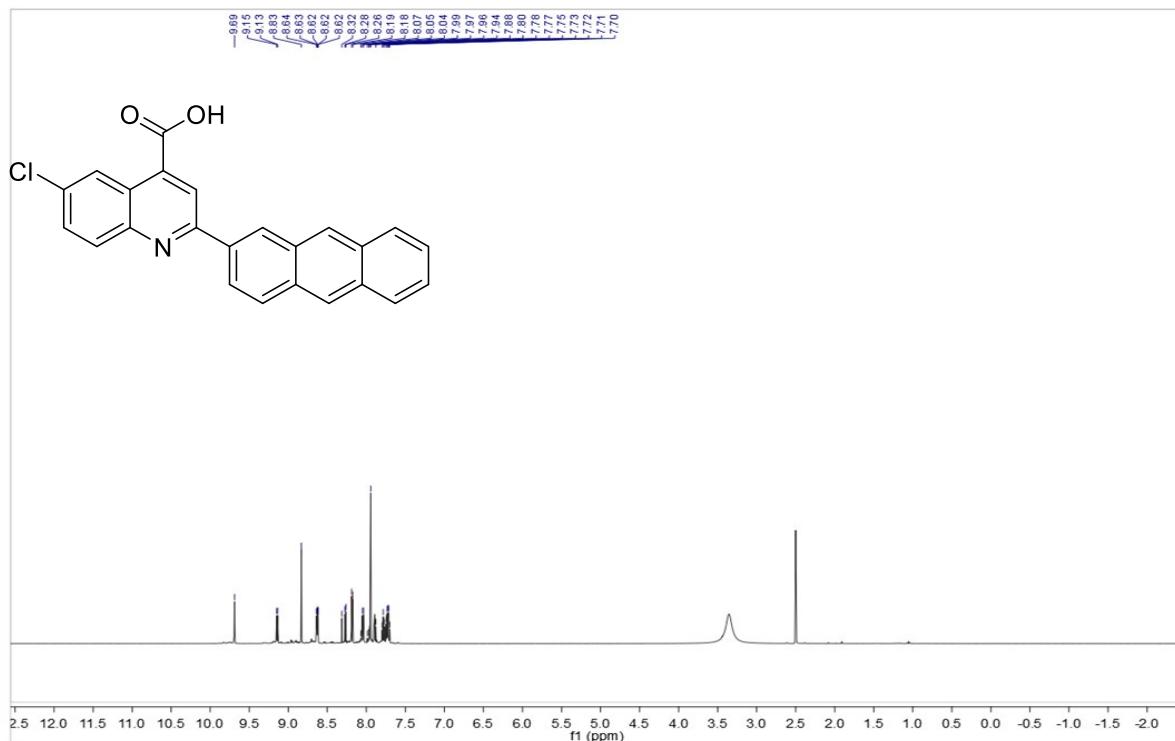


Figure S21. 600 MHz ^1H NMR spectrum of **6k** (DMSO- d_6)

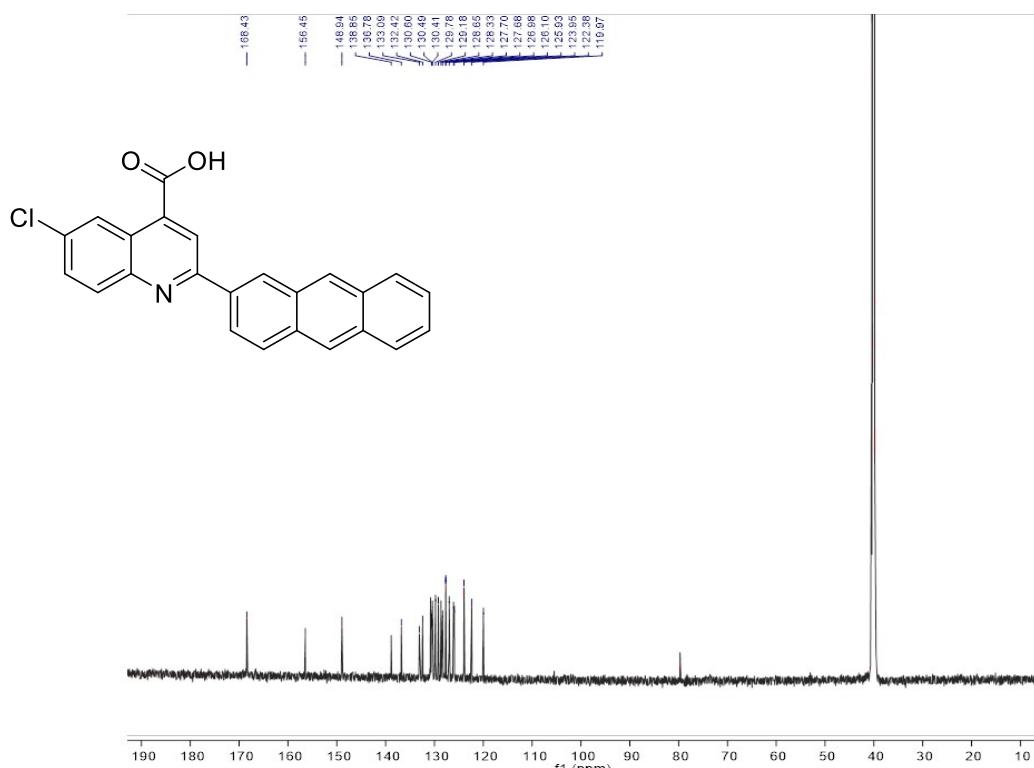


Figure S22. 151 MHz ^{13}C NMR spectrum of **6k** (DMSO- d_6)

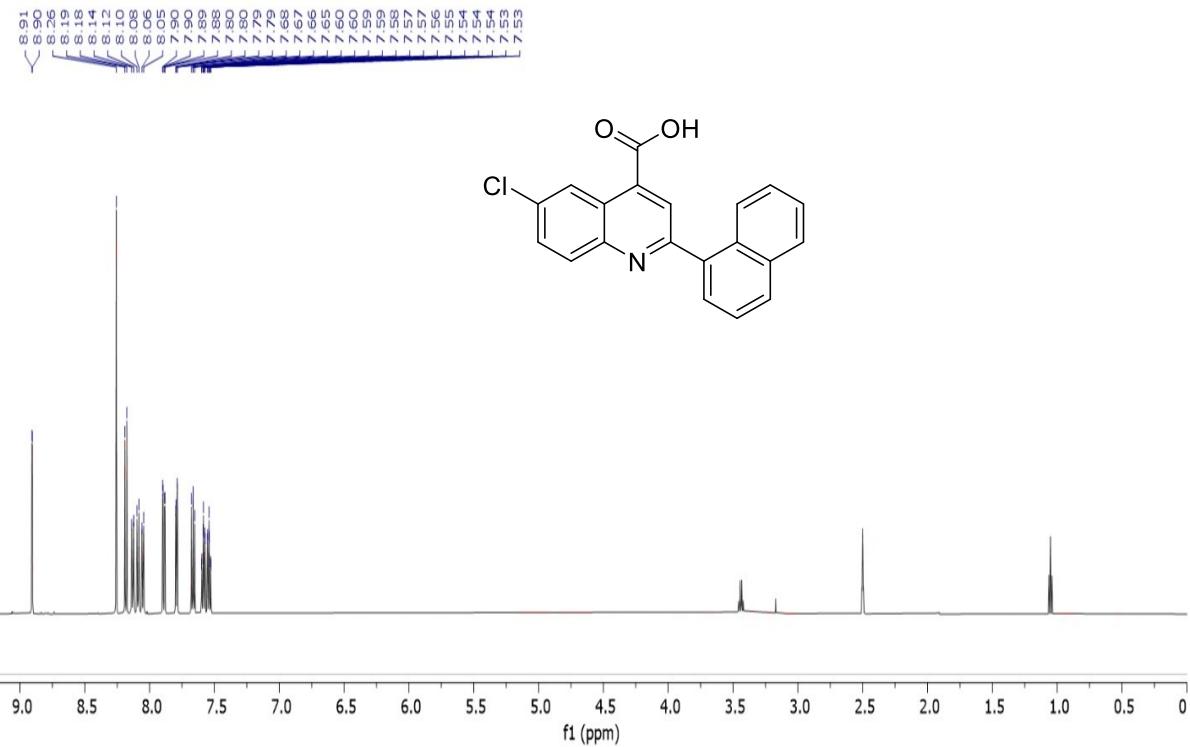


Figure S23. 600 MHz ^1H NMR spectrum of **6l** (DMSO- d_6)

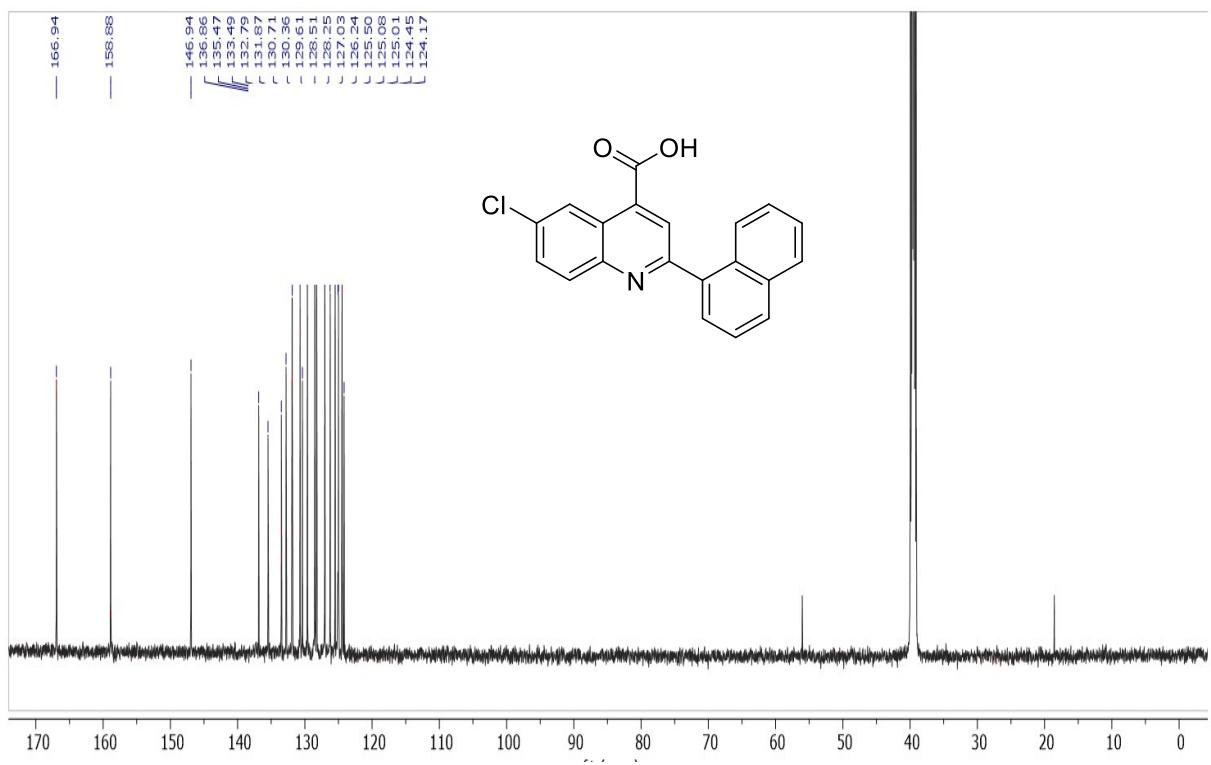


Figure S24. 151 MHz ^{13}C NMR spectrum of **6l** (DMSO- d_6)

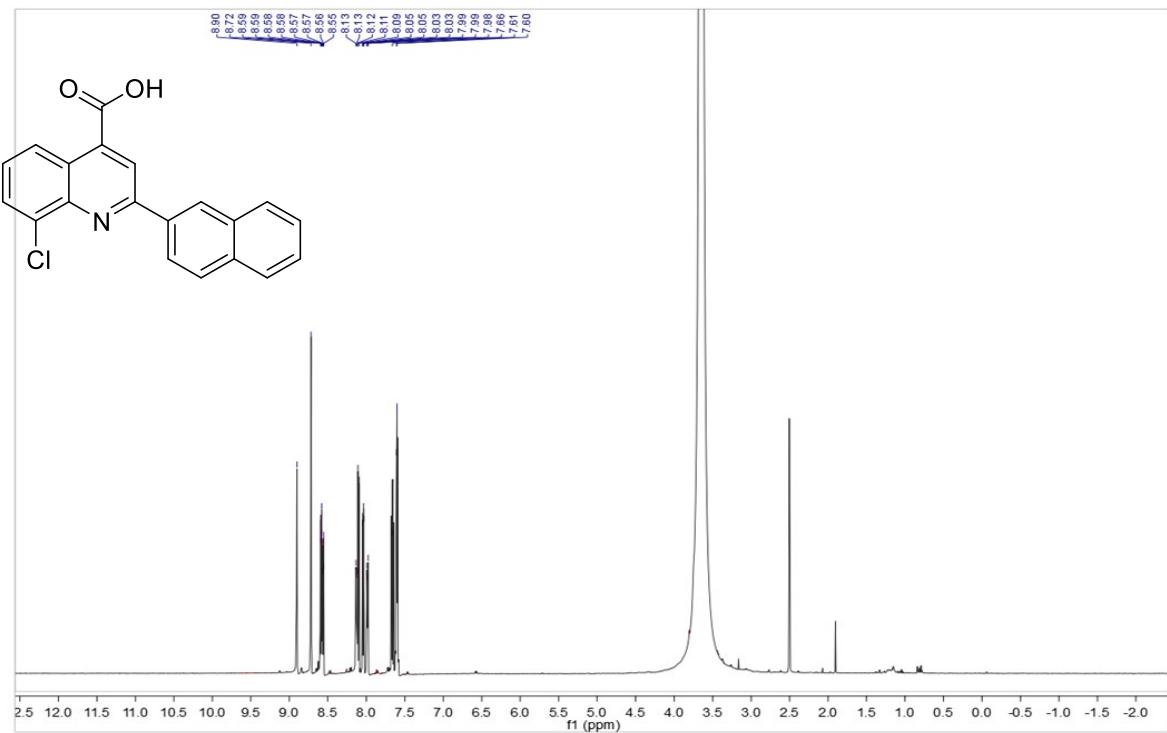


Figure S25. 600 MHz ^1H NMR spectrum of **6n** (DMSO- d_6)

