

*Supplementary Information*

# Synthesis of indole-coupled KYNA derivatives *via* C–N bond cleavage of Mannich bases

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Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-4-oxo-1,4-dihydroquinoline-2-carboxylate (7)

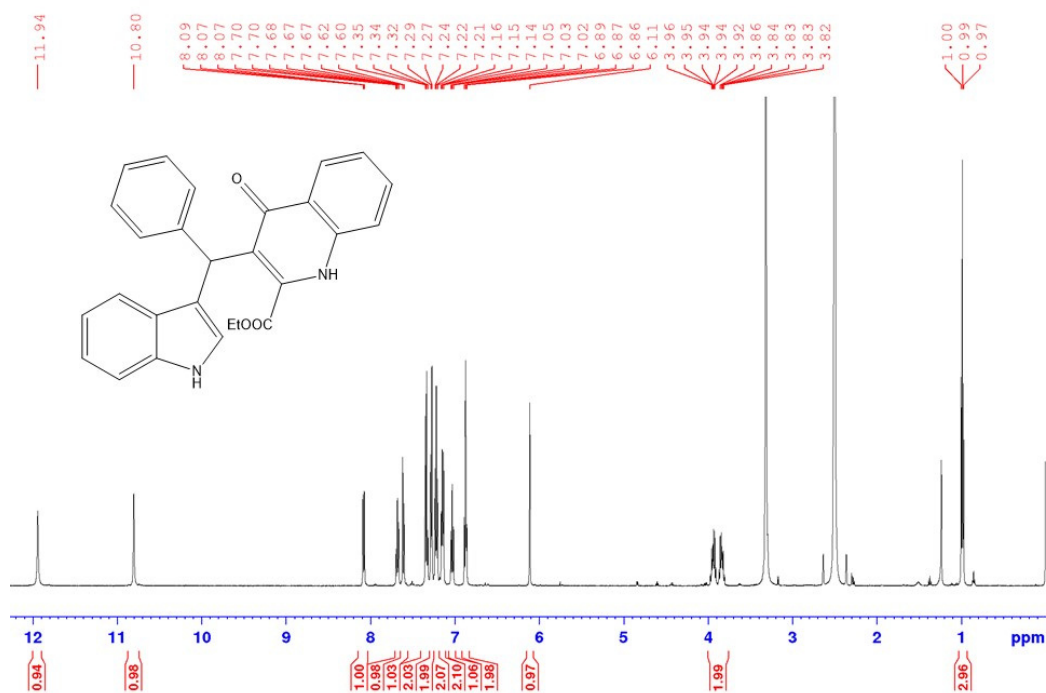


Figure S1. <sup>1</sup>H-NMR spectrum of 7

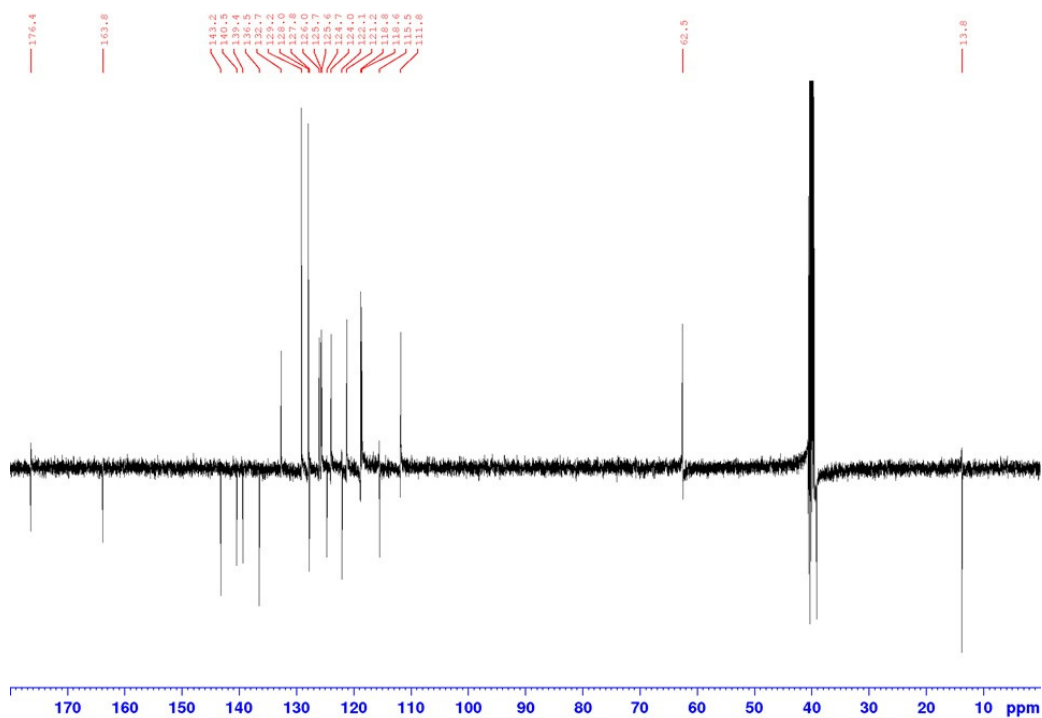


Figure S2. <sup>13</sup>C-NMR spectrum of 7

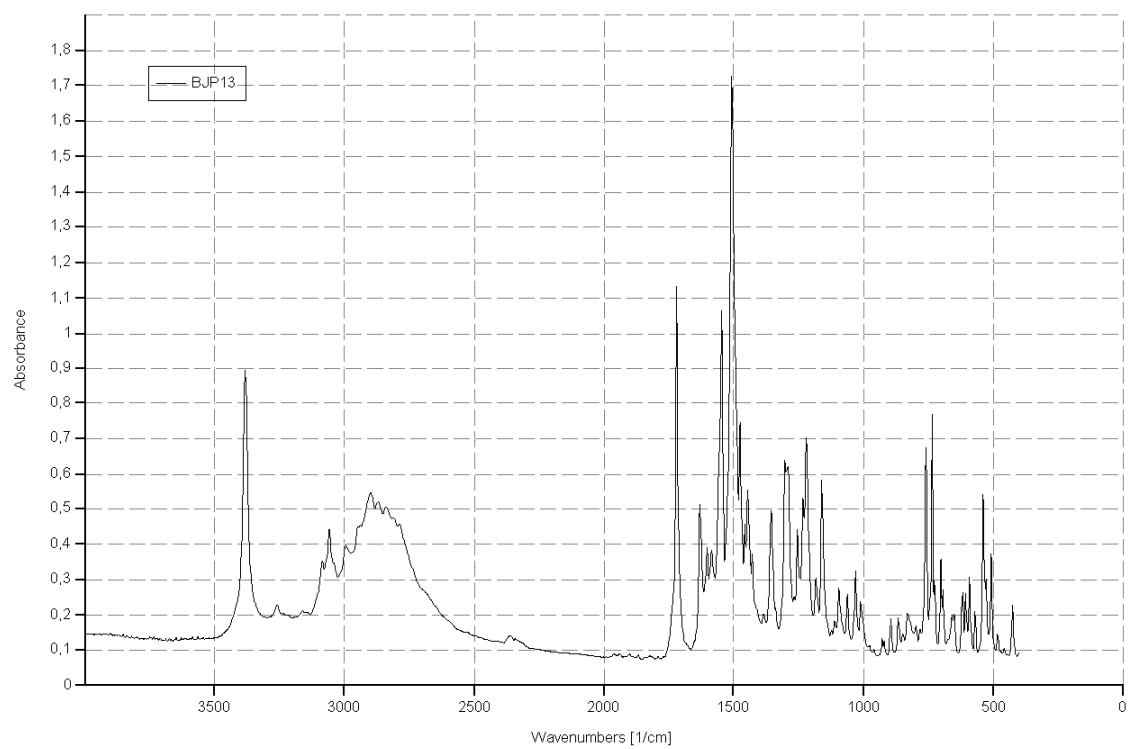


Figure S3. FTIR spectrum of 7

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-5-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20a**)

