**Synthesis, Antibacterial Activity and Docking Studies of Substituted Quinolone Thiosemicarbazones**

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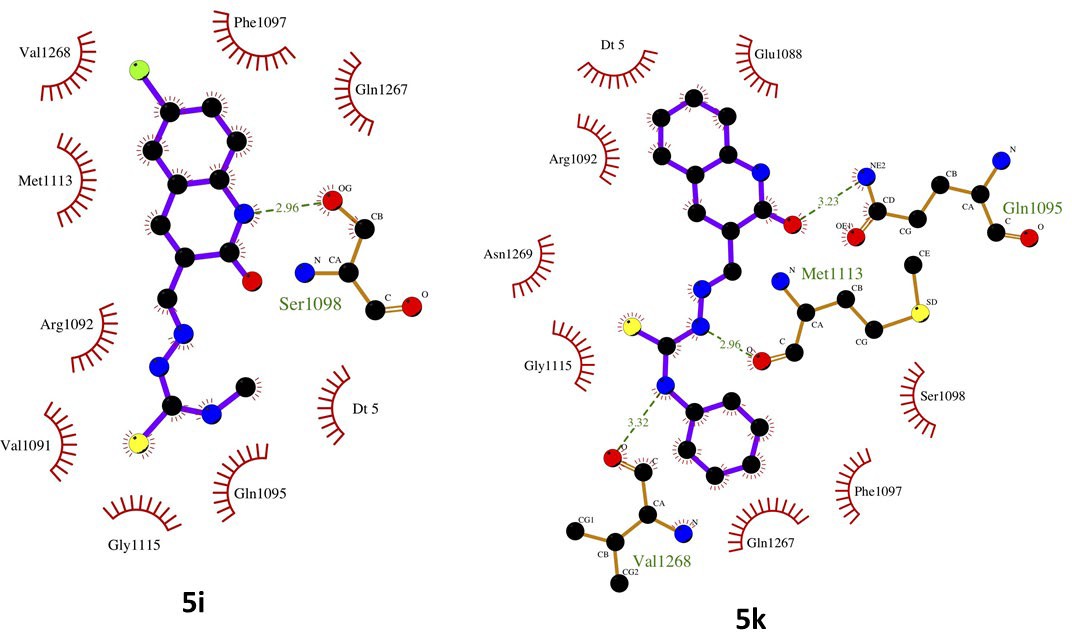
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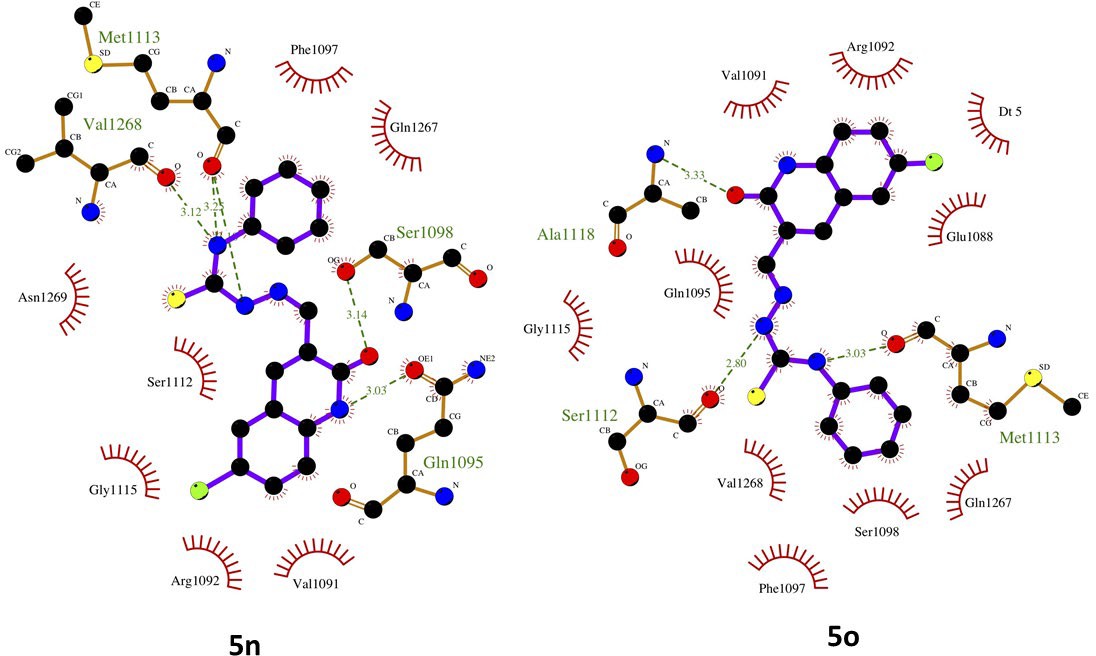
Email: [Koorbanally@ukzn.ac.za](mailto:Koorbanally@ukzn.ac.za)

**Supplemental Materials**

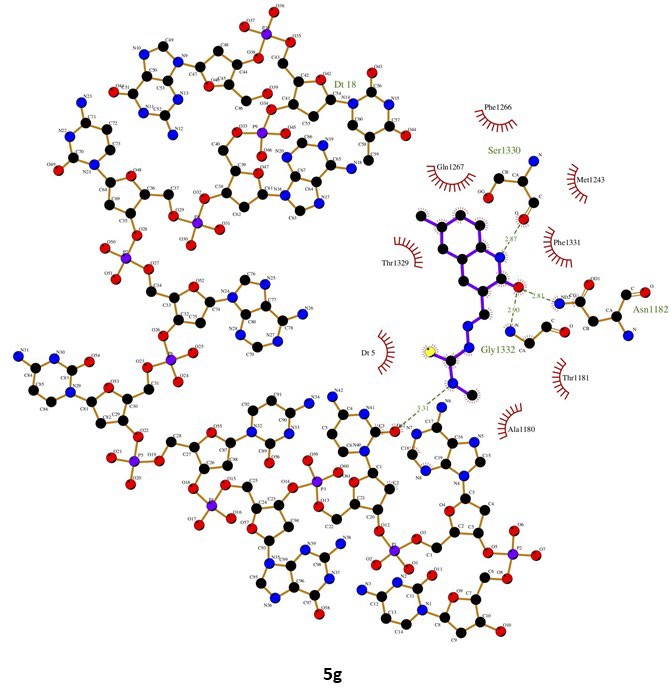
# Docking studies with the assistance of ligplot



**Figure S 1:** 3D Ligand residue interactions for **5i** and **5k** against DNA Gyrase. Oxygen = red spheres, nitrogen = blue spheres, carbon = black spheres, sulfur = yellow spheres, chlorine = green sphere, red arcs = hydrophobic interactions and green dashed lines = hydrogen bonds.

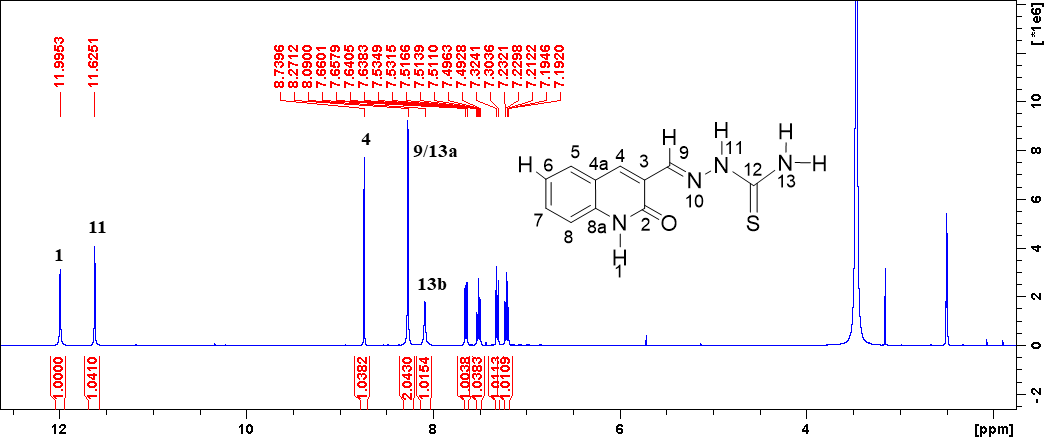


**Figure S 2:** 3D Ligand residue interactions for **5n** and **5o** against DNA Gyrase. Oxygen = red spheres, nitrogen = blue spheres, carbon = black spheres, sulfur = yellow spheres, chlorine = green sphere in **5n** and fluorine = green sphere in **5o**, red arcs = hydrophobic interactions and green dashed lines = hydrogen bonds.

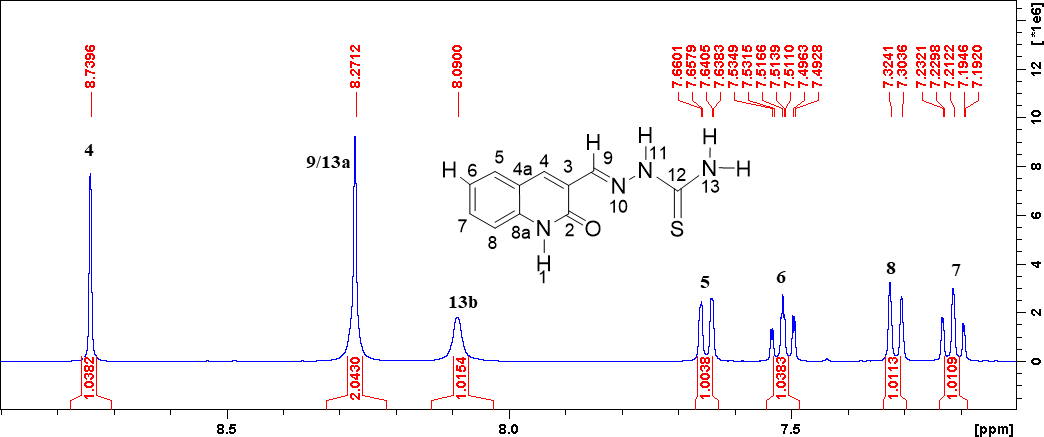


**Figure S 3** 3D Ligand residue interactions for **5g** against DNA Gyrase. Oxygen = red spheres, nitrogen = blue spheres, carbon = black spheres, sulfur = yellow spheres, red arcs = hydrophobic interactions and green dashed lines = hydrogen bonds.

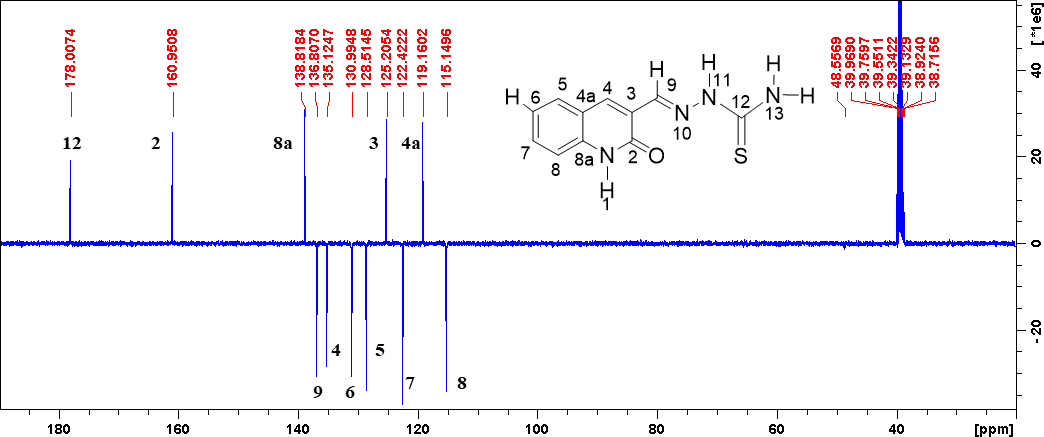
# NMR spectra



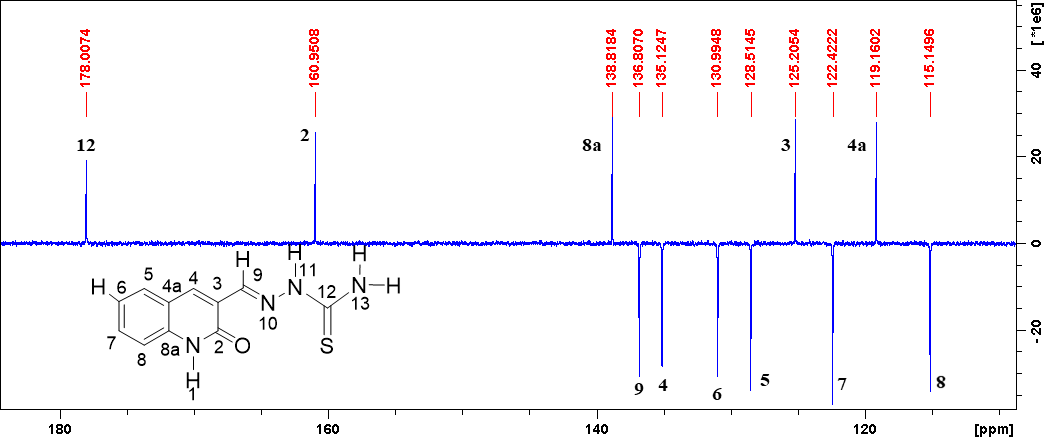
**Figure S 3** 1H NMR spectrum of **5a**