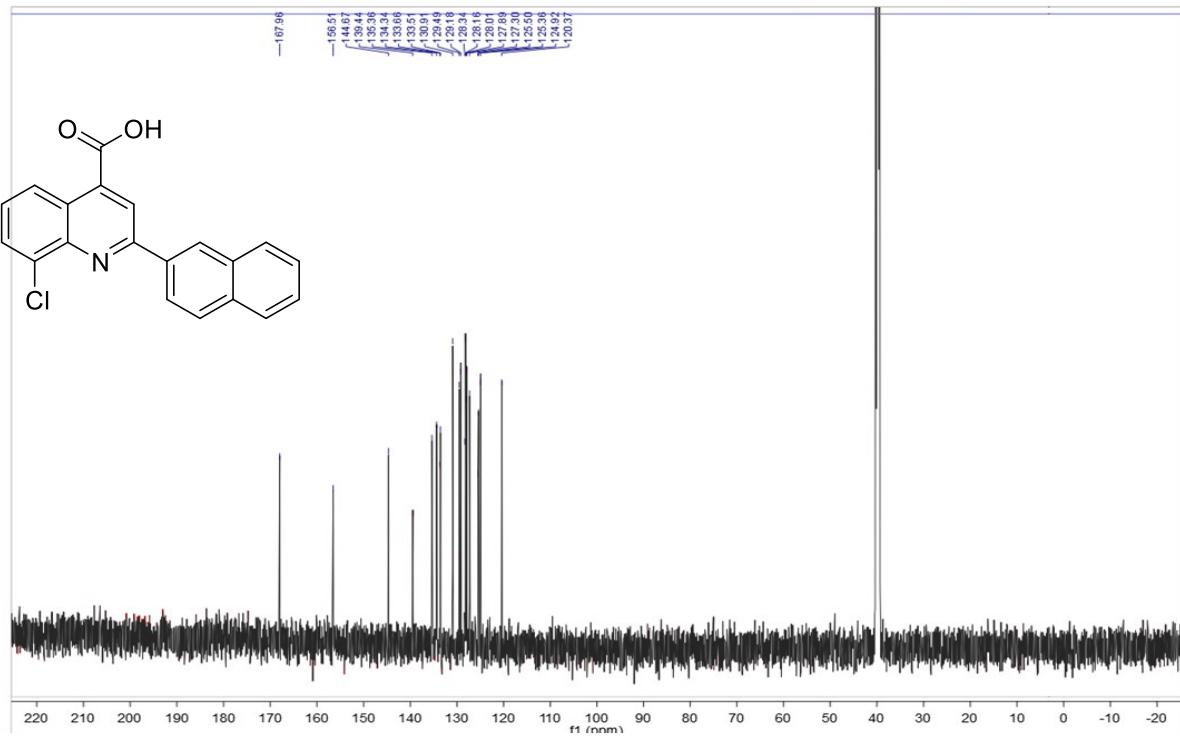


Figure S26. 151 MHz ^{13}C NMR spectrum of **6n** (DMSO- d_6)

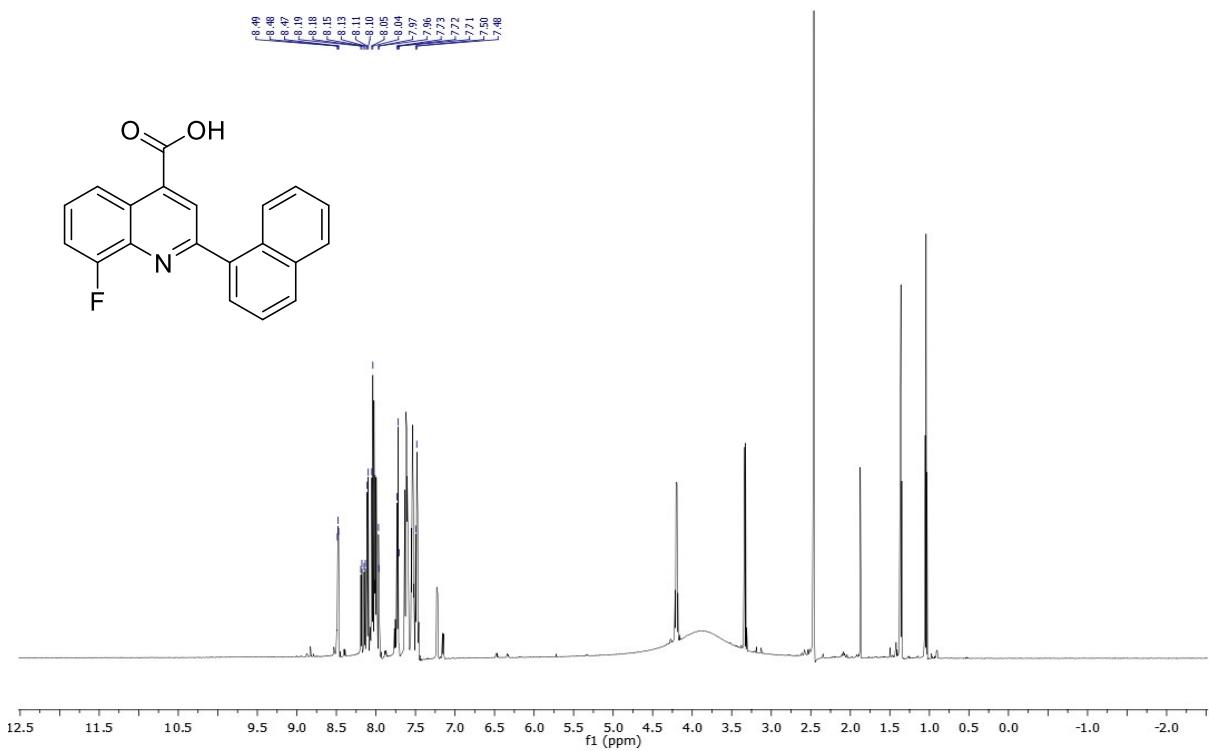


Figure S27. 600 MHz ^1H NMR spectrum of **6p** (DMSO- d_6)

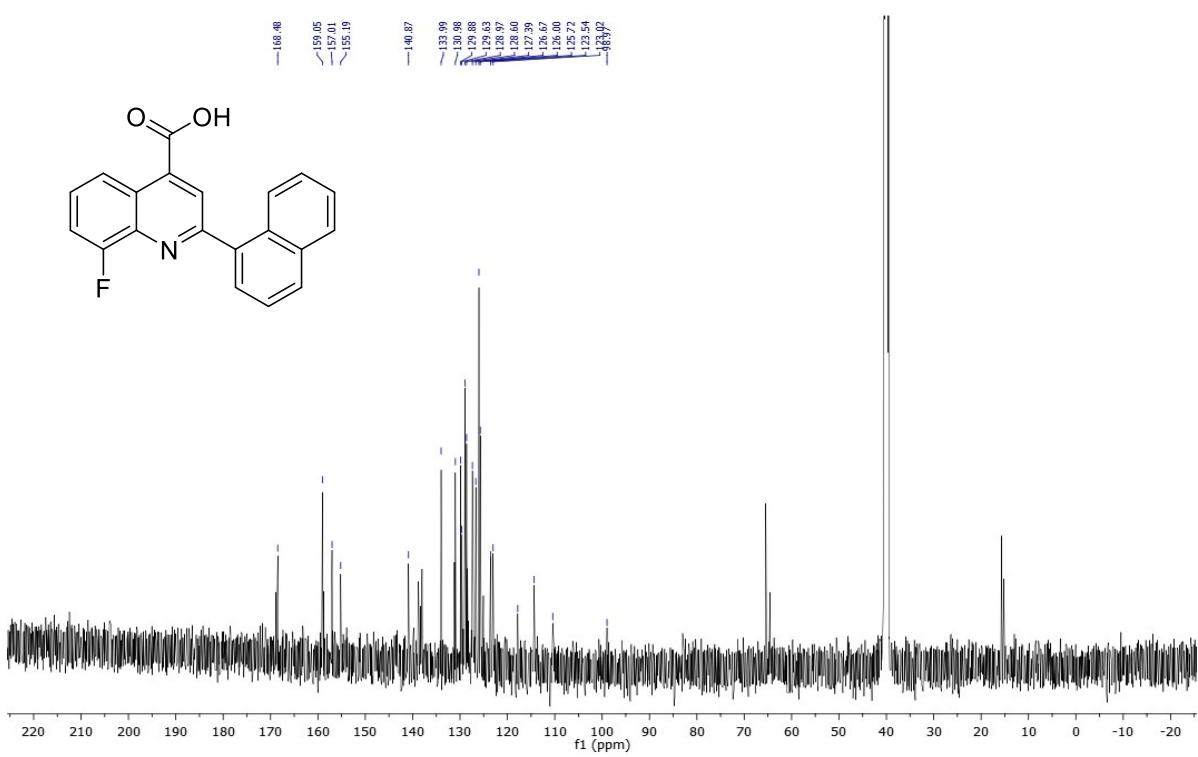


Figure S28. 151 MHz ^{13}C NMR spectrum of **6p** (DMSO-d₆)

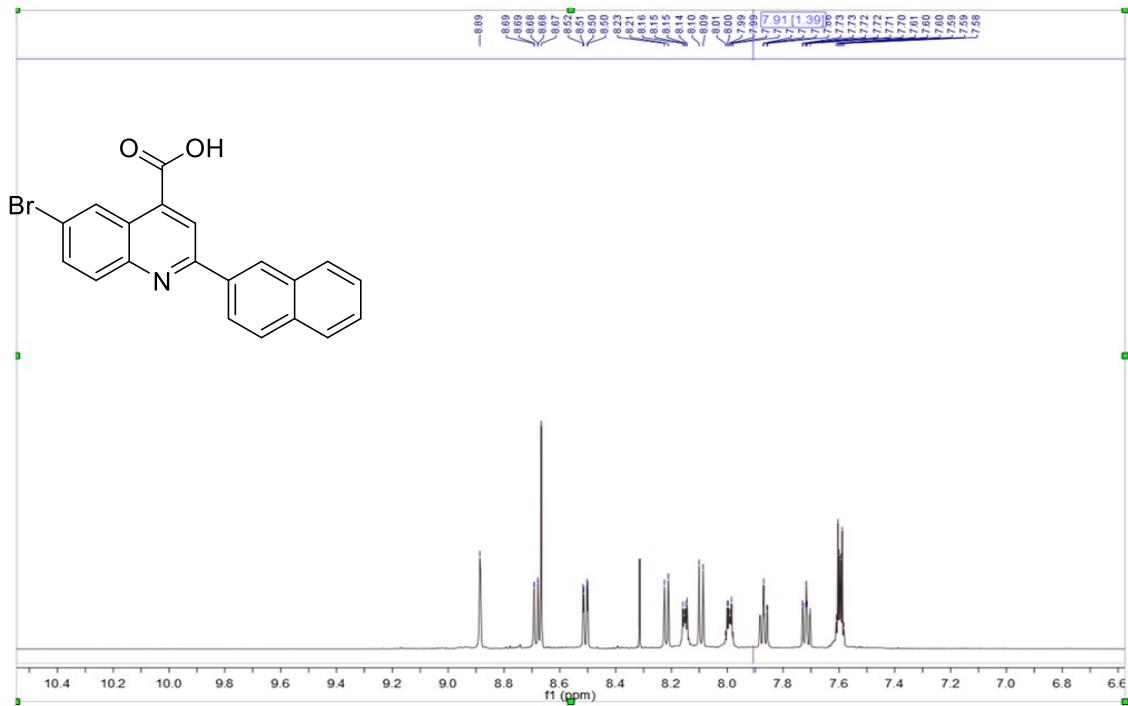


Figure S29. 600 MHz ^1H NMR spectrum of **6q** ($\text{DMSO}-d_6$)

