

CHEMISTRY

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Supporting Information

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Anion Binding of *N*-(*o*-Methoxybenzamido)thioureas: Contribution of the Intramolecular Hydrogen Bond in the *N*-Benzamide Moiety

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Supporting Information

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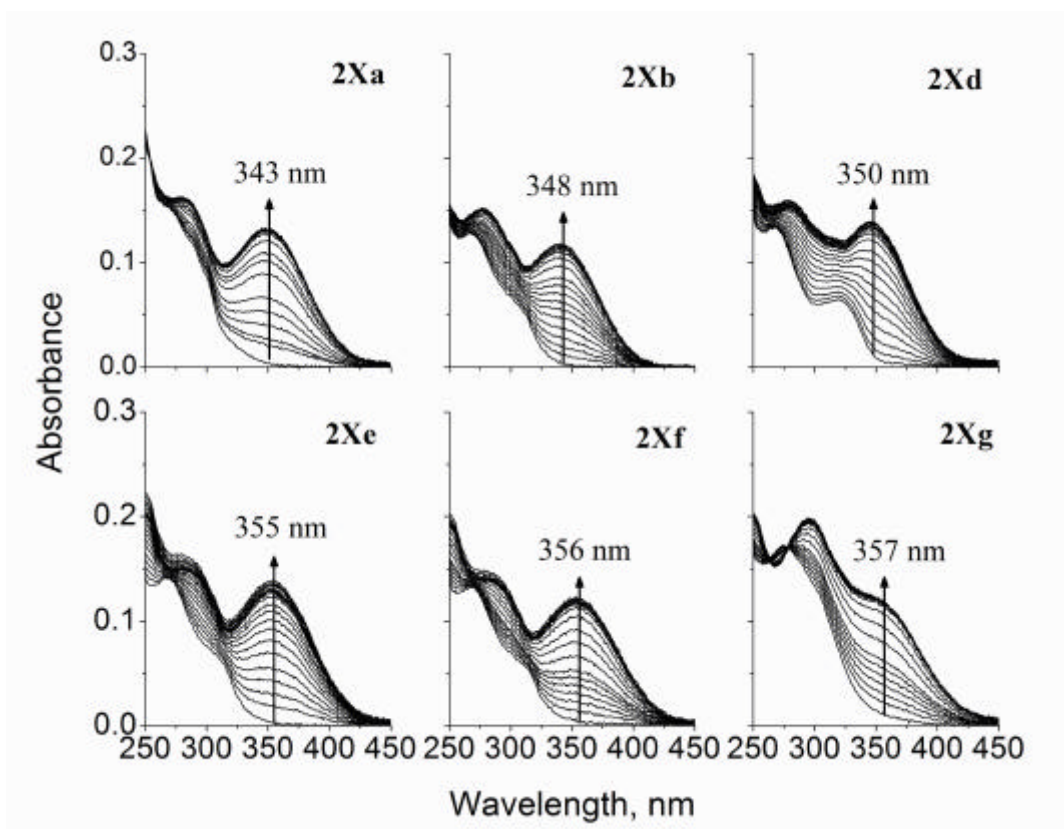


Figure S1. Absorption spectra of **2Xa-g** in MeCN in the presence of AcO^- of increasing concentration. $[\mathbf{2X}] = 1.0 \times 10^{-5} \text{ mol L}^{-1}$.

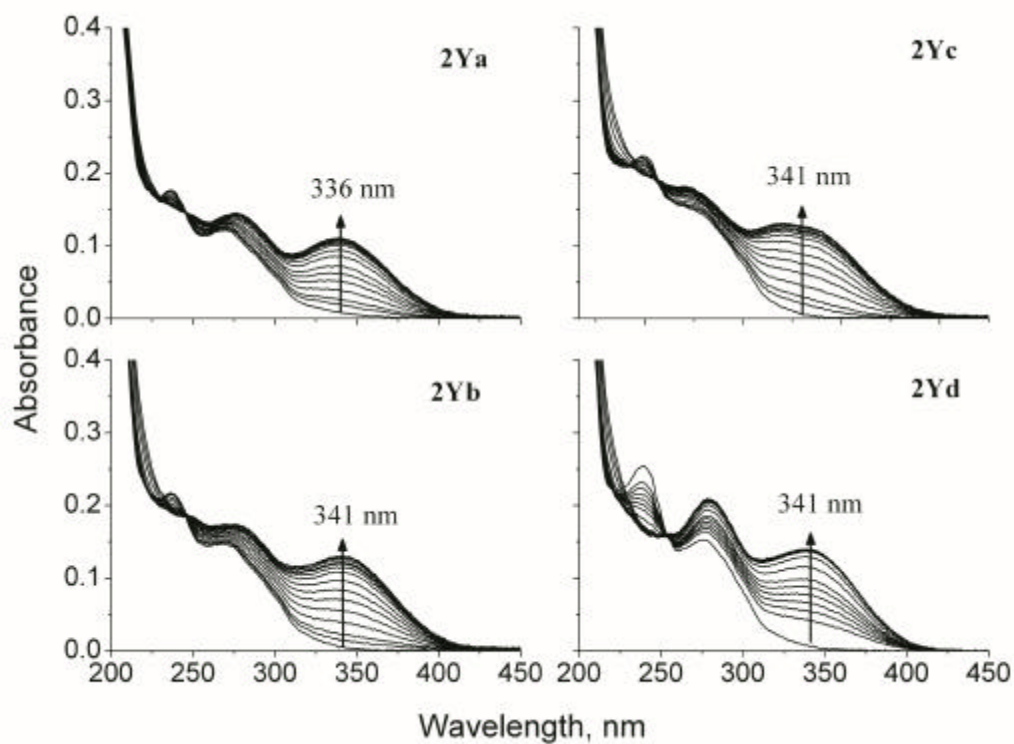
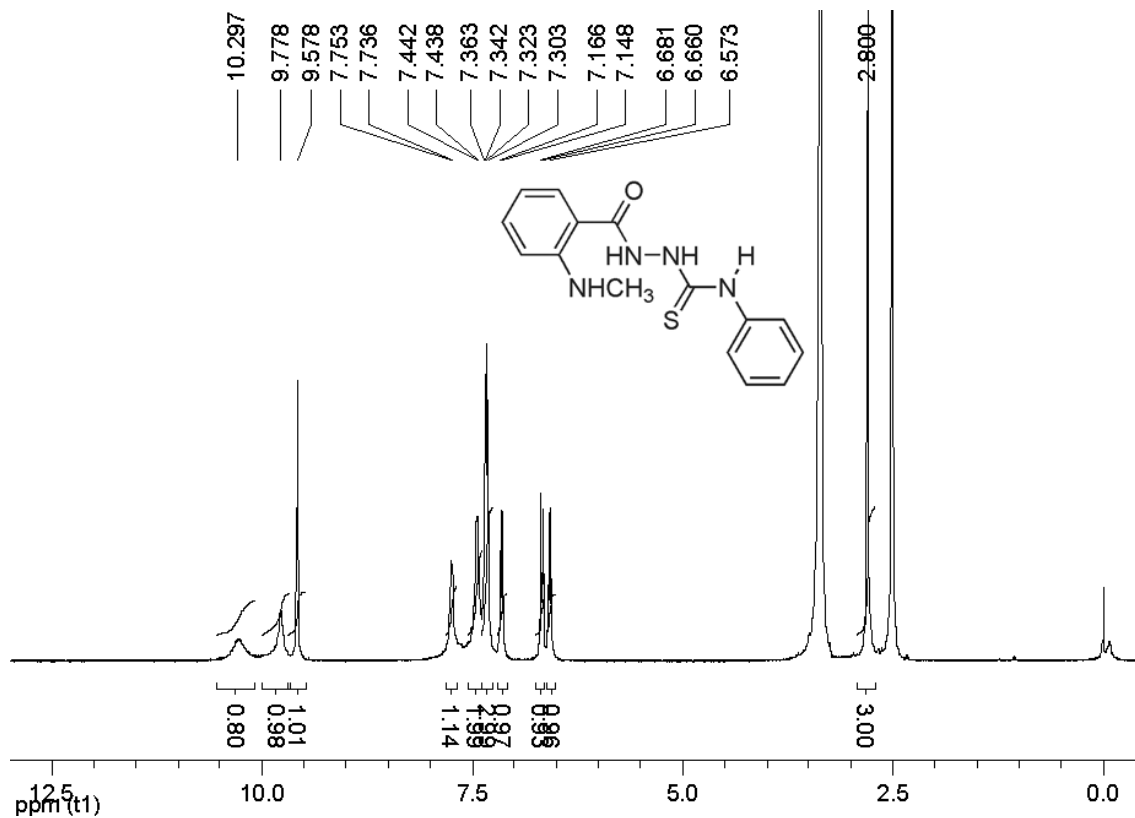


