

Catalysts

Supporting Information

Organic Base-Catalyzed C–S Bond Construction from CO₂: A New Route for the Synthesis of Benzothiazolones

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This file includes:

1. Effect of various reaction conditions on the yield of benzothiazolone, Figures S1–S4
2. ¹H and ¹³C NMR spectra of the substrates, Figures S5–S8
3. ¹H and ¹³C NMR spectra of the products, Figures S9–S13
4. References

1 Effect of various reaction conditions on the yield of benzothiazolone

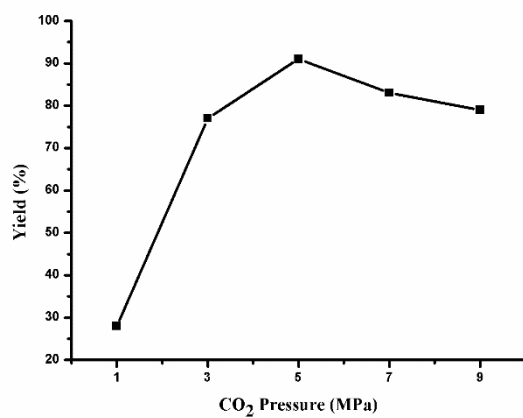


Figure S1. Effect of CO₂ pressure on the yield of benzothiazolone. Reaction conditions: 2-aminothiophenol, 2 mmol; DBN, 2 mmol; NMP, 2 mL; 150 °C; 24 h.

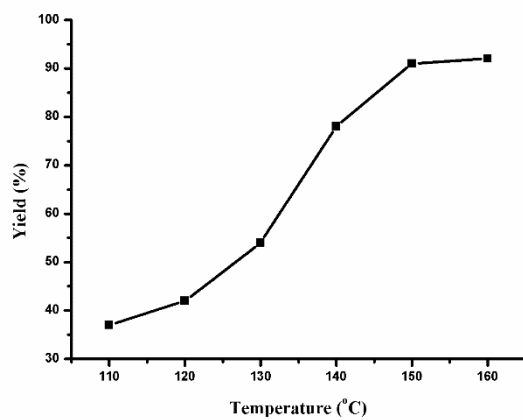


Figure S2. Reaction temperature dependence of benzothiazolone yield. Reaction conditions: 2-aminothiophenol, 2 mmol; DBN, 2 mmol; NMP, 2 mL; CO₂, 5 MPa; 24 h.

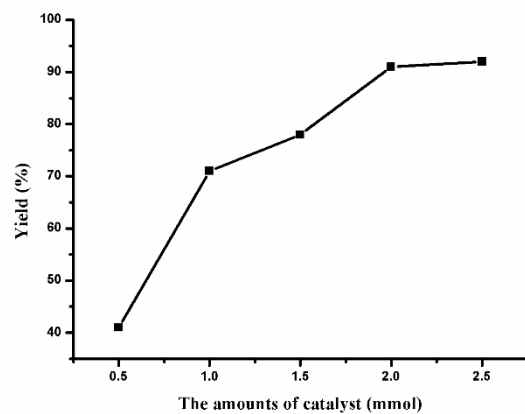


Figure S3. Influence of catalyst amount on the reaction outcome. Reaction conditions: 2-aminothiophenol, 2 mmol; NMP, 2 mL; CO₂, 5 MPa; 150 °C; 24 h.

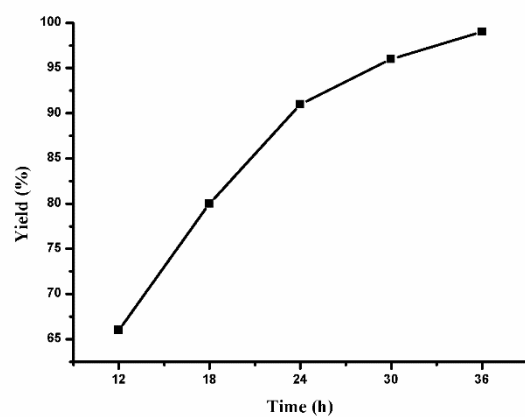


Figure S4. Dependence of benzothiazolone yield on reaction time. Reaction conditions: 2-aminothiophenol, 2 mmol; DBN, 2 mmol; NMP, 2 mL; CO₂, 5 MPa; 150 °C.

