

Antileishmanial potential of Thiourea-based derivatives: Design, synthesis and biological activity

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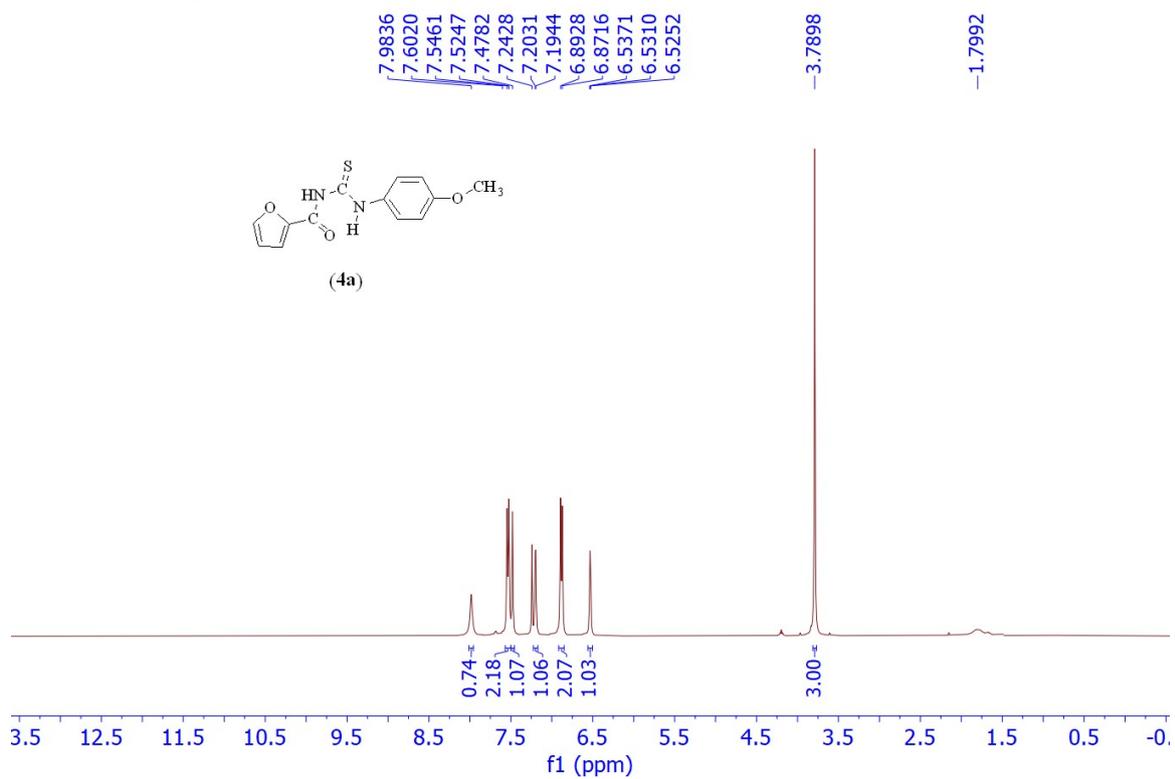


Figure S-1: ¹H NMR (400 MHz) spectrum of compound **4a** in CDCl₃

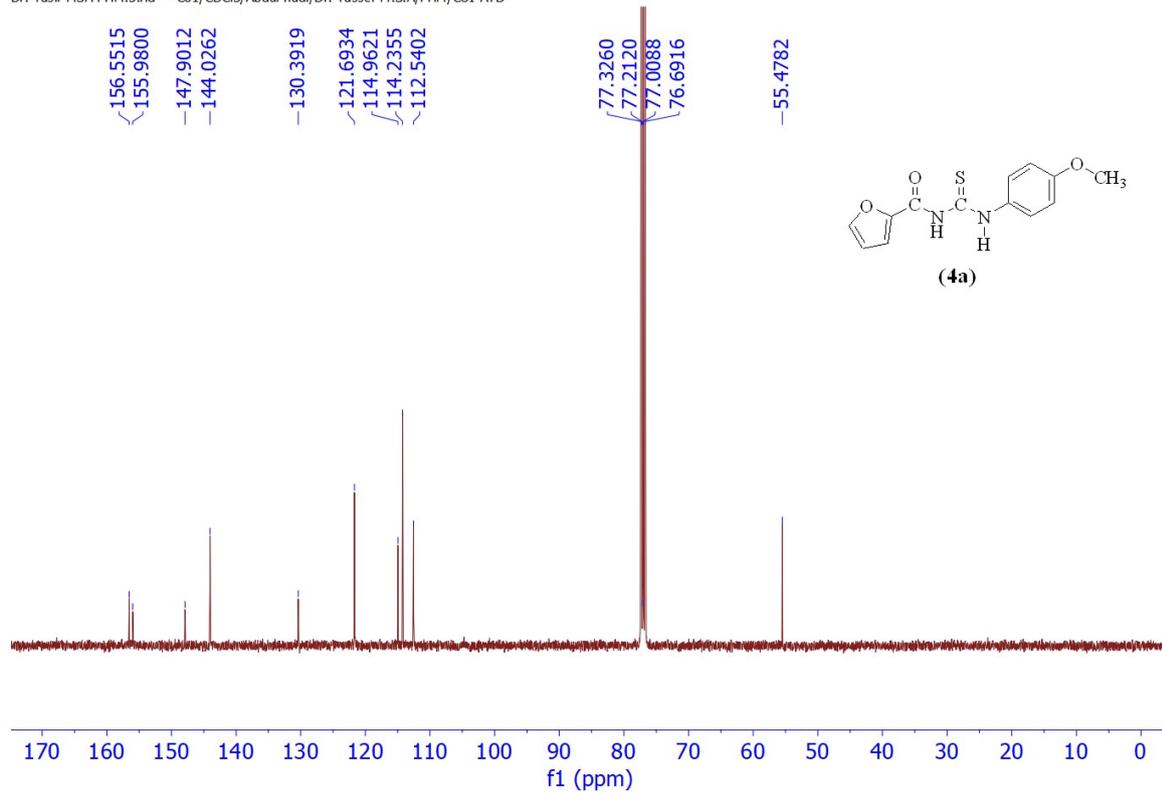


Figure S-2: ¹³C NMR (100 MHz) spectrum of compound **4a** in CDCl₃

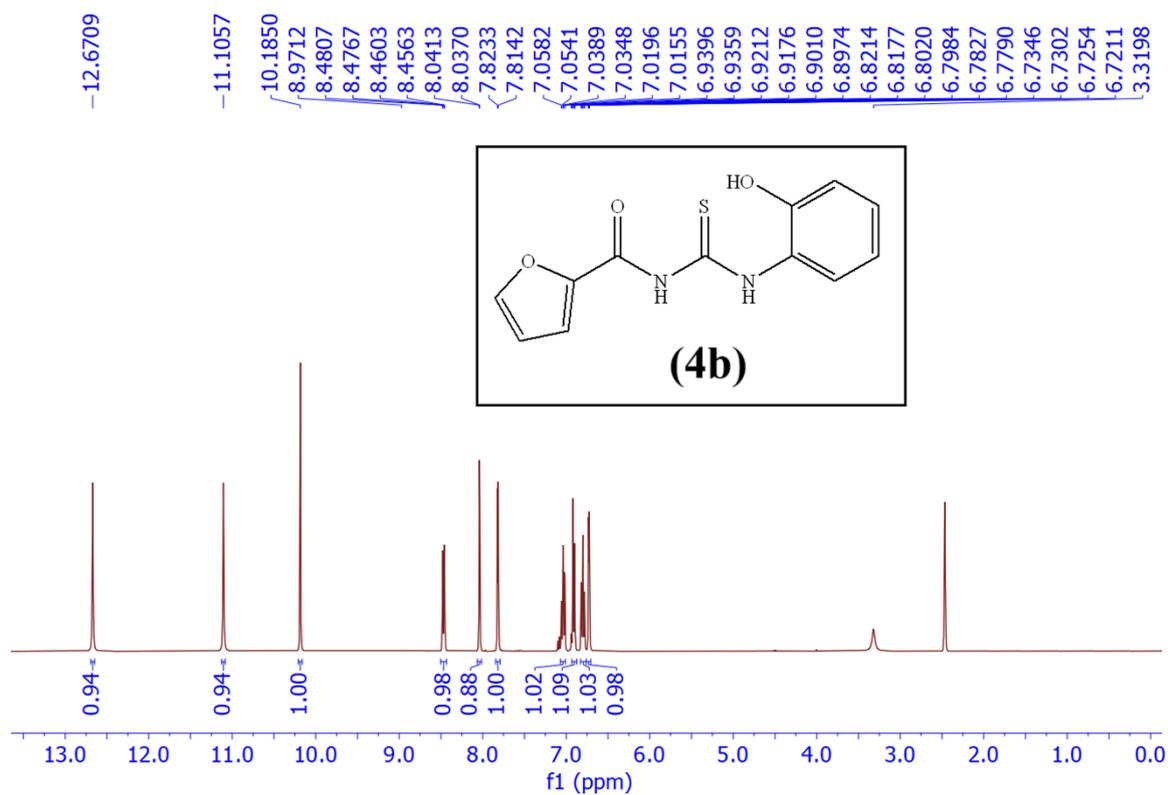


Figure S-3: ¹H NMR (400 MHz) spectrum of compound **4b** in CDCl₃

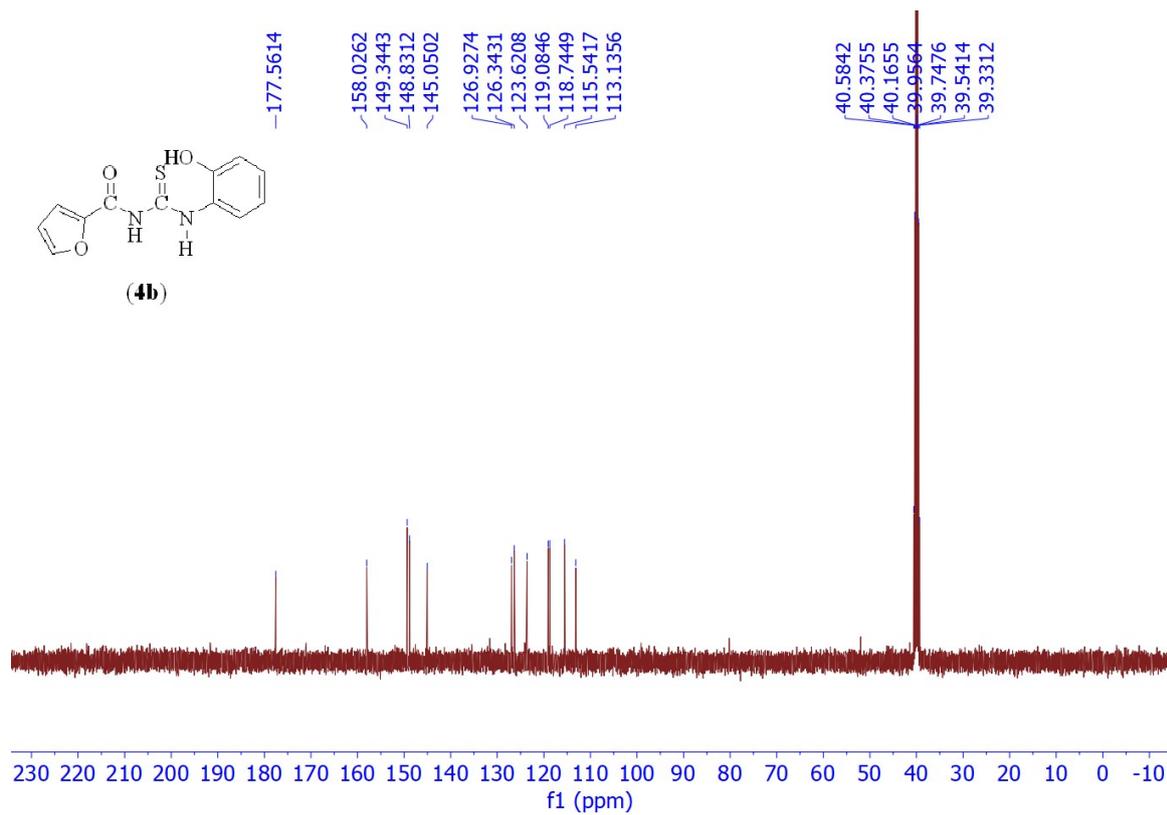


Figure S-4: ^{13}C NMR (100 MHz) spectrum of compound **4b** in $\text{DMSO-}d_6$

Display Report

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Sample Name	I3-N6FULL		
Comment	F3-PEG-3000Free format commentsFree format comments		