Figure S2. Absorption spectra of **2Ya-d** in MeCN in the presence of AcO^- of increasing
S2

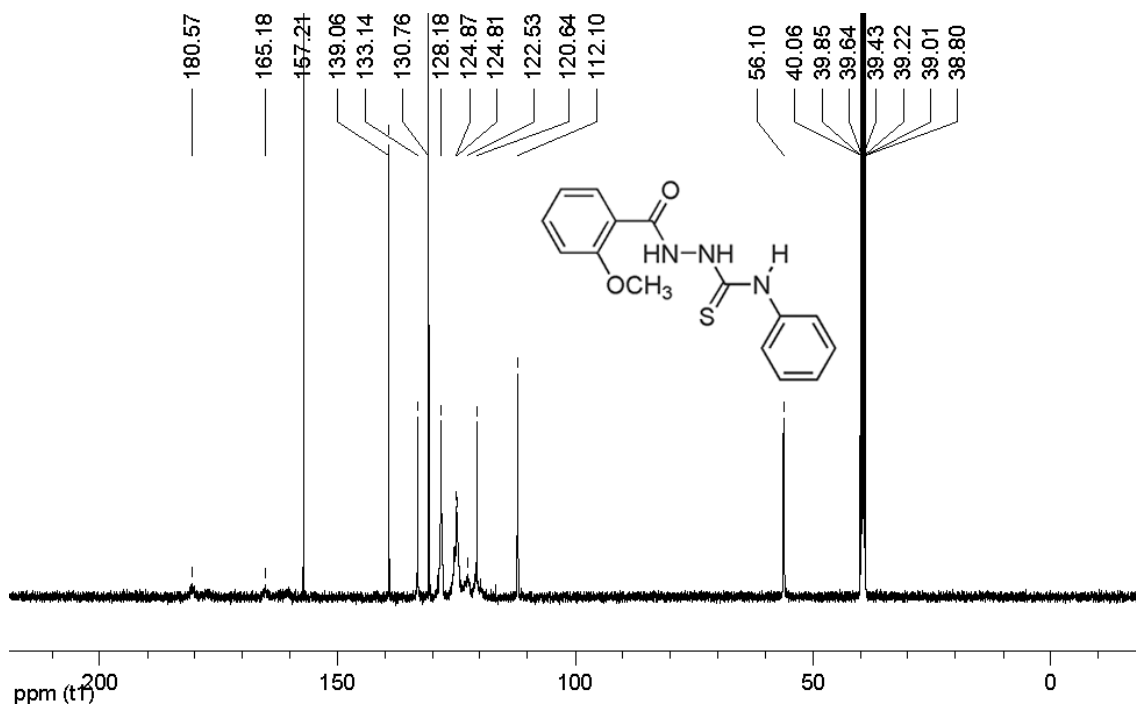
concentration. $[2\mathbf{Y}] = 1.0 \times 10^{-5} \text{ mol L}^{-1}$.

N-(2-Methylaminobenzamido)-*N'*-phenylthiourea (**2Za**)

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

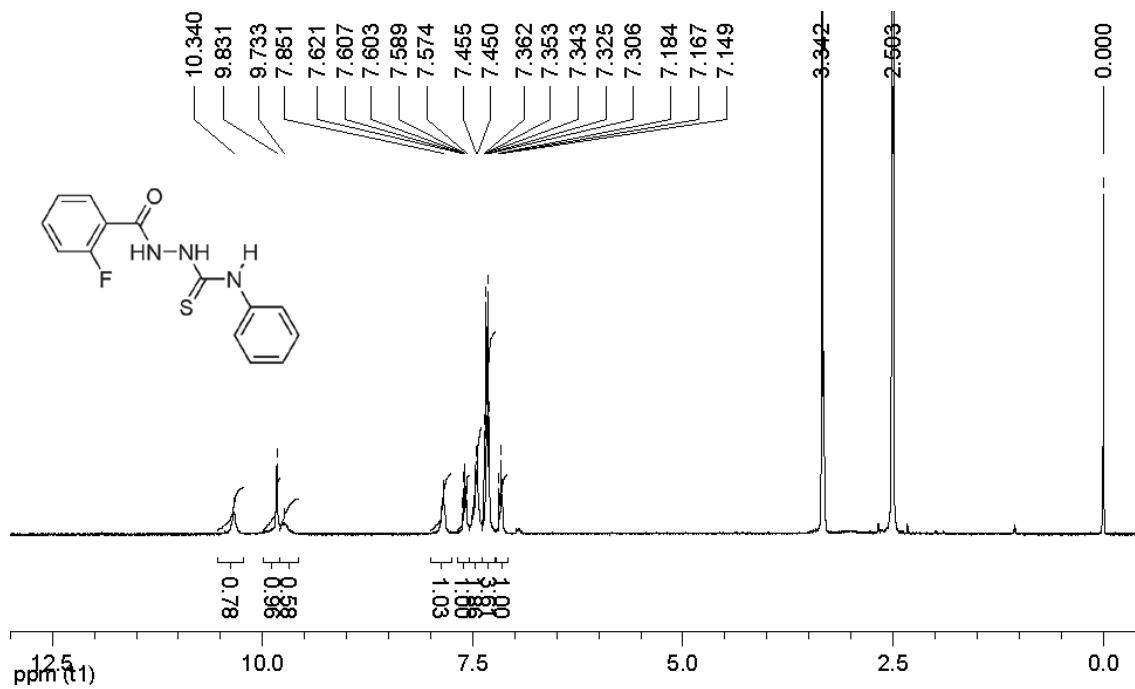


^{13}C NMR (100 MHz, DMSO- d_6)



