

## **Supporting information**

**For**

**Benzo[*d*]thiazole-2-thiol bearing 2-oxo-2-substituted-phenylethan-1-yl as potent selective *lasB* quorum sensing inhibitors of gram-negative bacteria.**

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## 1. Cytotoxicity Assay.

The method was described previously [1]. Firstly, the stock solution of the active compounds **3**, **6**, **7** was prepared in DMSO as 200 µg/mL. The testing concentrations were prepared from stock solution by diluting in growth medium (90% high glucose medium supplemented with 10% fetal bovine serum). The HeLa cells were grown as monolayers in the growth medium at 37°C (atmosphere containing 5% CO<sub>2</sub>). When cells reached 70% confluence were detached from the culture flask with 5% trypsin-EDTA and resuspended in fresh culture media at a density of 5 x 10<sup>4</sup> cells/mL. By use of a Falcon 24-well, flat bottom plate, 500 µL of the cell suspension was added to each of the wells, and the cells were incubated for 24h at 37°C. Then the active compounds (with concentrations of 1 to 200 µg/mL) were added to each cell in triplicates and incubated for 24 h. The cytotoxicity was performed using the in vitro toxicology assay kit, MTT based (Sigma). Absorbance values were measured at 570 nm and 690 nm. The absorbance values measured at 690 nm were subtracted from the values measured at 570 nm when the data was analyzed. Data were normalized by subtracting the absorbance values of the growth medium treated equally than the rest of the samples.

[1] Truong-Thanh Tung, Trong T Dao, Marta G Junyent, Michael Palmgren, Thomas Günther-Pomorski, Anja T Fuglsang, Søren B Christensen, John Nielsen, *ChemMedChem*, **2018**, 13(1):37-47

