

Synthesis and antiproliferative potency of 1,3,4-thiadiazole and 1,3-thiazolidine-4-one based new binary heterocyclic molecules: *in vitro* cell-based anticancer studies

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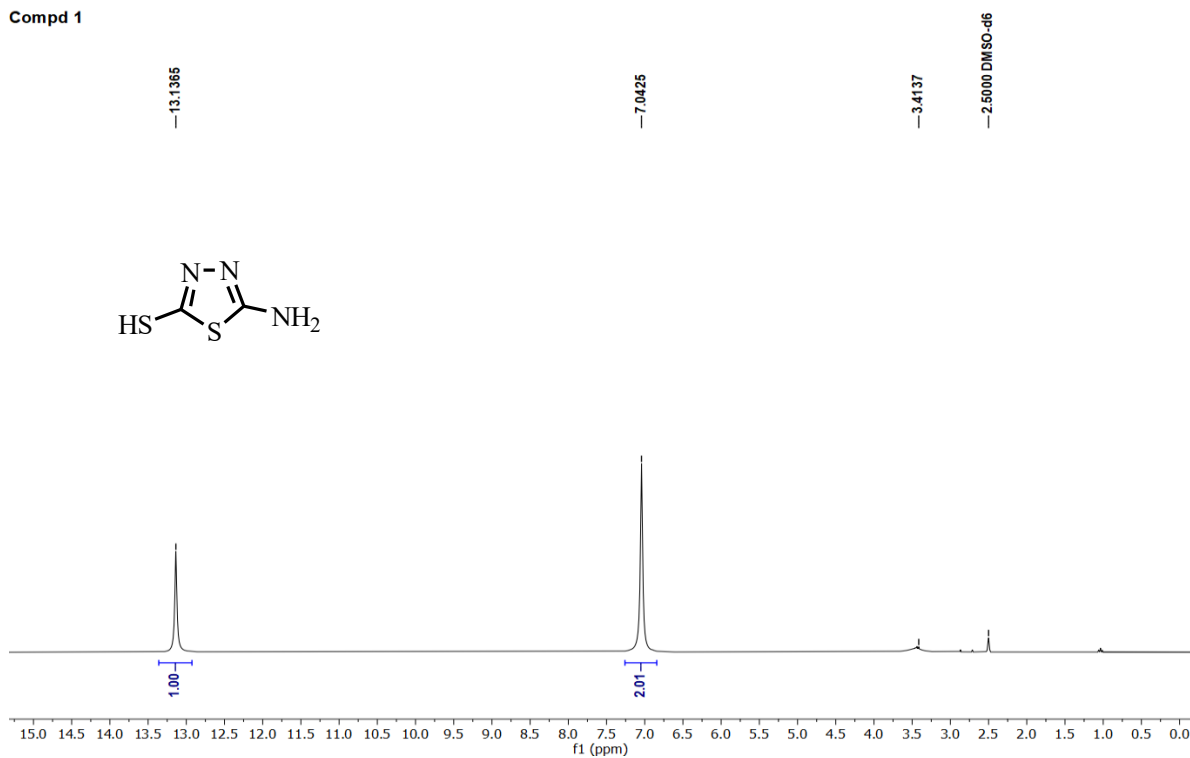
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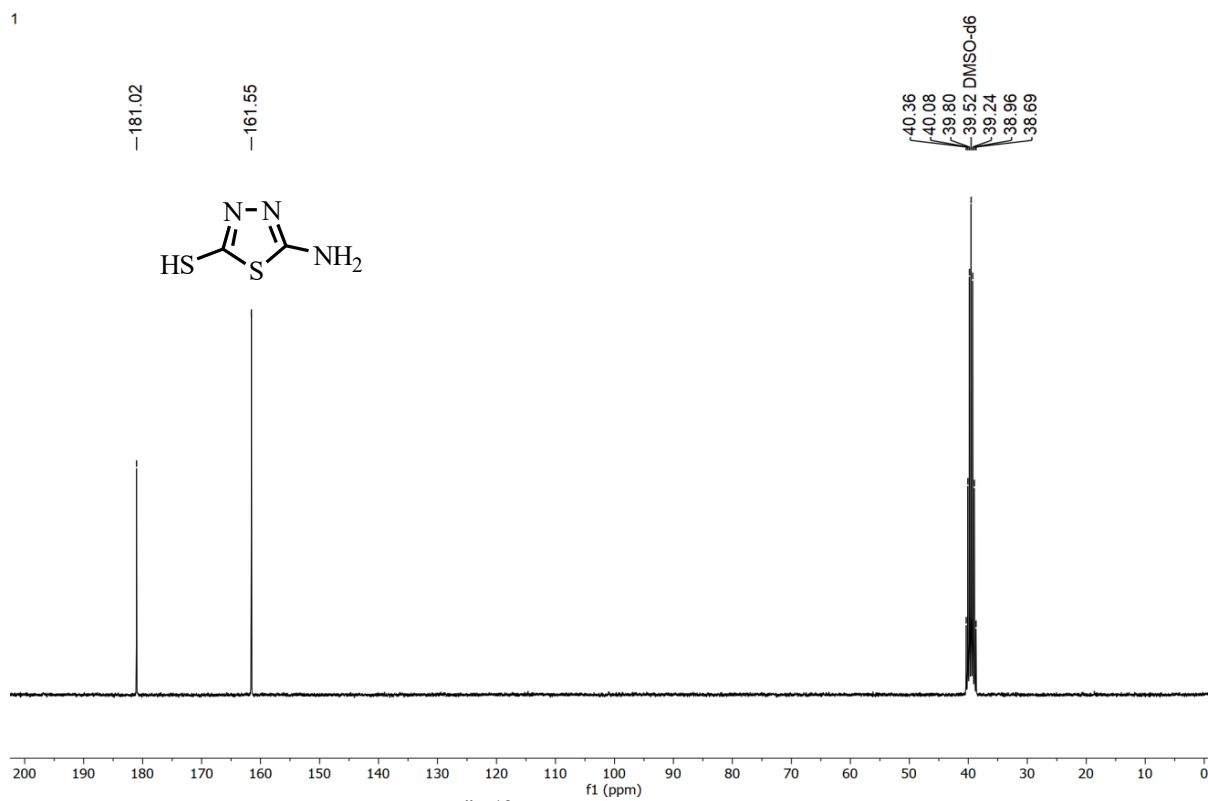
Copy of ^1H , ^{13}C and ^{19}F NMR data:

Compd 1



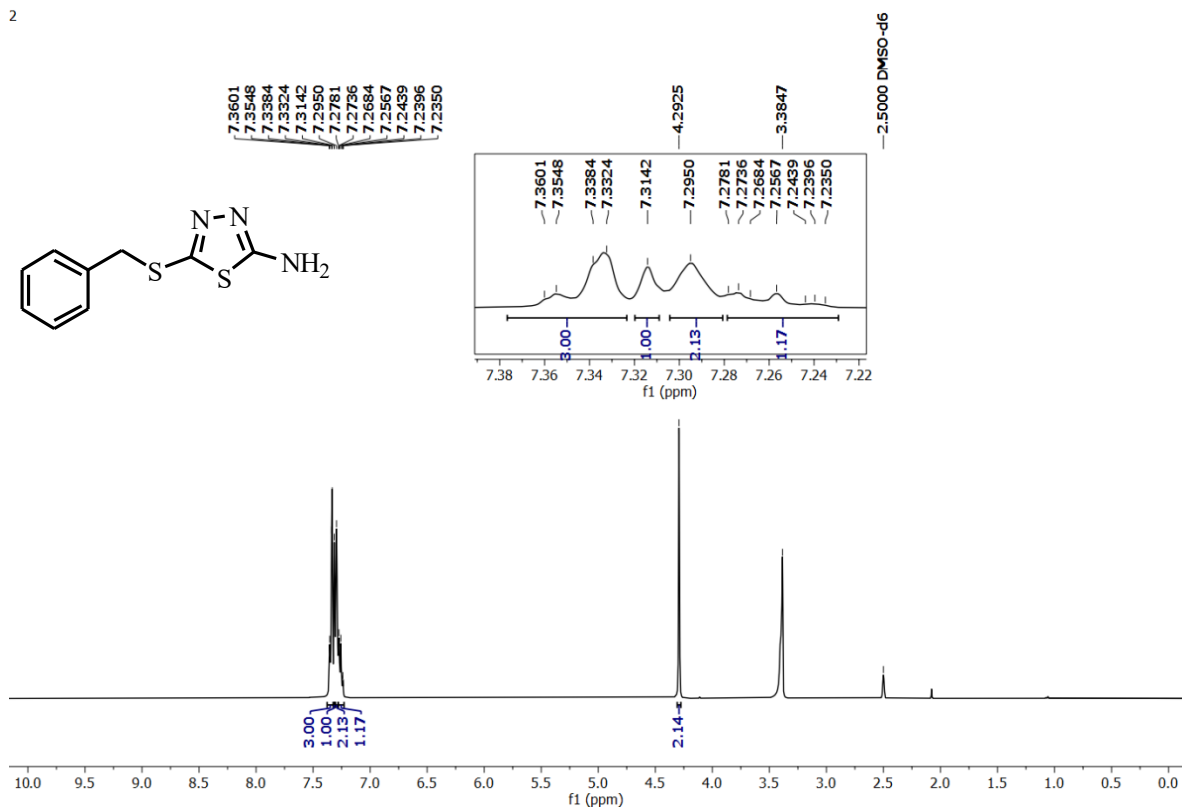
S.F1': ^1H NMR of compound 1

1

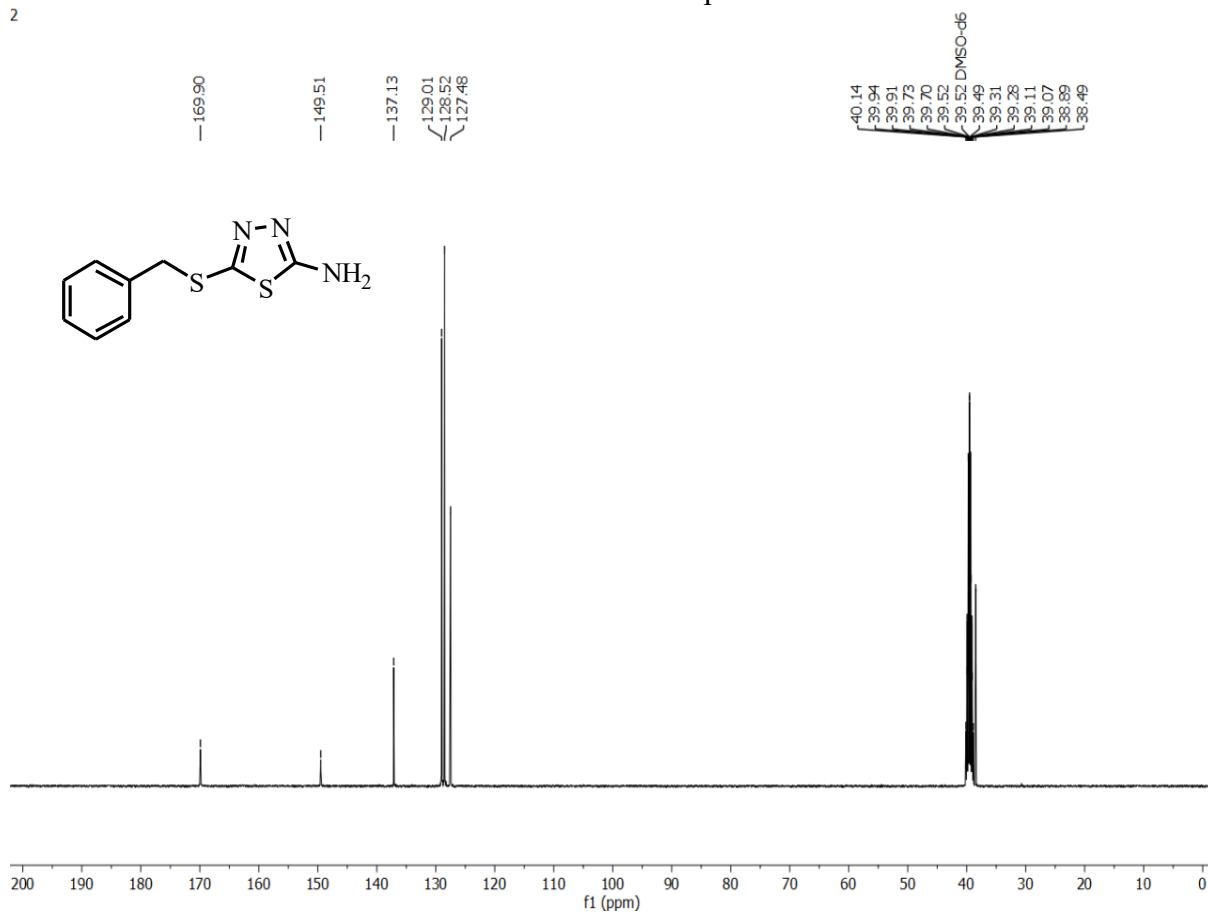


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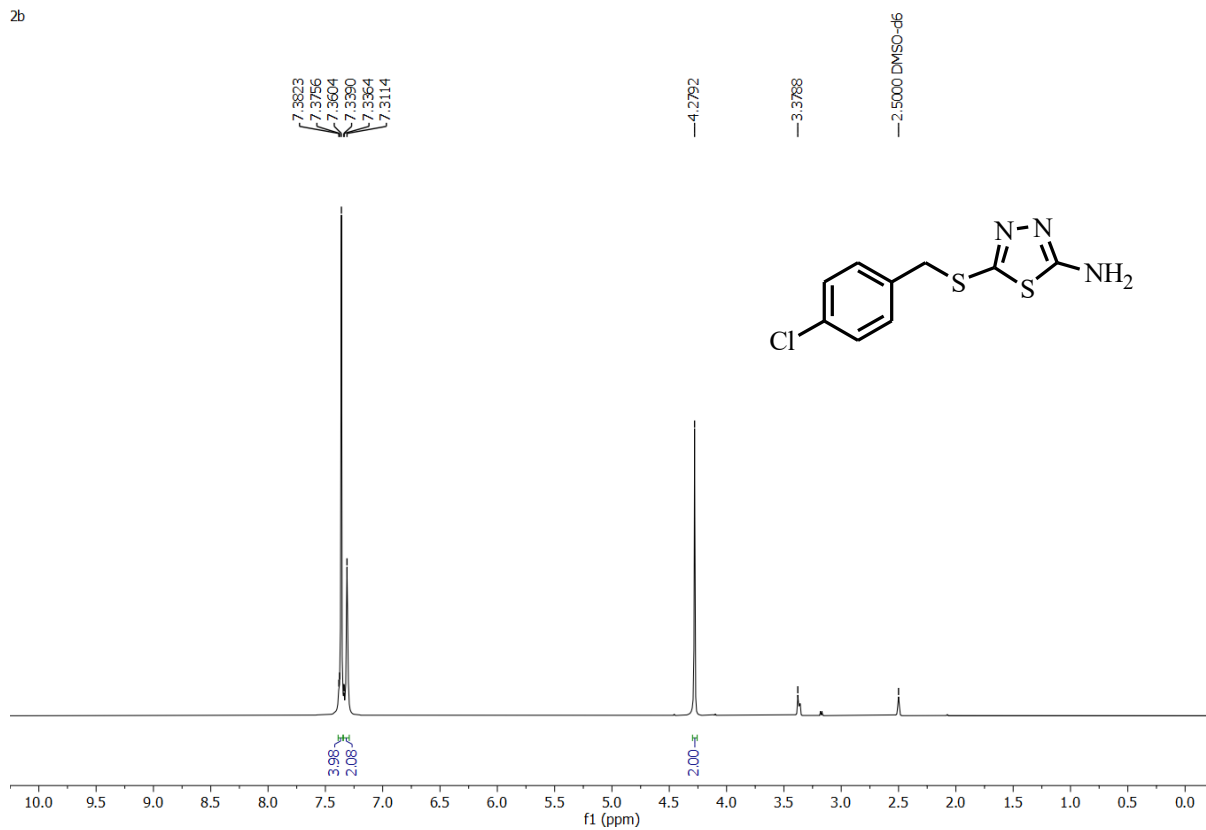
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S.F2': ¹H NMR of compound 2a