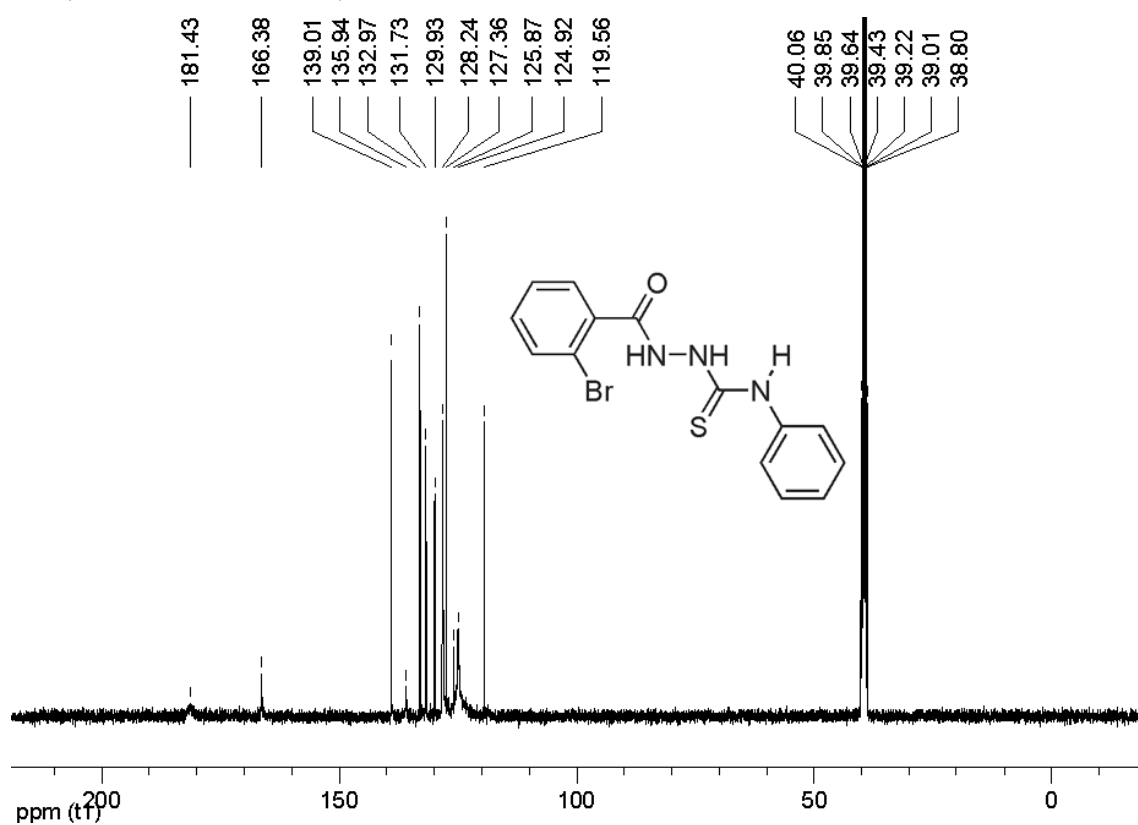
N-(2-Fluorobenzamido)-*N'*-phenylthiourea (**2Zd**)

¹H NMR (400 MHz, DMSO-*d*₆)



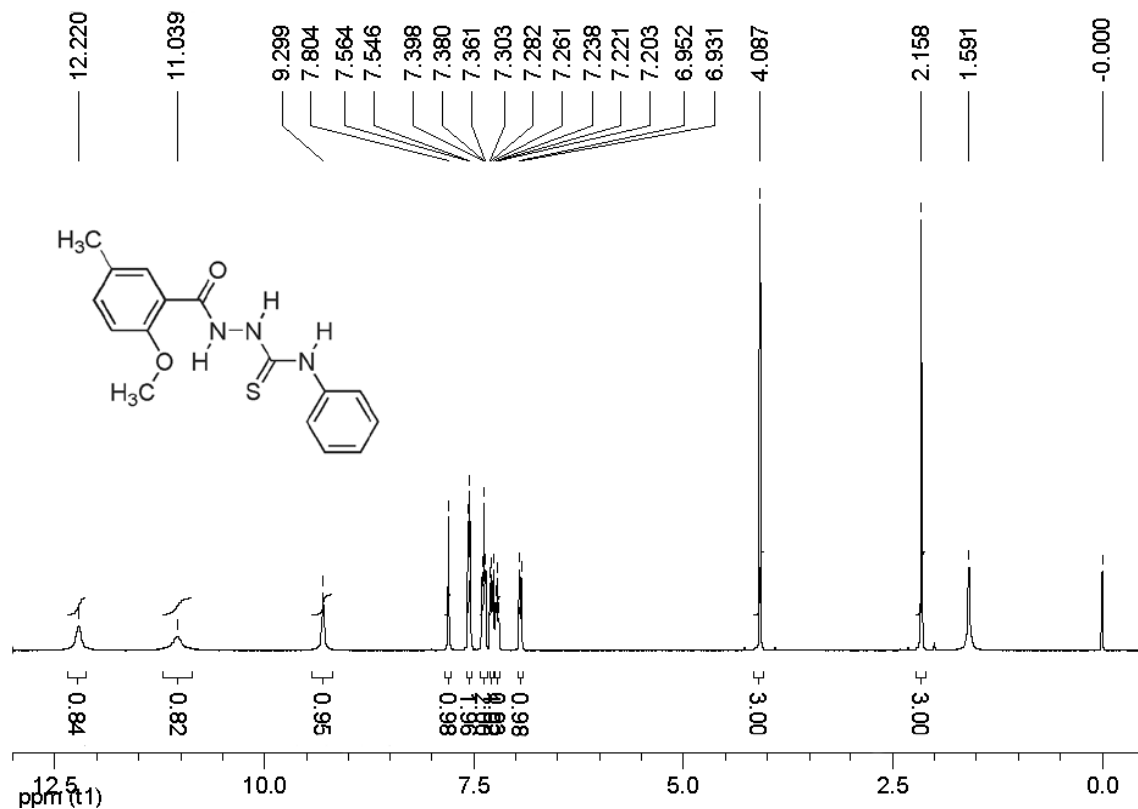
¹³C NMR (100 MHz, DMSO-*d*₆)