## 2. Copy of NMR spectra of library compounds

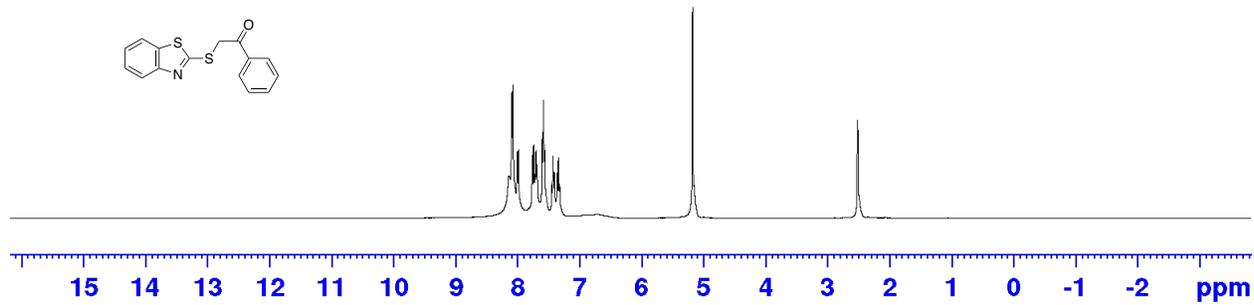


Figure S1. <sup>1</sup>H of compound 1

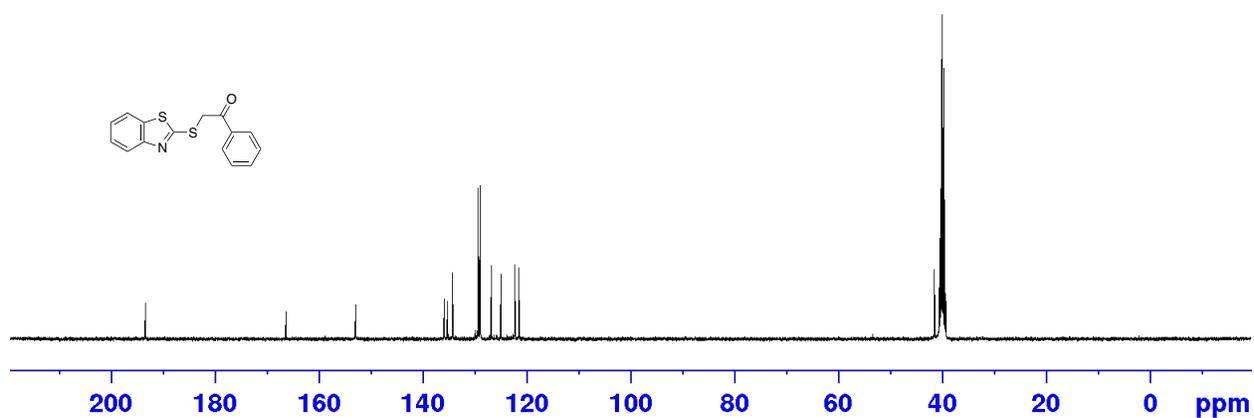


Figure S2. <sup>13</sup>C of compound 1

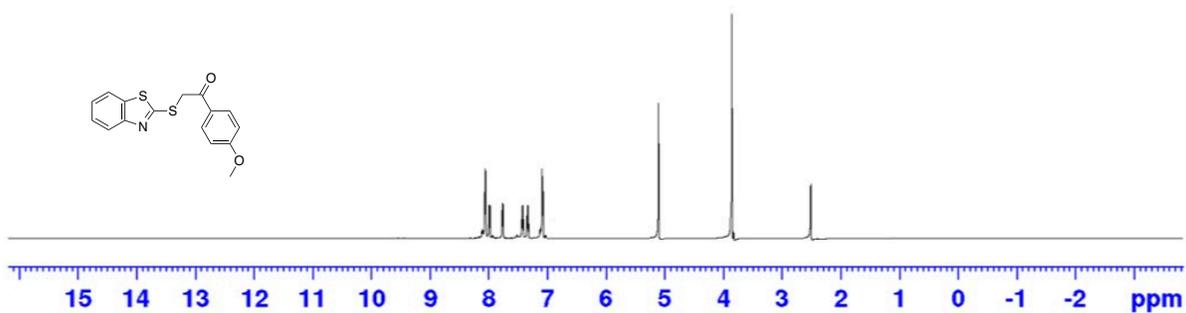
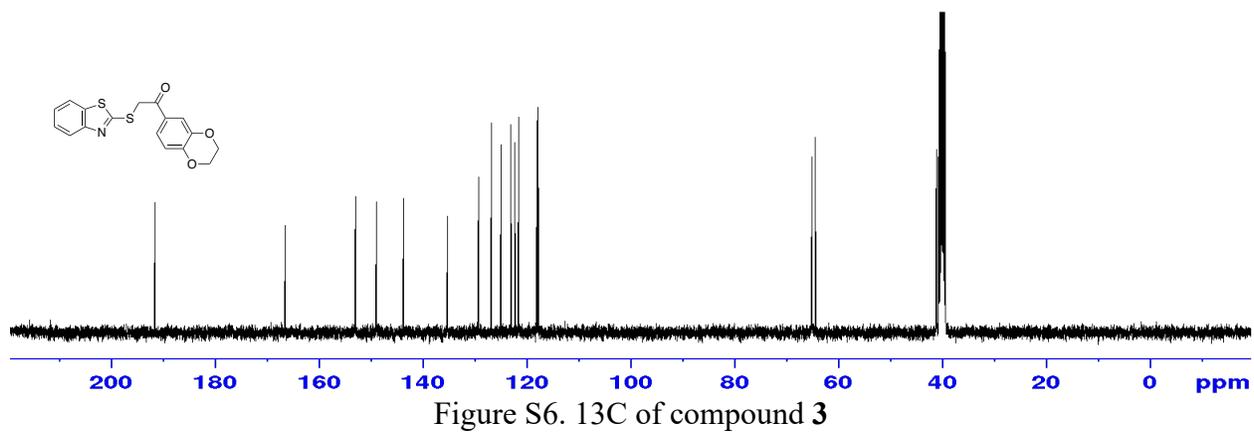
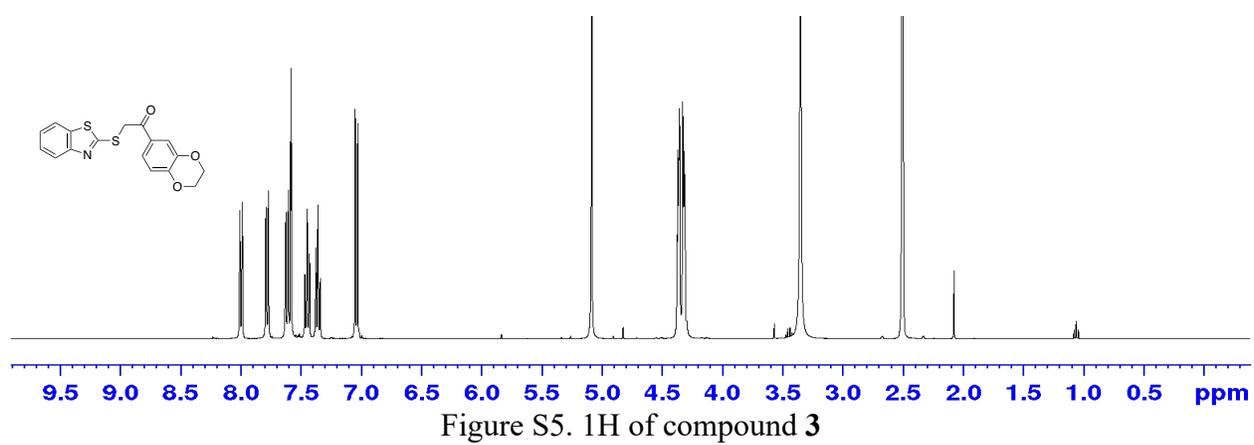
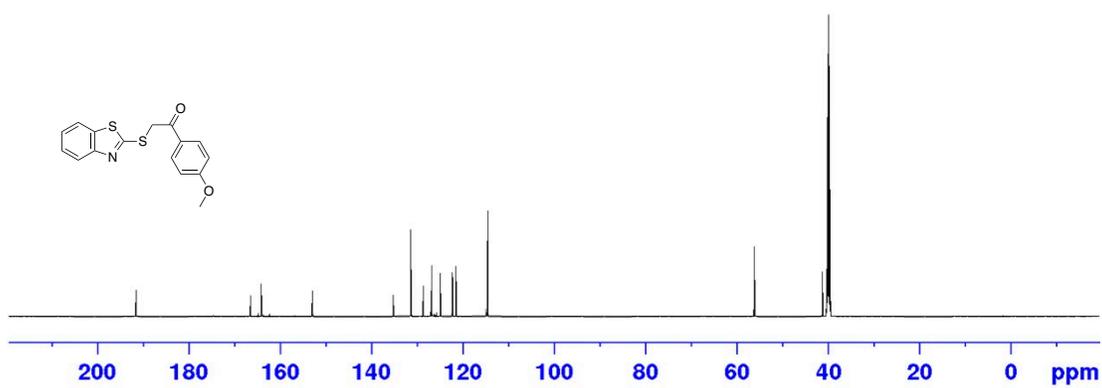


