N-(Acetamido)thiourea Based Simple Neutral Hydrogen-Bonding Receptors for Anions

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Electronic Supplementary Information (ESI)

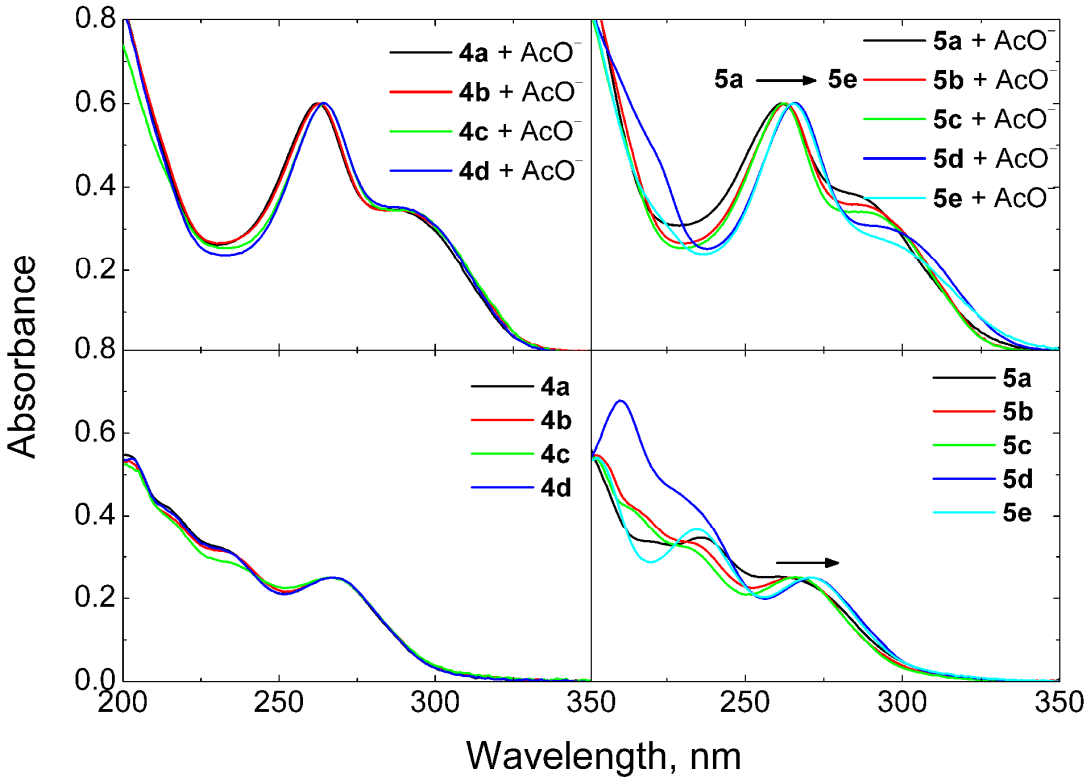


Figure S1. Absorption spectra of **4** and **5** and their AcO^- complexes in acetonitrile

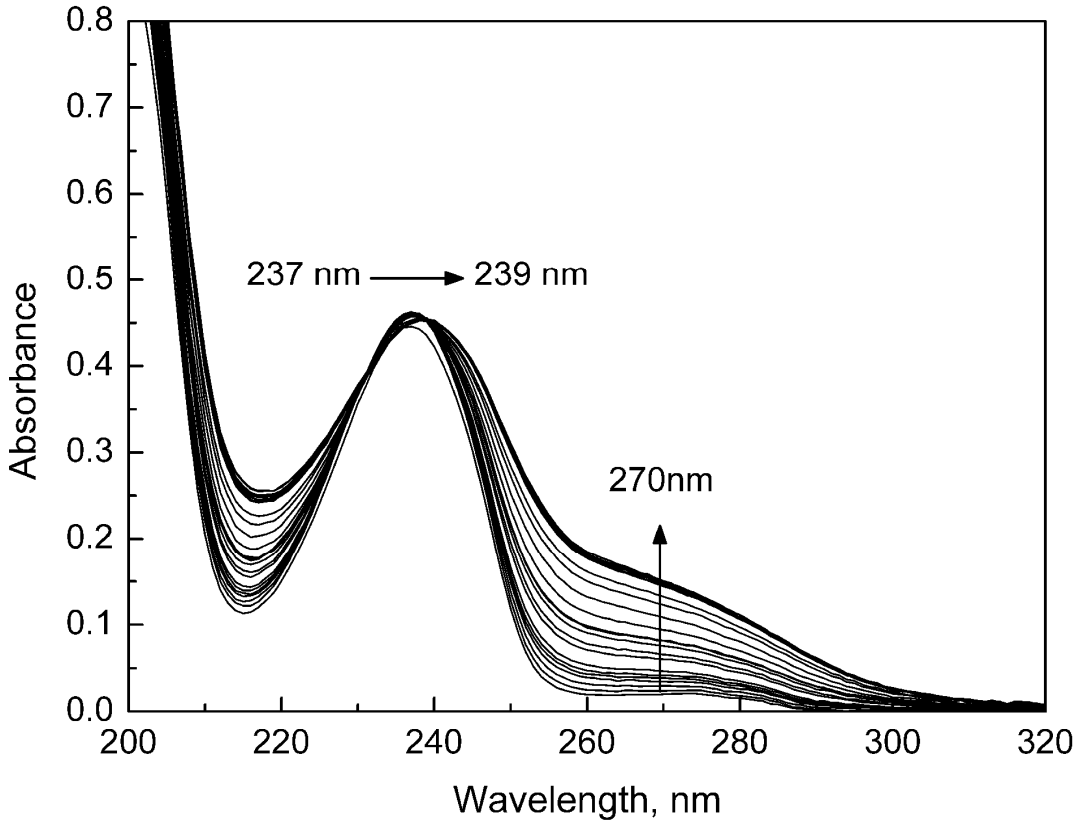
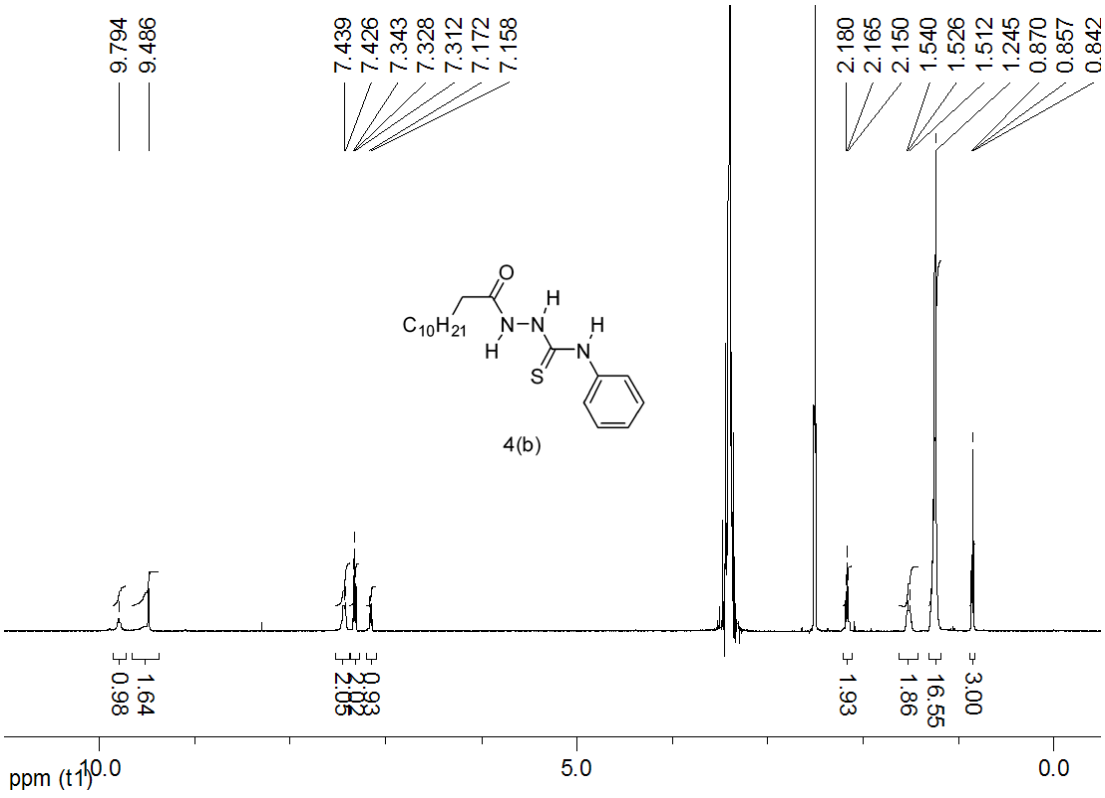


Figure S2. Absorption spectra of **7** in acetonitrile in the presence of F^- over 0 to 5.0×10^{-4} mol L^{-1}. [**7**] = 1.0×10^{-5} mol L^{-1}.