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

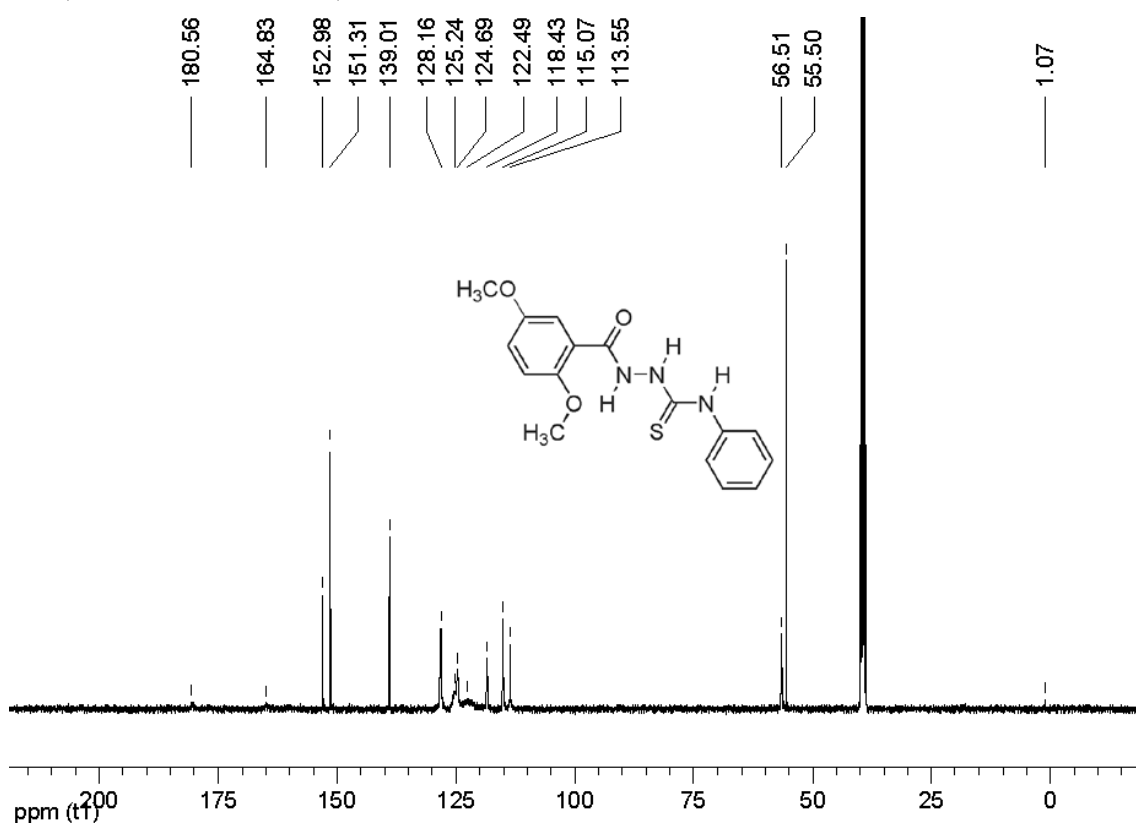


N-(2-Methoxy-5-methylbenzamido)-*N'*-phenylthiourea (**2Xa**)

^1H NMR (400 MHz, CDCl_3)

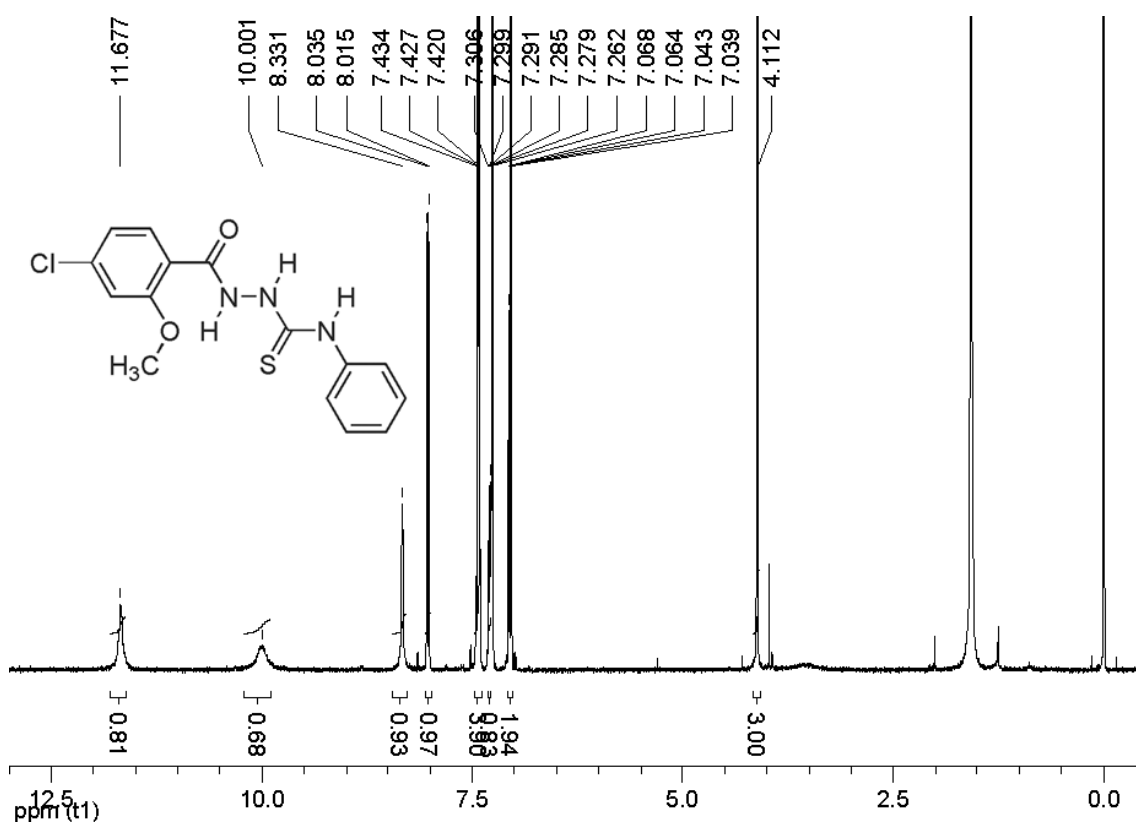


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

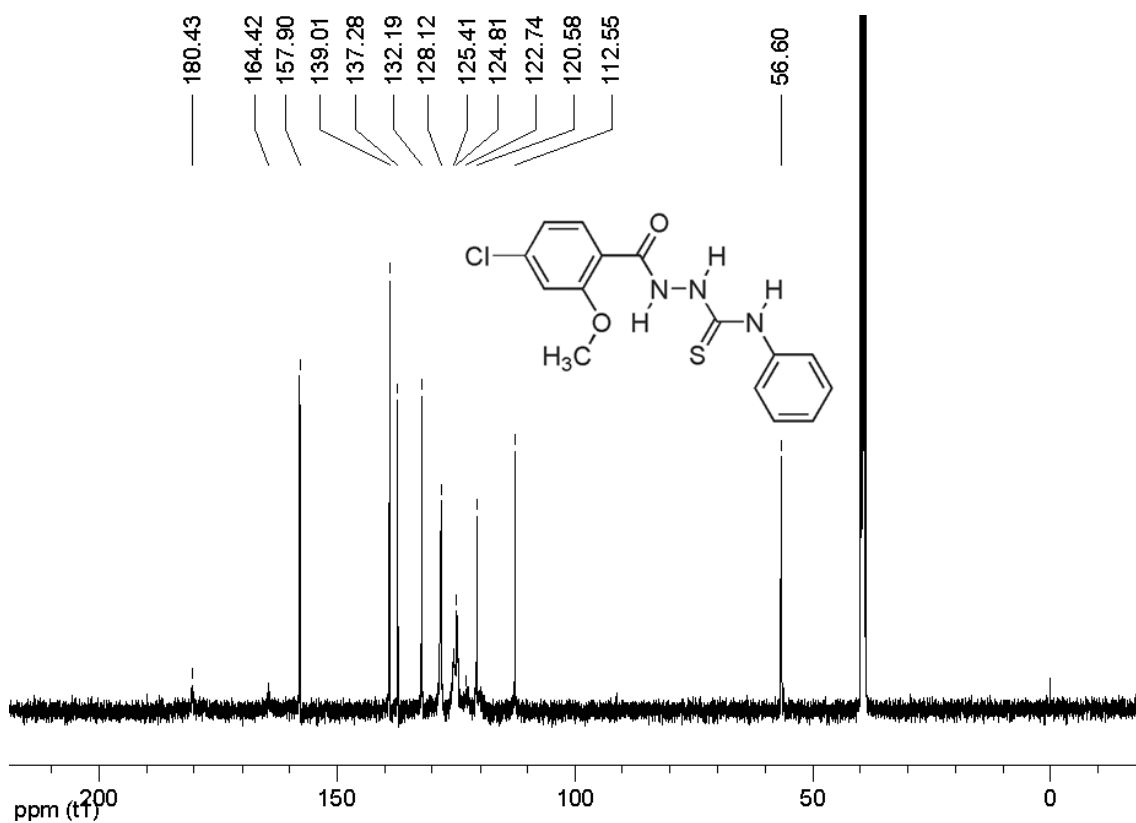


N-(2-Methoxy-4-chlorobenzamido)-*N'*-phenylthiourea (**2Xd**)