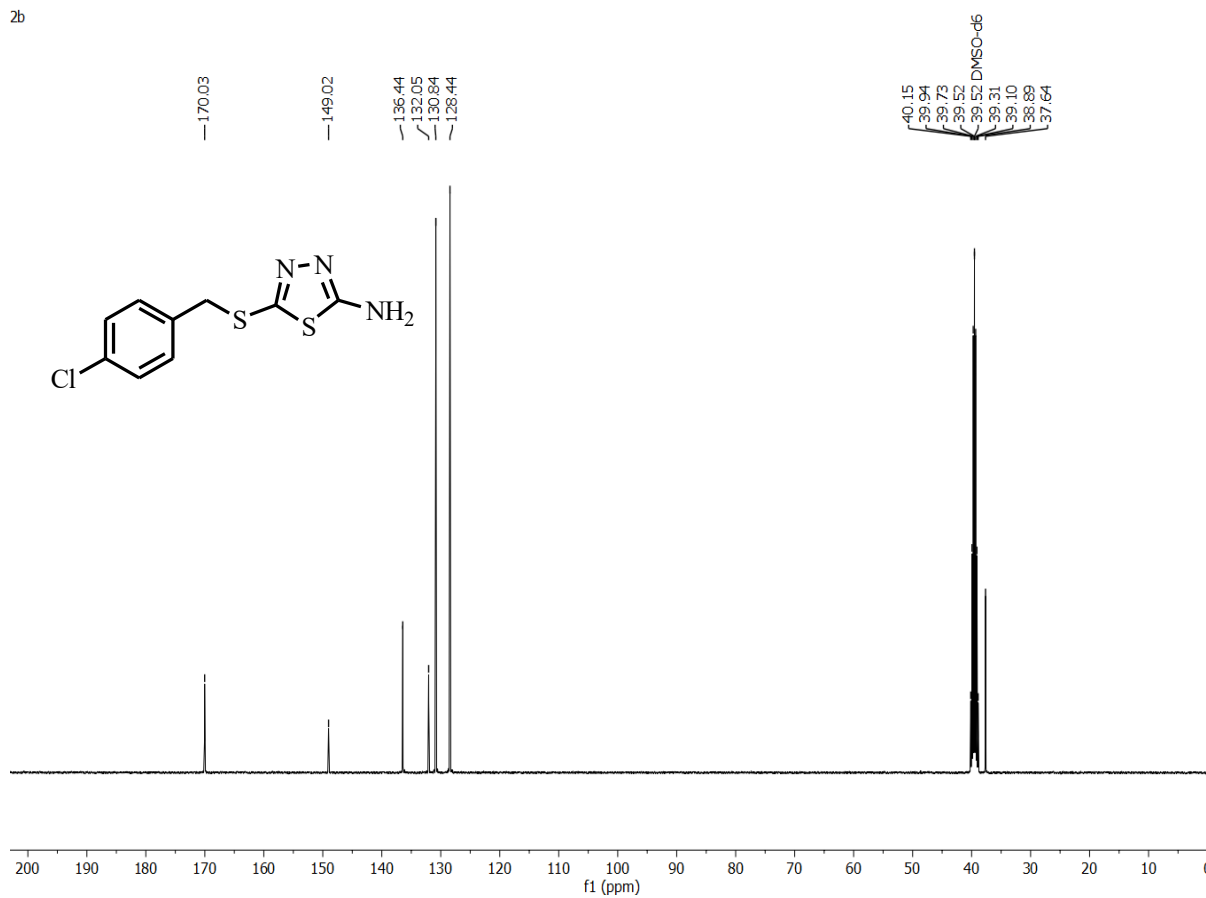
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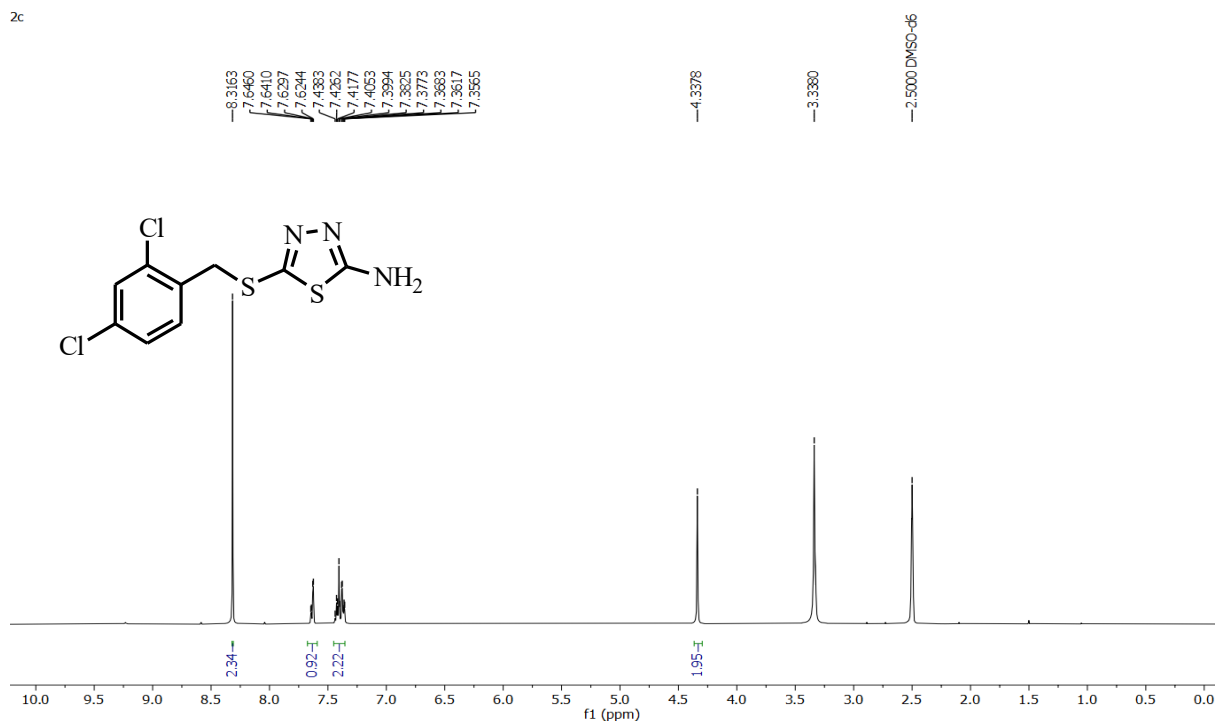
2b

S.F3': $^1\text{H NMR}$ of compound 2b

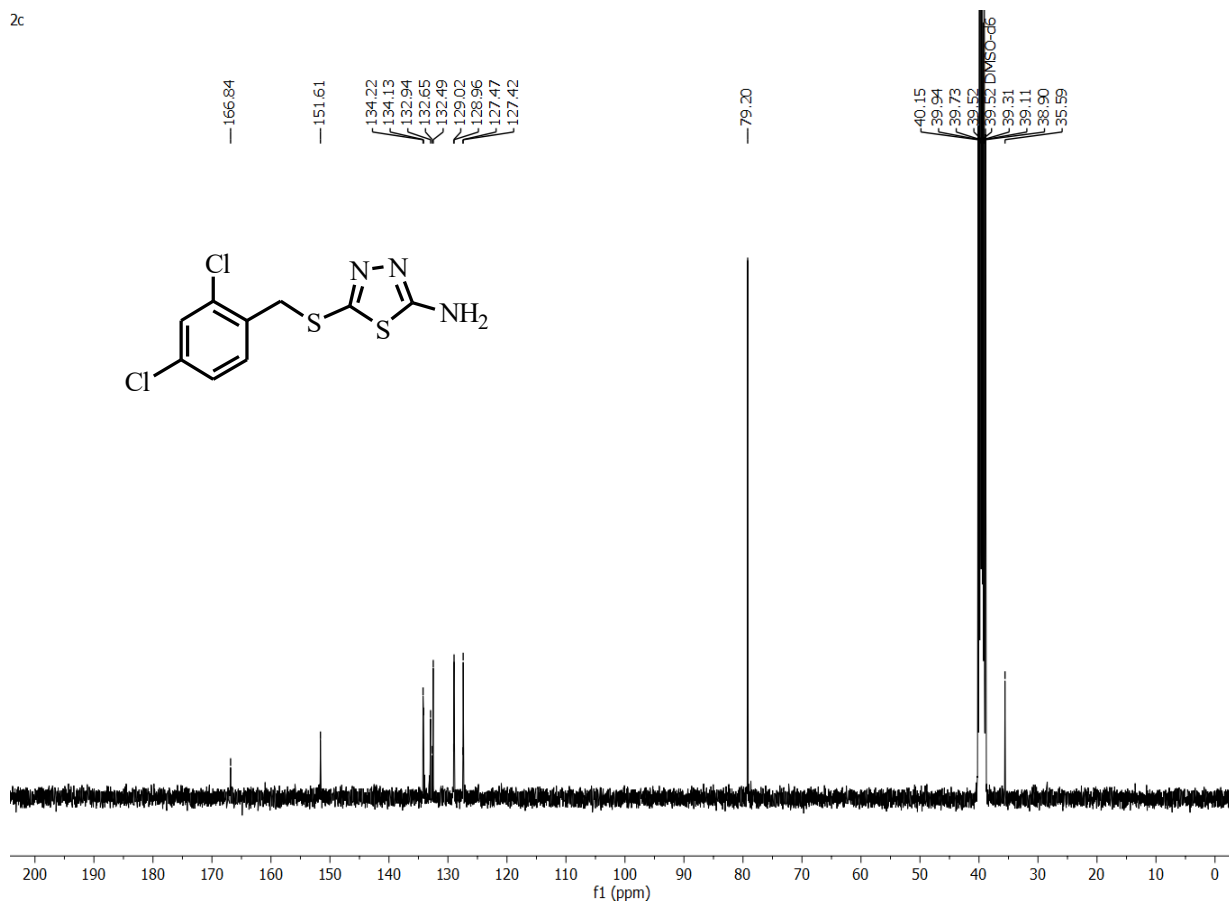
2b

S.F3'': $^{13}\text{C NMR}$ of compound 2b

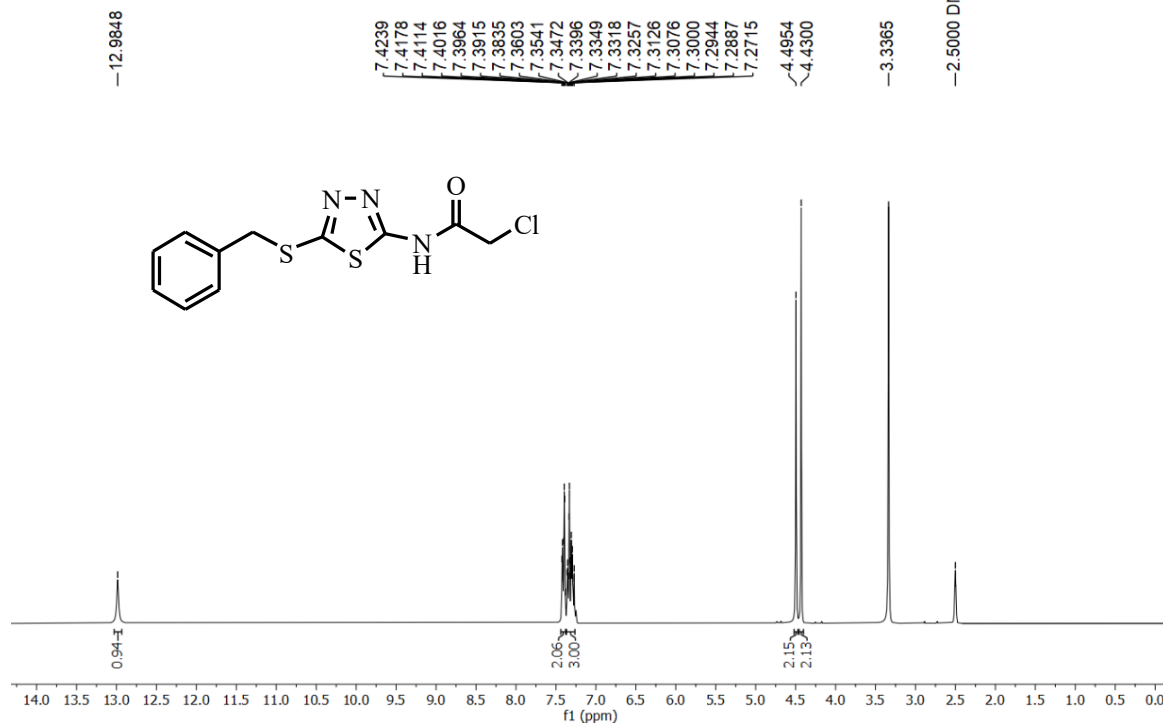
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S.F4': ¹H NMR of compound 2c

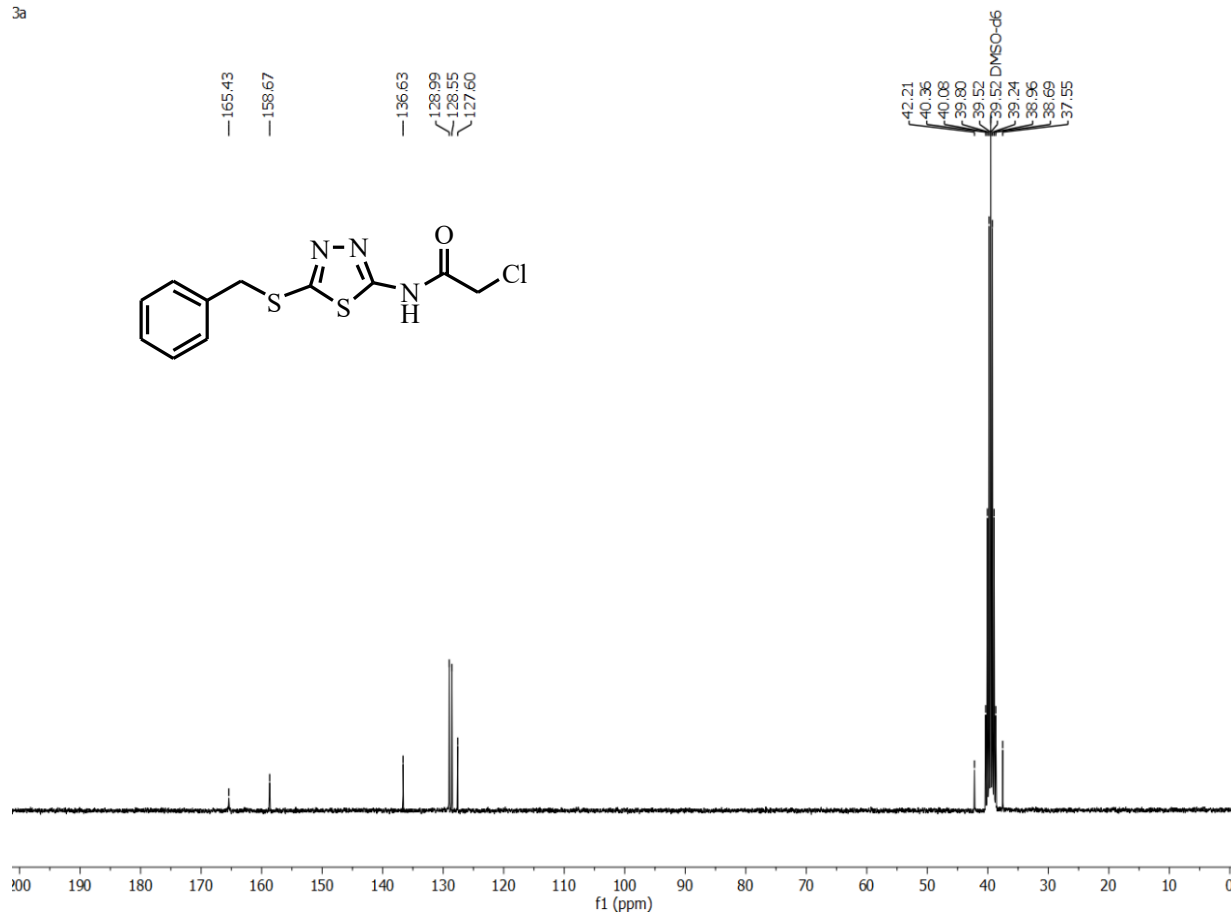
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S.F4'': ¹³C NMR of compound 2c

