

Research Article

Haleema Ali, Rasool Khan*, Xiandao Pan, Farzana Shaheen, Almas Jabeen, Abdur Rauf*, Muhammad Shah, Umer Rashid, Yahya S. Al-Awthan, Omar S. Bahattab, Mohammed A. Al-Duais, and Mohammad S. Mubarak

Synthesis, characterization, anti-cancer, anti-inflammatory activities, and docking studies of 3,5-disubstituted thiadiazine-2-thiones

Supplementary material

* **Corresponding author: Rasool Khan**, Institute of Chemical Sciences, University of Peshawar, Peshawar-25120, Khyber Pakhtunkhwa, Pakistan, e-mail: rasoolkhan1@hotmail.com

* **Corresponding author: Abdur Rauf**, Department of Chemistry University of Swabi, Swabi, Anbar, 23561, Khyber Pakhtunkhwa, Pakistan, e-mail: mashaljcs@yahoo.com

Haleema Ali: Institute of Chemical Sciences, University of Peshawar, Peshawar-25120, Khyber Pakhtunkhwa, Pakistan

Xiandao Pan: Beijing Key Laboratory of Active Substance Discovery and Drug ability Evaluation Institute of Material Medical, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, China

Farzana Shaheen: HEJ Research Institute of Chemistry, International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi 75270, Pakistan

Almas Jabeen: Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi, 75270, Pakistan

Muhammad Shah, Umer Rashid: Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, 22060 Abbottabad, Pakistan

Yahya S. Al-Awthan: Department of Biology, Faculty of Science, University of Tabuk, Tabuk 71421, Saudi Arabia; Department of Biology, Faculty of Science, Ibb University, Ibb 70270, Yemen

Omar S. Bahattab: Department of Biology, Faculty of Science, University of Tabuk, Tabuk 71421, Saudi Arabia

Mohammed A. Al-Duais: Department of Biochemistry, Faculty of Science, University of Tabuk, Tabuk 71421, Saudi Arabia; Biochemistry Unit, Chemistry Department, Faculty of Science, Ibb University, Ibb 70270, Yemen

Mohammad S. Mubarak: Department of Chemistry, The University of Jordan, Amman 11942, Jordan

1. nmr

¹H NMR (600 MHz, DMSO)

Chemical structure of the compound is shown. The structure is a thiazolidine derivative with a thiazolidine ring fused to a five-membered ring containing a carbonyl group and a hydroxyl group. The thiazolidine ring has a propyl group attached to the nitrogen atom.

The ¹H NMR spectrum (600 MHz, DMSO) is displayed. The x-axis represents the chemical shift in ppm (f1), ranging from 0.8 to 4.8. The y-axis represents the intensity, ranging from -2.0E+09 to 3.4E+10. The spectrum shows several peaks, with integration values provided for some of them:

- Peak at ~4.5 ppm: Integration 3.08
- Peak at ~3.9 ppm: Integration 1.01
- Peak at ~3.7 ppm: Integration 1.00
- Peak at ~3.4 ppm: Integration 1.24
- Peak at ~2.8 ppm: Integration 0.53
- Peak at ~1.6 ppm: Integration 4.99
- Peak at ~1.3 ppm: Integration 2.03
- Peak at ~0.9 ppm: Integration 9.00

Additional chemical shift values (ppm) are listed at the top of the spectrum:

- 4.64, 4.61, 4.57, 4.55, 4.50, 4.45, 3.98, 3.97, 3.96, 3.95, 3.93, 3.83, 3.82, 3.81, 3.80, 3.79, 3.53, 3.52, 3.51, 3.49, 3.37 H₂O, 3.34 H₂O, 2.56 DMSO, 1.63, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.54, 1.53, 1.52, 1.50, 1.31, 1.30, 1.29, 1.28, 1.26, 1.25, 0.90, 0.89, 0.88, 0.86

1-88 ¹³C NMR (151 MHz, DMSO)

CCCCN1CN(C(=O)C(C)C)S1=S

C13H24N2O2S2

190.56
173.44
67.60
60.77
55.74
51.47
51.44
39.93 DMSO
39.74 DMSO
39.64 DMSO
39.52 DMSO
39.37 DMSO
39.24 DMSO
28.37
28.25
24.86
24.63
23.43
22.40
22.40
19.69
13.97

f1 (ppm)

Figure S2: C13 NMR spectra of compound 1.

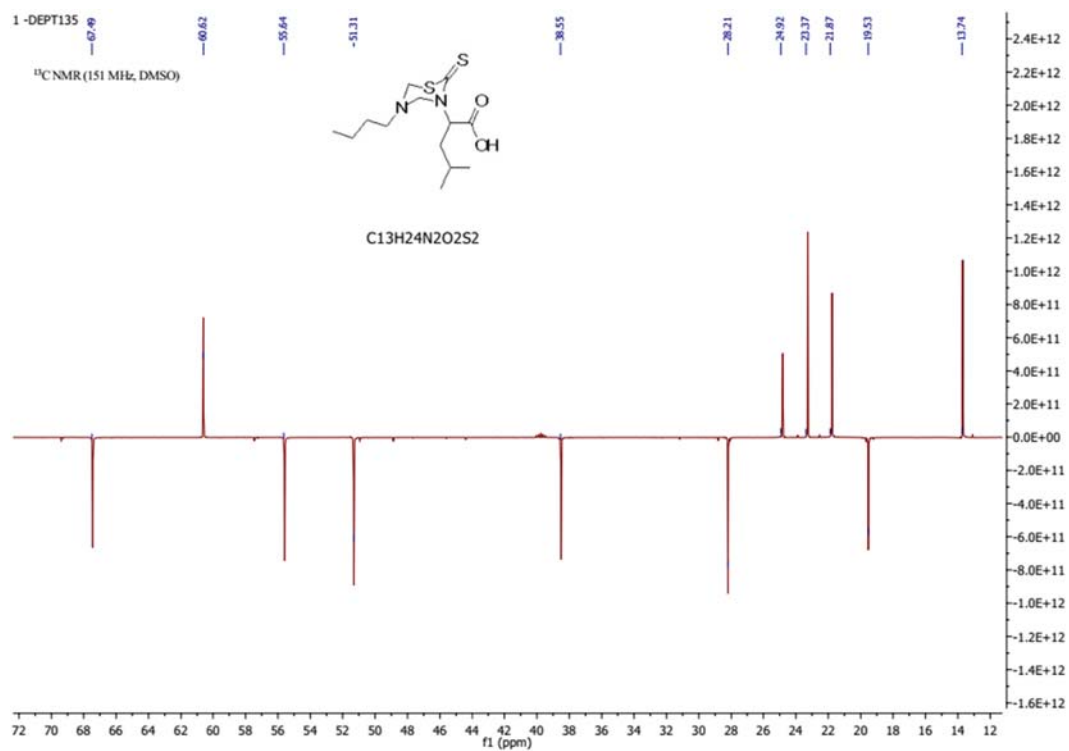


Figure S3: Dept 135 C13 spectra of compound 1.

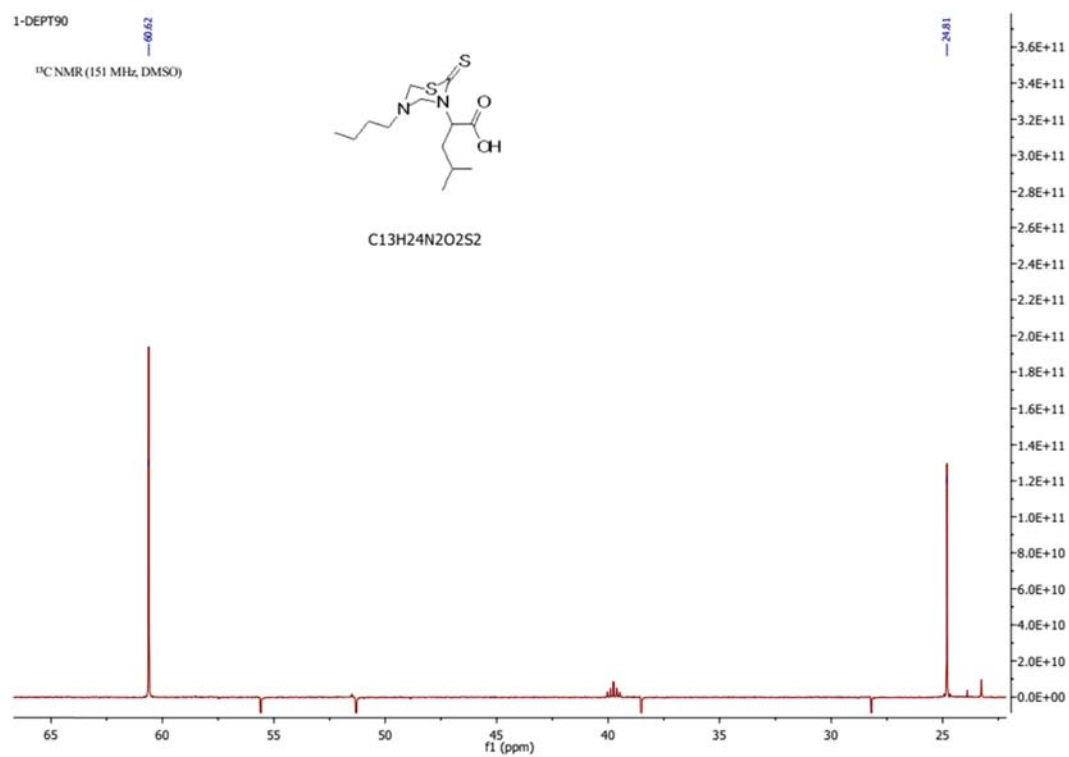


Figure S4: Dept 90 C13 spectra of compound 1.

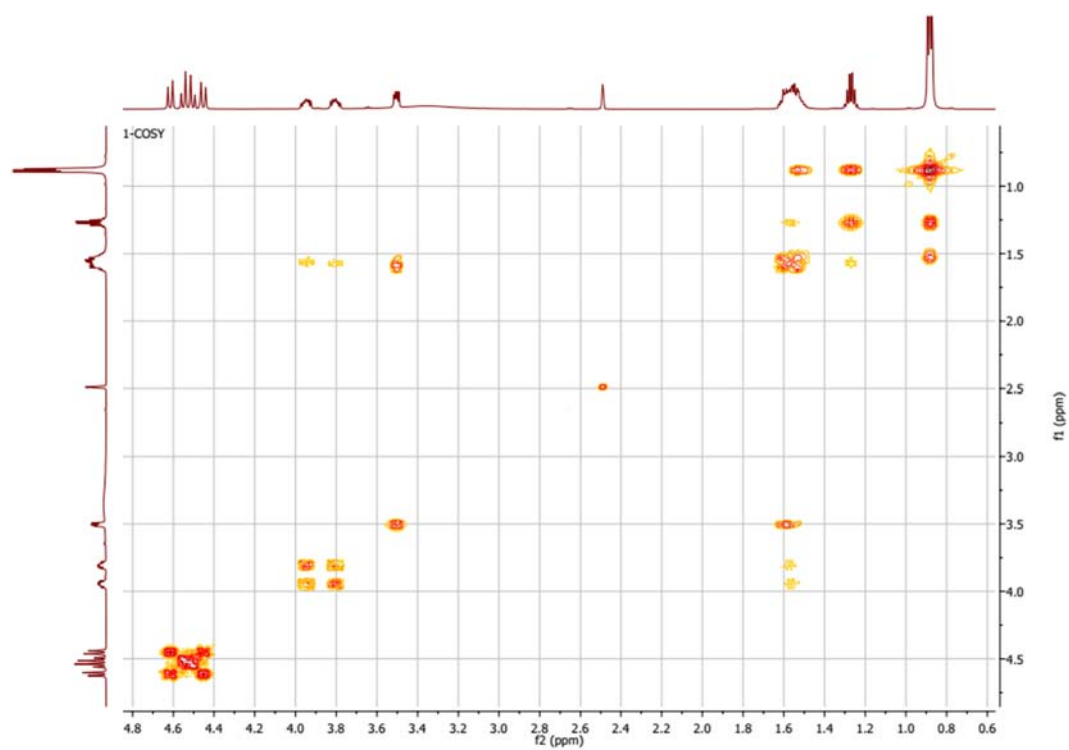


Figure S5: Cosy spectra of compound 1.

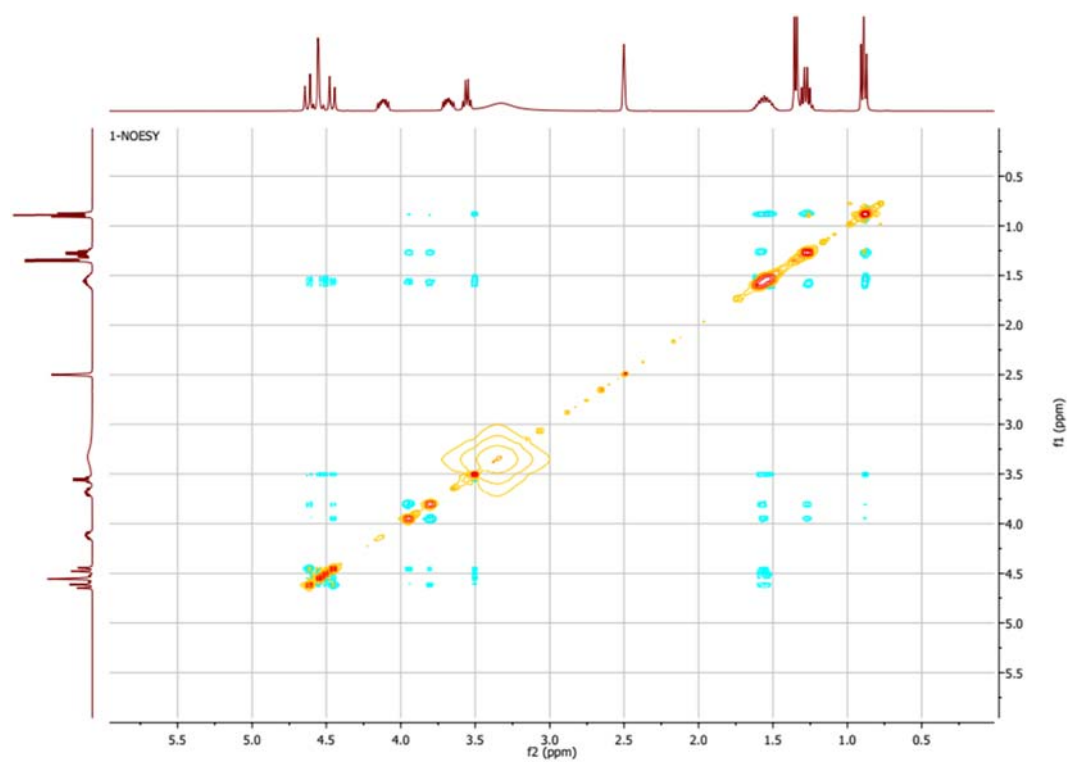


Figure S6: Nesy spectra of compound 1.