^1H NMR (400 MHz, CDCl_3)

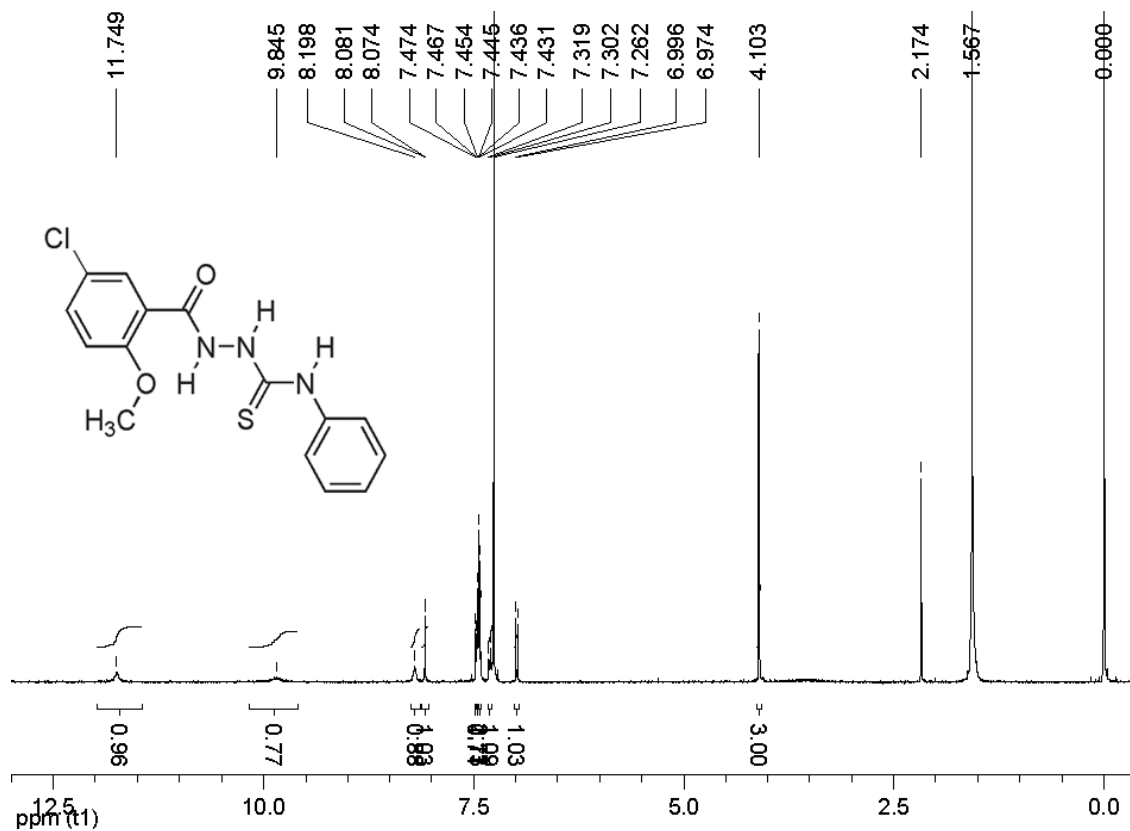


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

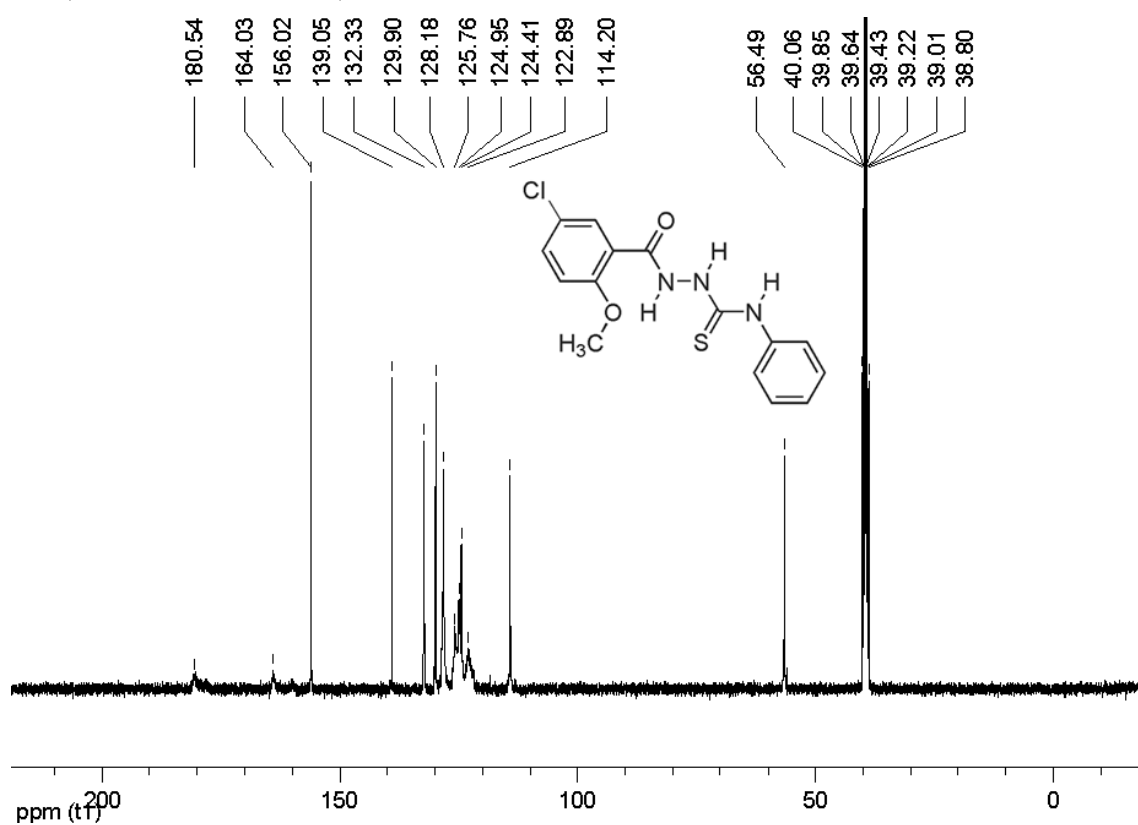


N-(2-Methoxy-5-chlorobenzamido)-*N'*-phenylthiourea (2Xe)

^1H NMR (400 MHz, CDCl_3)