3a

S.F5': $^1\text{H NMR}$ of compound 3a

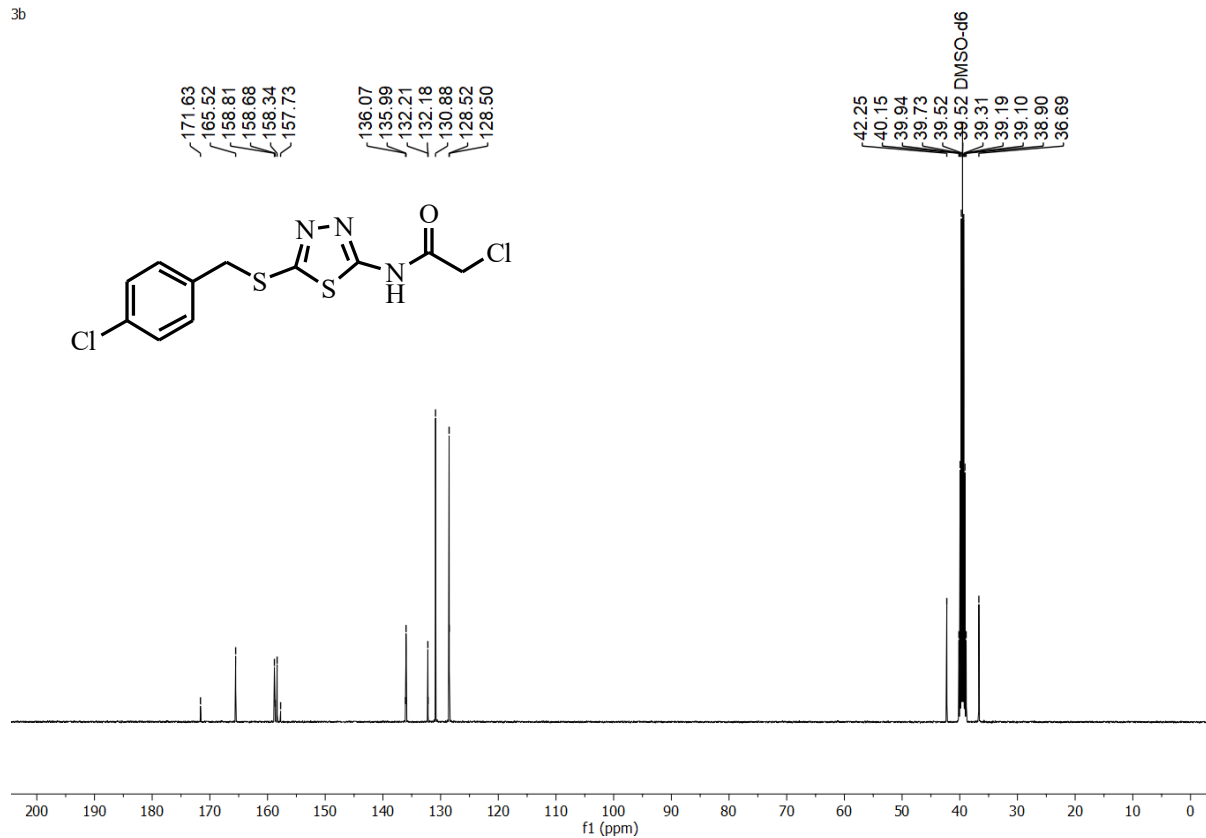
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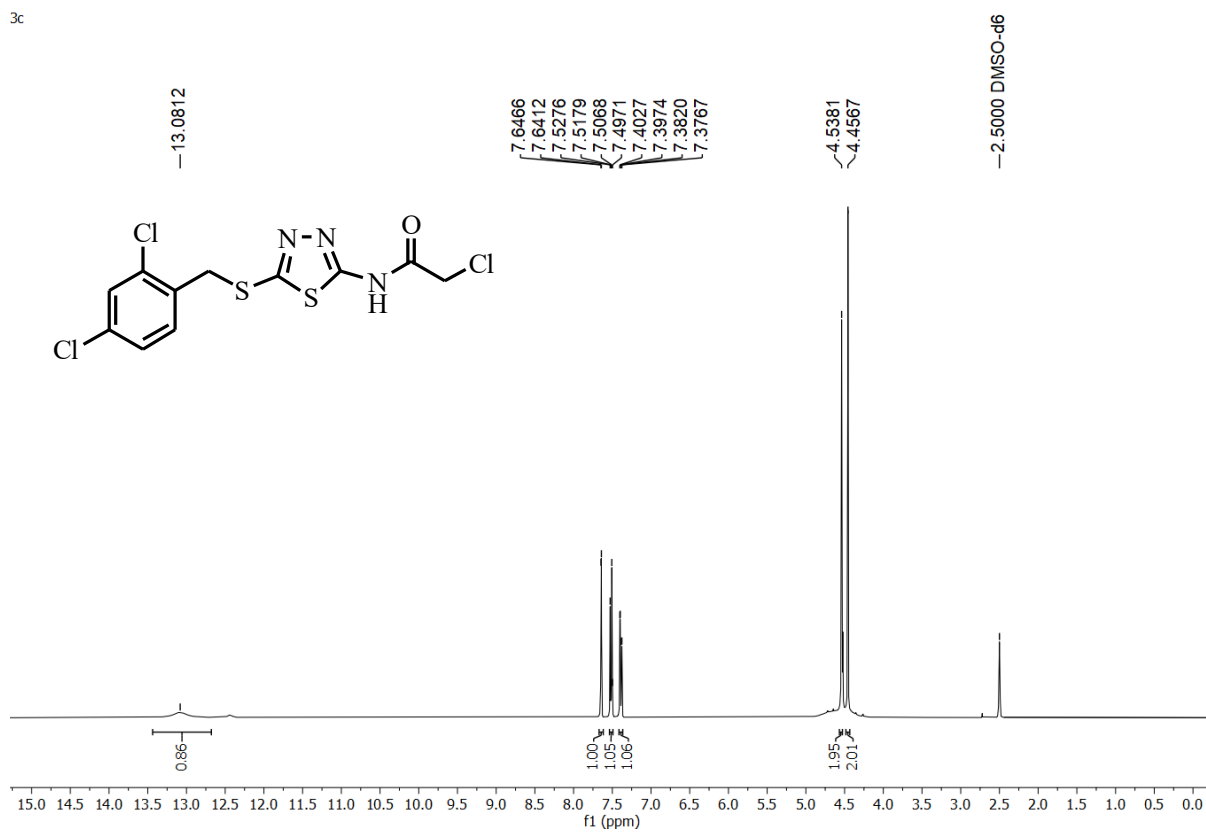
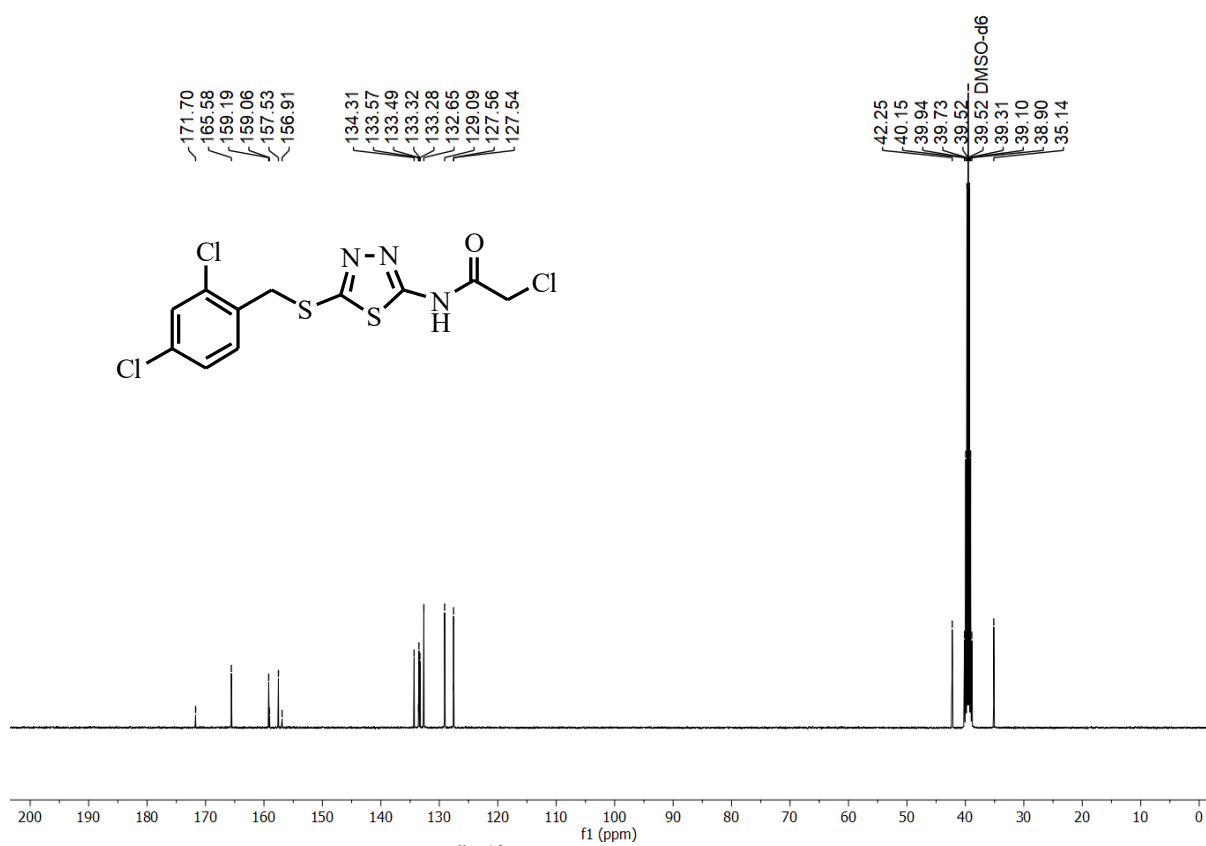
S.F5'': $^{13}\text{C NMR}$ of compound 3a