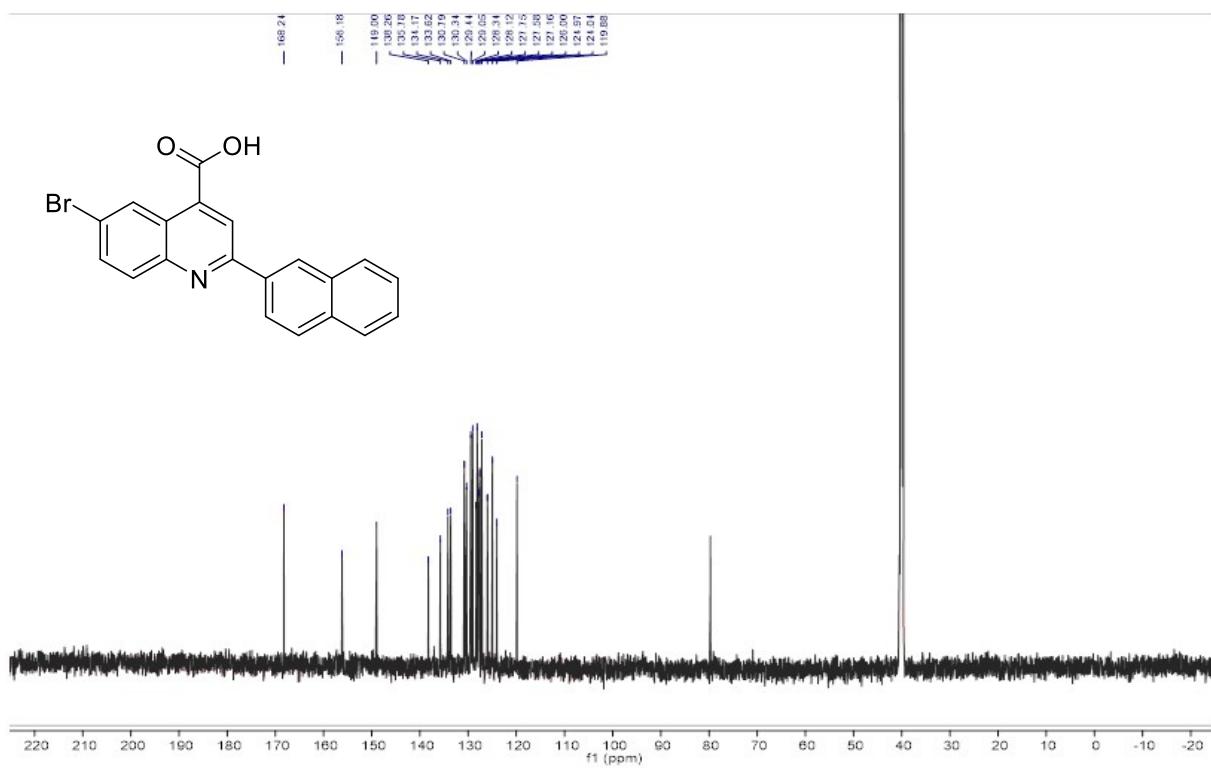
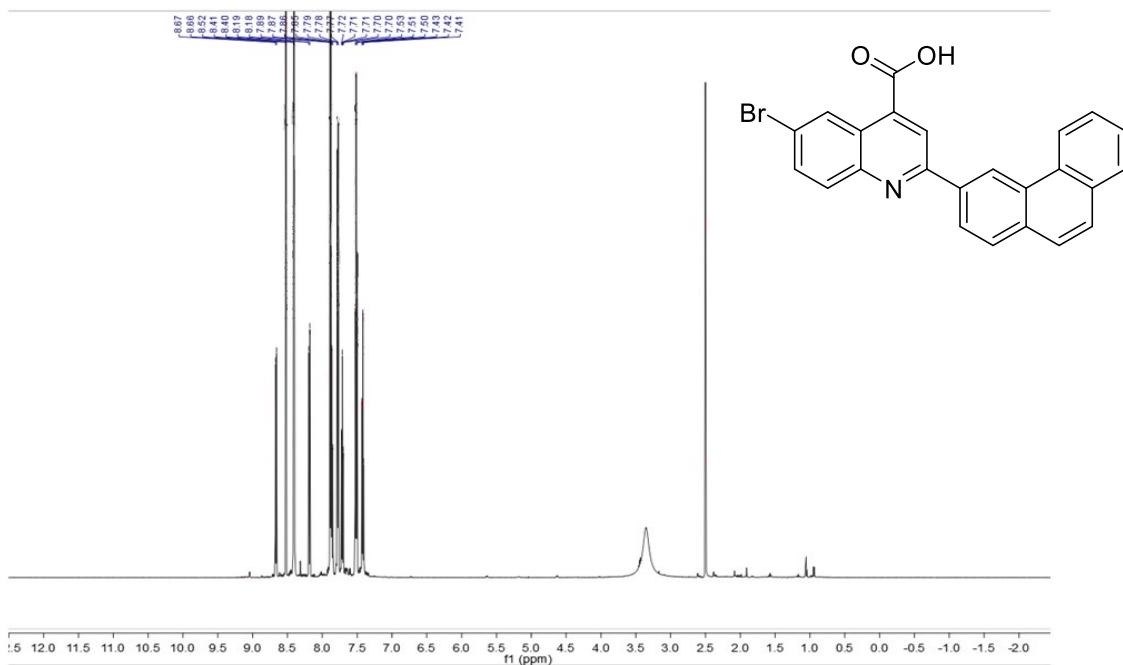


Figure S30. 151 MHz ^{13}C NMR spectrum of **6q** ($\text{DMSO}-d_6$)



S31. 600 MHz ^1H NMR spectrum of **6r** (DMSO- d_6)

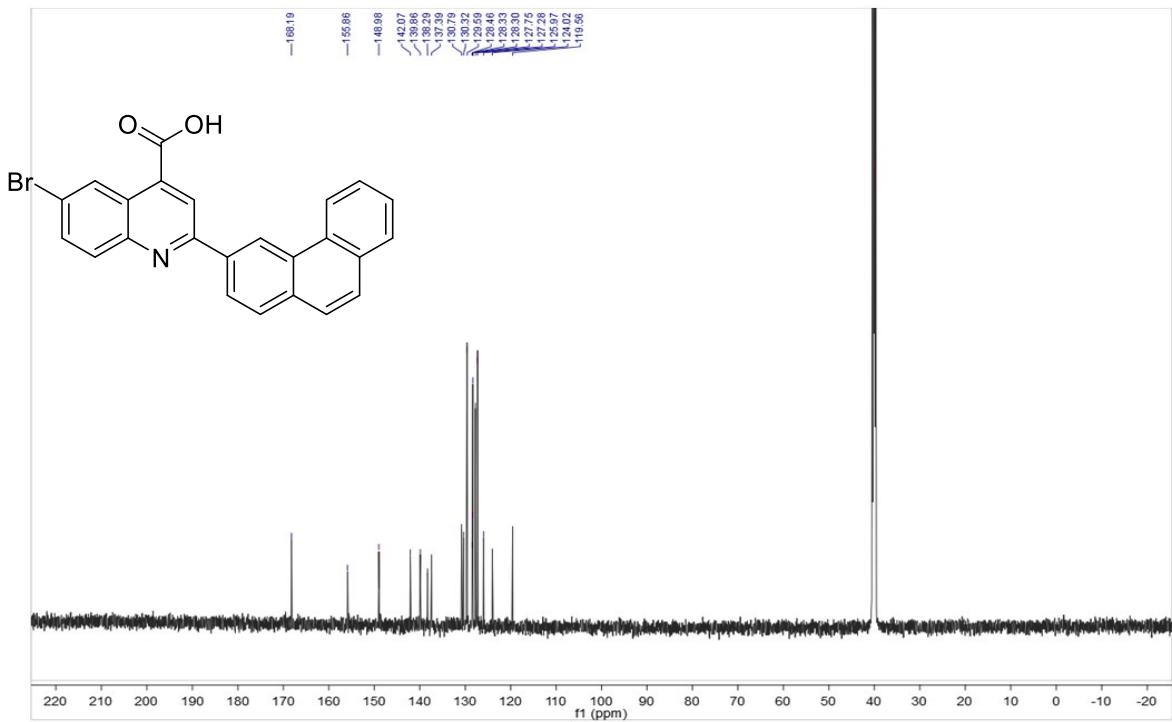


Figure S32. 151 MHz ^{13}C NMR spectrum of **6r** (DMSO- d_6)

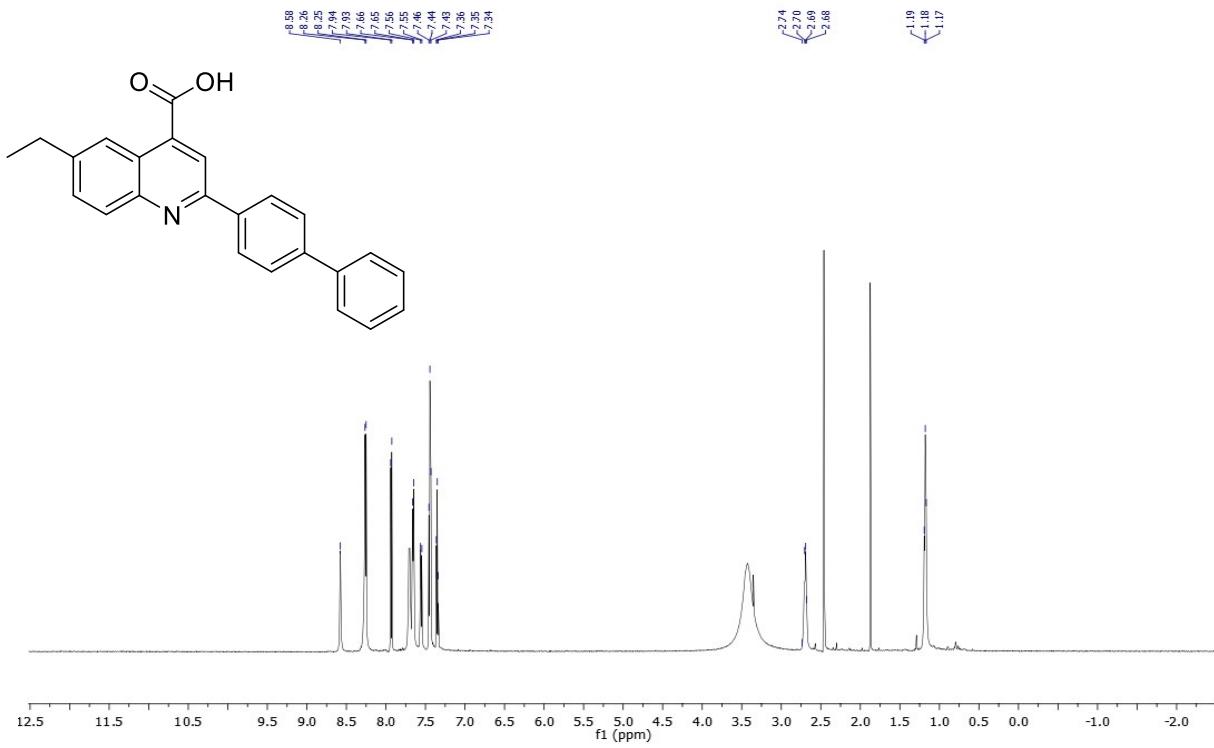


Figure S33. 600 MHz ¹H NMR spectrum of **7b** (DMSO-*d*₆)

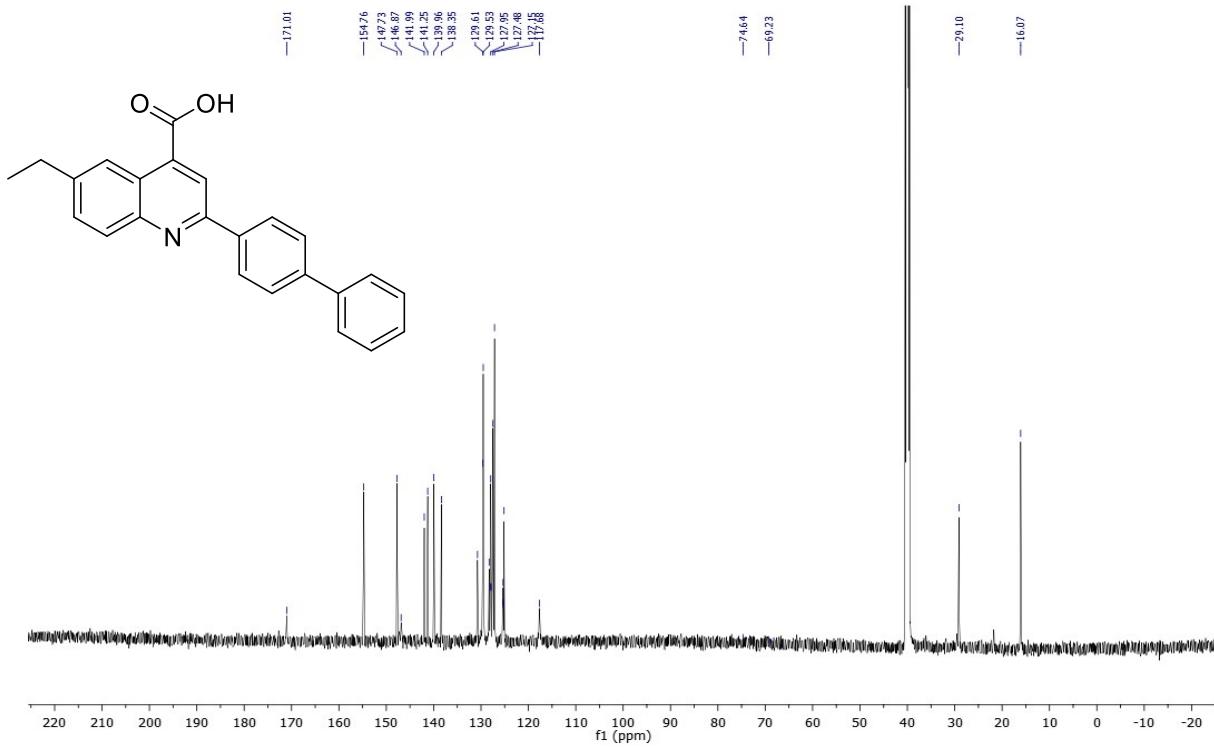


Figure S34. 151 MHz ¹³C NMR spectrum of **7b** (DMSO-*d*₆)