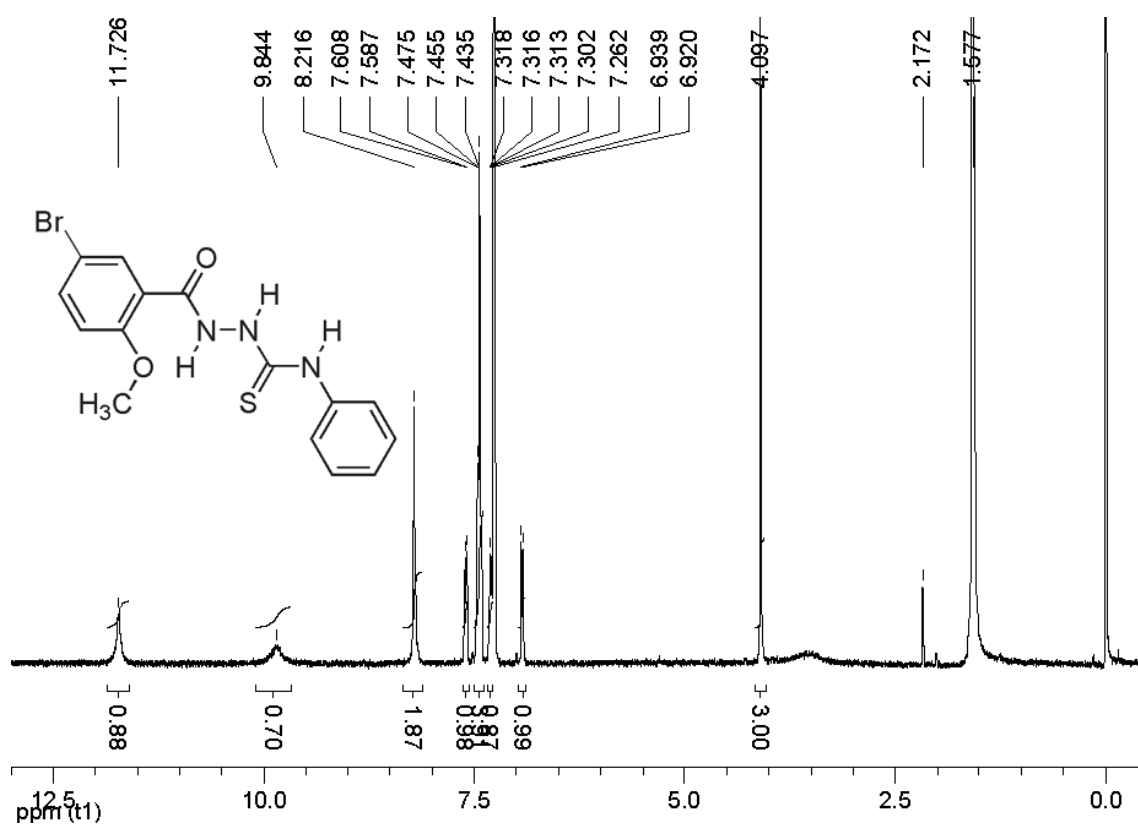


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

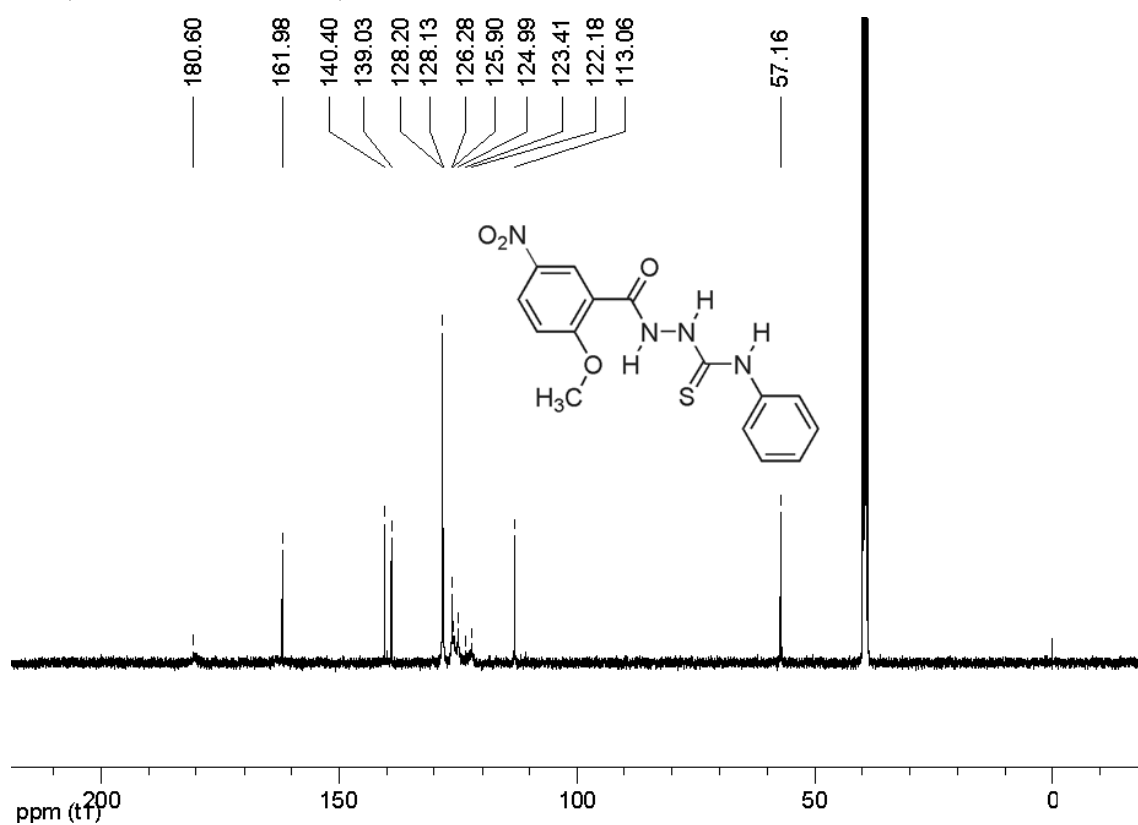


N-(2-Methoxy-5-bromobenzamido)-*N'*-phenylthiourea (**2Xf**)

^1H NMR (400 MHz, CDCl_3)

