

Supporting Information

TITLE : TRANSNITROSATION OF ALICYCLIC *N*-NITRSAMINES CONTAINING SULFUR ATOMS IN FIVE- OR SIX-MEMBERED RINGS

Noriko Usui, Masataka Mochizuki, and Keiko Inami*

Division of Pharmaceutical Organic Chemistry, Faculty of Pharmaceutical Sciences, Sanyo-Onoda City University, 1-1- Daigakudori, Sanyo-Onoda-shi, Yamaguchi 756-0884, Japan. E-mail: inami@rs.socu.ac.jp

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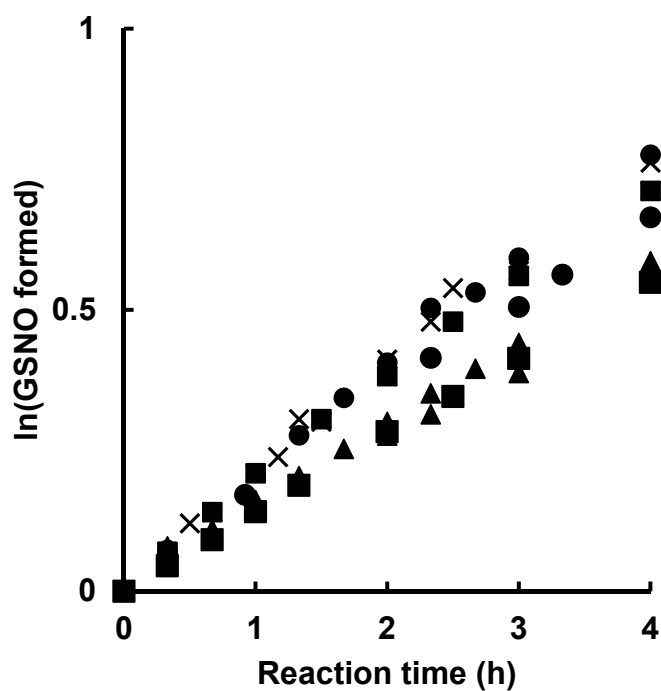


Figure S1. Formation of GSNO for pH-profile by reaction of **2**.
 Reaction conditions are as follows: compound **2**, 0.45 mM; GSH, 5.0 mM; pH2.0;
 phosphate buffer concentration, 50 mM(●), 100 mM(▲), 200 mM(■), 500 mM(×);
 37 °C

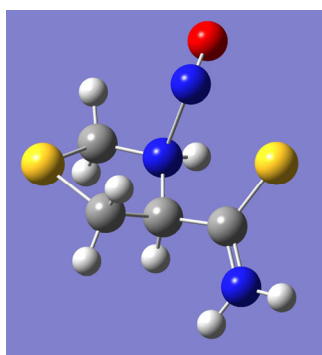
Table S1. k_{obs} for GSNO formation under the acidic conditions.

Concentration (mM)	$k_{obs} (\times 10^{-7}/s)$
50	372
50	384
100	391
100	364
200	342
200	372
500	365
500	404

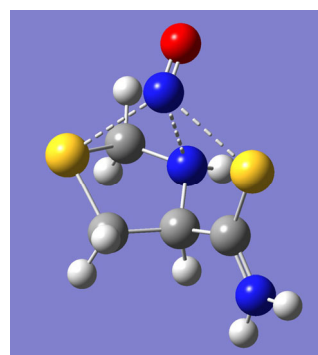
Table S2. DFT calculations of protonated and transition state structures.