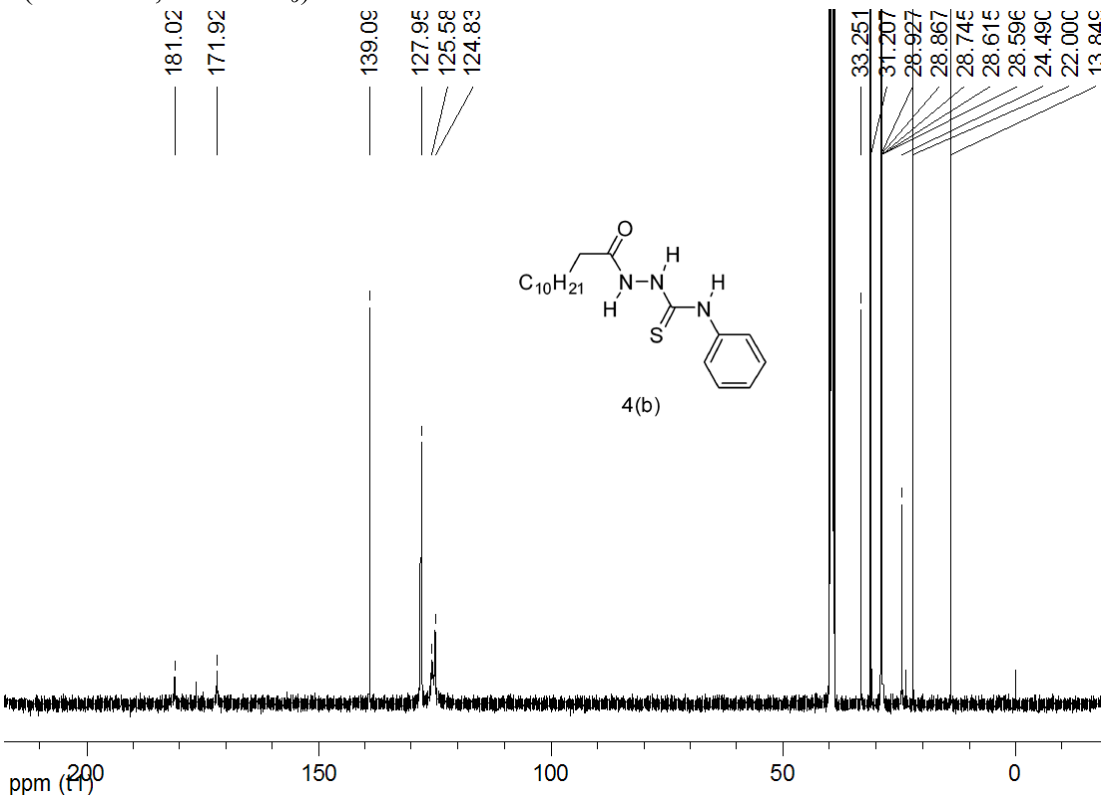
^{1}H NMR and ^{13}C NMR spectra of 4b-4d (4a = 5c), 5a-5f, 6 and 7

2-Dodecanoyl-*N*-phenylhydrazinecarbothioamide (4b)

^{1}H NMR (500 MHz, DMSO-d_6)

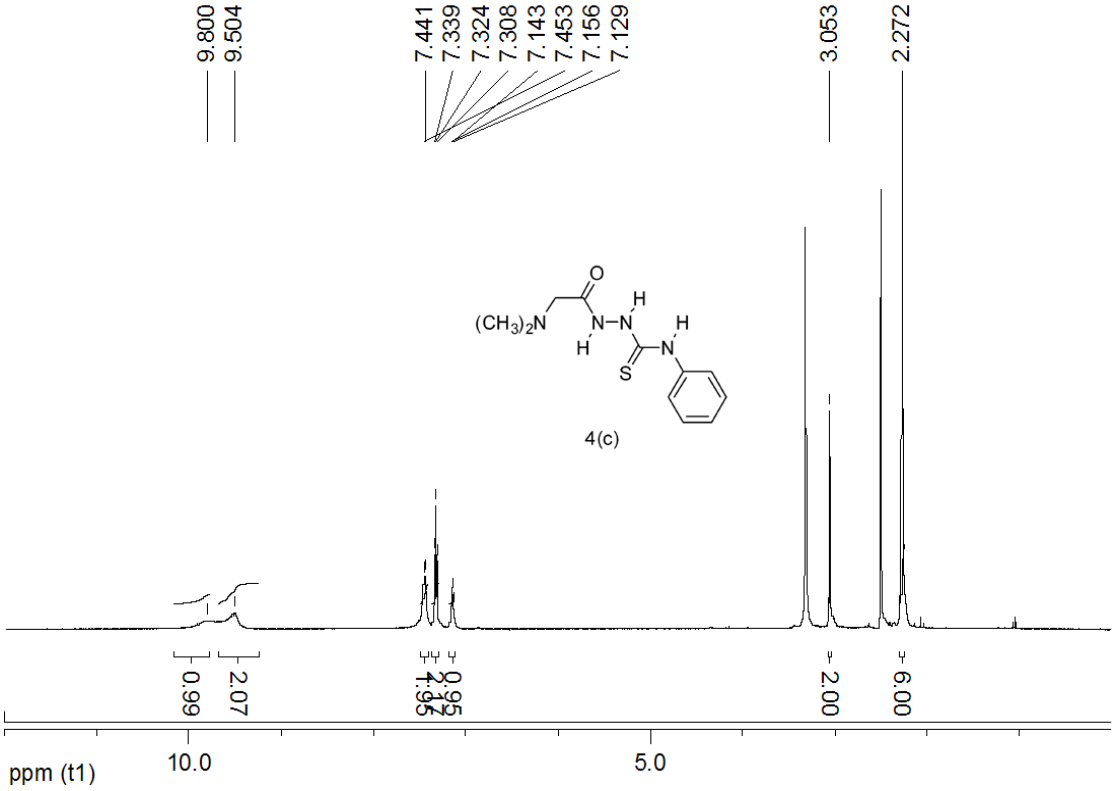


^{13}C NMR (125 MHz, DMSO-d_6)

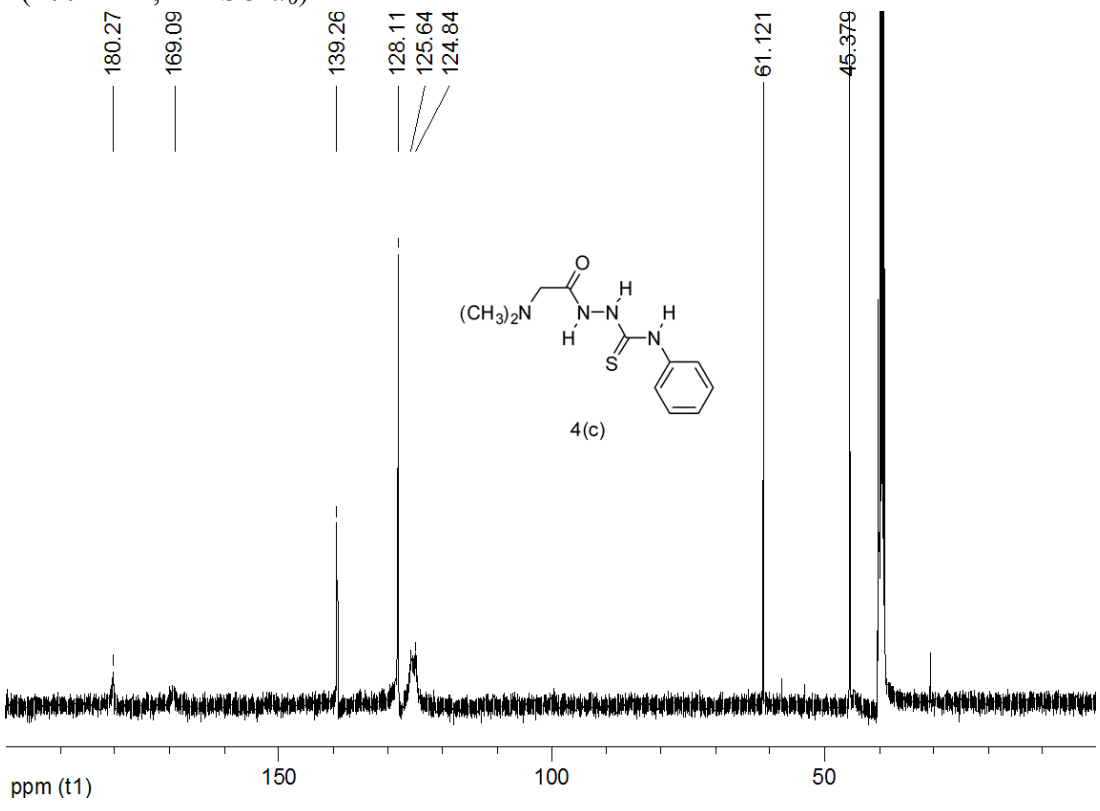


2-(2-(Dimethylamino)acetyl)-*N*-phenylhydrazinecarbothioamide (4c)