Figure S3. <sup>1</sup>H of compound 2



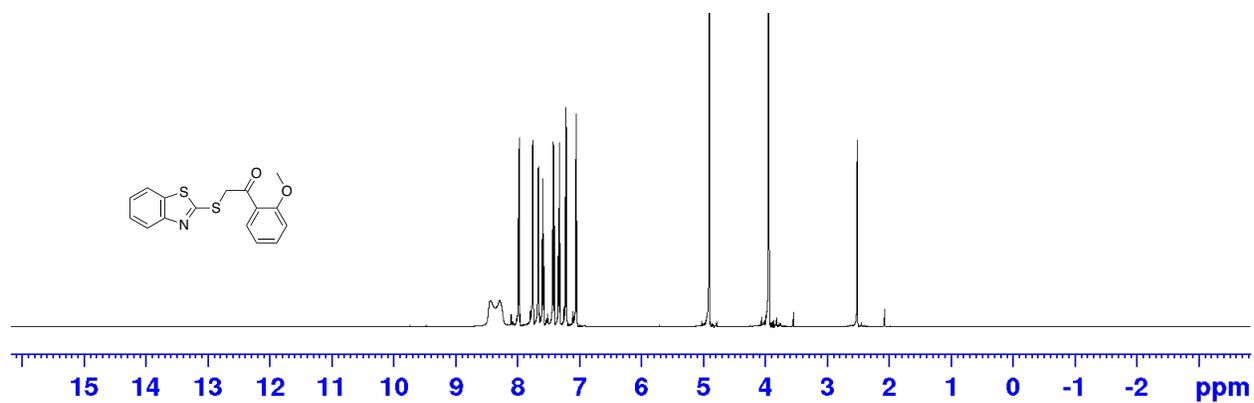


Figure S7. <sup>1</sup>H of compound 4

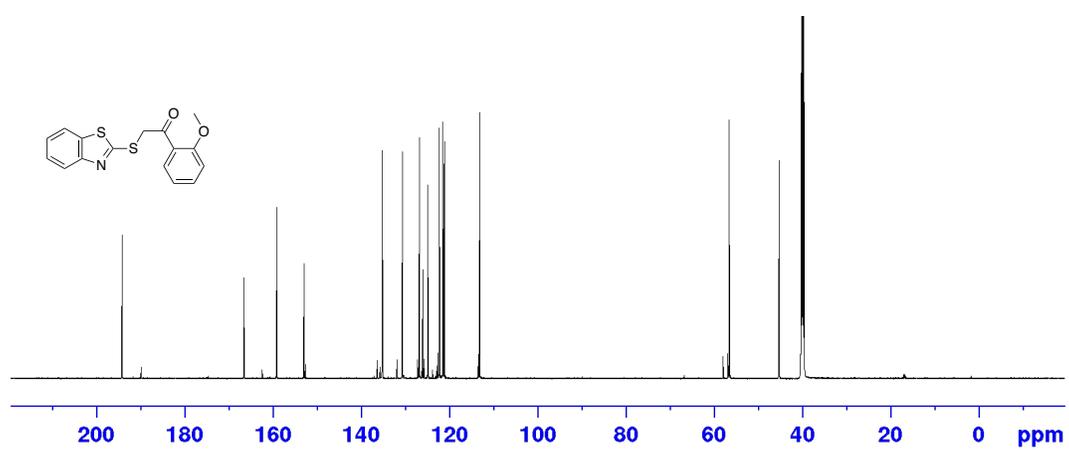


Figure S8. <sup>13</sup>C of compound 4

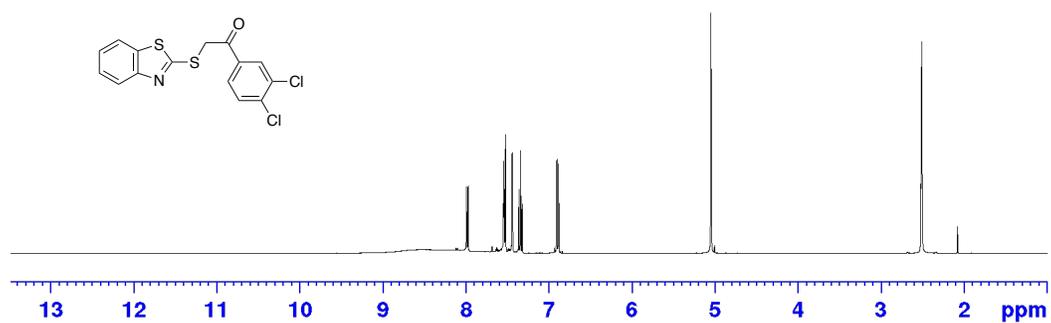


Figure S9. <sup>1</sup>H of compound 5