Compound	(Hartree)		
	1	2	3
Protonated	-1192.884823	-1232.198647	-1232.210297
Transition state	-1192.873349	-1232.194334	-1232.188797
Δ Energy	0.011474	0.004313	0.021500
Δ Energy (kcal/mol)	7.20	2.71	13.49

Compound 1

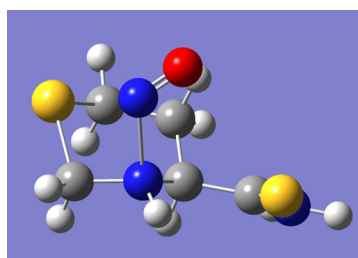


Protonated 1

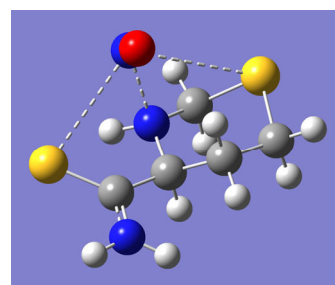


Transition state

Compound 2

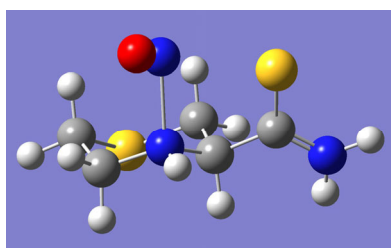


Protonated 2

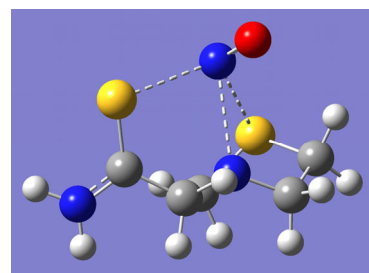


Transition state

Compound 3



Protonated 3



Transition state

Figure S2. The DFT optimized structures.

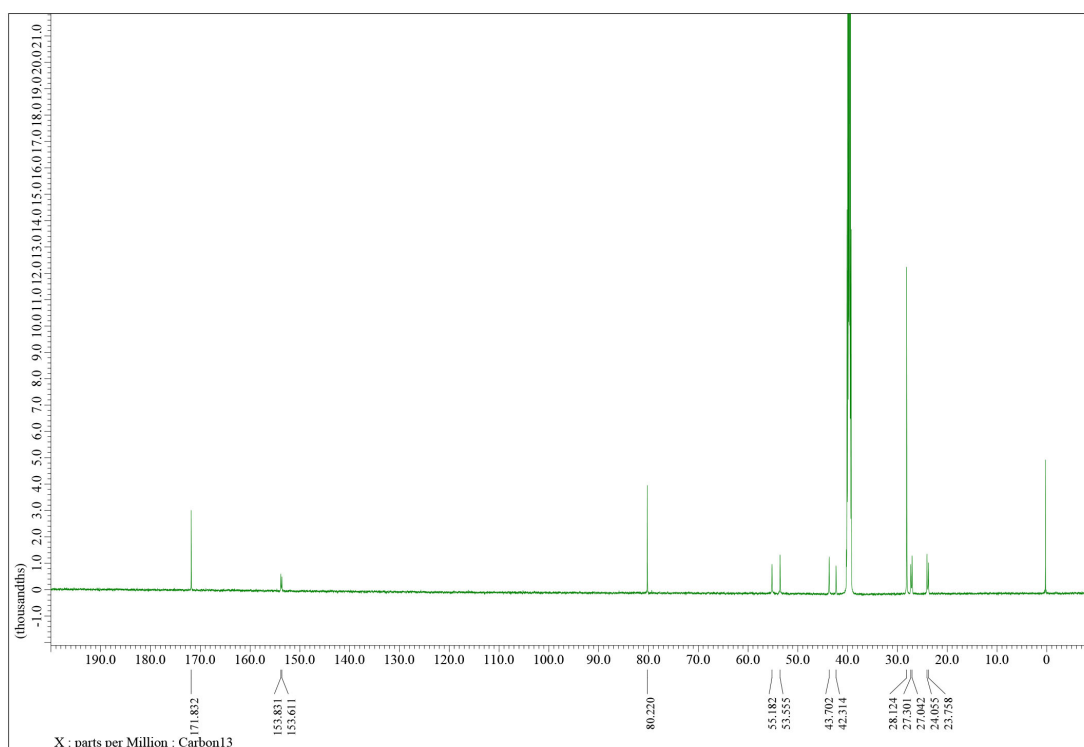
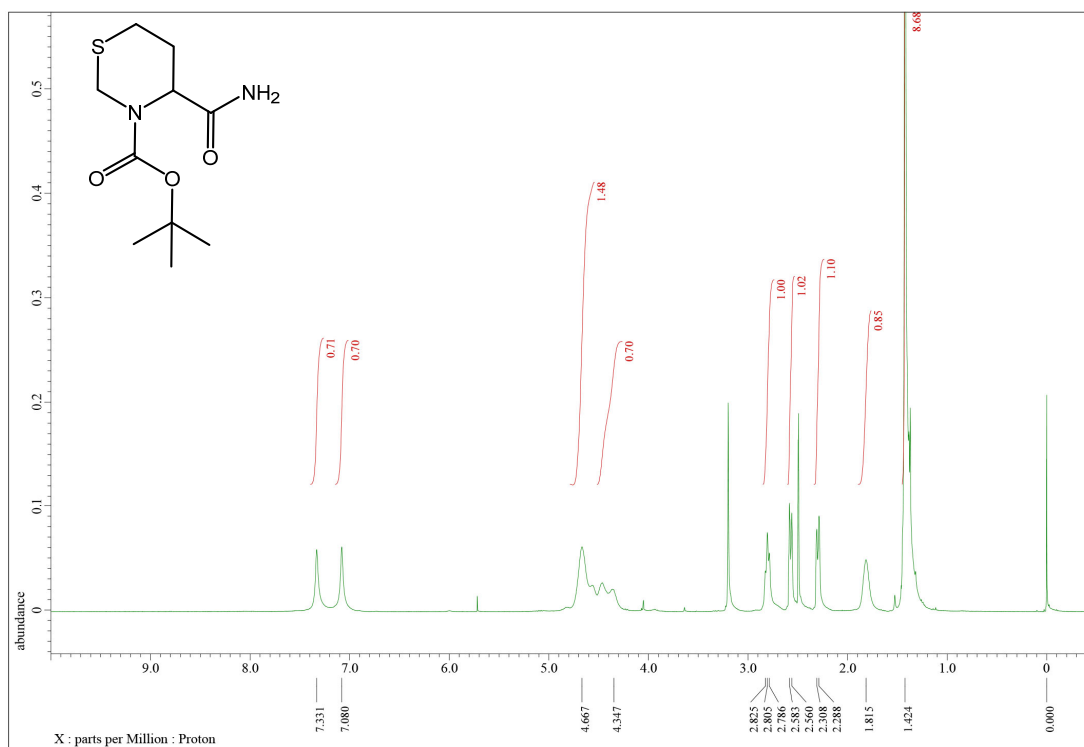