^{1}H NMR (400 MHz, DMSO-d_6)

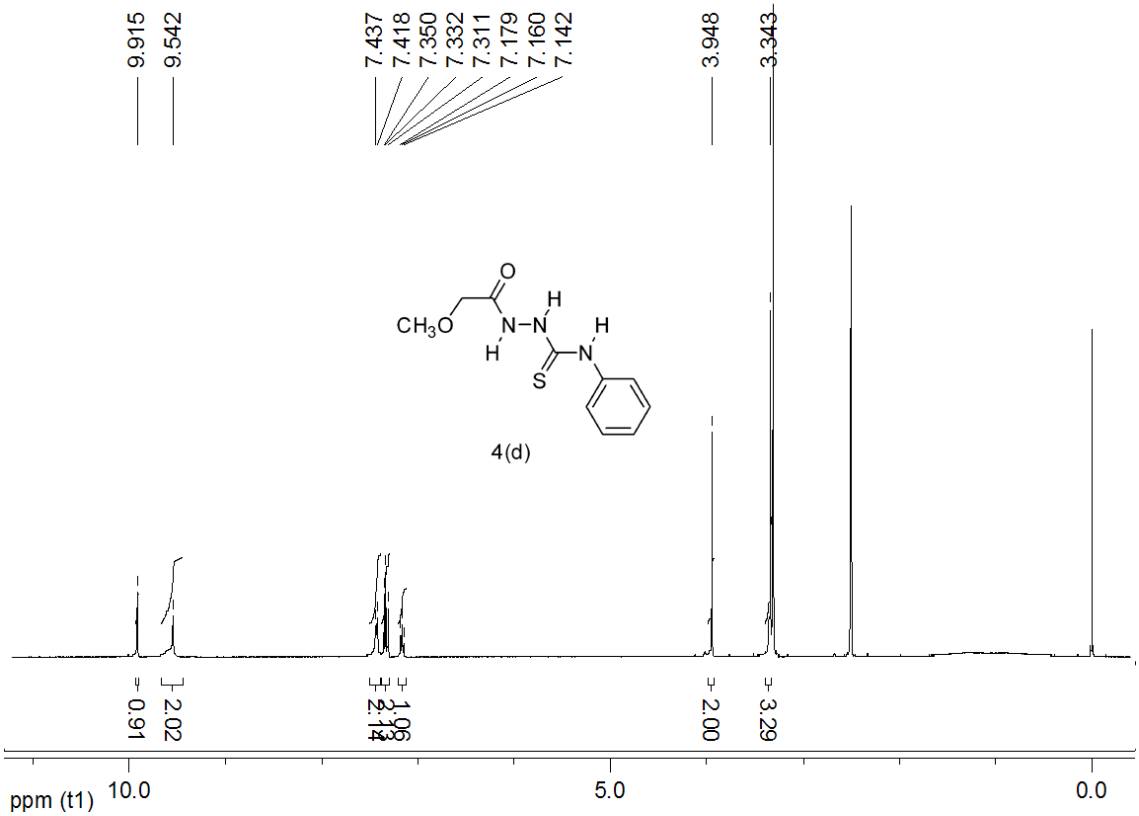


^{13}C NMR (100 MHz, DMSO-d_6)

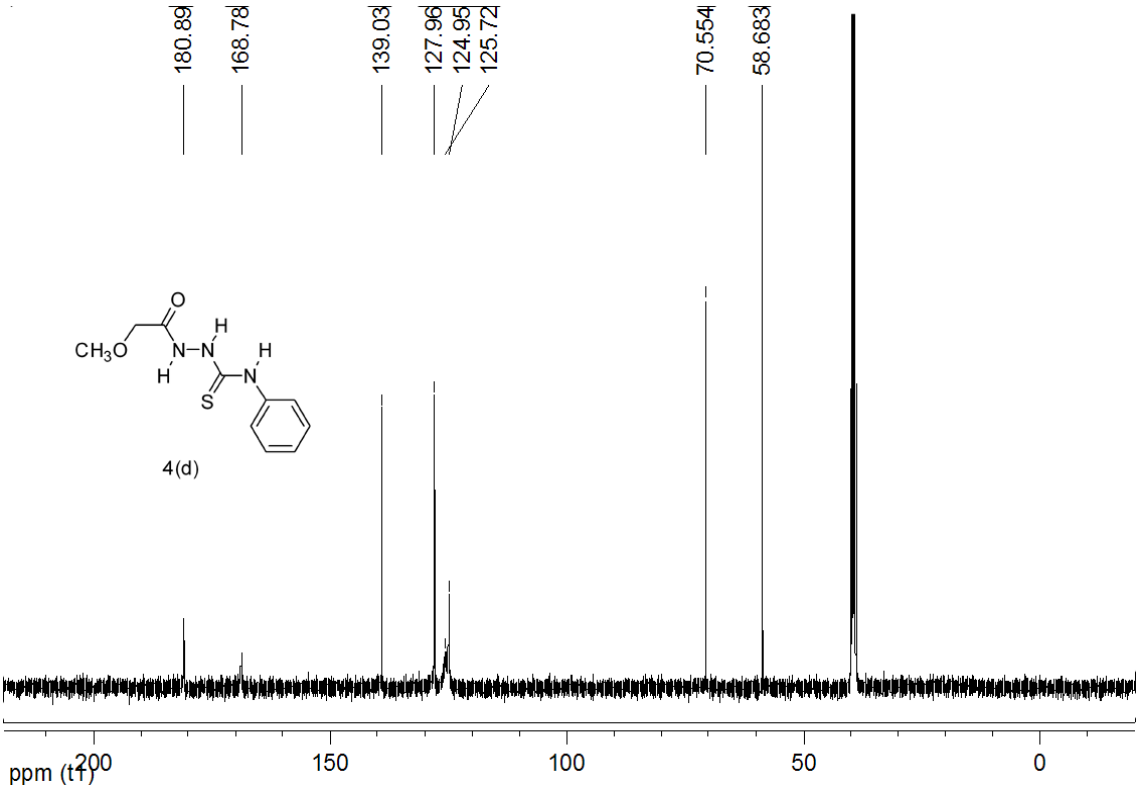


2-Methoxyacetyl-*N*-phenylhydrazinecarbothioamide (4d)

^{1}H NMR (400 MHz, DMSO-d_6)

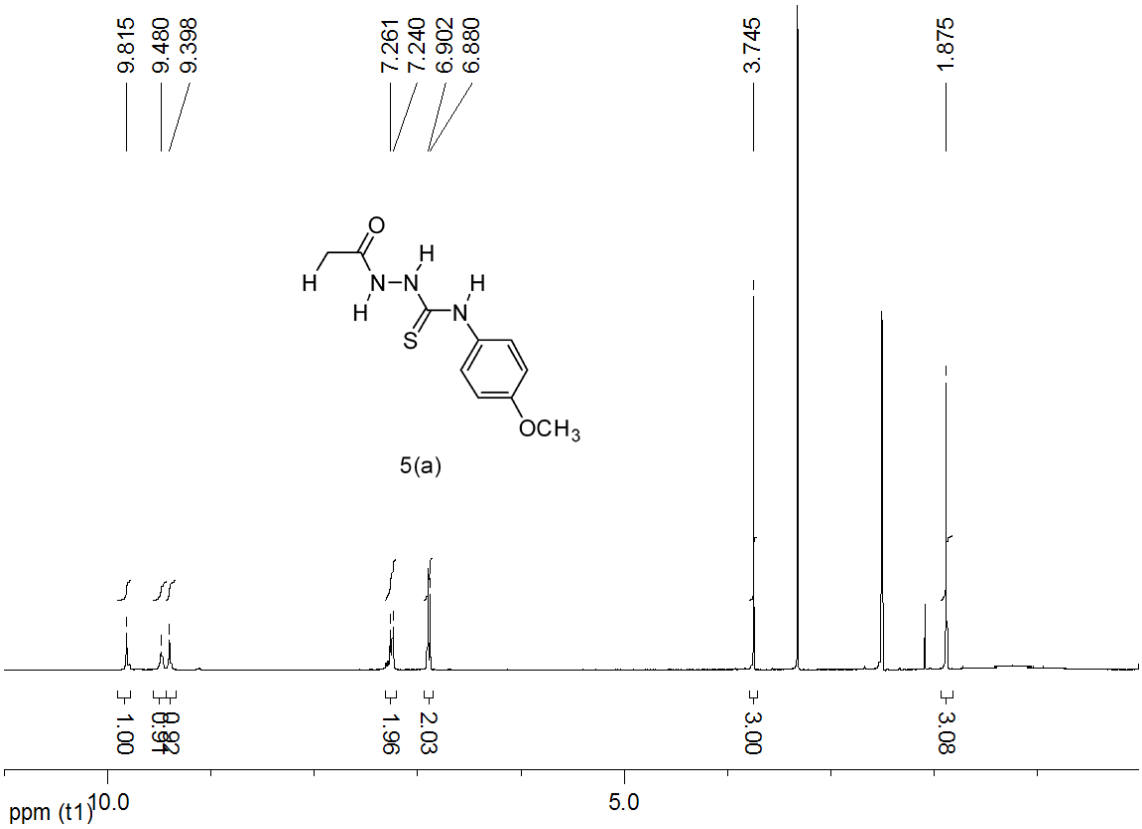


^{13}C NMR (100 MHz, DMSO-d_6)