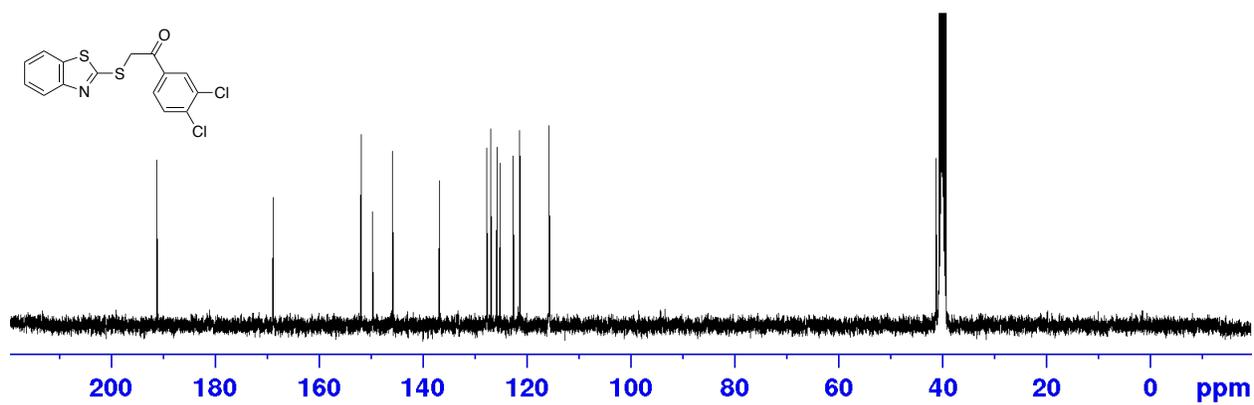


Figure S10. <sup>13</sup>C of compound 5

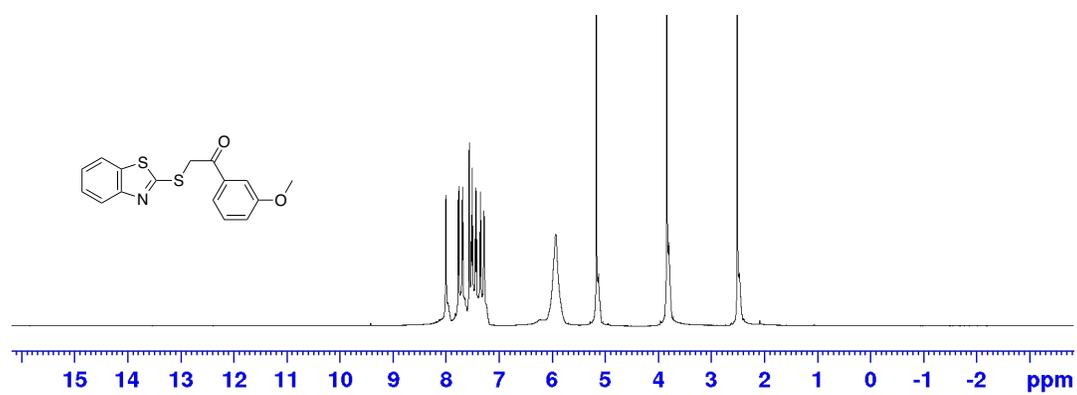


Figure S11. <sup>1</sup>H of compound 6

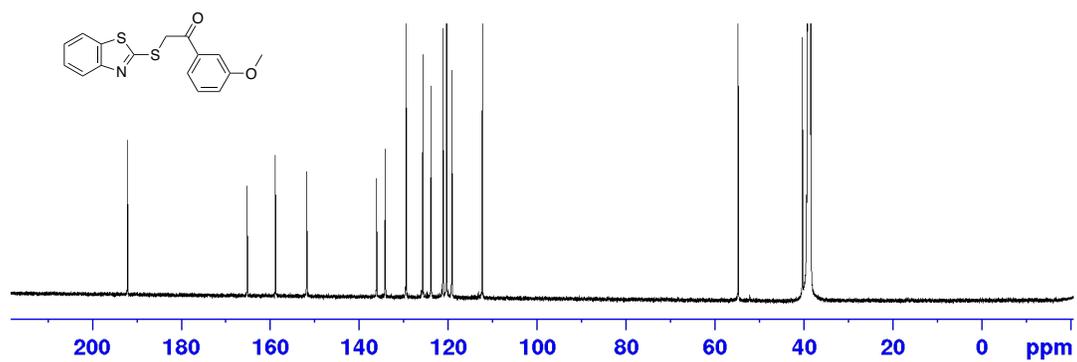


Figure S12. <sup>13</sup>C of compound 6