Figure S3. ¹H (600 MHz, 50 °C) and ¹³C (150 MHz) spectra of *t*-butyl 4-carbamoyl-1,3-thiazinane-3-carboxylate in DMSO-*d*₆.

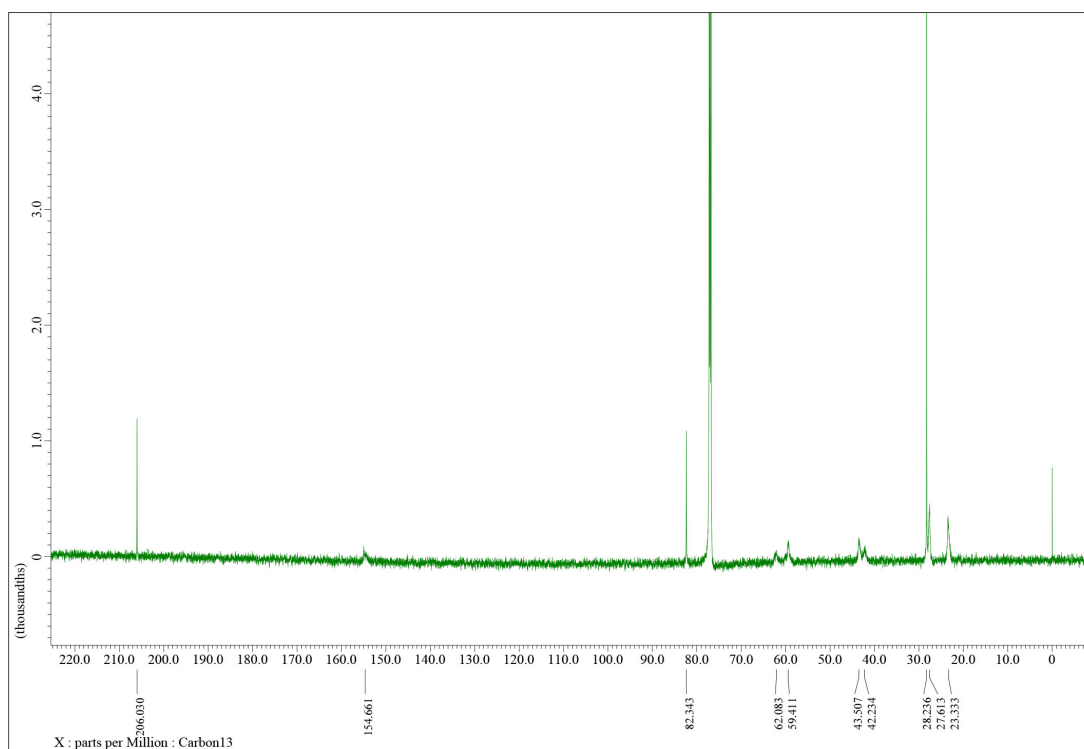