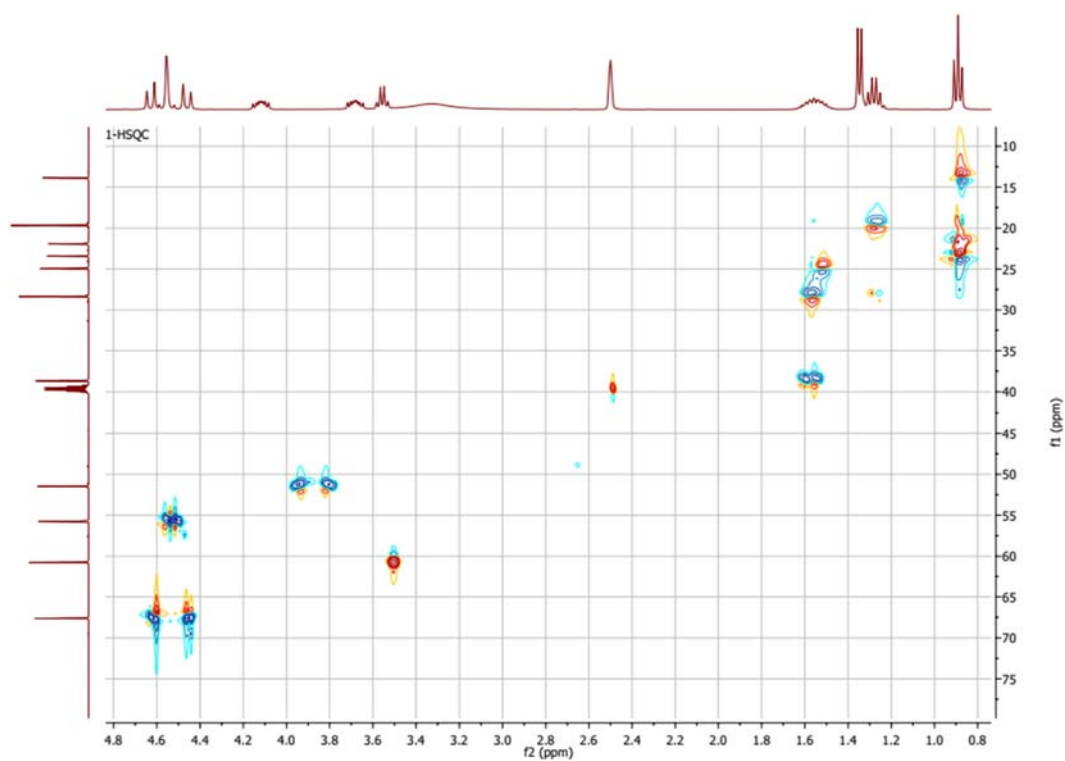


Figure S7: HSQC spectra of compound 1.

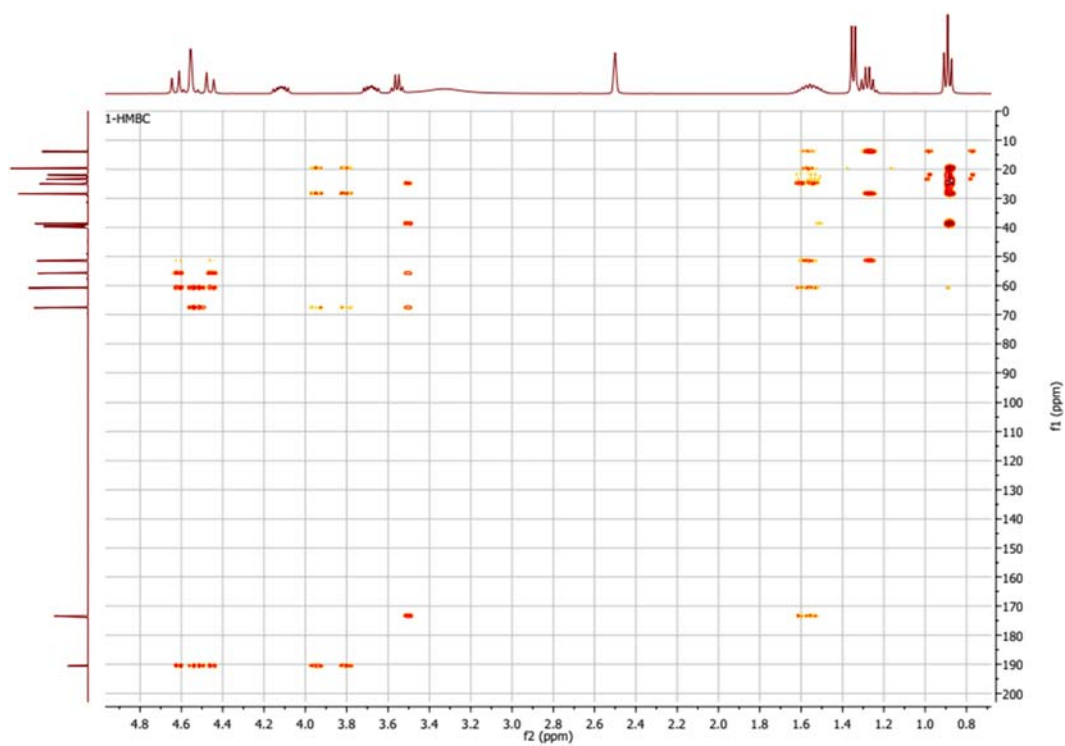


Figure S8: HMBC spectra of compound 1.

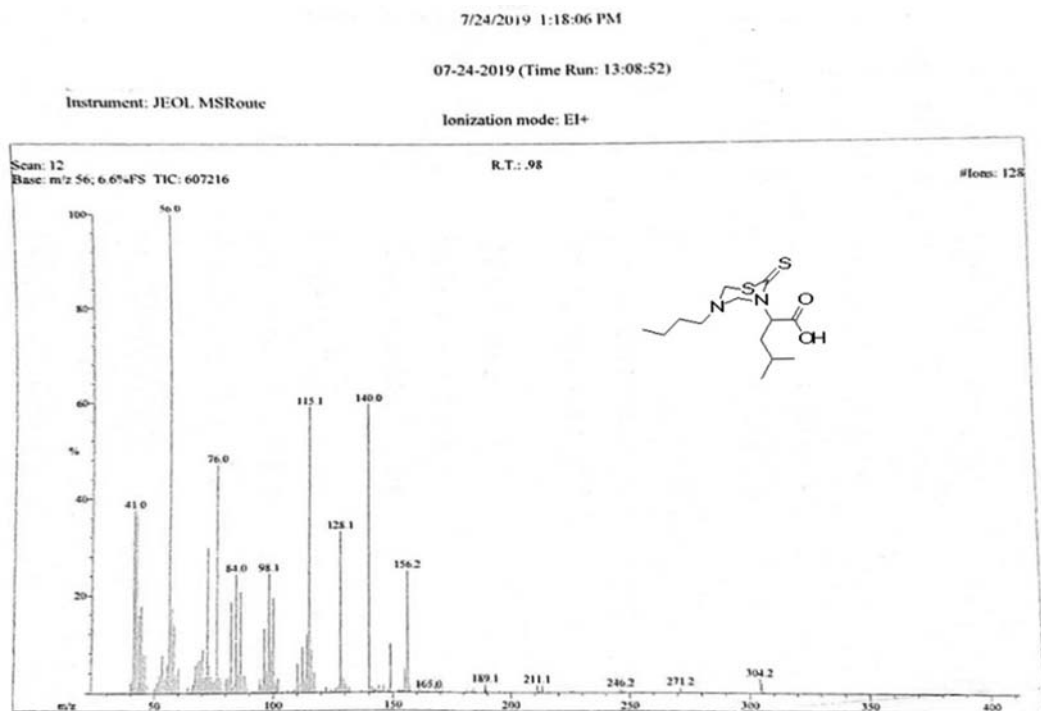


Figure S9: Mass spectra of compound 1.

S2 Compound 2

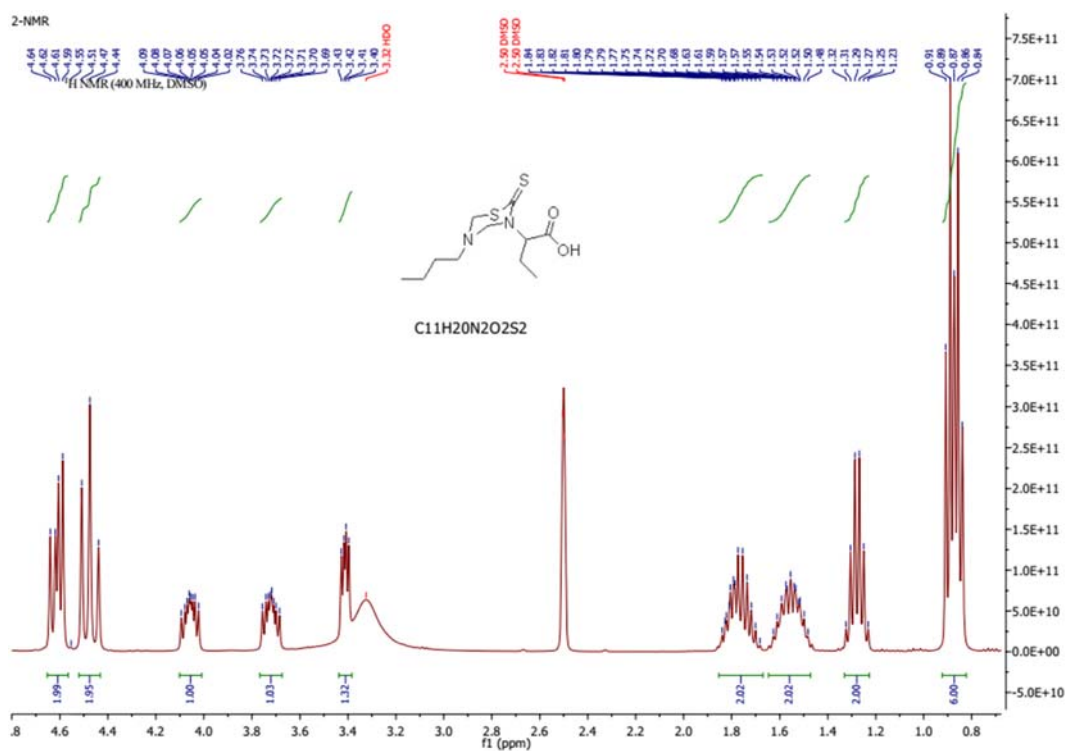


Figure S10: H-NMR spectra of compound 2.

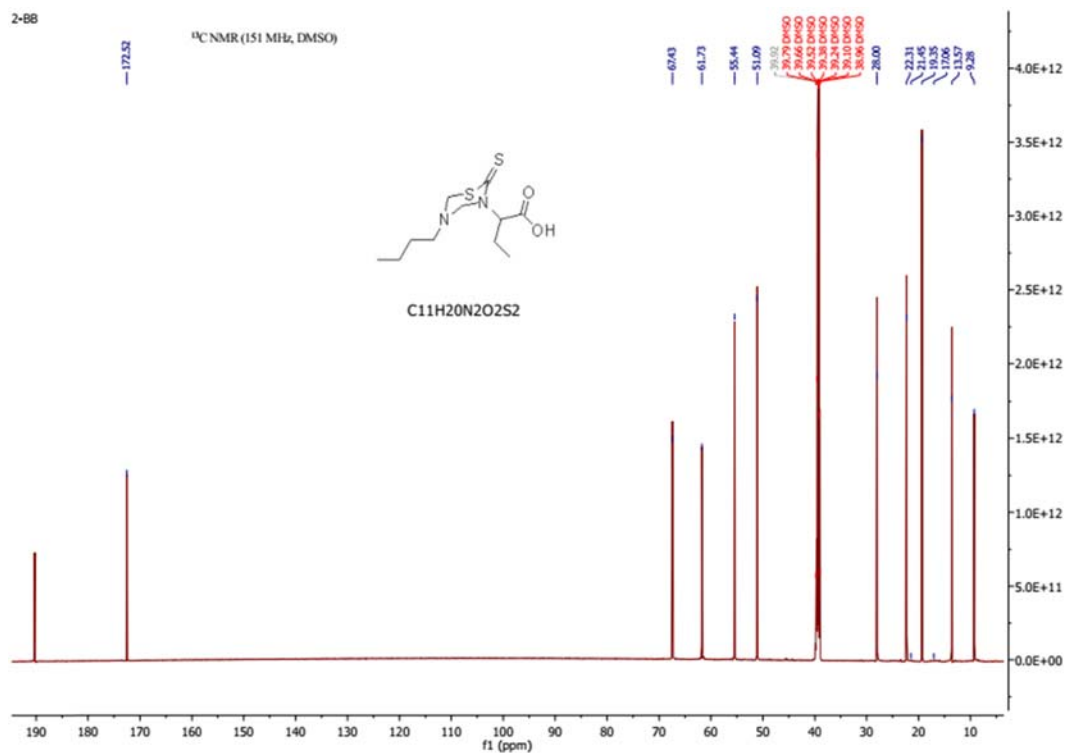


Figure S11: C13NMR spectra of compound 2.

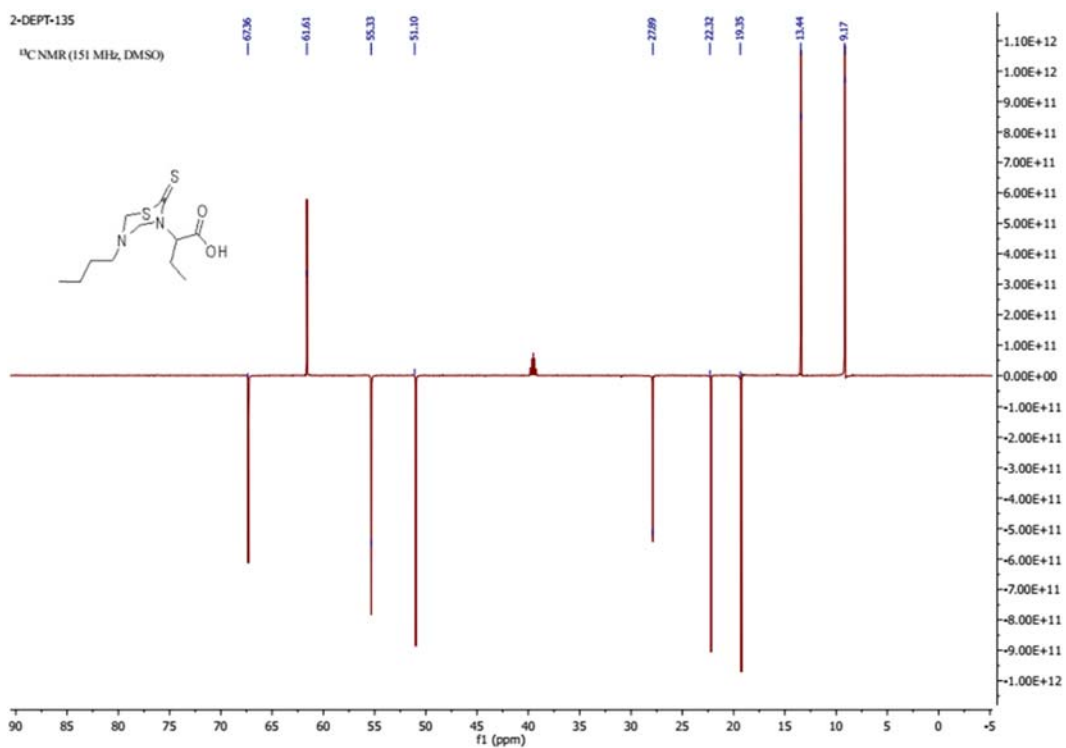


Figure S12: Dept 135 spectra of compound 2.