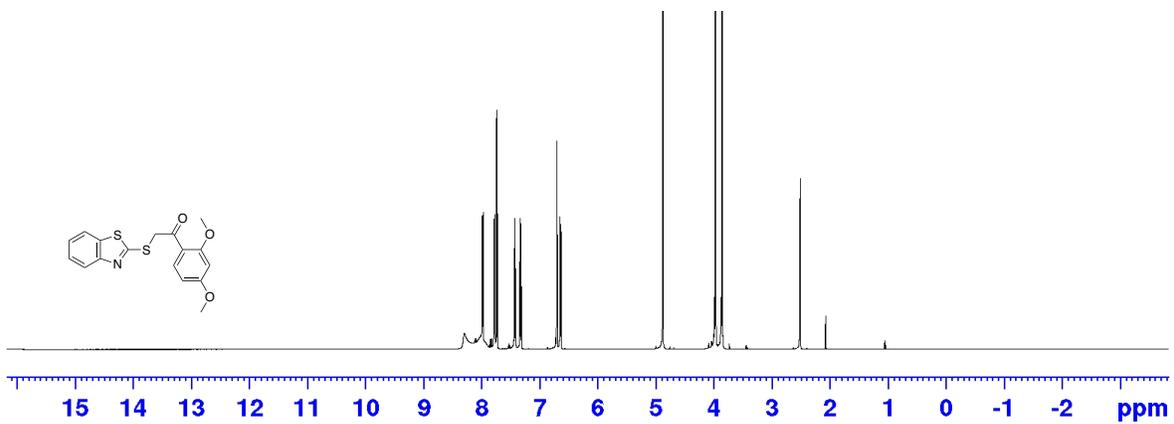


Figure S13. <sup>1</sup>H of compound 7

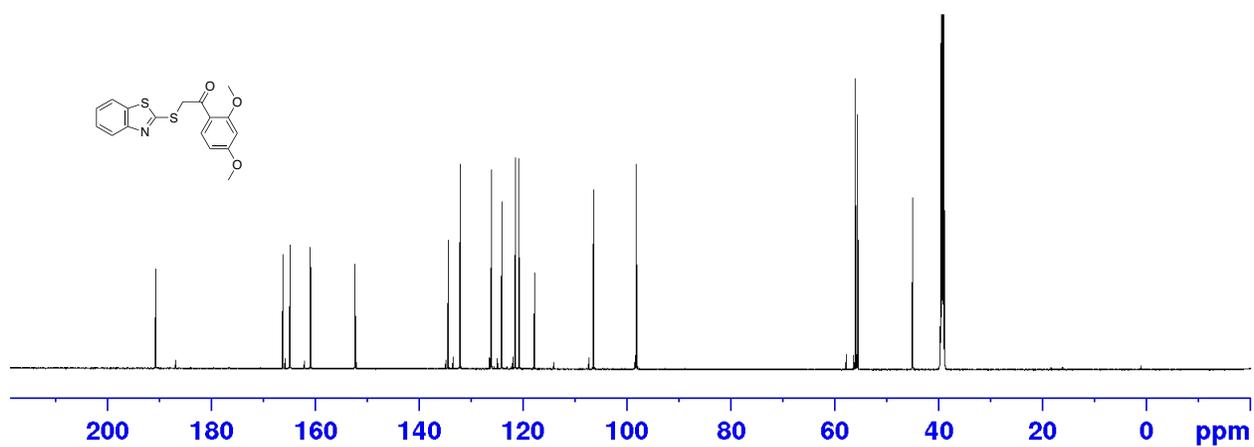


Figure S14. <sup>13</sup>C of compound 7

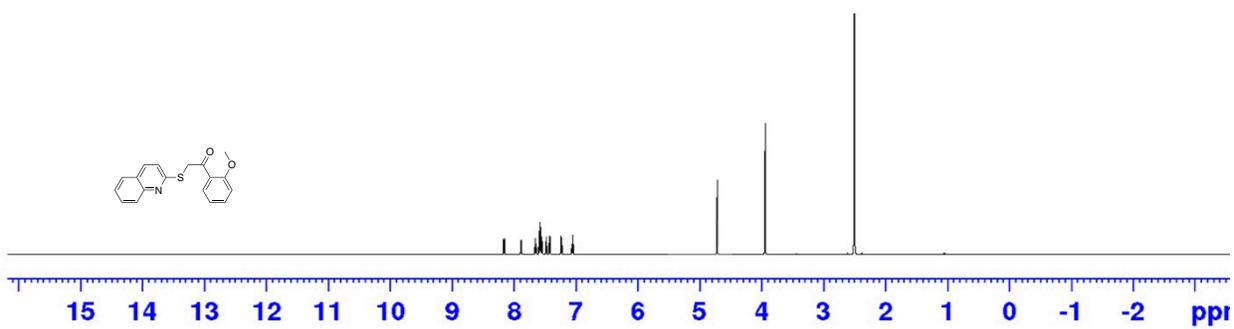


Figure S15. <sup>1</sup>H of compound 8

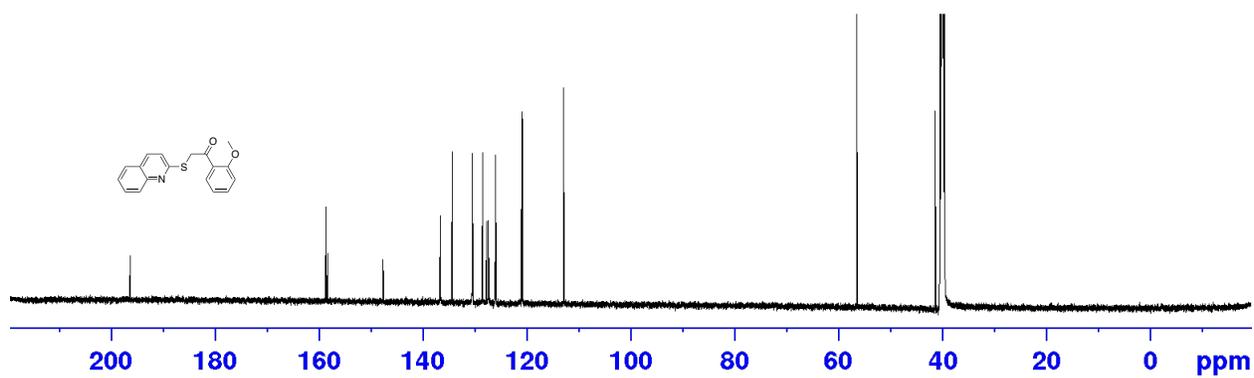