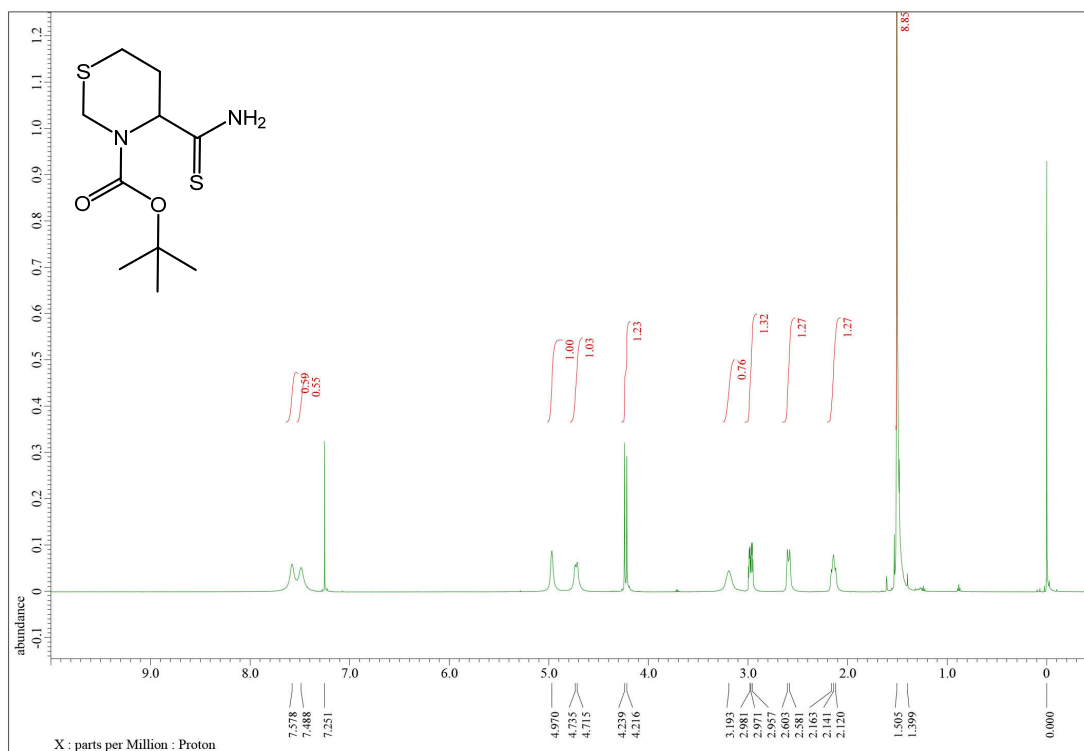


Figure S4. ¹H (600 MHz, 50 °C) and ¹³C (150 MHz) spectra of *t*-butyl 4-carbamothioyl-1,3-thiazinane-3-carboxylate in CDCl₃.