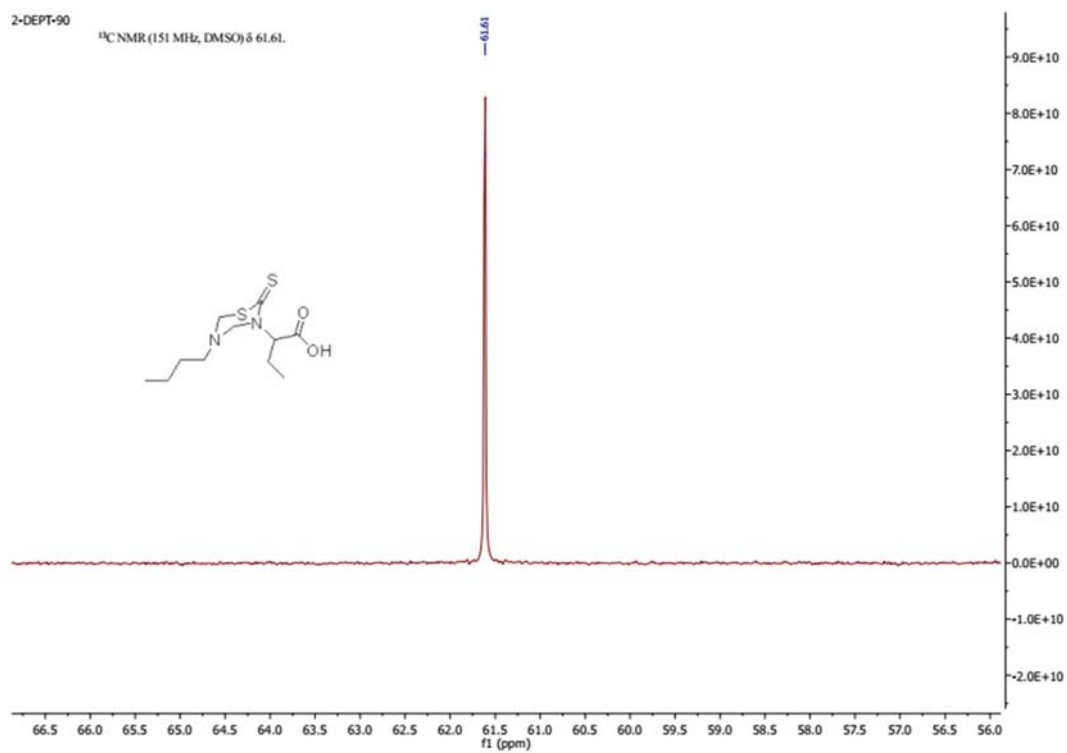


Figure S13: Dept 90 spectra of compound 2.

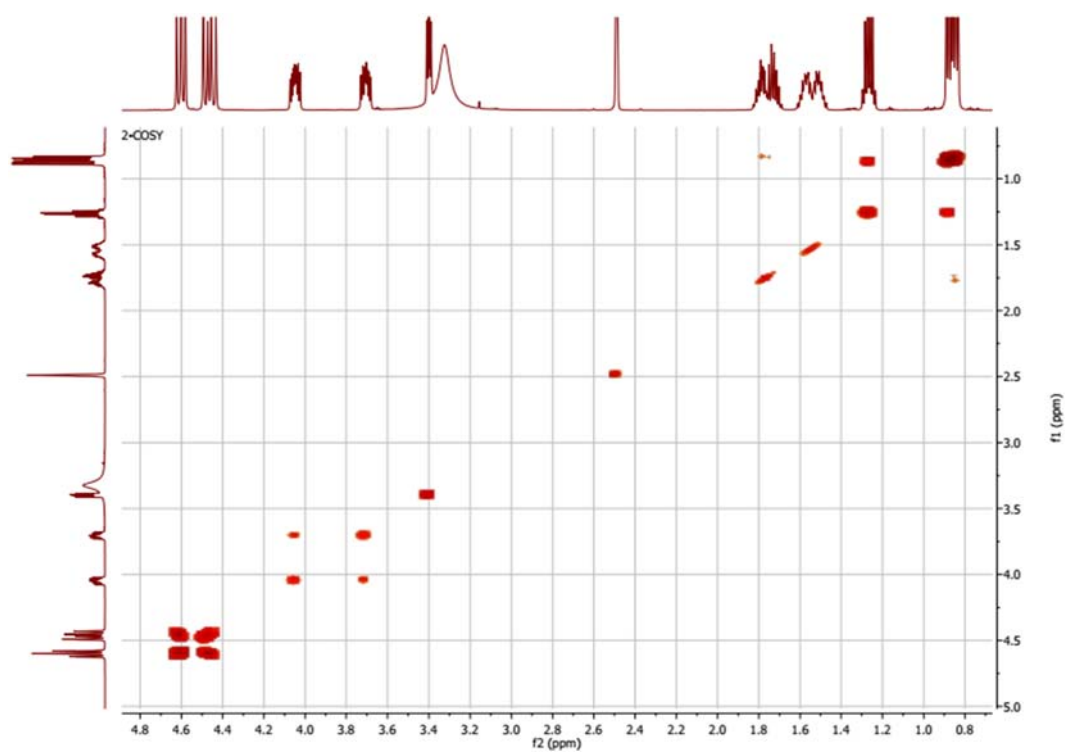


Figure S14: COSY spectra of compound 2.

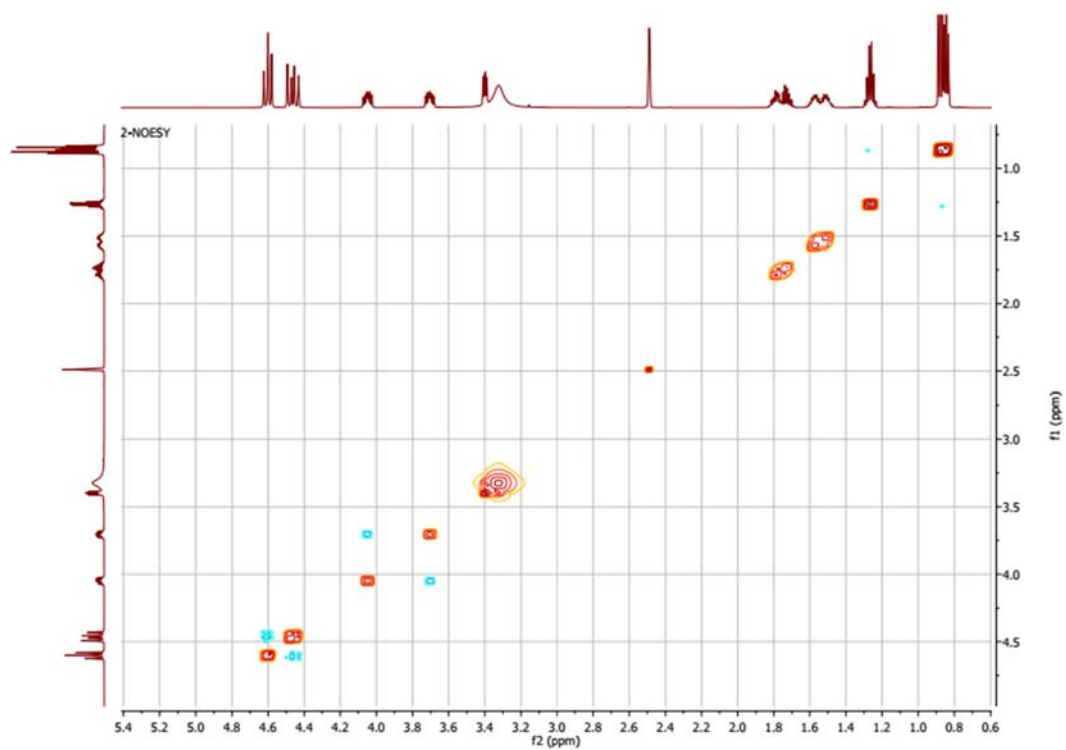


Figure S15: NQSY spectra of compound 2.

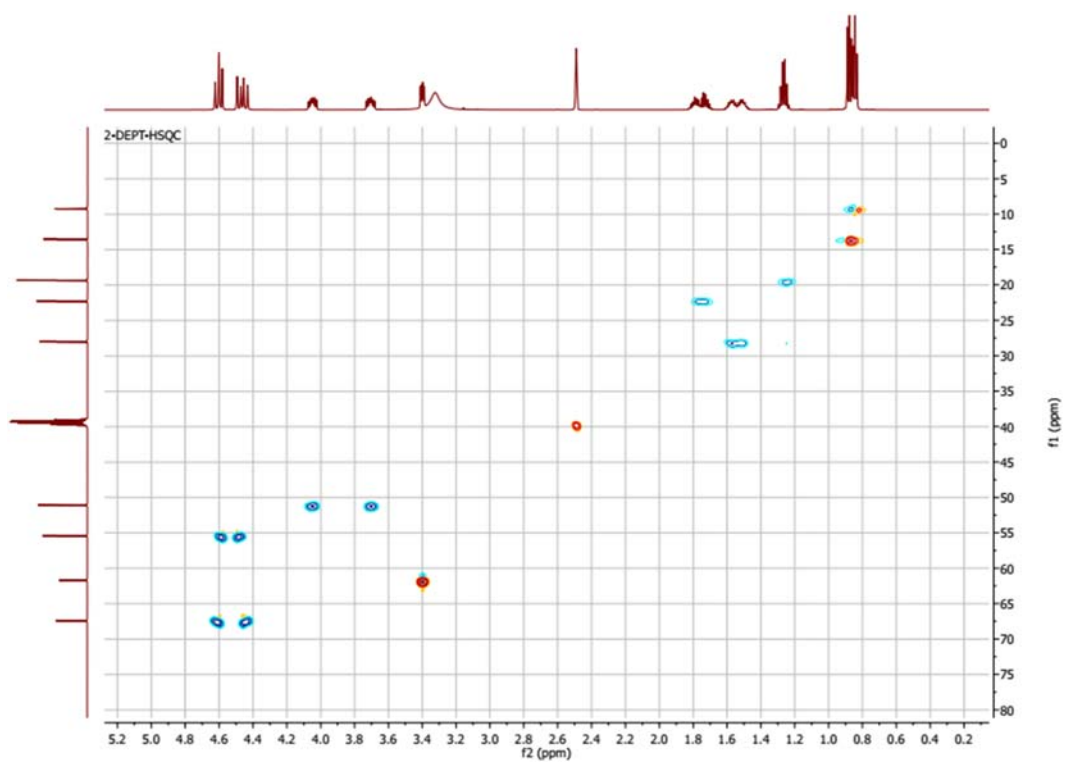


Figure S16: HSQC spectra of compound 2.

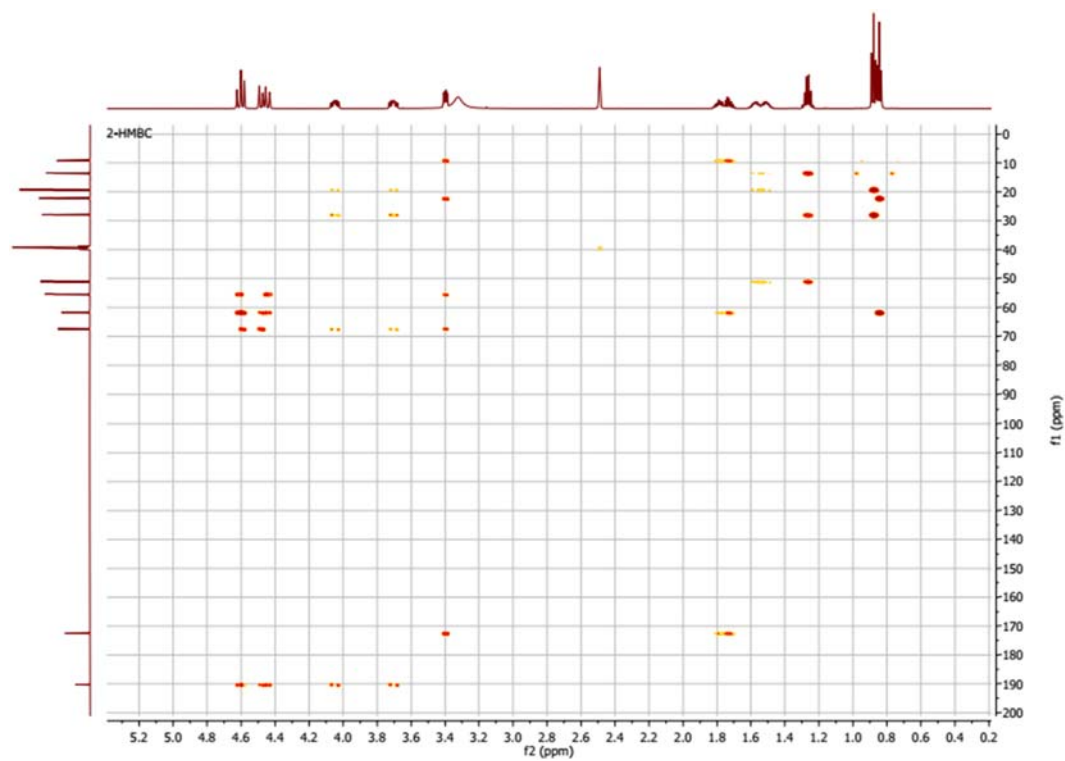


Figure S17: HMBC spectra of compound 2.