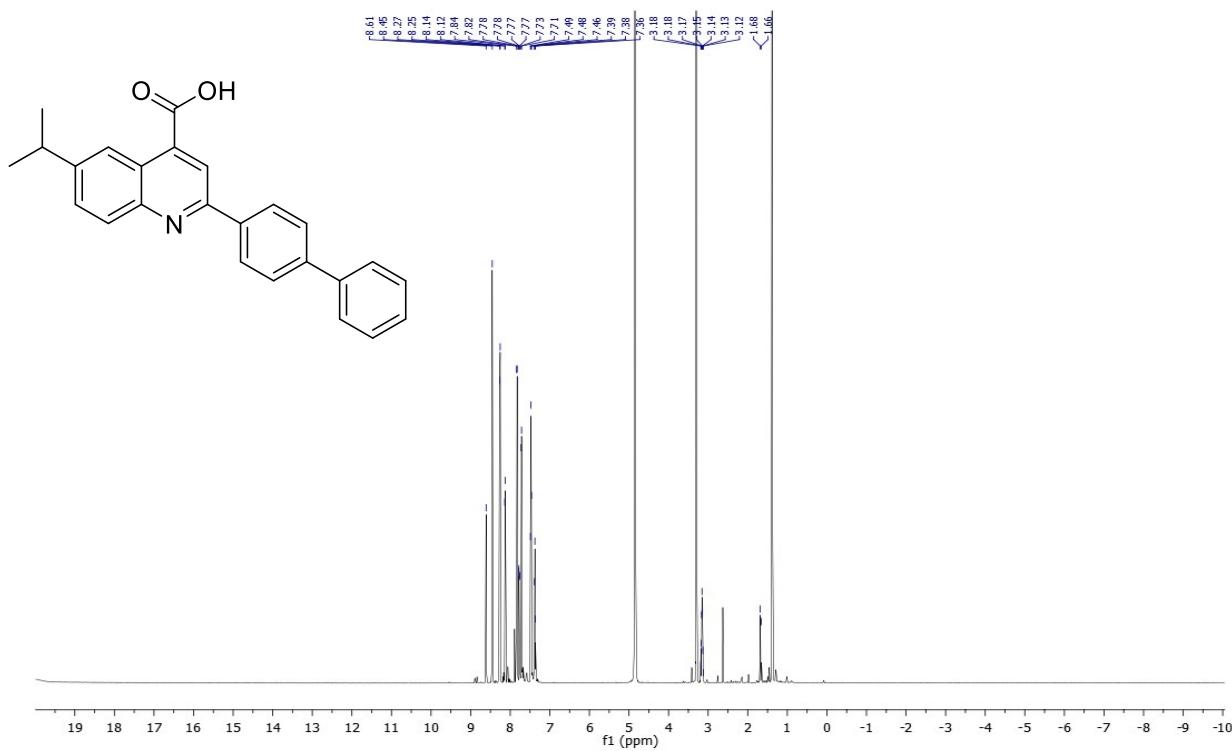


Figure S35. 600 MHz ^1H NMR spectrum of **7c** (MeOH- d_7)

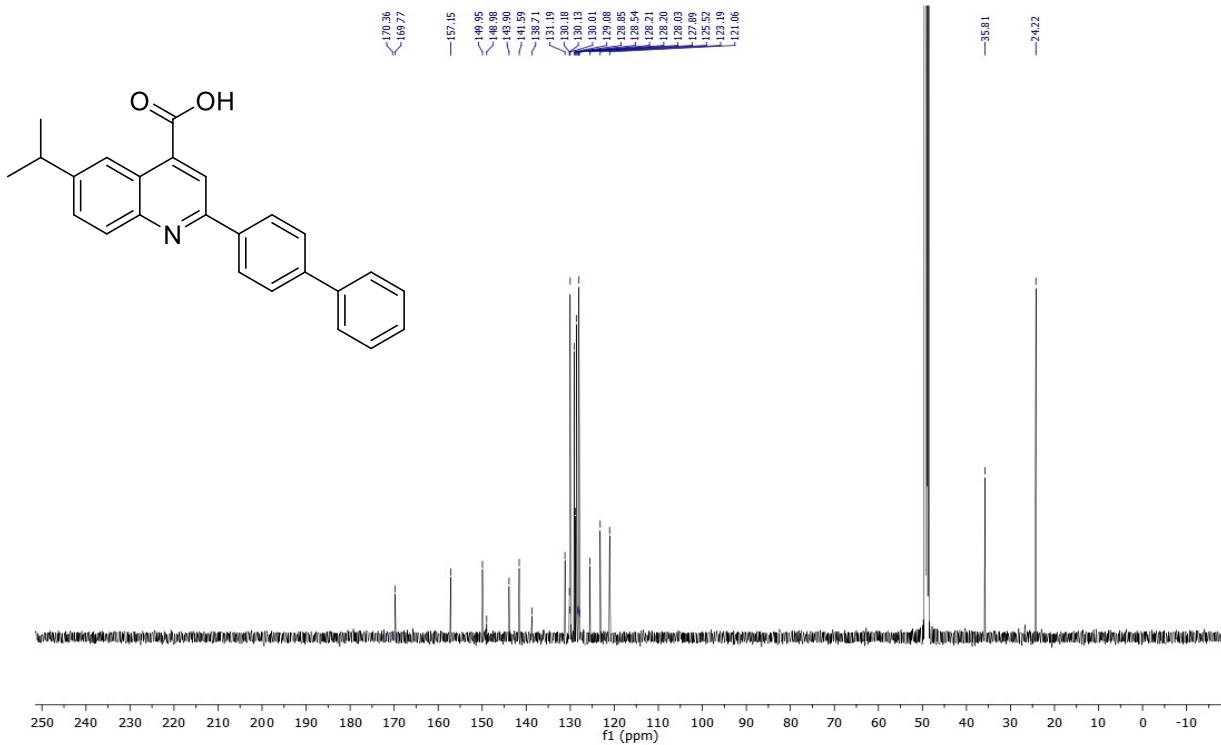


Figure S36. 151 MHz ^{13}C NMR spectrum of **7c** (MeOH- d_7)

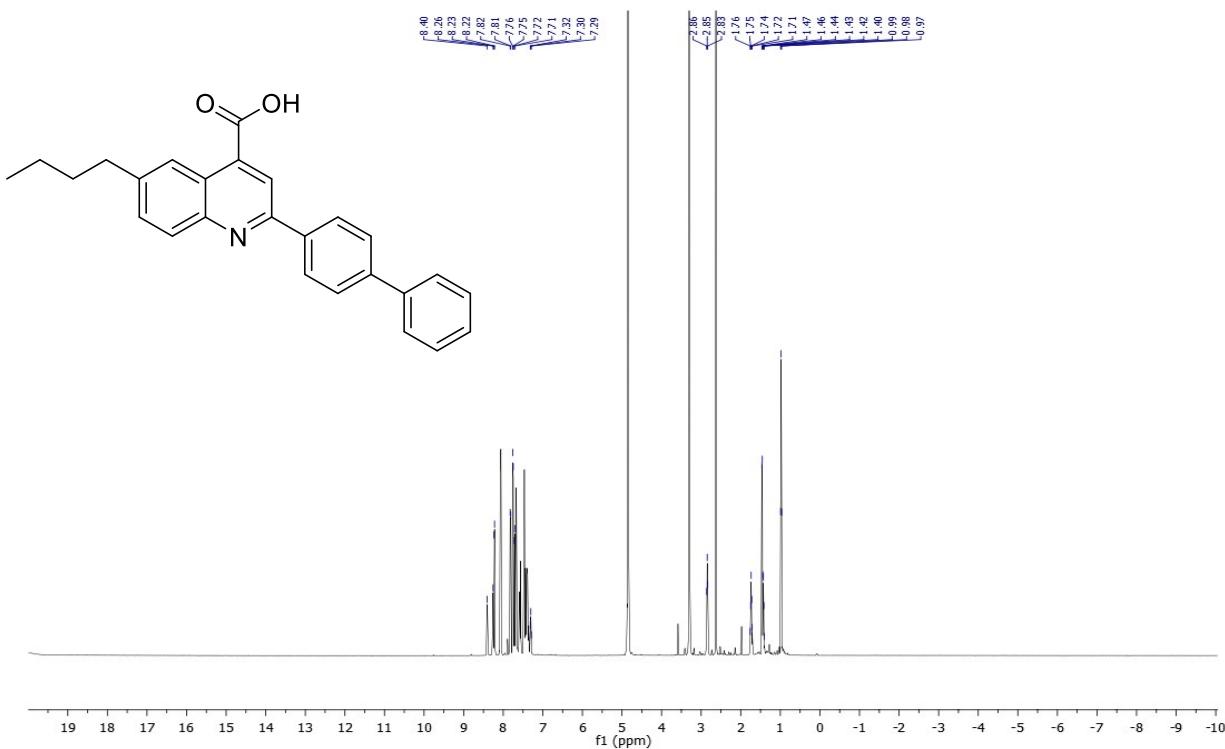


Figure S37. 600 MHz ¹H NMR spectrum of **7d** (MeOH-*d*₄)

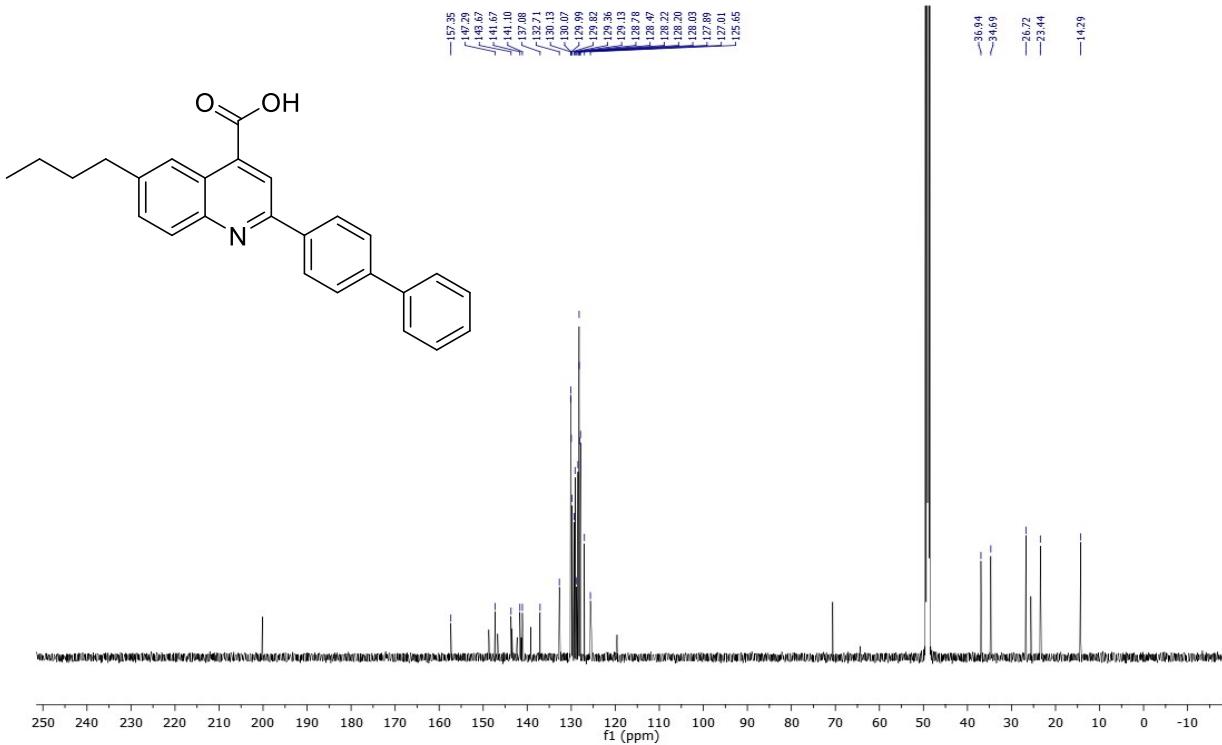


Figure S38. 151 MHz ¹³C NMR spectrum of **7d** (MeOH-*d*₄)