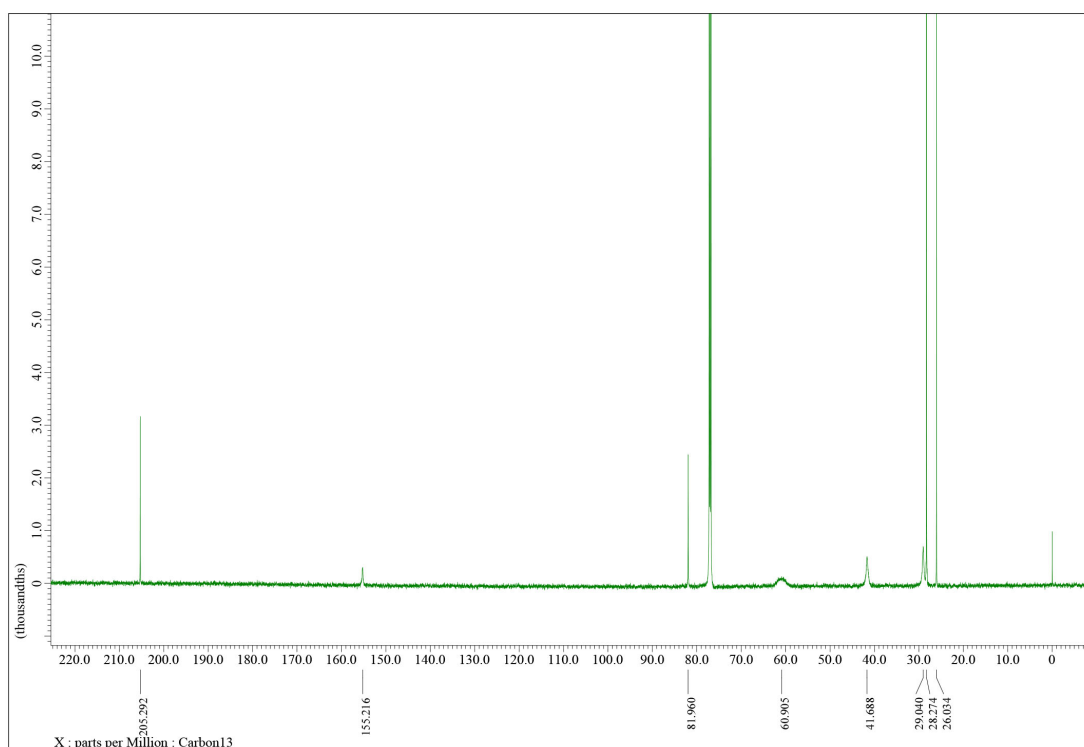
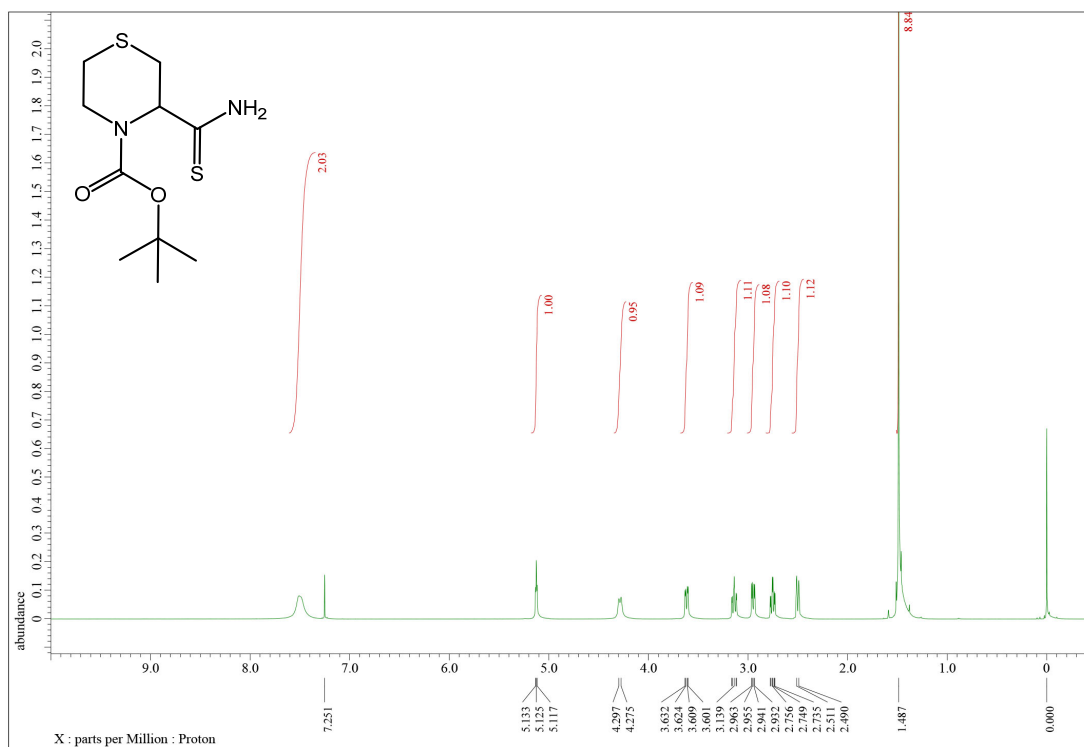