3b

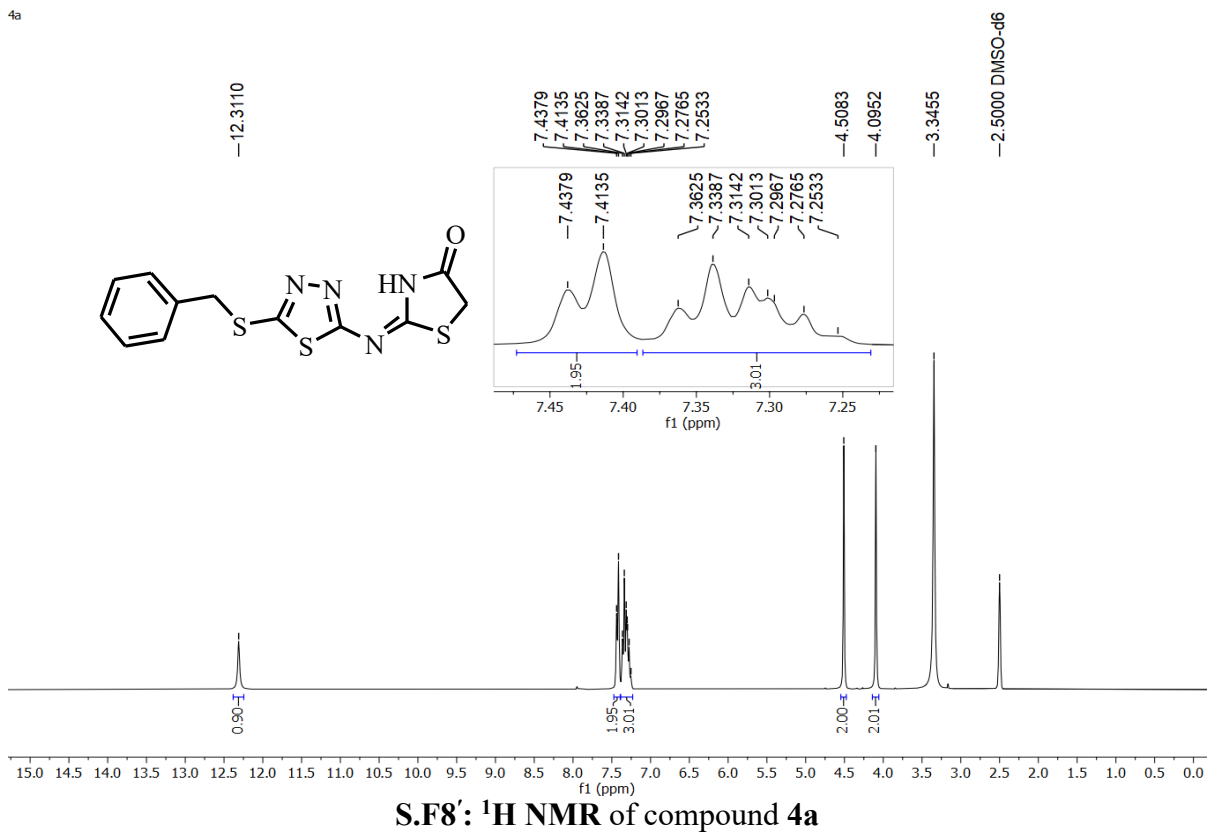
S.F6': $^1\text{H NMR}$ of compound 3b

3b

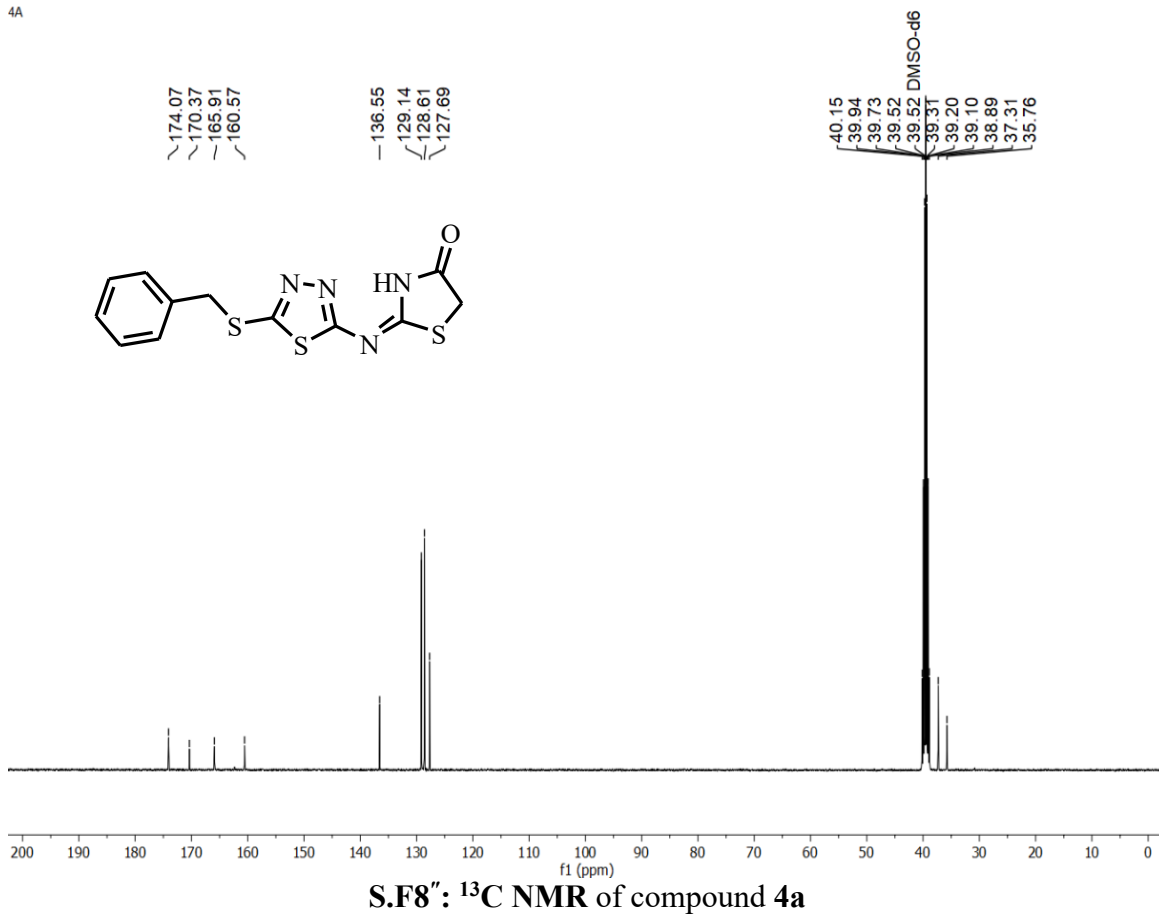
S.F6'': $^{13}\text{C NMR}$ of compound 3b

S.F7': $^1\text{H NMR}$ of compound 3cS.F7'': $^{13}\text{C NMR}$ of compound 3c

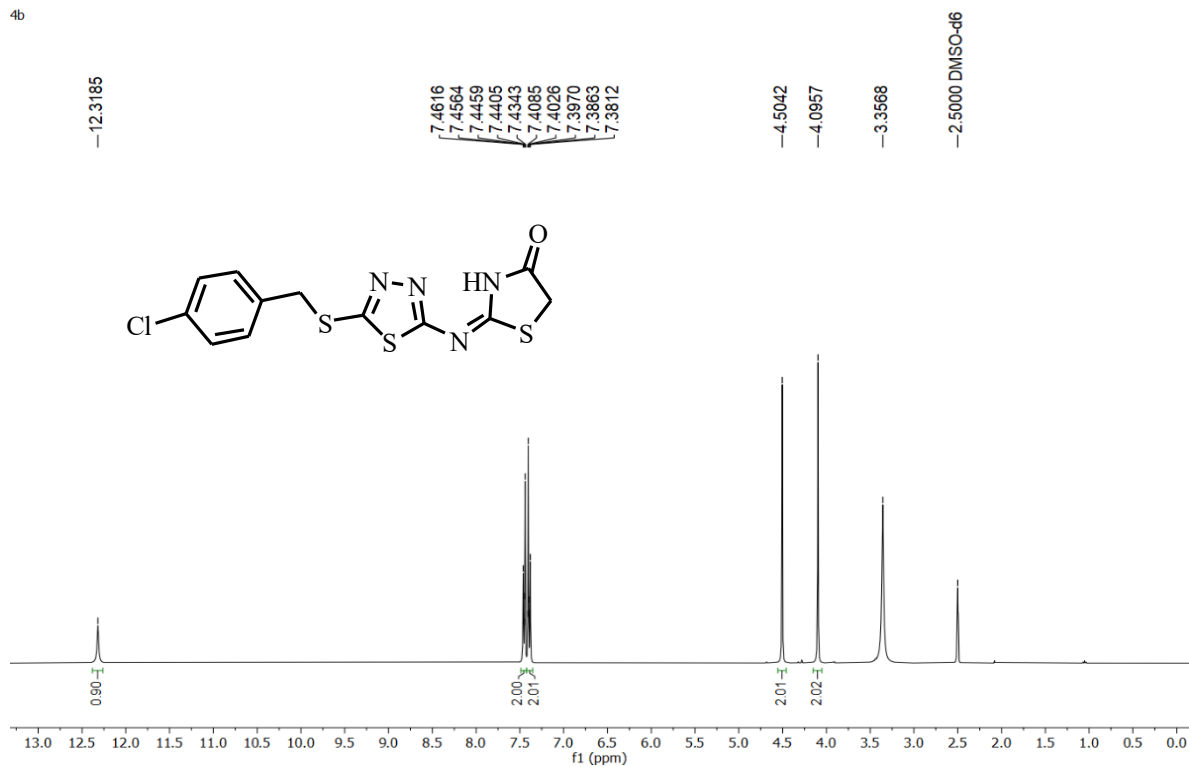
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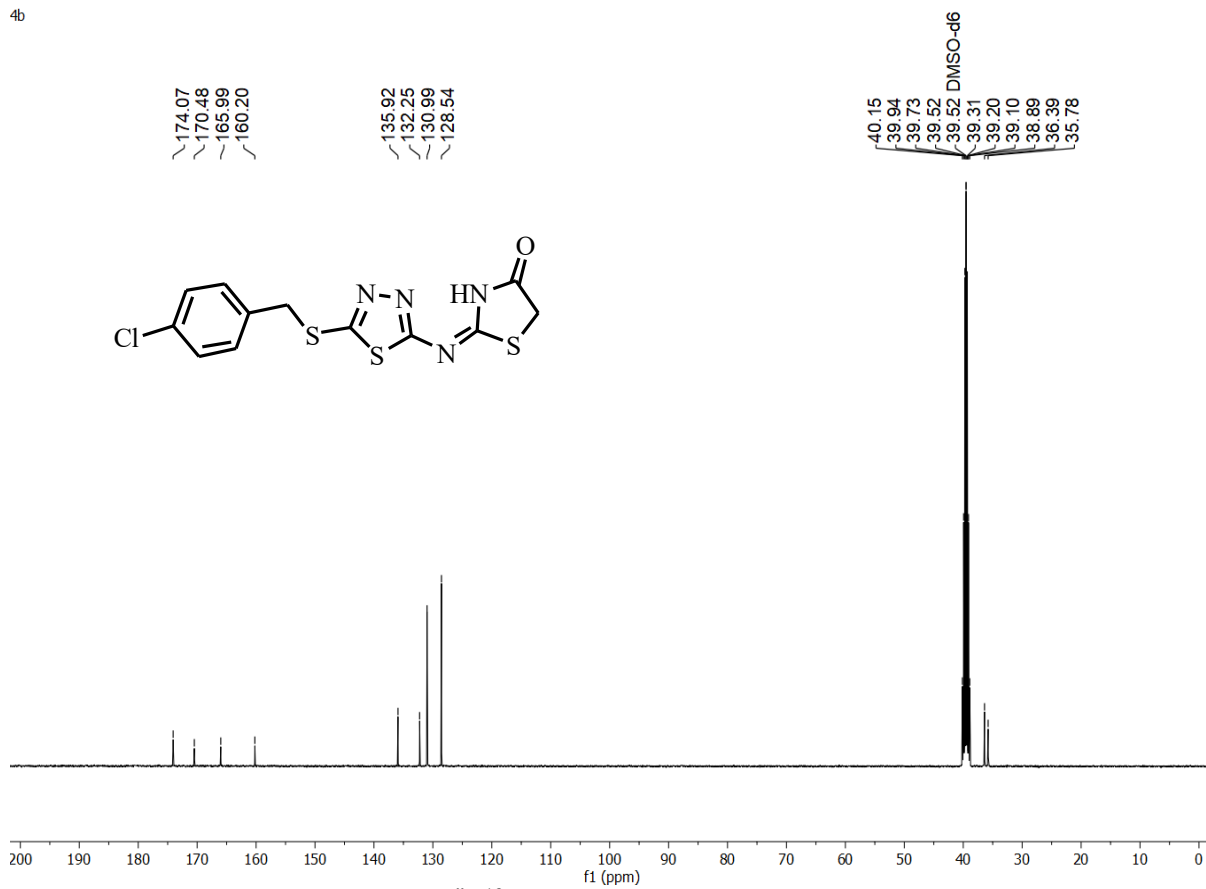
4A



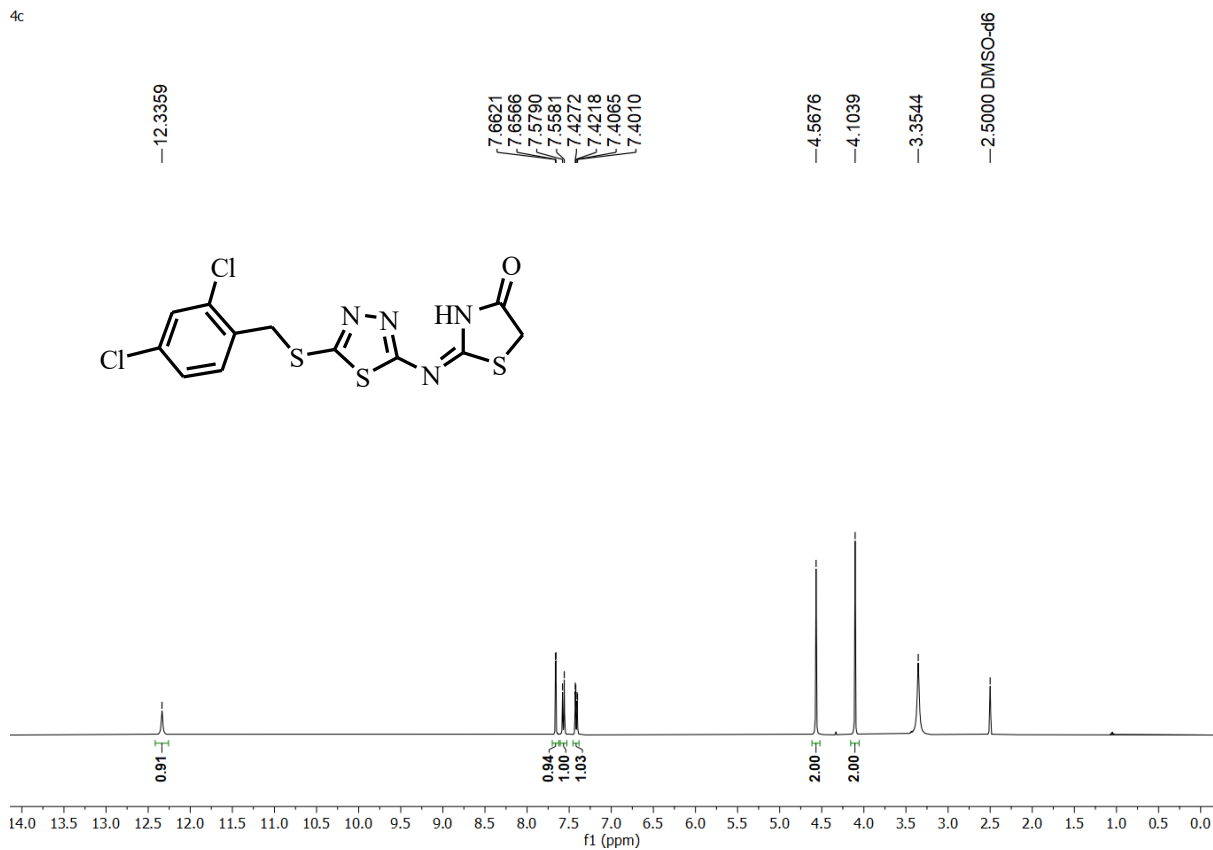
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S.F9': $^1\text{H NMR}$ of compound 4b