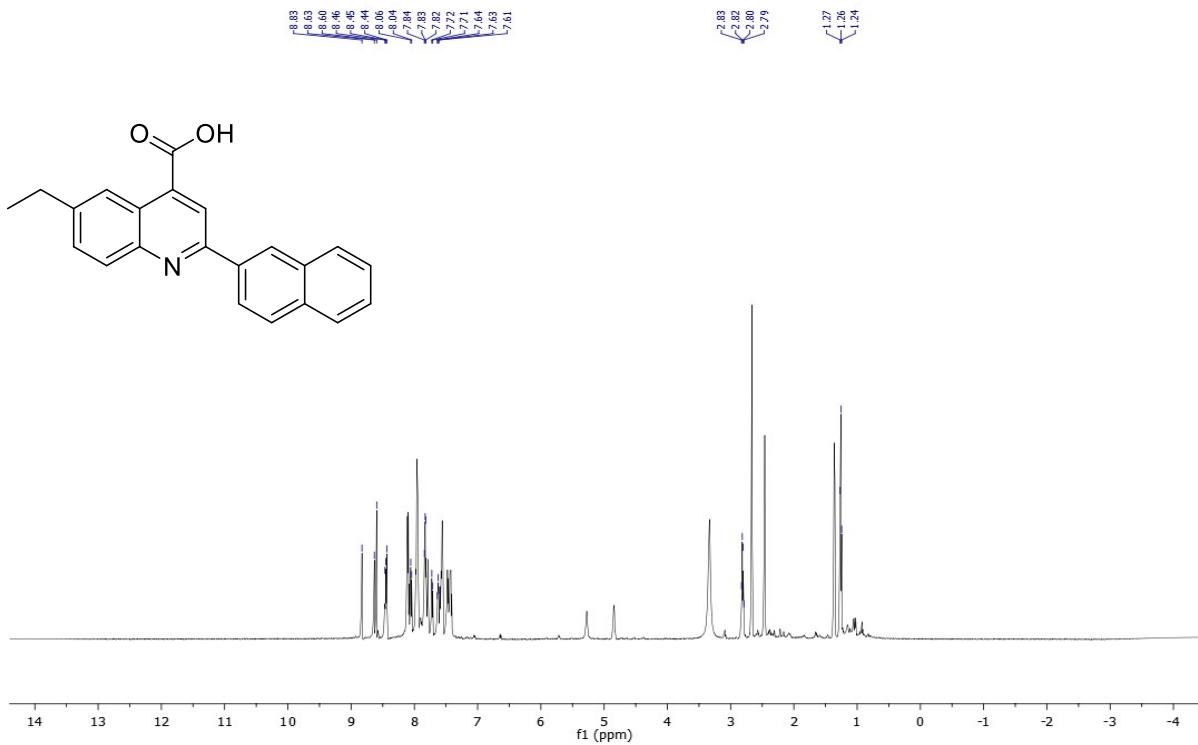


Figure S39. 600 MHz ^1H NMR spectrum of **7g** (DMSO- d_6)

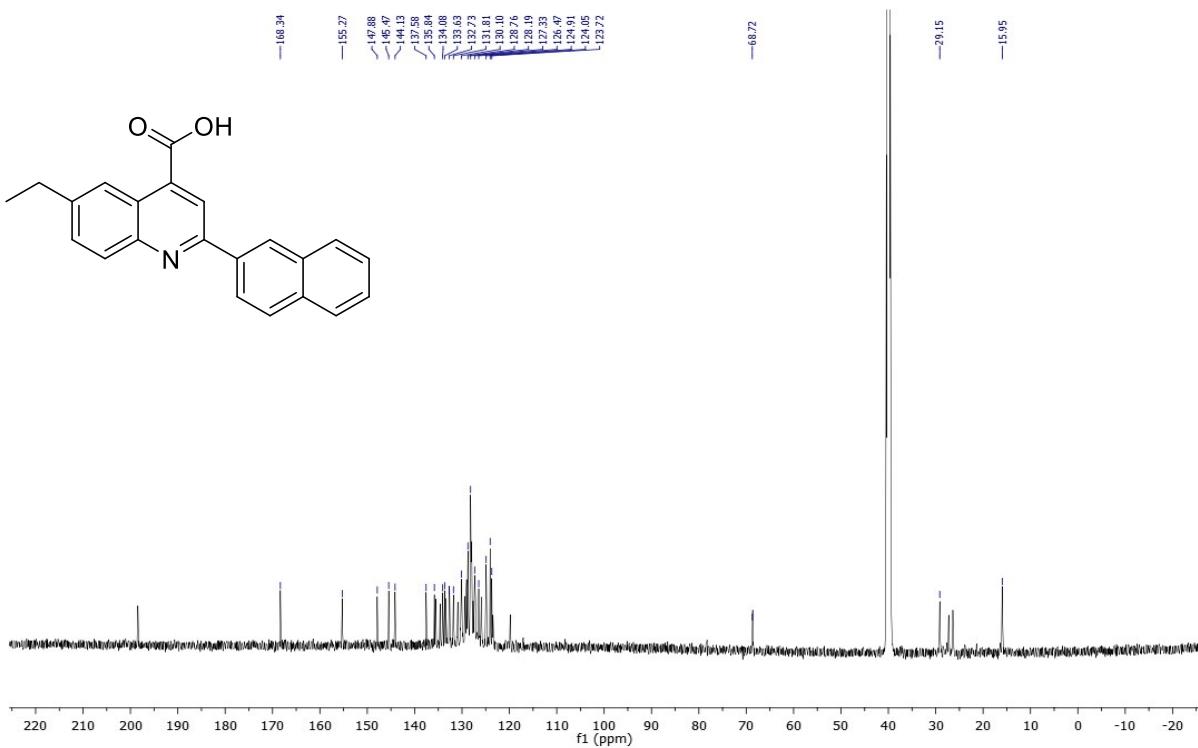


Figure S40. 151 MHz ^{13}C NMR spectrum of **7g** (DMSO- d_6)

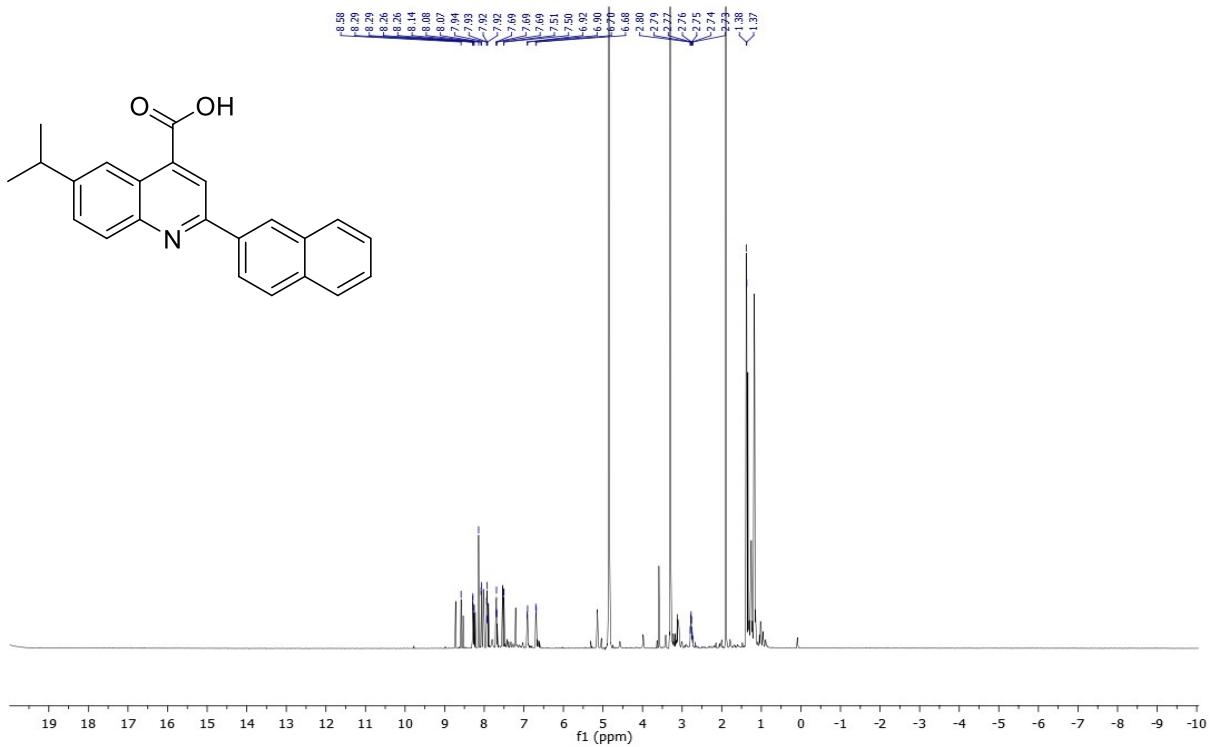


Figure S41. 600 MHz ^1H NMR spectrum of **7h** ($\text{MeOH}-d_4$)

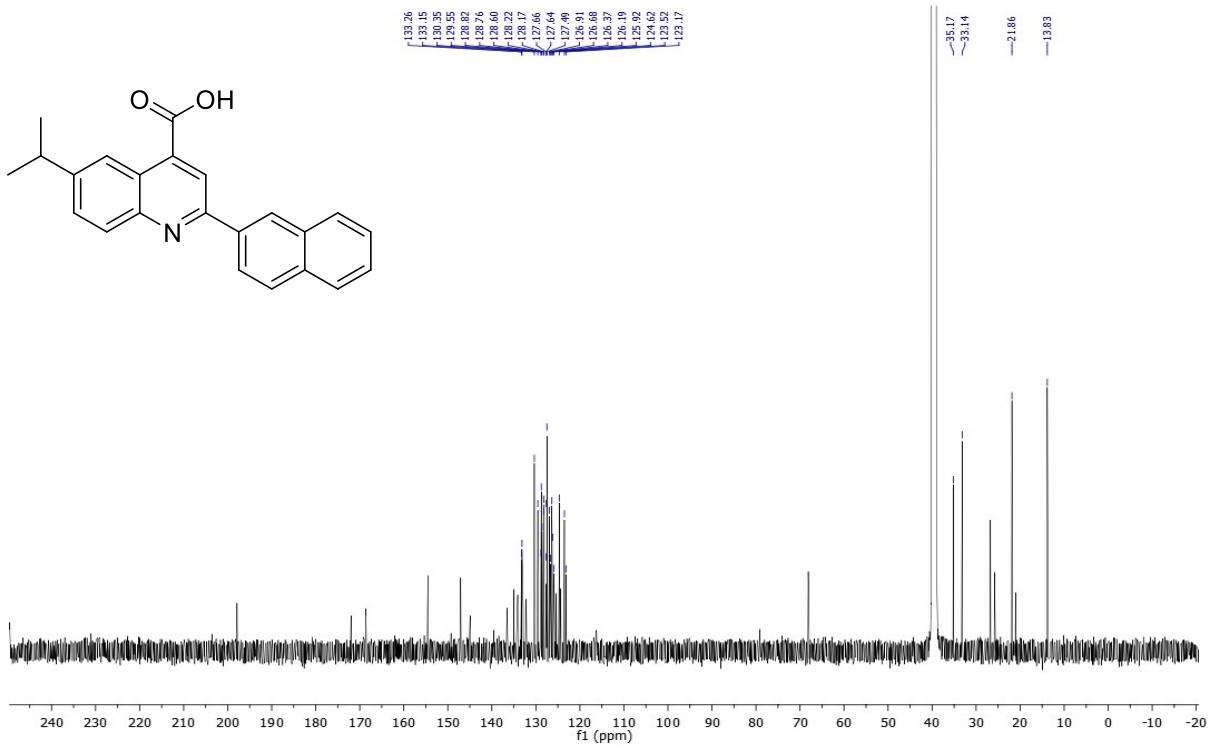


Figure S42. 151 MHz ^{13}C NMR spectrum of **7h** (MeOH- d_4)