2 ¹H and ¹³C NMR spectra of the substrates

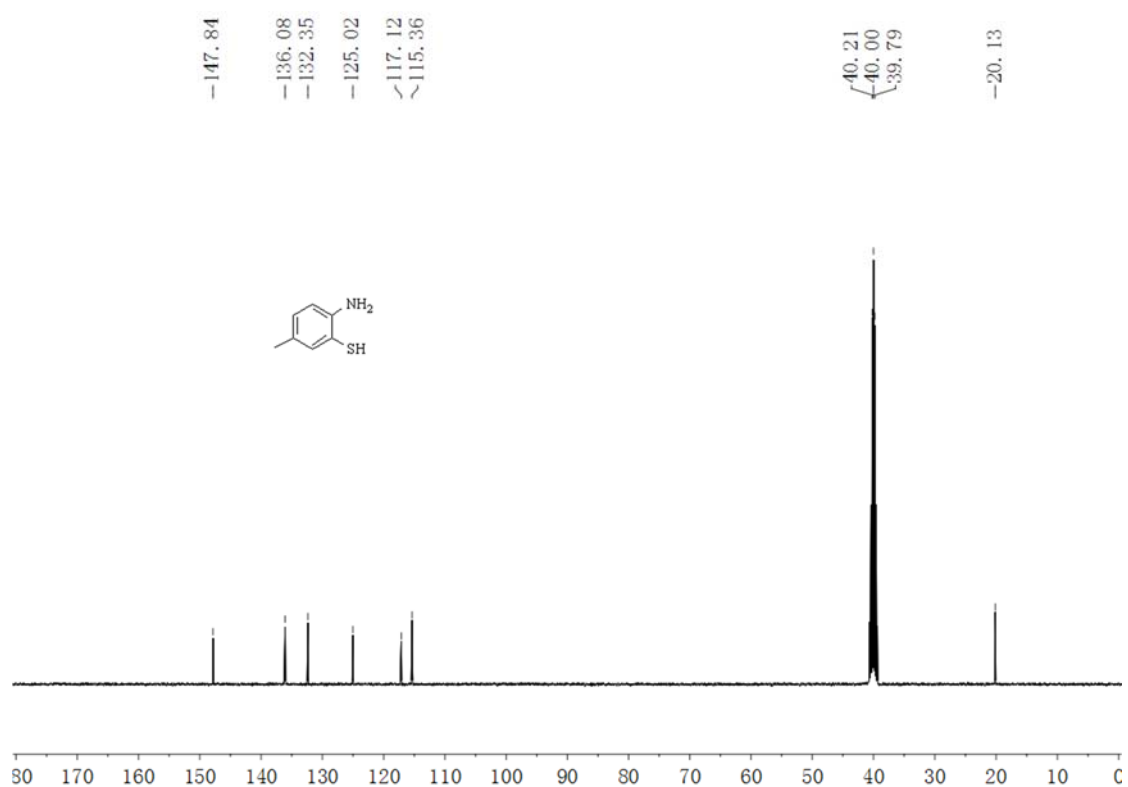
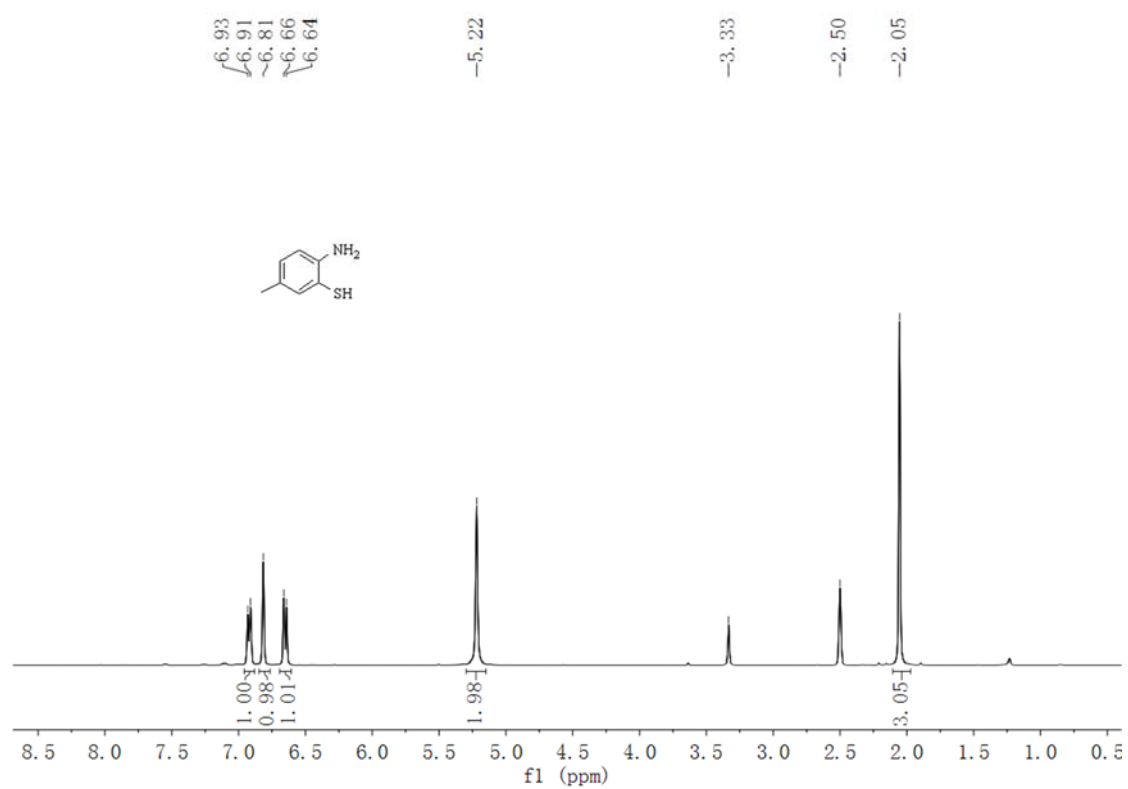