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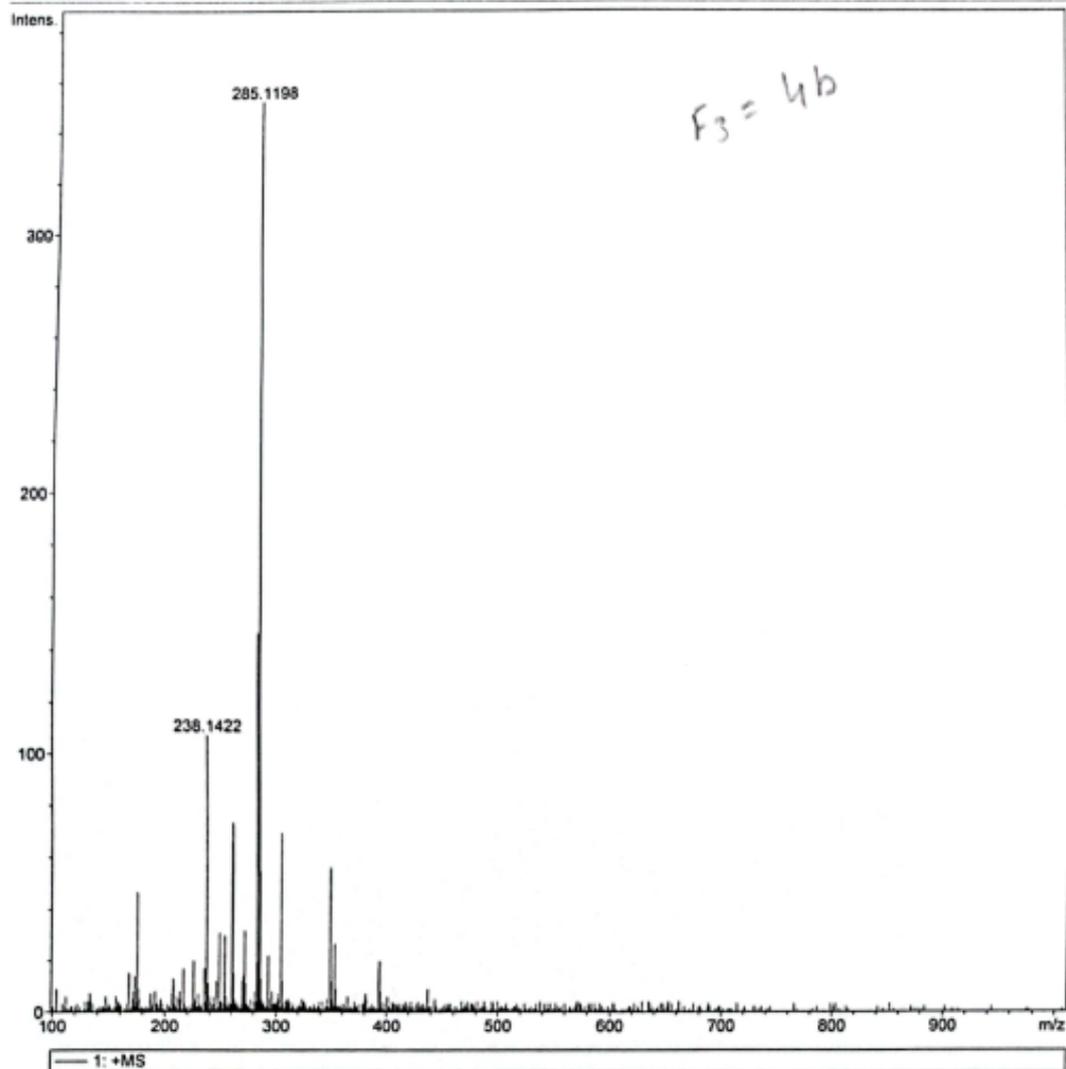


Figure S-5: HRMS of compound **4b**

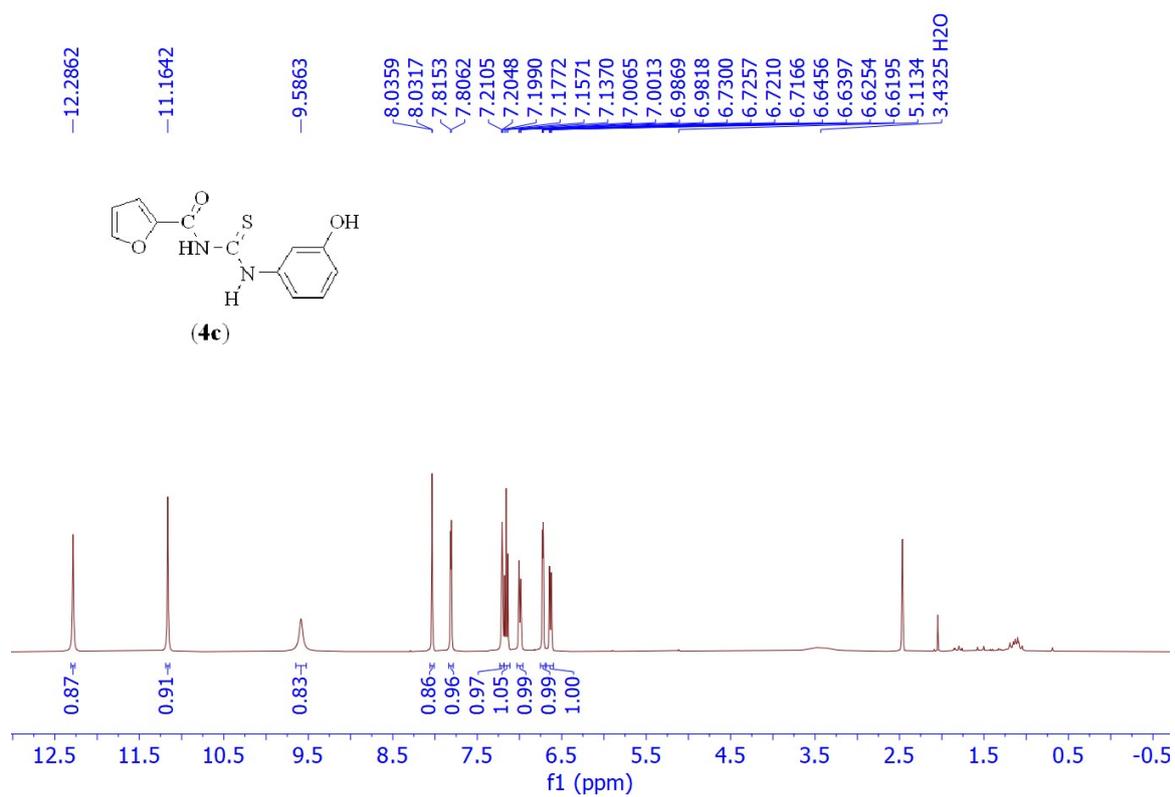


Figure S-6: ¹H NMR (400 MHz) spectrum of compound **4c** in DMSO-*d*₆

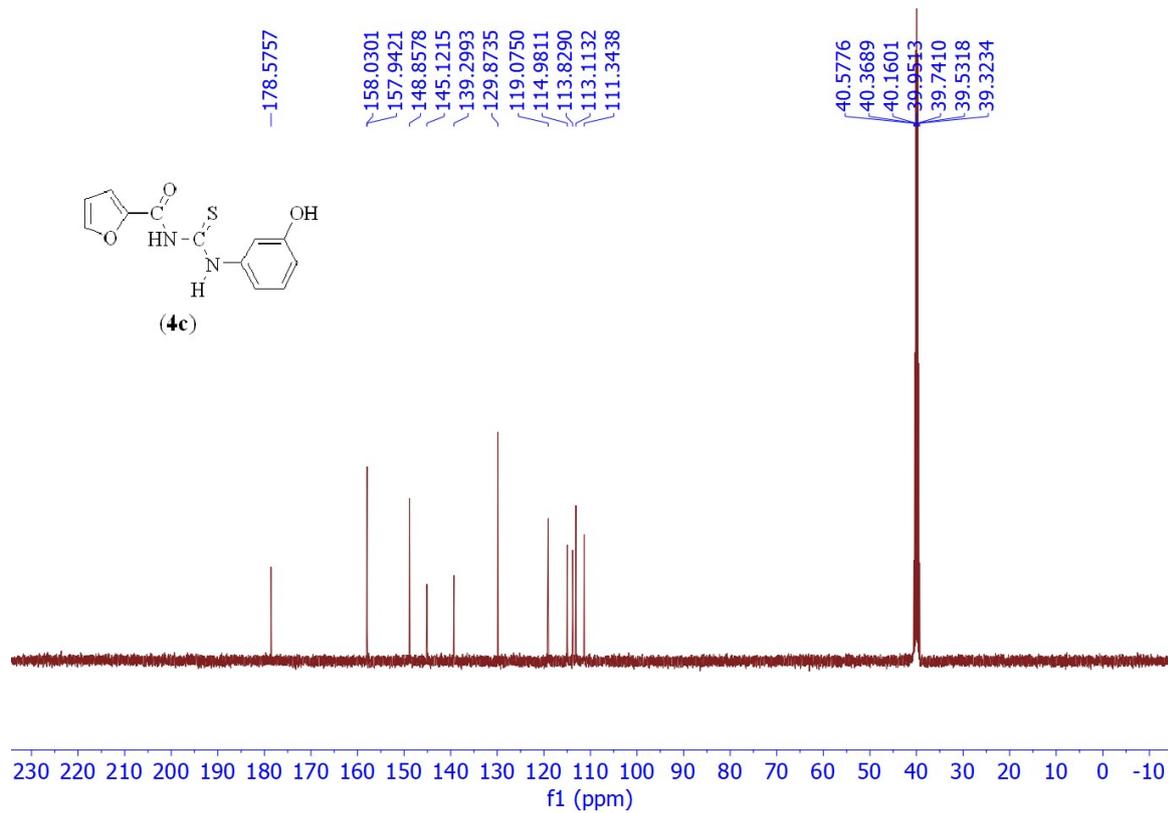
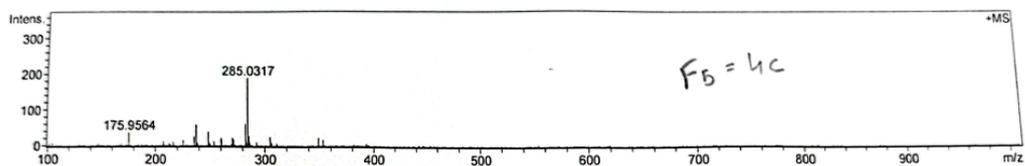


Figure S-7: ^{13}C NMR (100 MHz) spectrum of compound **4c** in $\text{DMSO-}d_6$

Mass Spectrum Report

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Method	positive_03102022.tofpar	Instrument / Ser#	BioTOF II 1.11
Sample Name	F5-3		
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Full Mass Spectrum



Spectrum Region of Interest

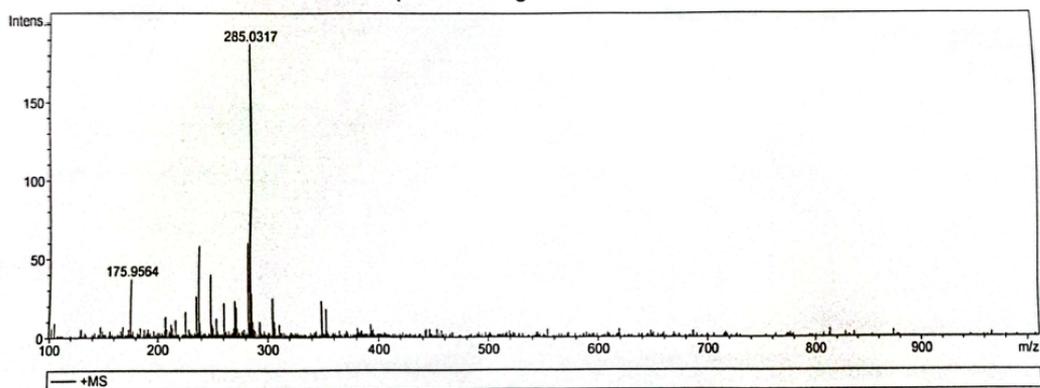


Figure S-8: HRMS of compound 4c

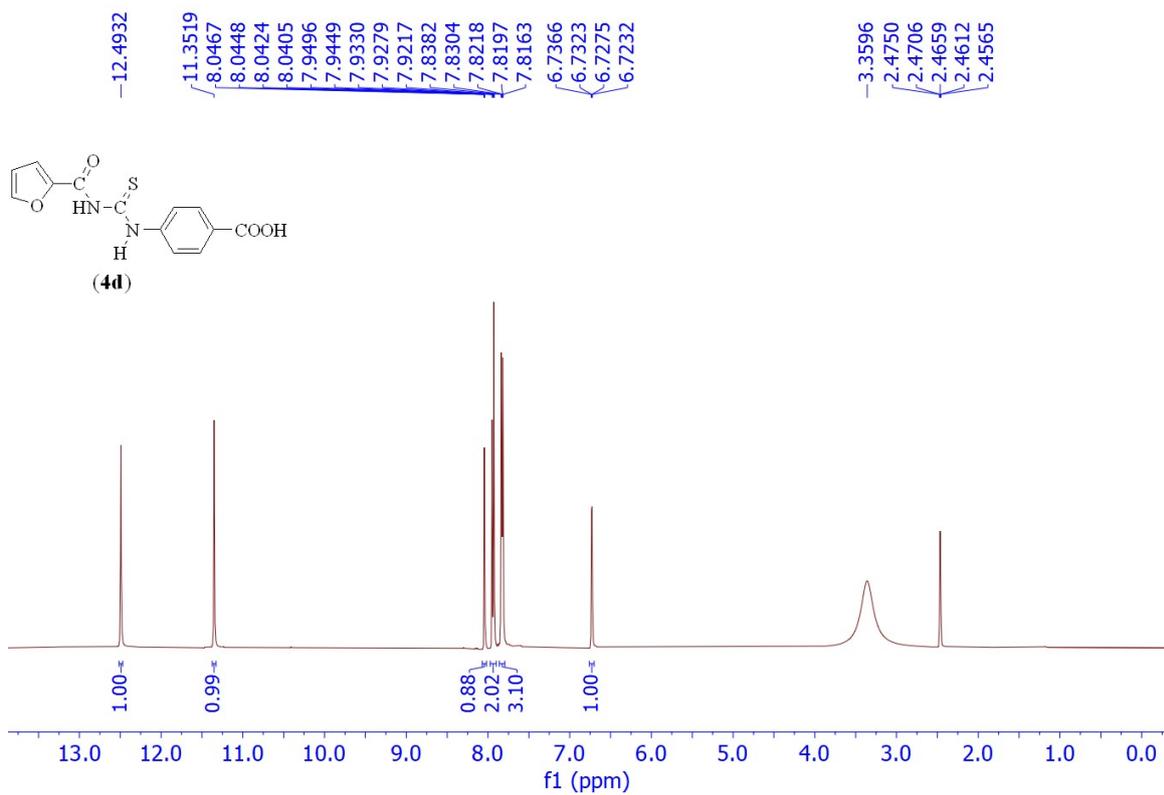


Figure S-9: $^1\text{H NMR}$ (400 MHz) spectrum of compound **4d** in $\text{DMSO-}d_6$