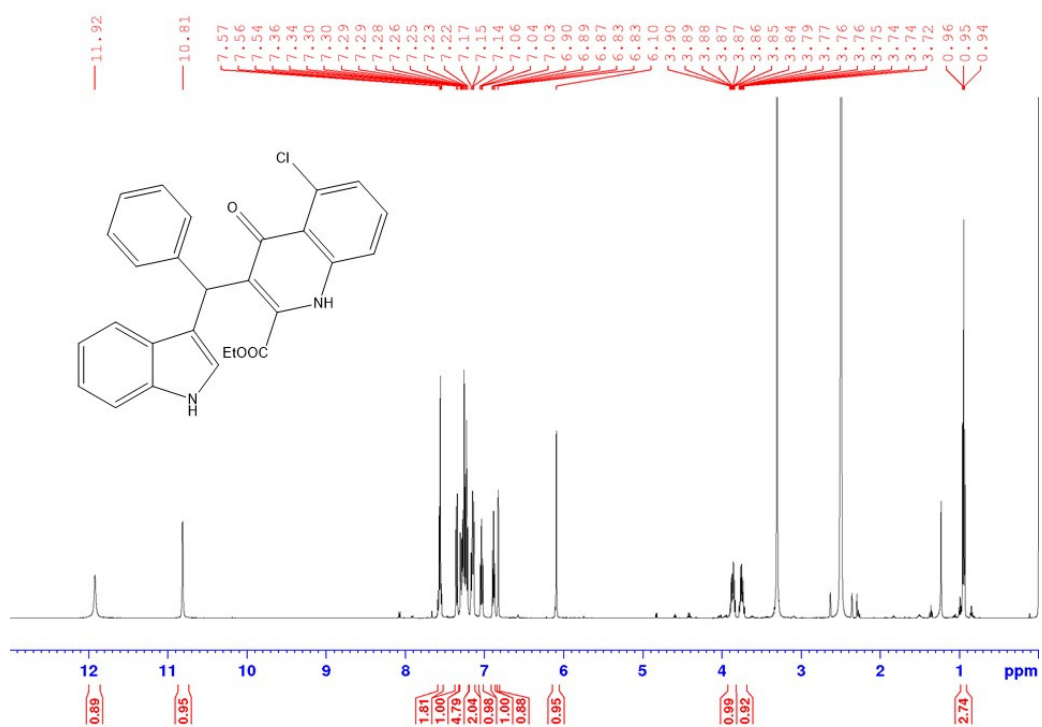


Figure S4. <sup>1</sup>H-NMR spectrum of **20a**

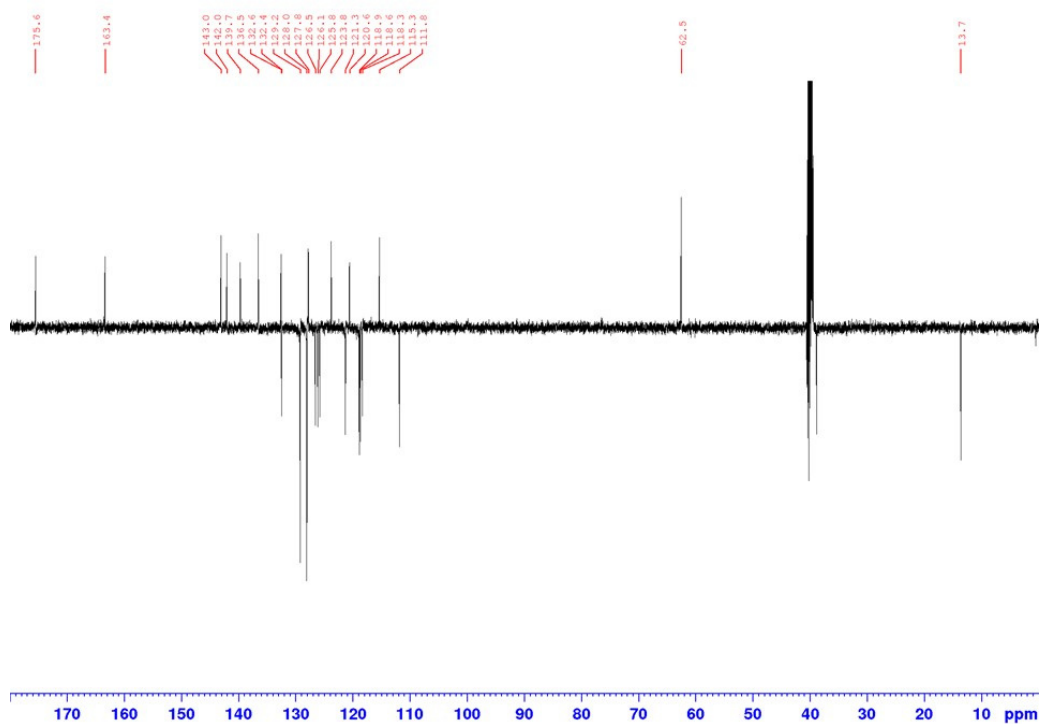


Figure S5. <sup>13</sup>C-NMR spectrum of **20a**

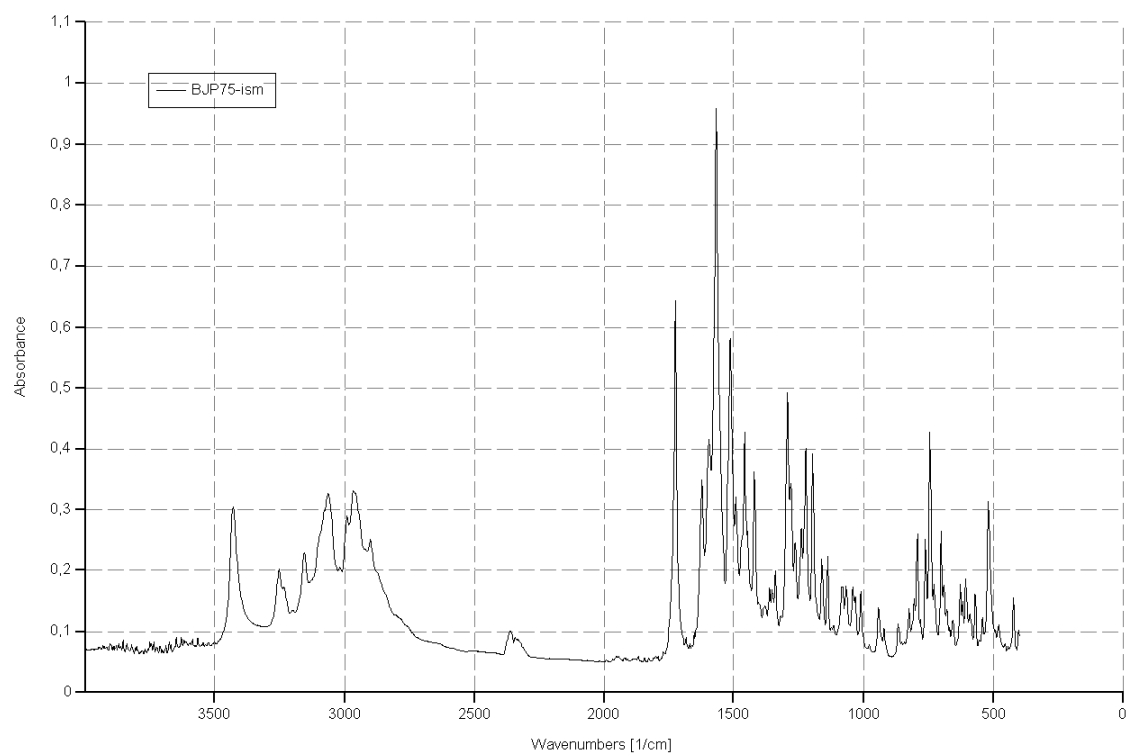


Figure S6. FTIR spectrum of **20a**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-6-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20b**)

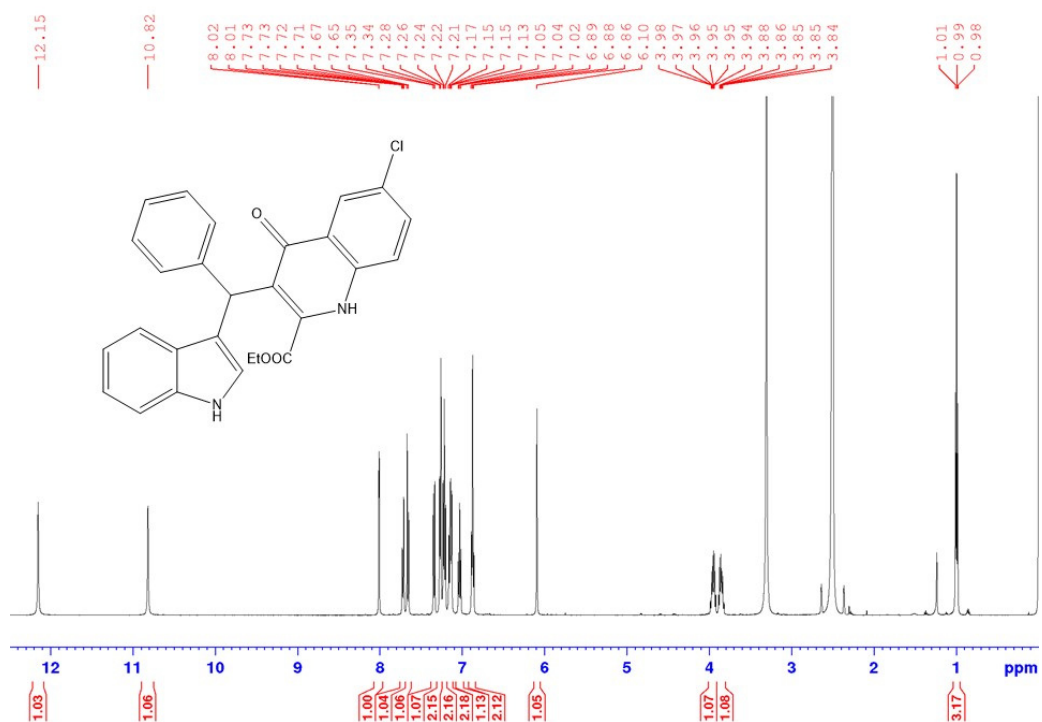


Figure S7. <sup>1</sup>H-NMR spectrum of **20b**

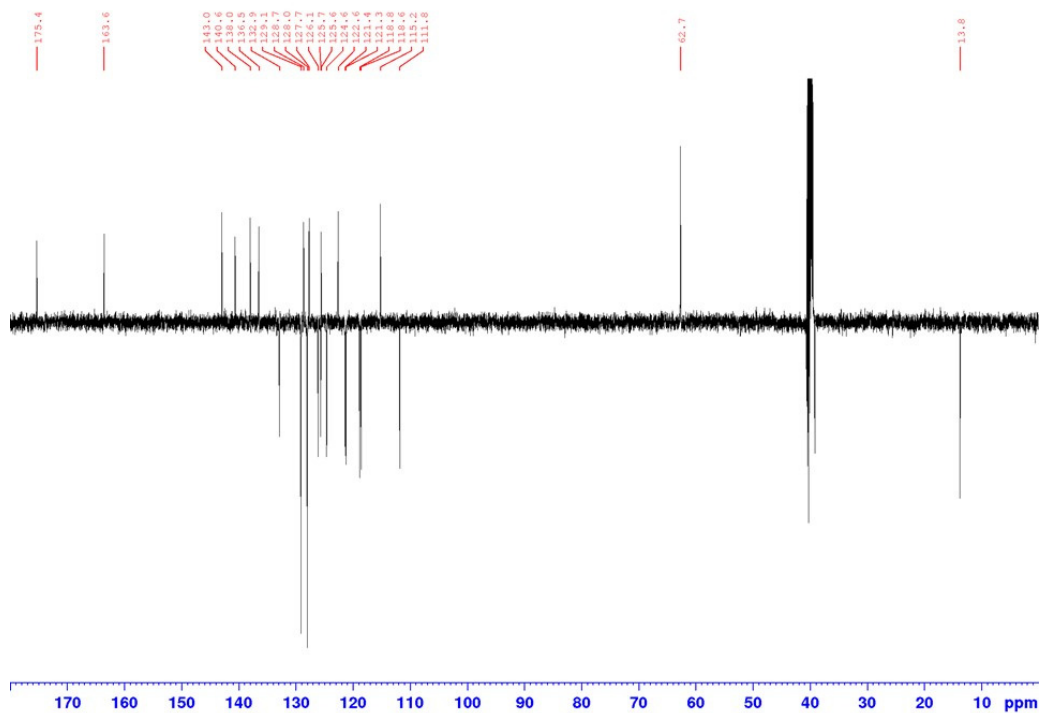


Figure S8. <sup>13</sup>C-NMR spectrum of **20b**

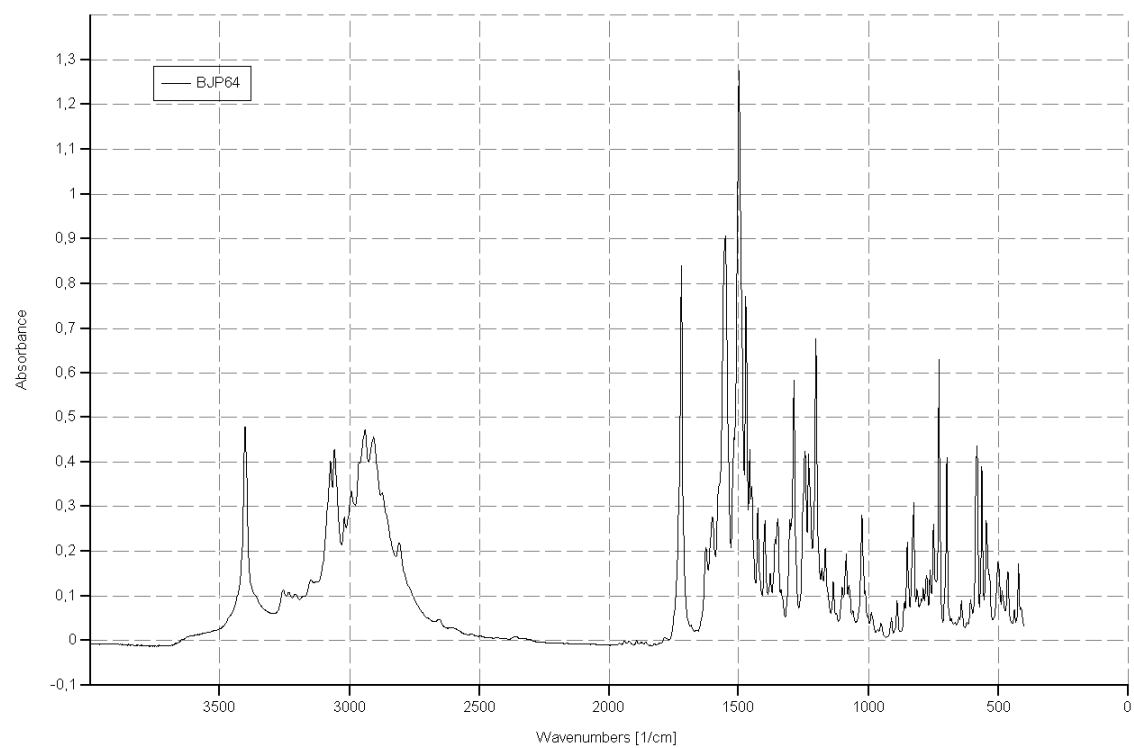


Figure S9. FTIR spectrum of **20b**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-7-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20c**)