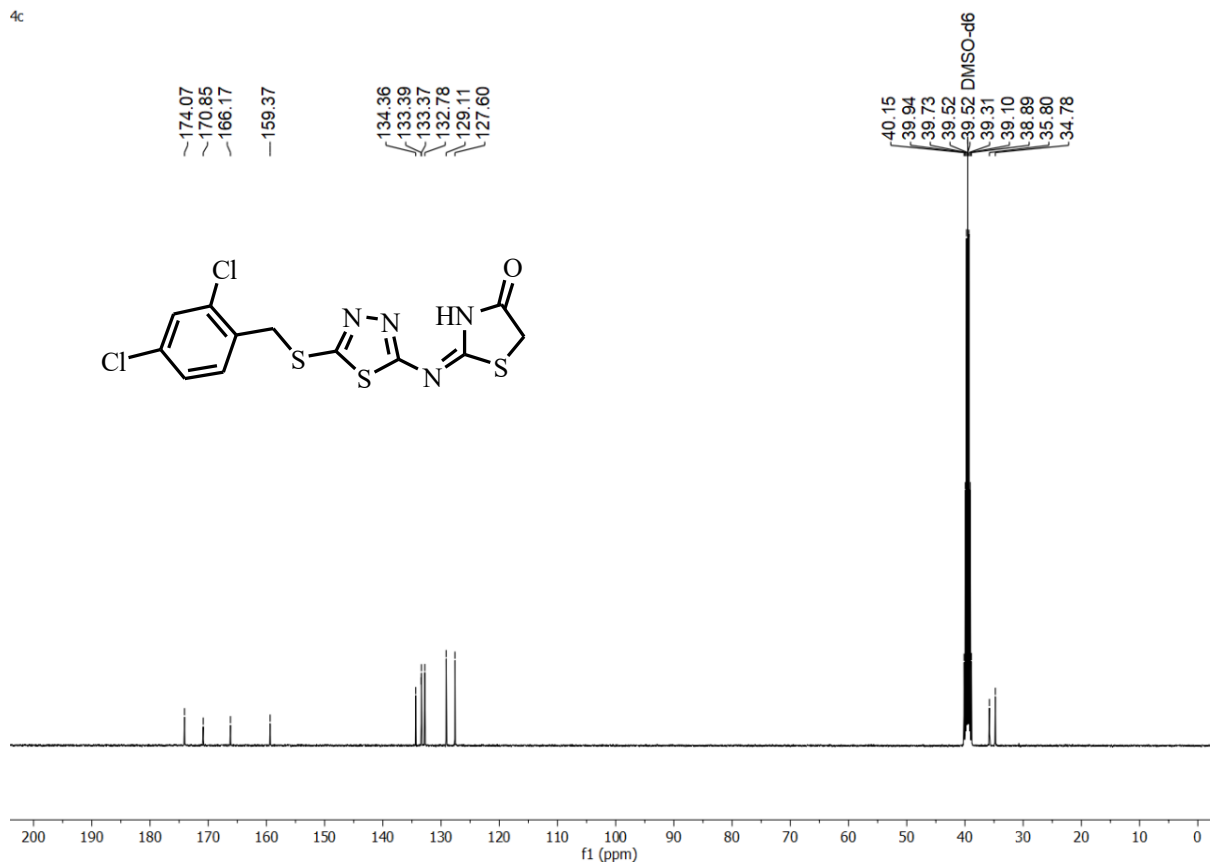
4b

S.F9'': $^{13}\text{C NMR}$ of compound 4b

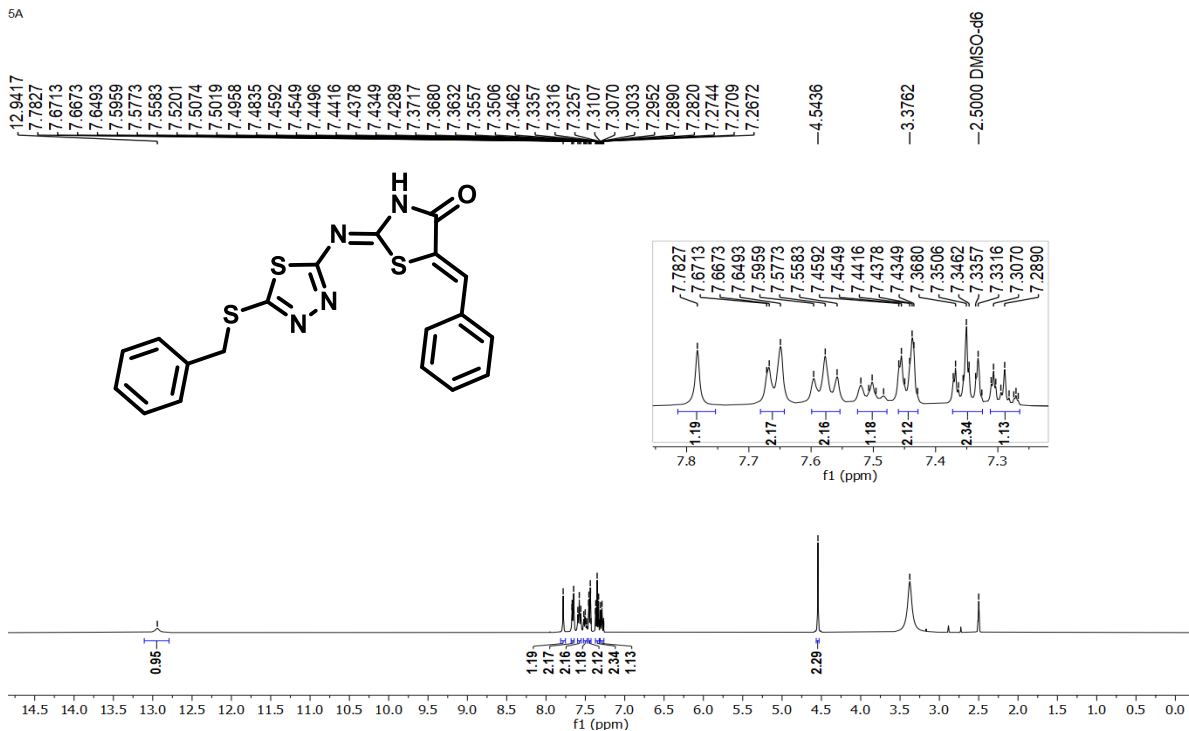
4c

S.F10': ¹H NMR of compound 4c

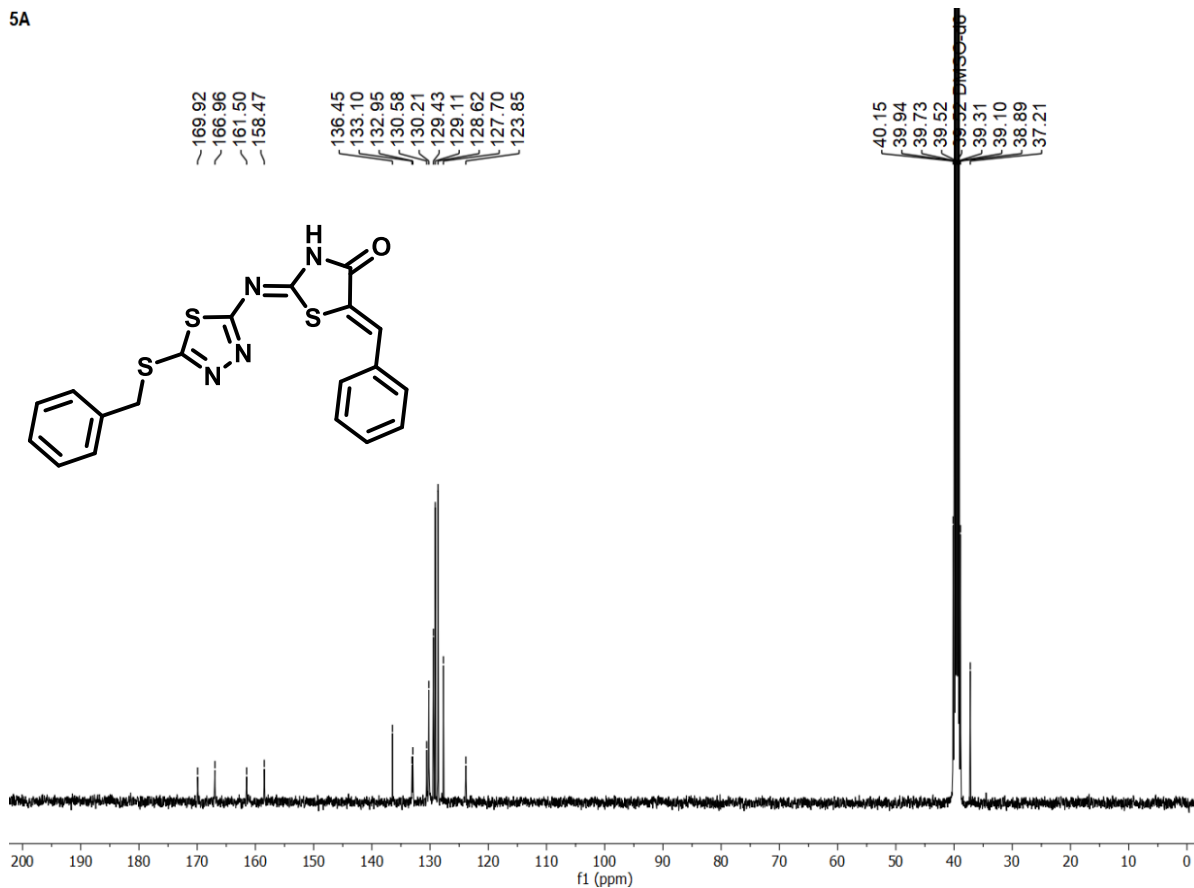
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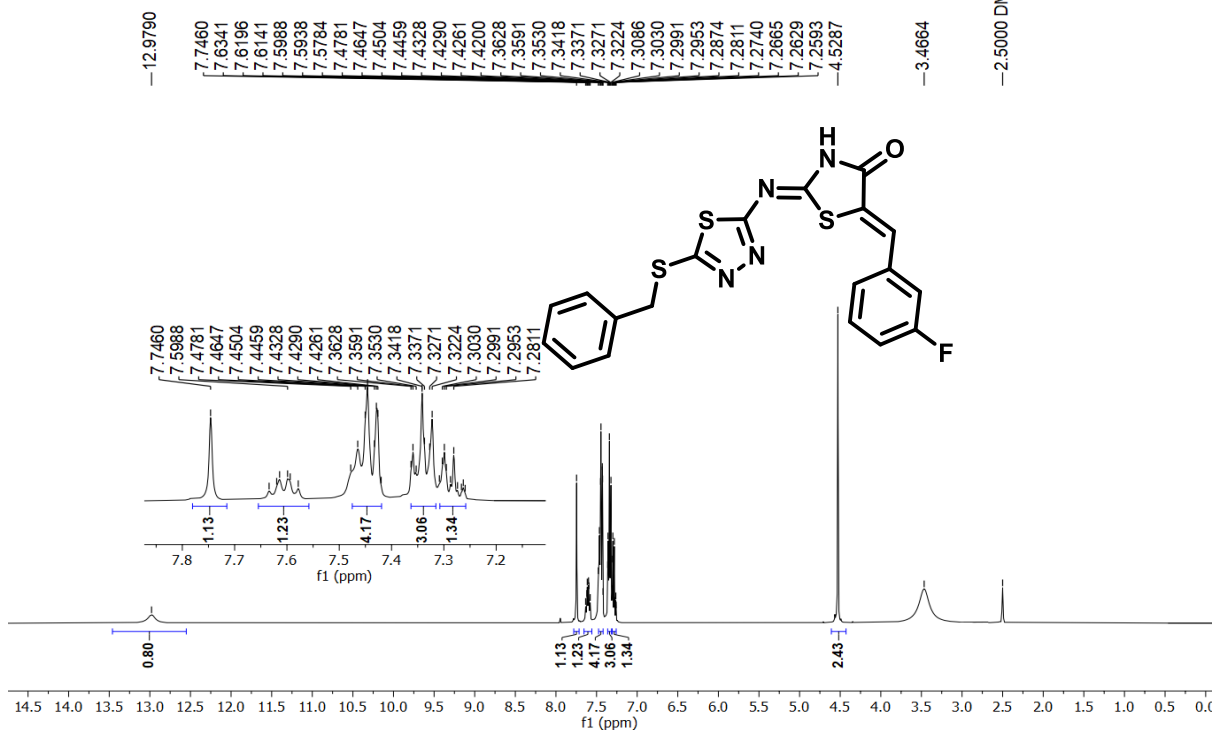
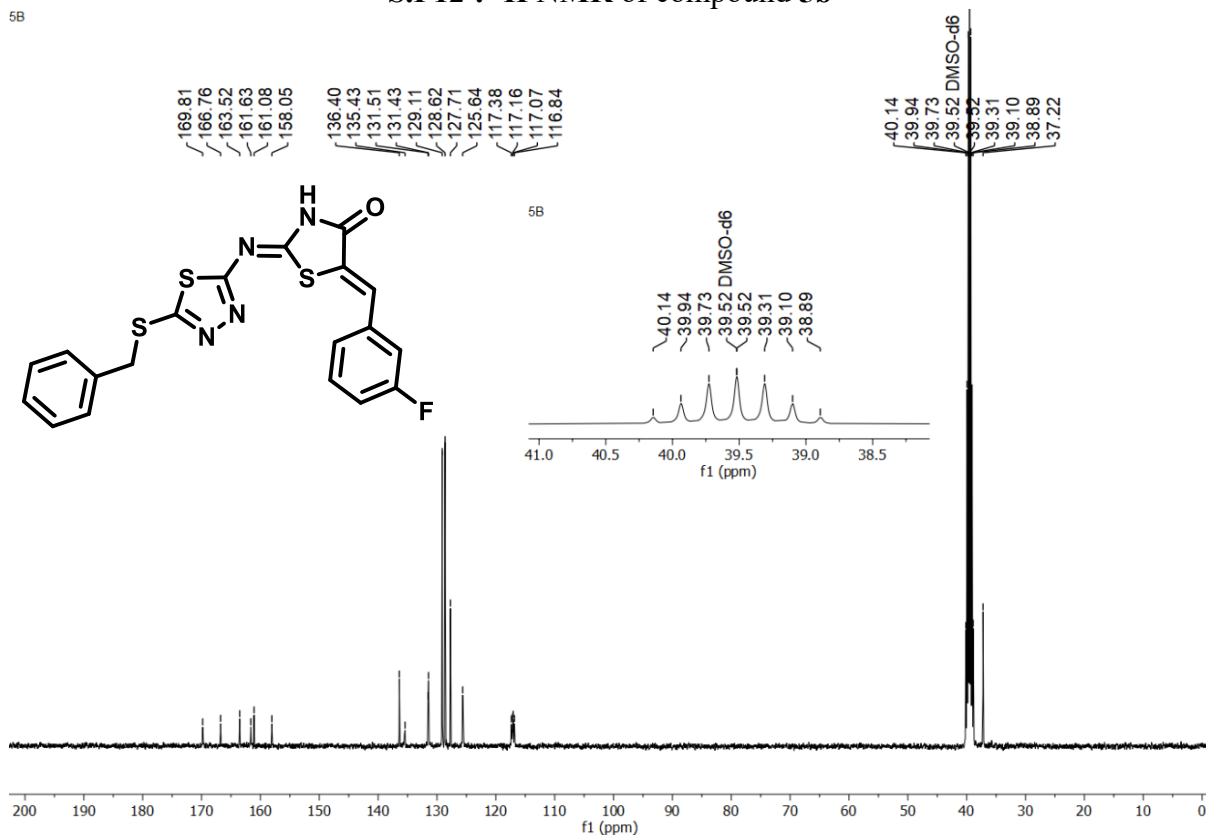
S.F10'': ¹³C NMR of compound 4c