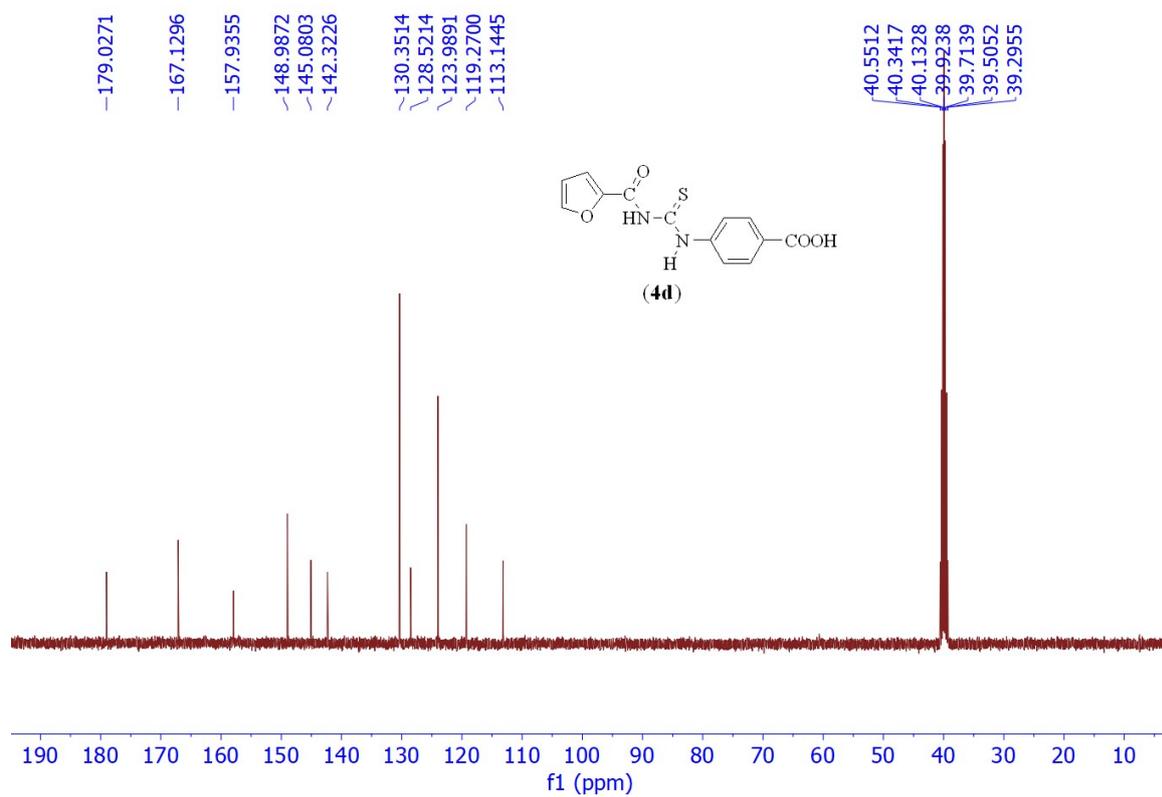
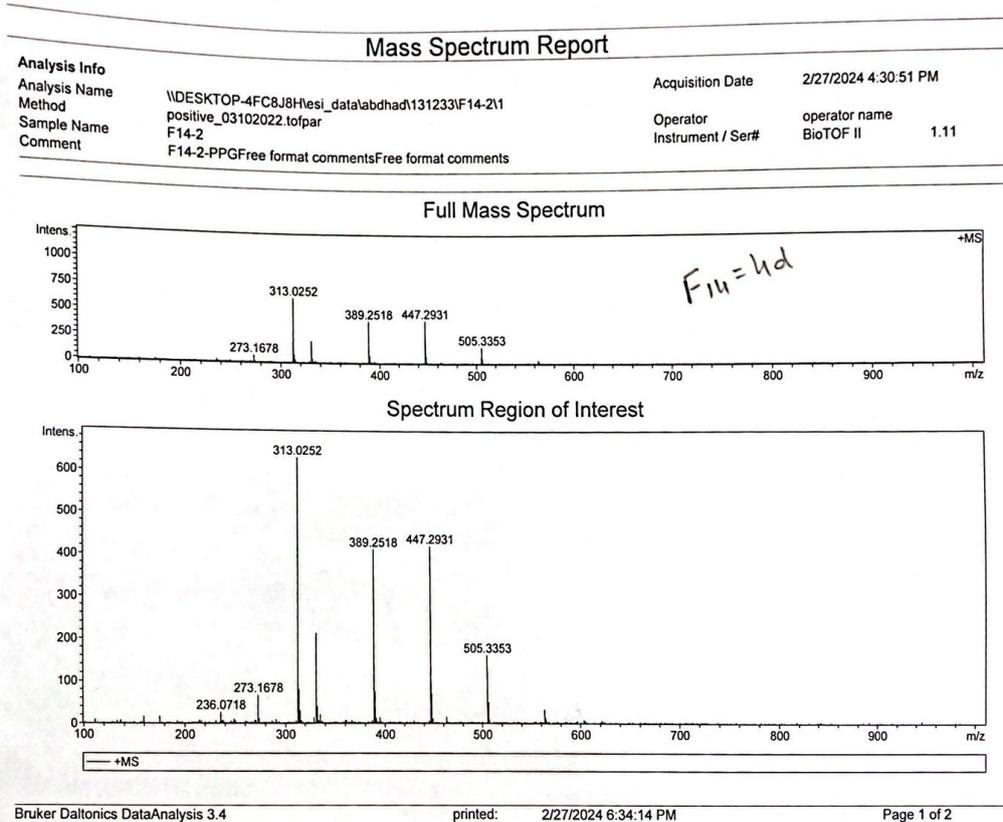


Figure S-10: ¹³C NMR (100 MHz) spectrum of compound **4d** in DMSO-*d*₆

Figure S-11: HRMS of compound **1**



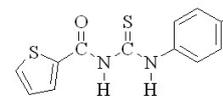
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Page 1 of 2

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(4e)

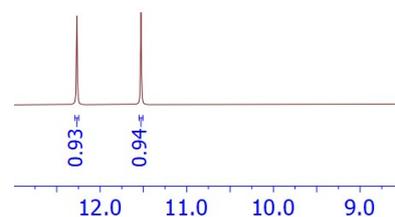


Figure S-12: ^1H NMR (400 MHz) spectrum of compound **4e** in $\text{DMSO}-d_6$

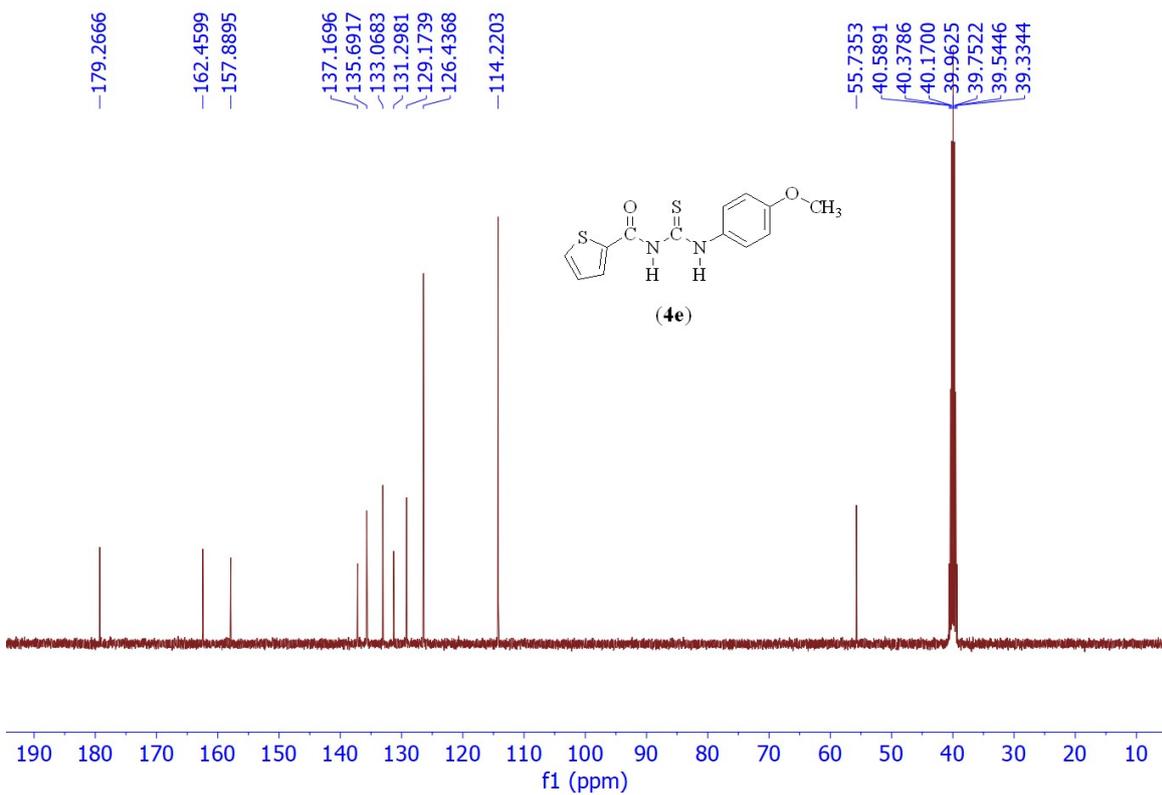
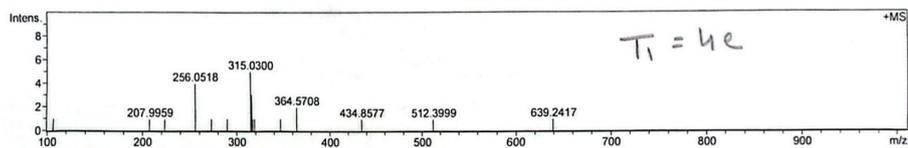


Figure S-13: ^{13}C NMR (100 MHz) spectrum of compound **4e** in $\text{DMSO-}d_6$

Mass Spectrum Report

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Sample Name	T1-4		
Comment	PPGFree format commentsFree format comments		

Full Mass Spectrum



Spectrum Region of Interest

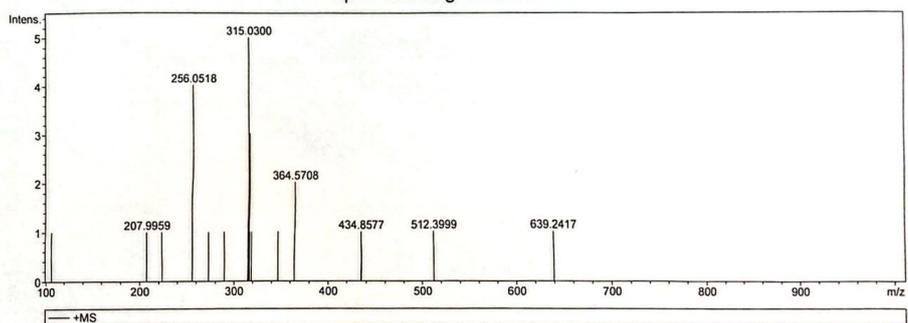


Figure S-14: HRMS of compound **4e**

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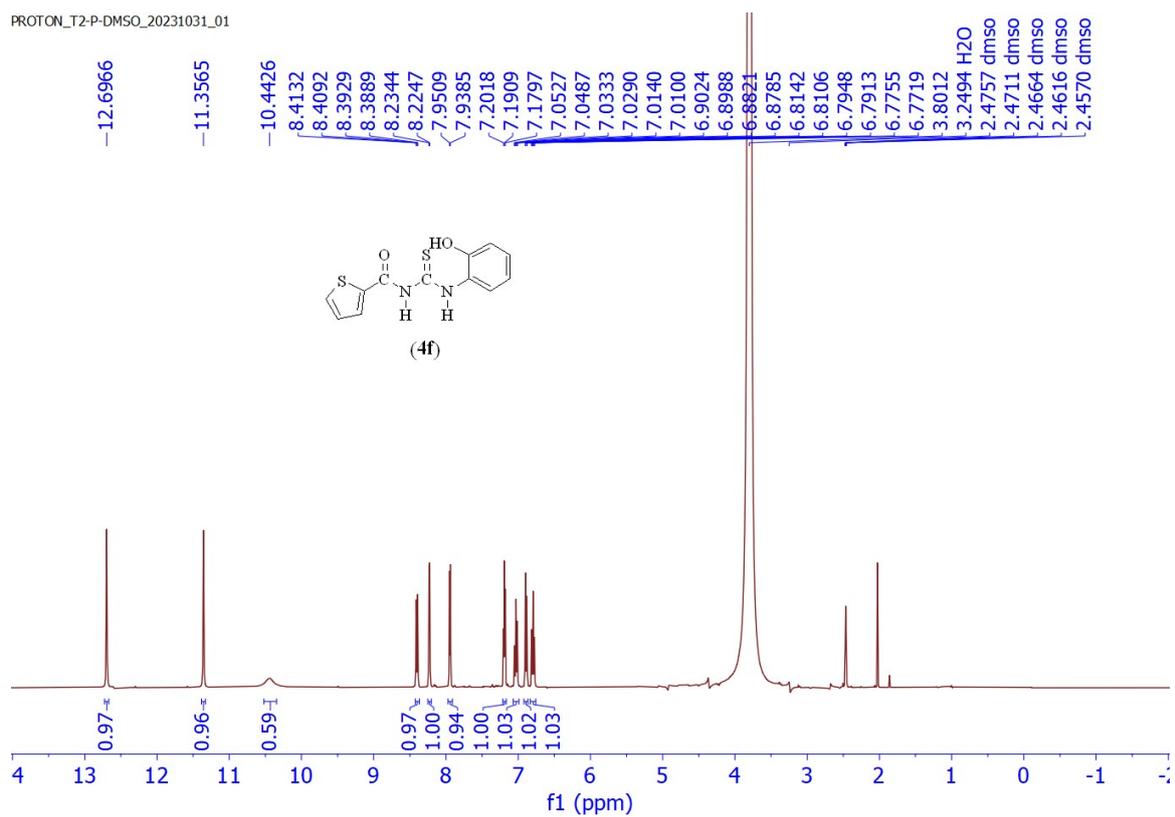