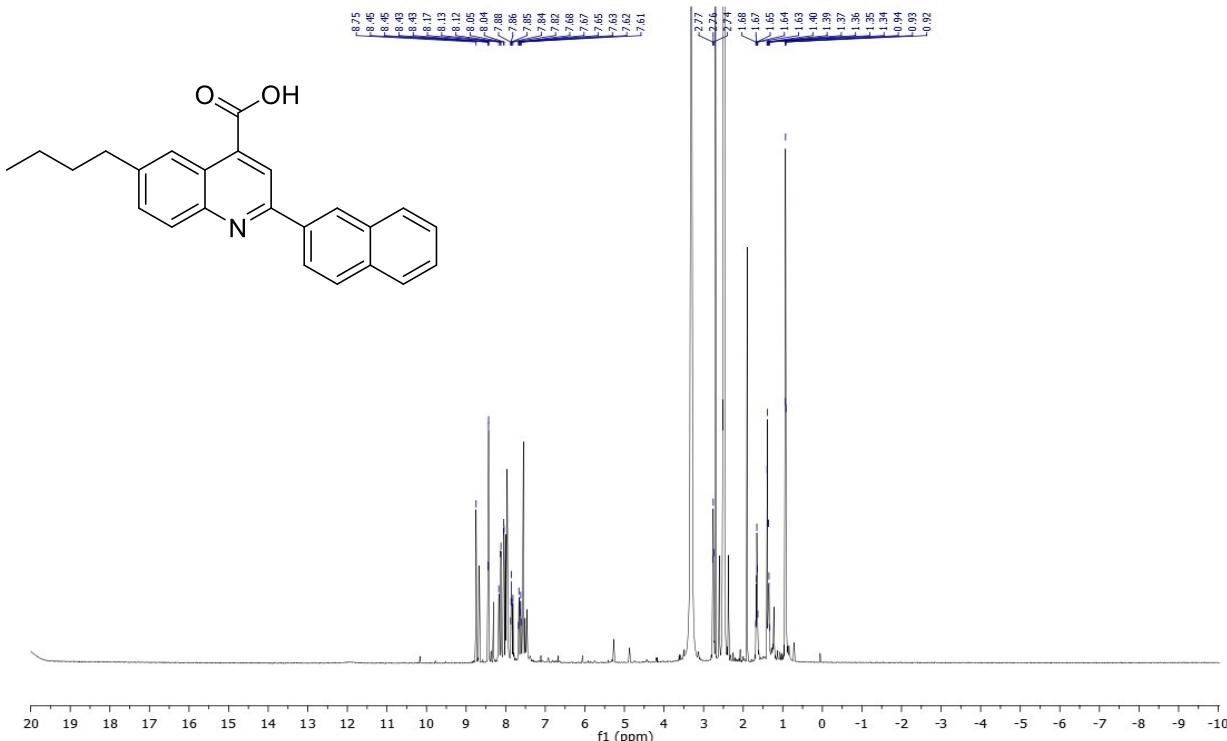


Figure S43. 600 MHz ^1H NMR spectrum of **7i** (DMSO-d₆)

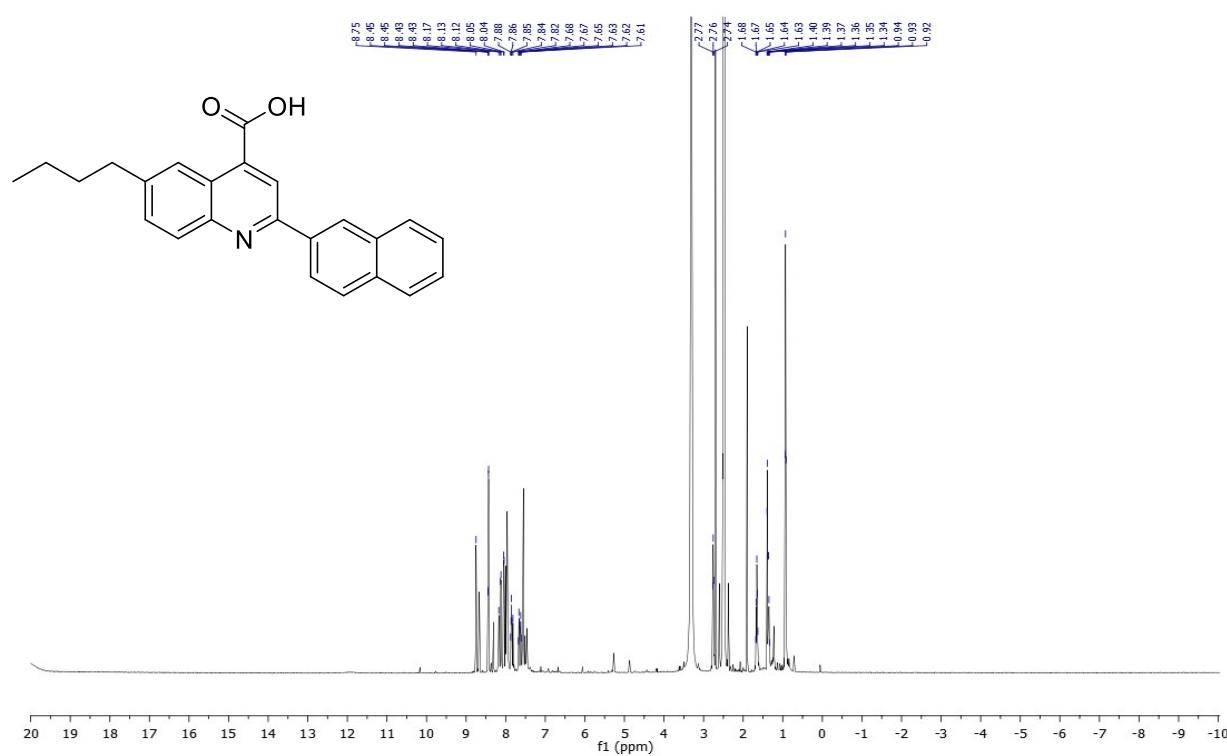


Figure S44. 151 MHz ^{13}C NMR spectrum of **7i** (DMSO- d_6)

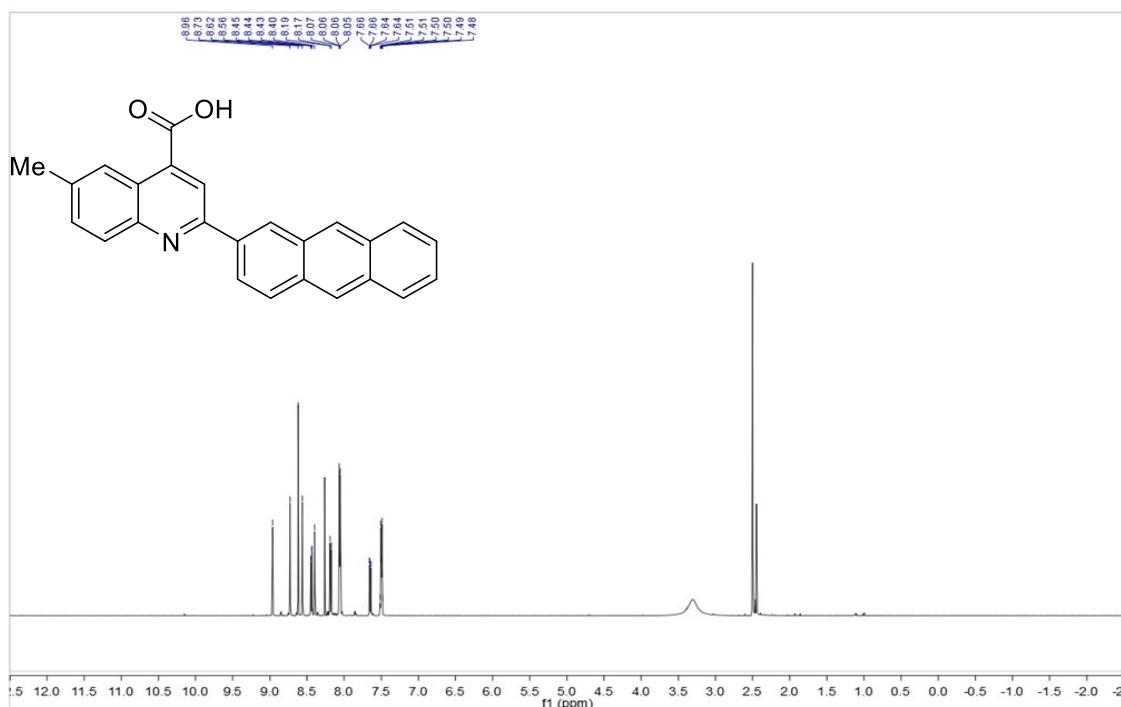


Figure S45. 600 MHz ^1H NMR spectrum of **7j** (DMSO- d_6)

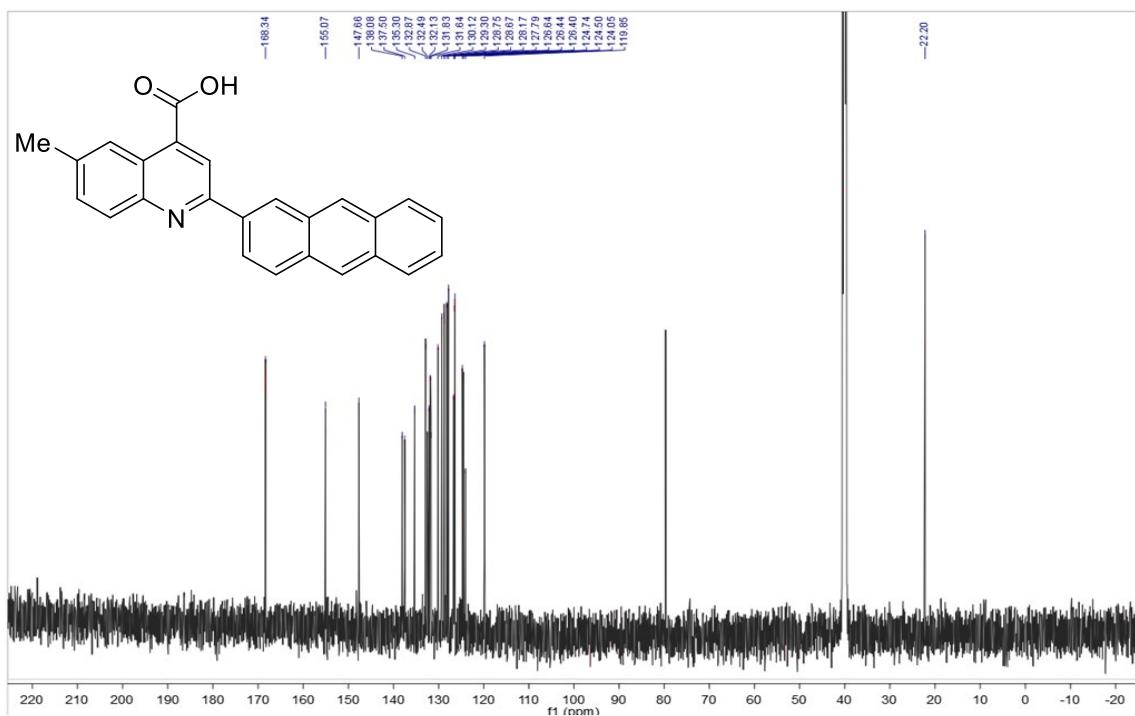


Figure S46. 151 MHz ^{13}C NMR spectrum of **7j** (DMSO- d_6)

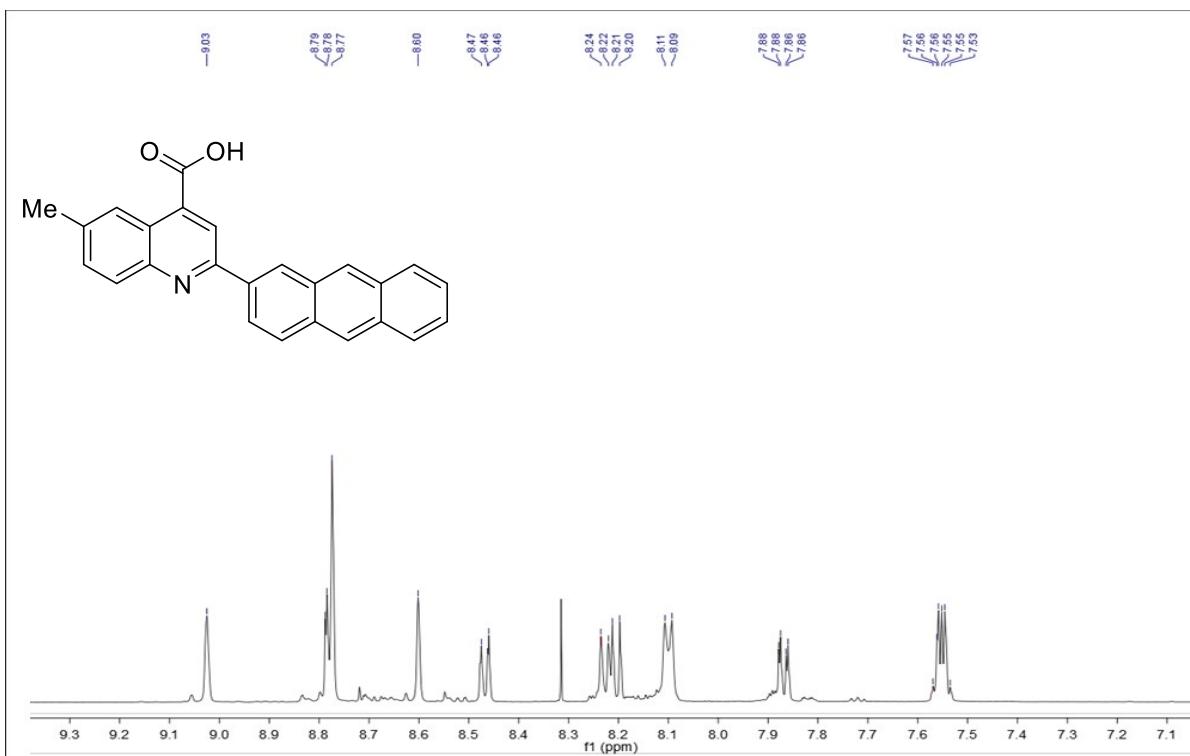


Figure S47. 600 MHz ^1H NMR spectrum of 7k (DMSO- d_6)