5A

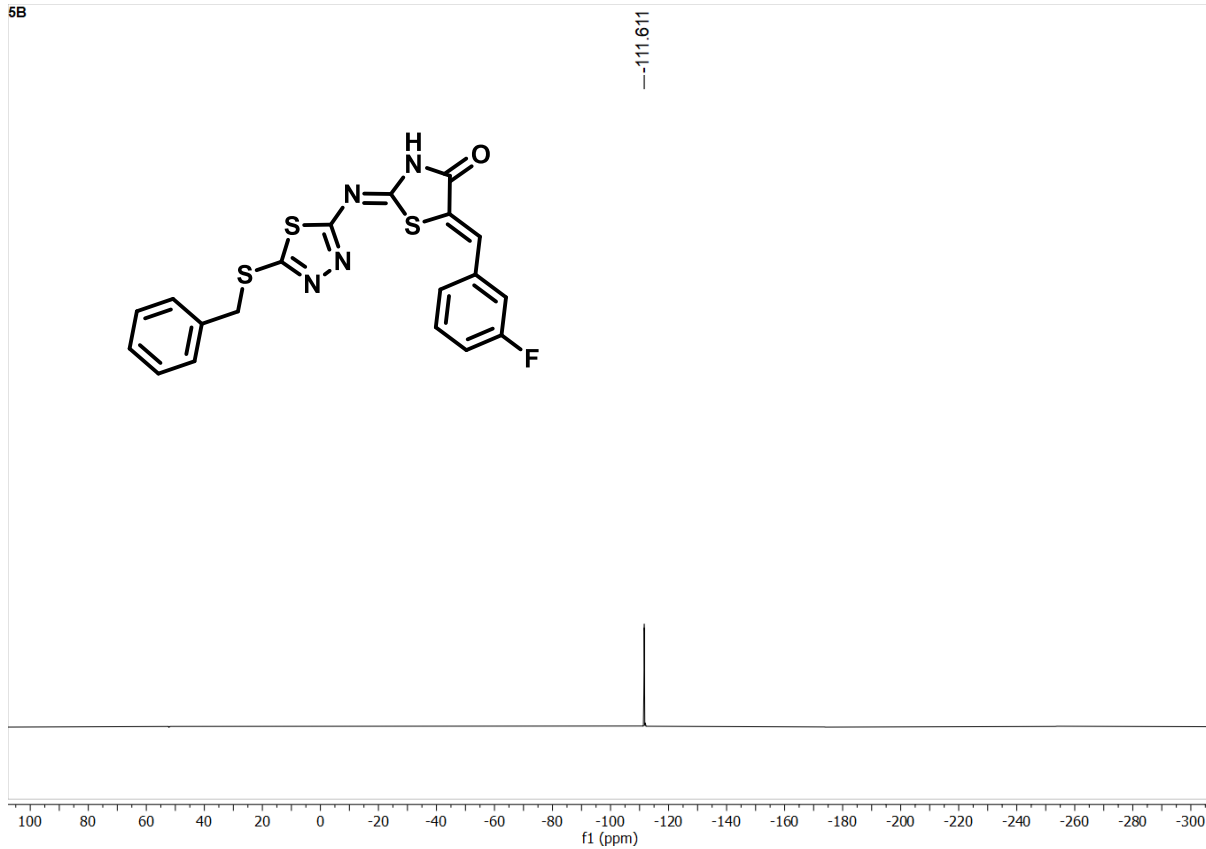
S.F11': $^1\text{H NMR}$ of compound 5a

5A

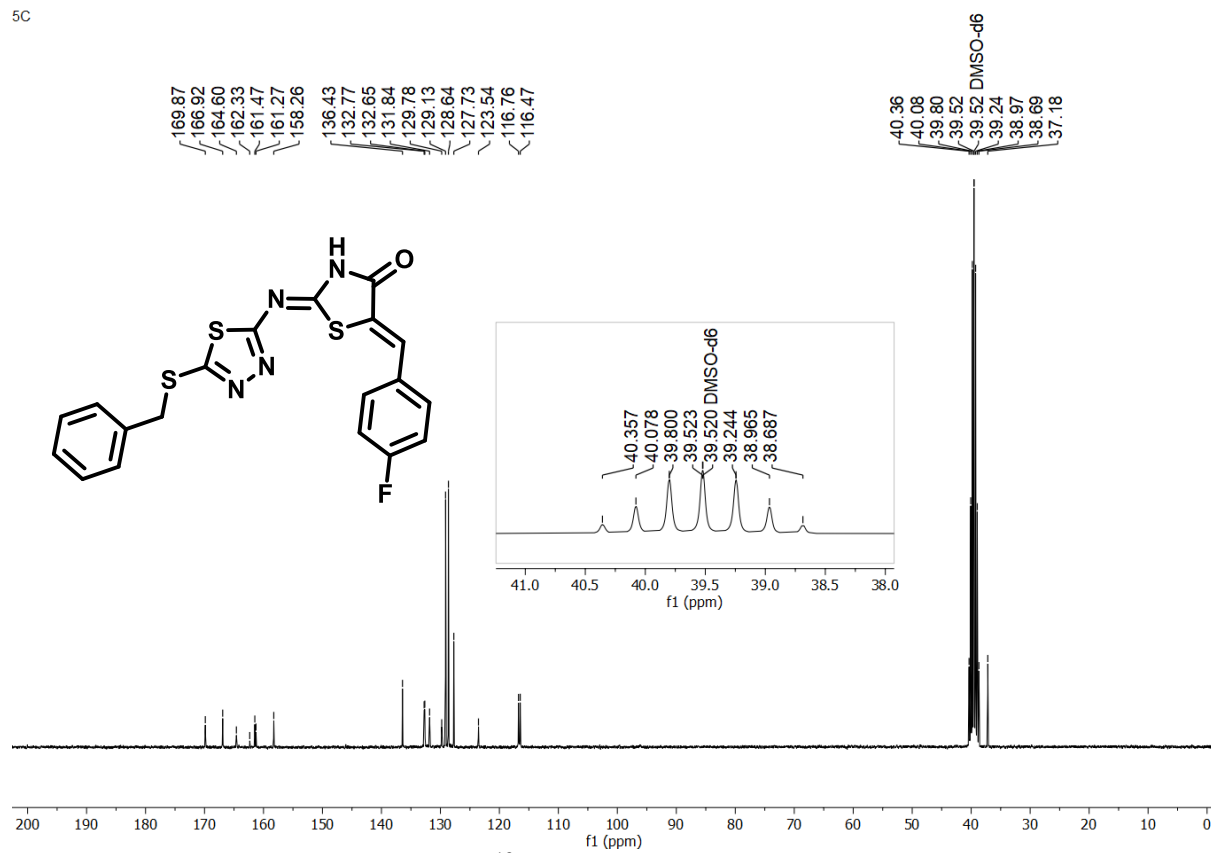
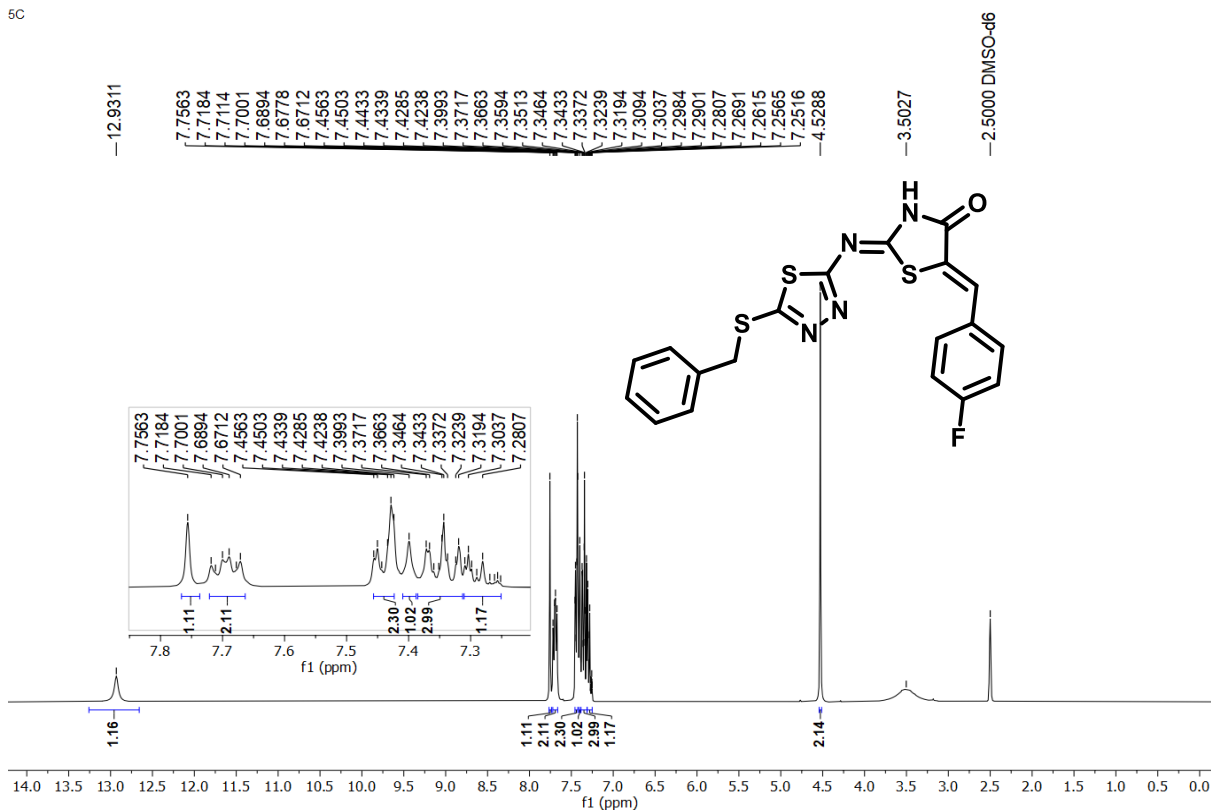
S.F11'': $^{13}\text{C NMR}$ of compound 5a

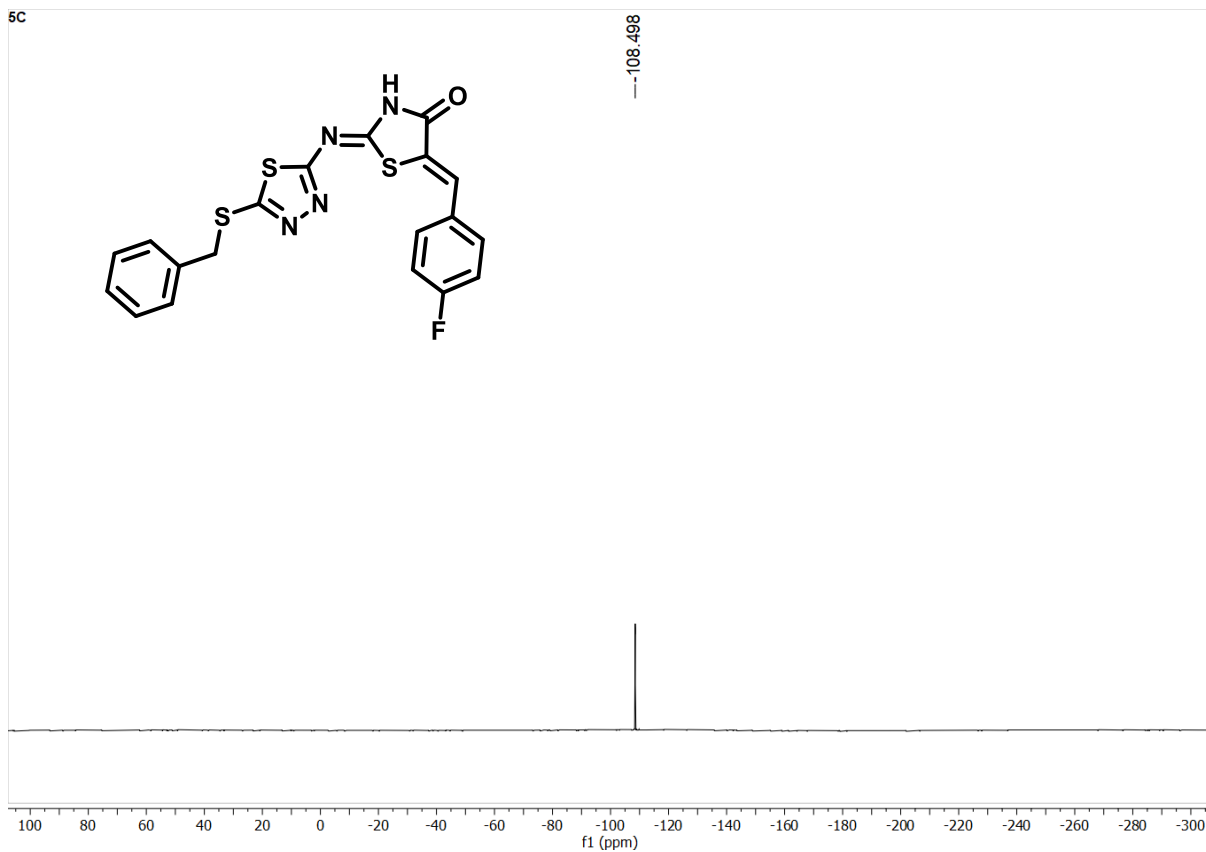
S.F12': ¹H NMR of compound 5bS.F12'': ¹³C NMR of compound 5b