Figure S5. ¹H (600 MHz, 50 °C) and ¹³C (150 MHz) spectra of *t*-butyl 3-carbamthiylthiomorpholine-4-carboxylate in CDCl₃.

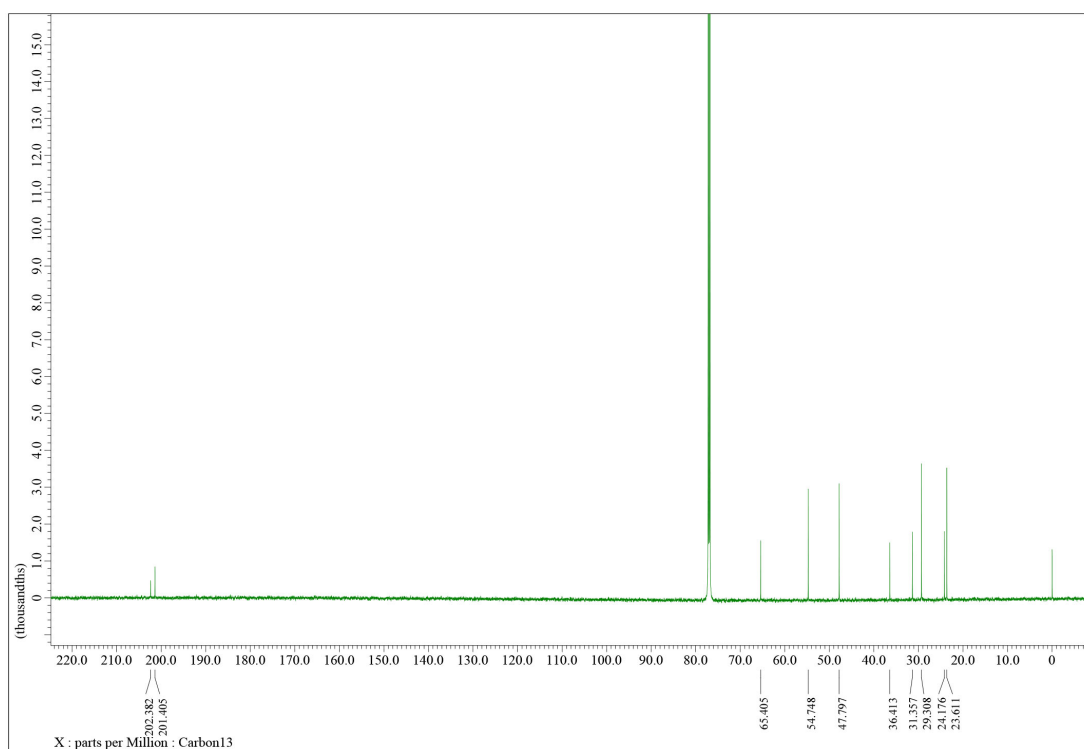
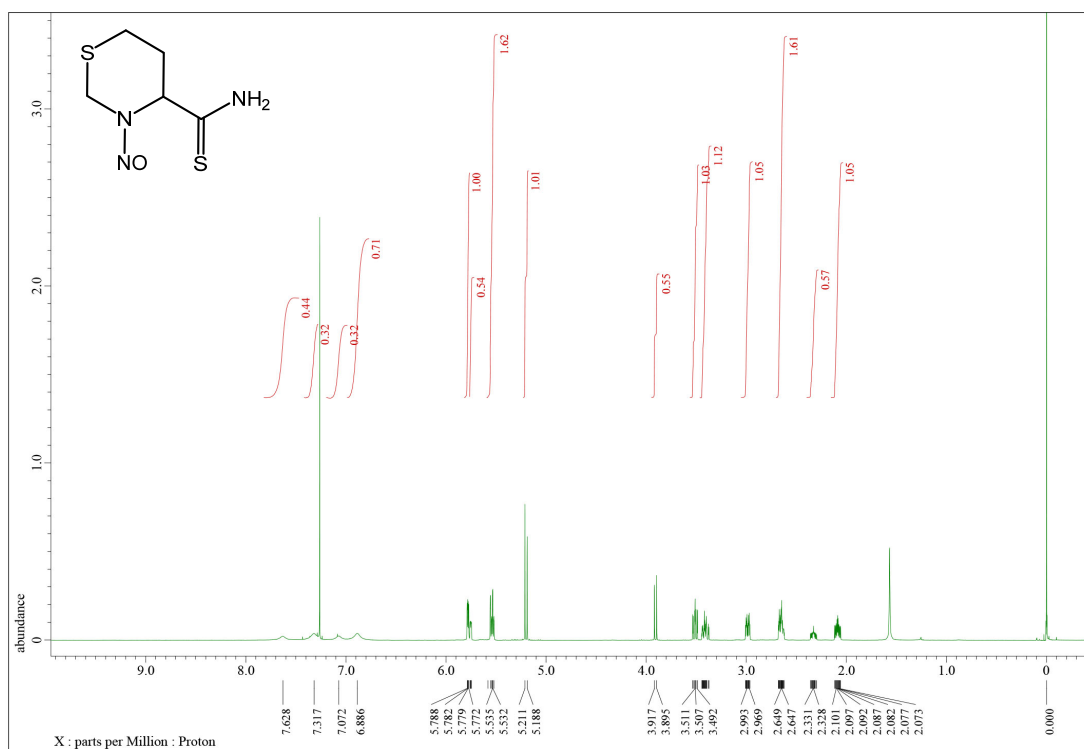