Figure S5. ¹H NMR and ¹³C NMR spectra of 2-amino-5-methylbenzenethiol

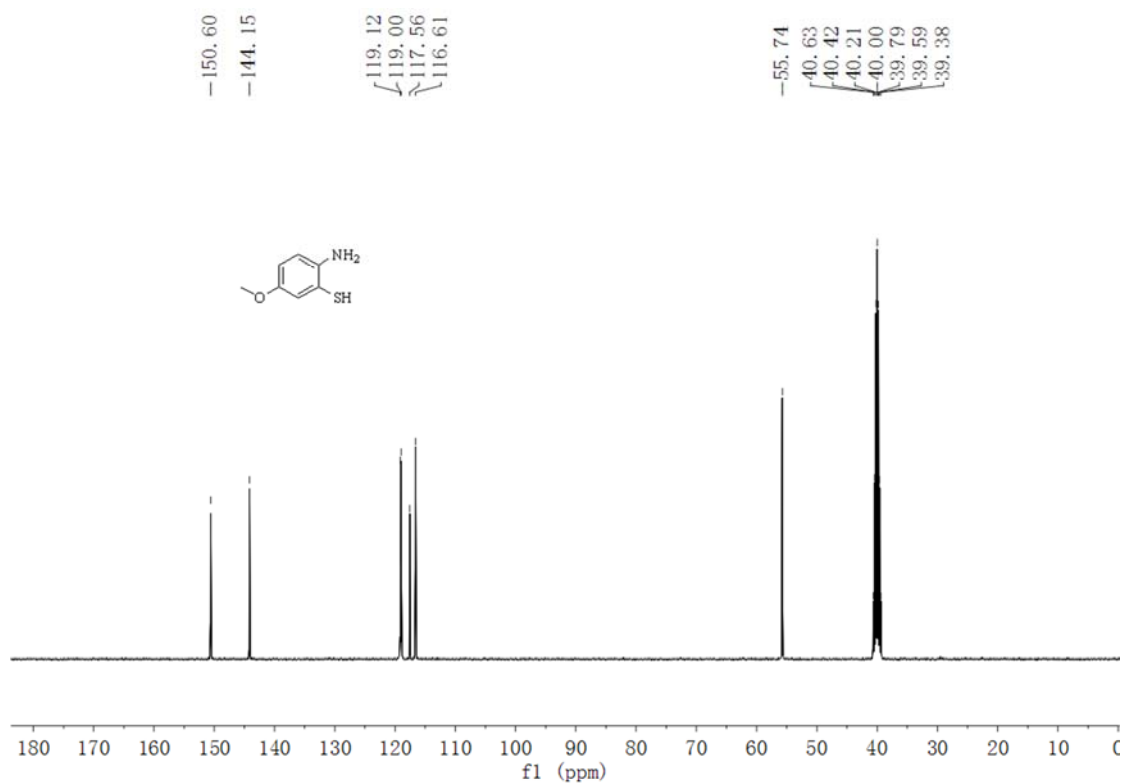
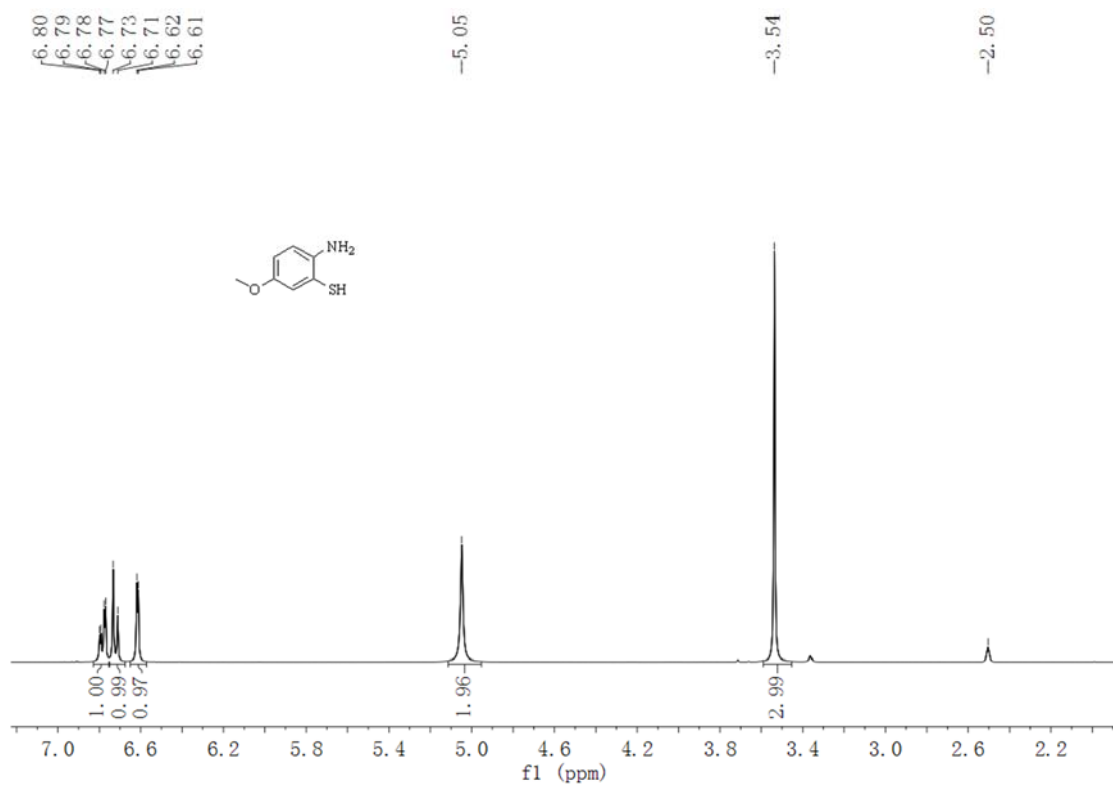