Figure S16. <sup>13</sup>C of compound 8

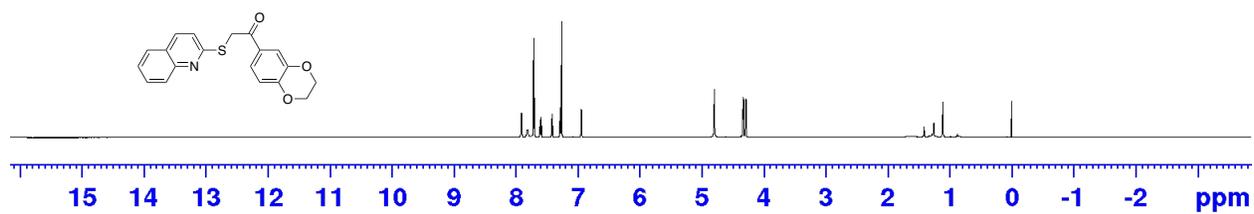


Figure S17. <sup>1</sup>H of compound 9

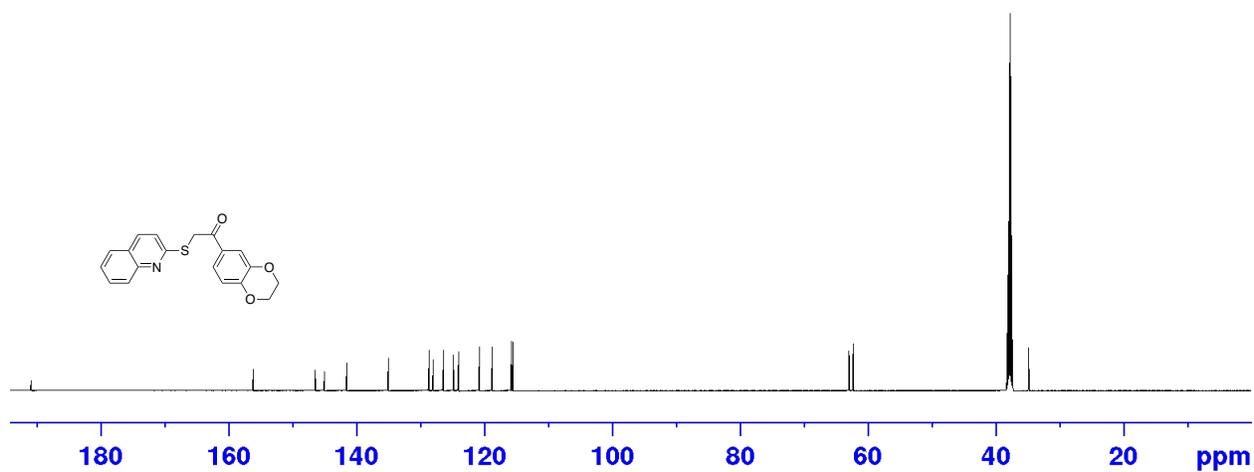


Figure S18. <sup>13</sup>C of compound 9

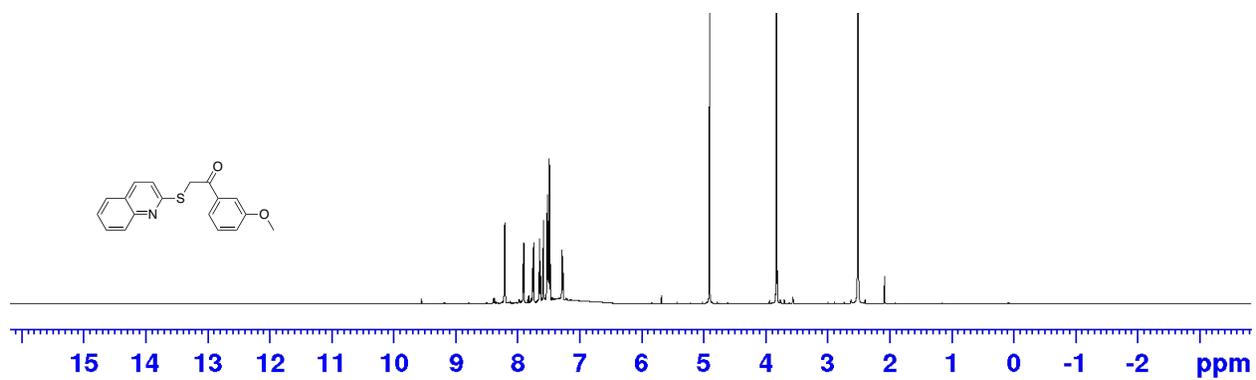