Figure S-15: ¹H NMR (400 MHz) spectrum of compound **4f** in DMSO-*d*₆

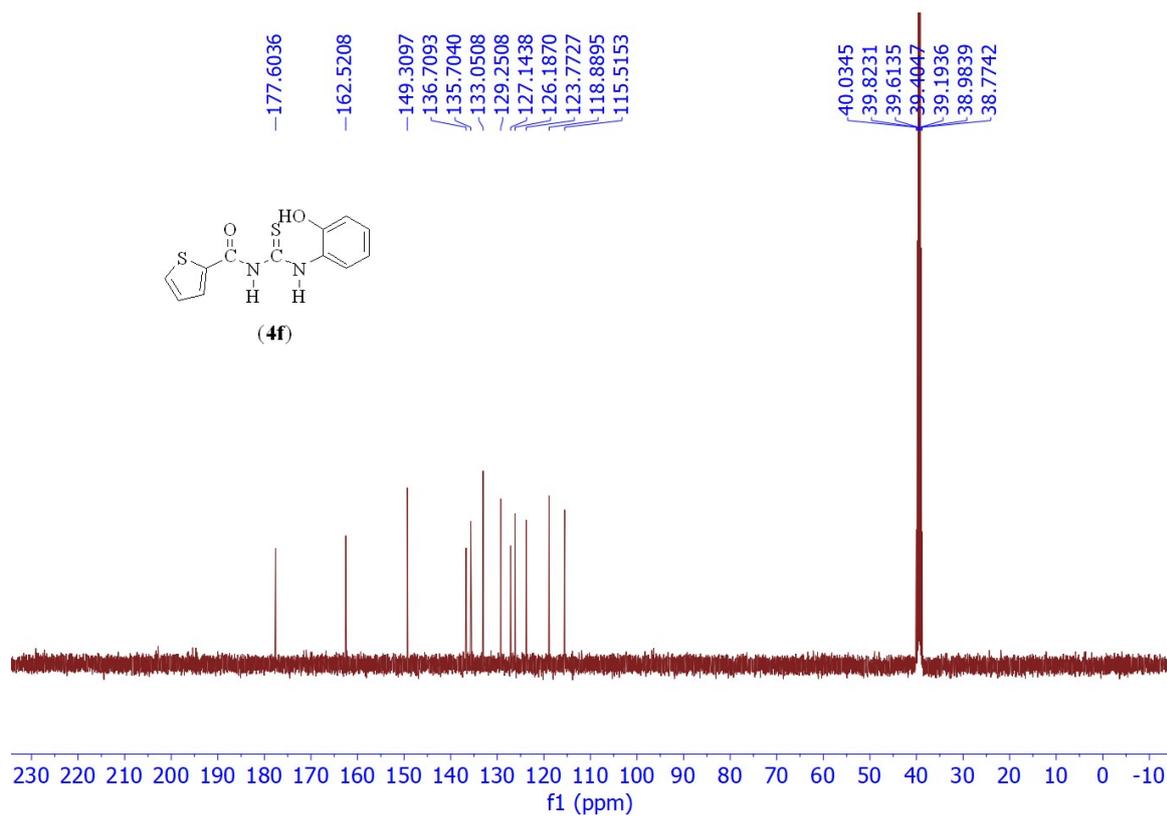
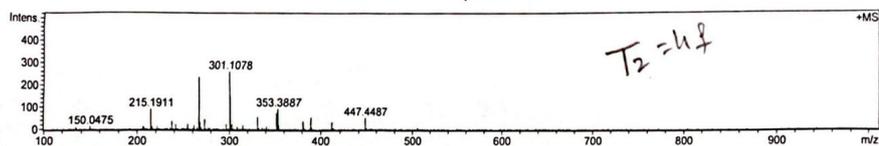


Figure S-16: ^{13}C NMR (100 MHz) spectrum of compound **4f** in $\text{DMSO-}d_6$

Mass Spectrum Report

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Sample Name	T2-2		
Comment	P PGFree format commentsFree format comments		