Figure S6. ¹H NMR and ¹³C NMR spectra of 2-amino-5-methoxybenzenethiol

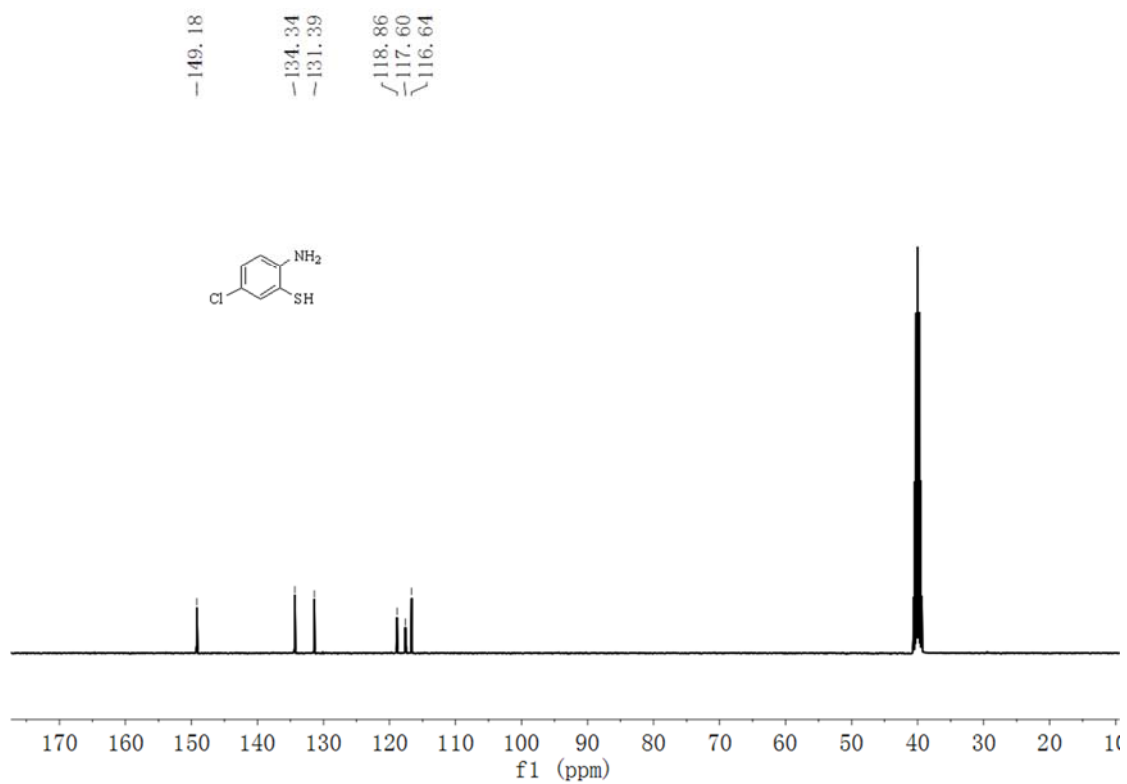
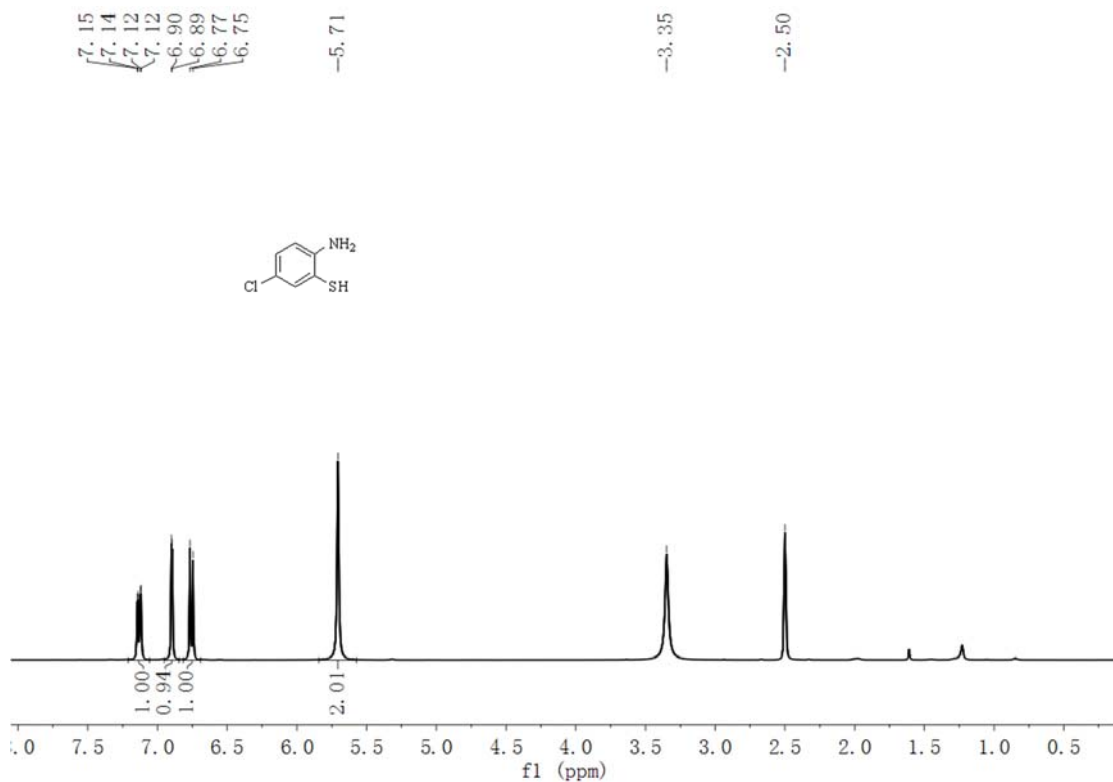