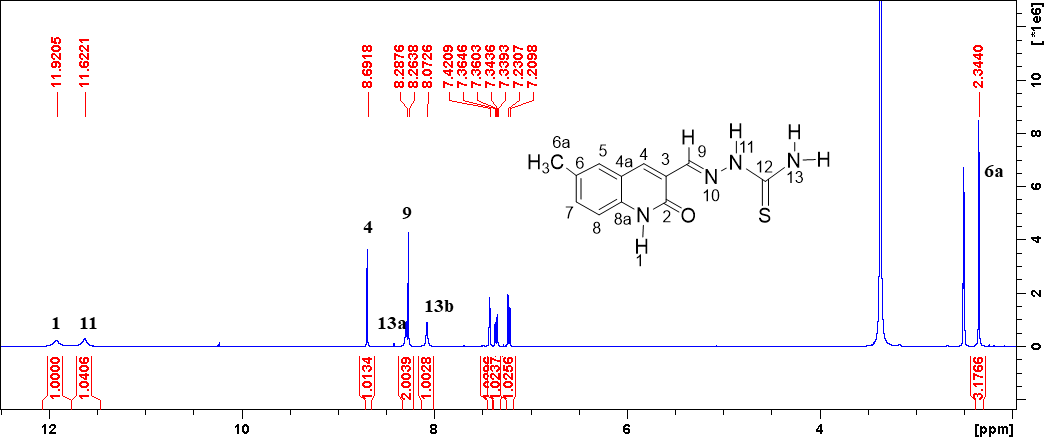
**Figure S 4** Expanded 1H NMR spectrum of **5a**



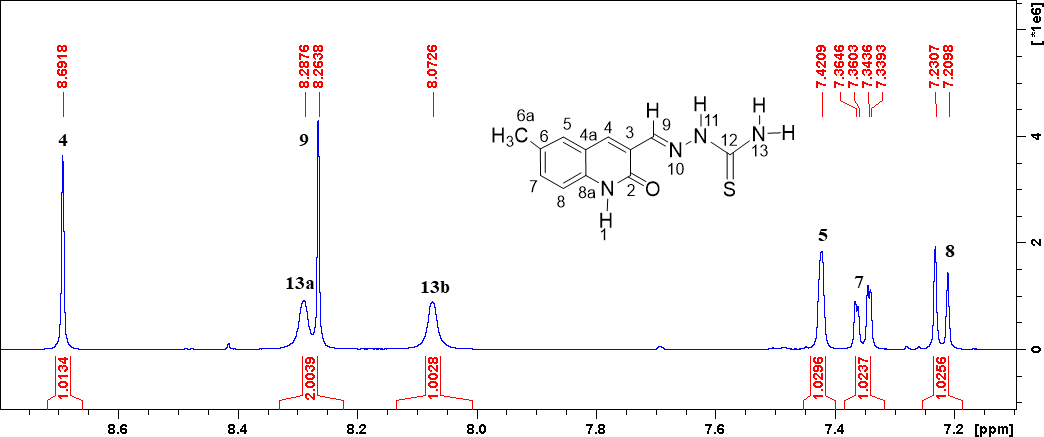
**Figure S 5** 13C NMR spectrum of **5a**



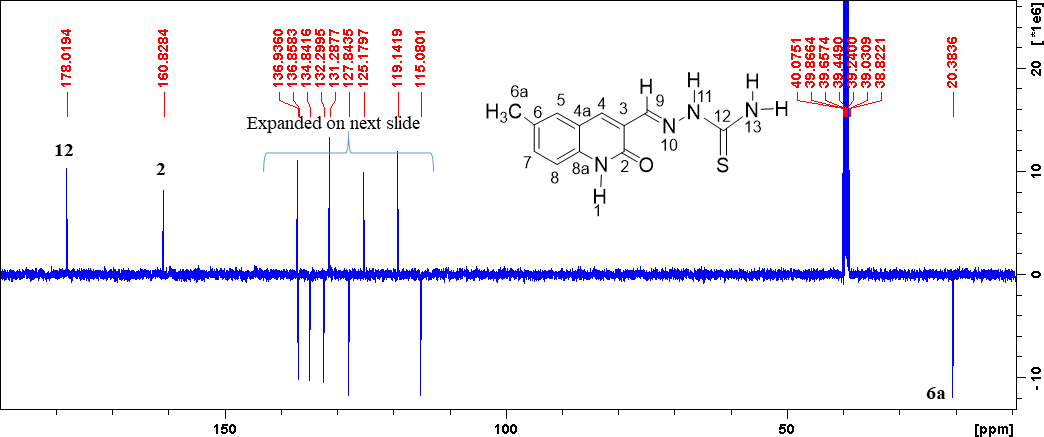
**Figure S 6** Expanded 13C NMR spectrum of **5a**



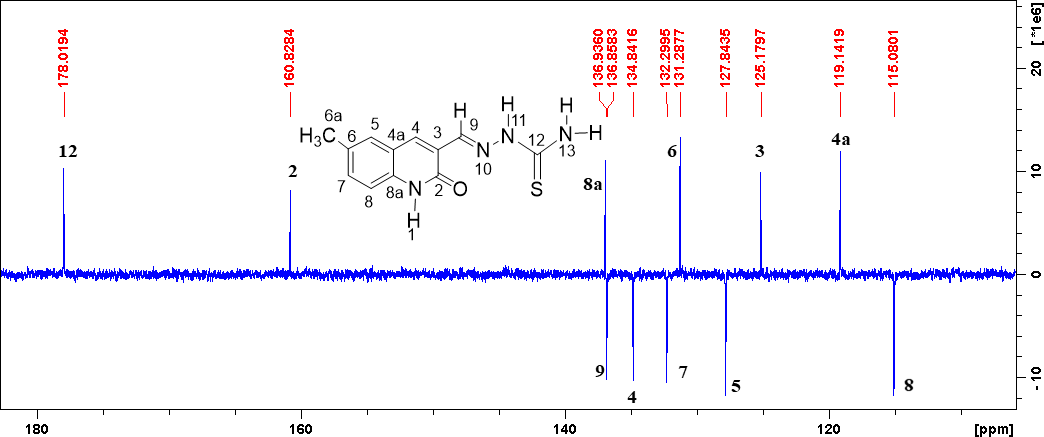
**Figure S 7** 1H NMR spectrum of **5b**



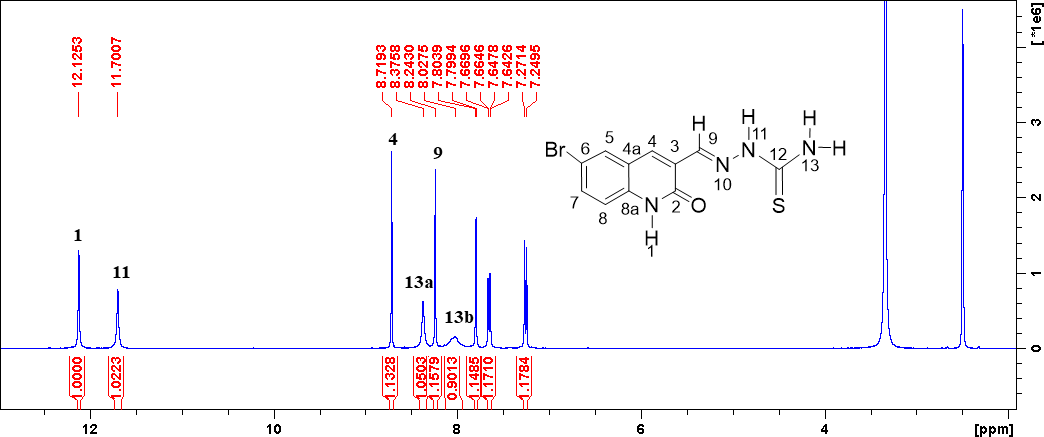
**Figure S 8** Expanded 1H NMR spectrum of **5b**



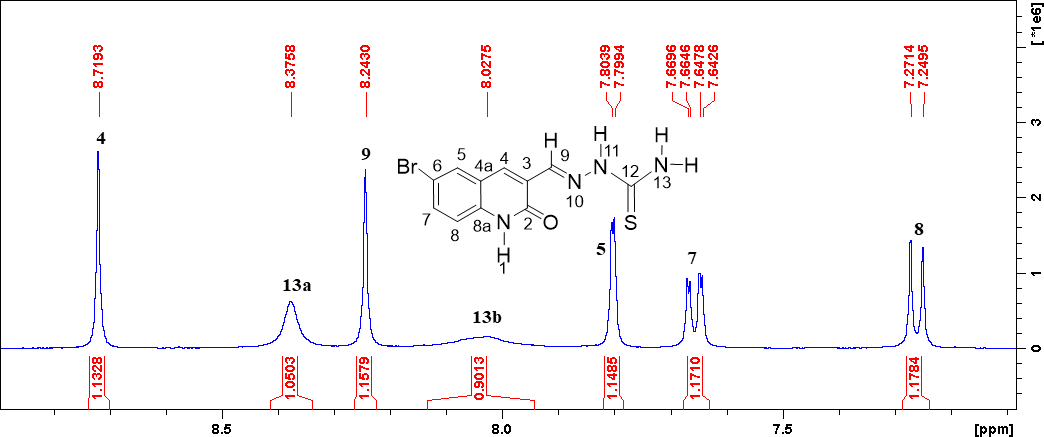
**Figure S 9** 13C NMR spectrum of **5b**



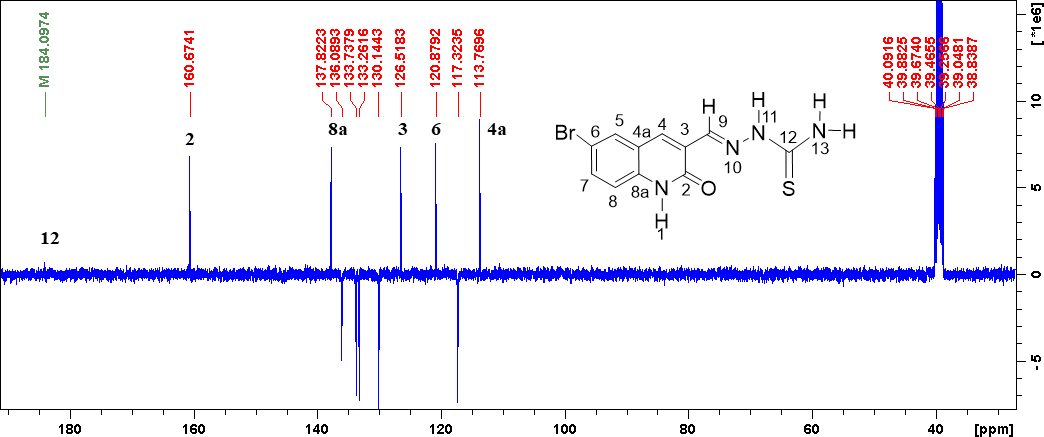
**Figure S 10** Expanded 13C NMR spectrum of **5b**