Full Mass Spectrum



Spectrum Region of Interest

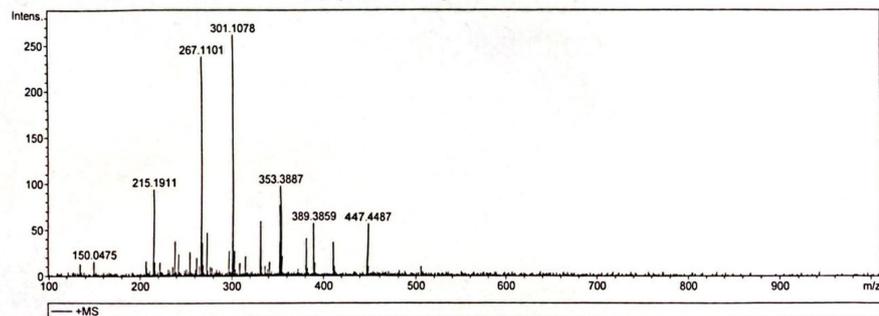


Figure S-17: HRMS of compound **4f**

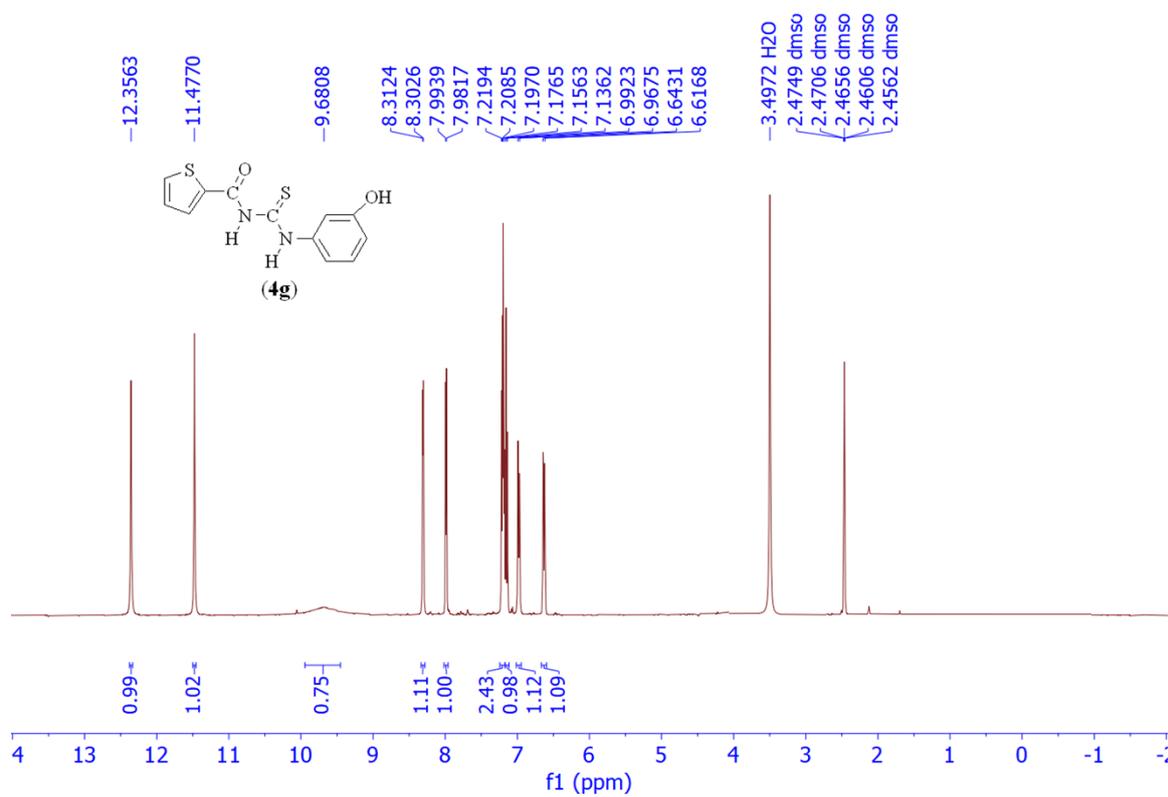


Figure S-18: ¹H NMR (400 MHz) spectrum of compound **4g** in DMSO-*d*₆

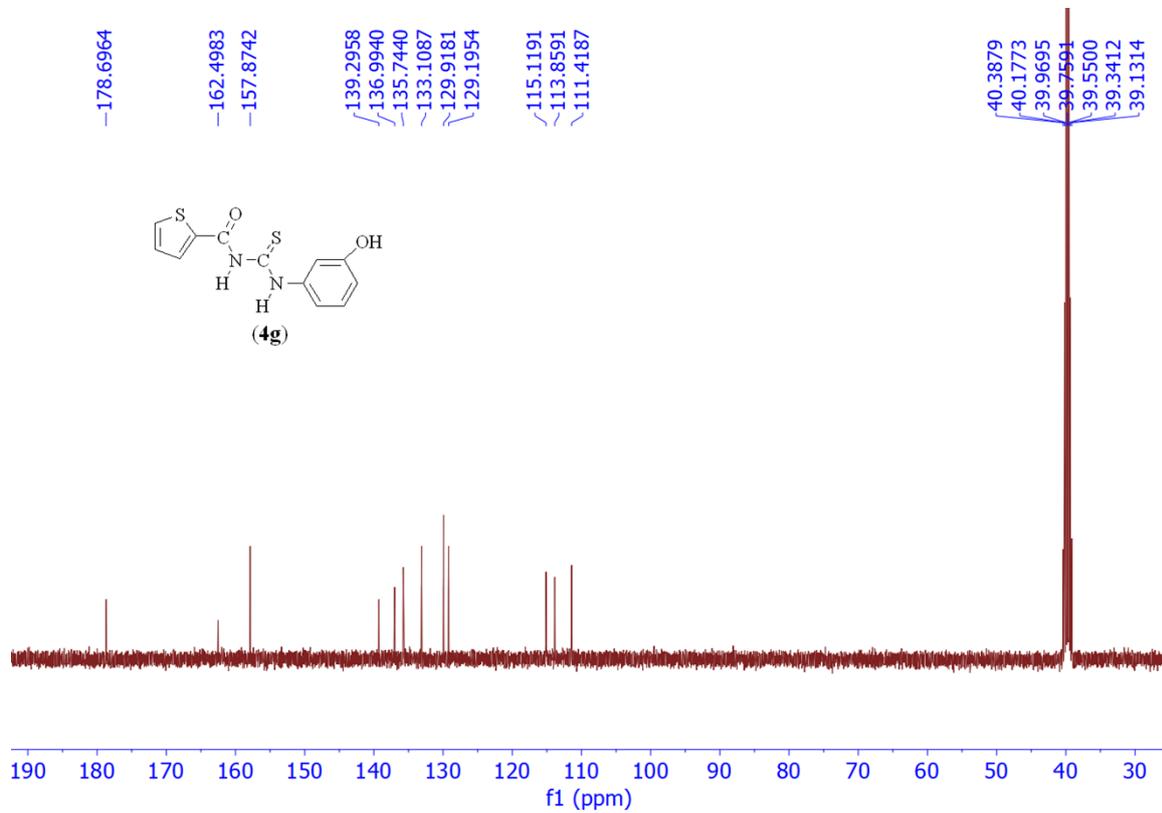


Figure S-19: ¹³C NMR (100 MHz) spectrum of compound **4g** in DMSO-*d*₆

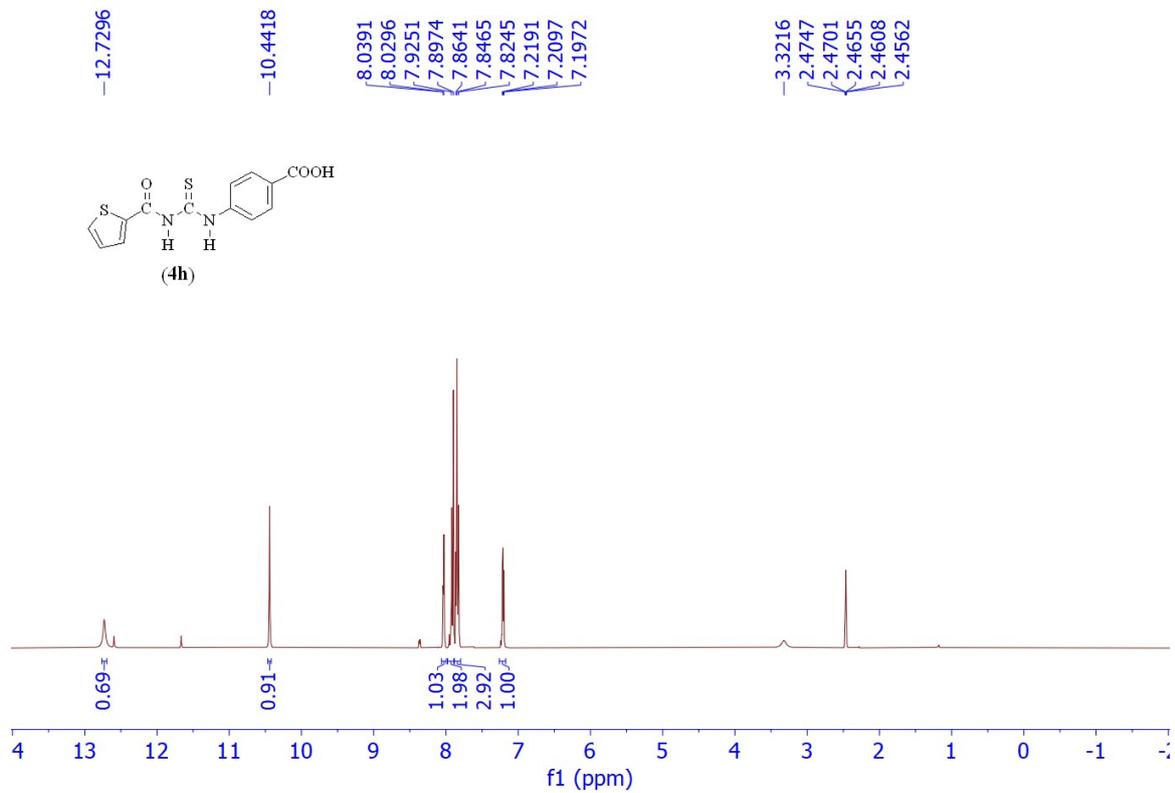


Figure S-20: ¹H NMR (400 MHz) spectrum of compound **4h** in DMSO-*d*₆

CARBON_T8n-carbon_20240119_01 --

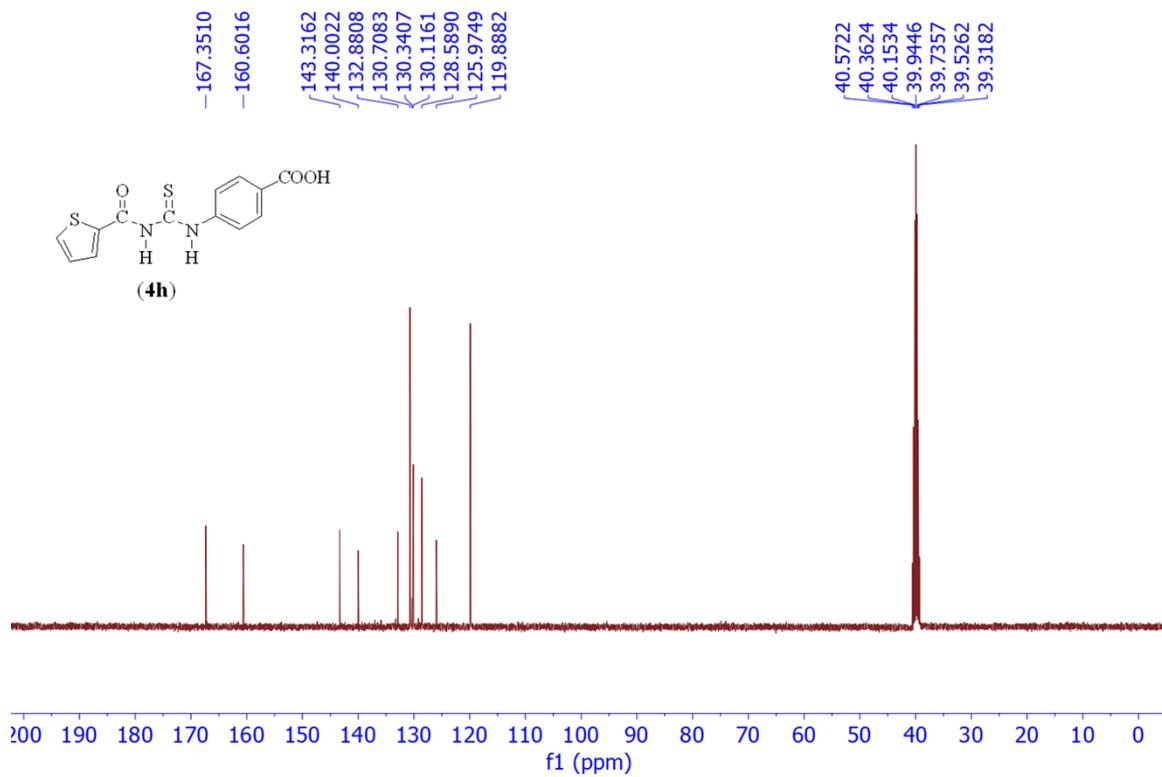


Figure S-21: ^{13}C NMR (100 MHz) spectrum of compound **4h** in $\text{DMSO-}d_6$