Figure S7. ^1H NMR and ^{13}C NMR spectra of 2-amino-5-chlorobenzenethiol

3 ^1H and ^{13}C NMR spectra of the products

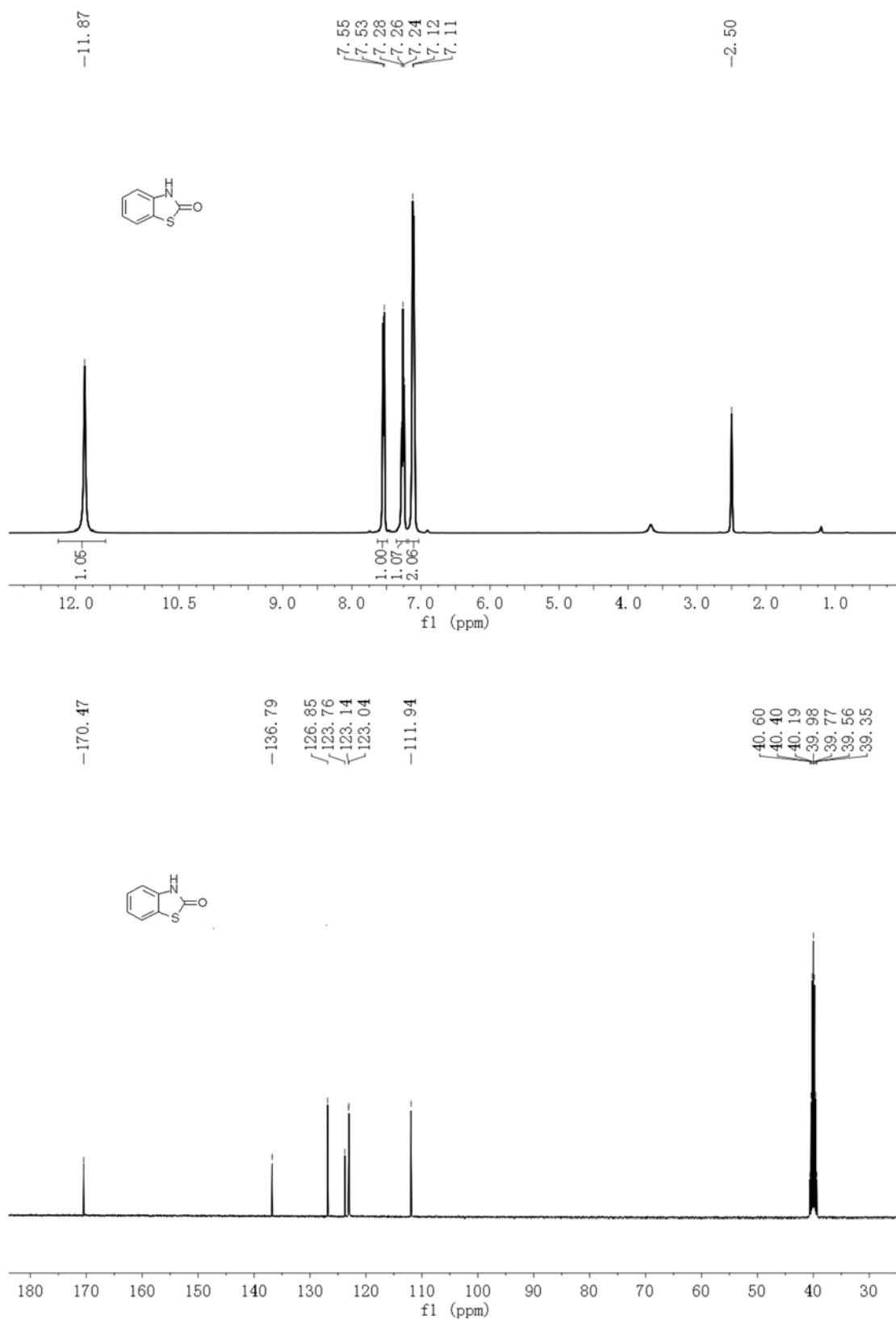


Figure S9. ^1H NMR and ^{13}C NMR spectra of benzothiazolone