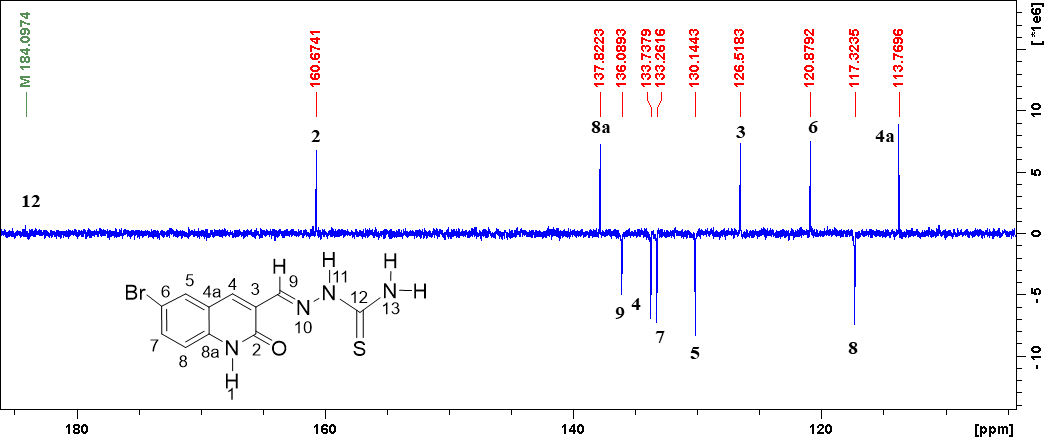
**Figure S 11** 1H NMR spectrum of **5c**



**Figure S 12** Expanded 1H NMR spectrum of **5c**



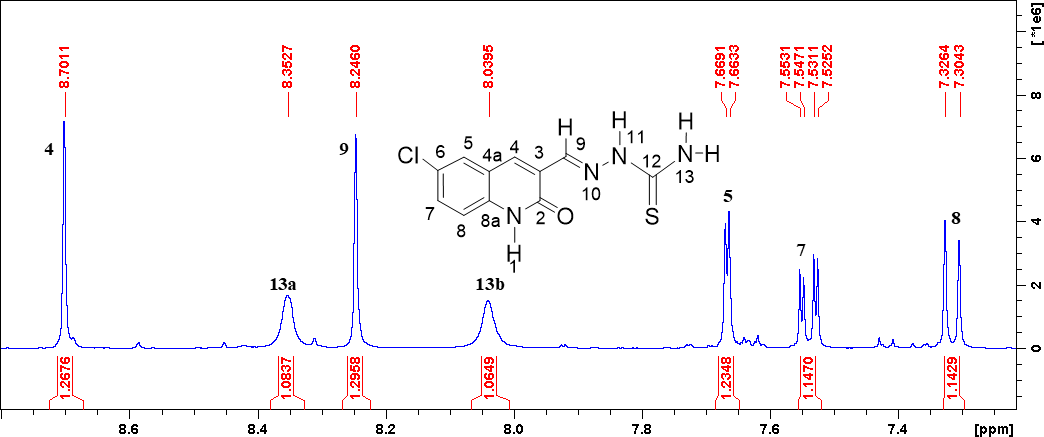
**Figure S 13** 13C NMR spectrum of **5c**



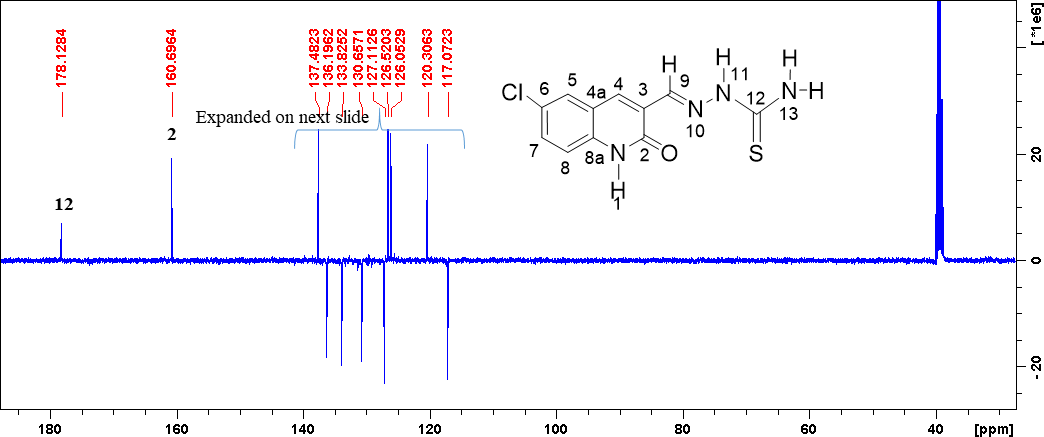
**Figure S 14** Expanded 13C NMR spectrum of **5c**



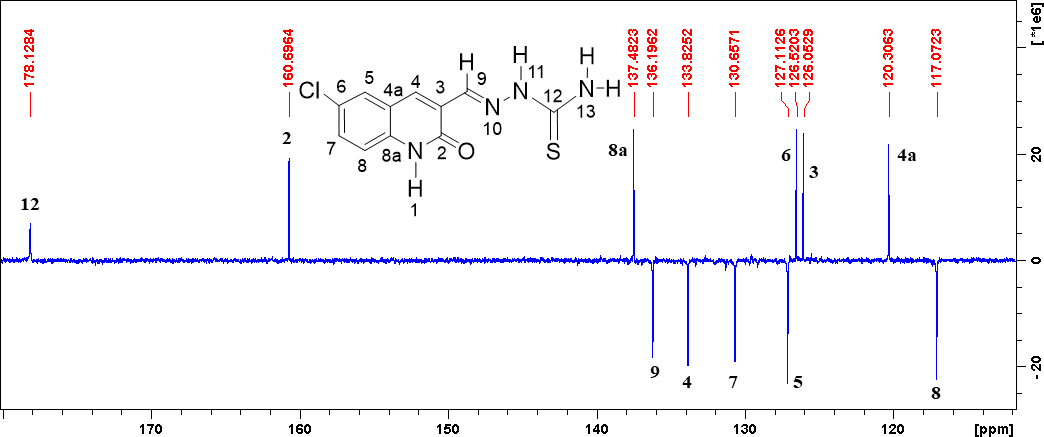
**Figure S 15** 1H NMR spectrum of **5d**



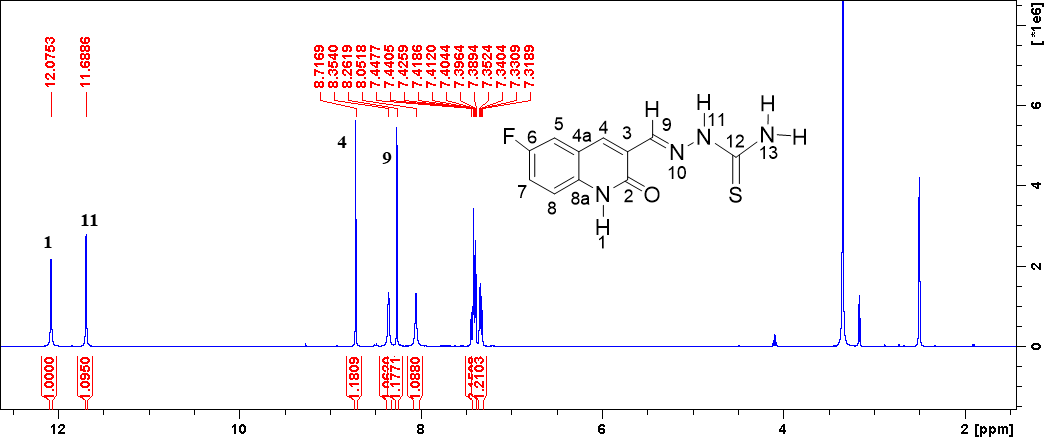
**Figure S 16** Expanded 1H NMR spectrum of **5d**



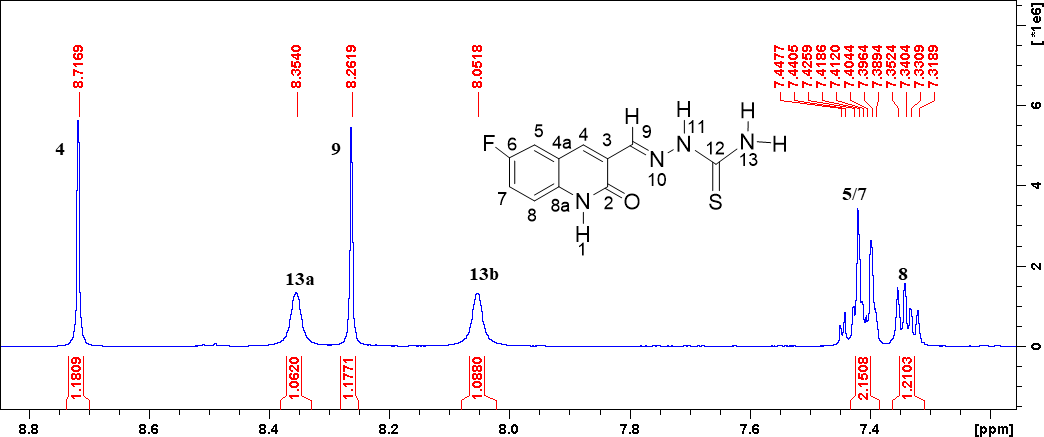
**Figure S 17** 13C NMR spectrum of **5d**



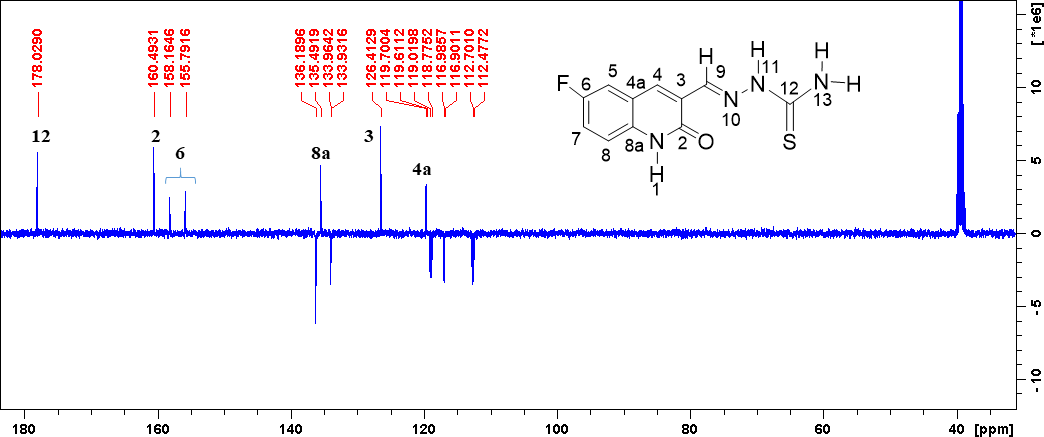
**Figure S 18** Expanded 13C NMR spectrum of **5d**



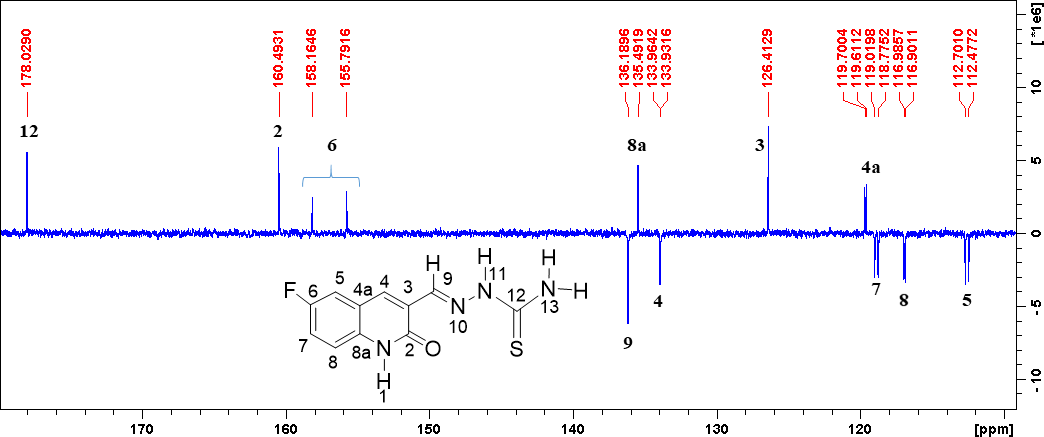
**Figure S 19** 1H NMR spectrum of **5e**