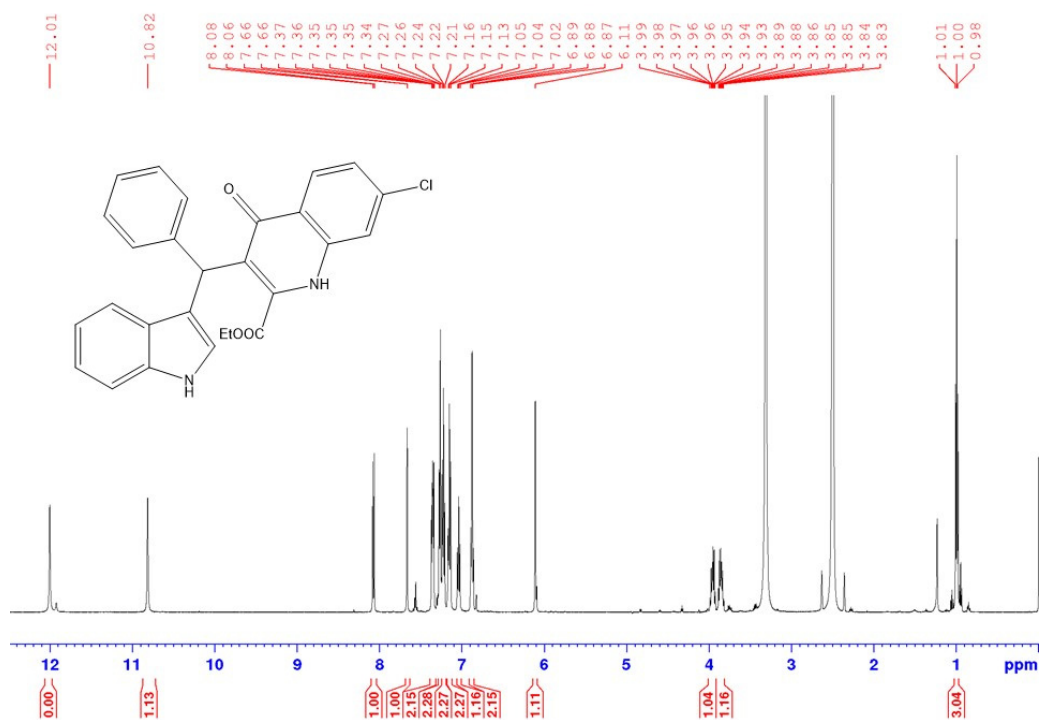


Figure S10. <sup>1</sup>H-NMR spectrum of **20c**

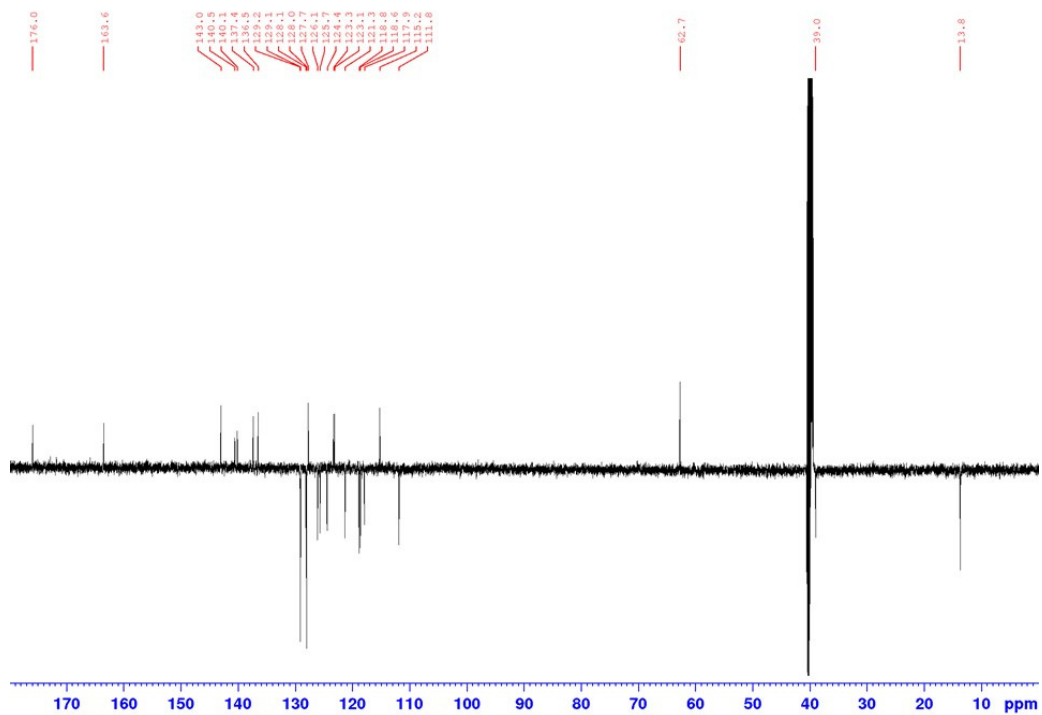


Figure S11. <sup>13</sup>C-NMR spectrum of **20c**



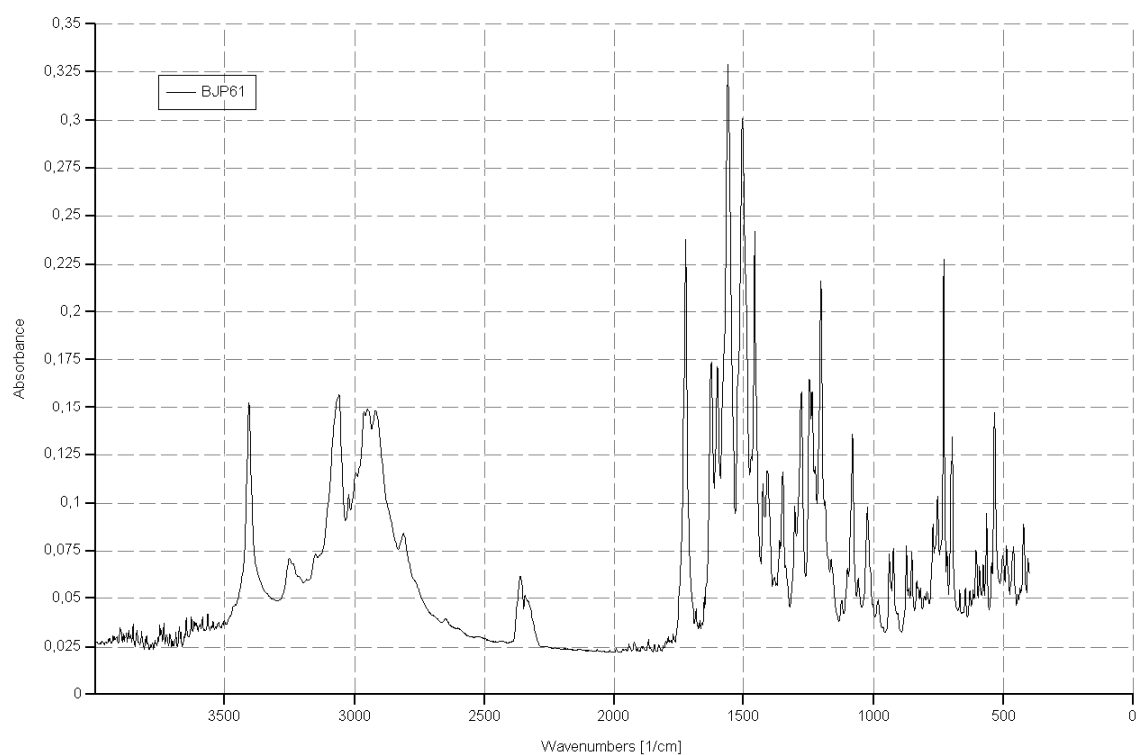


Figure S12. FTIR spectrum of **20c**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-8-chloro-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20d**)