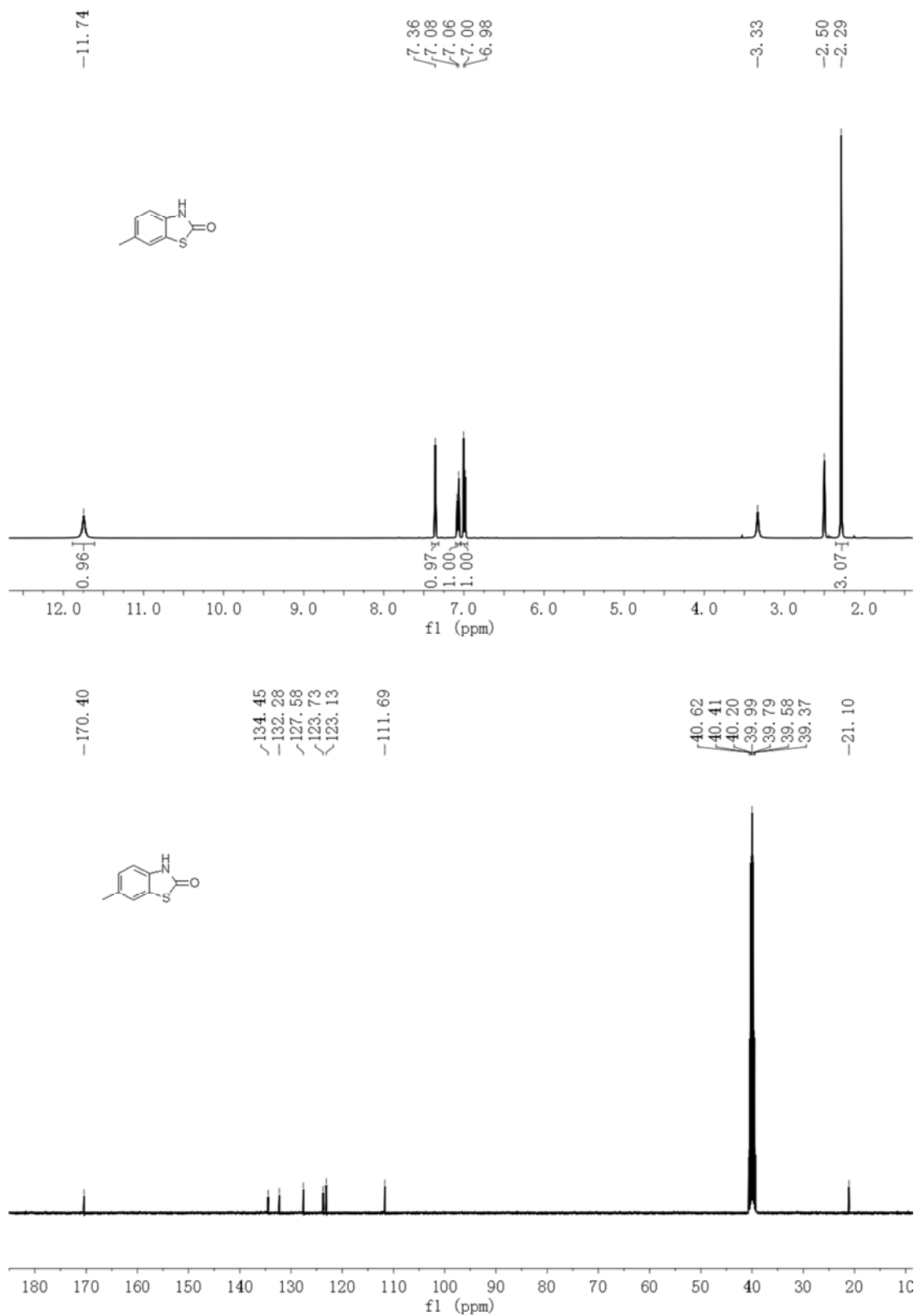


Figure S10. ¹H NMR and ¹³C NMR spectra of 6-methylbenzothiazolone

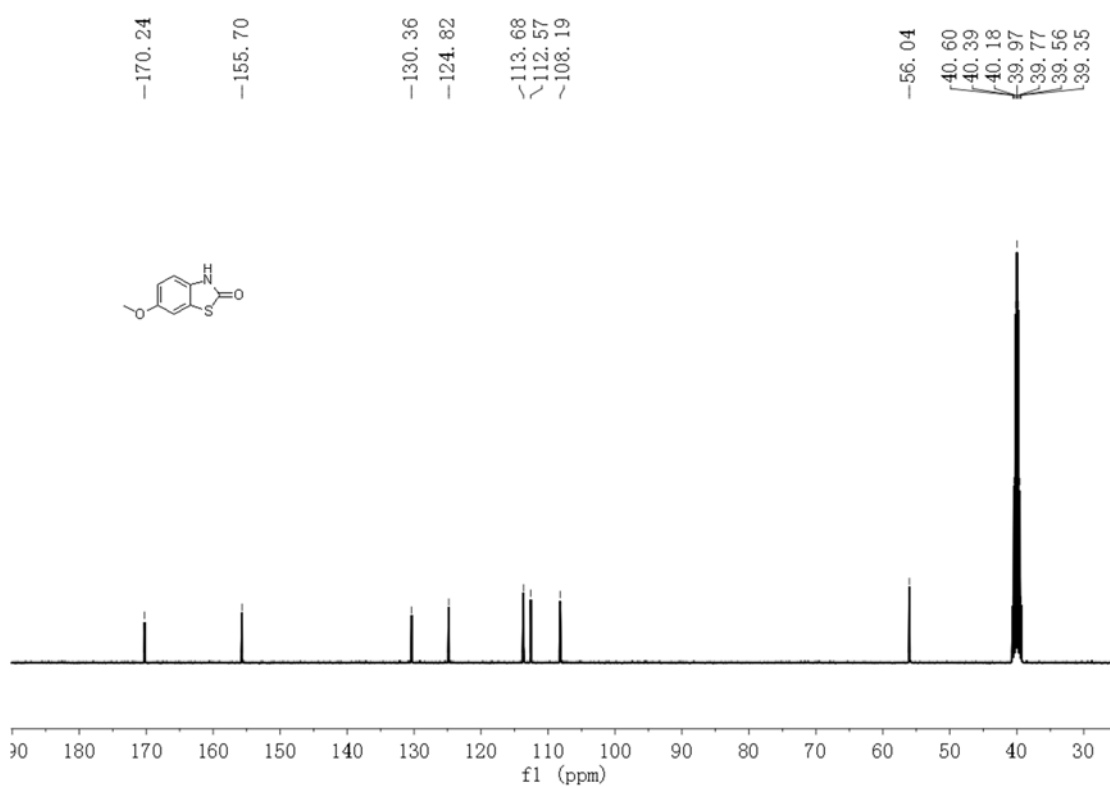
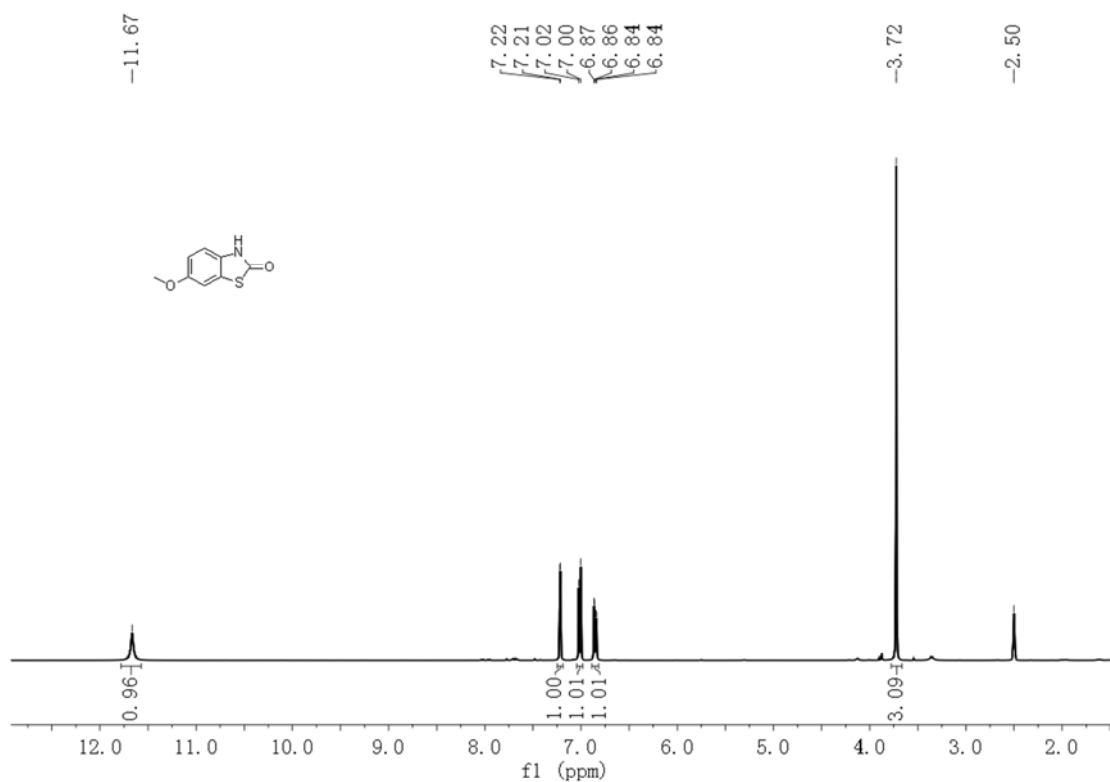