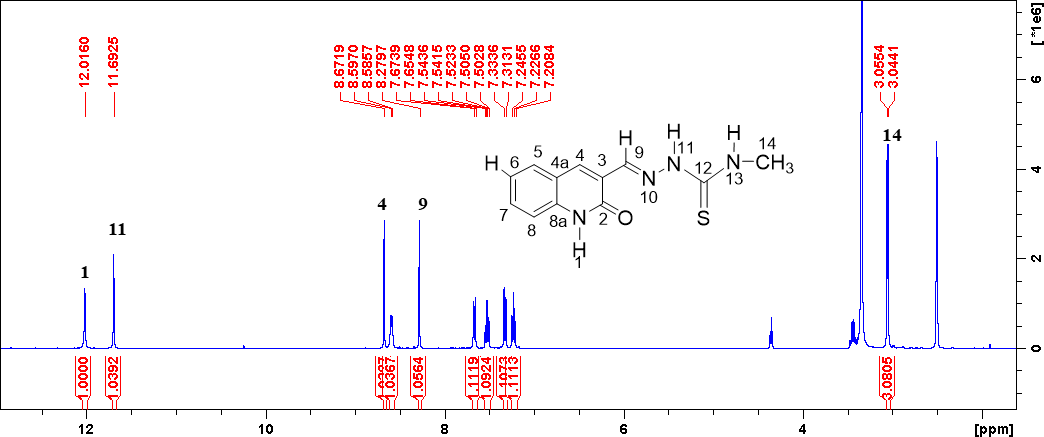
**Figure S 20** Expanded 1H NMR spectrum of **5e**



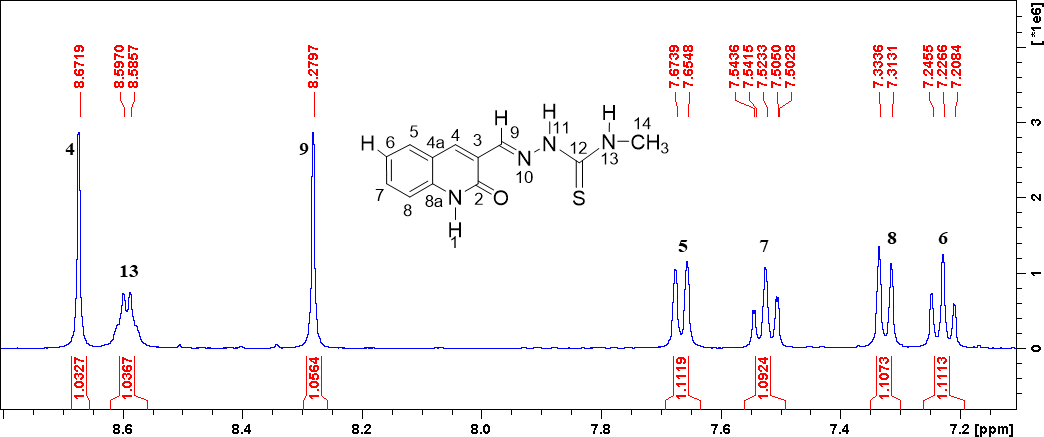
**Figure S 21** 13C NMR spectrum of **5e**



**Figure S 22** Expanded 13C NMR spectrum of **5e**



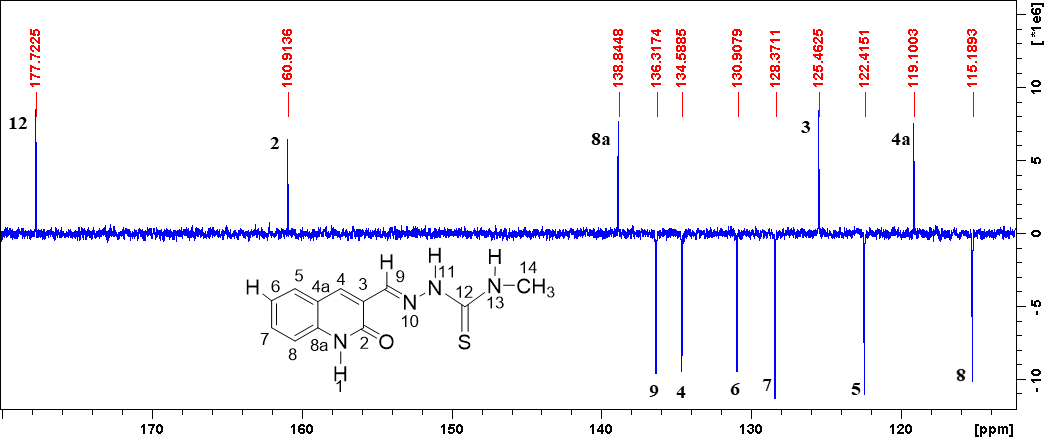
**Figure S 23** 1H NMR spectrum of **5f**



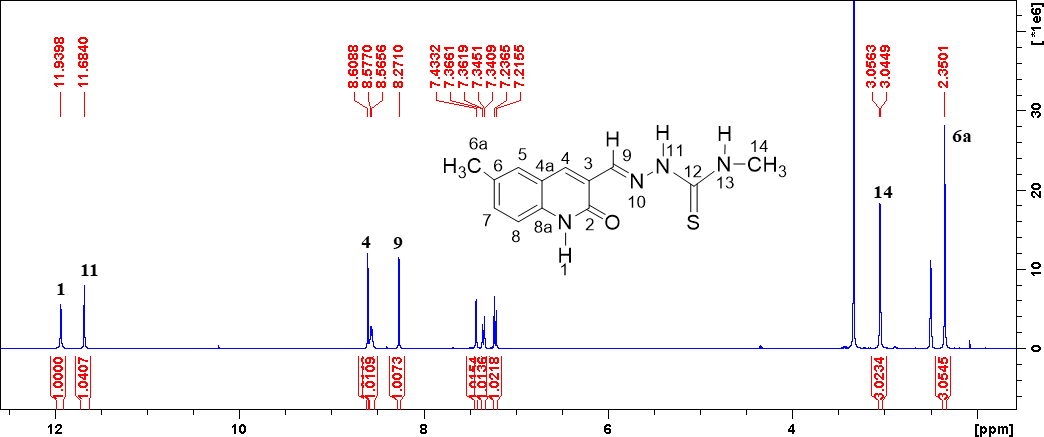
**Figure S 24** Expanded 1H NMR spectrum of **5f**



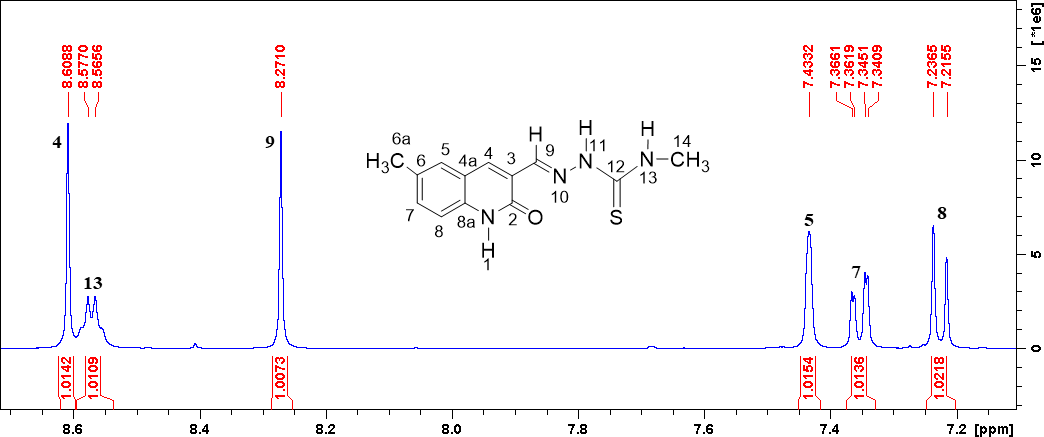
**Figure S 25** 13C NMR spectrum of **5f**



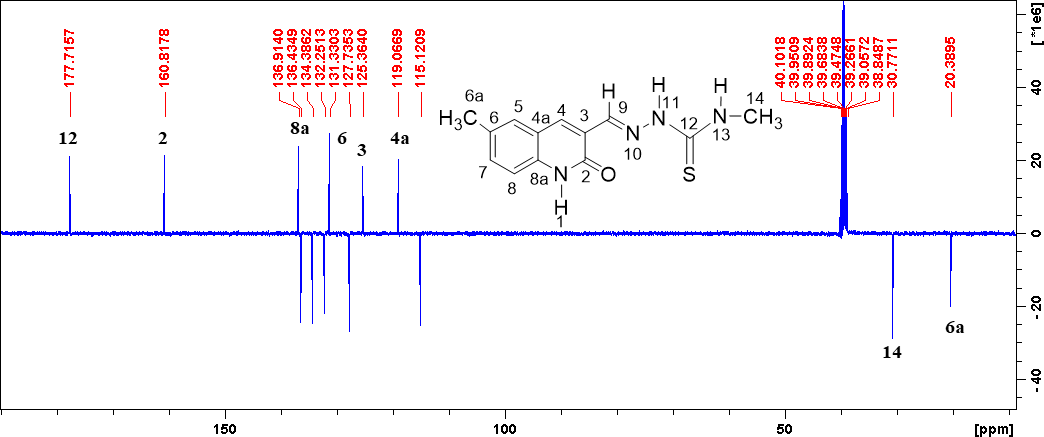
**Figure S 26** Expanded 13C NMR spectrum of **5f**



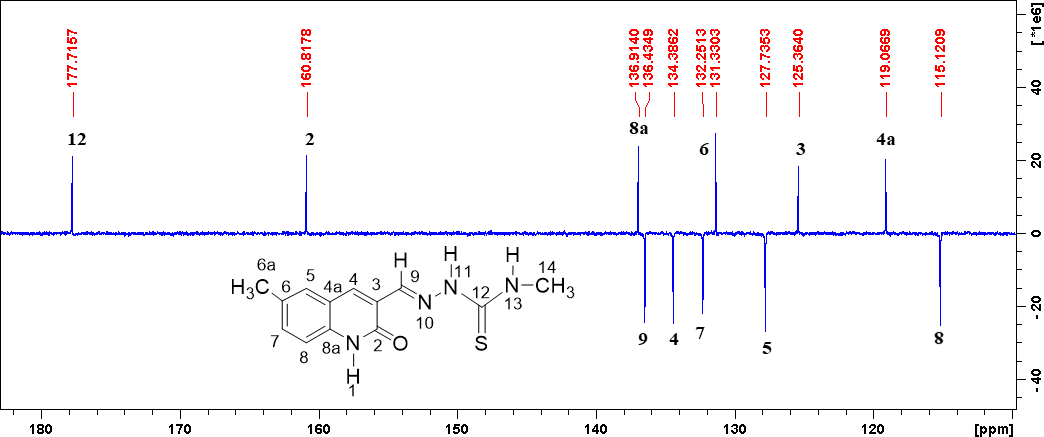
**Figure S 27** 1H NMR spectrum of **5g**



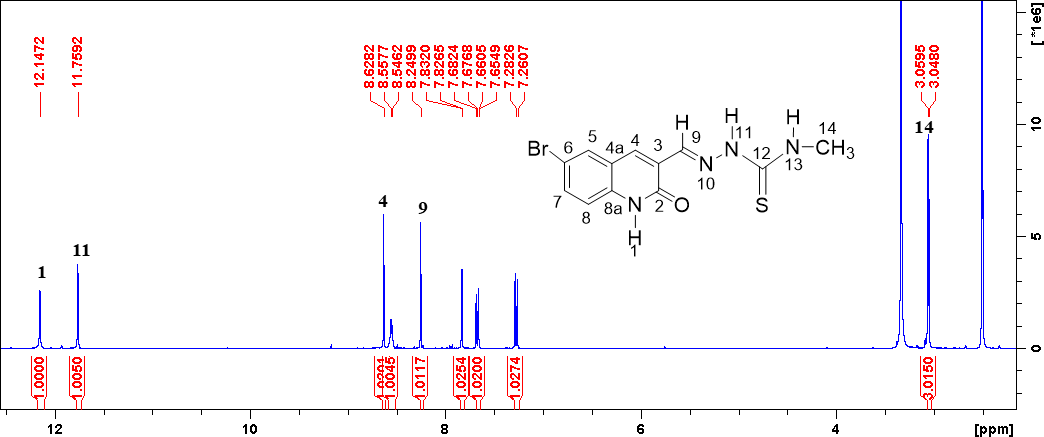
**Figure S 28** Expanded 1H NMR spectrum of **5g**