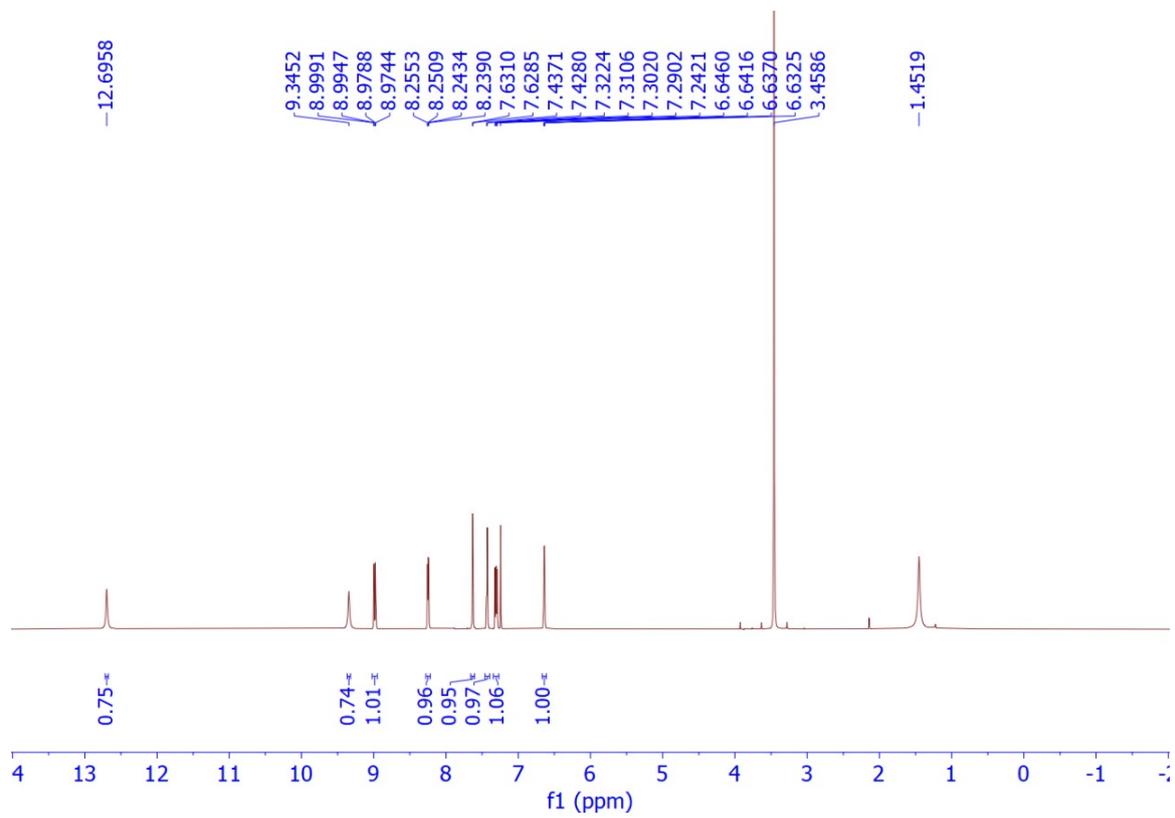


Figure S-22: ^1H NMR (400 MHz) spectrum of compound **5a** in CDCl_3

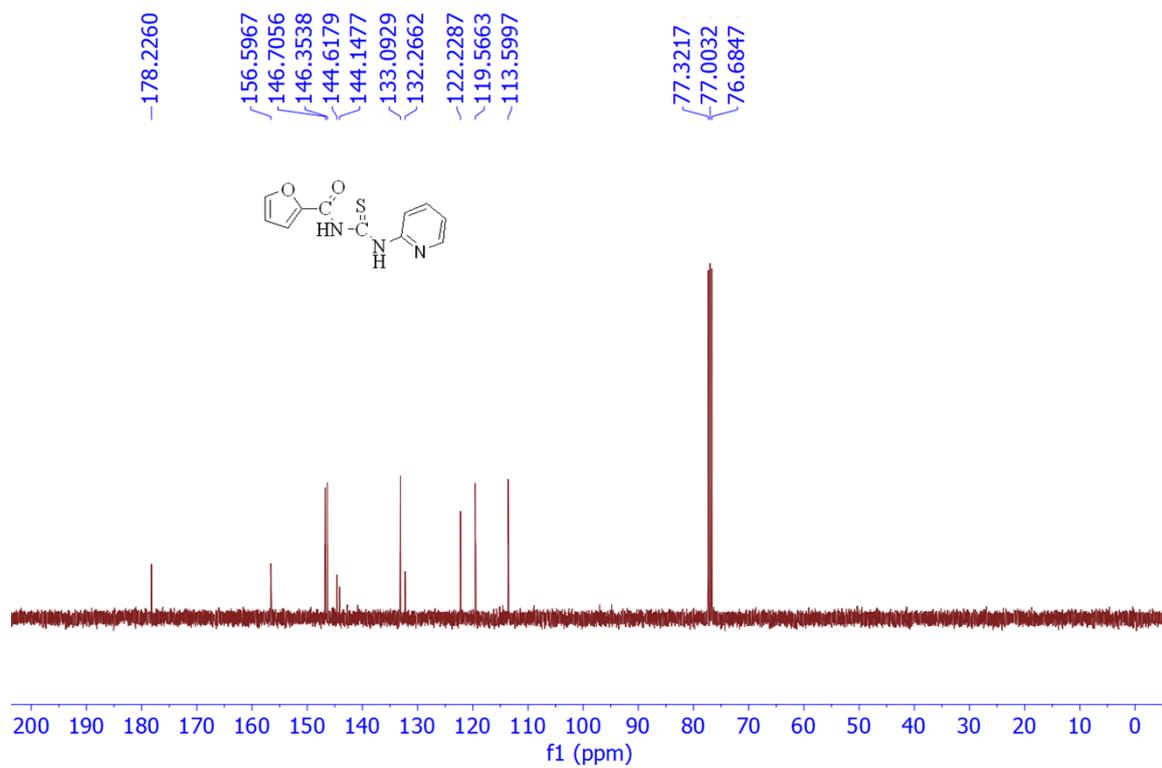


Figure S-23: ¹³C NMR (100 MHz) spectrum of compound **5a** in CDCl₃

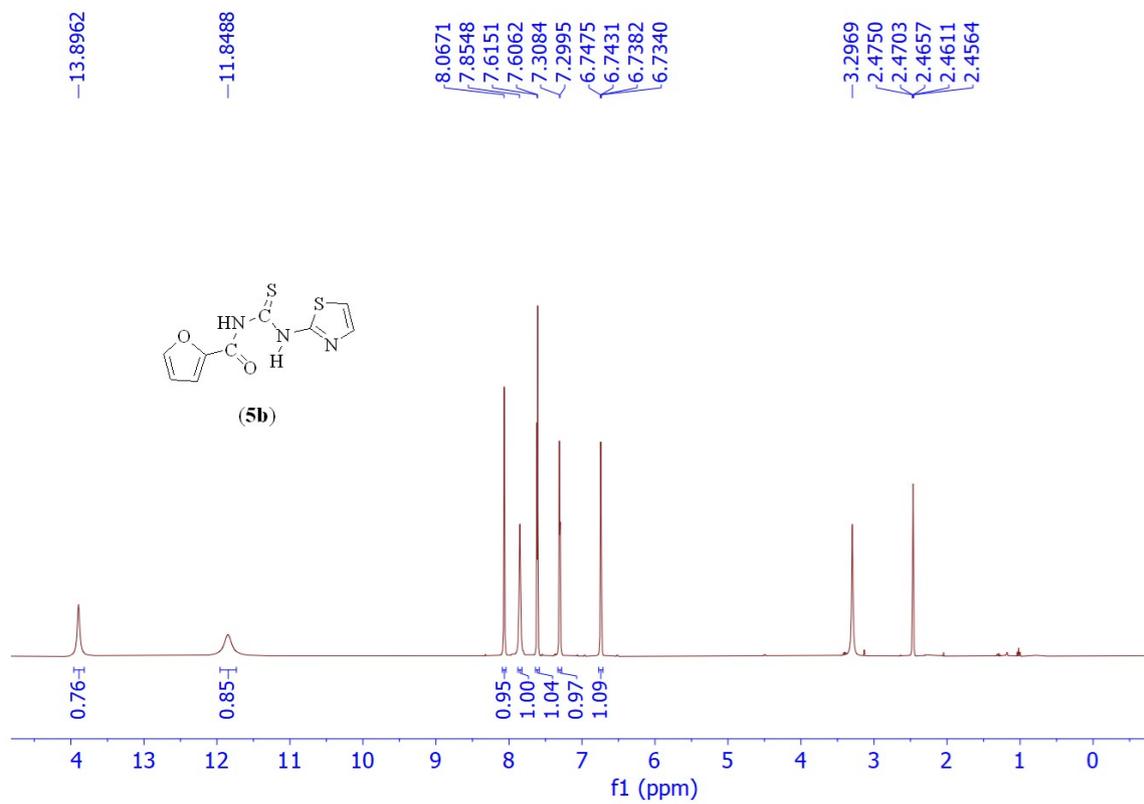


Figure S-24: ¹H NMR (400 MHz) spectrum of compound **5b** in DMSO-*d*₆

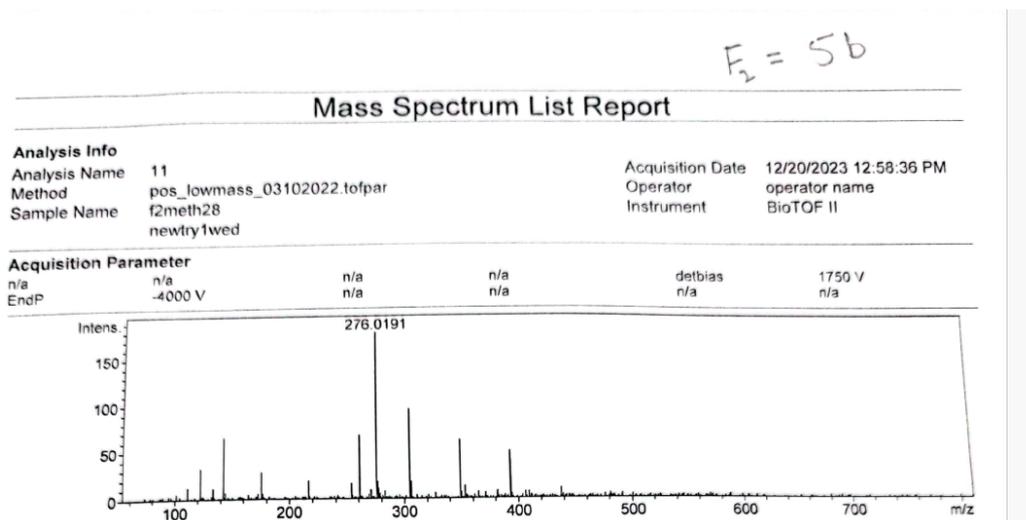
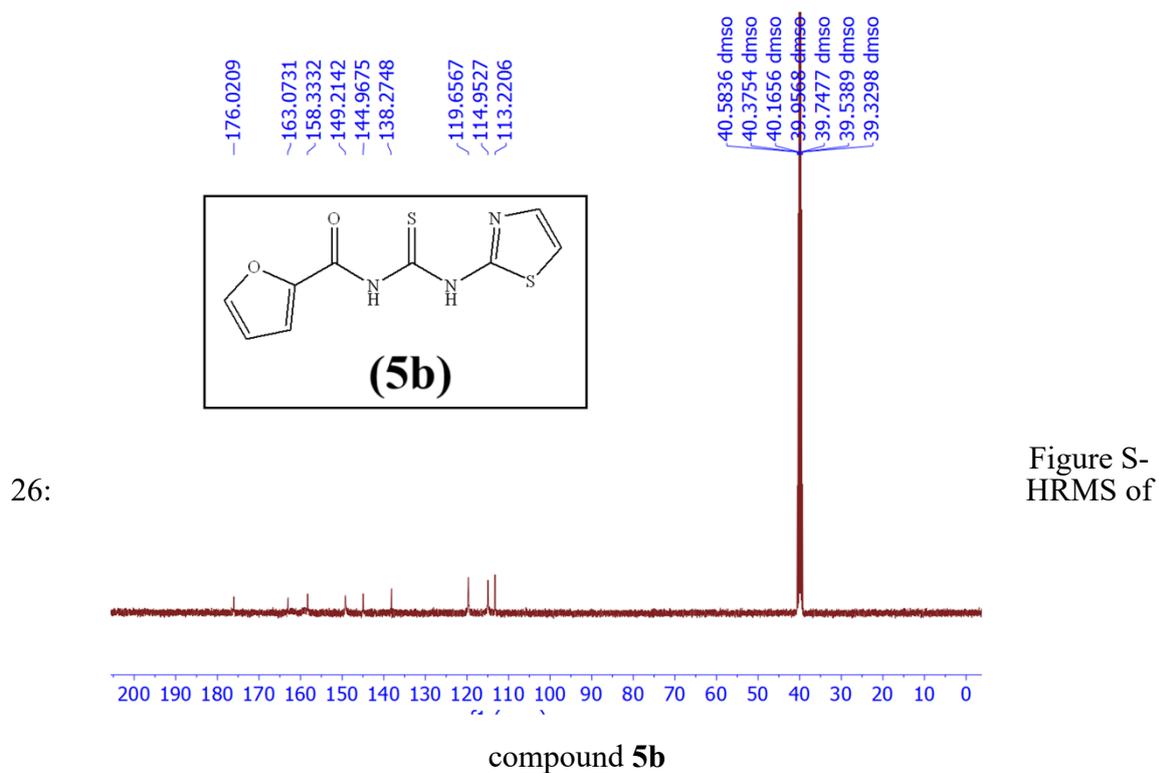


Figure S-25: ¹³C NMR (100 MHz) spectrum of compound **5b** in DMSO-*d*₆



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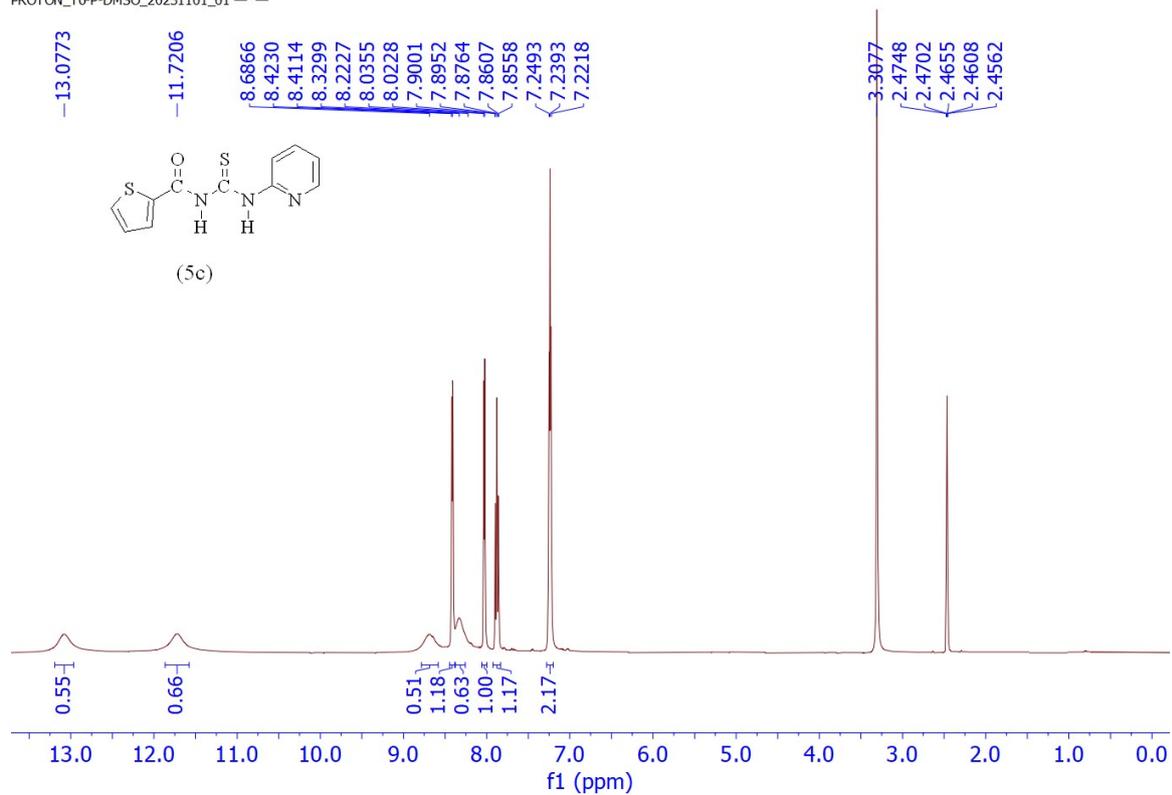


Figure S-27: ¹H NMR (400 MHz) spectrum of compound **5c** in DMSO-*d*₆

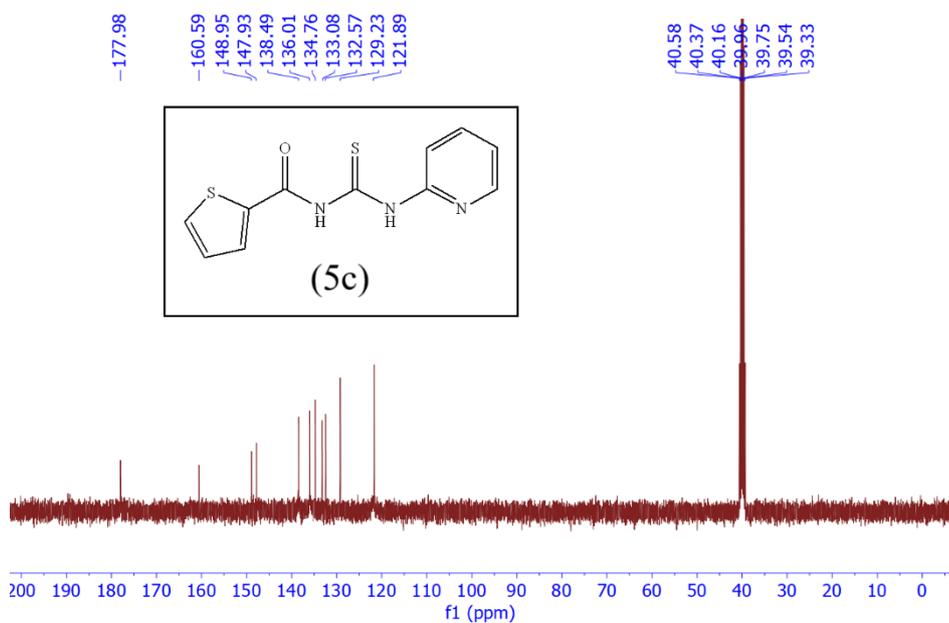


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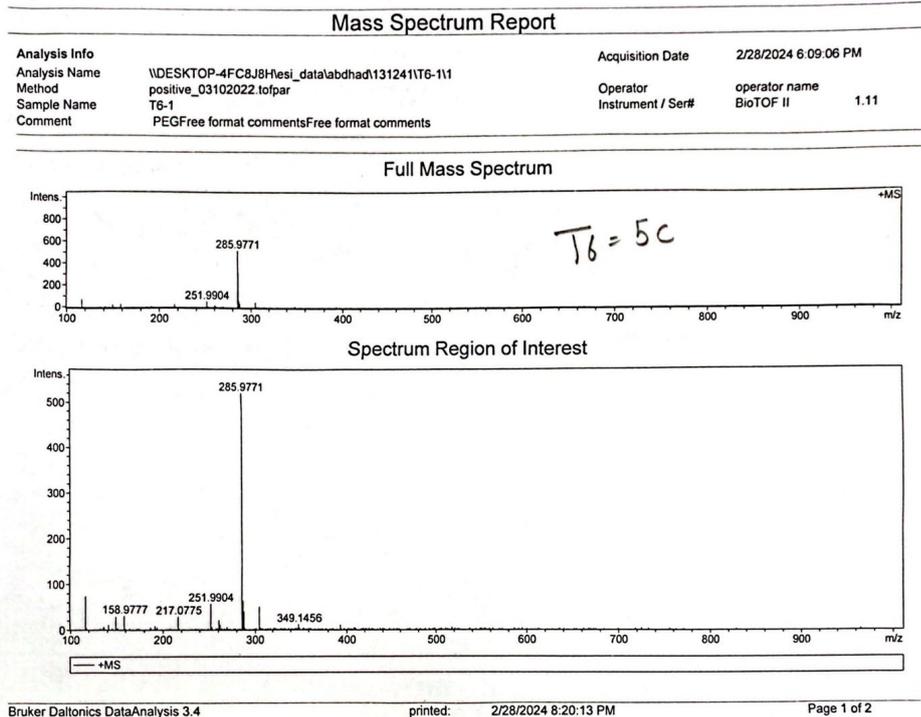