Figure S11. ^1H NMR and ^{13}C NMR spectra of 6-methoxybenzothiazolone

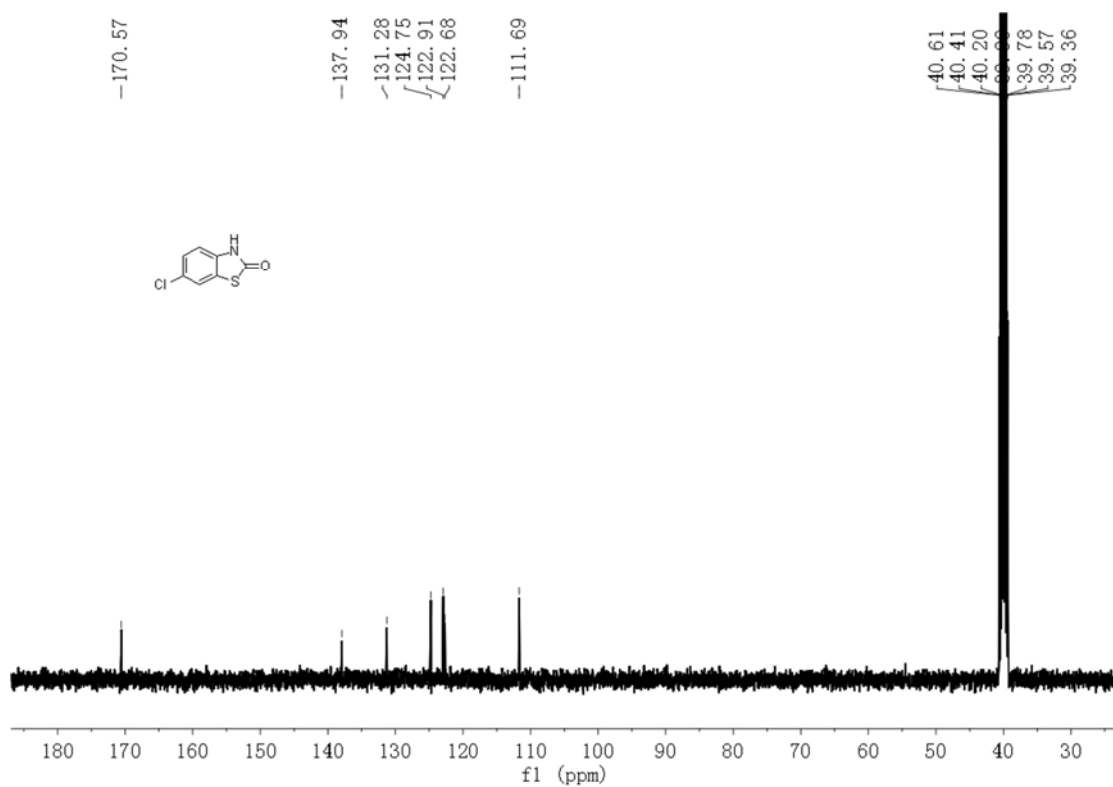
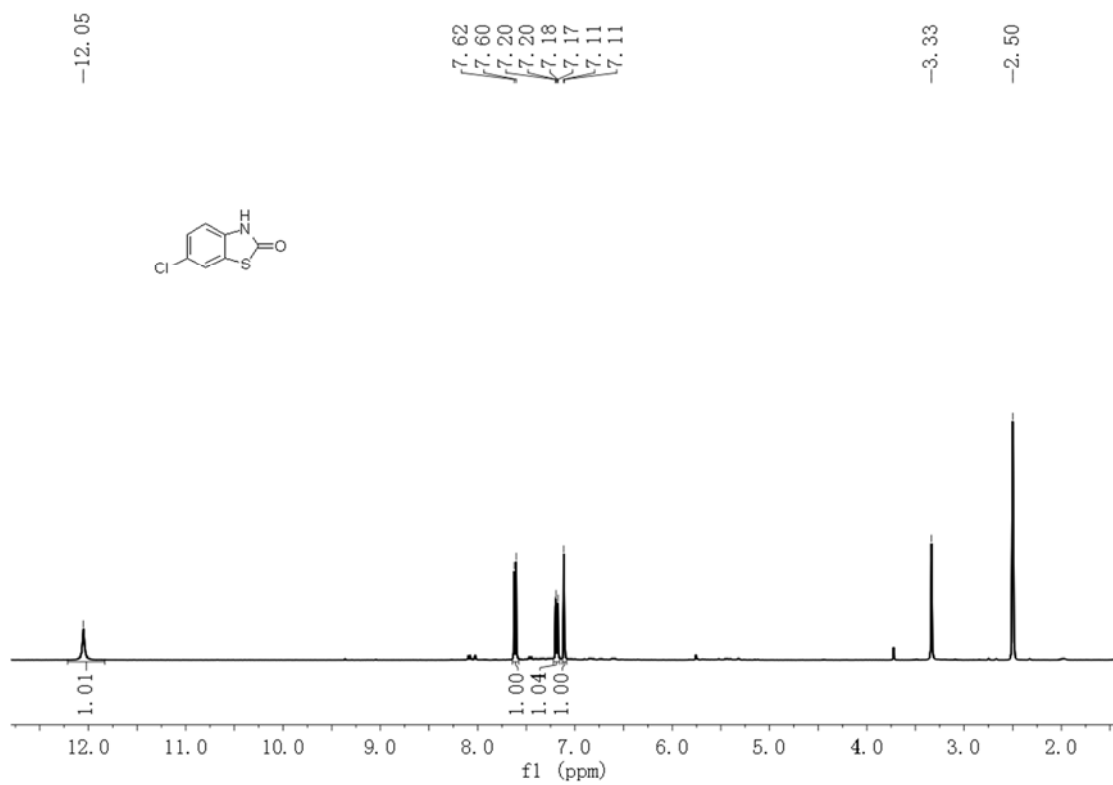