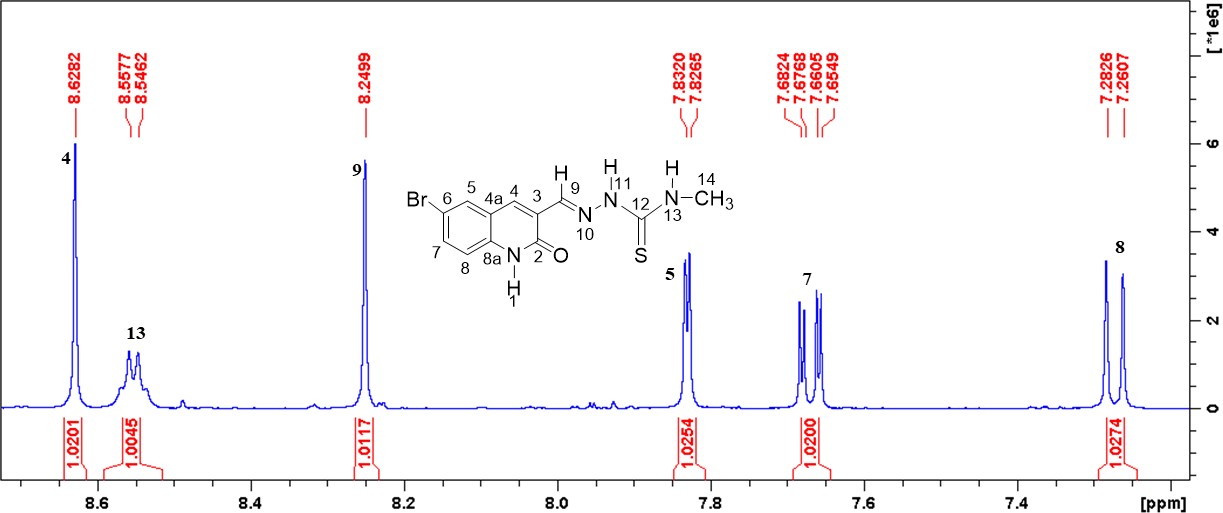
**Figure S 29** 13C NMR spectrum of **5g**



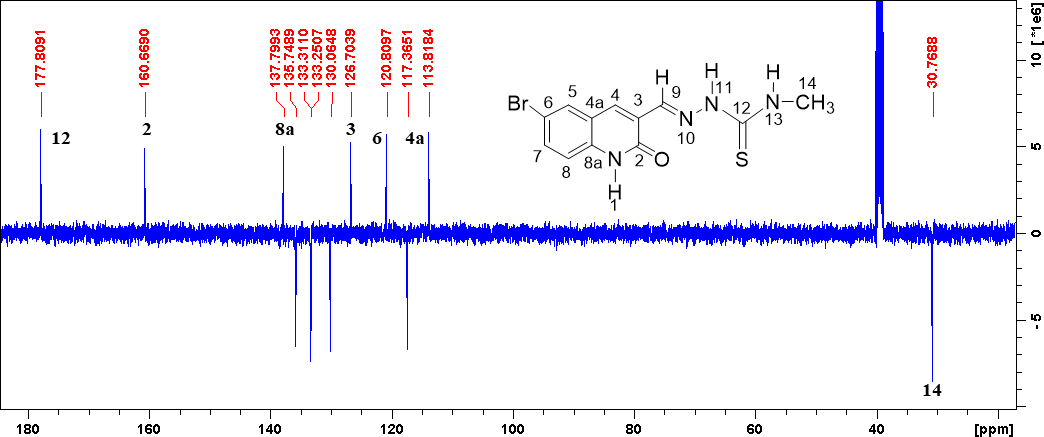
**Figure S 30** Expanded 13C NMR spectrum of **5g**



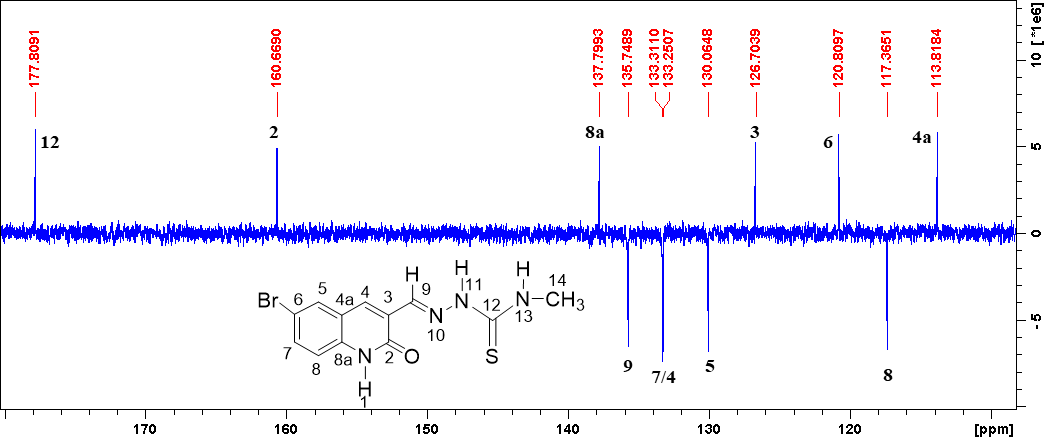
**Figure S 31** 1H NMR spectrum of **5h**



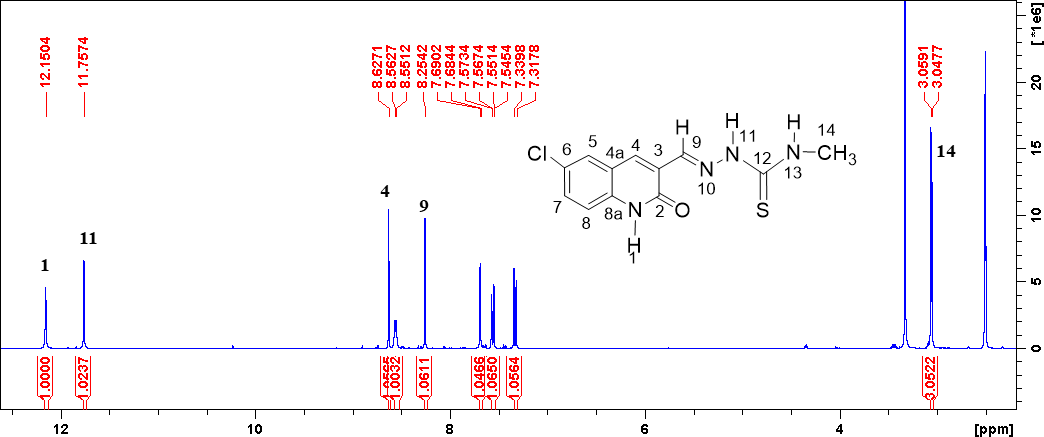
**Figure S 32** Expanded 1H NMR spectrum of **5h**



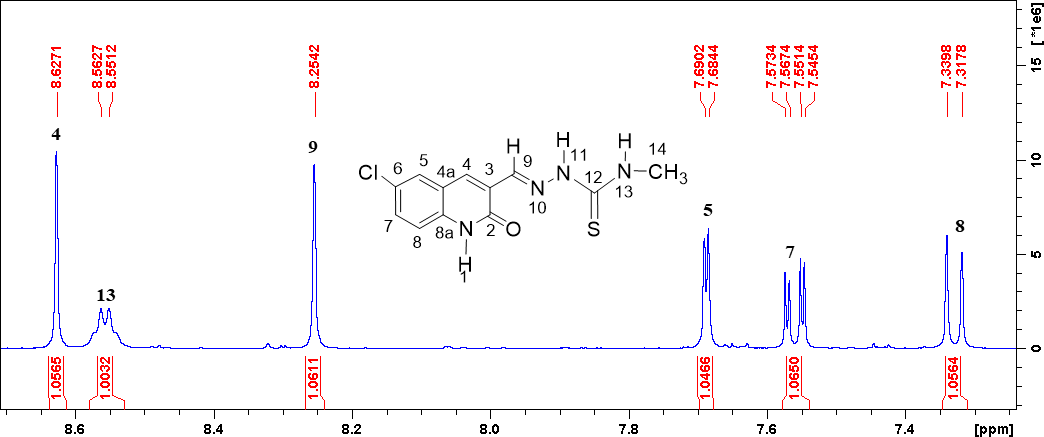
**Figure S 33** 13C NMR spectrum of **5h**



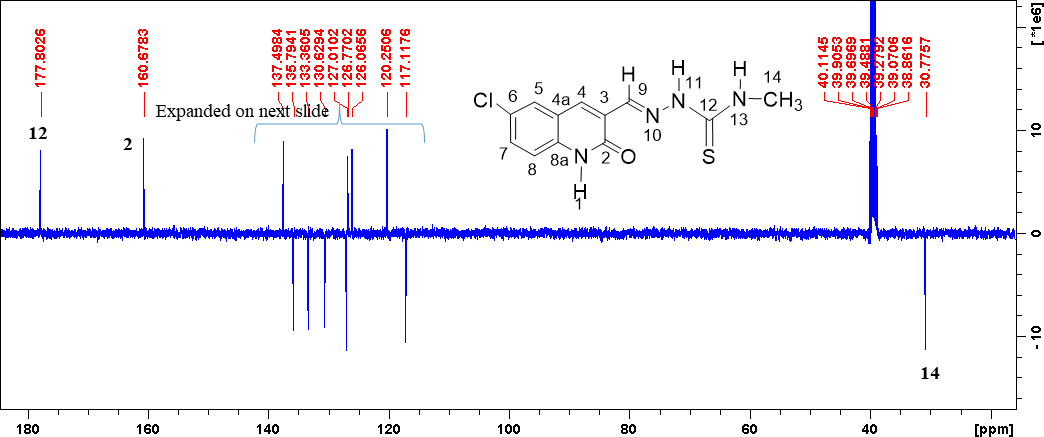
**Figure S 34** Expanded 13C NMR spectrum of **5h**



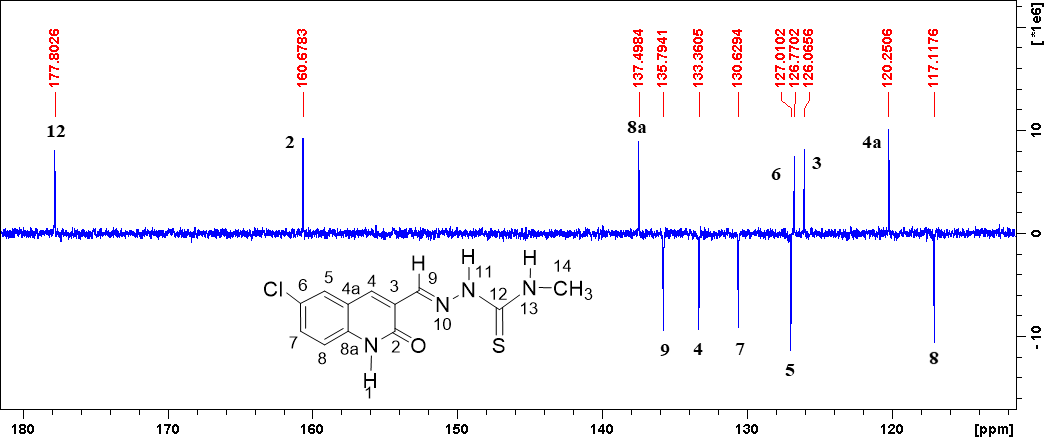
**Figure S 35** 1H NMR spectrum of **5i**