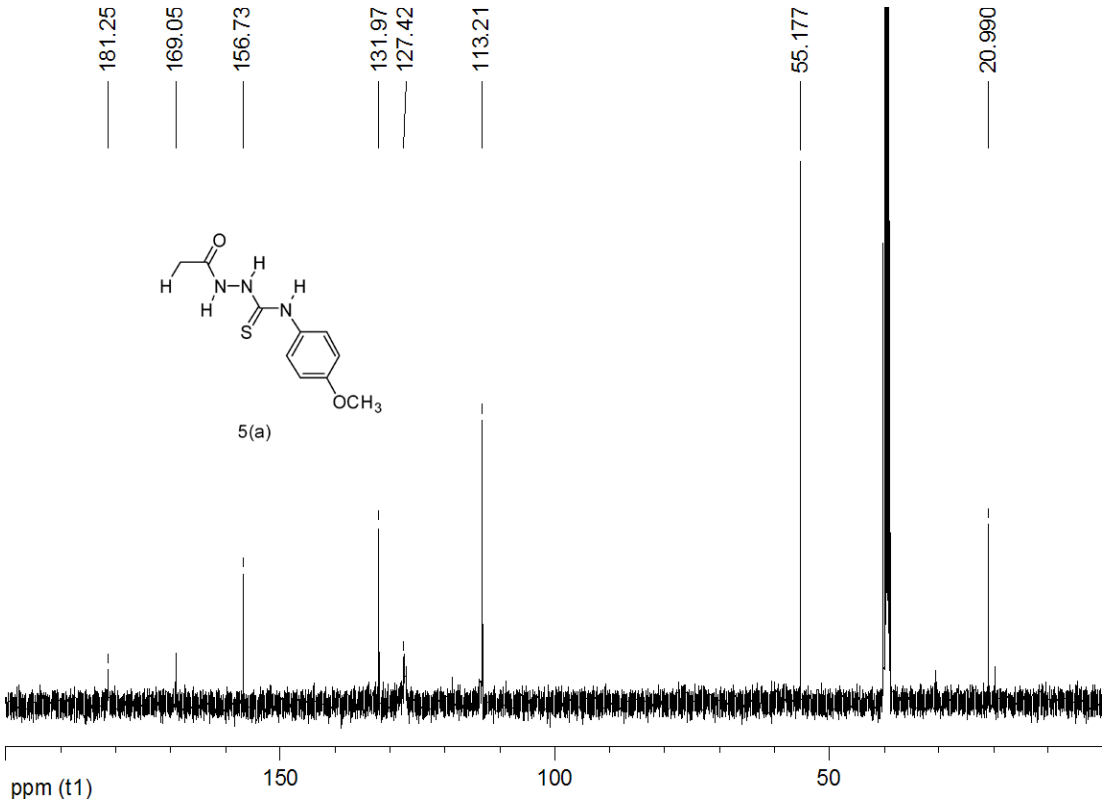


2-Acetyl-*N*-(4-methoxyphenyl)hydrazinecarbothioamide (5a)

^{1}H NMR (400 MHz, DMSO-d_6)

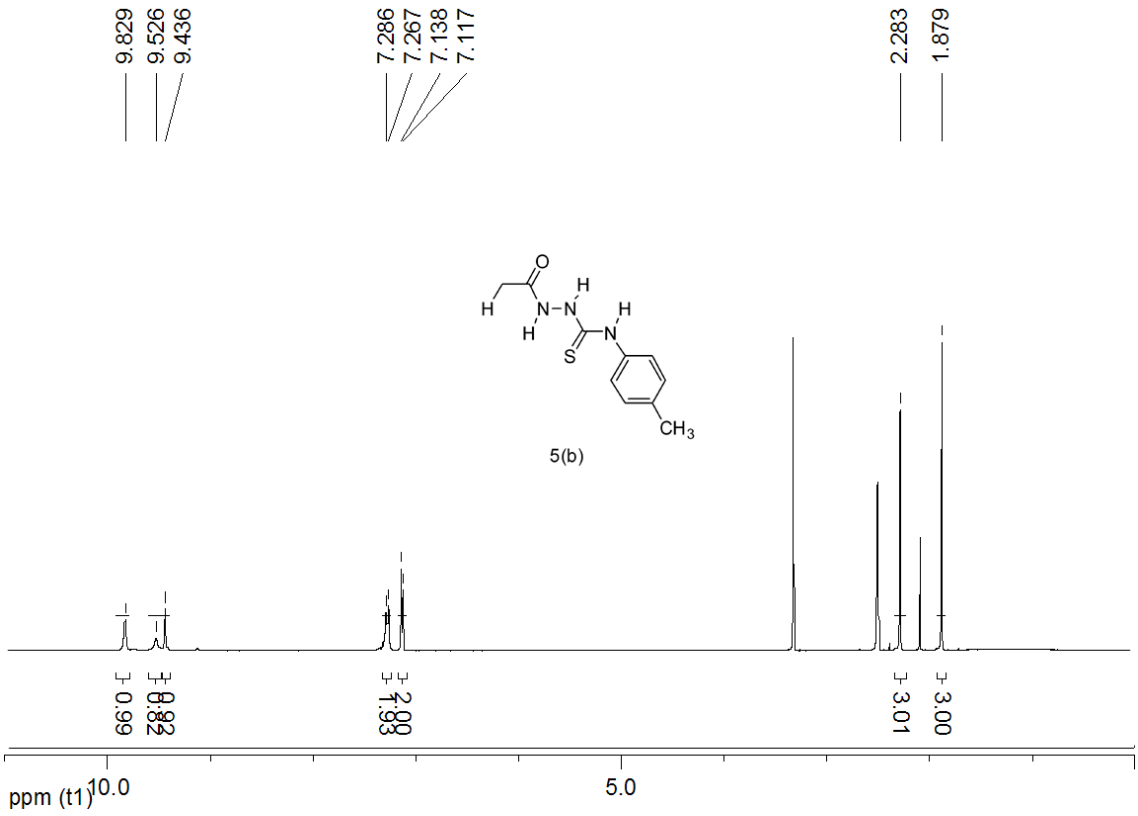


^{13}C NMR (100 MHz, DMSO-d_6)

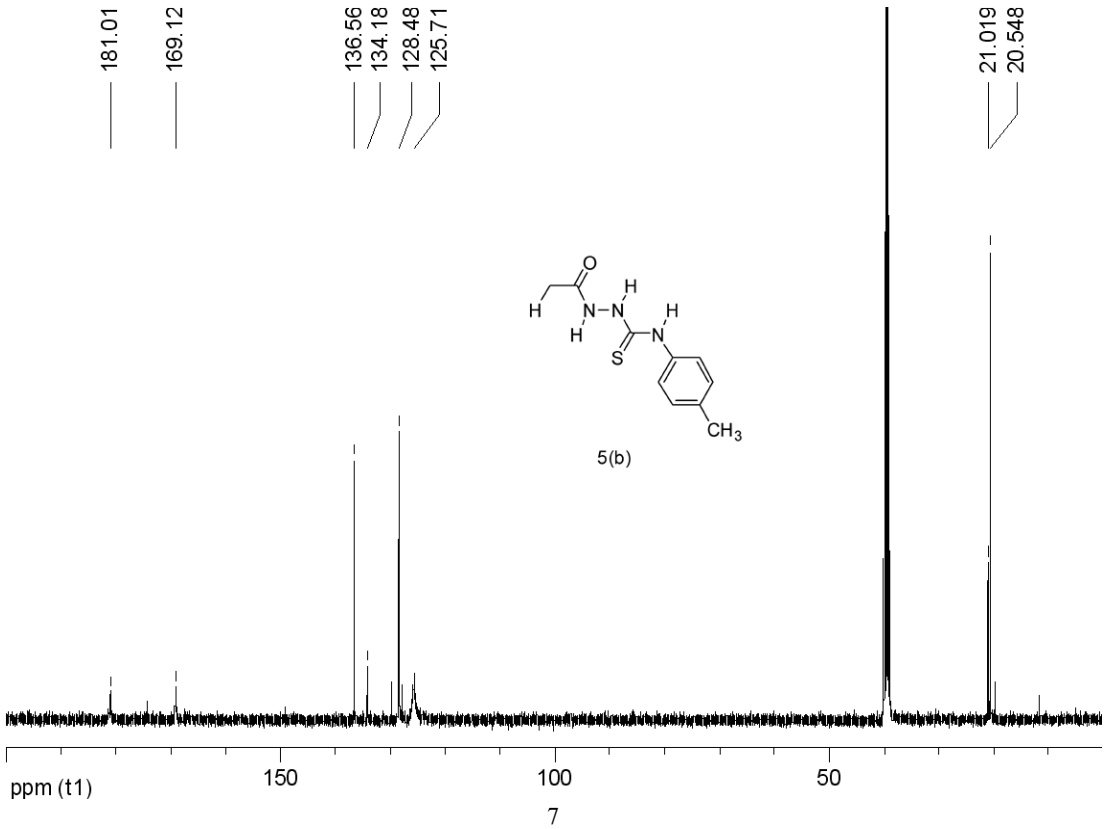


2-Acetyl-*N*-(*p*-tolyl)hydrazinecarbothioamide (5b)