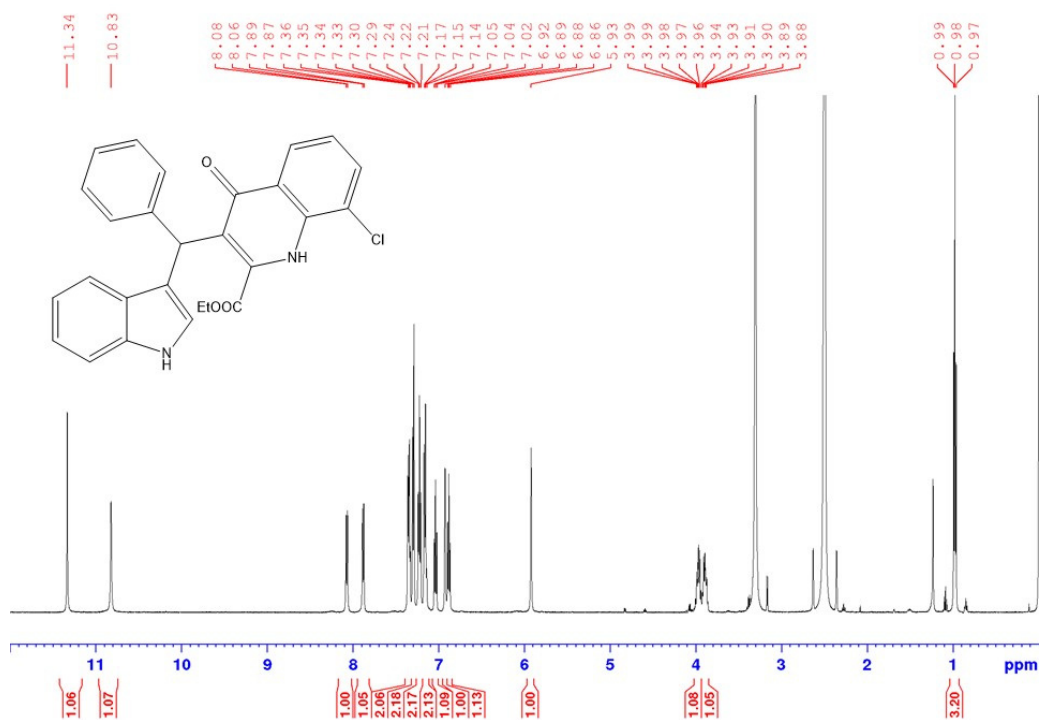


Figure S13. <sup>1</sup>H-NMR spectrum of **20d**

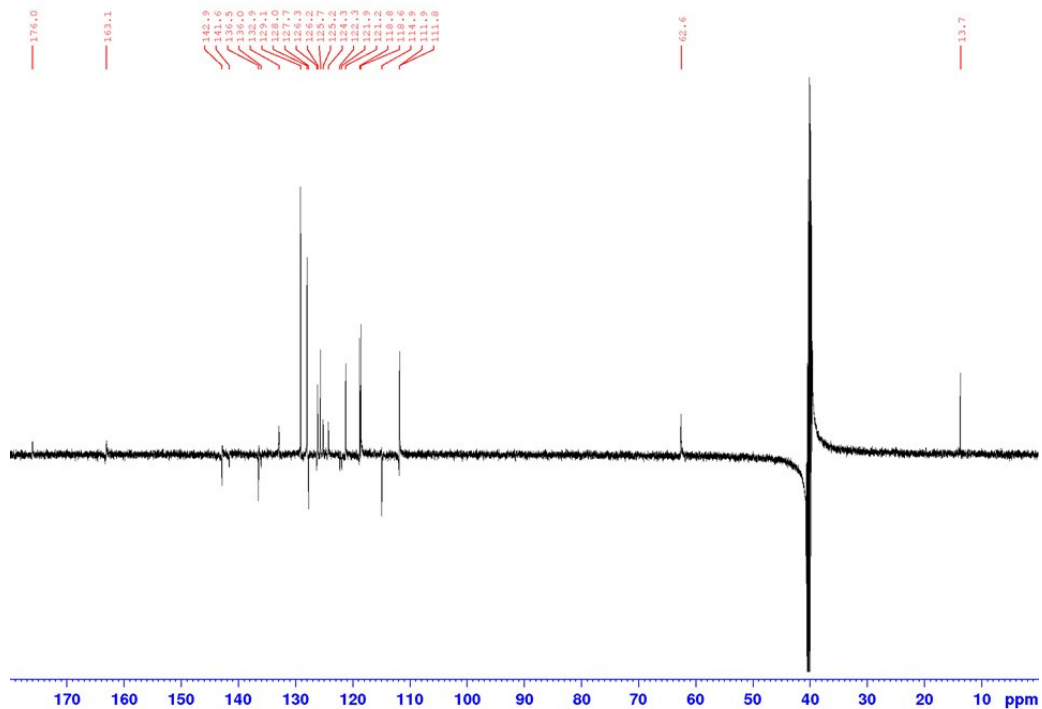


Figure S14. <sup>13</sup>C-NMR spectrum of **20d**

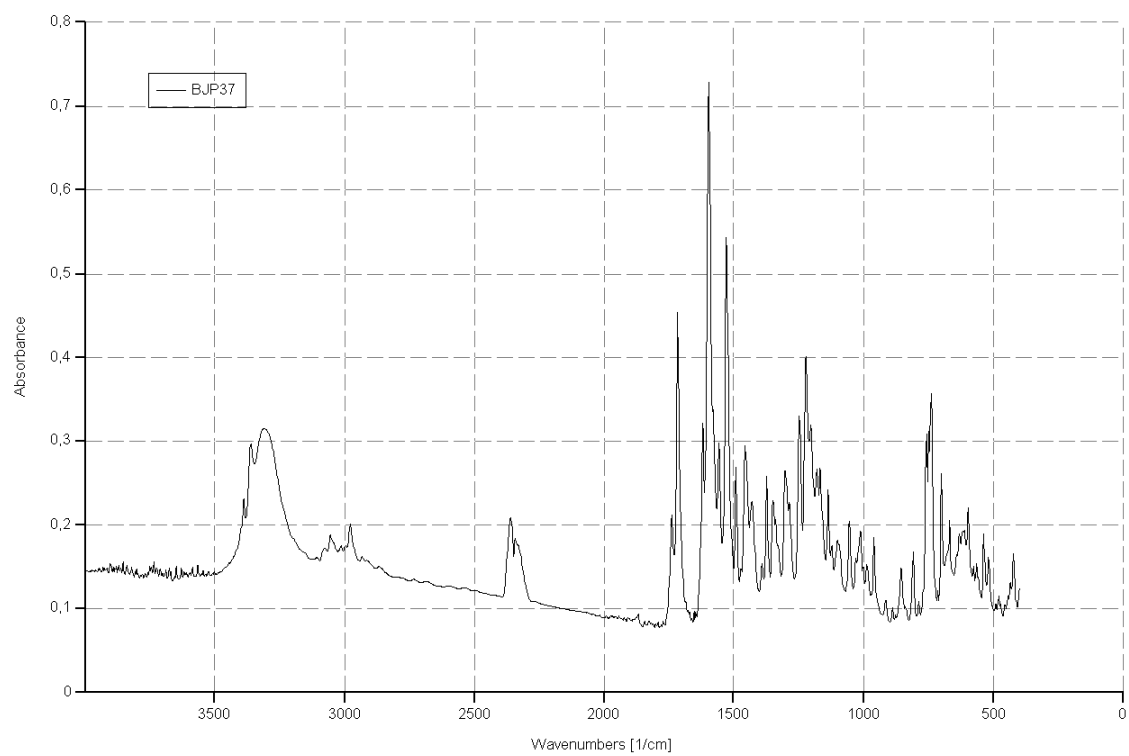


Figure S15. FTIR spectrum of **20d**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-5-methoxy-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20e**)

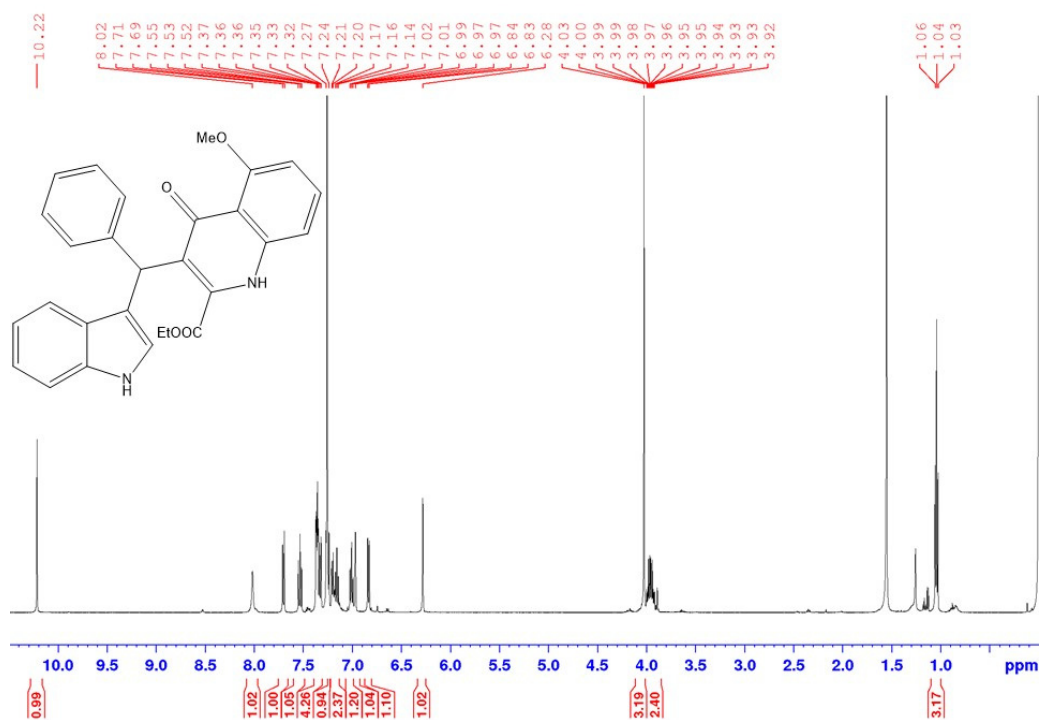


Figure S16. <sup>1</sup>H-NMR spectrum of **20e**

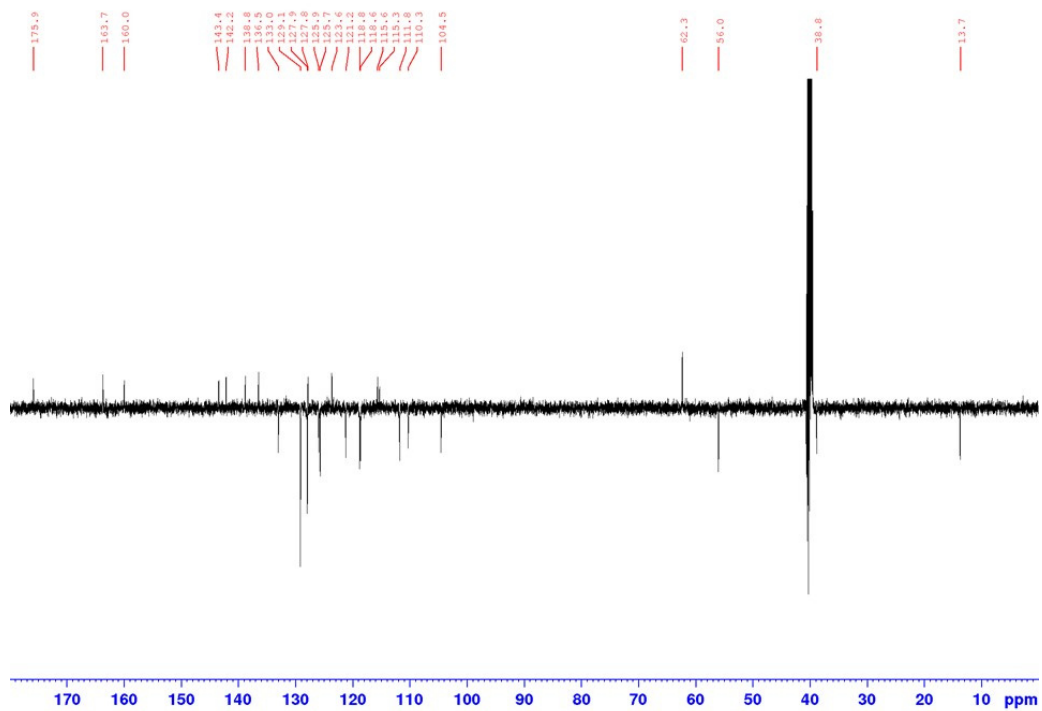


Figure S17. <sup>13</sup>C-NMR spectrum of **20e**

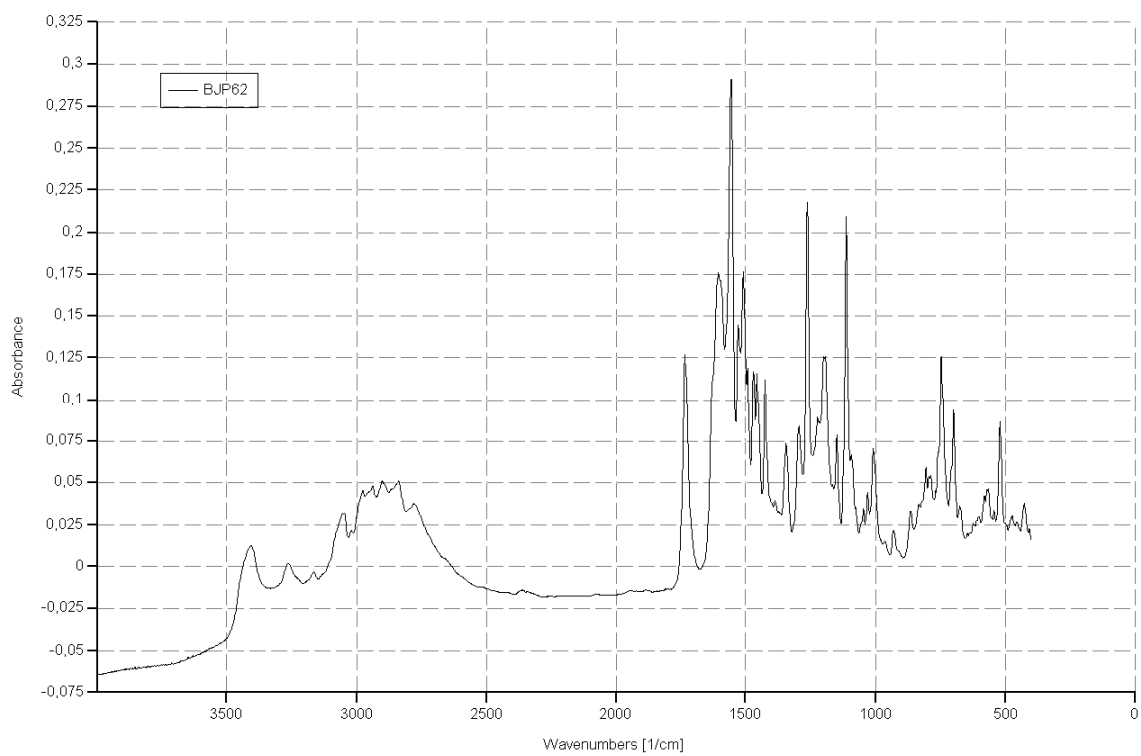


Figure S18. FTIR spectrum of **20e**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-6-methoxy-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20f**)