Figure S19. <sup>1</sup>H of compound **10**

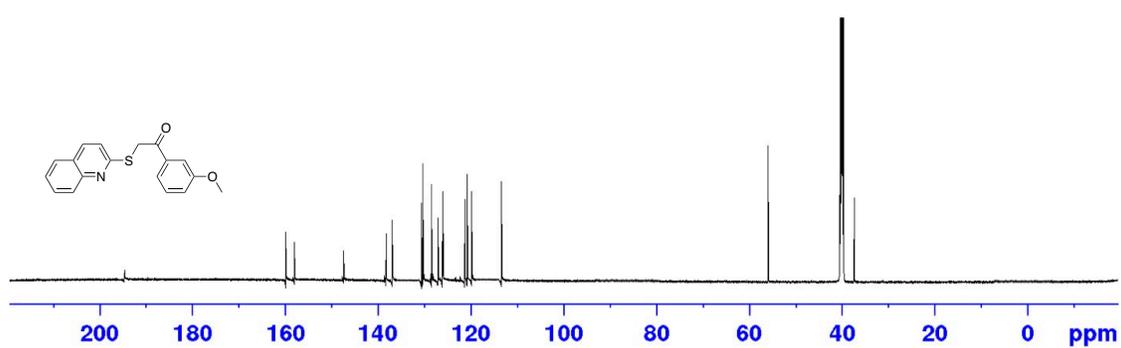


Figure S20. <sup>13</sup>C of compound **10**

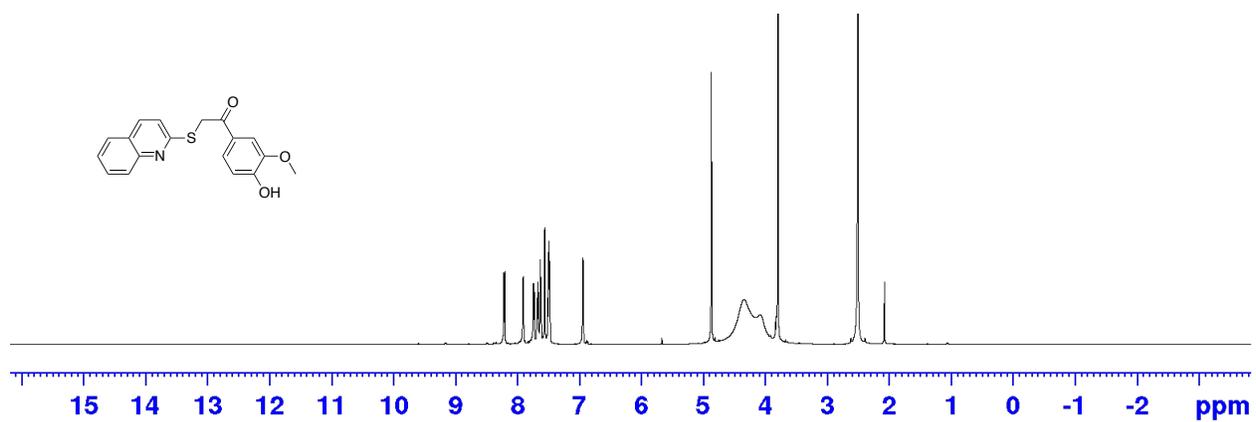
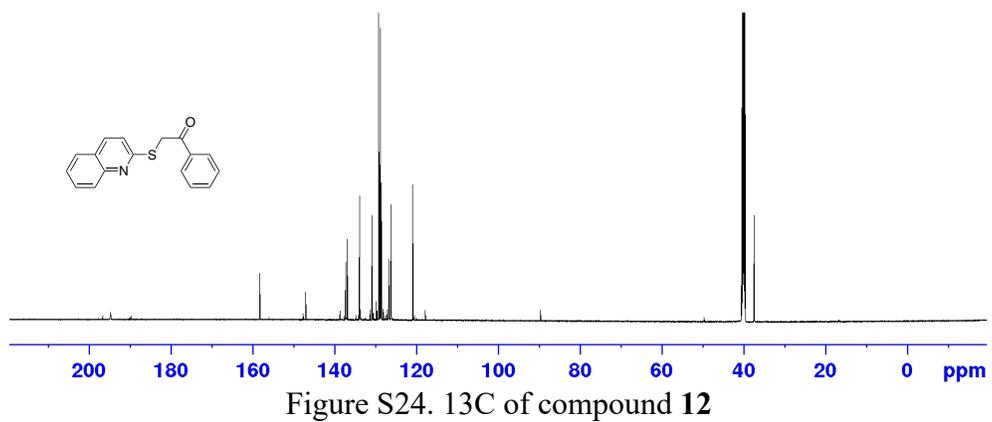
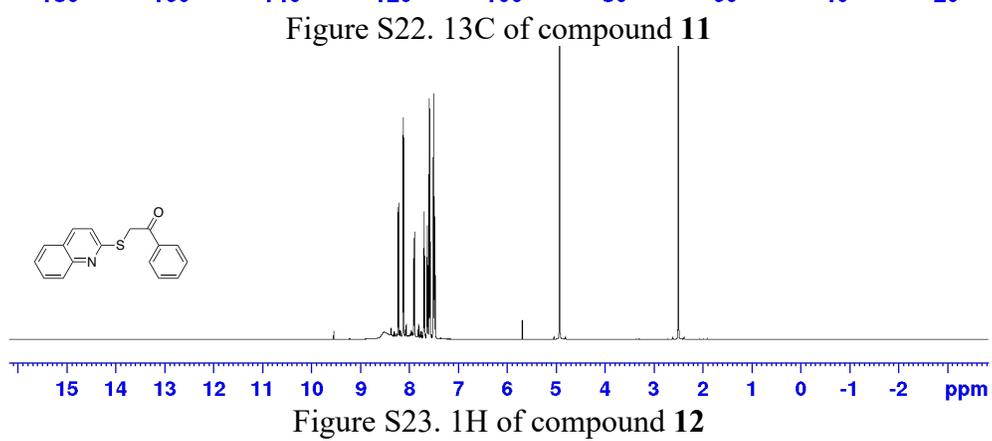
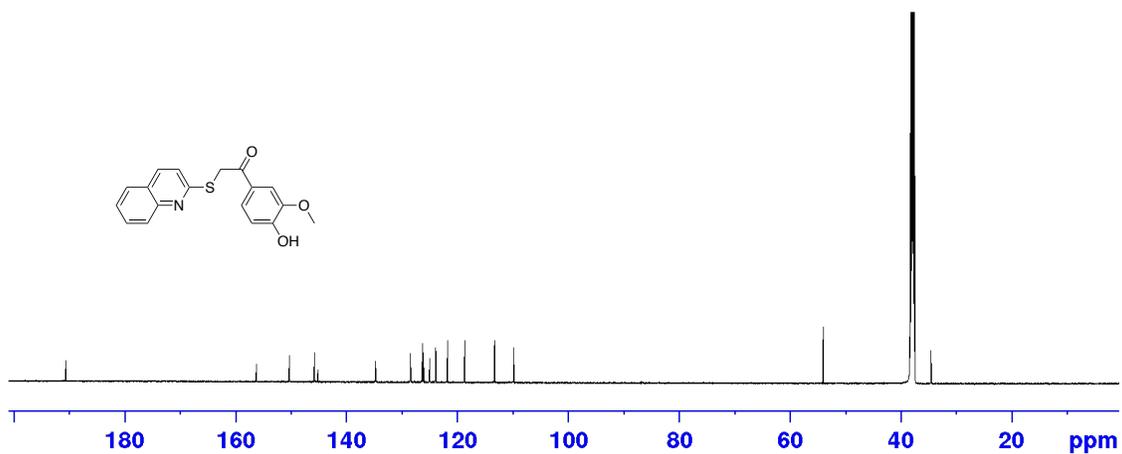