^{1}H NMR (400 MHz, DMSO-d_6)

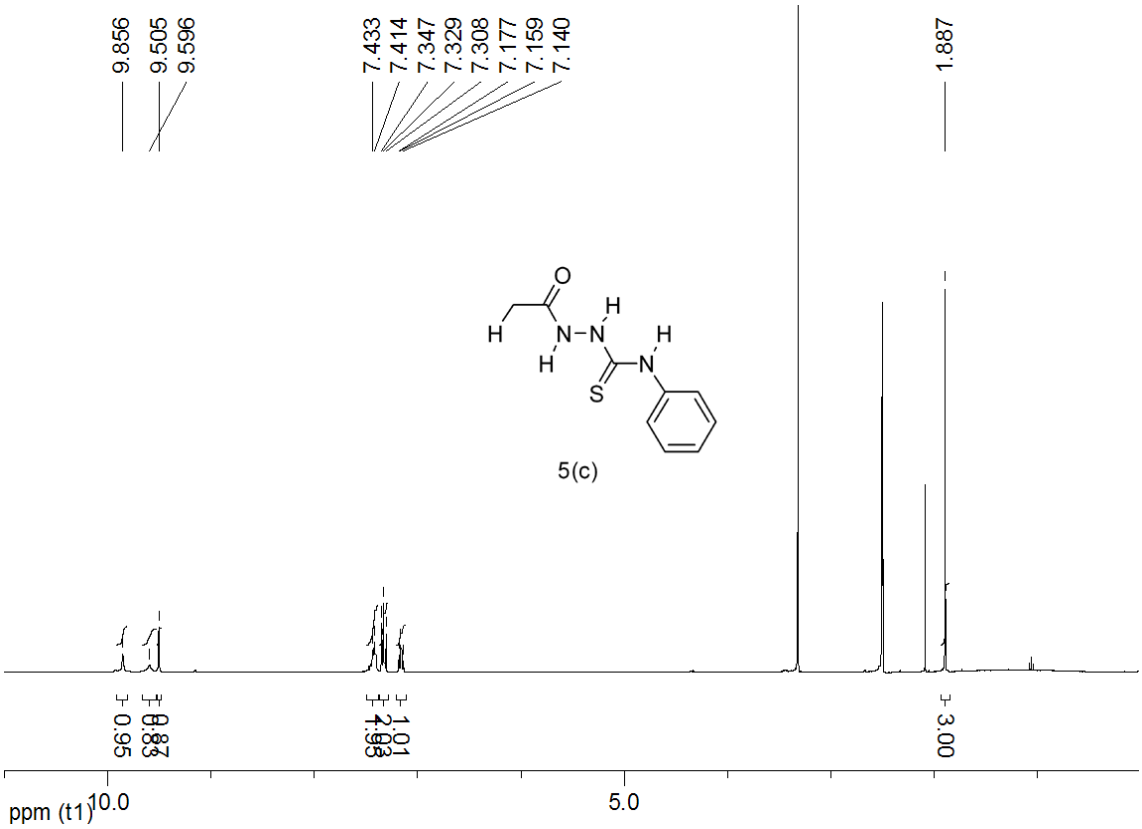


^{13}C NMR (100 MHz, DMSO-d_6)

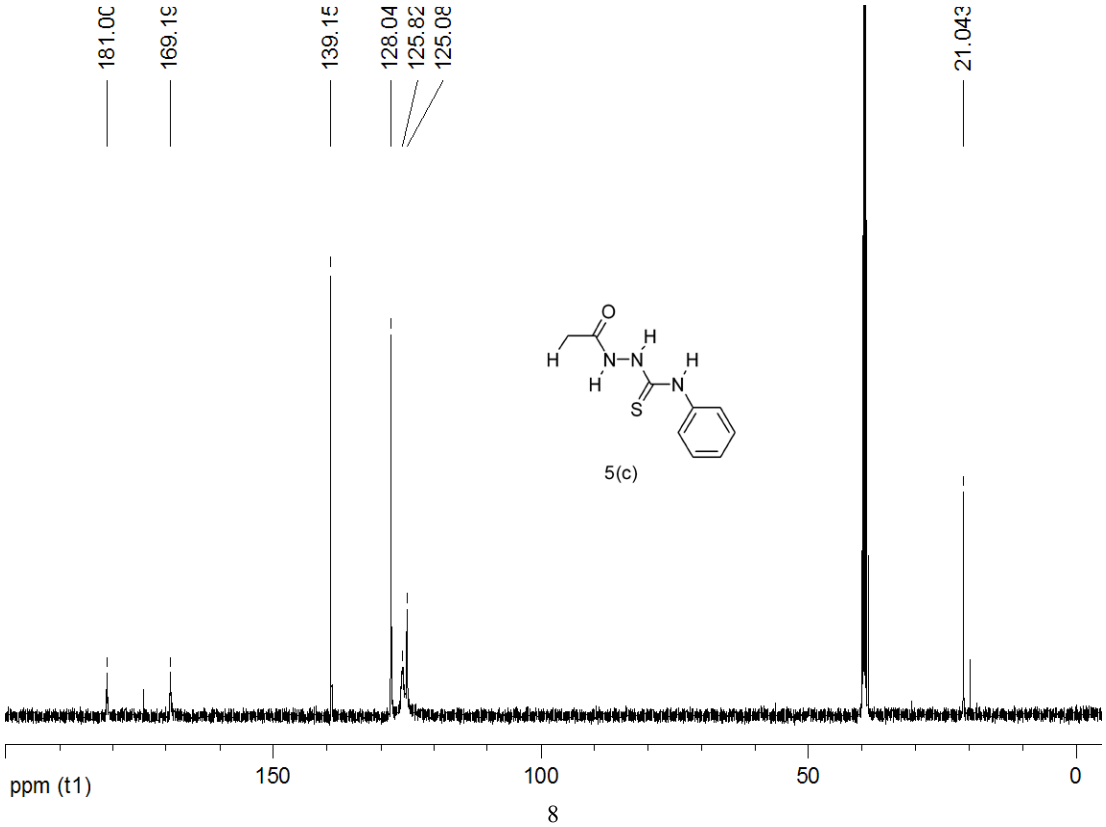


2-Acetyl-*N*-phenylhydrazinecarbothioamide (5c)

^{1}H NMR (400 MHz, DMSO-d_6)