5B

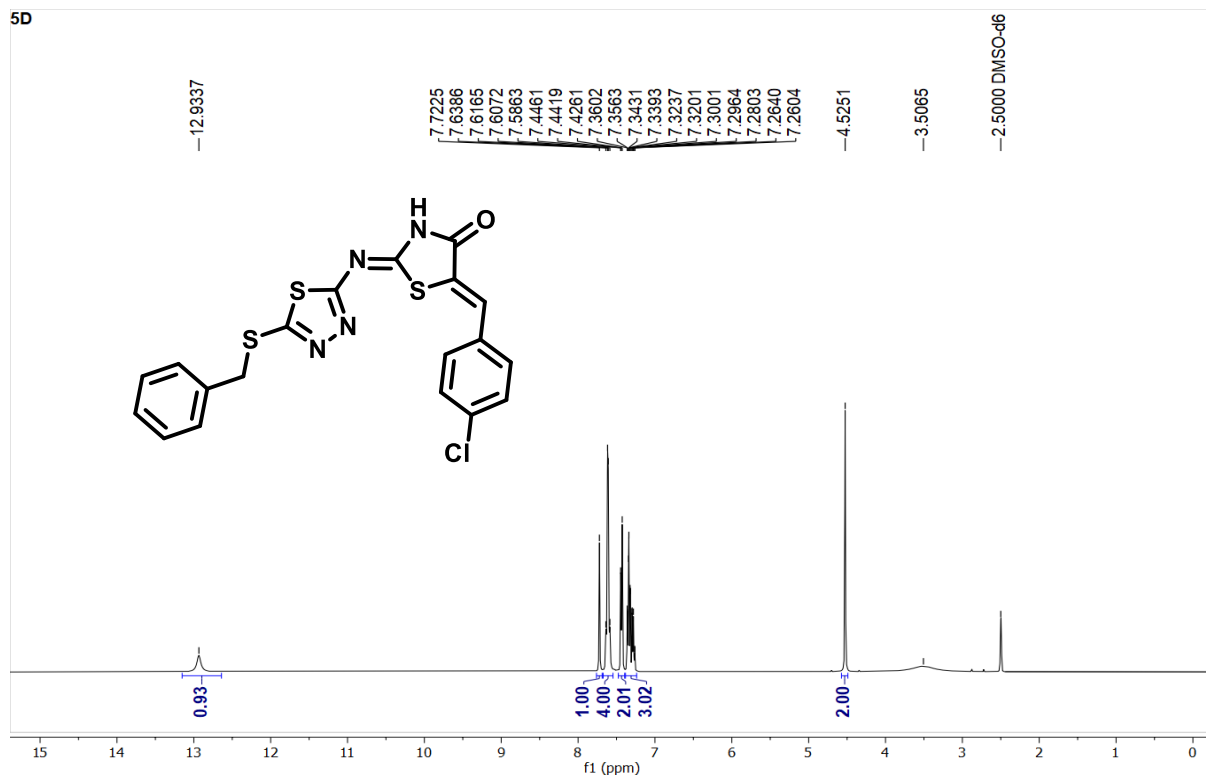


S.F12''': ^{19}F NMR of compound 5b

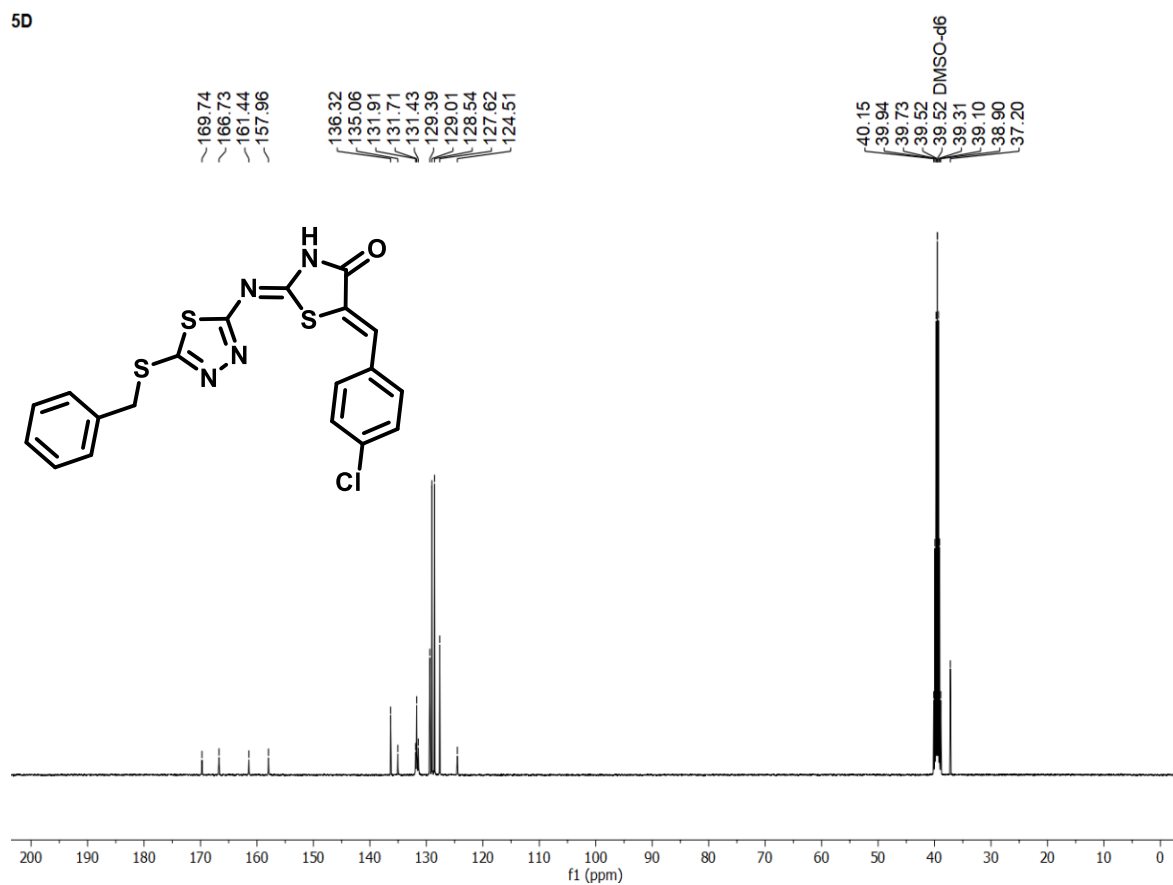




S.F13''': ^{19}F NMR of compound 5c

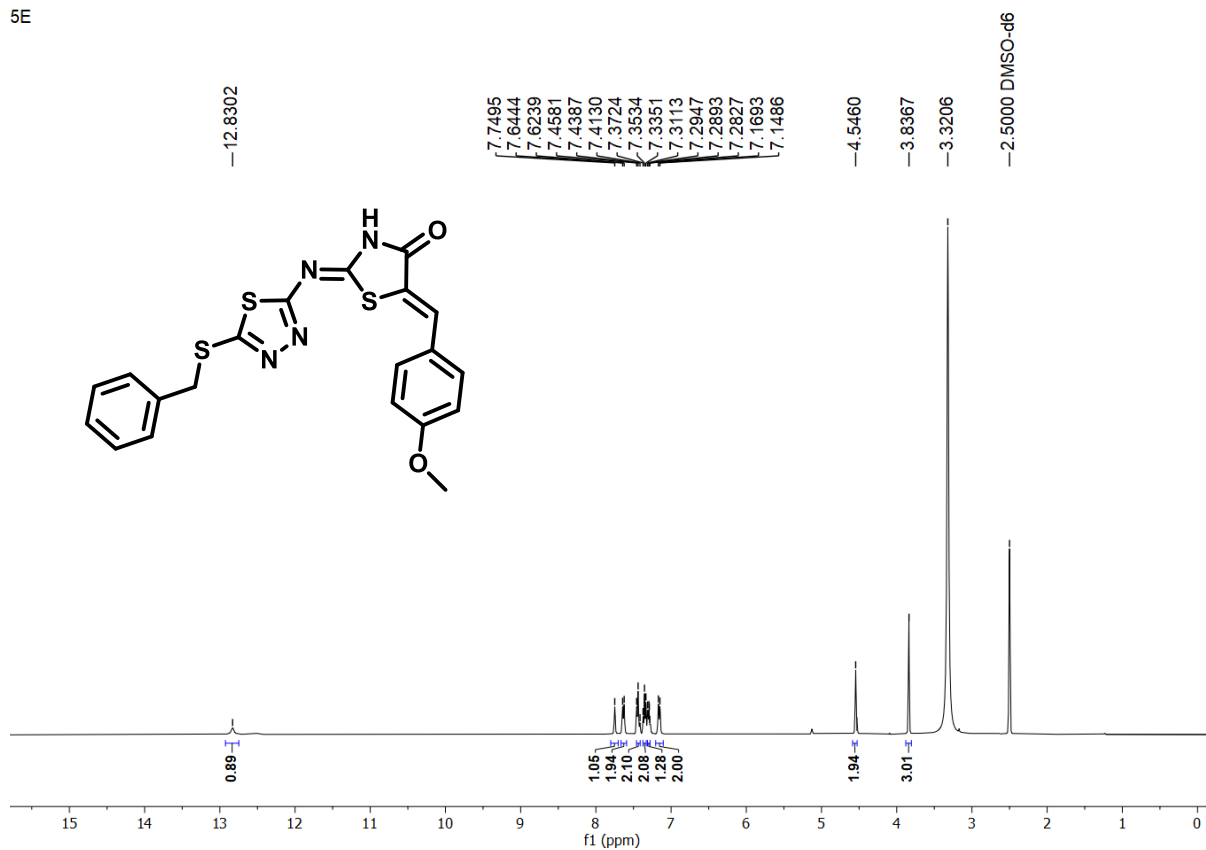


S.F14': ^1H NMR of compound 5d

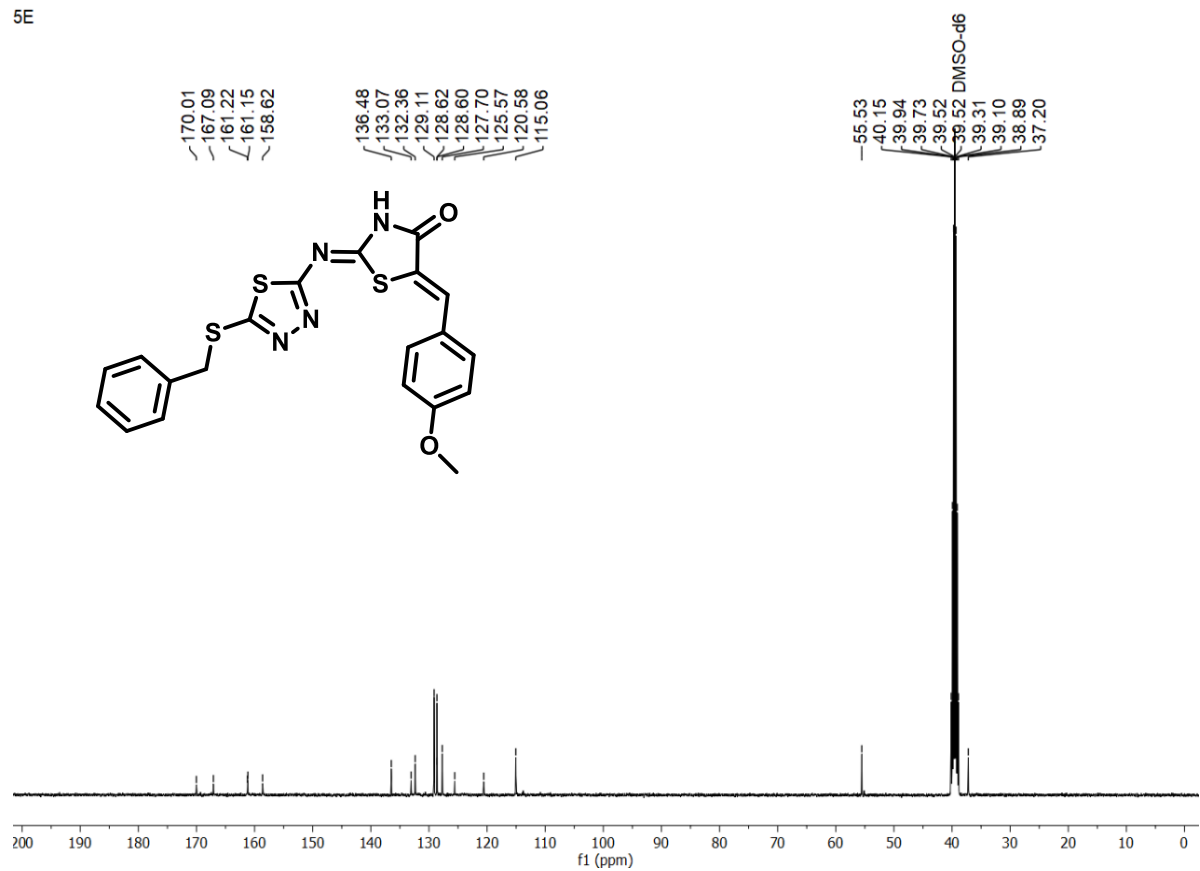


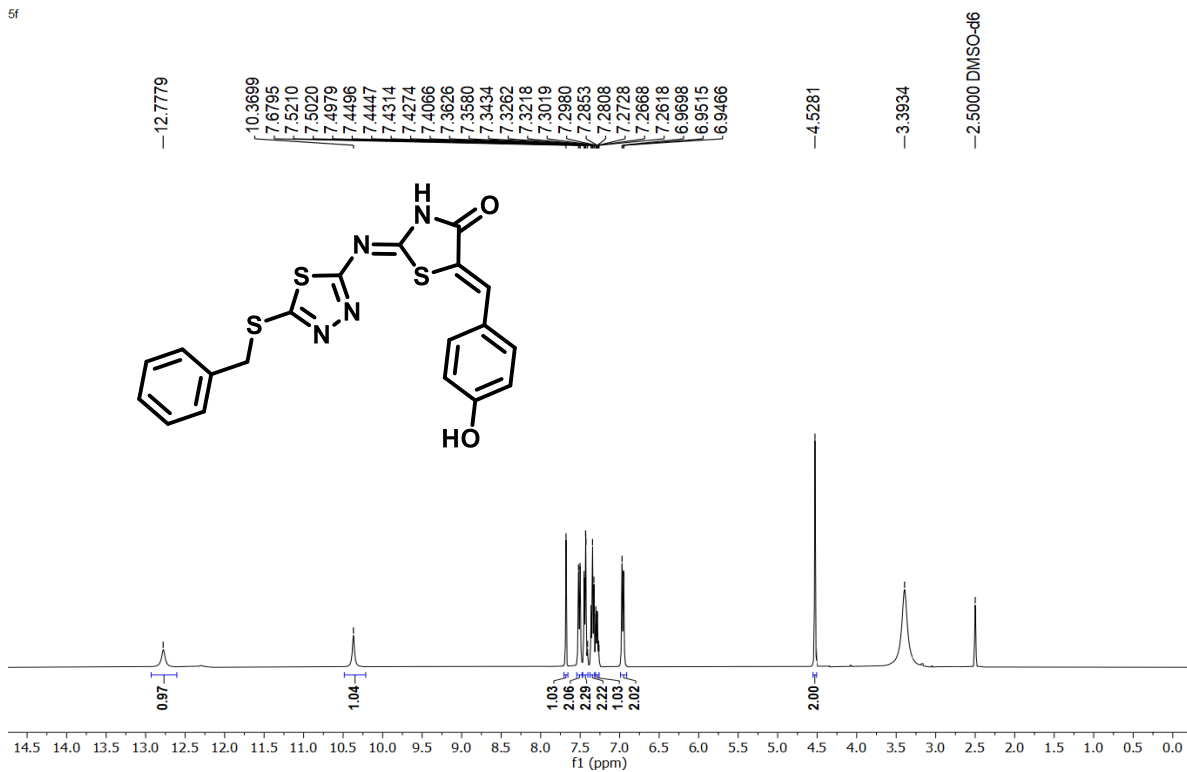
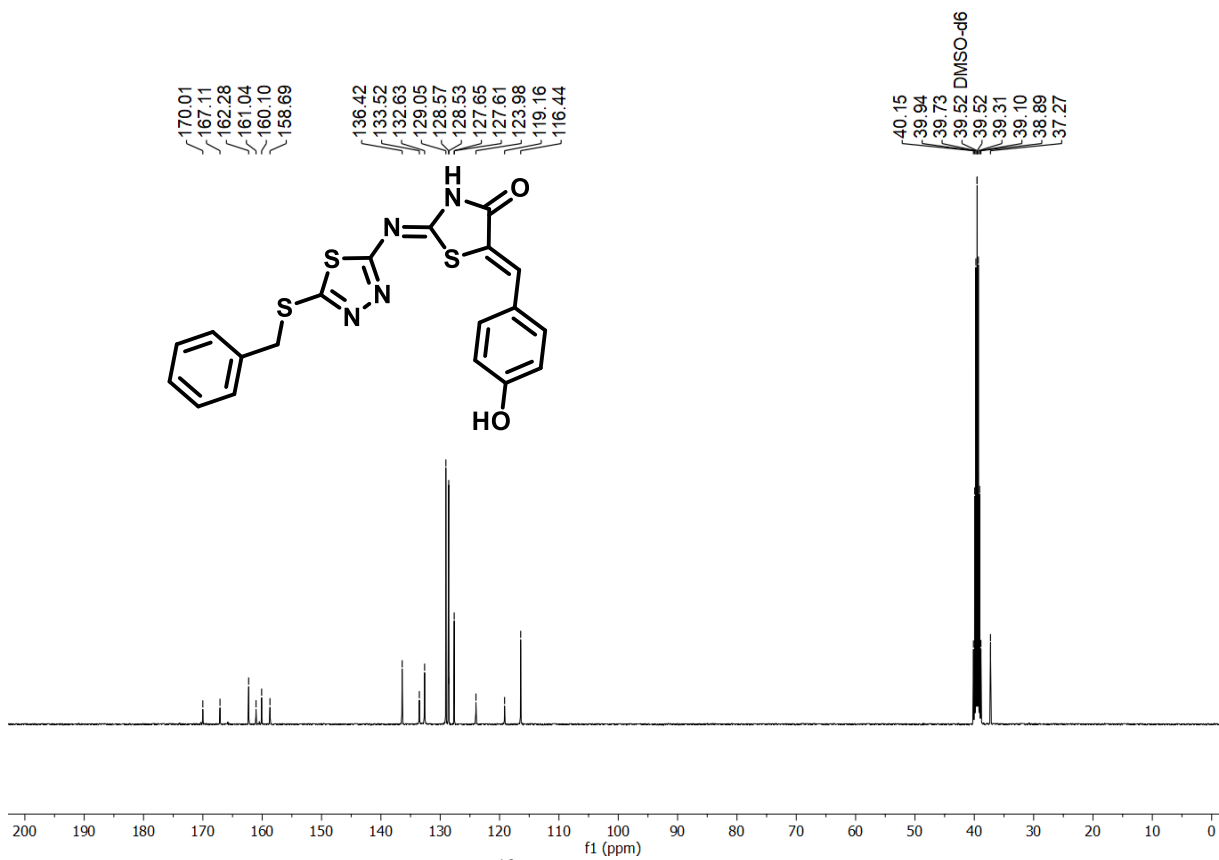
S.F14'': ^{13}C NMR of compound 5d