Figure S21. <sup>1</sup>H of compound **11**



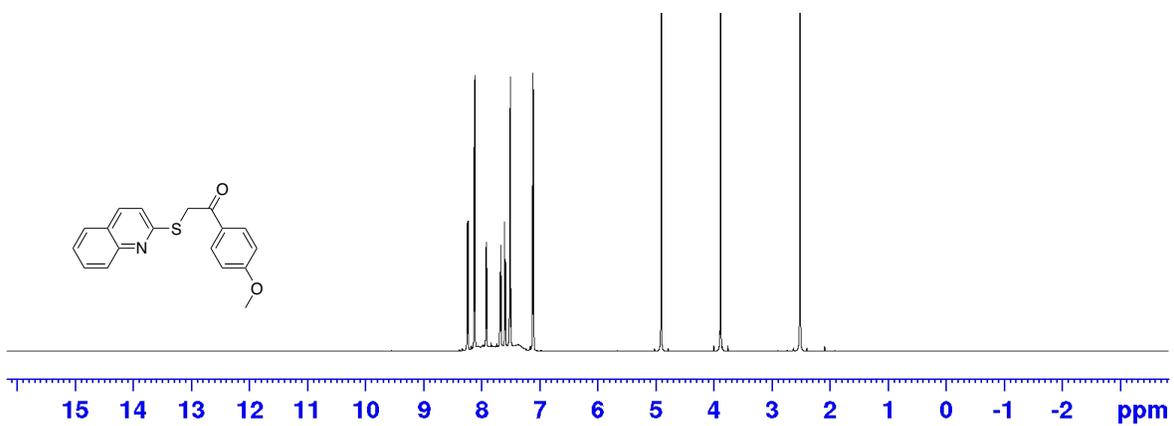


Figure S25. <sup>1</sup>H of compound **13**

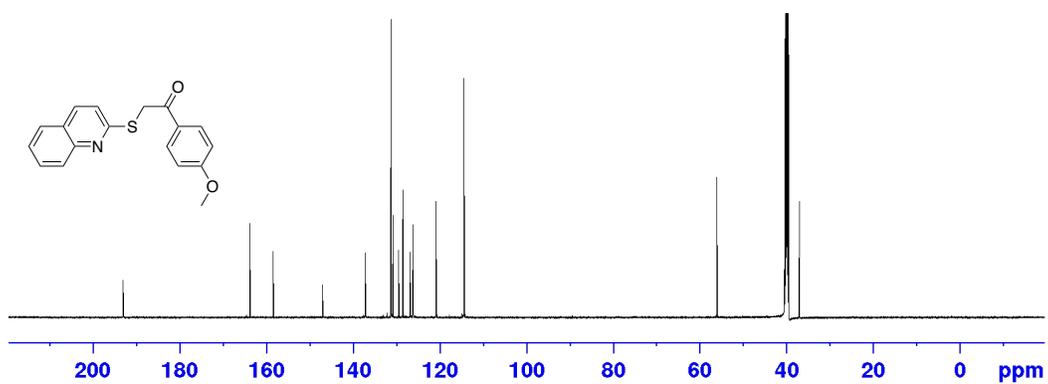


Figure S26. <sup>13</sup>C of compound **13**

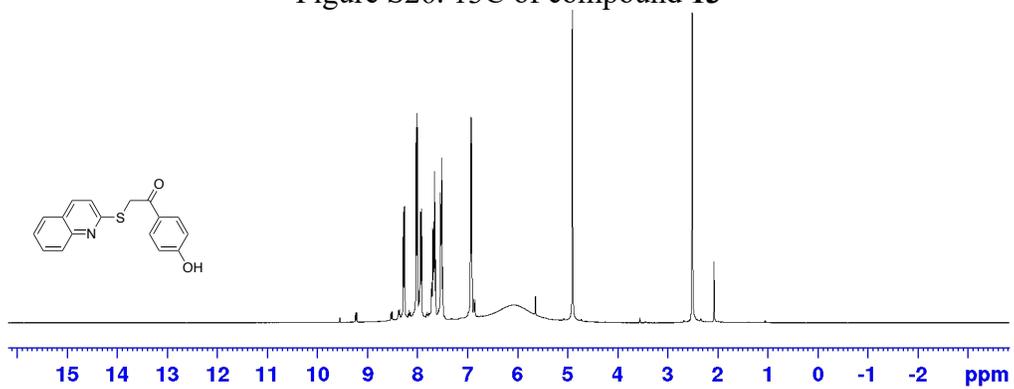


Figure S27. <sup>1</sup>H of compound **14**