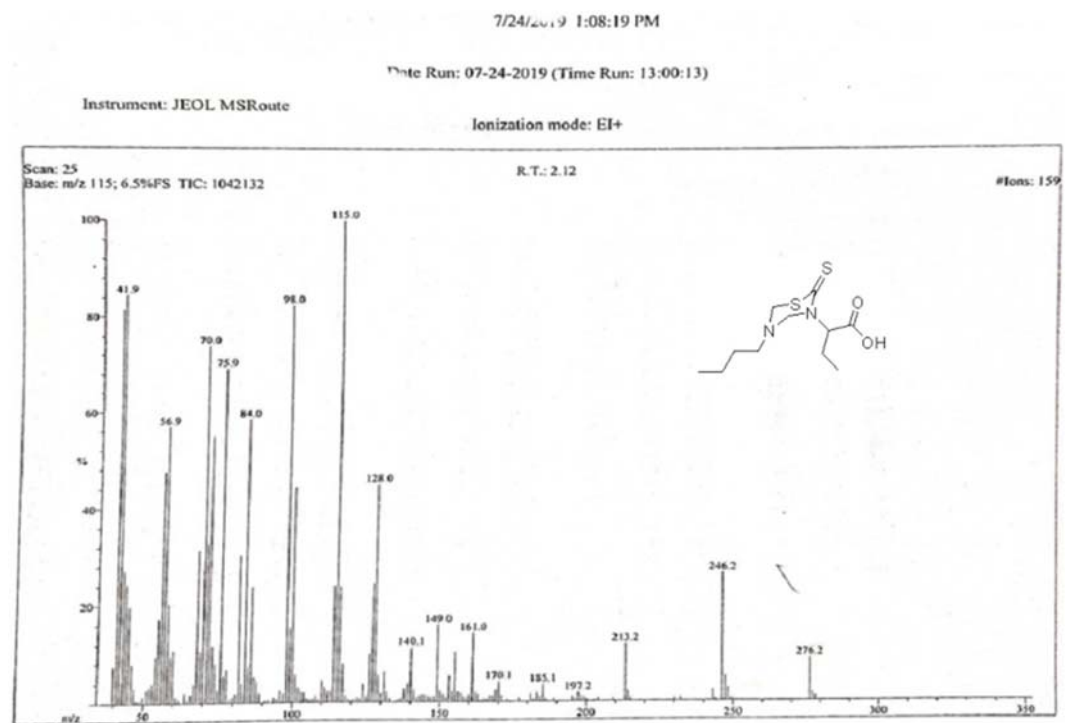


Figure S18: Mass spectra of compound 2.

S3 Compound 3

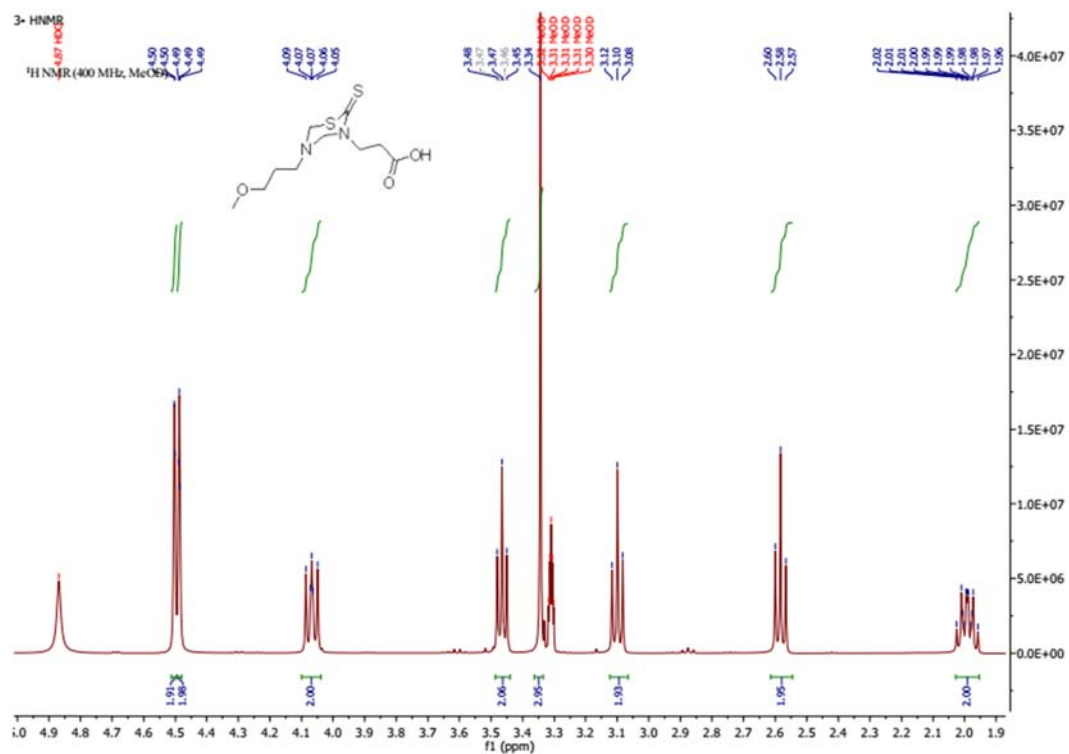


Figure S19: H-NMR spectra of compound 3.

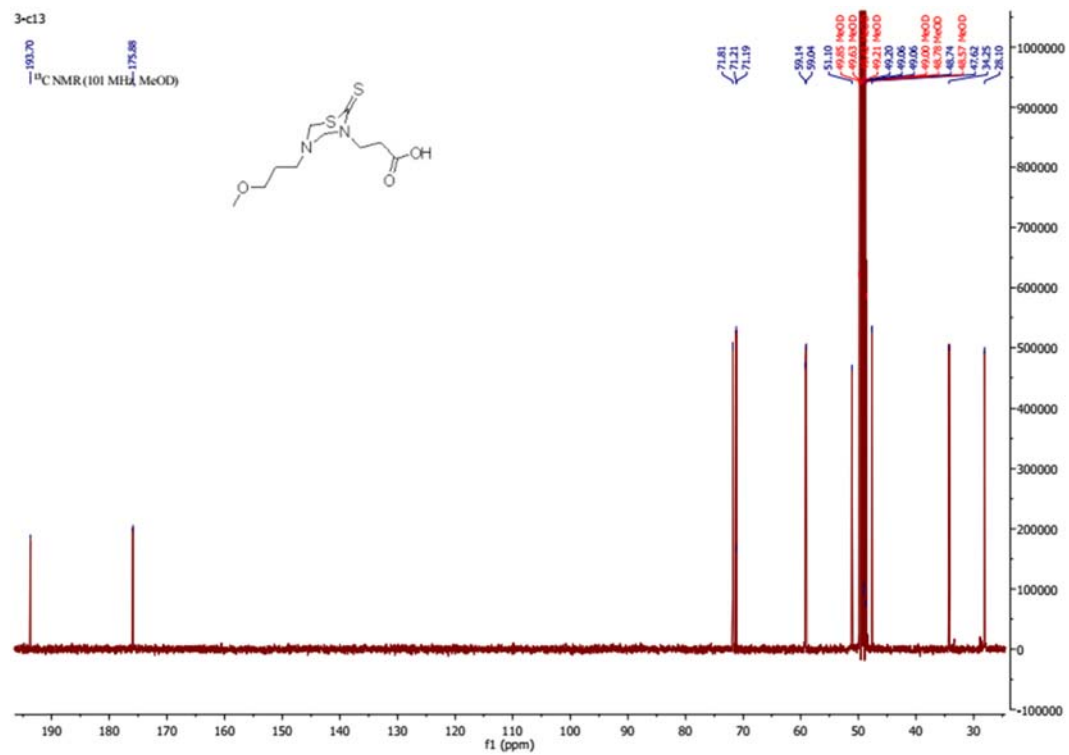


Figure S20: C13 NMR spectra of compound 3.

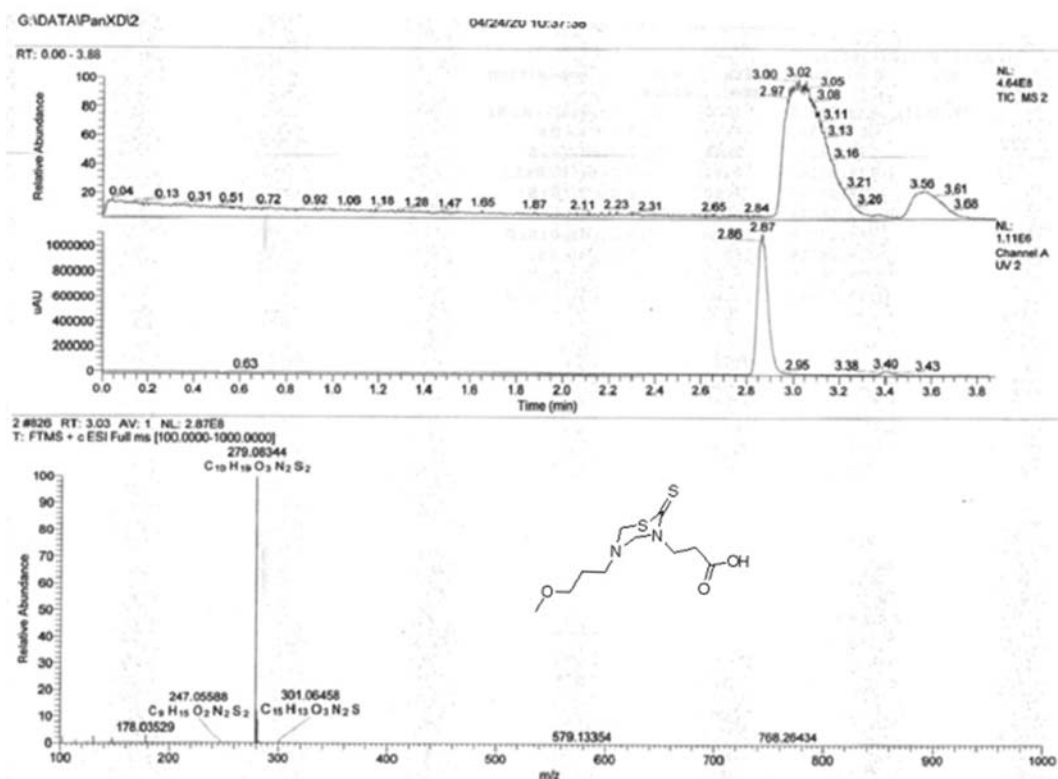


Figure S21: HRMS spectra of compound 3.

S4 Compound 4

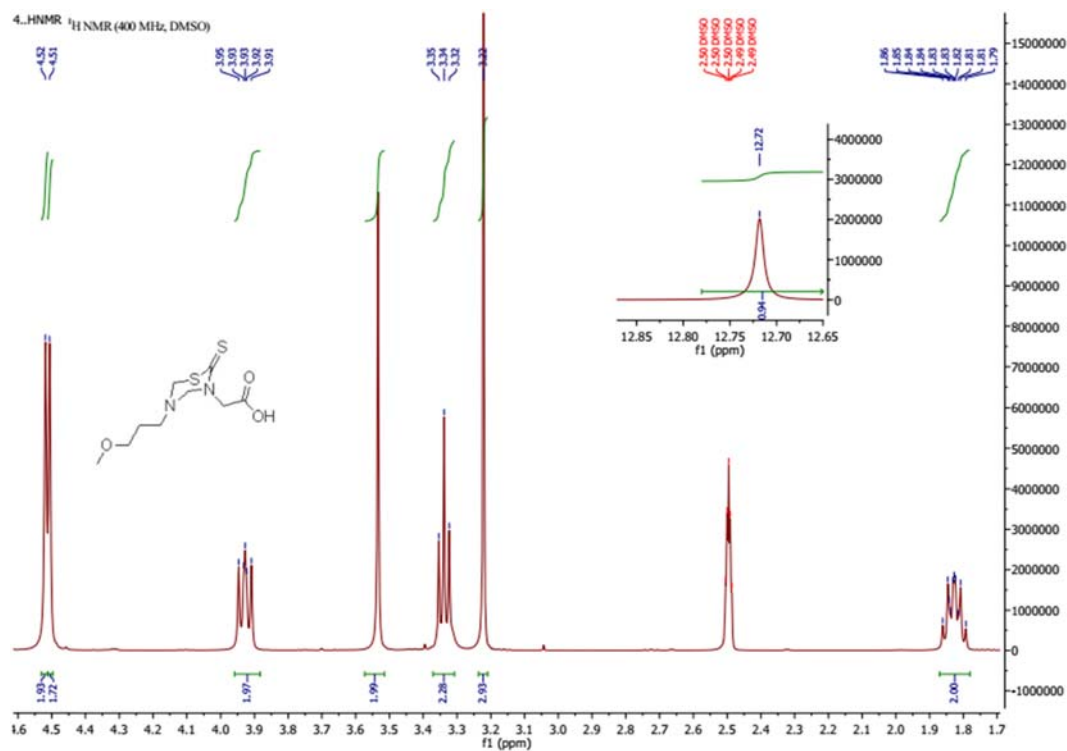


Figure S22: H-NMR spectra of compound 4.

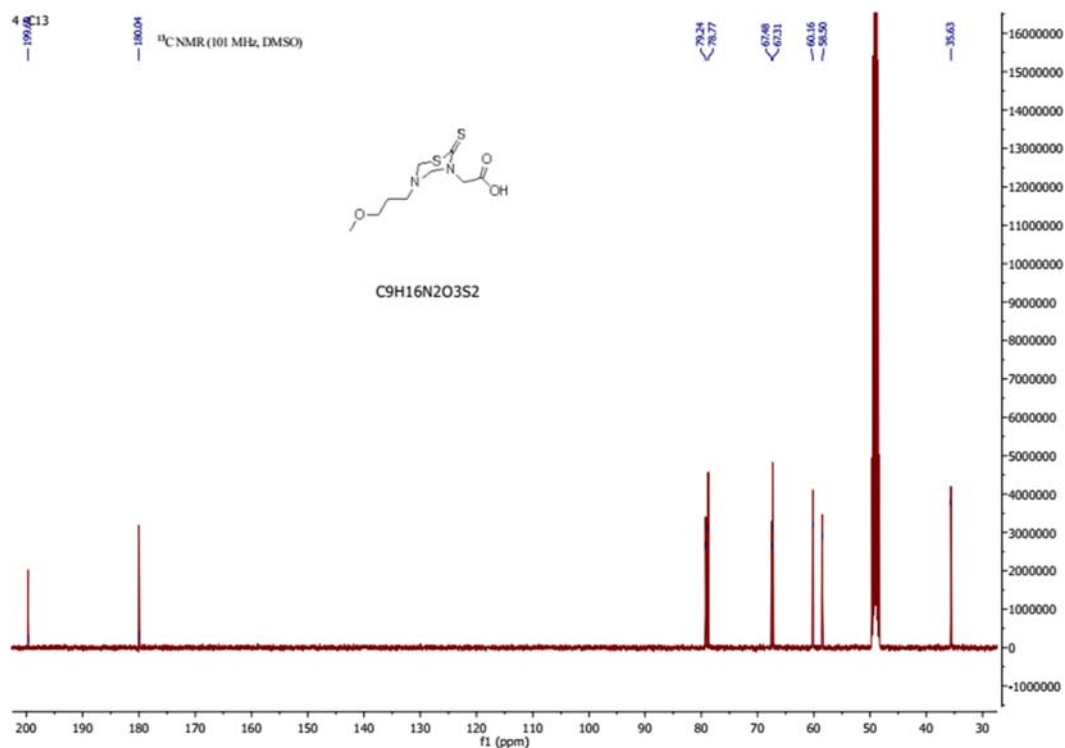


Figure S23: C13 NMR spectra of compound 4.