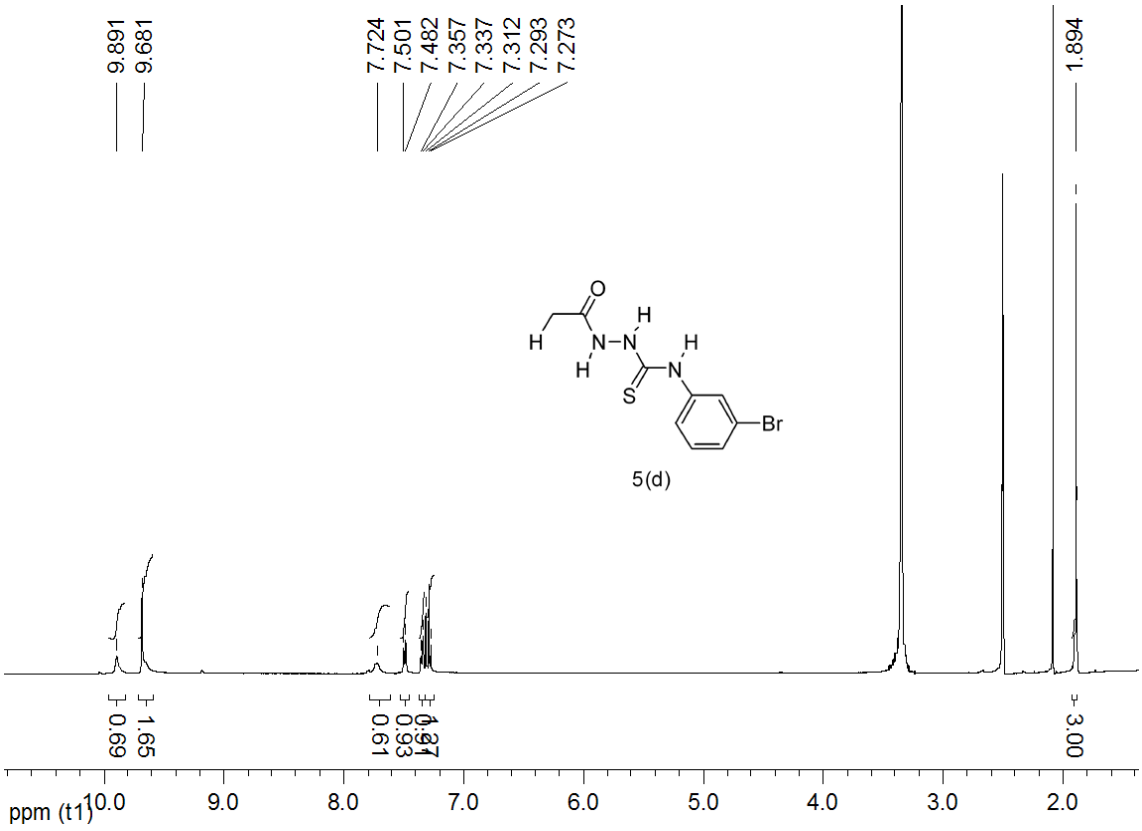


^{13}C NMR (100 MHz, DMSO-d_6)

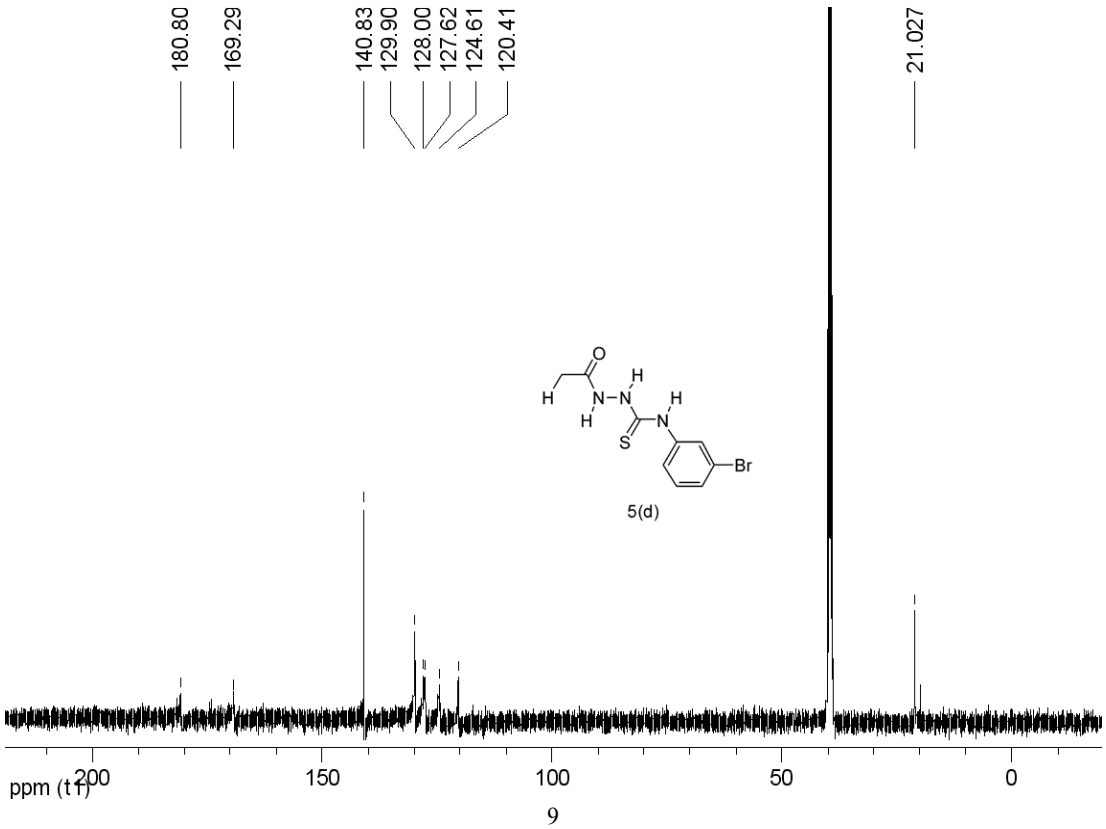


2-Acetyl-*N*-(3-bromophenyl)hydrazinecarbothioamide (5d)

^{1}H NMR (400 MHz, DMSO-d_6)

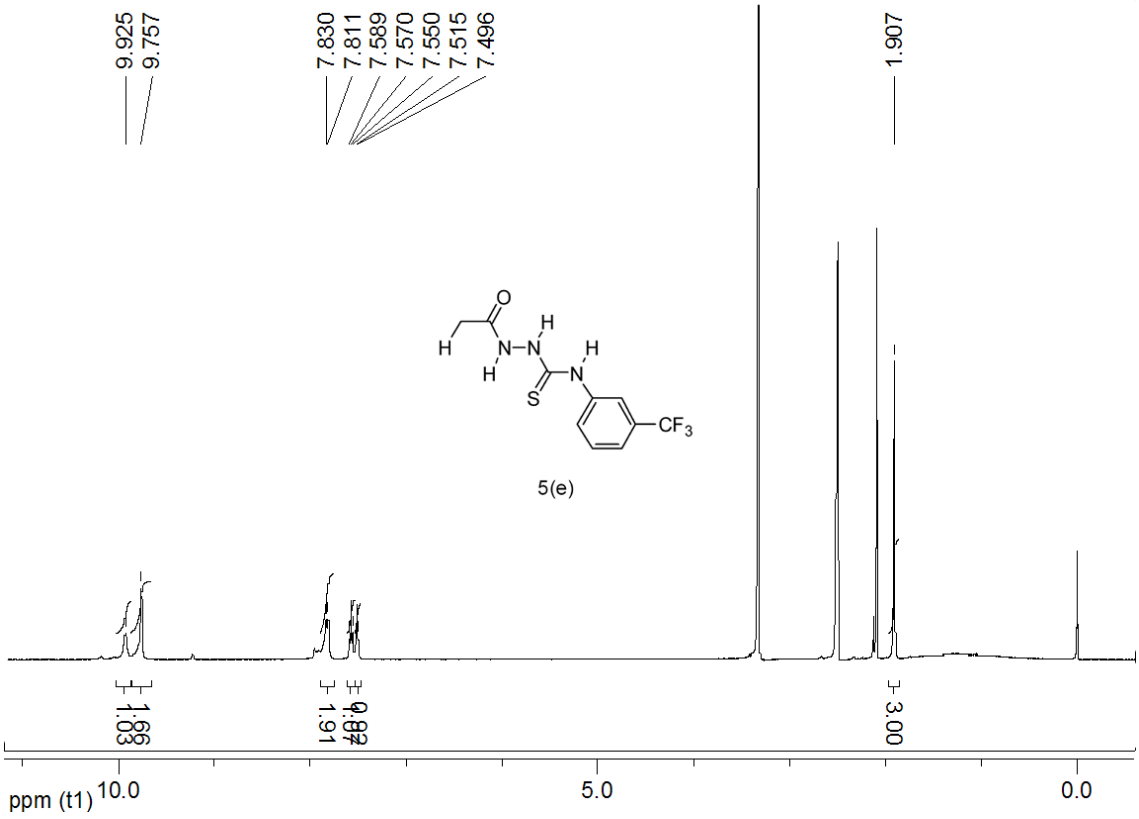


^{13}C NMR (100 MHz, DMSO-d_6)