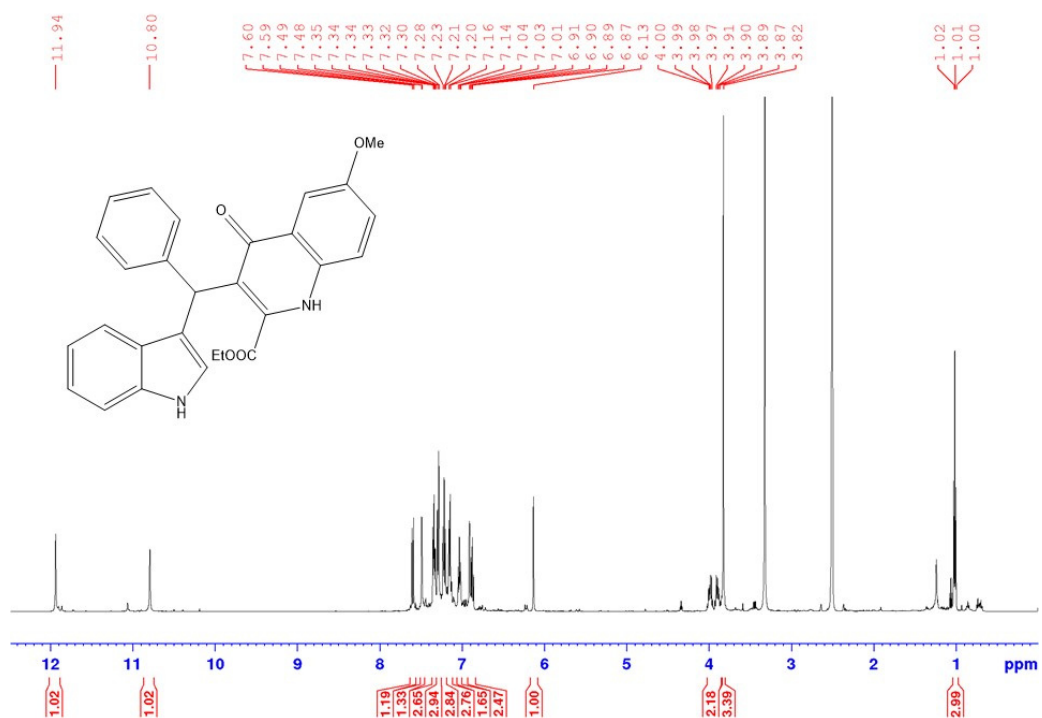


Figure S19.  $^1\text{H}$ -NMR spectrum of **20f**

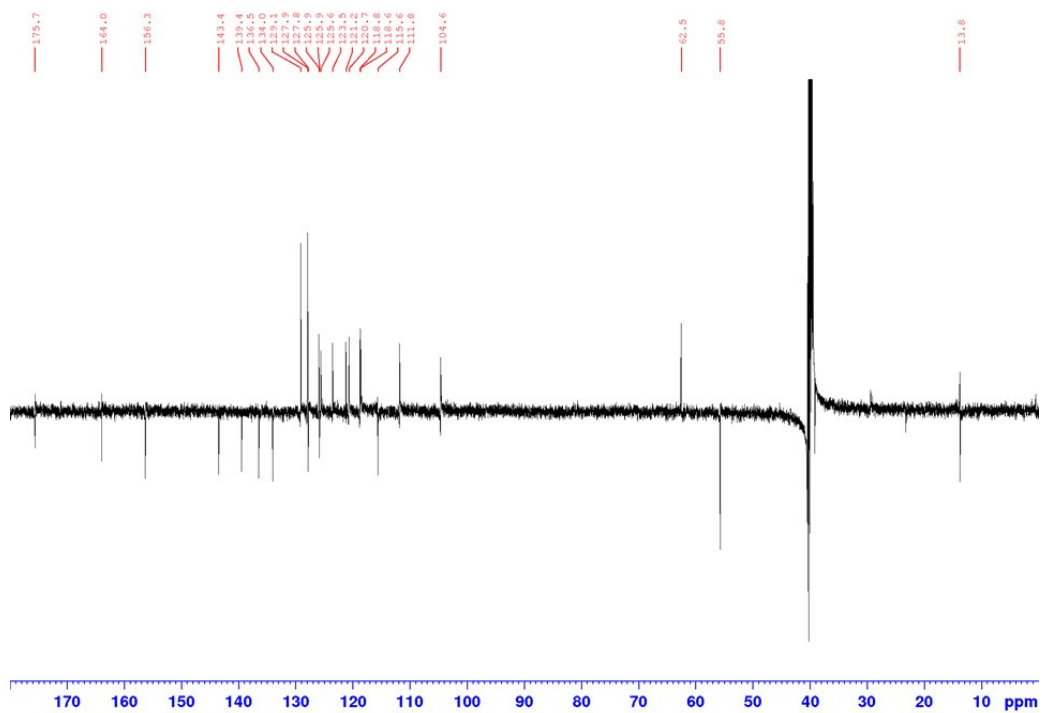


Figure S20.  $^{13}\text{C}$ -NMR spectrum of **20f**

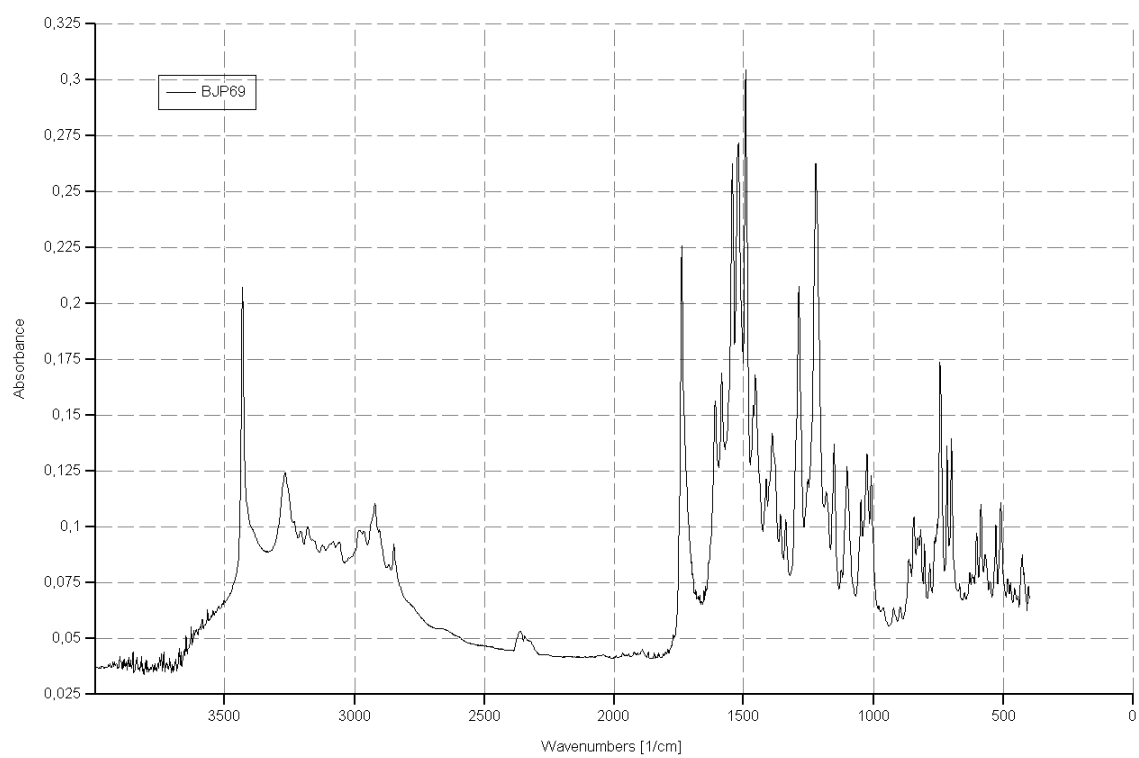


Figure S21. FTIR spectrum of **20f**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-7-methoxy-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20g**)

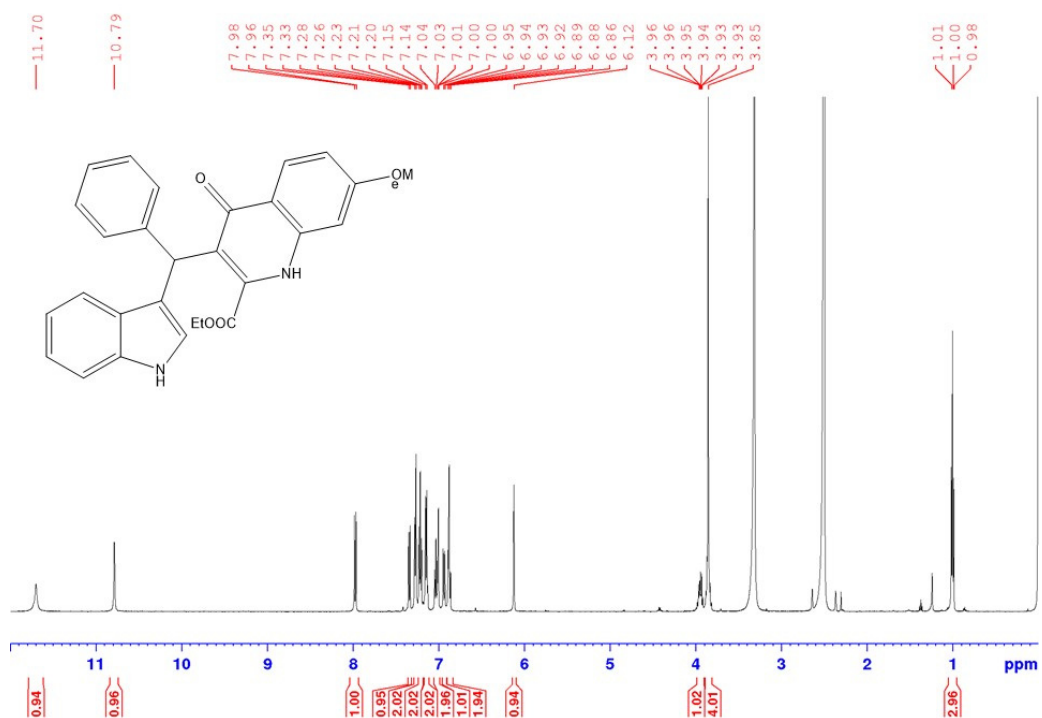


Figure S22. <sup>1</sup>H-NMR spectrum of **20g**

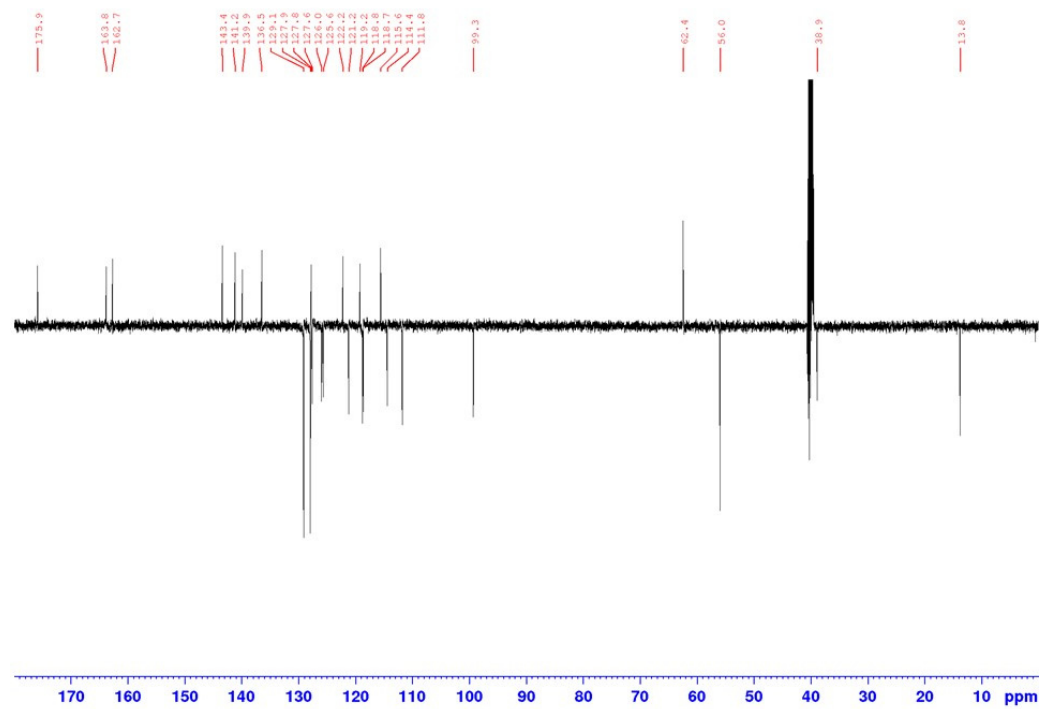


Figure S23. <sup>13</sup>C-NMR spectrum of **20g**



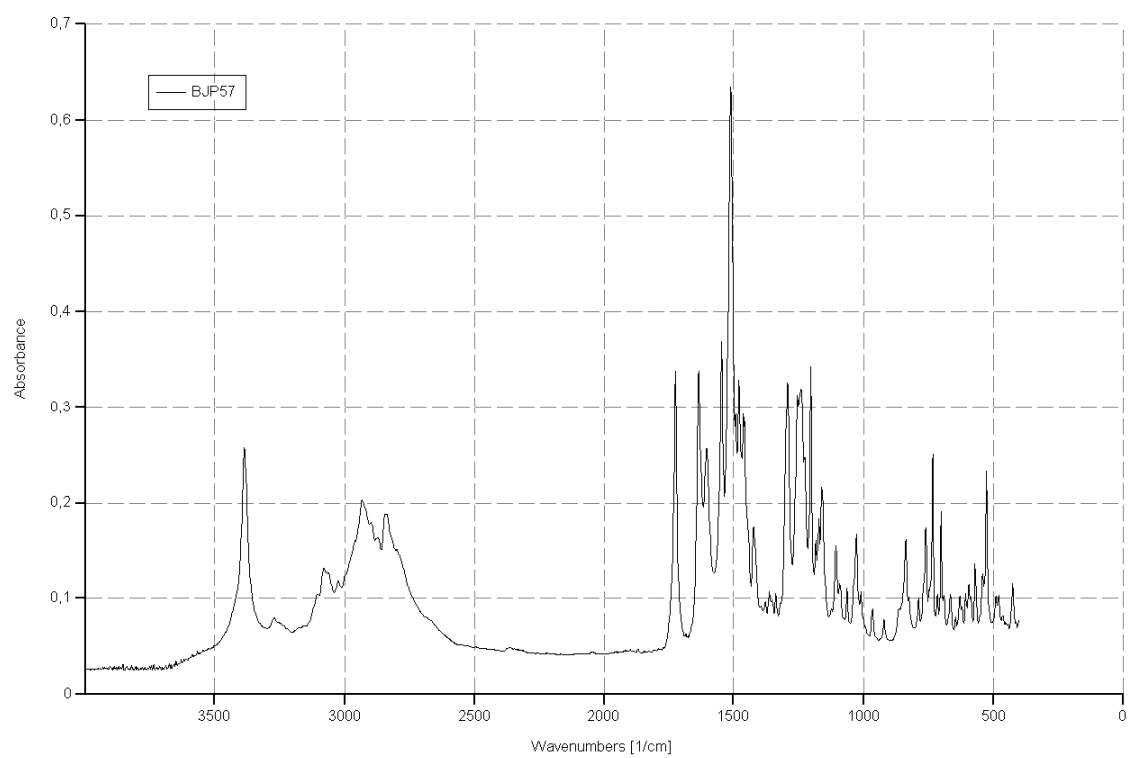


Figure S24. FTIR spectrum of **20g**

Ethyl 3-((1H-indol-3-yl)(phenyl)methyl)-8-methoxy-4-oxo-1,4-dihydroquinoline-2-carboxylate (**20h**)