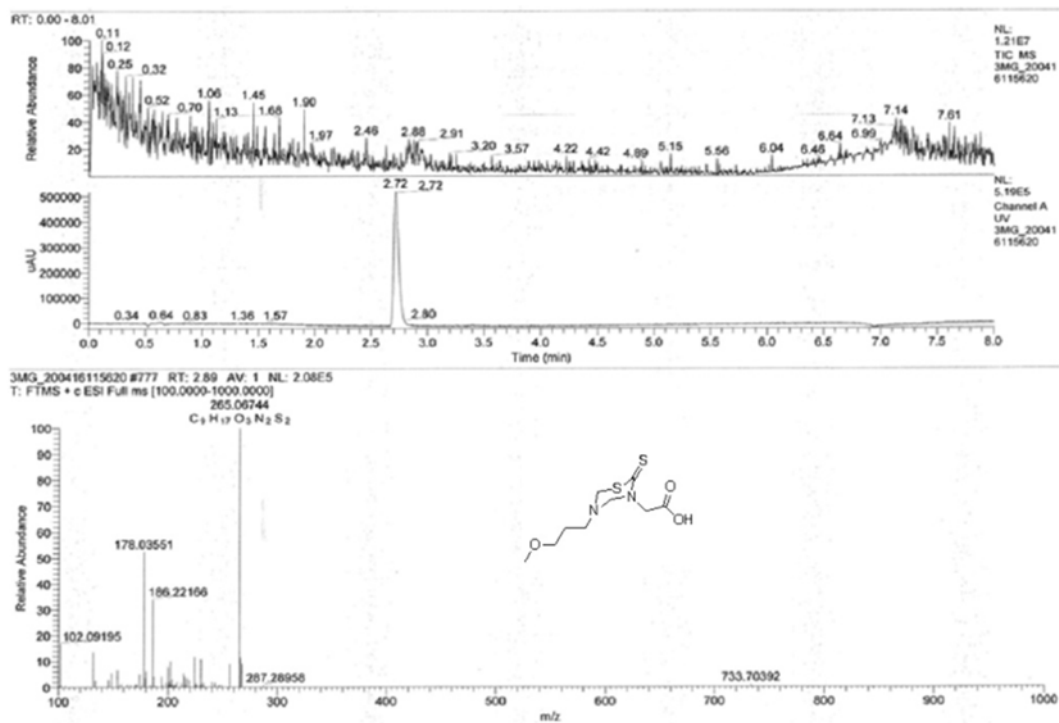


Figure S24: HRMS spectra of compound 4.

S5 Compound 5

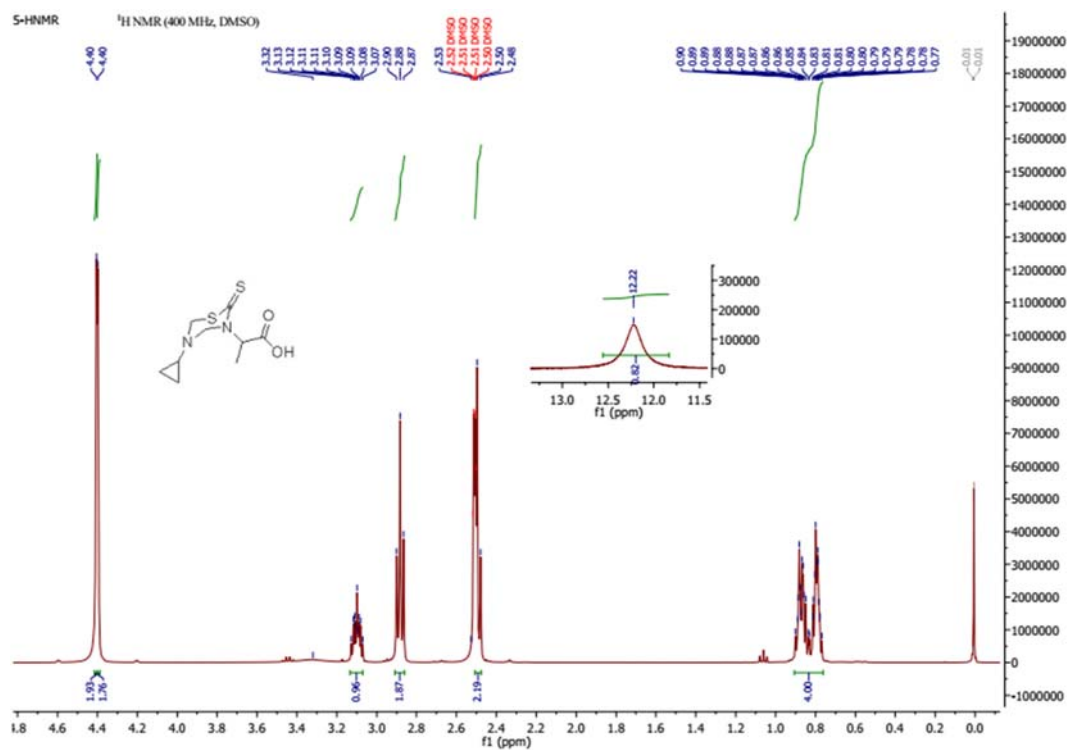


Figure S25: H-NMR spectra of compound 5.

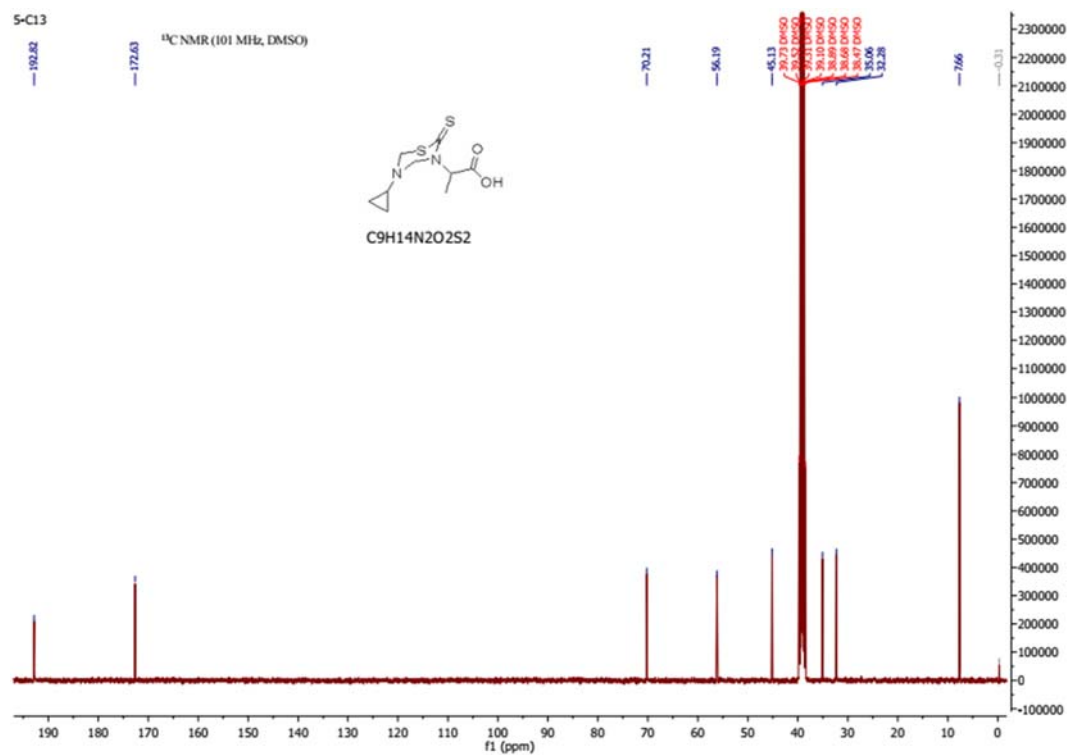


Figure S26: C13 NMR spectra of compound 5.

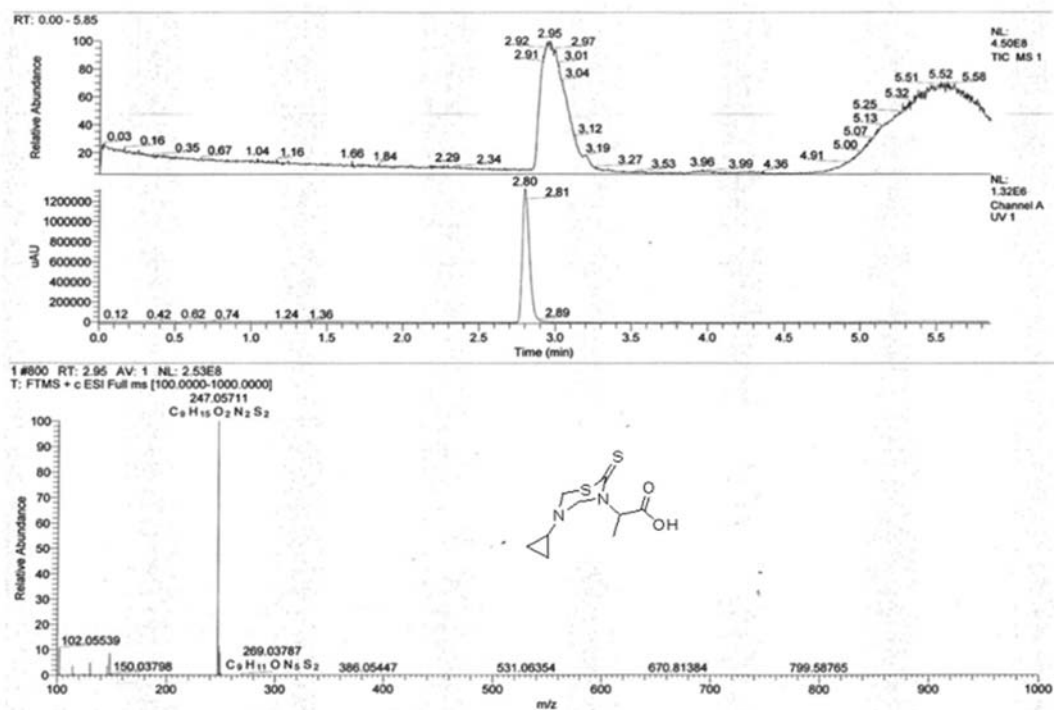
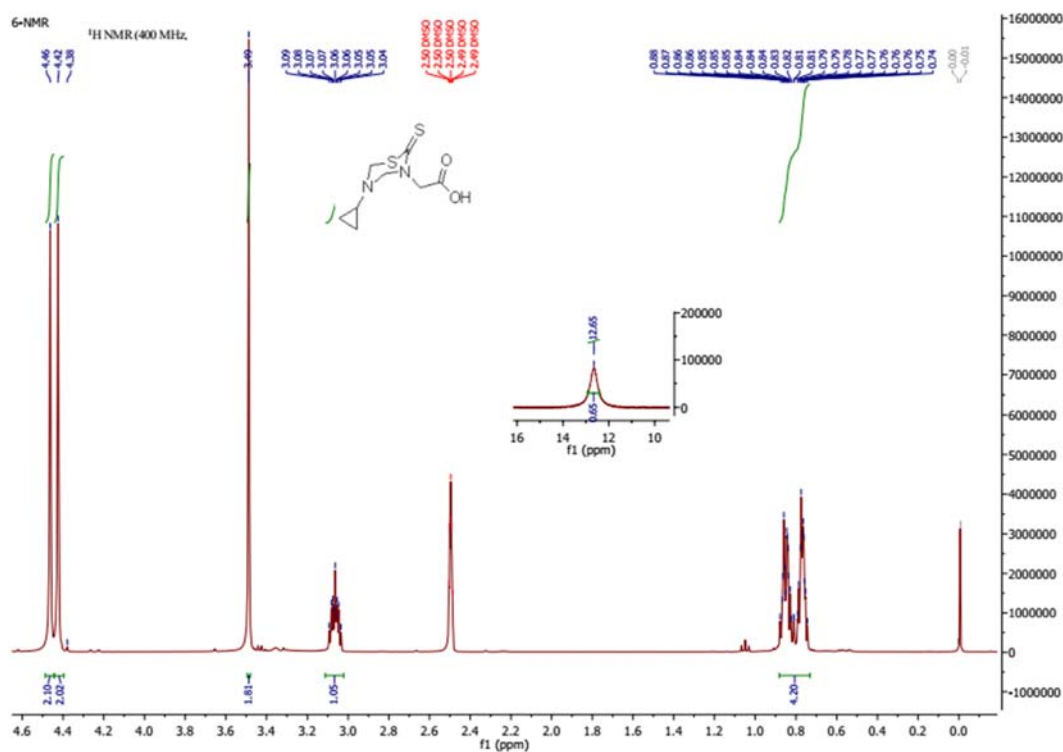


Figure S27: HRMS spectra of compound 5.

S6 Compound 6

Figure S28: ^1H -NMR spectra of compound 6.