Figure S12. ^1H NMR and ^{13}C NMR spectra of 6-chlorobenzothiazolone

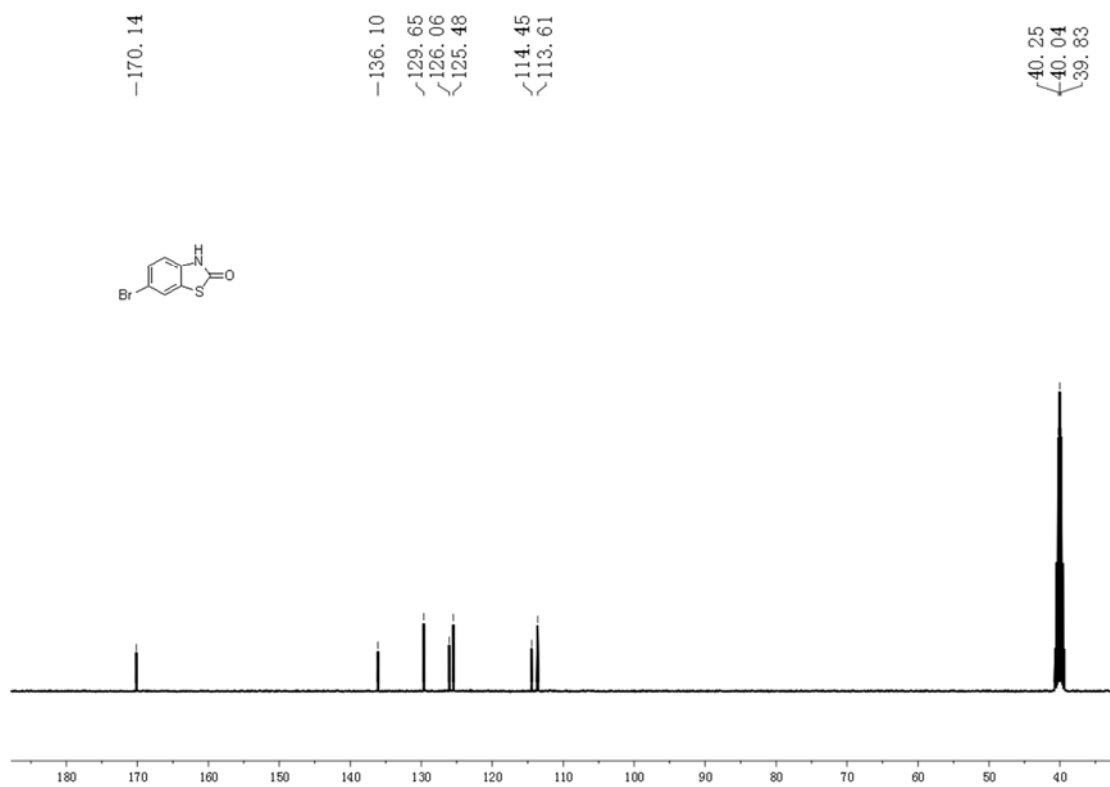
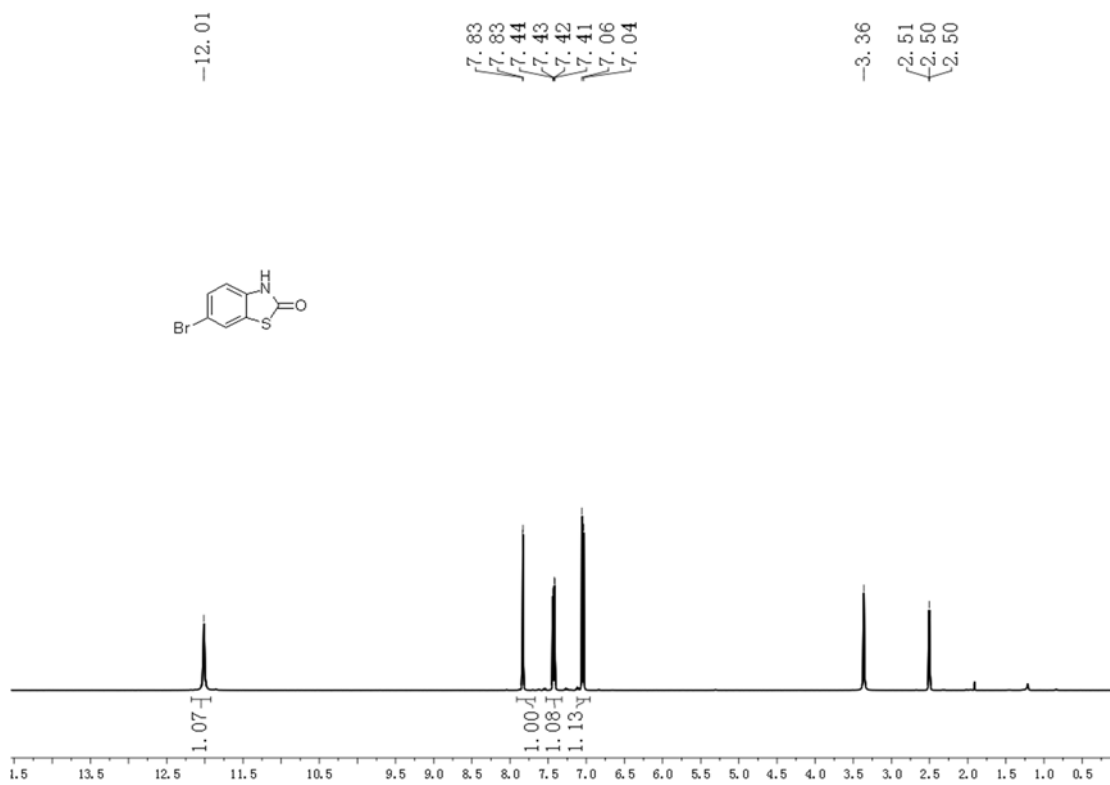


Figure S13. ^1H NMR and ^{13}C NMR spectra of 6-bromobenzothiazolone

4. References

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