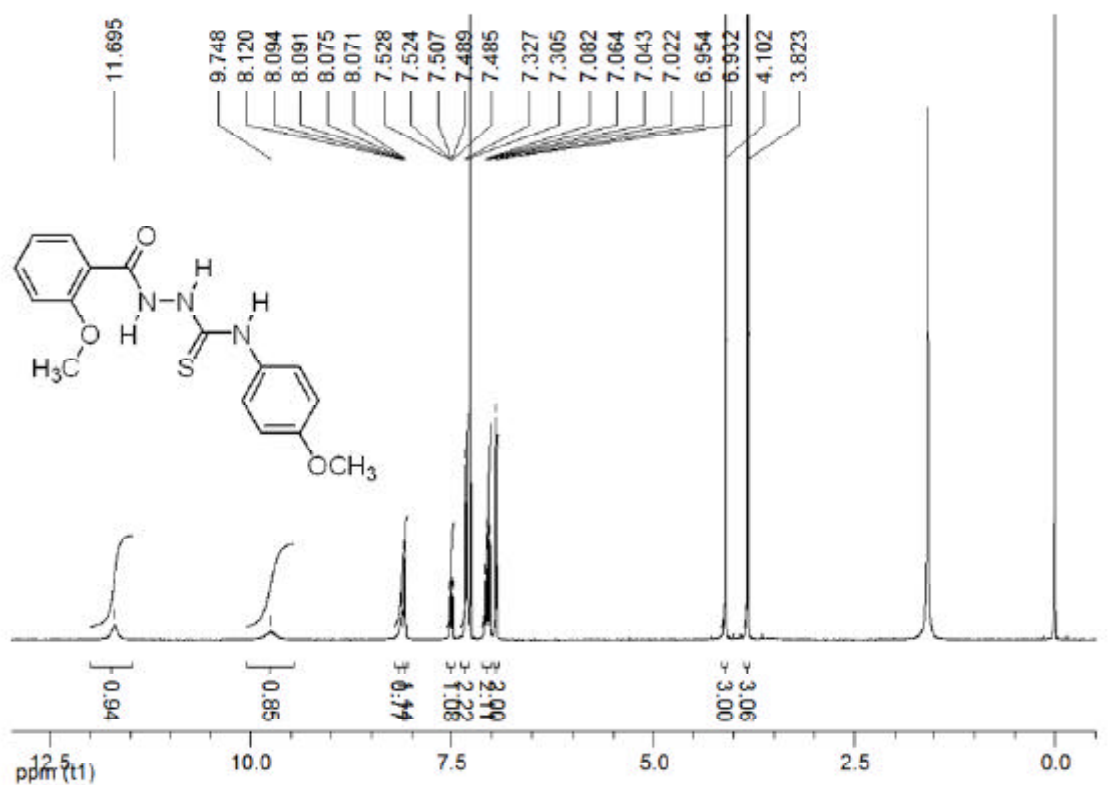


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

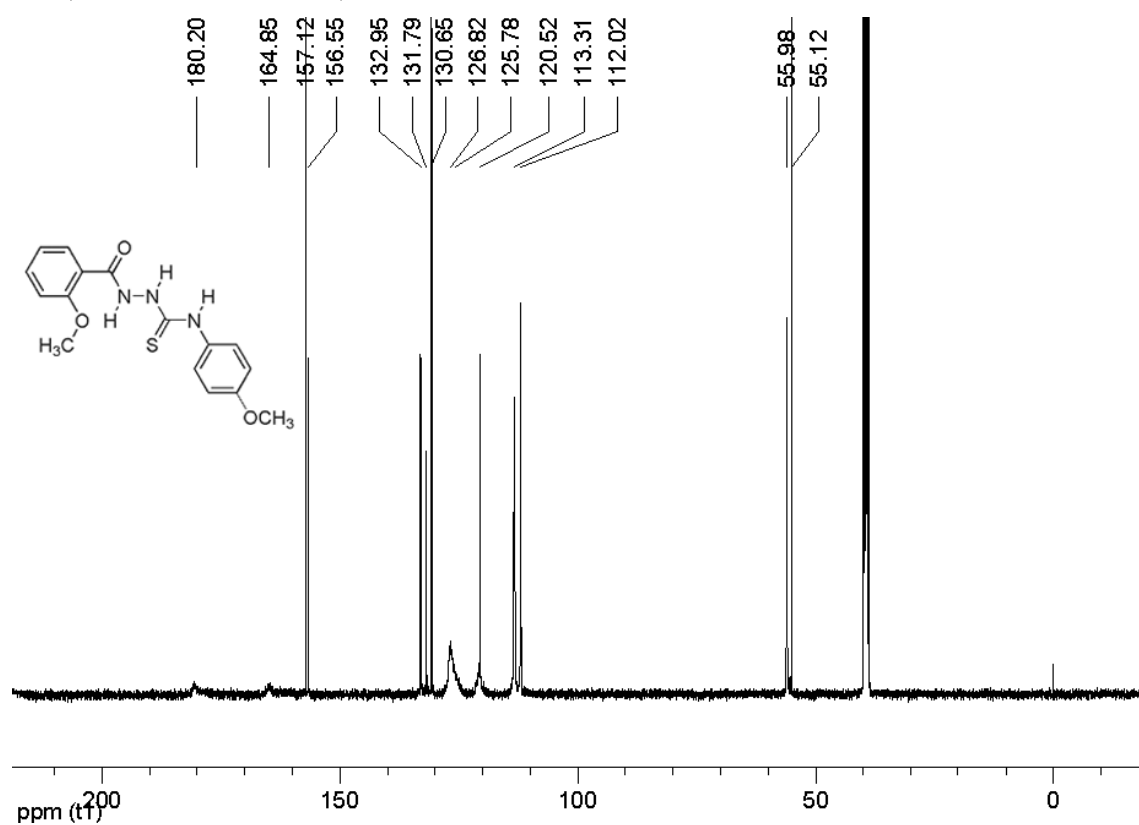


N-(2-Methoxybenzamido)-*N'*-(4'-methoxyphenyl)thiourea (**2Ya**)

^1H NMR (400 MHz, CDCl_3)

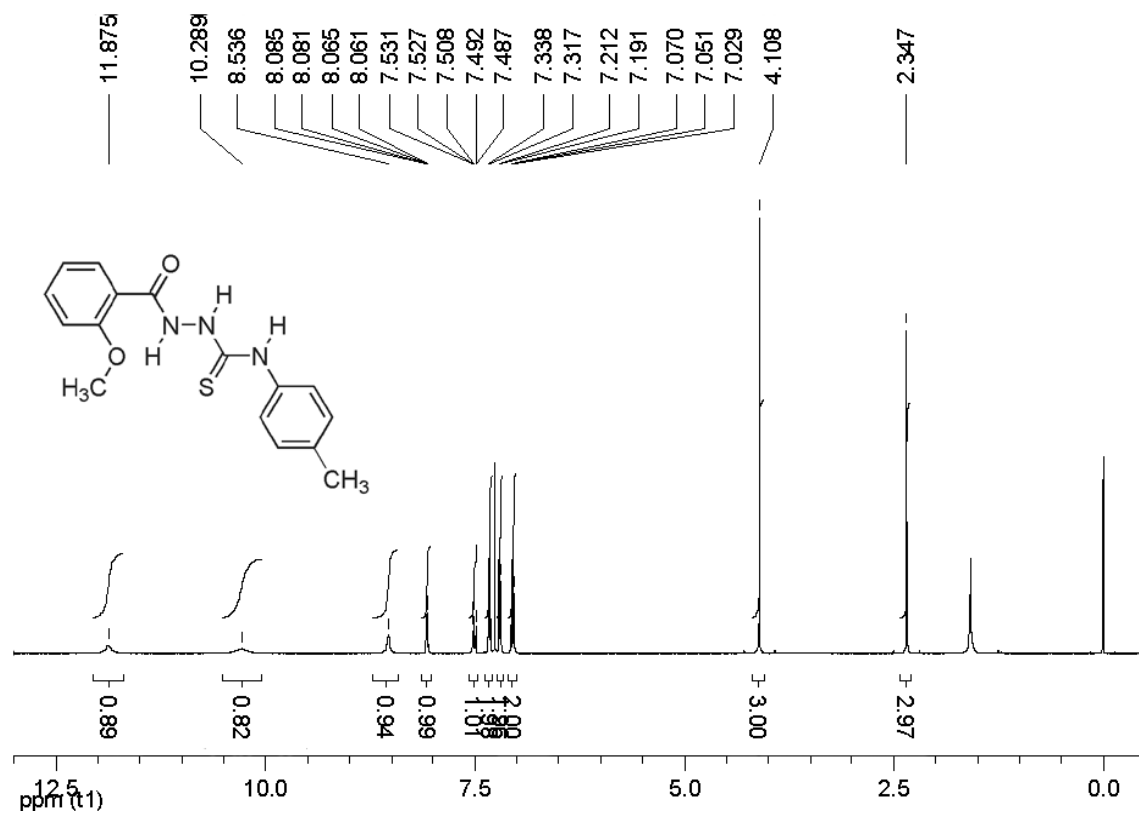


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)