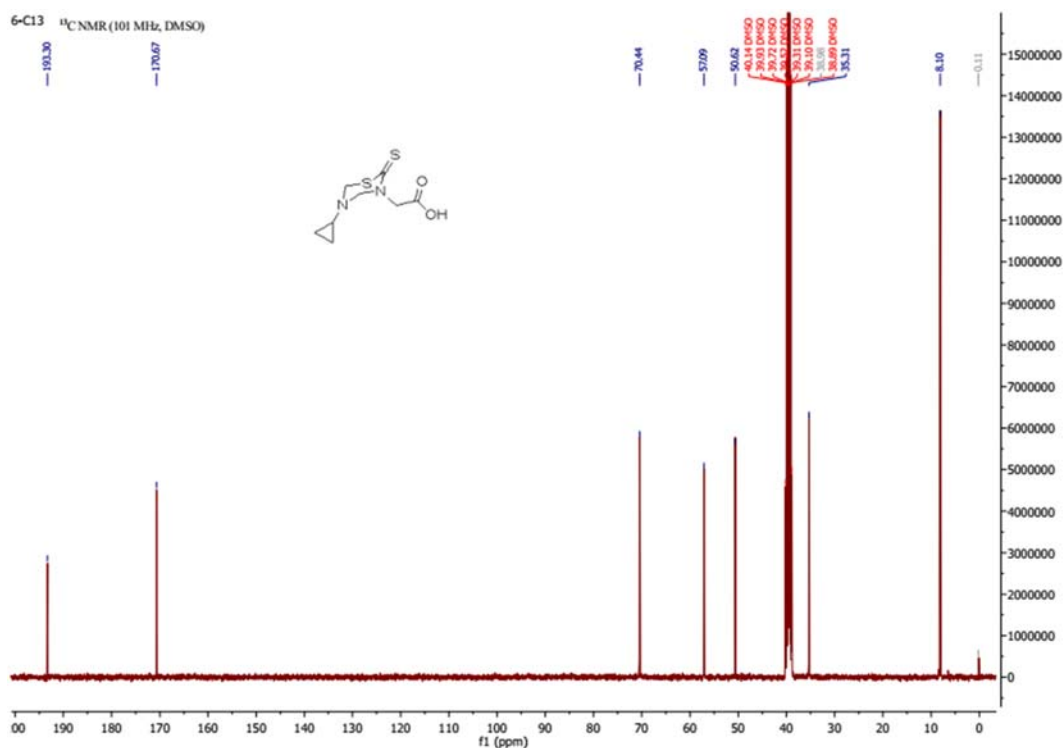
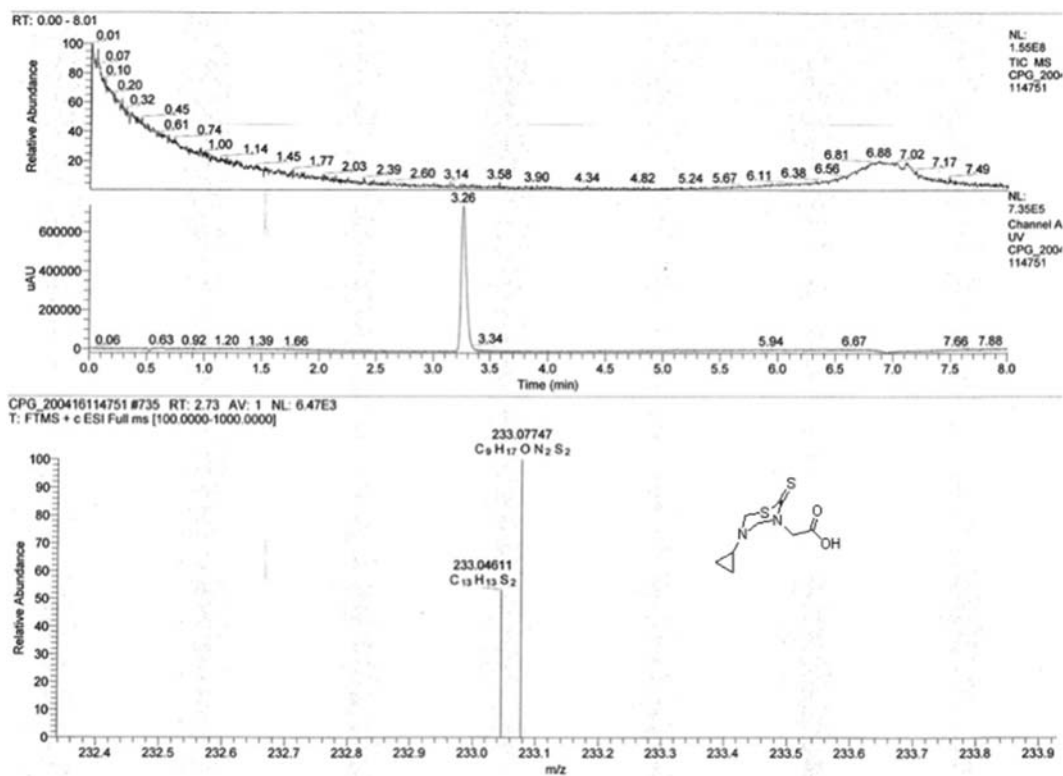
Figure S29: ¹³C NMR spectra of compound 6.

Figure S30: HRMS spectra of compound 6.

S7 Compound 7

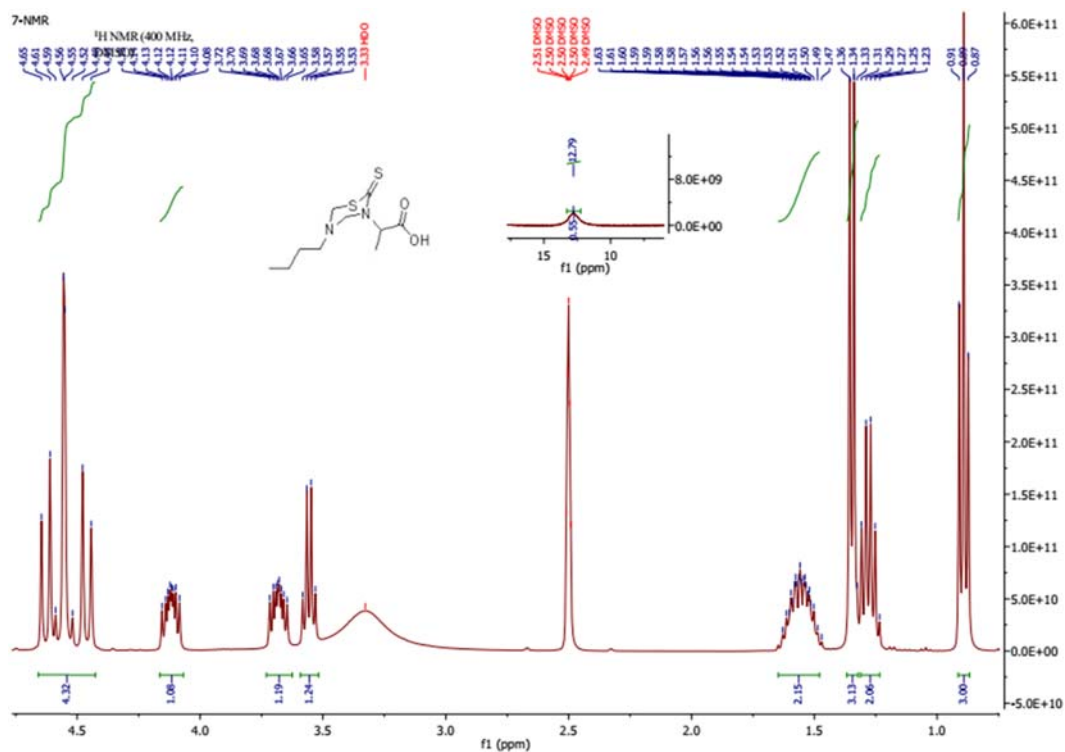


Figure S31: H-NMR spectra of compound 7.

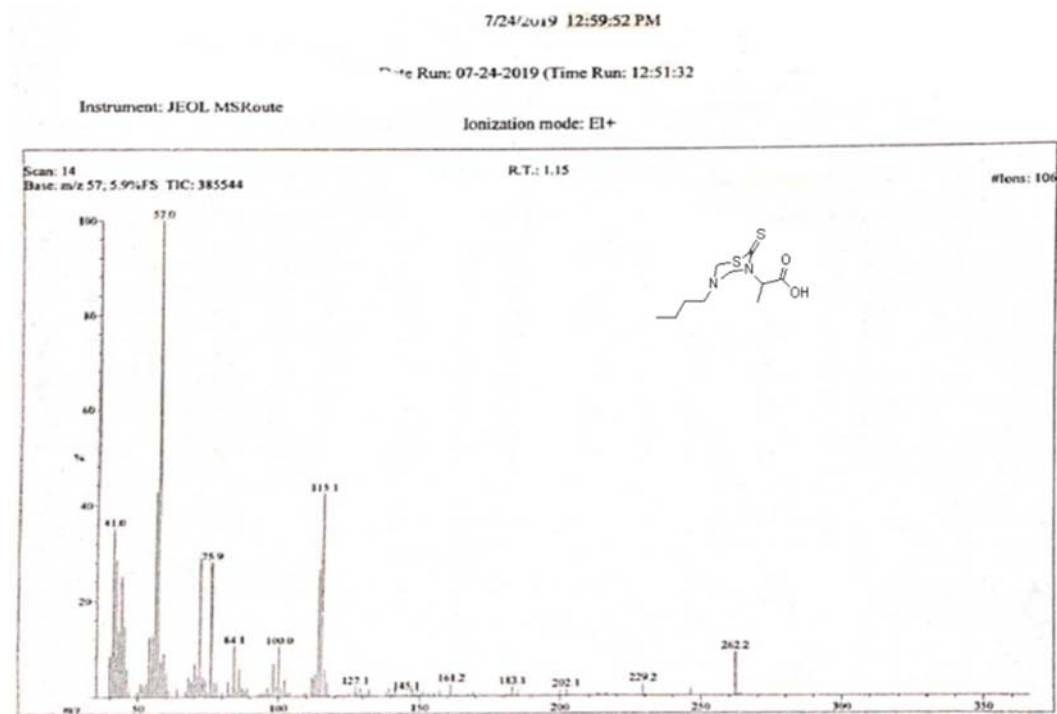


Figure S32: Mass spectra of compound 7.

S8 Compound 8

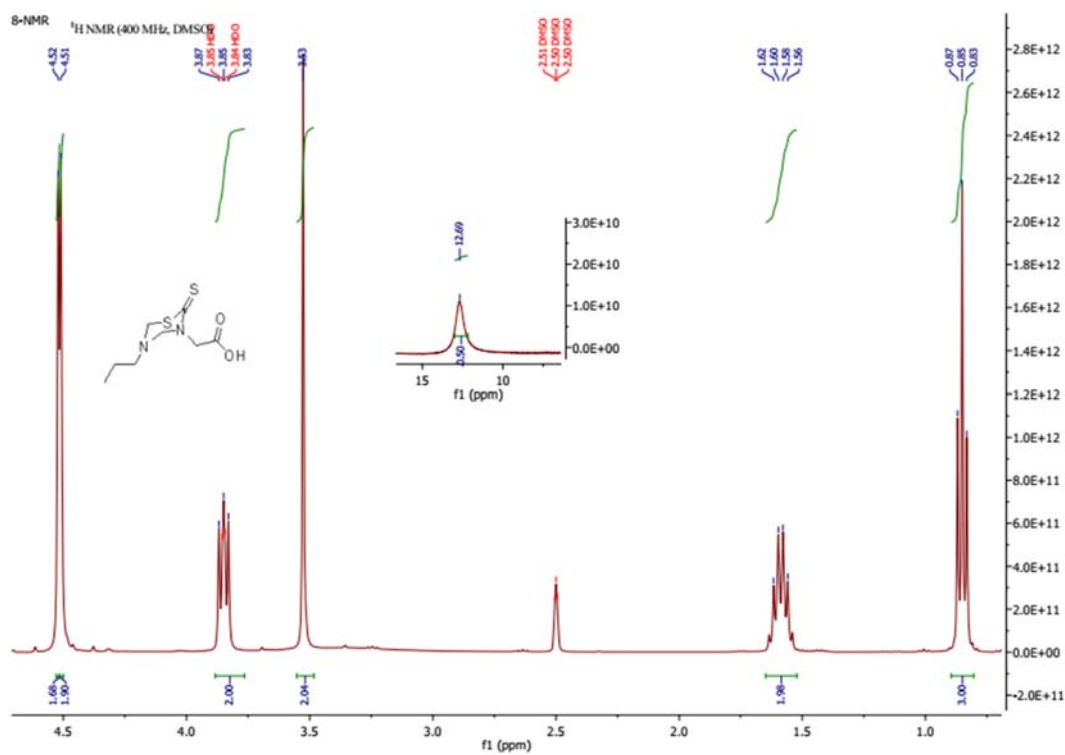


Figure S33: H-NMR spectra of compound 8.