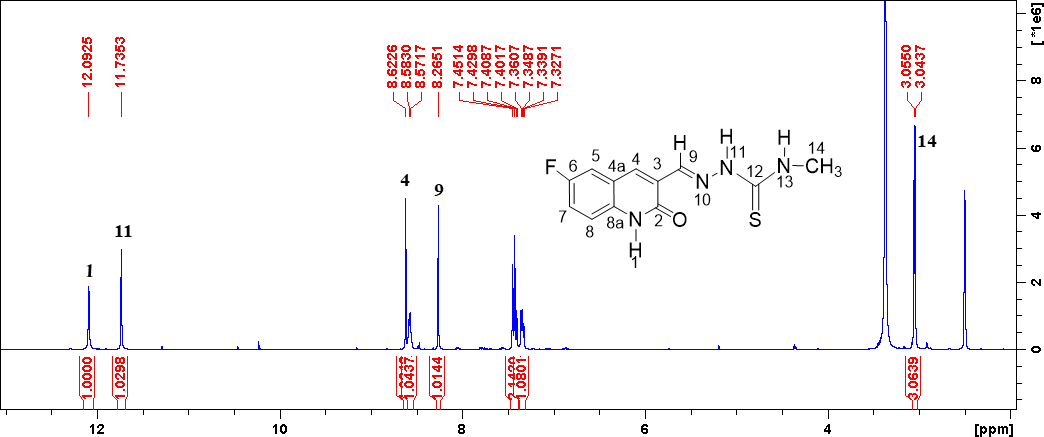
**Figure S 36** Expanded 1H NMR spectrum of **5i**



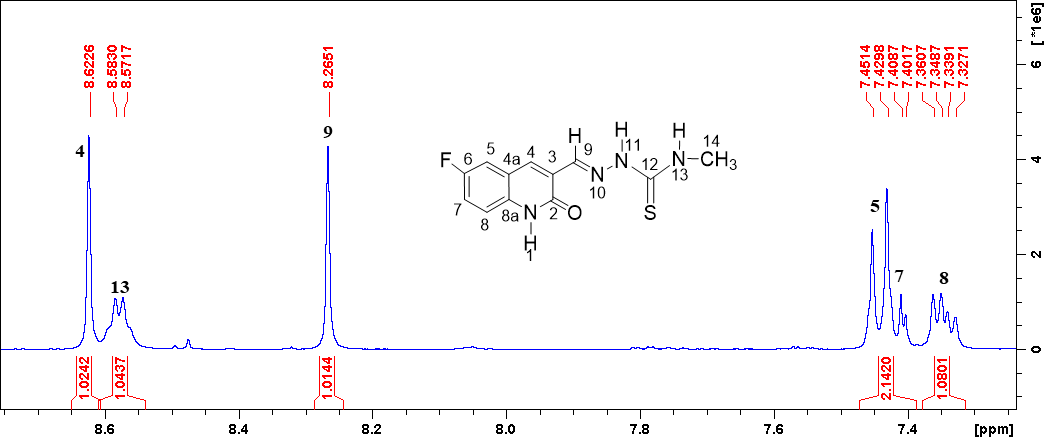
**Figure S 37** 13C NMR spectrum of **5i**



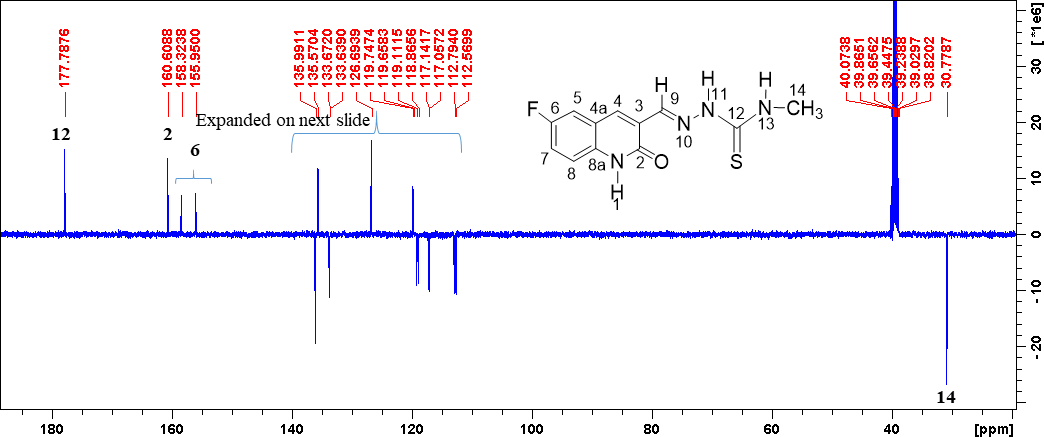
**Figure S 38** Expanded 13C NMR spectrum of **5i**



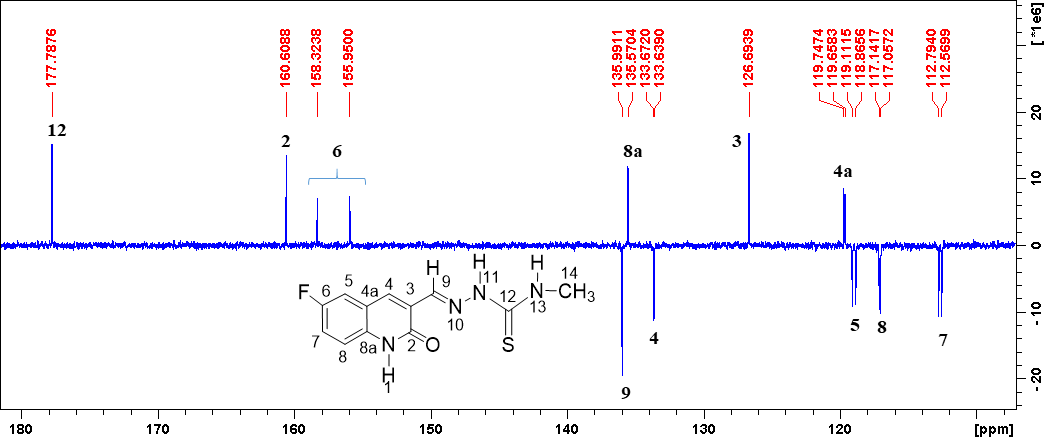
**Figure S 39** 1H NMR spectrum of **5j**



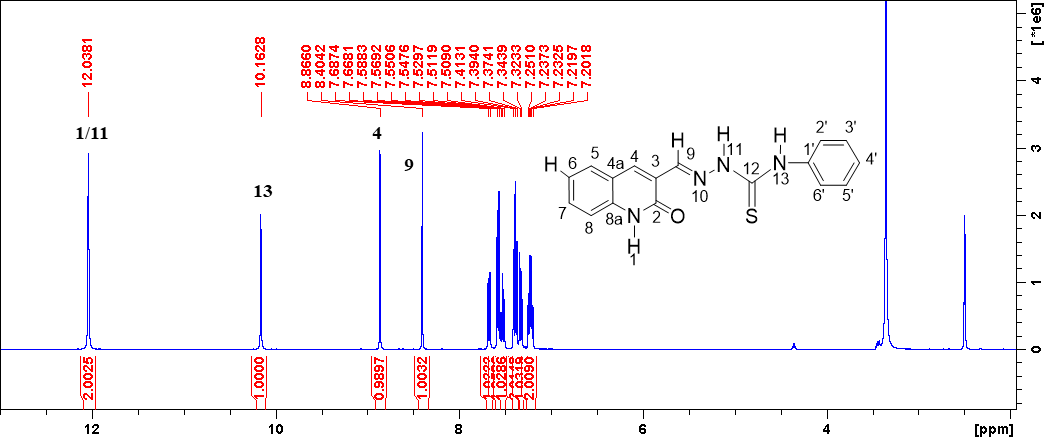
**Figure S 40** Expanded 1H NMR spectrum of **5j**



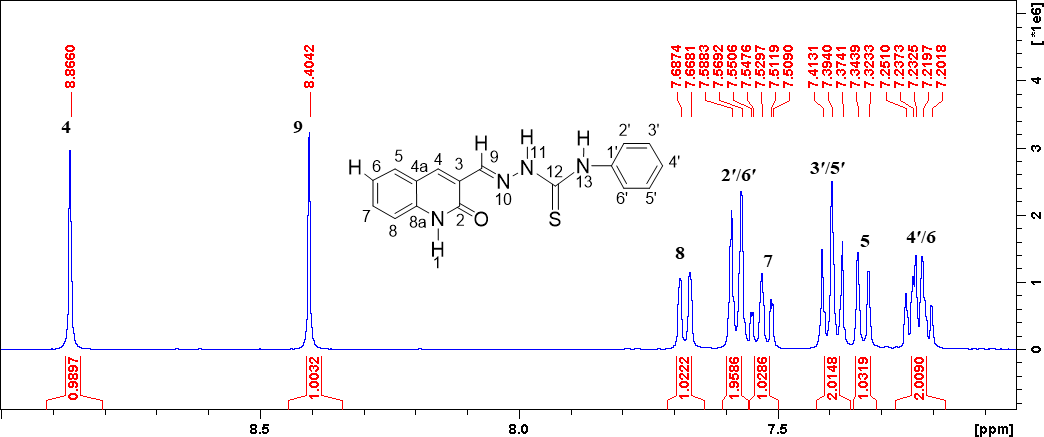
**Figure S 41** 13C NMR spectrum of **5j**



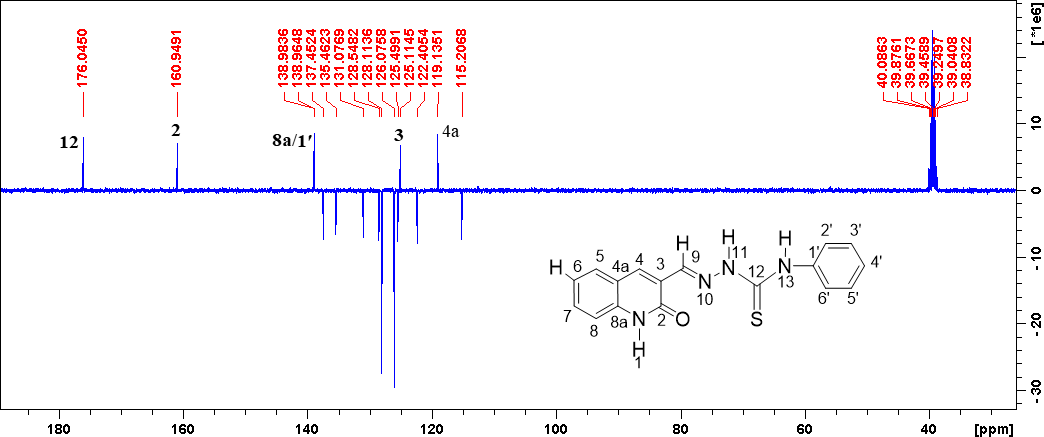
**Figure S 42** Expanded 13C NMR spectrum of **5j**



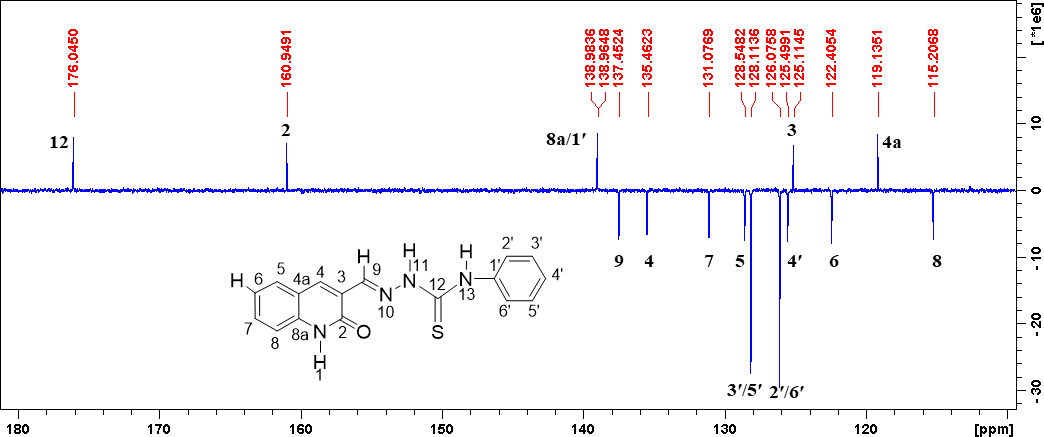
**Figure S 43** 1H NMR spectrum of **5k**