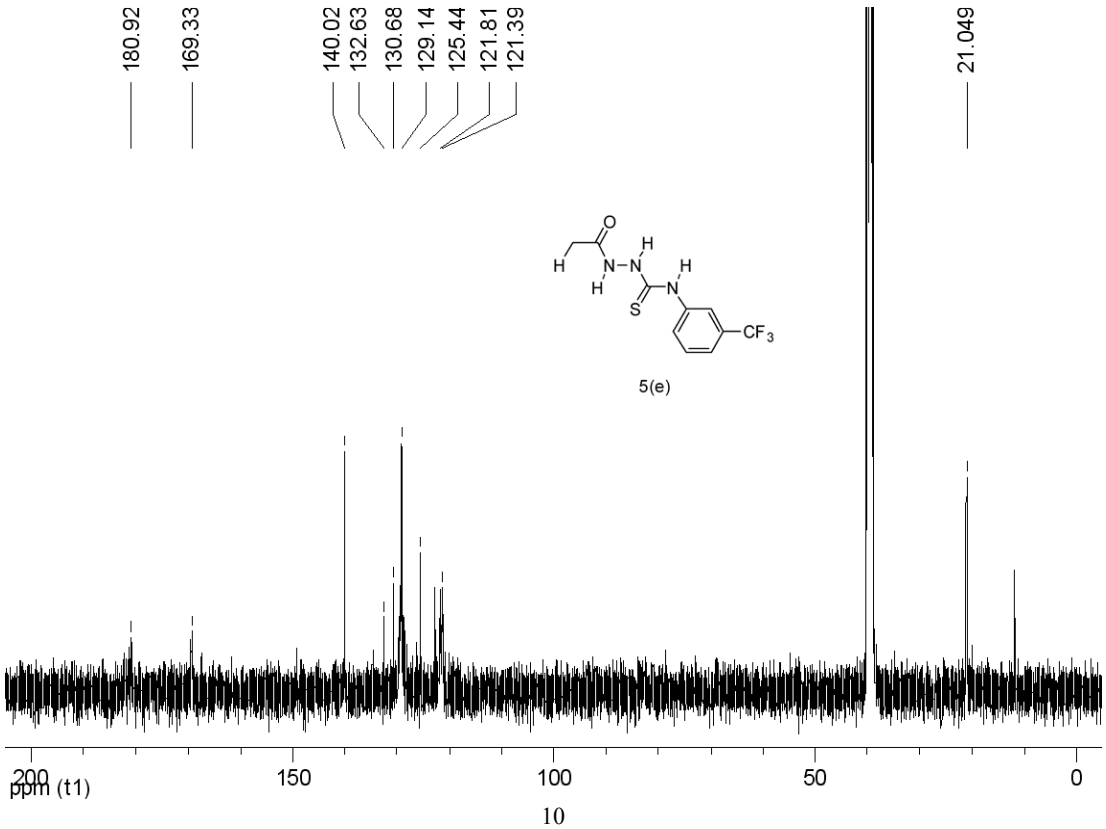


2-Acetyl-*N*-(3-(trifluoromethyl)phenyl)hydrazinecarbothioamide (5e)

^{1}H NMR (400 MHz, DMSO-d_6)

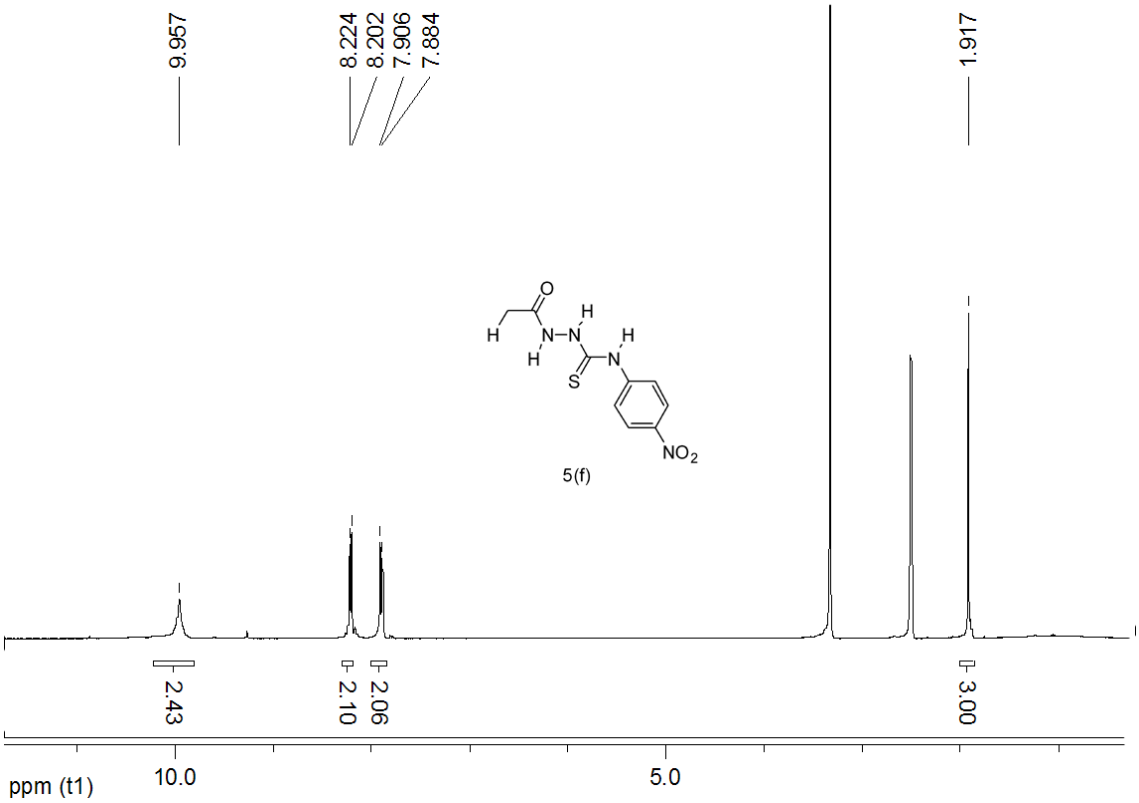


^{13}C NMR (100 MHz, DMSO-d_6)

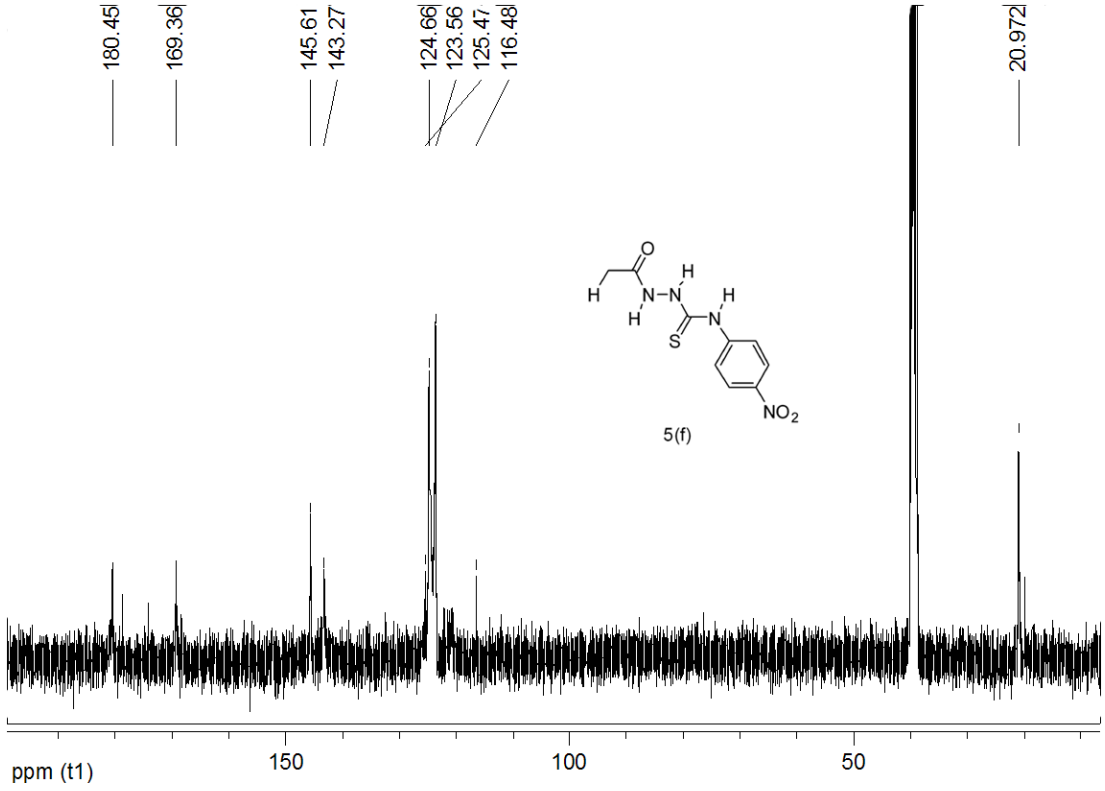


2-Acetyl-*N*-(4-nitrophenyl)hydrazinecarbothioamide (5f)

^{1}H NMR (400 MHz, DMSO-d_6)