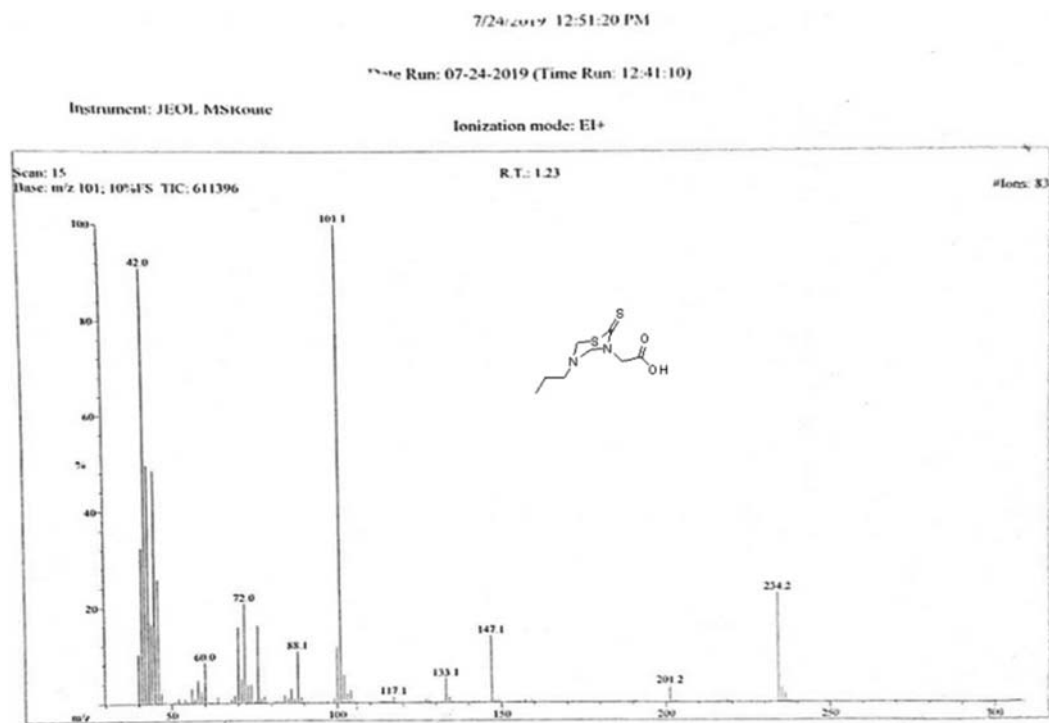
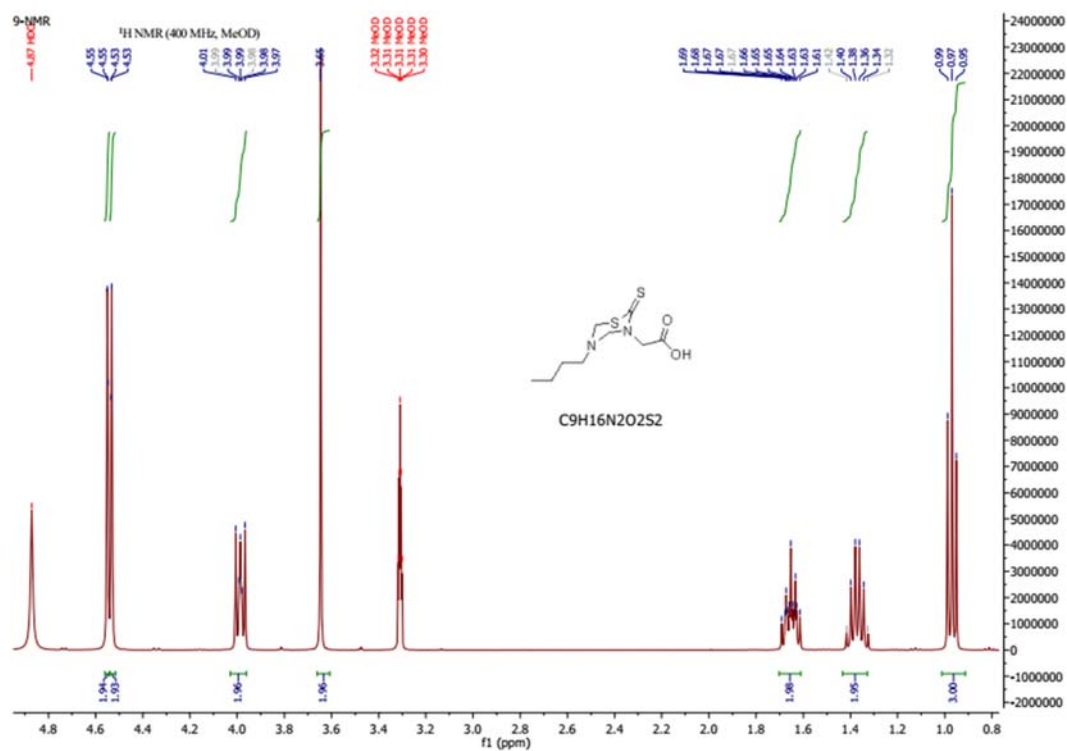
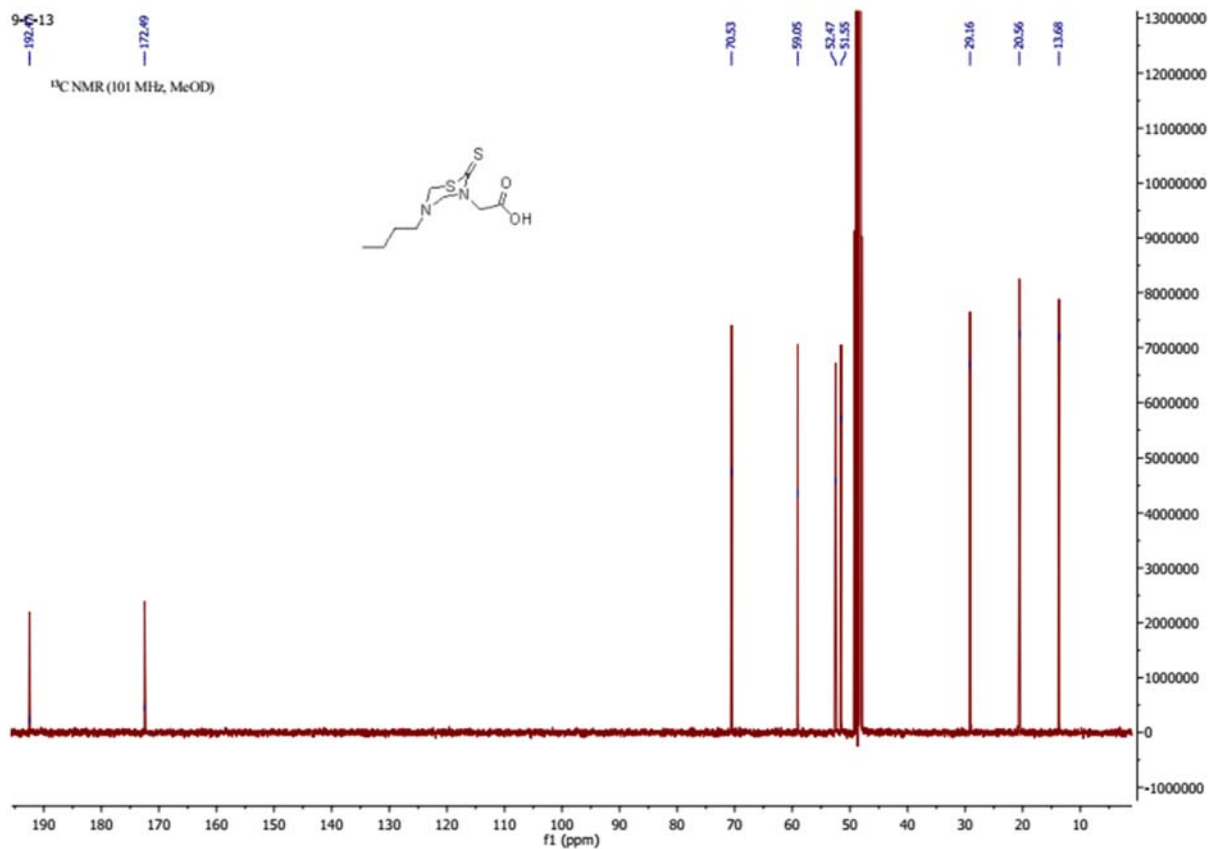
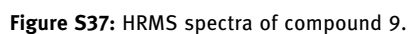


Figure S34: Mass spectra of compound 8.

S9 Compound 9

Figure S35: ¹H-NMR spectra of compound 9.Figure S36: ¹³C NMR spectra of compound 9.



10 nmr

¹H NMR (400 MHz, DMSO-d₆)

O=S1N(Cc2ccccc2)N(CO)S1

7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4

f1 (ppm)

4.8 4.0 1.6 3.33H₂O 1.5 2.50DMSO-d₆

Figure S38: H-NMR spectra of compound 10.

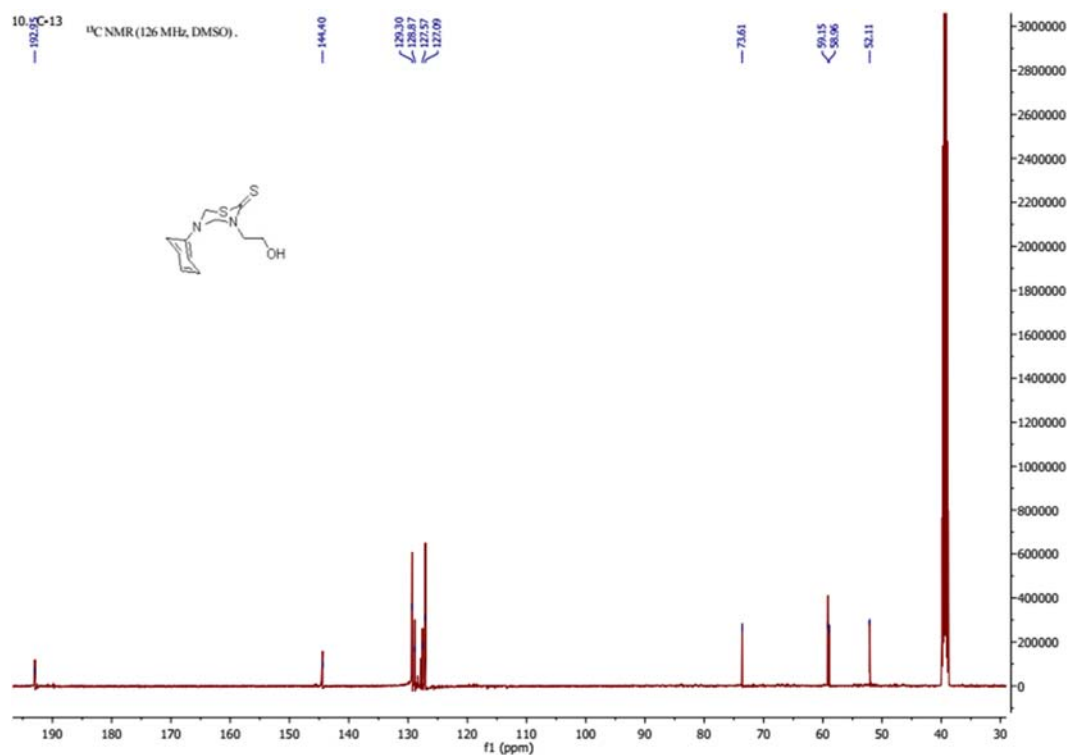


Figure S39: C13 NMR spectra of compound 10.

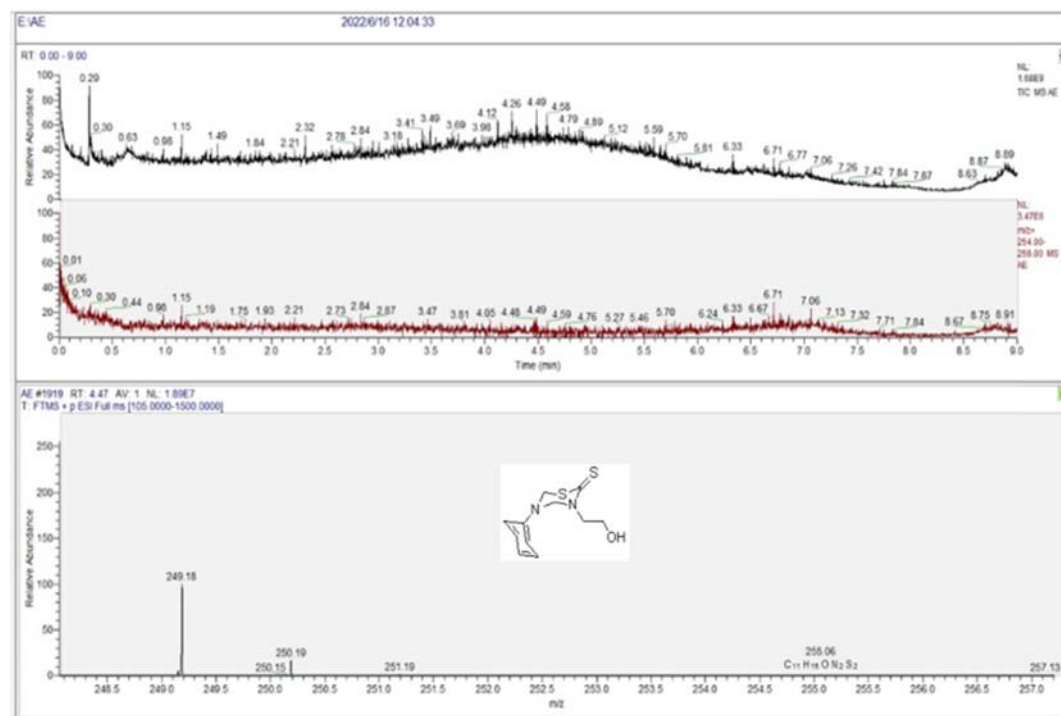


Figure S40: HRMS spectra of compound 10.

Figure S42: C13 NMR spectra of compound 11.

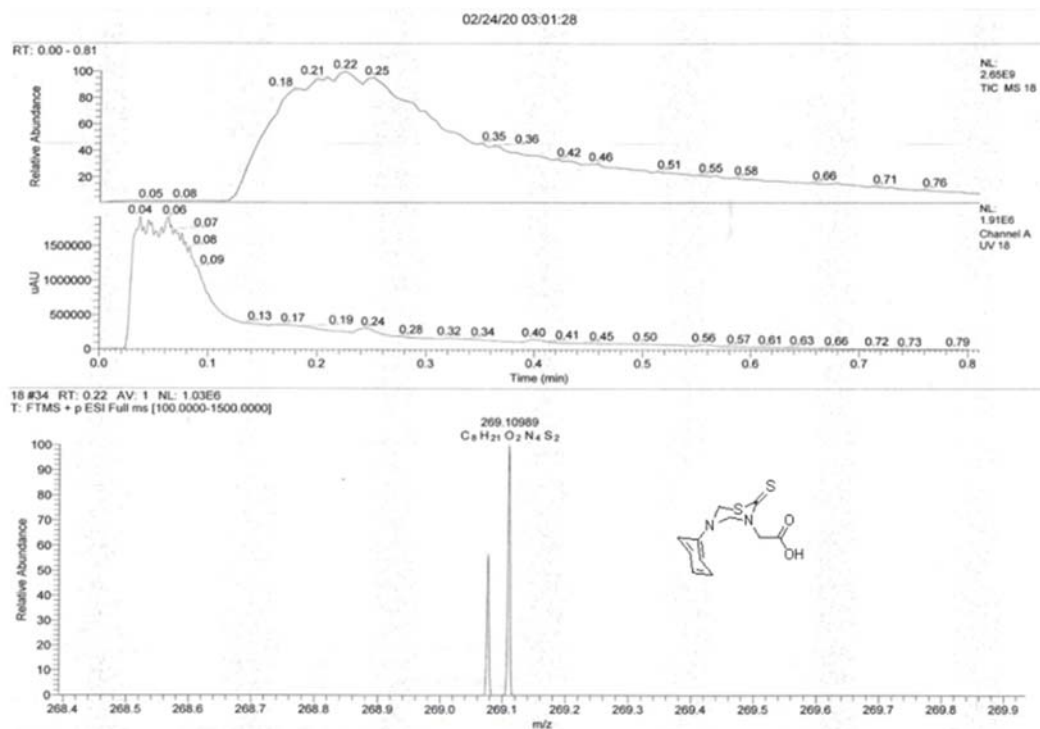
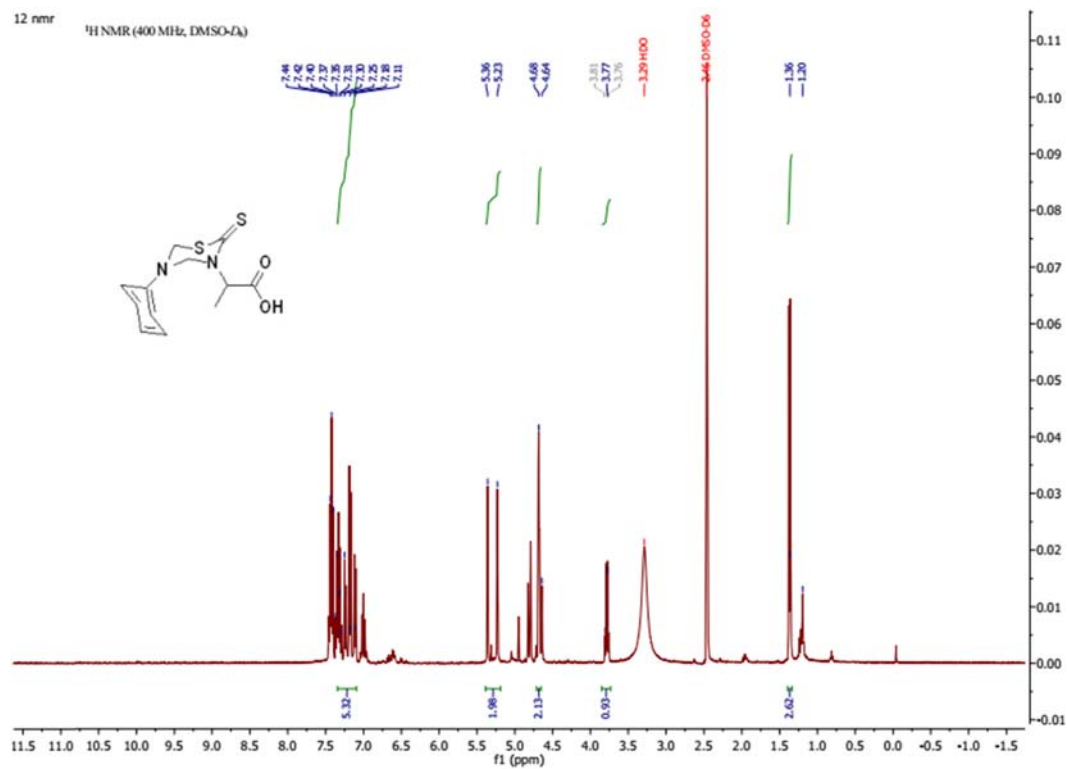


Figure S43: HRMS spectra of compound 11.