Figure S6. ¹H (600 MHz) and ¹³C (150 MHz) spectra of *N*-nitroso-1,3-thiazinane-4-carbothioamide in CDCl₃.

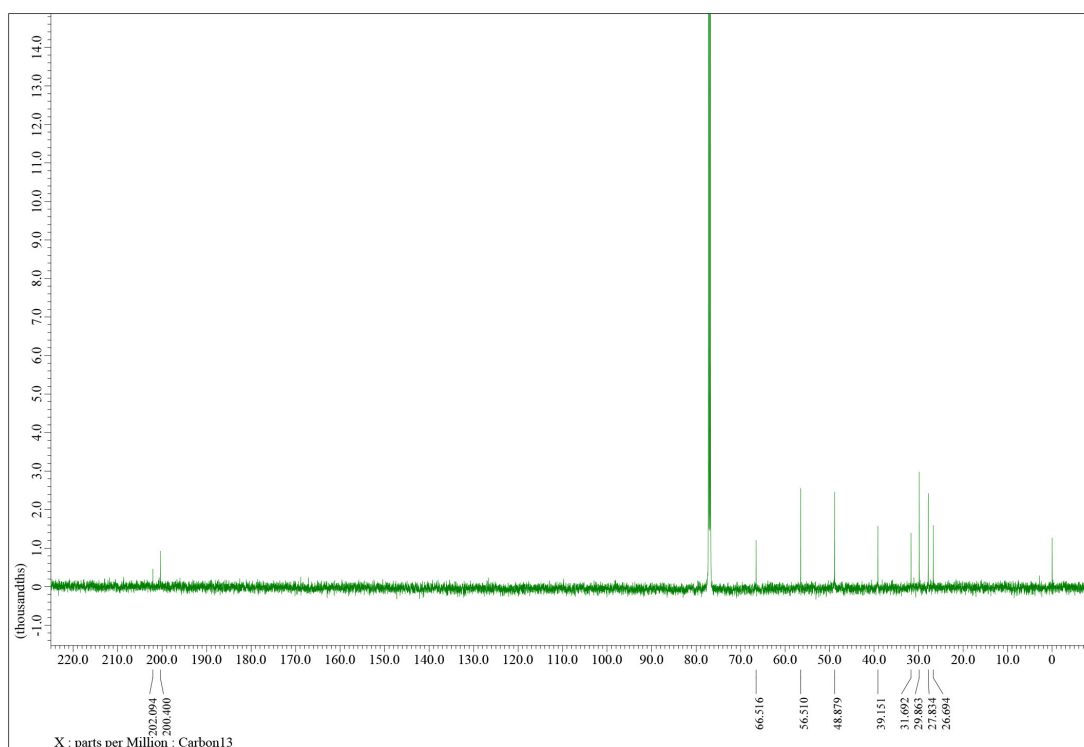
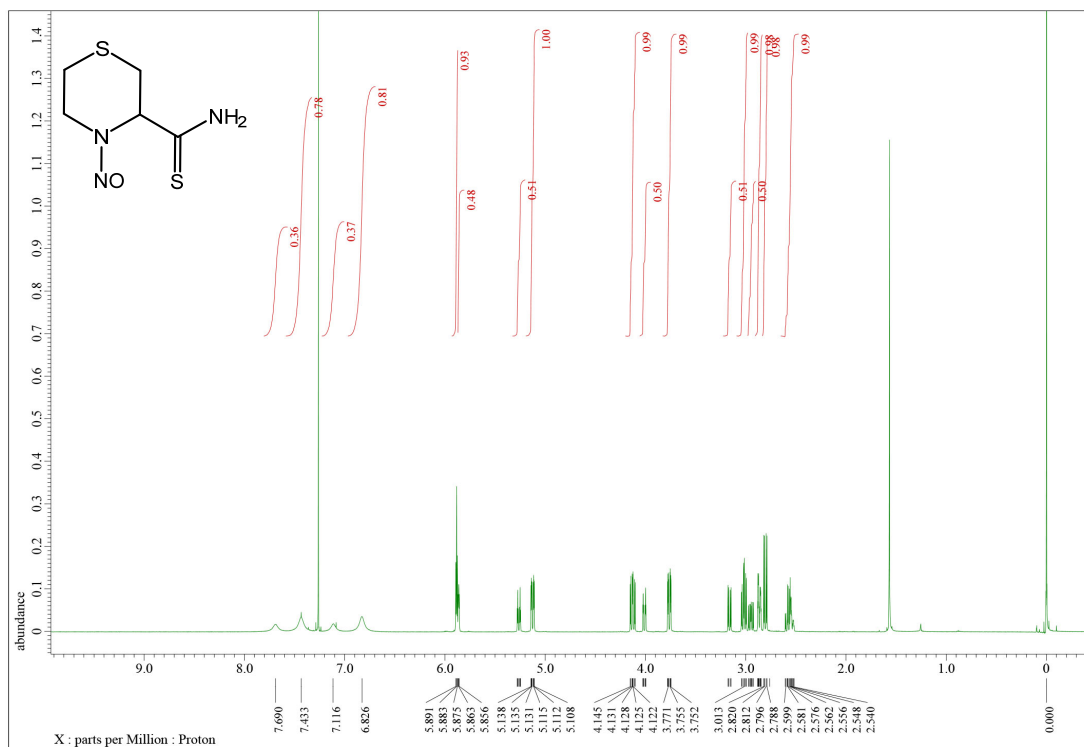


Figure S7. ¹H (600 MHz,) and ¹³C (150 MHz) spectra of *N*-nitrosothiomorpholine-3-carbothioamide in CDCl₃.