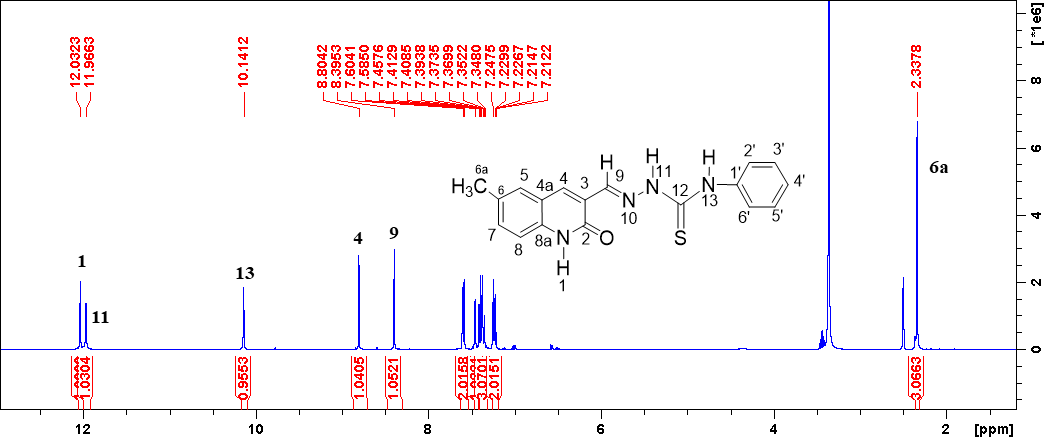
**Figure S 44** Expanded 1H NMR spectrum of **5k**



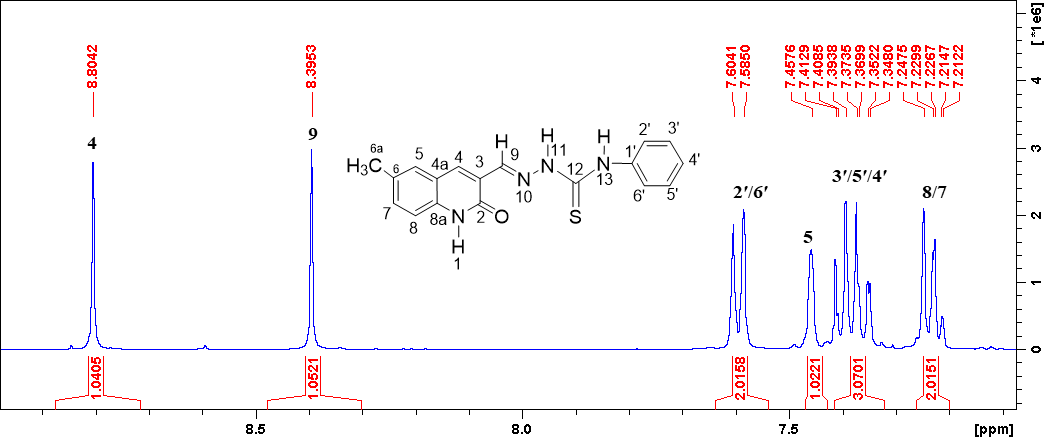
**Figure S 45** 13C NMR spectrum of **5k**



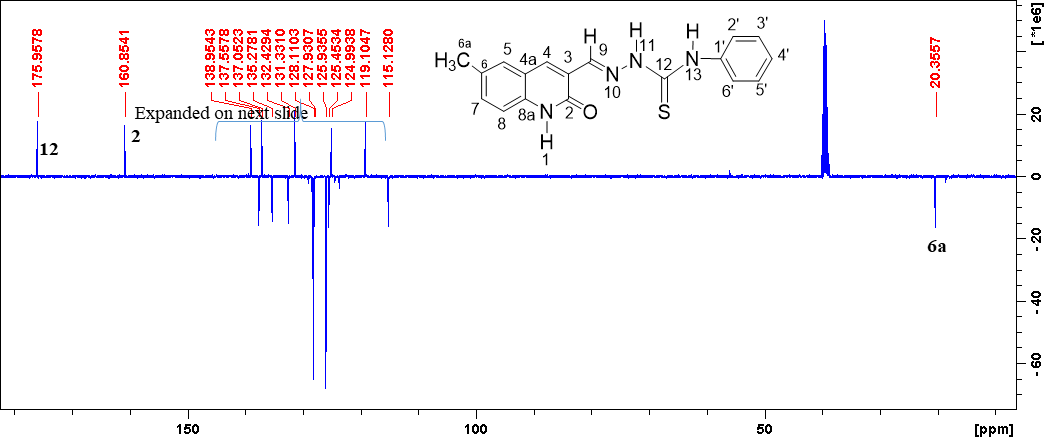
**Figure S 46** Expanded 13C NMR spectrum of **5k**



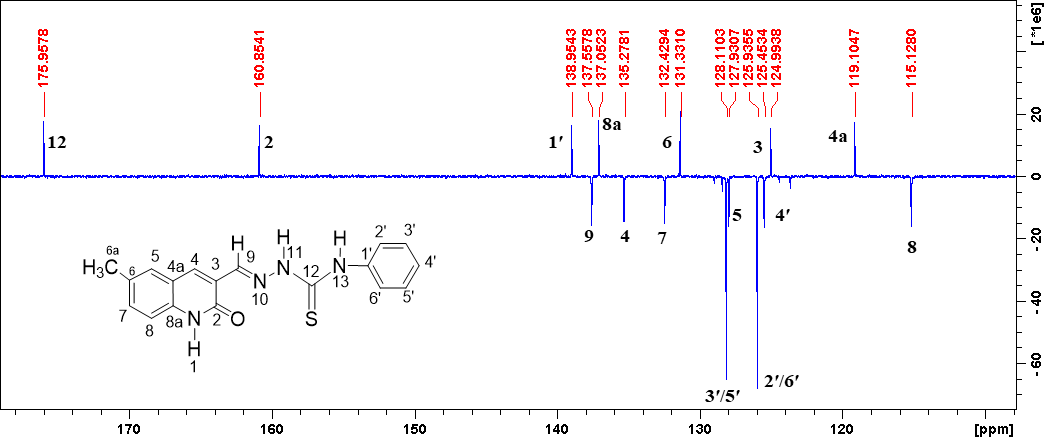
**Figure S 47** 1H NMR spectrum of **5l**



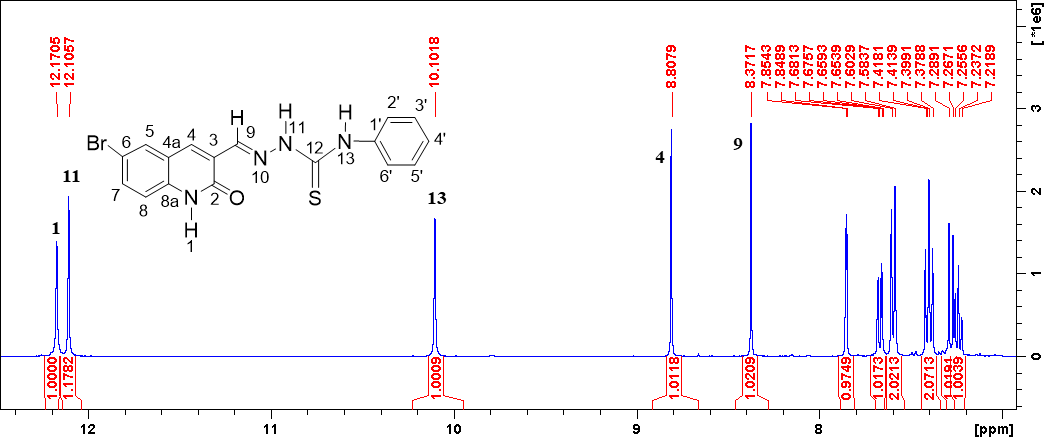
**Figure S 48** Expanded 1H NMR spectrum of **5l**



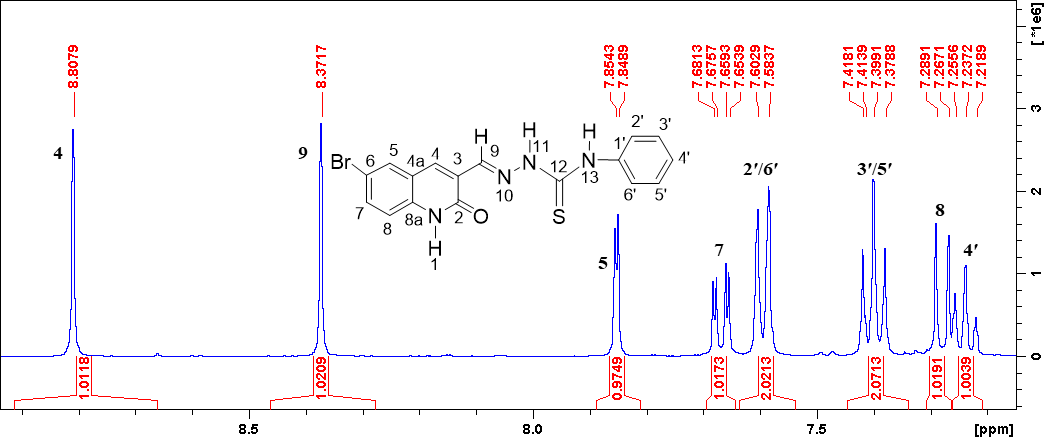
**Figure S 49** 13C NMR spectrum of **5l**



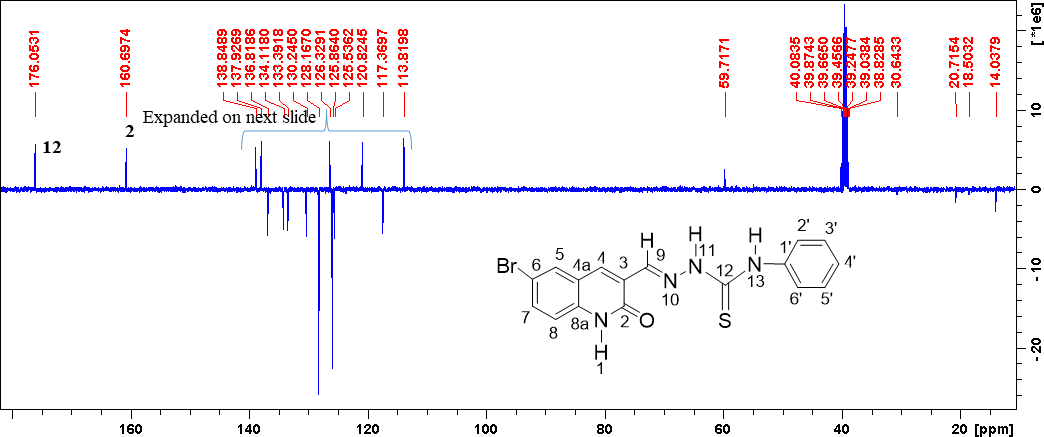
**Figure S 50** Expanded 13C NMR spectrum of **5l**



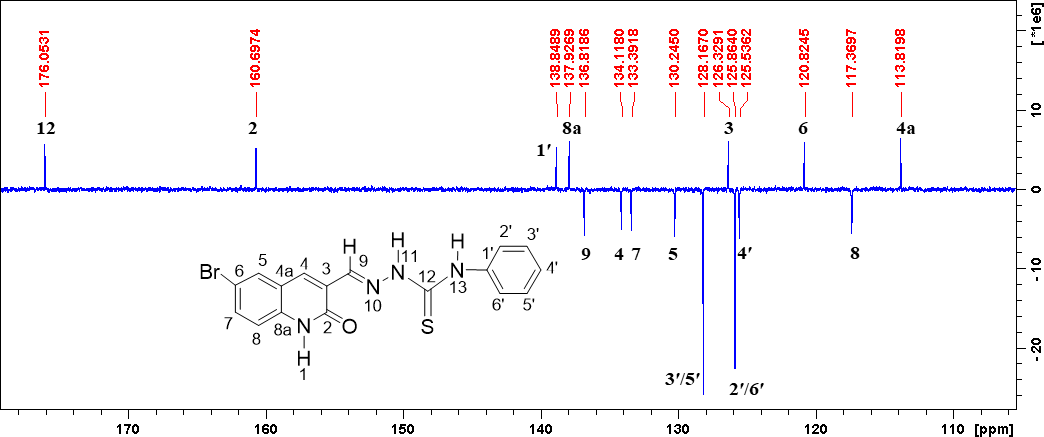
**Figure S 51** 1H NMR spectrum of **5m**