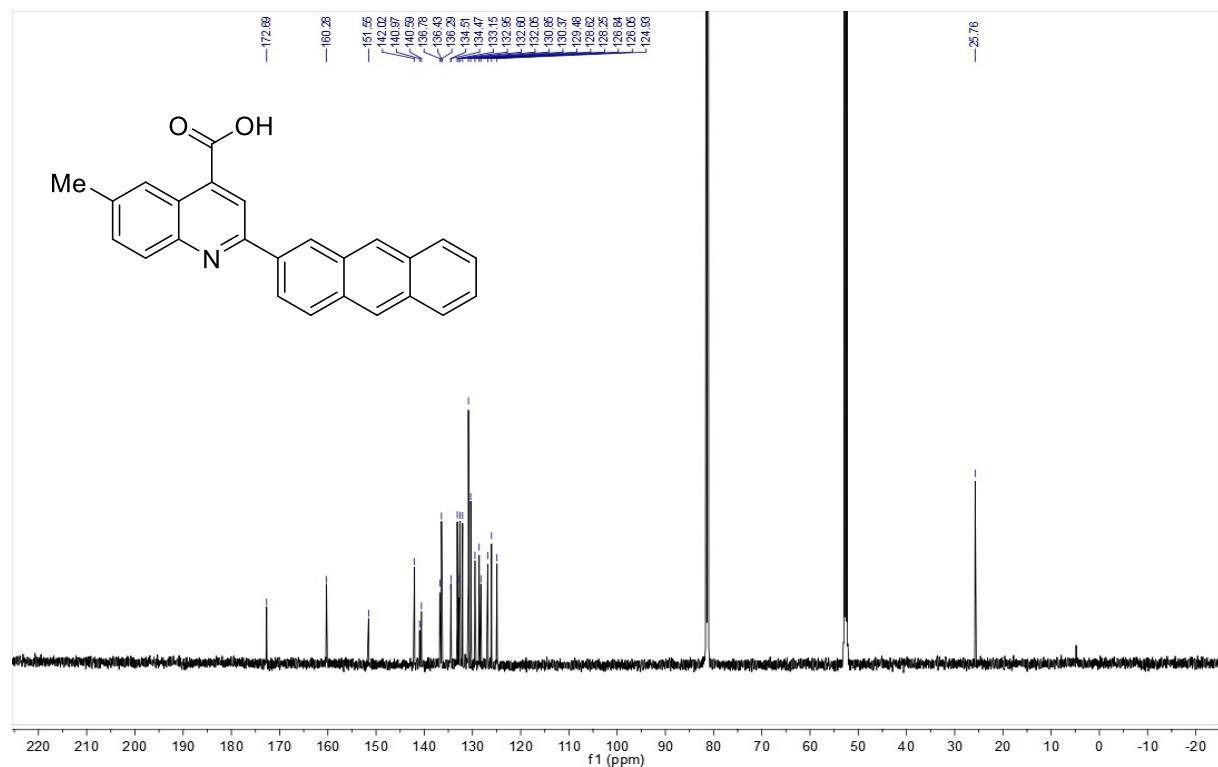


Figure S48. 151 MHz ^{13}C NMR spectrum of 7k (DMSO- d_6)

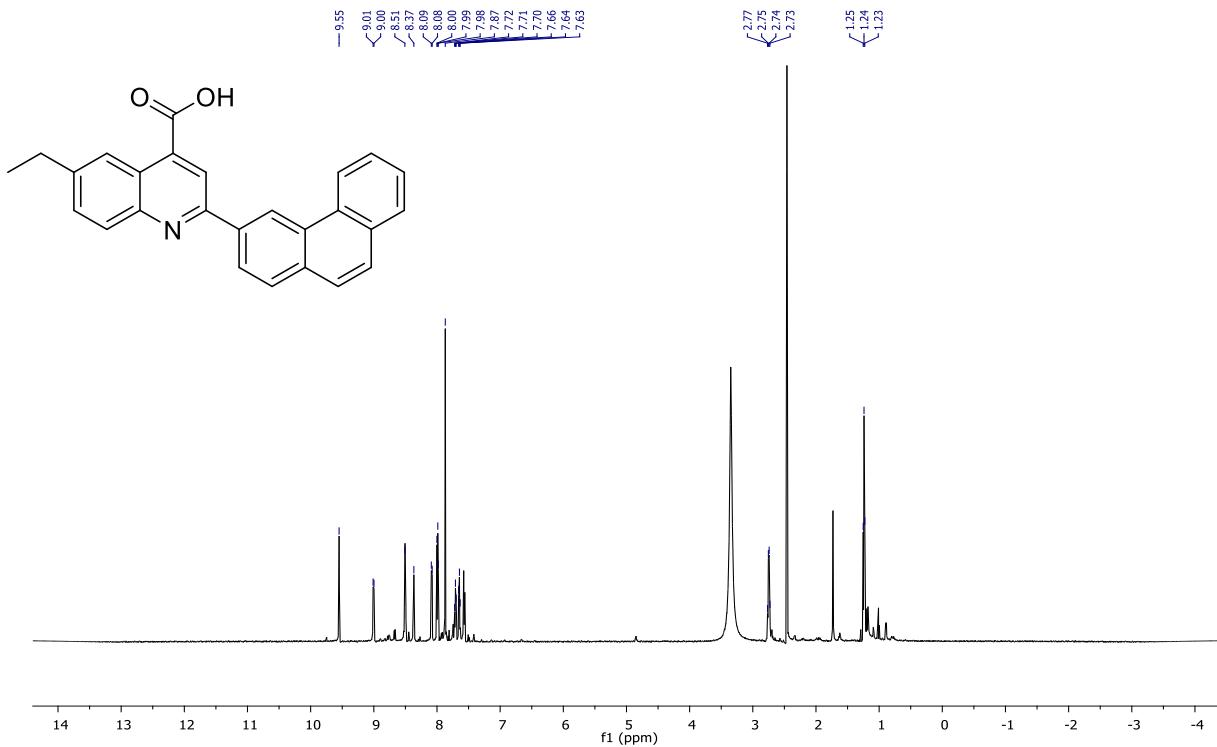


Figure S49. 600 MHz ^1H NMR spectrum of **7I** (DMSO- d_6)

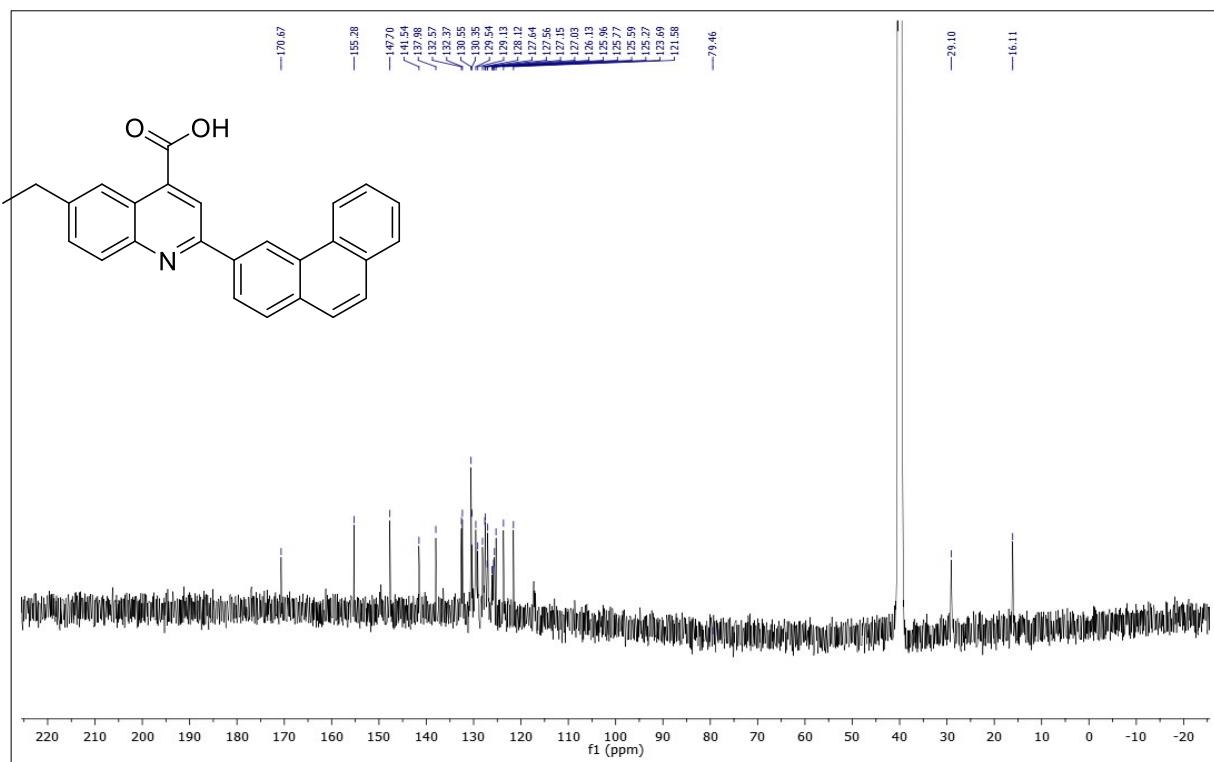
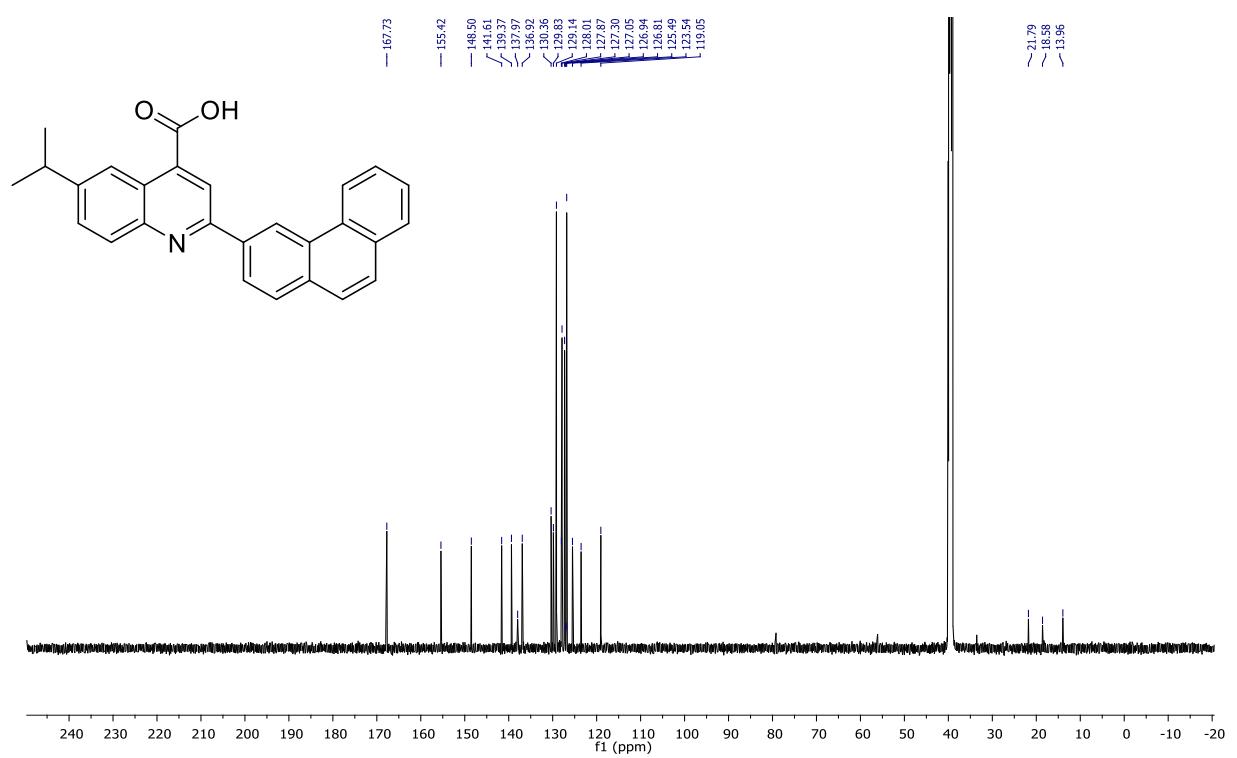
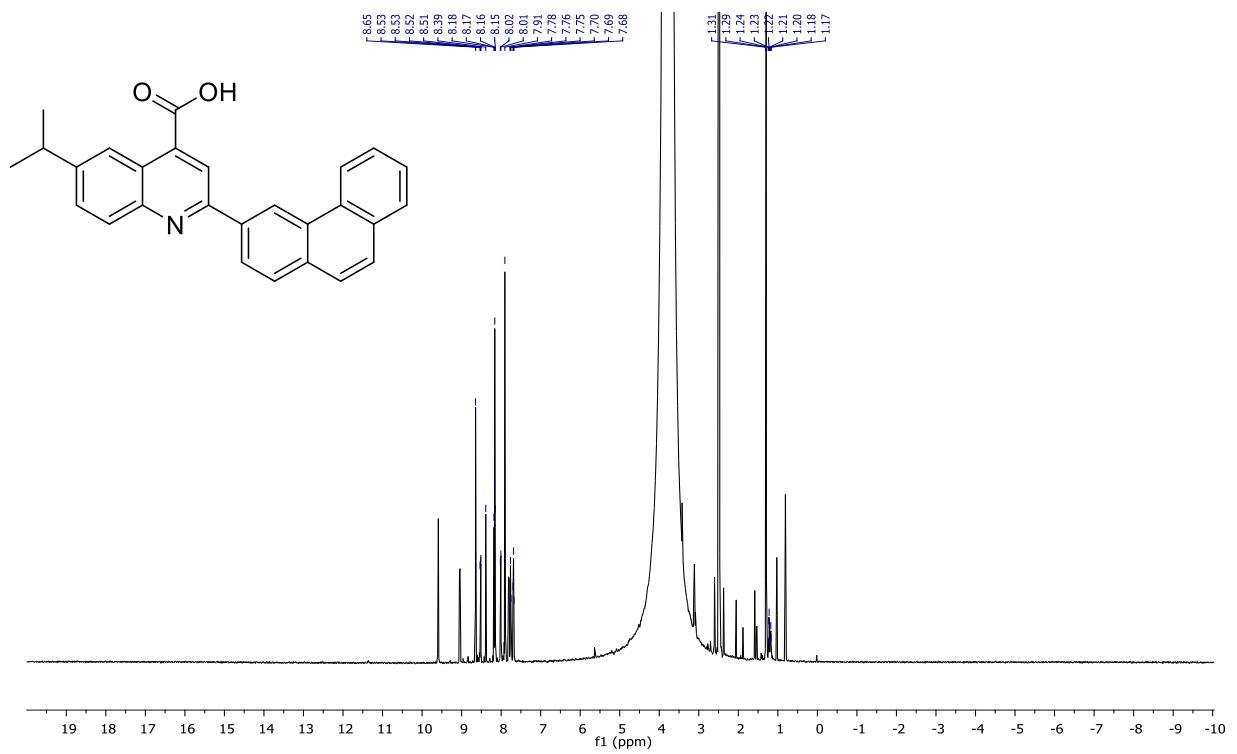