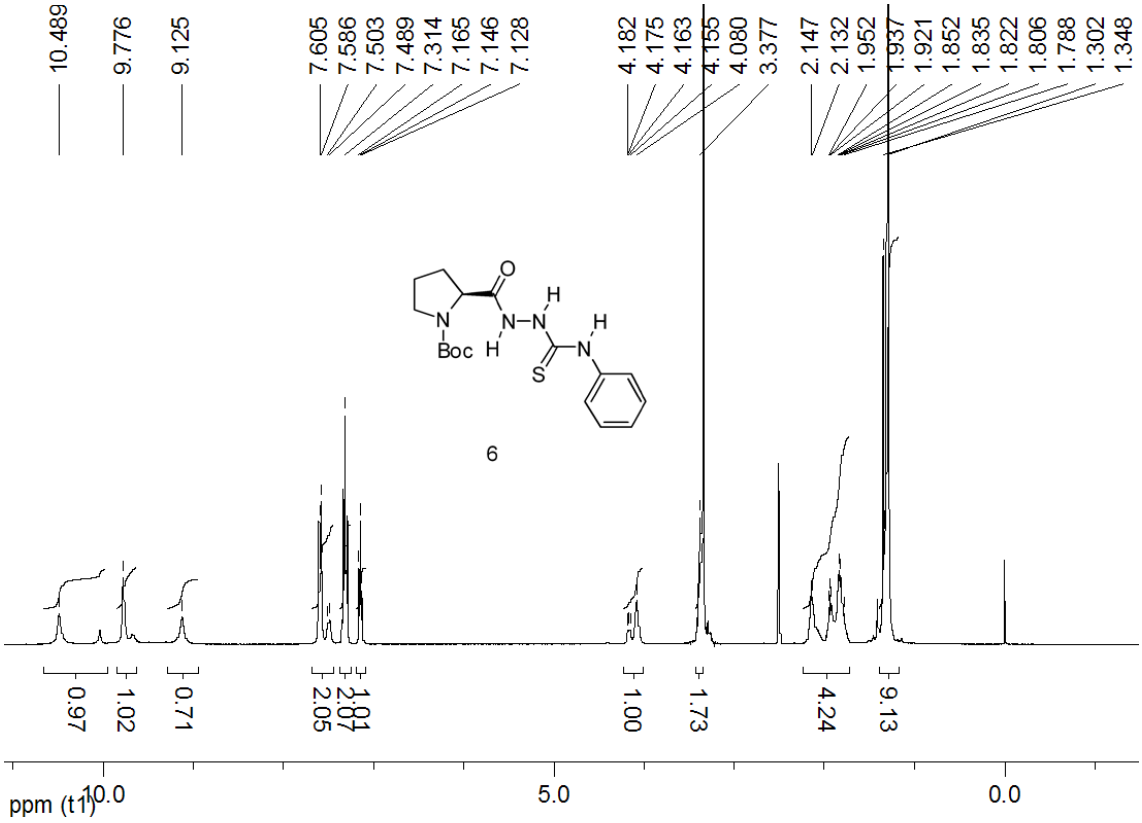


^{13}C NMR (100 MHz, DMSO-d_6)

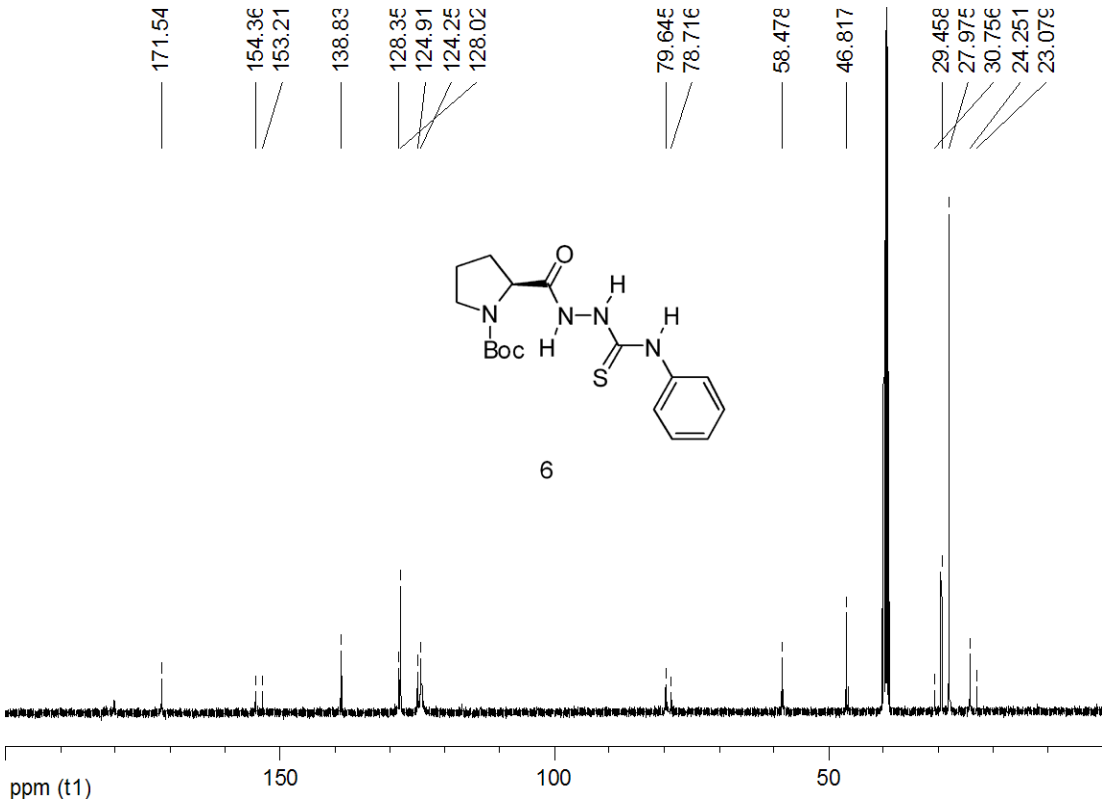


tert-Butyl 2-(2-(phenylcarbamothioyl)hydrazinecarbonyl)pyrrolidine-1-carboxylate (6)

^{1}H NMR (400 MHz, DMSO-d_6). Several small peaks were noted in repeated experiments from differing samples, that were tentatively attributed to the minor enantiomer.

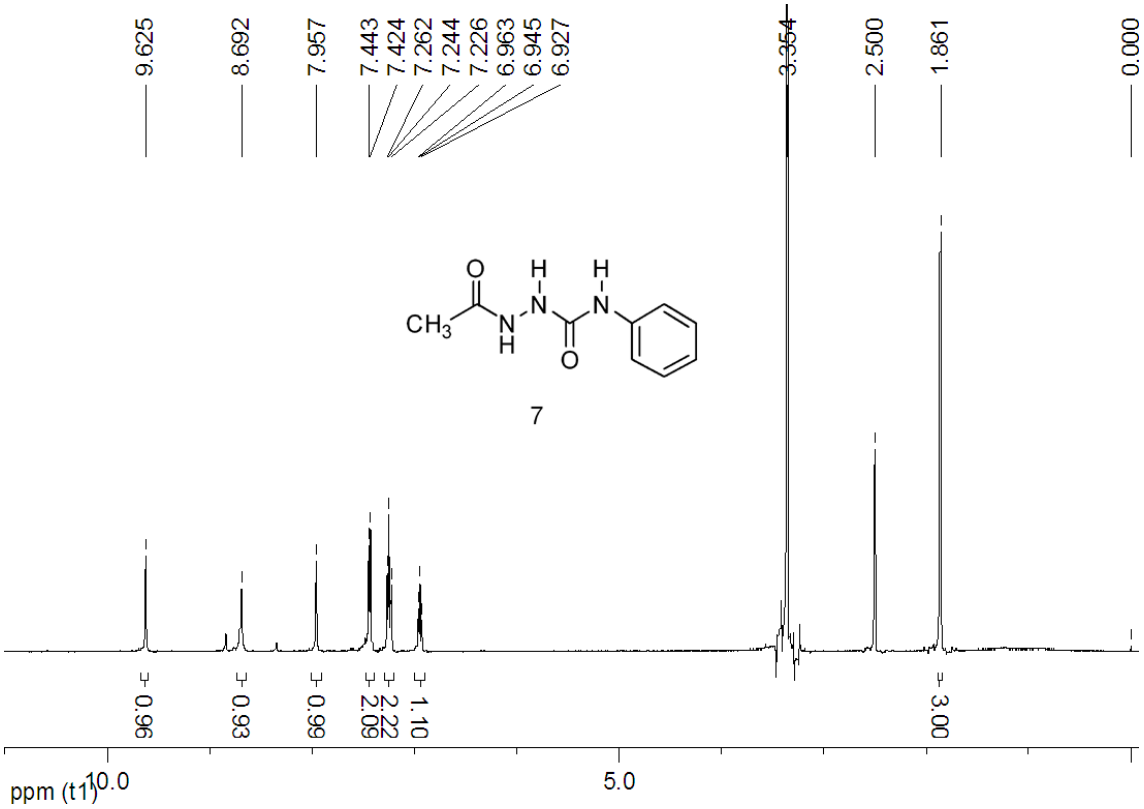


^{13}C NMR (100 MHz, DMSO-d_6)



2-Acetyl-*N*-phenylhydrazinecarboxamide (7)

^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)