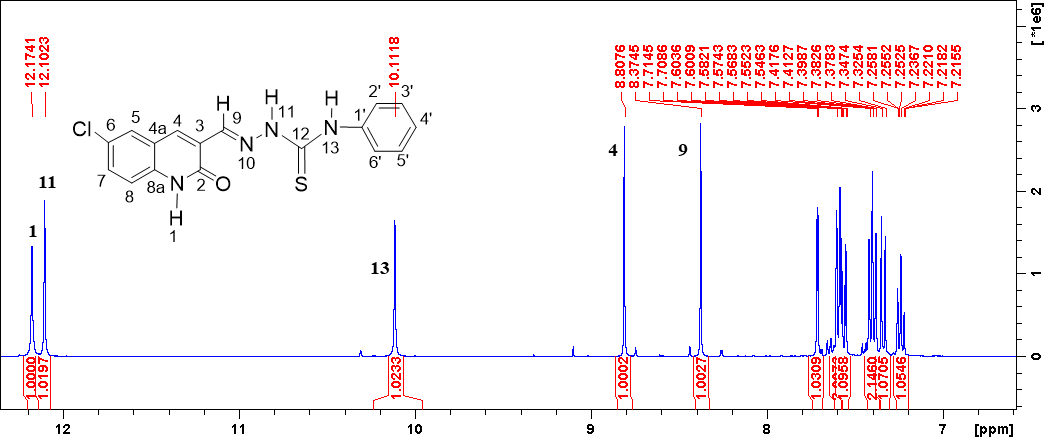
**Figure S 52** Expanded 1H NMR spectrum of **5m**



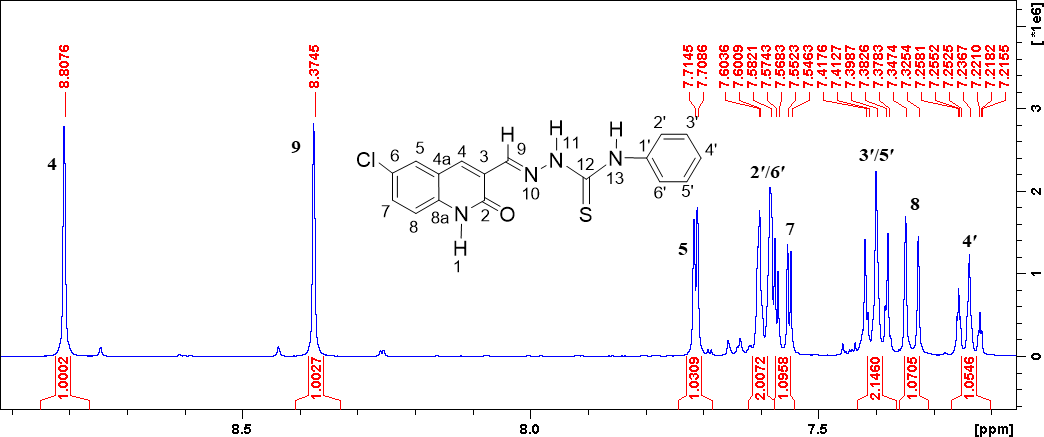
**Figure S 53** 13C NMR spectrum of **5m**



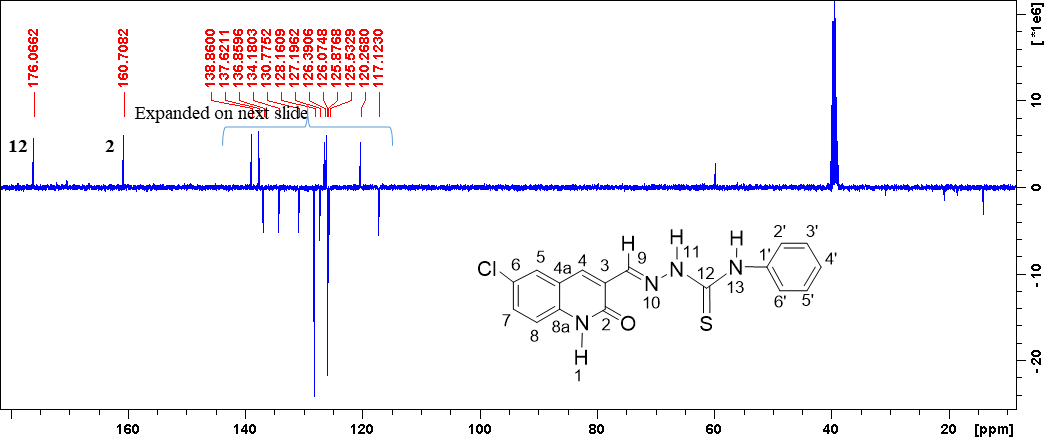
**Figure S 54** Expanded 13C NMR spectrum of **5m**



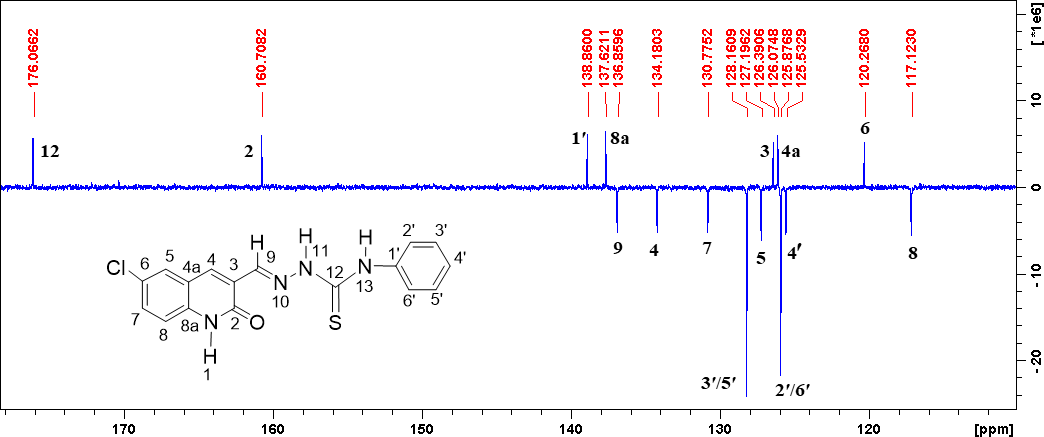
**Figure S 55** 1H NMR spectrum of **5n**



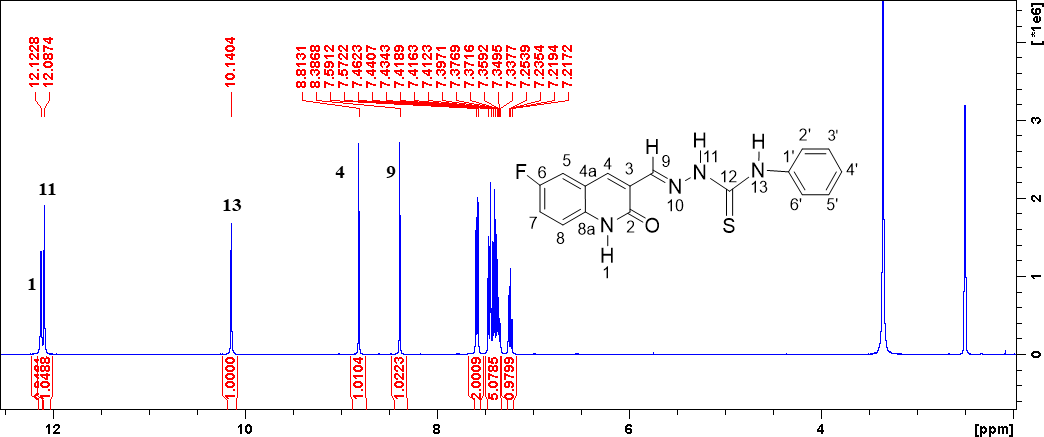
**Figure S 56** Expanded 1H NMR spectrum of **5n**



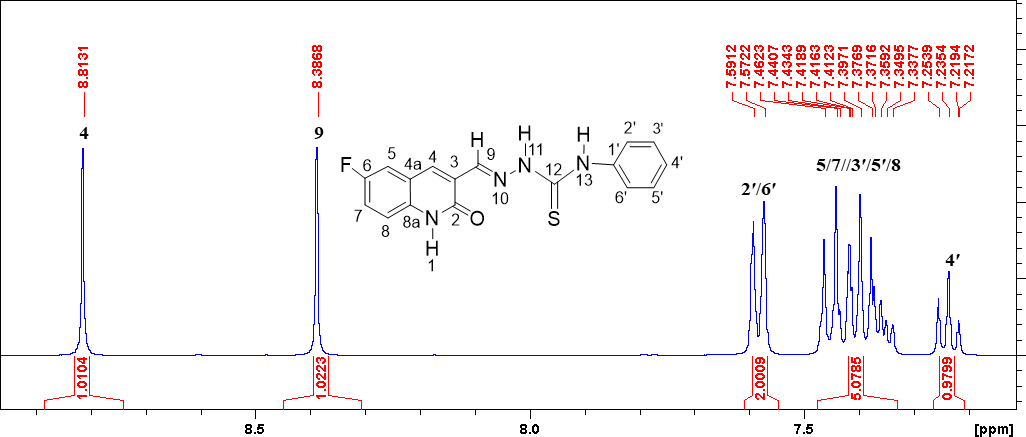
**Figure S 57** 13C NMR spectrum of **5n**



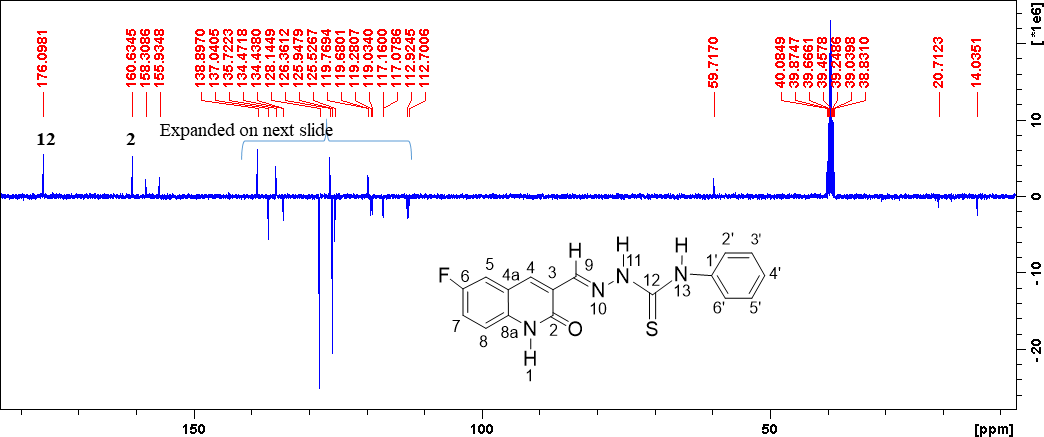
**Figure S 58** Expanded 13C NMR spectrum of **5n**



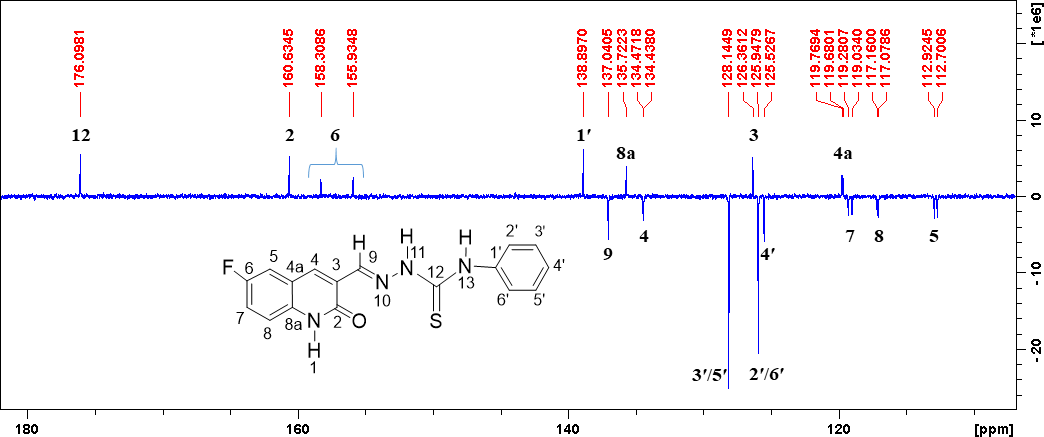
**Figure S 59** 1H NMR spectrum of **5o**



**Figure S 60** Expanded 1H NMR spectrum of **5o**



**Figure S 61** 13C NMR spectrum of **5o**



**Figure S 62** Expanded 13C NMR spectrum of **5o**