Figure S-29: HRMS of compound **5c**

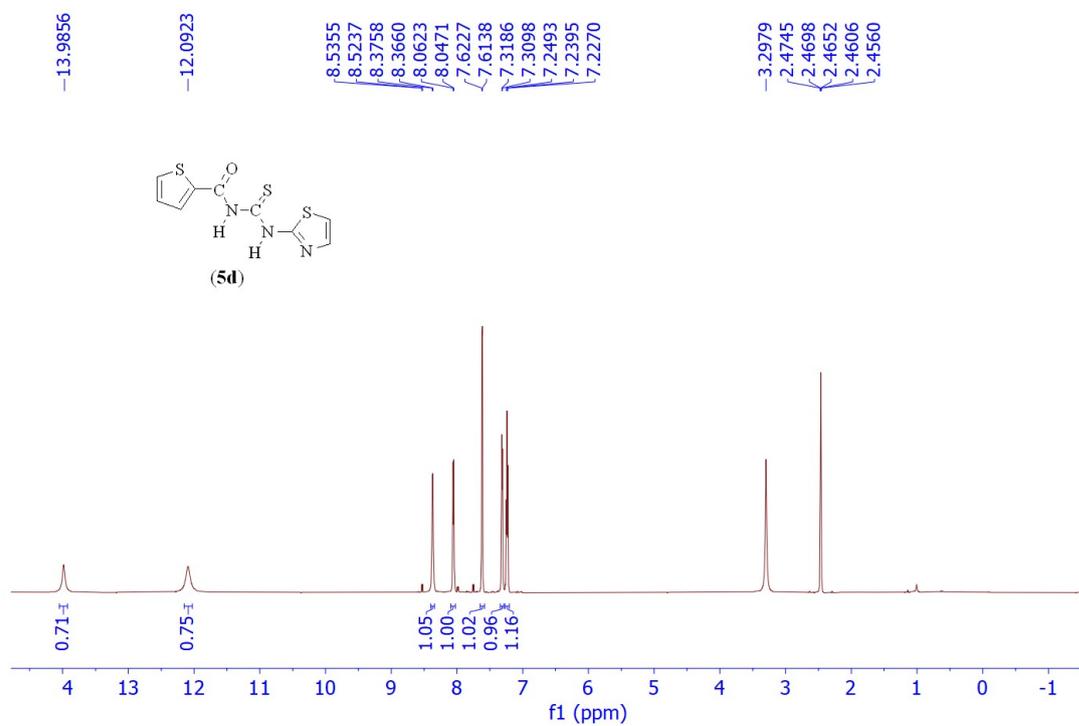
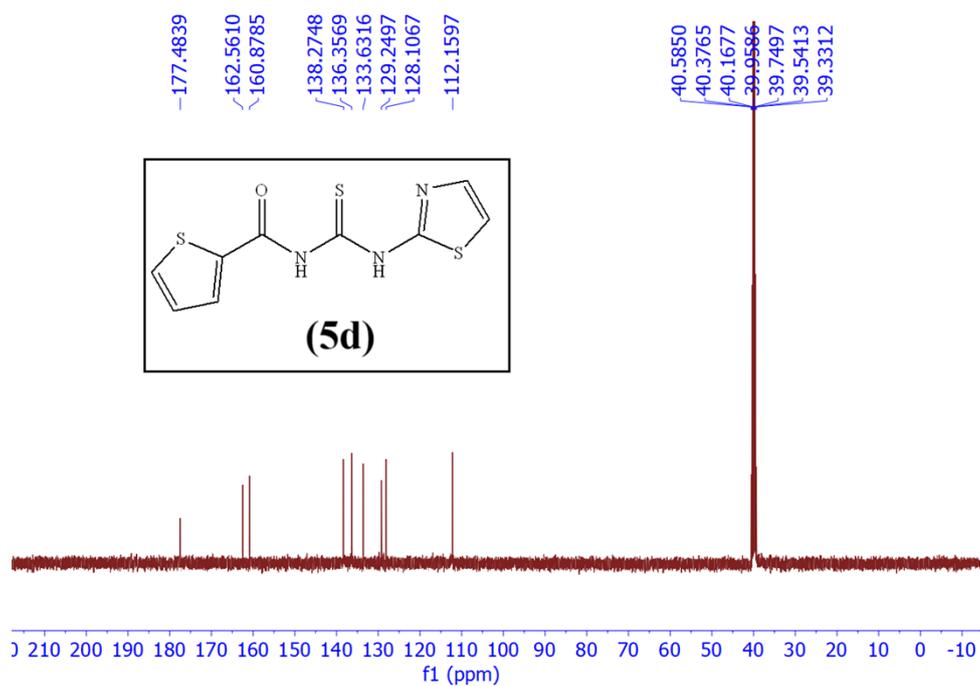
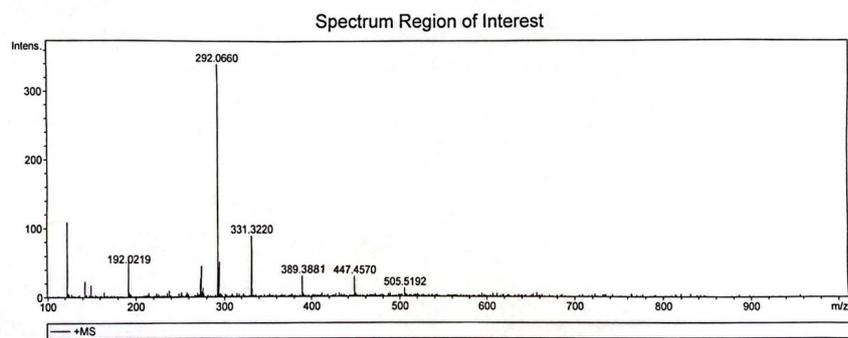
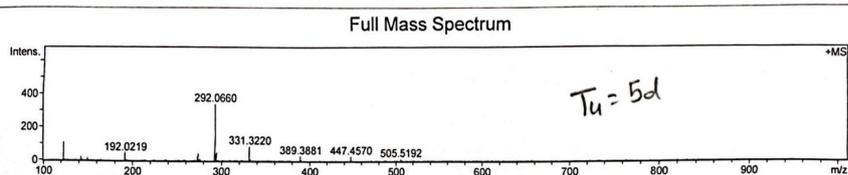


Figure S-30: ¹H NMR (400 MHz) spectrum of compound **5d** in DMSO-*d*₆



Mass Spectrum Report			
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Method	positive_03102022.tofpar	Instrument / Ser#	BioTOF II 1.11
Sample Name	T4-1		
Comment	PPGFree format commentsFree format comments		



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Figure S-32: HRMS of compound **5d**