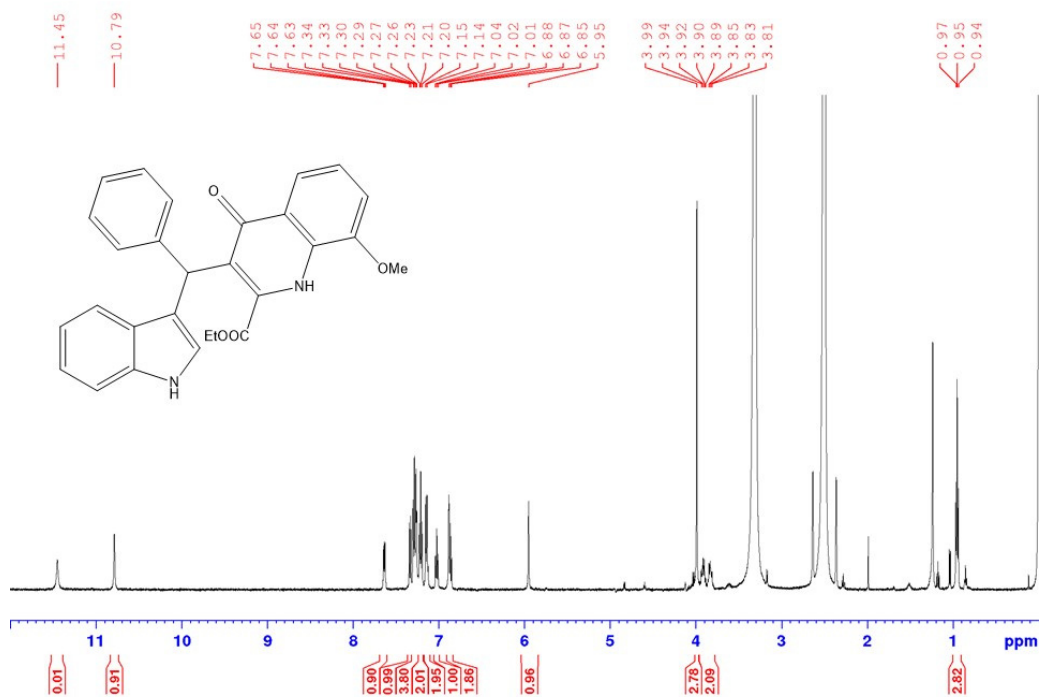


Figure S25. <sup>1</sup>H-NMR spectrum of **20h**

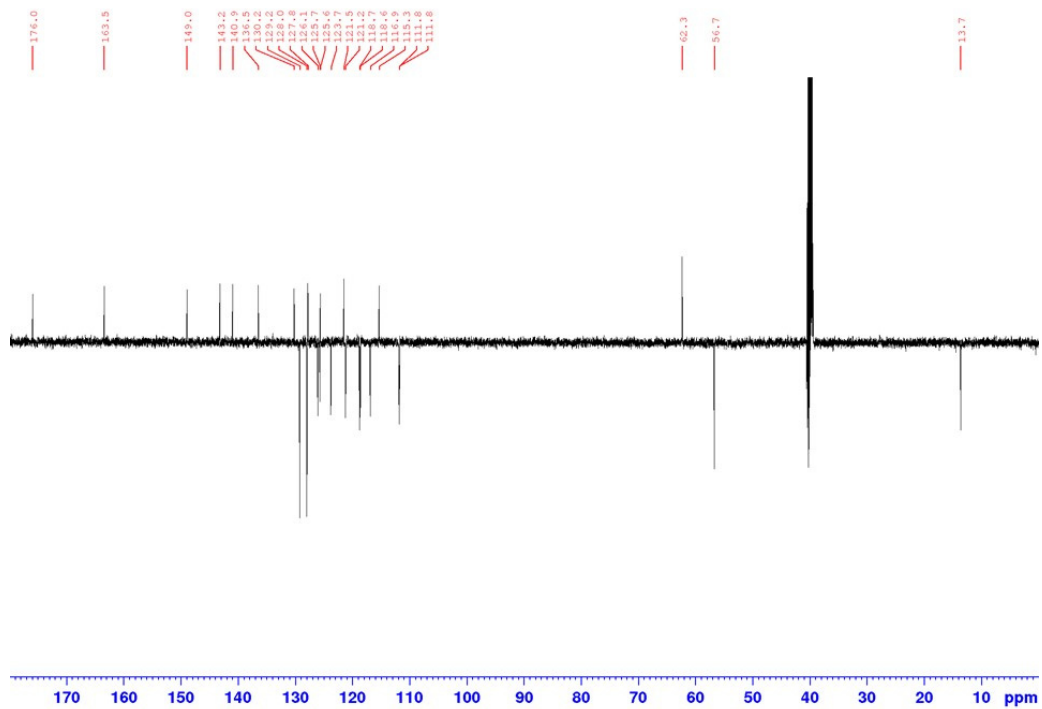


Figure S26. <sup>13</sup>C-NMR spectrum of **20h**

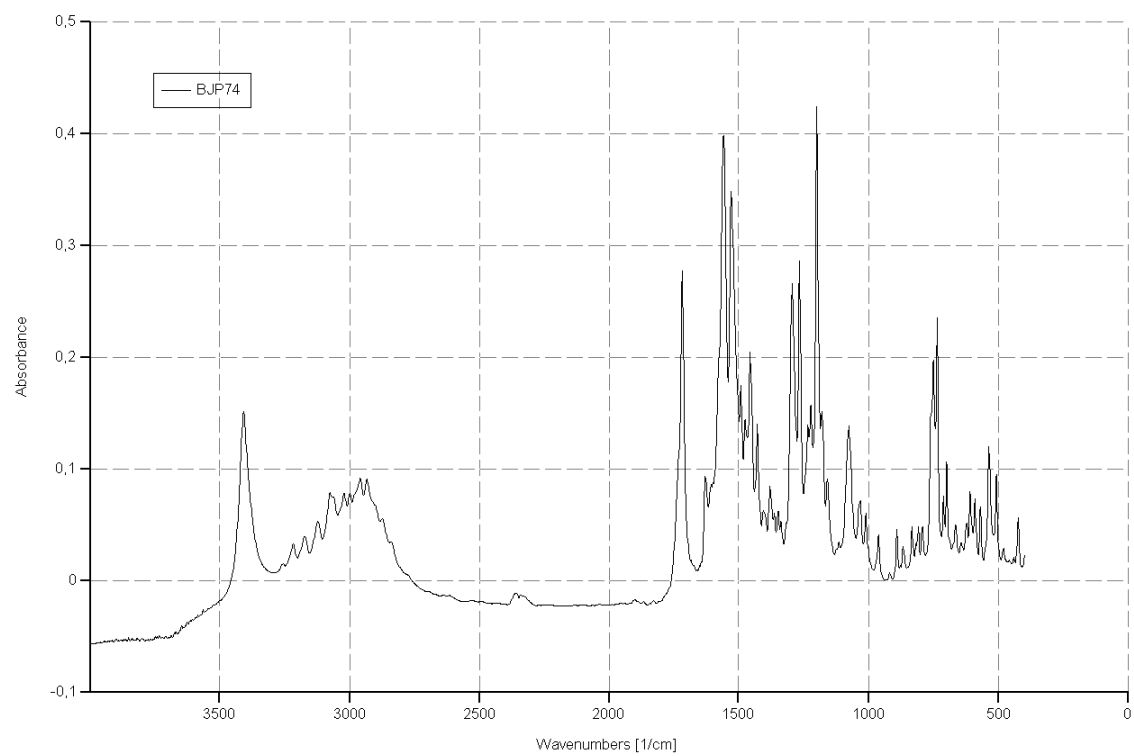


Figure S27. FTIR spectrum of **20h**

2-(((2-(Dimethylamino)ethyl)amino)(phenyl)methyl)naphthalen-1-ol (**16b**)