S12 Compound 12

Figure S44: 1H -NMR spectra of compound 12.

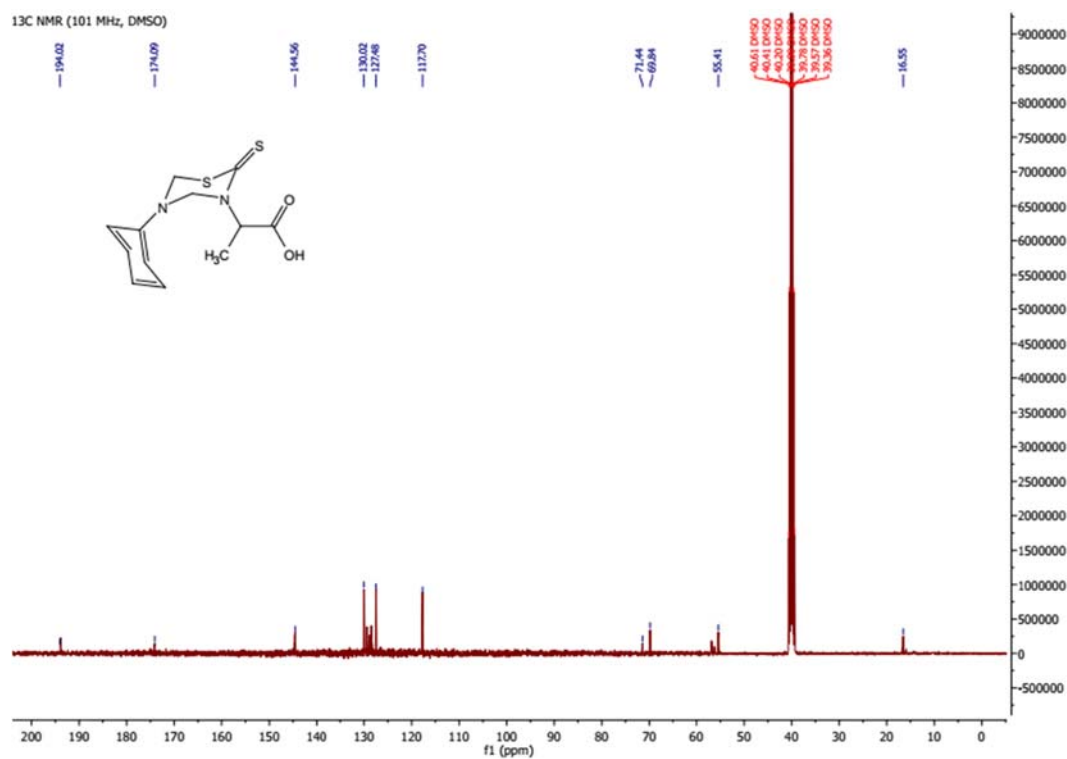


Figure S45: C13 NMR spectra of compound 12.

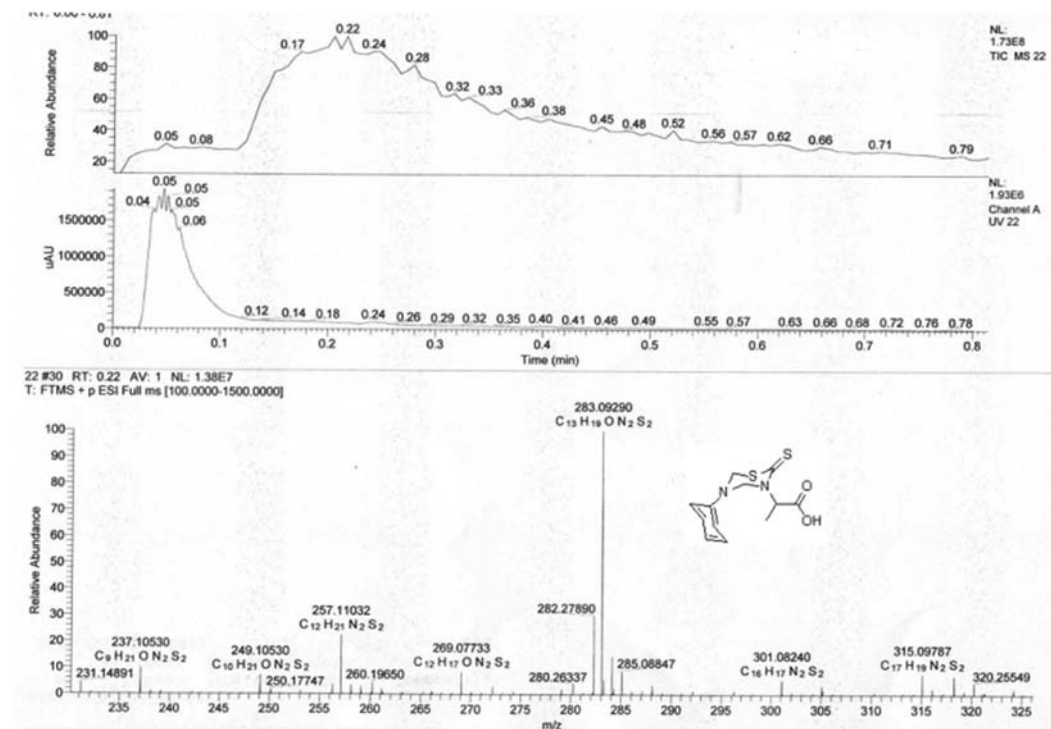


Figure S46: HRMS spectra of compound 12.

S13 Compound 13

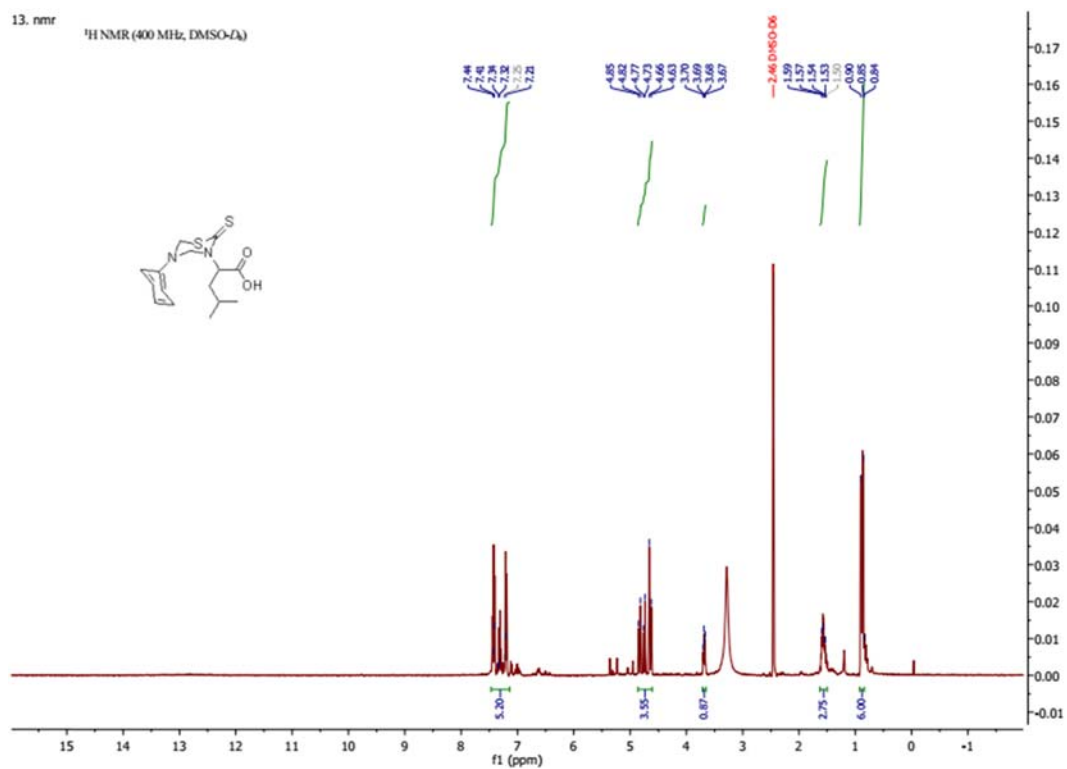


Figure S47: HNMR spectra of compound 13.

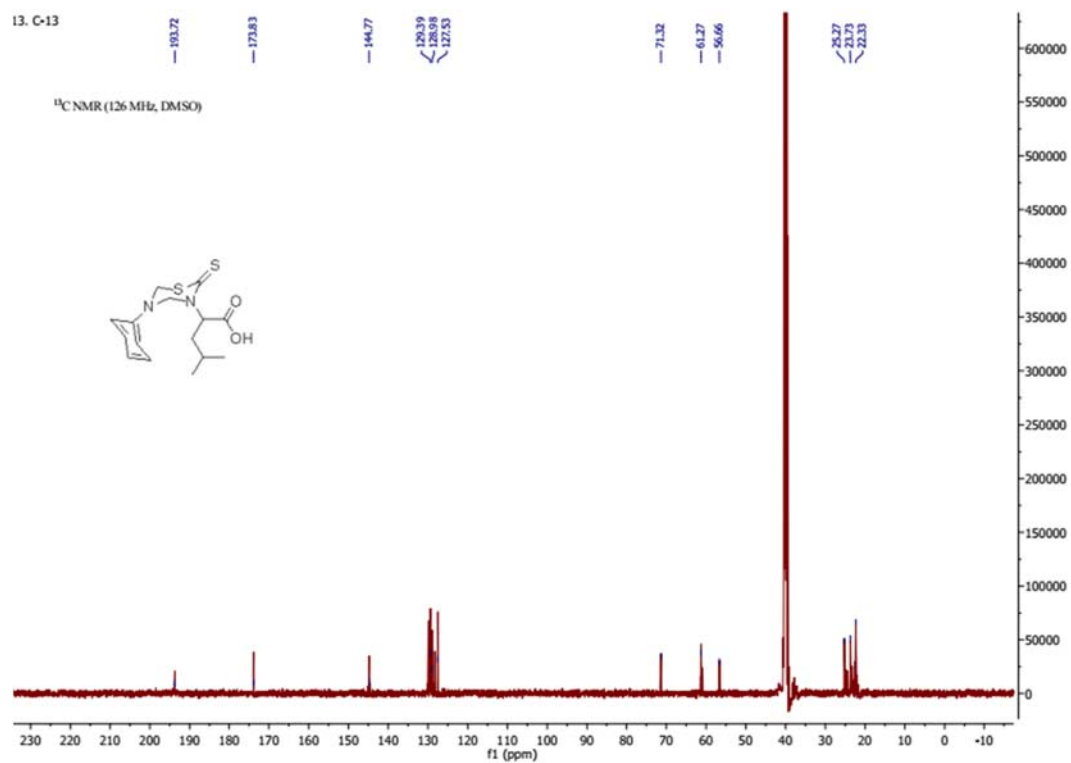


Figure S48: C13 NMR spectra of compound 13.

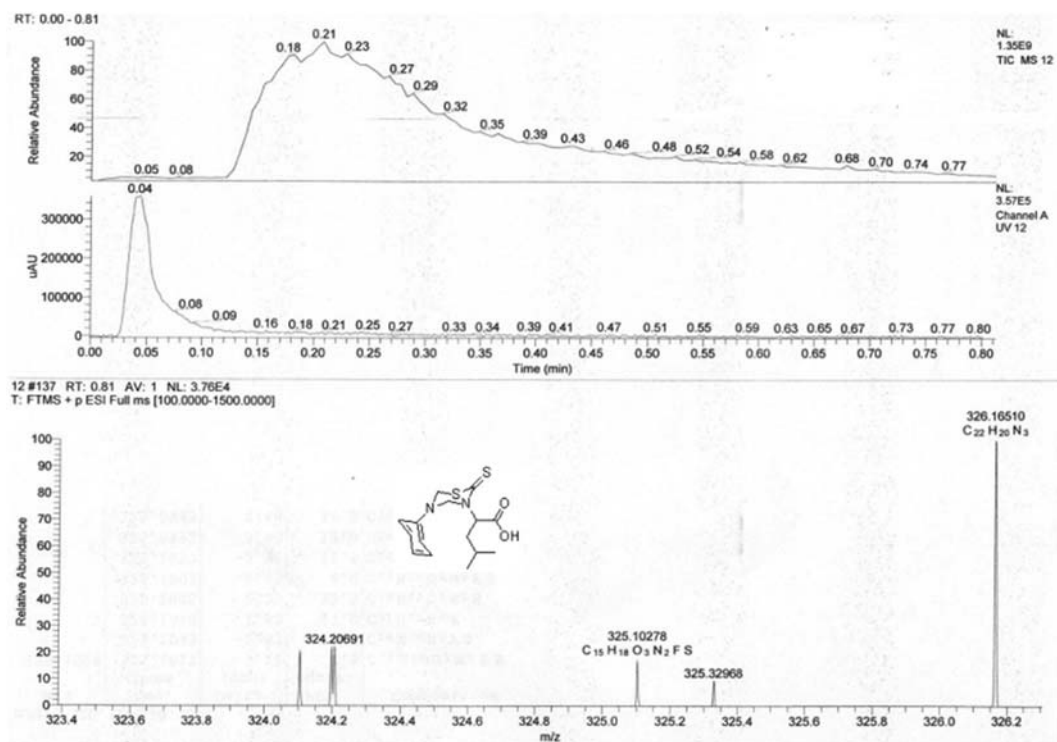


Figure S49: HRMS spectra of compound 13.