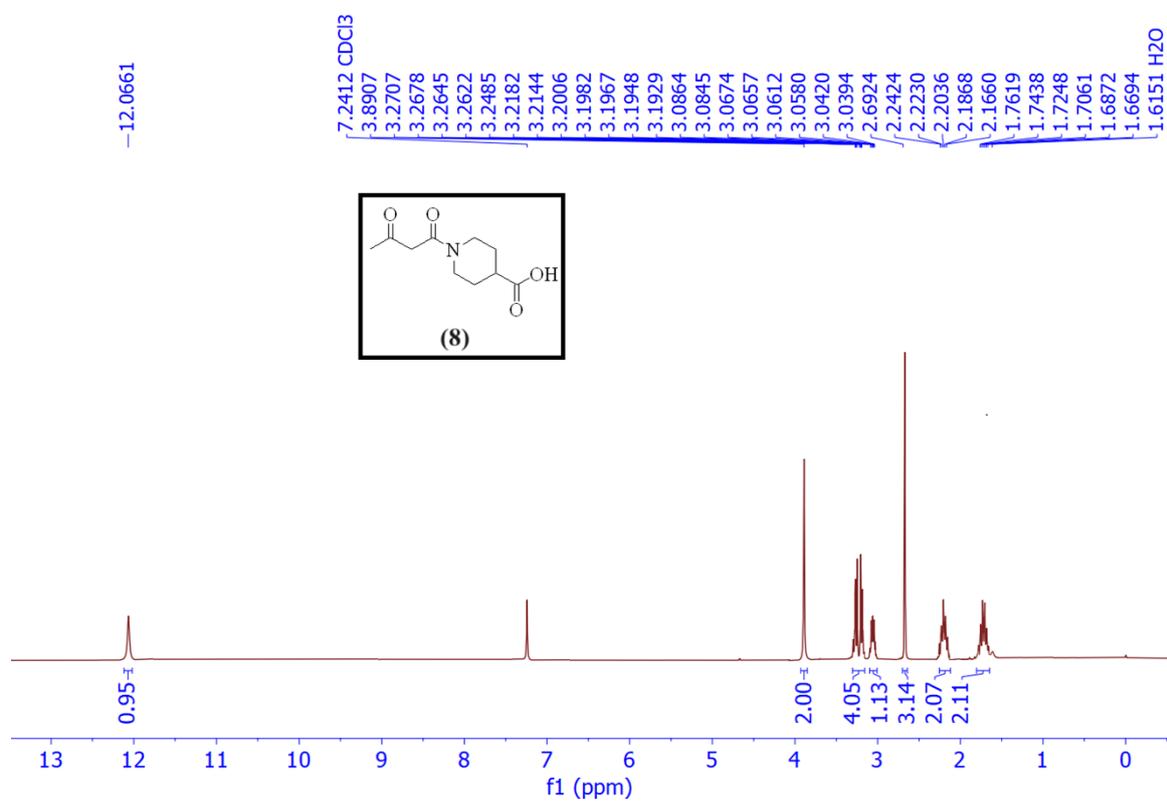


Figure S-33: ¹H NMR (400 MHz) spectrum of compound **8** in CDCl₃

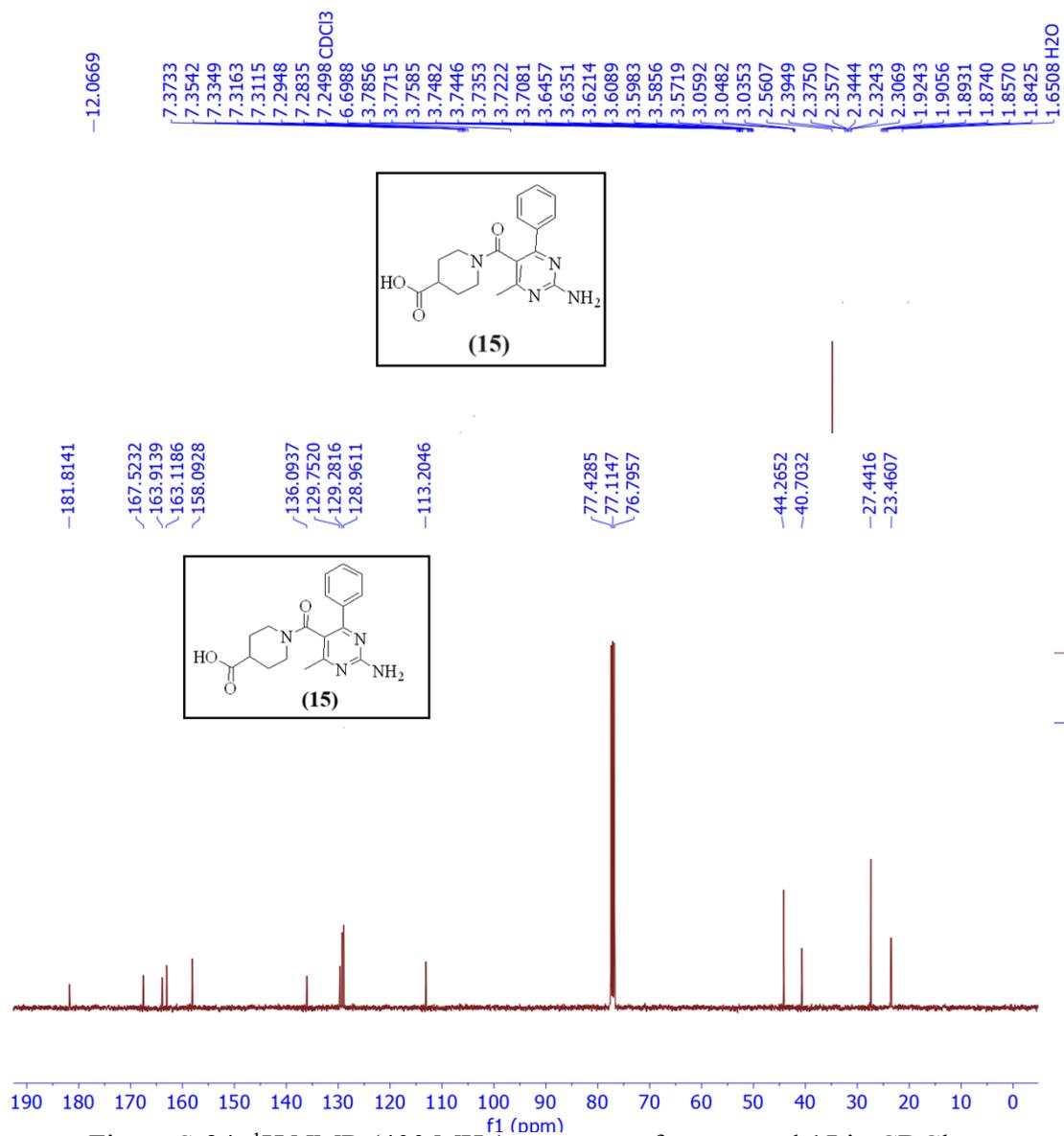


Figure S-34: ¹H NMR (400 MHz) spectrum of compound **15** in CDCl₃

Figure S-35: ^{13}C NMR (100 MHz) spectrum of compound **15** in CDCl_3

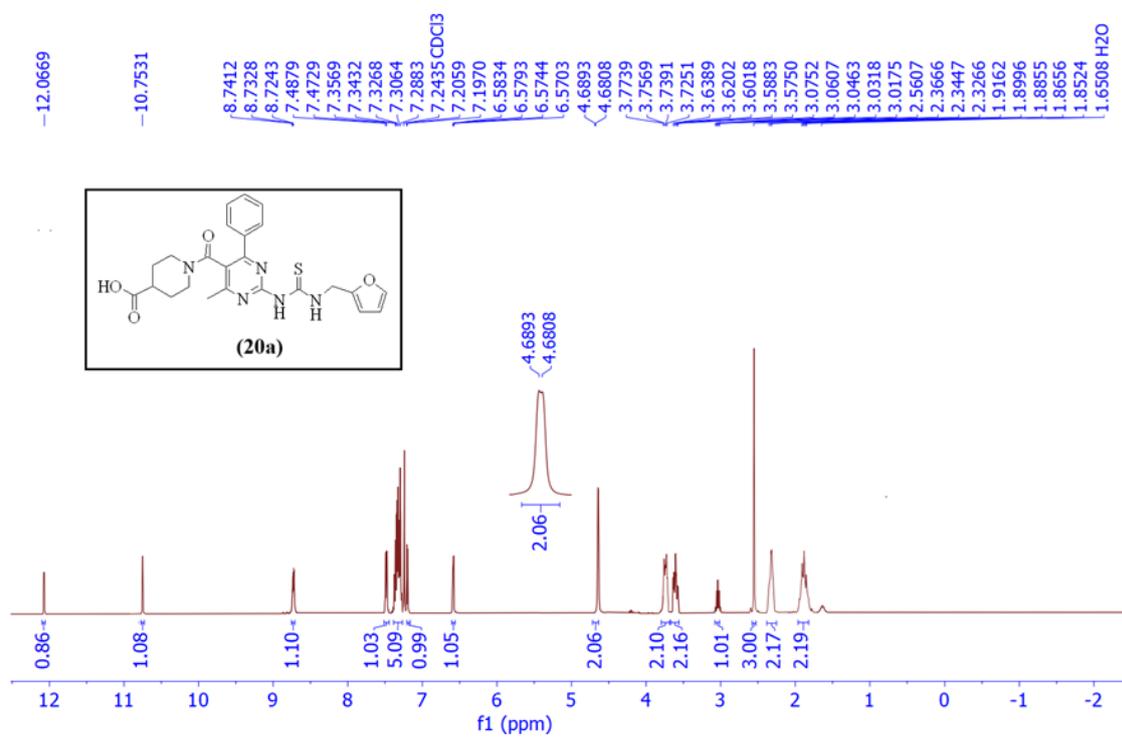


Figure S-36: ^1H NMR (400 MHz) spectrum of compound **20a** in CDCl_3

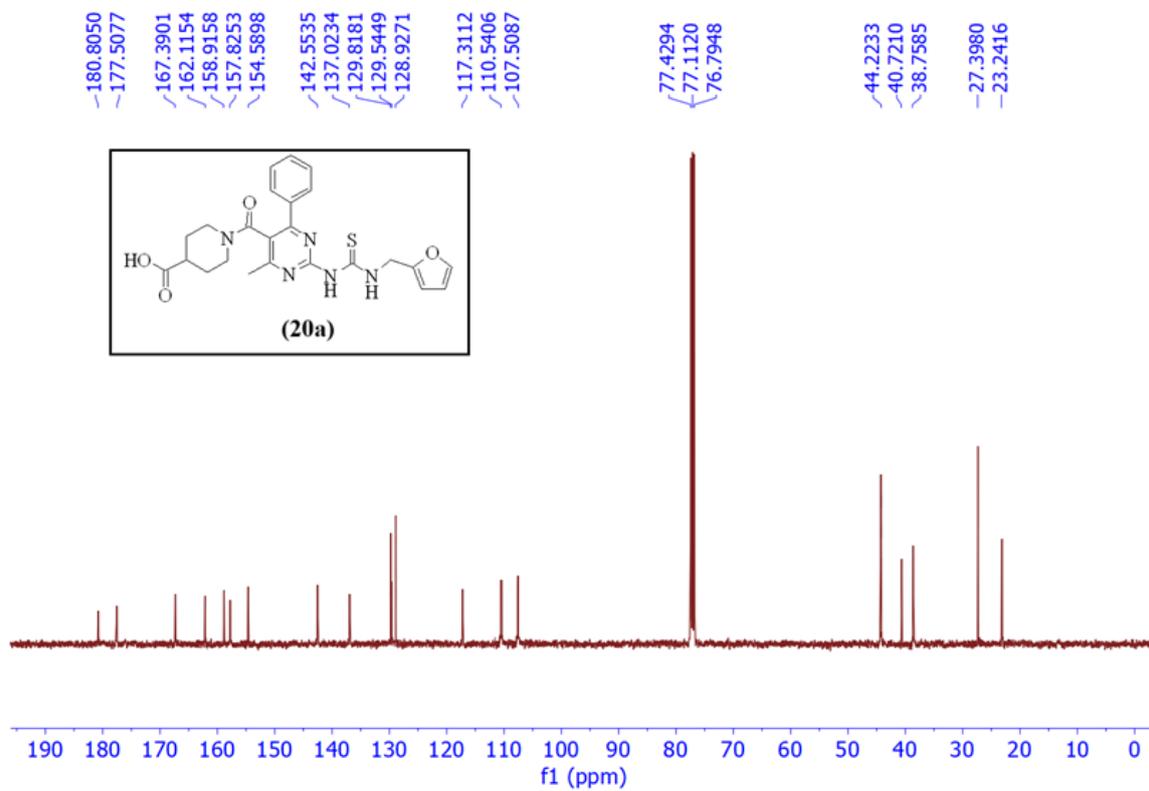


Figure S-37: ^{13}C NMR (100 MHz) spectrum of compound **20a** in CDCl_3

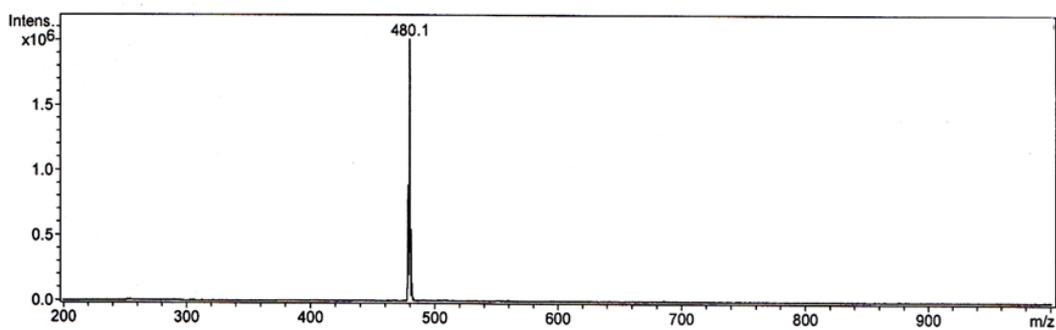


Figure S-38: LCMS Chromatogram of compound **20a**

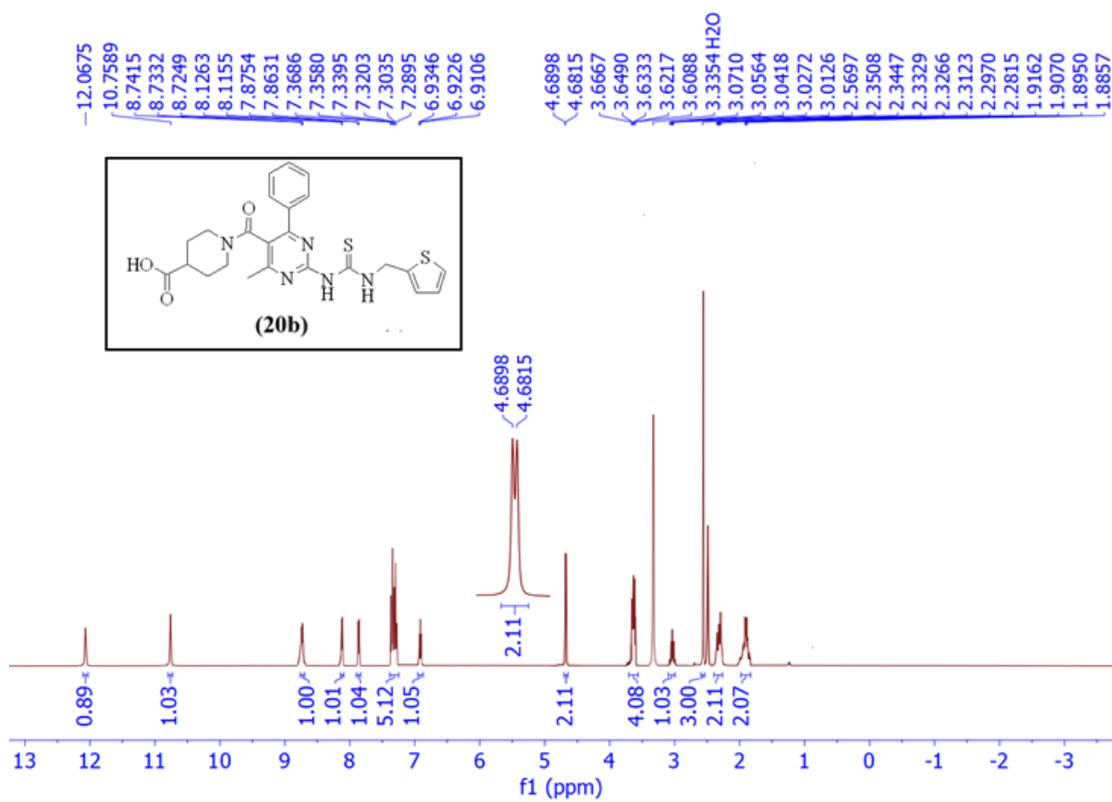


Figure S-39: ¹H NMR (400 MHz) spectrum of compound **20b** in DMSO-d₆

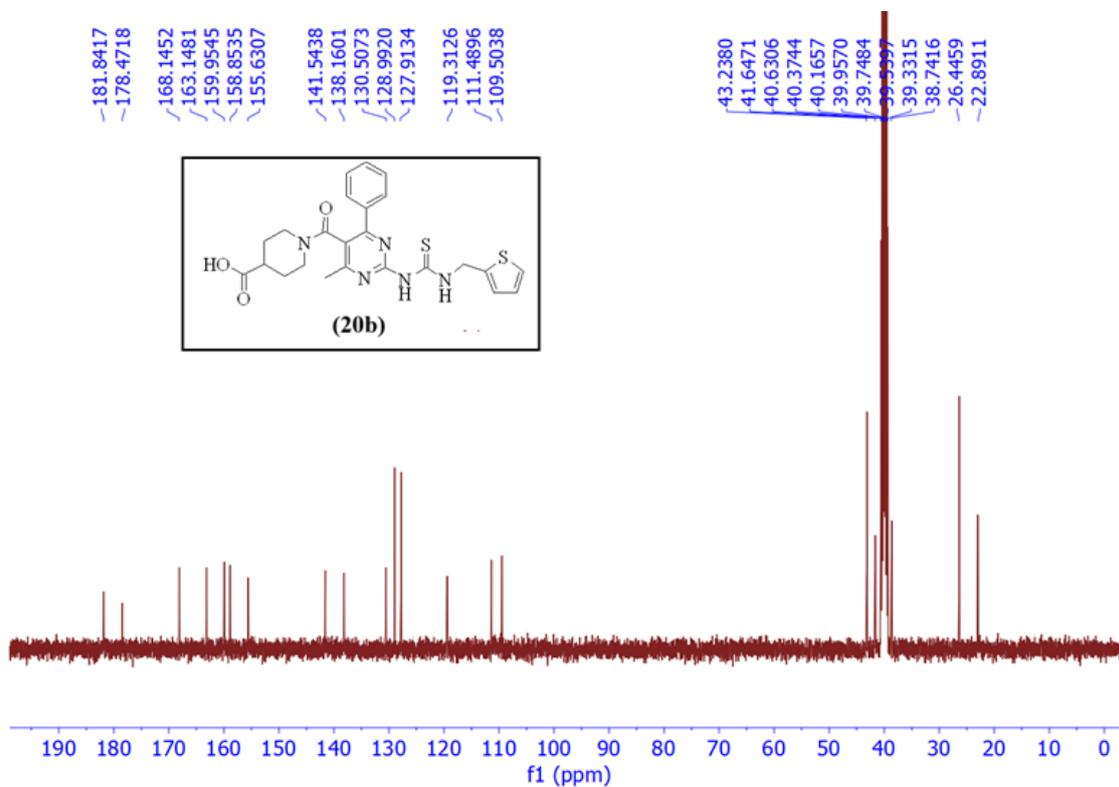


Figure S-40: ¹³C NMR (100 MHz) spectrum of compound **20b** in DMSO-d₆

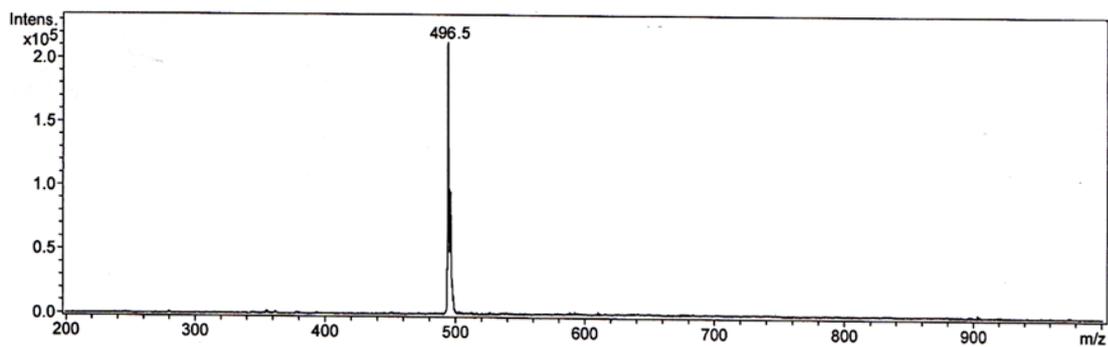


Figure S-41: LCMS Chromatogram of compound **20b**