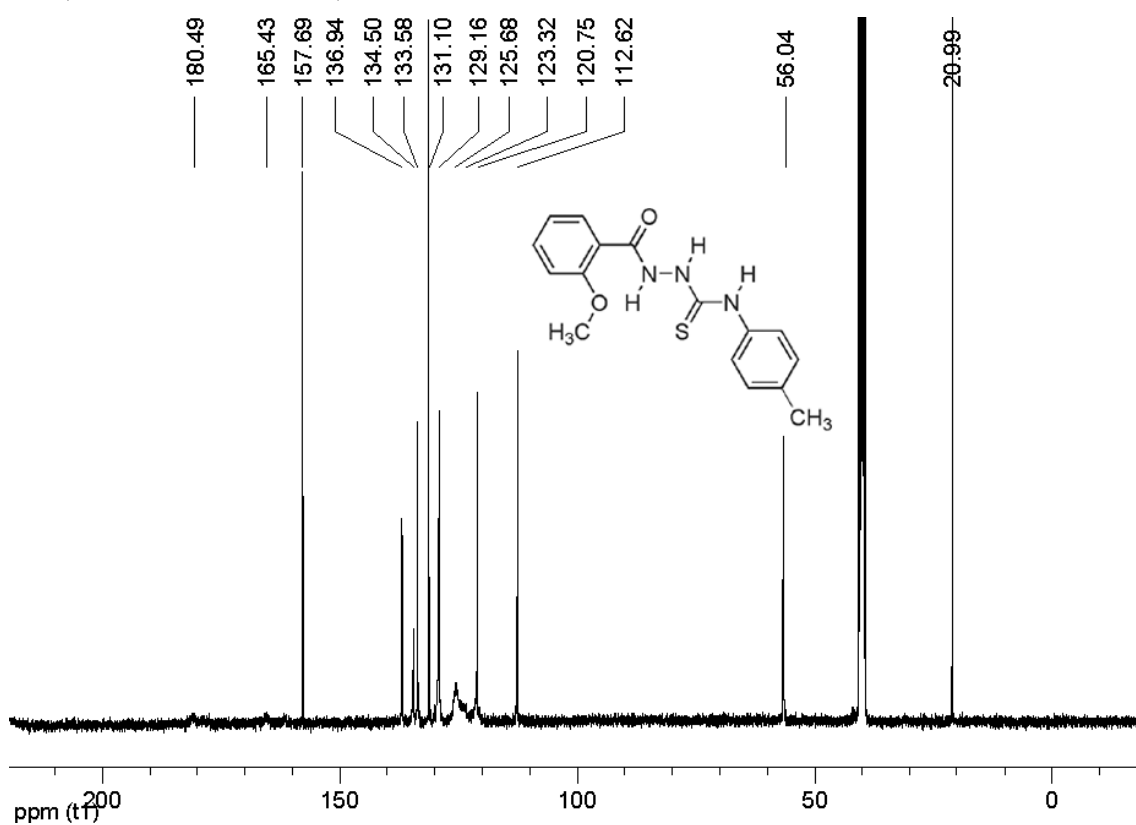


N-(2-Methoxybenzamido)-*N'*-(4'-methylphenyl)thiourea (**2Yb**)

^1H NMR (400 MHz, CDCl_3)

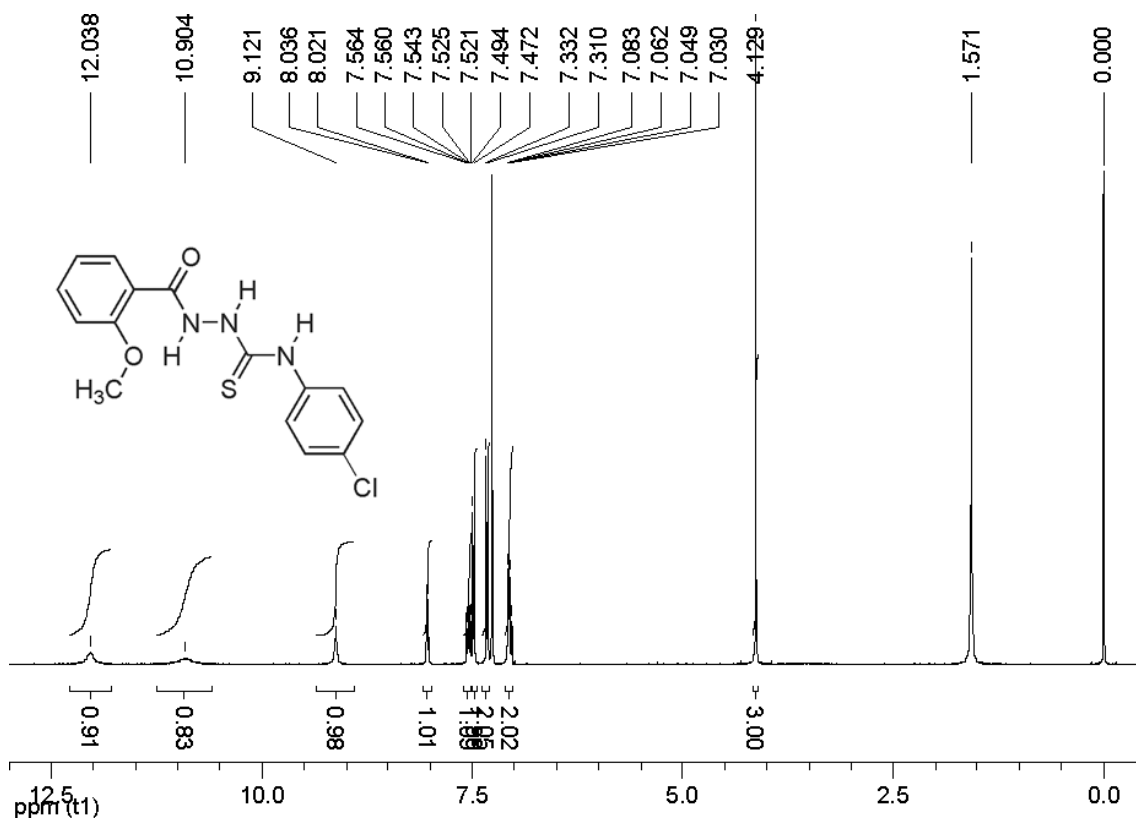


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$)



N-(2-Methoxybenzamido)-*N'*-(4'-chlorophenyl)thiourea (**2Yd**)

^1H NMR (400 MHz, CDCl_3)



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