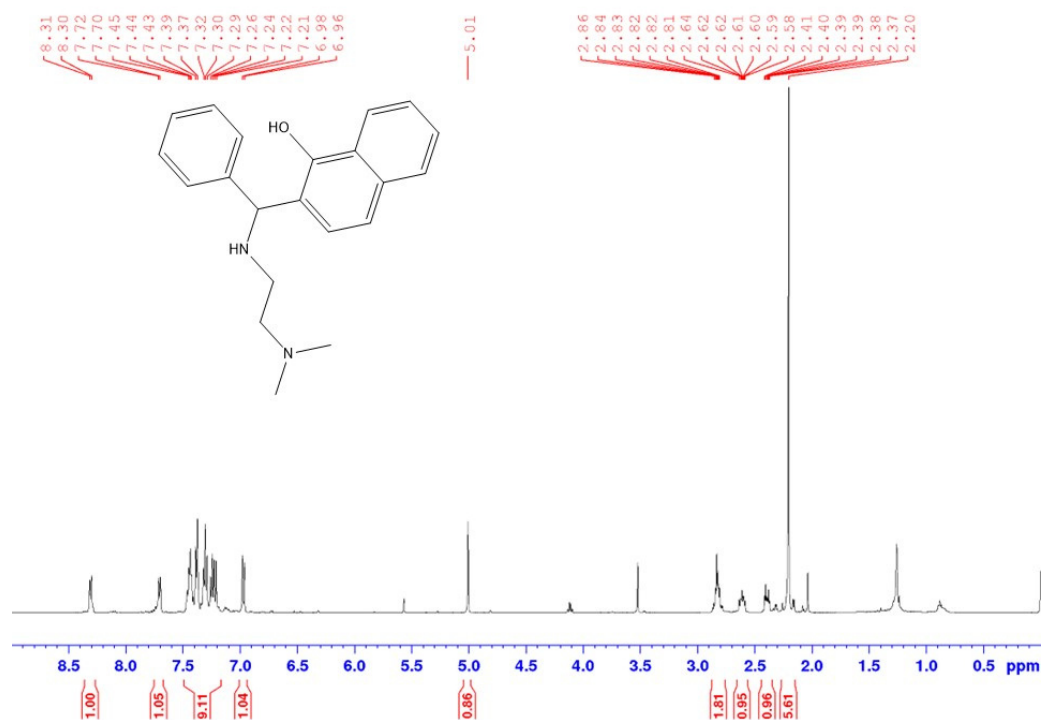


Figure S28. <sup>1</sup>H-NMR spectrum of **16b**

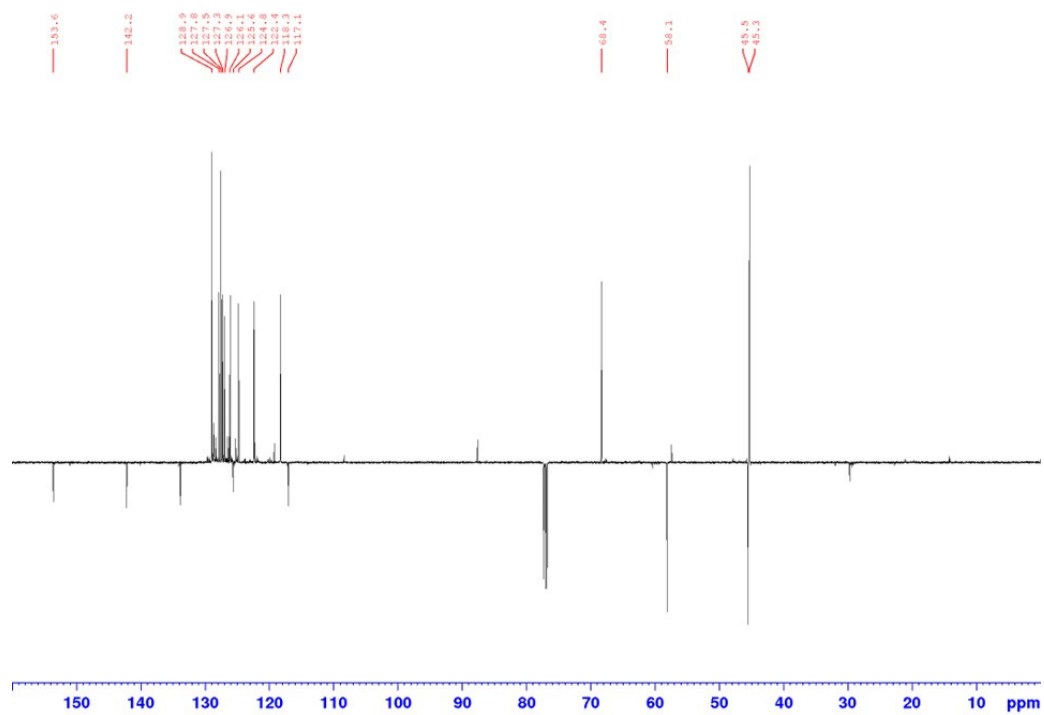


Figure S29. <sup>13</sup>C-NMR spectrum of **16b**

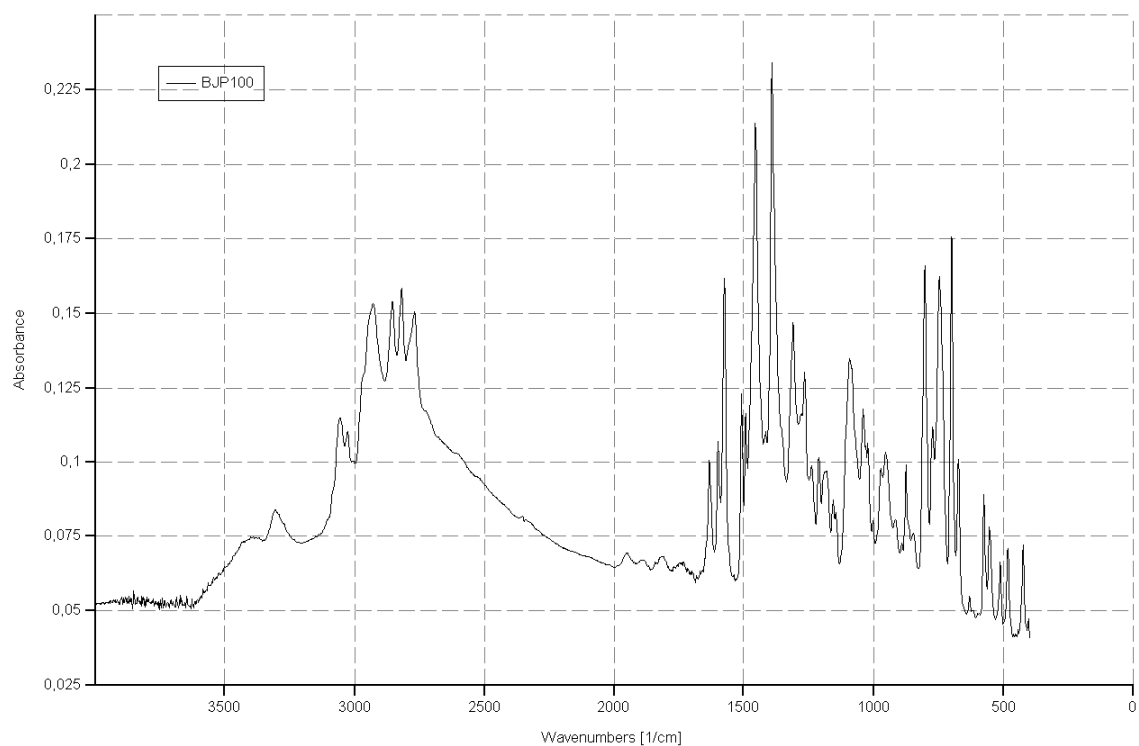


Figure S30. FTIR spectrum of **16b**

Chemical structure: Oc1ccc2cc(ccc2c1)C(c3ccccc3)C4C=CNc5ccccc45

<sup>1</sup>H NMR spectrum (ppm):

- 10.87
- 10.01
- 8.24
- 8.23
- 8.22
- 8.22
- 8.12
- 8.12
- 8.10
- 7.47
- 7.46
- 7.45
- 7.45
- 7.41
- 7.40
- 7.35
- 7.33
- 7.31
- 7.30
- 7.25
- 7.24
- 7.17
- 7.16
- 7.11
- 7.09
- 7.08
- 6.92
- 6.90
- 6.89
- 6.87
- 6.80
- 6.78
- 6.60
- 6.60
- 6.36

Integration values (from left to right): 1.00, 0.99, 1.00, 1.02, 1.12, 1.36, 1.23, 1.13, 1.11, 1.19, 1.14, 1.06, 1.00, 1.04.

Chemical shifts (ppm) listed on the left:

- 152.3
- 144.9
- 137.2
- 132.8
- 130.5
- 129.2
- 128.6
- 128.3
- 127.9
- 127.0
- 126.5
- 125.9
- 125.5
- 125.1
- 124.4
- 123.0
- 121.5
- 119.8
- 118.7
- 116.0
- 107.7

Chemical shifts (ppm) labeled on the right:

- 67.8
- 43.9
- 23.3

Figure S32.  $^{13}\text{C}$ -NMR spectrum of **18**

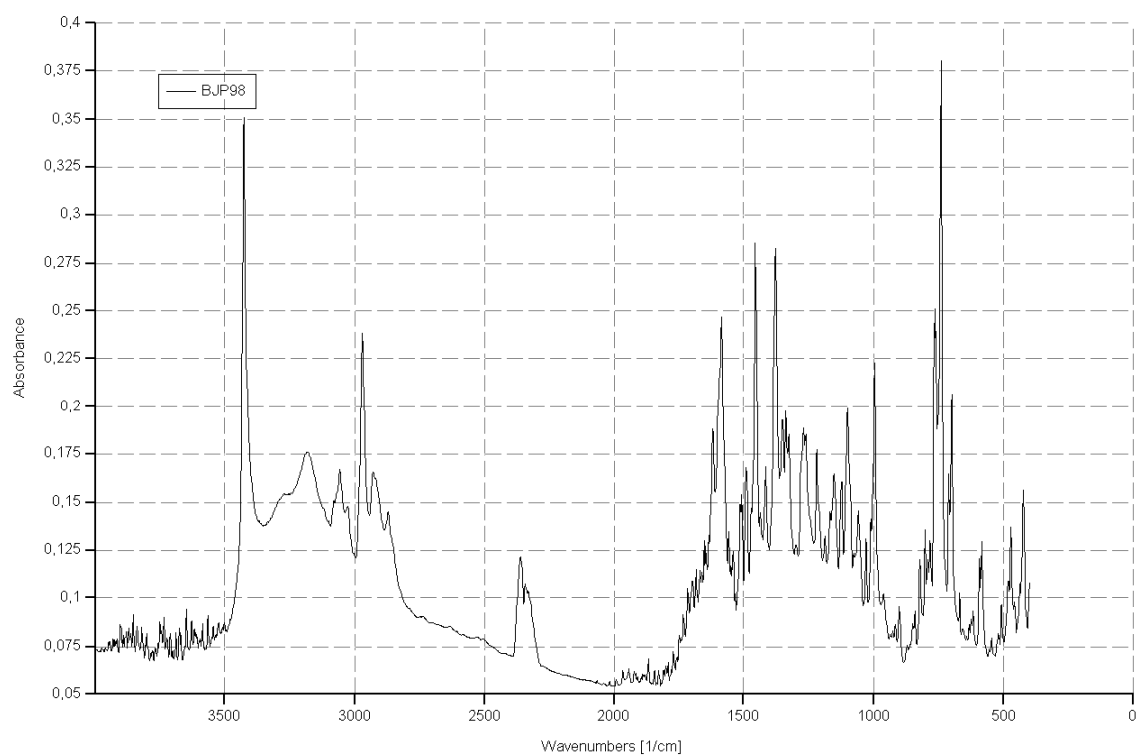


Figure S33. FTIR spectrum of **18**

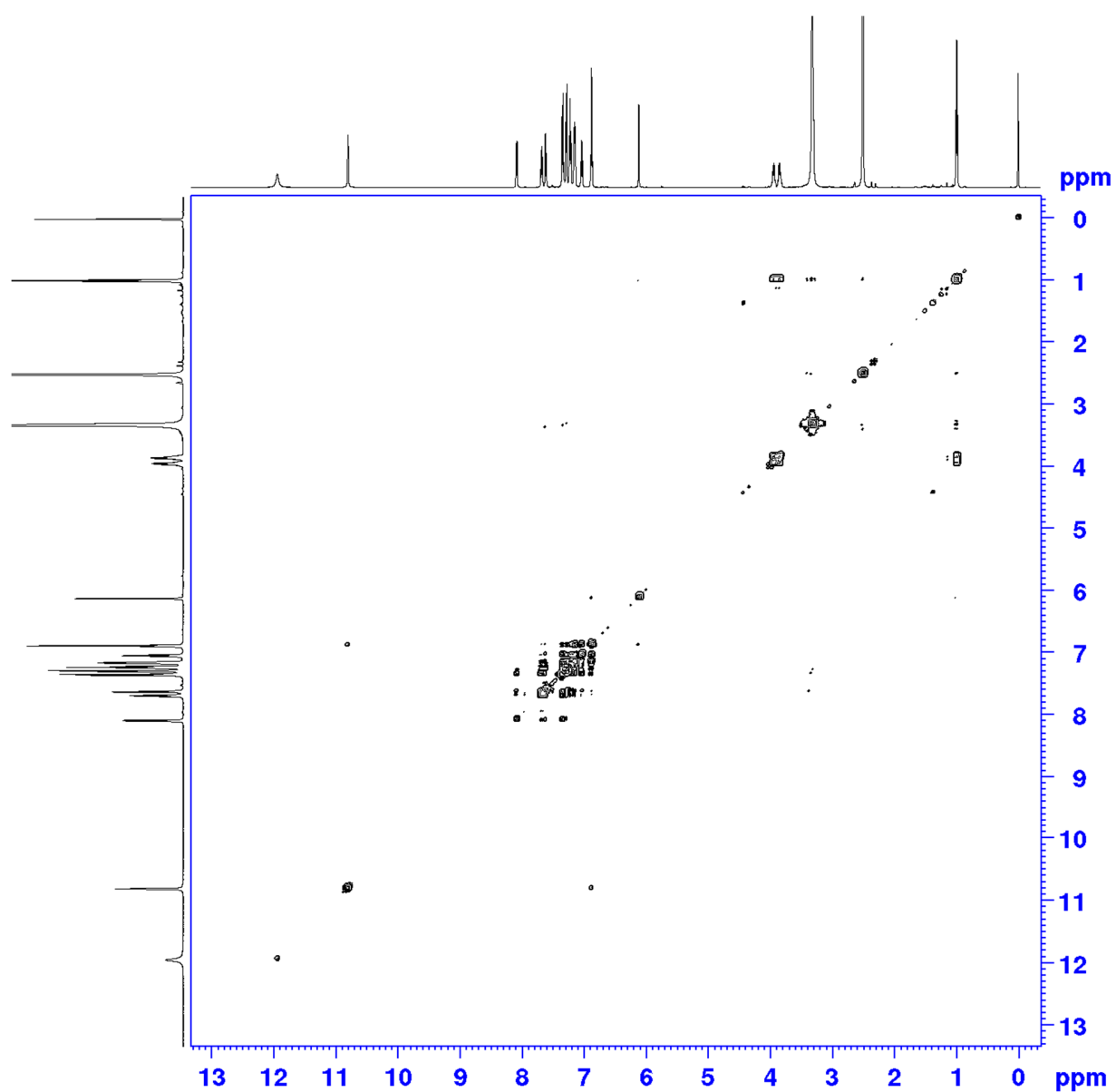


Figure S34. COSY spectrum of 7



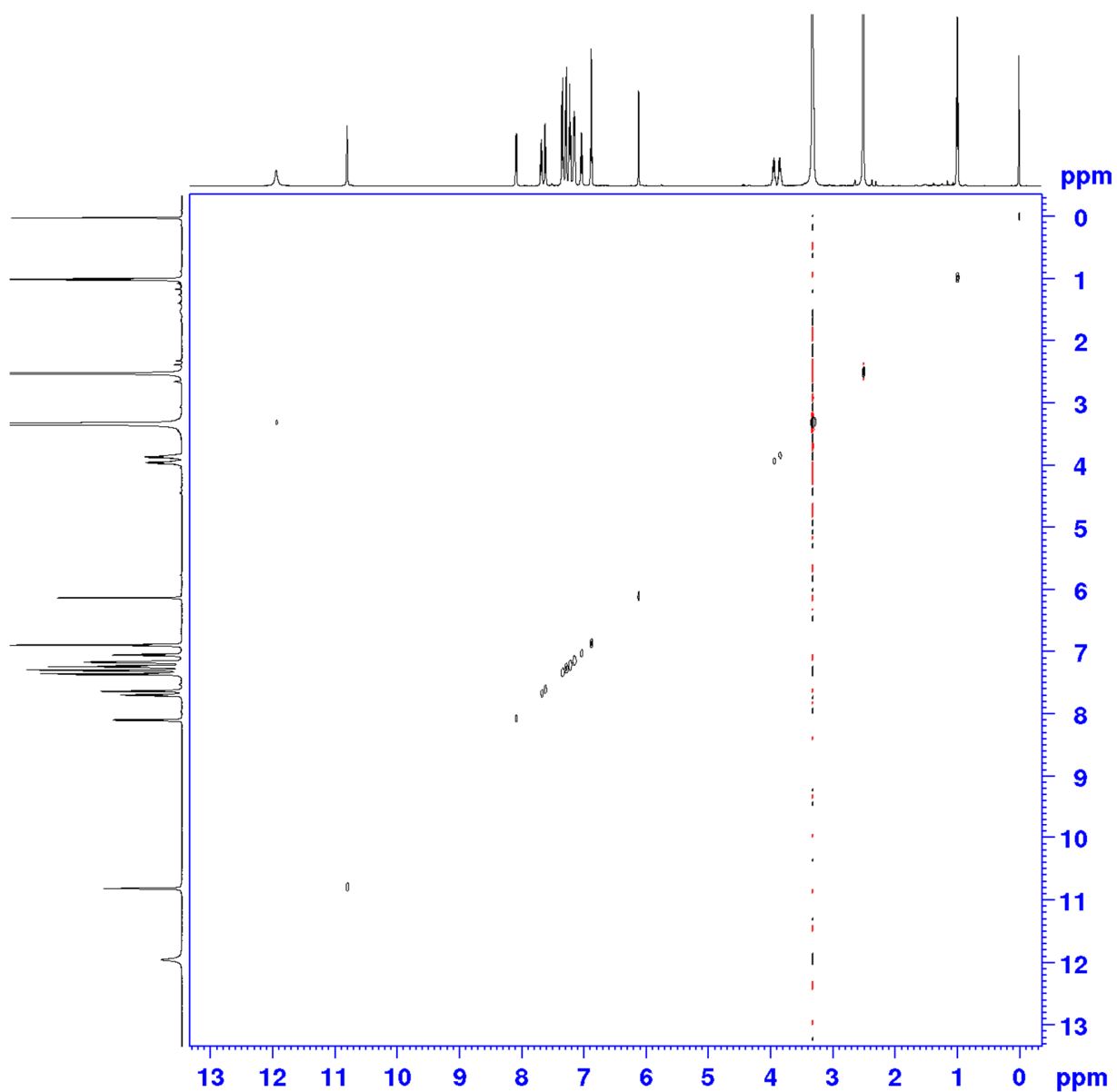


Figure S35. NOESY spectrum of 7

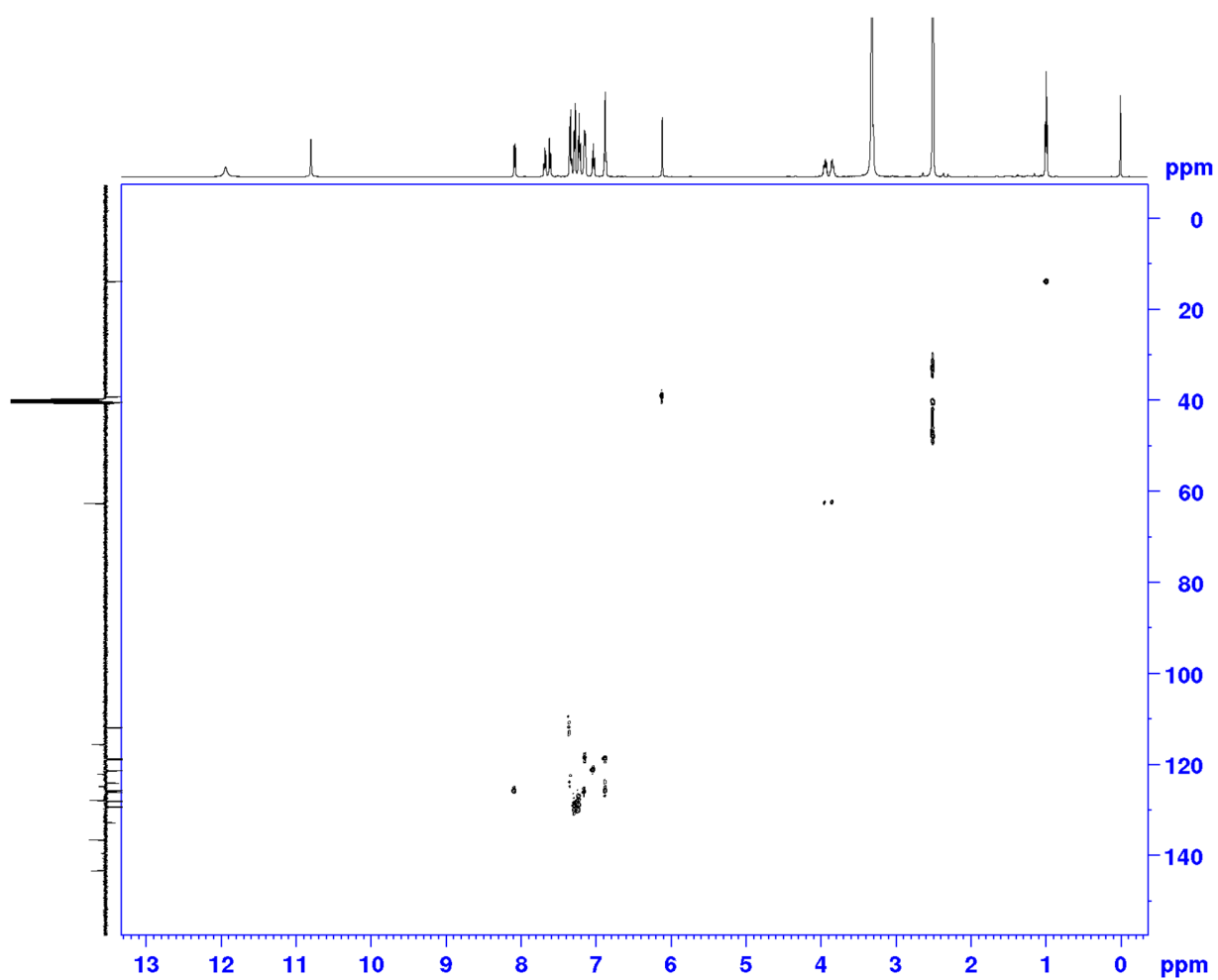


Figure S36. HSQC spectrum of 7

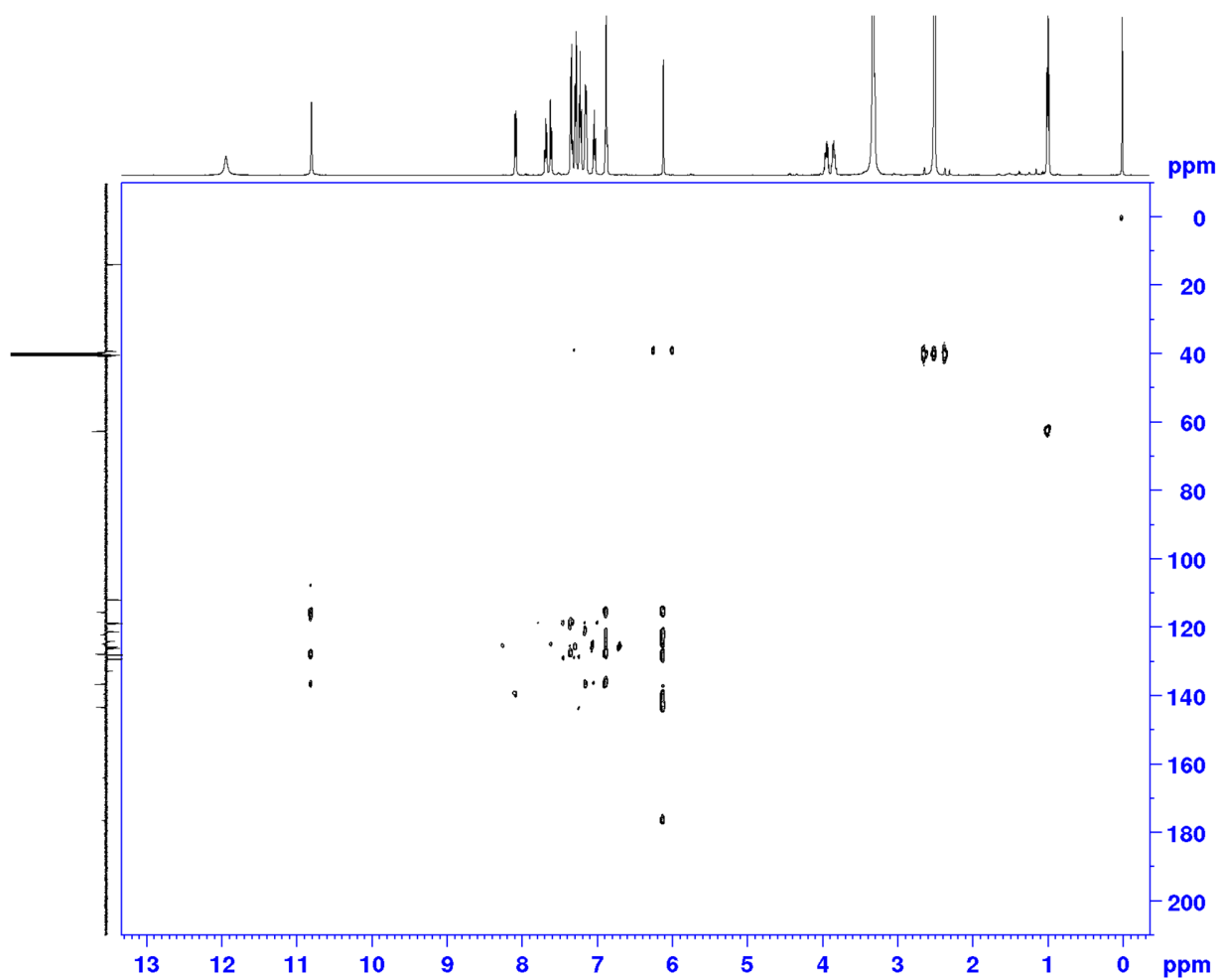


Figure S37. HMBC spectrum of 7