Figure S50. 151 MHz ^{13}C NMR spectrum of **7I** (DMSO- d_6)



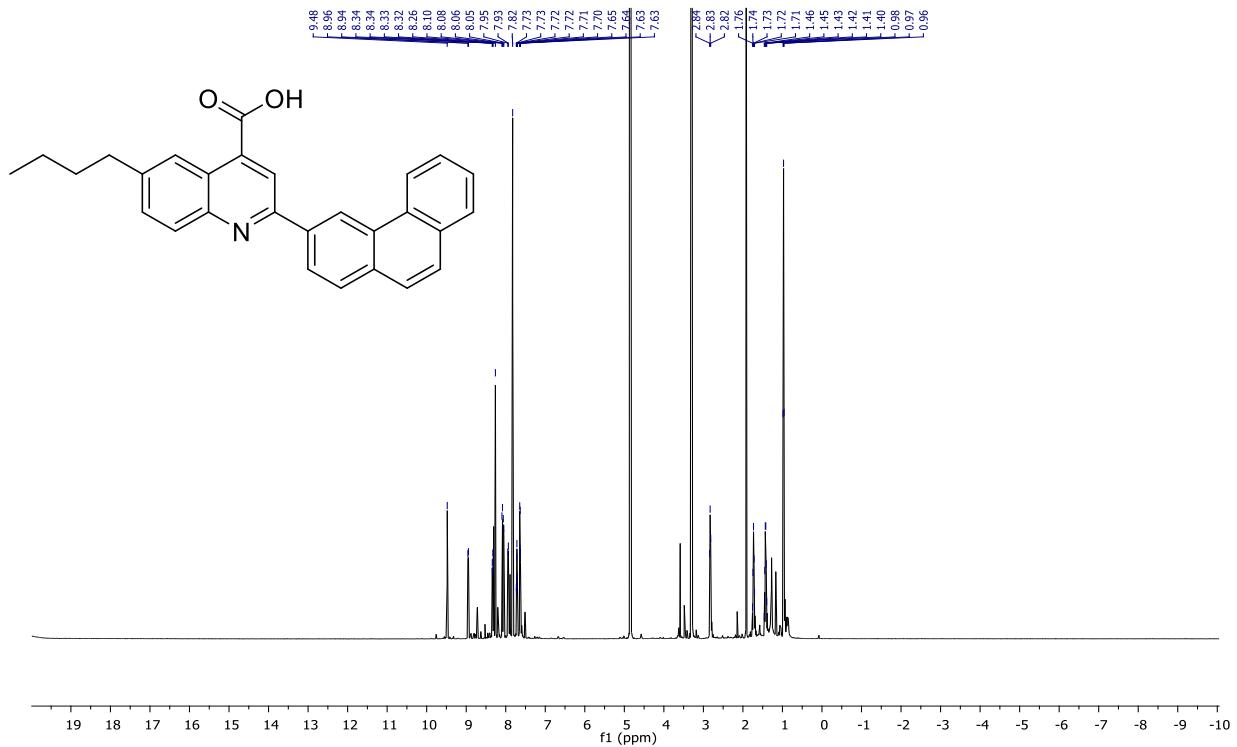


Figure S53. 600 MHz ^1H NMR spectrum of **7n** ($\text{MeOH-}d_4$)

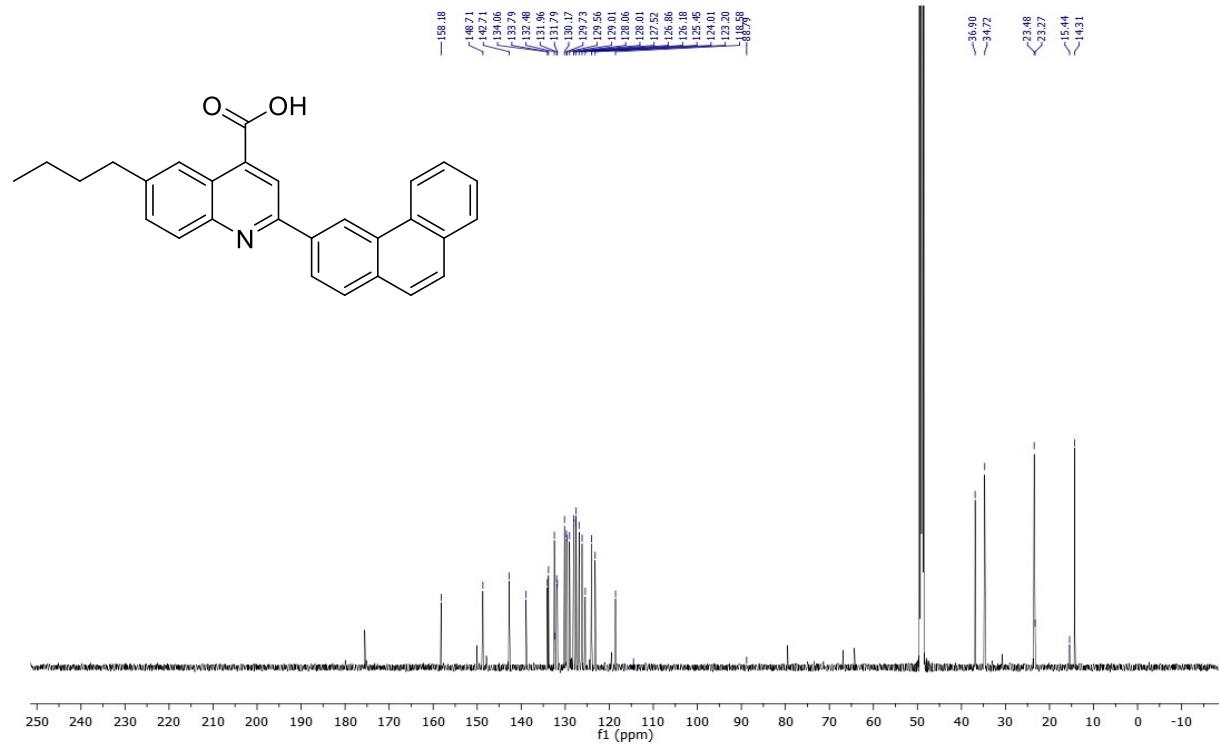


Figure S54. 151 MHz ^{13}C NMR spectrum of **7n** (MeOH- d_4)

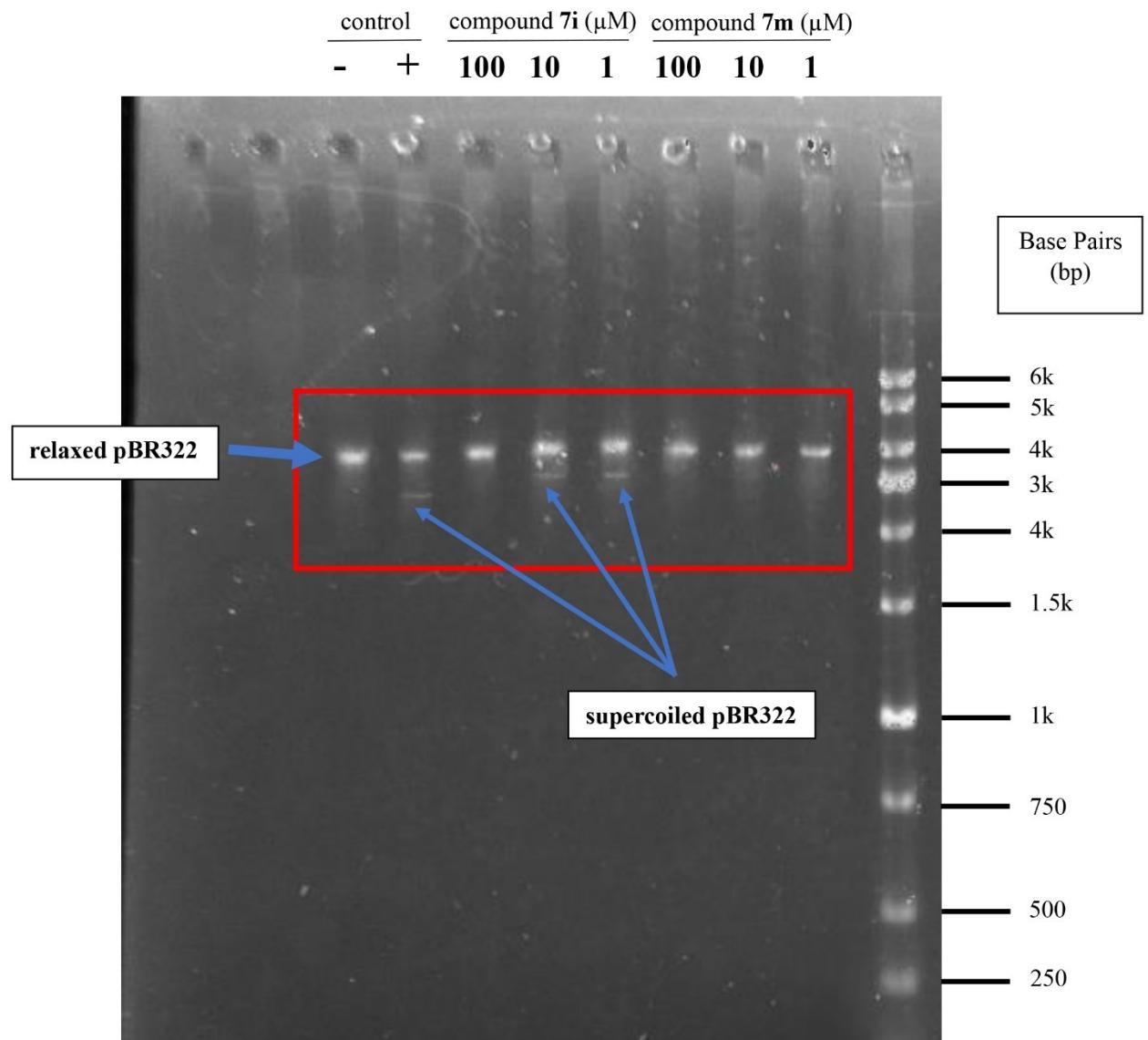


Figure S55. Agarose gel electrophoresis result showing inhibition of QCA **7i** and **7m** against *Mtb* DNA gyrase; (-) negative control without gyrase; (+) positive control with gyrase.