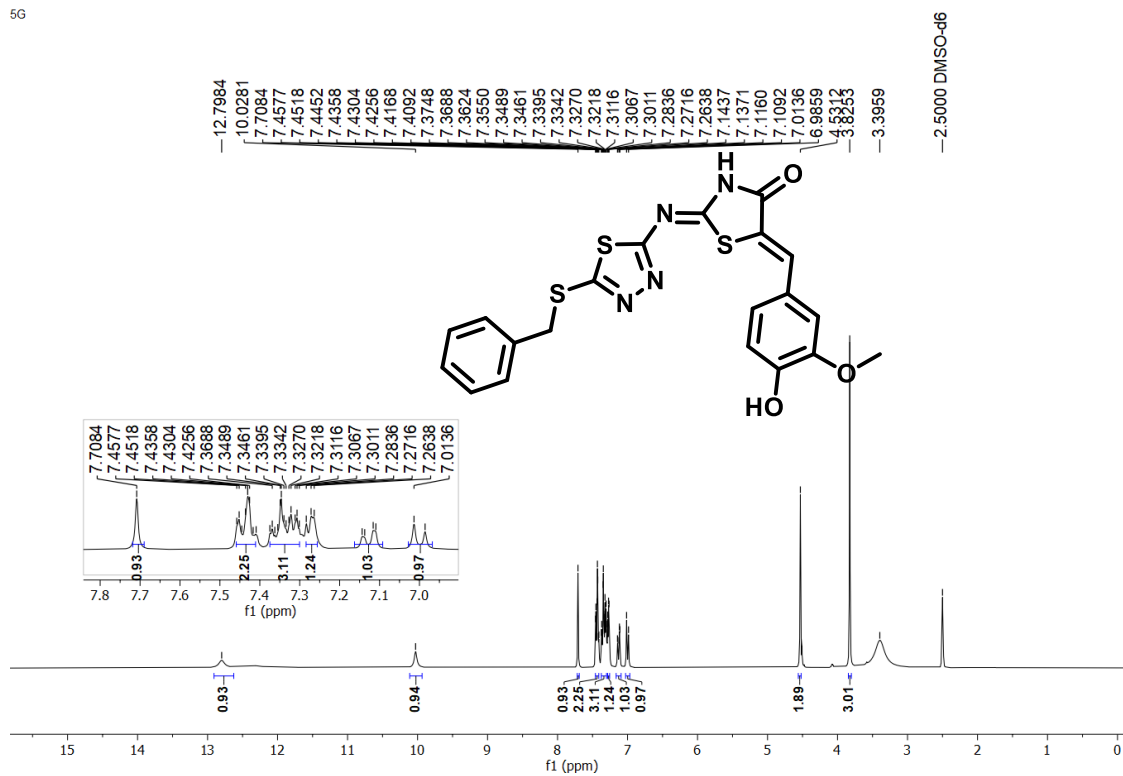
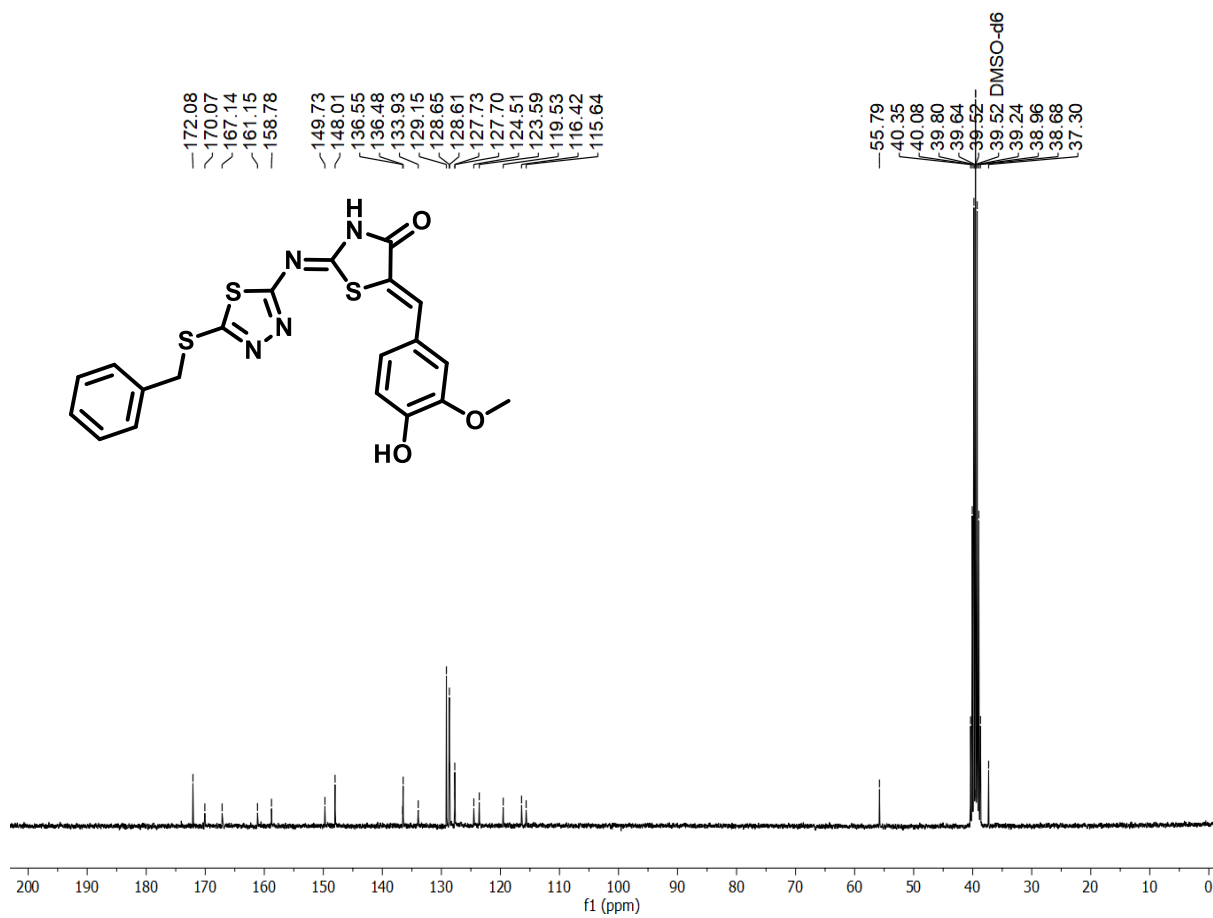
5E

S.F15': ^1H NMR of compound 5e

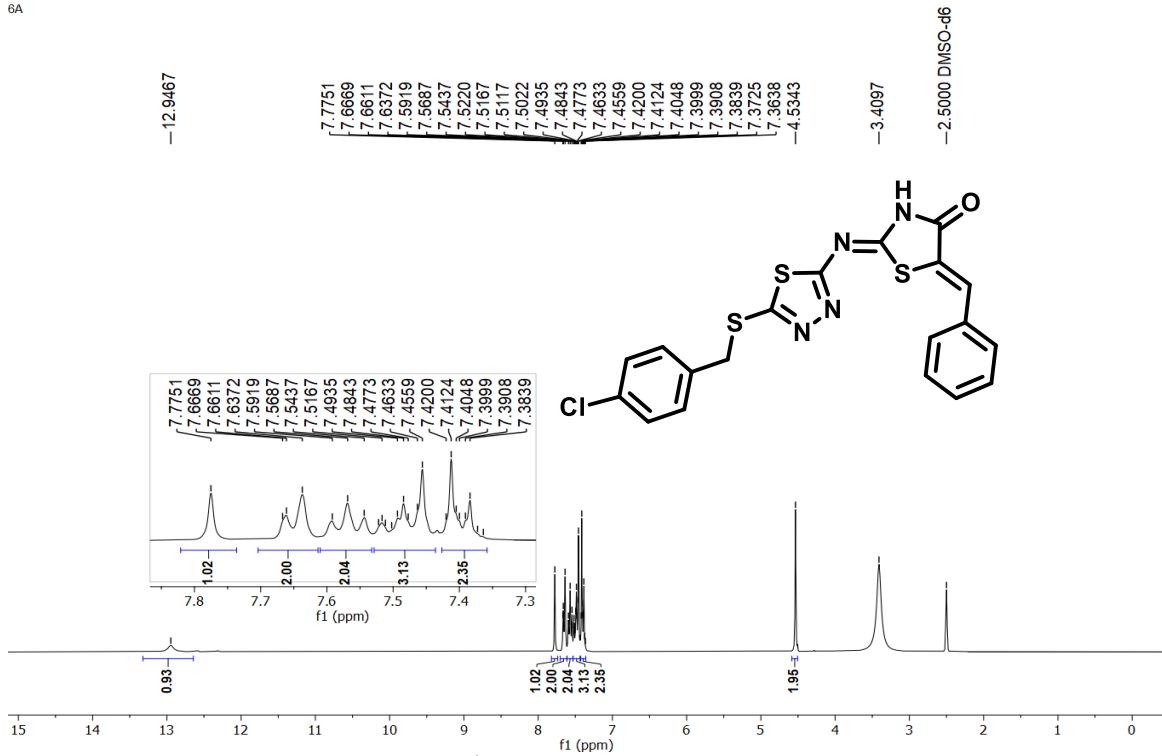
5E

S.F15'': ^{13}C NMR of compound 5e

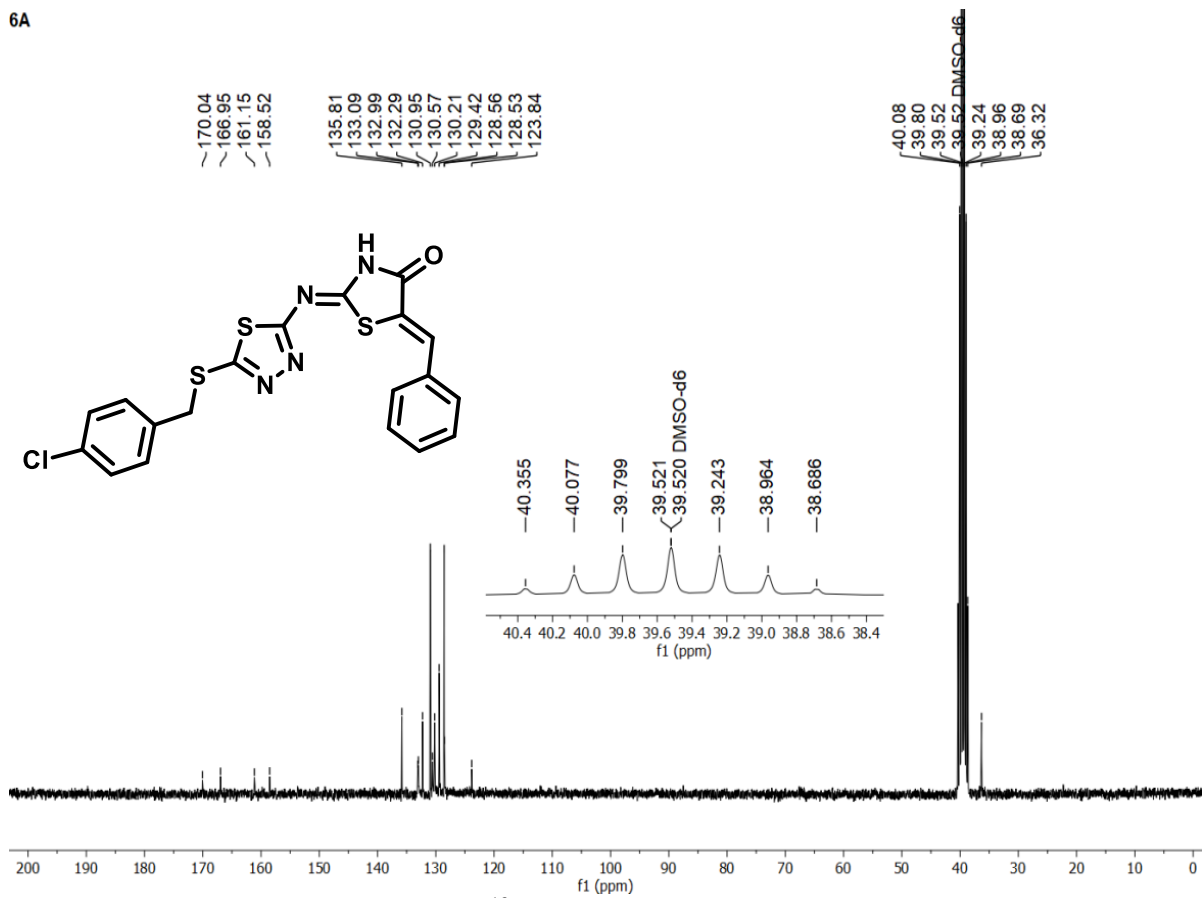
S.F16': $^1\text{H NMR}$ of compound 5fS.F16'': $^{13}\text{C NMR}$ of compound 5f

S.F17': $^1\text{H NMR}$ of compound 5gS.F17'': $^{13}\text{C NMR}$ of compound 5g

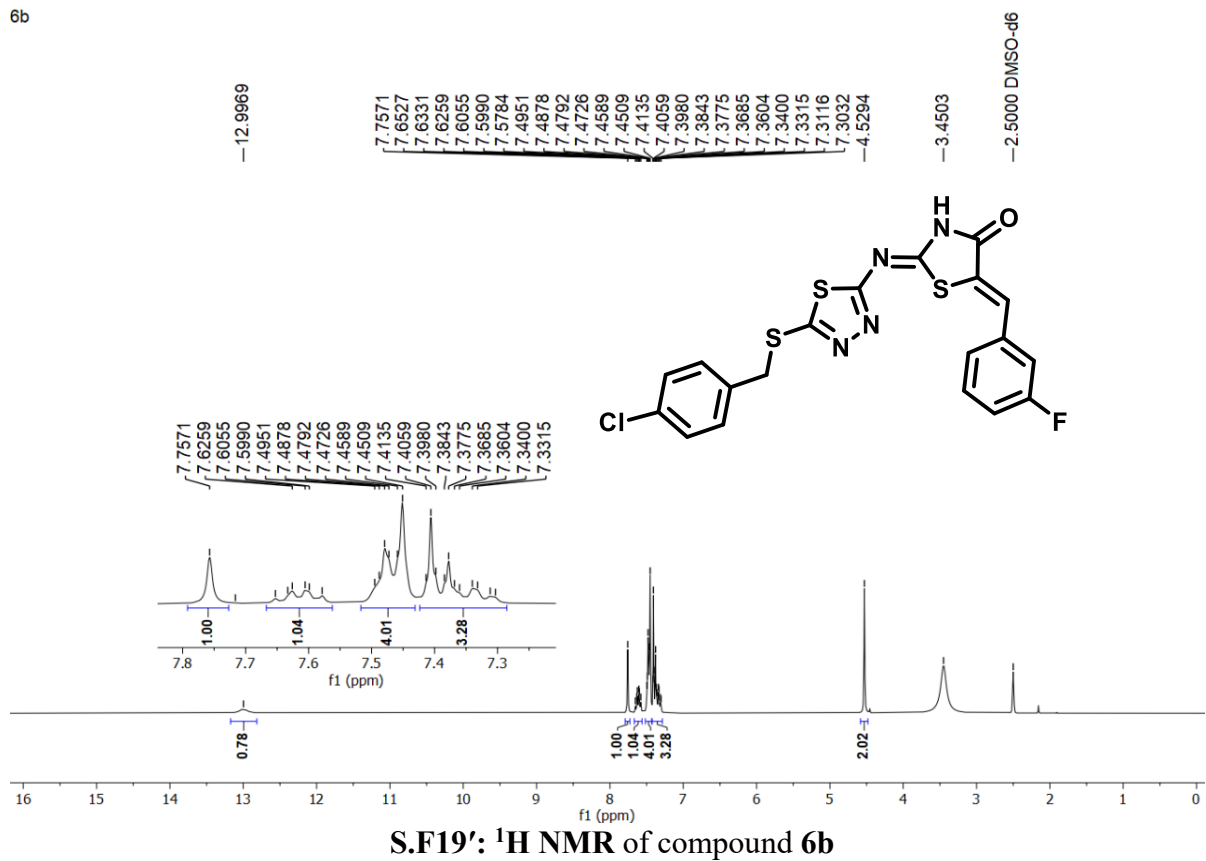
6A

S.F18': ¹H NMR of compound 6a

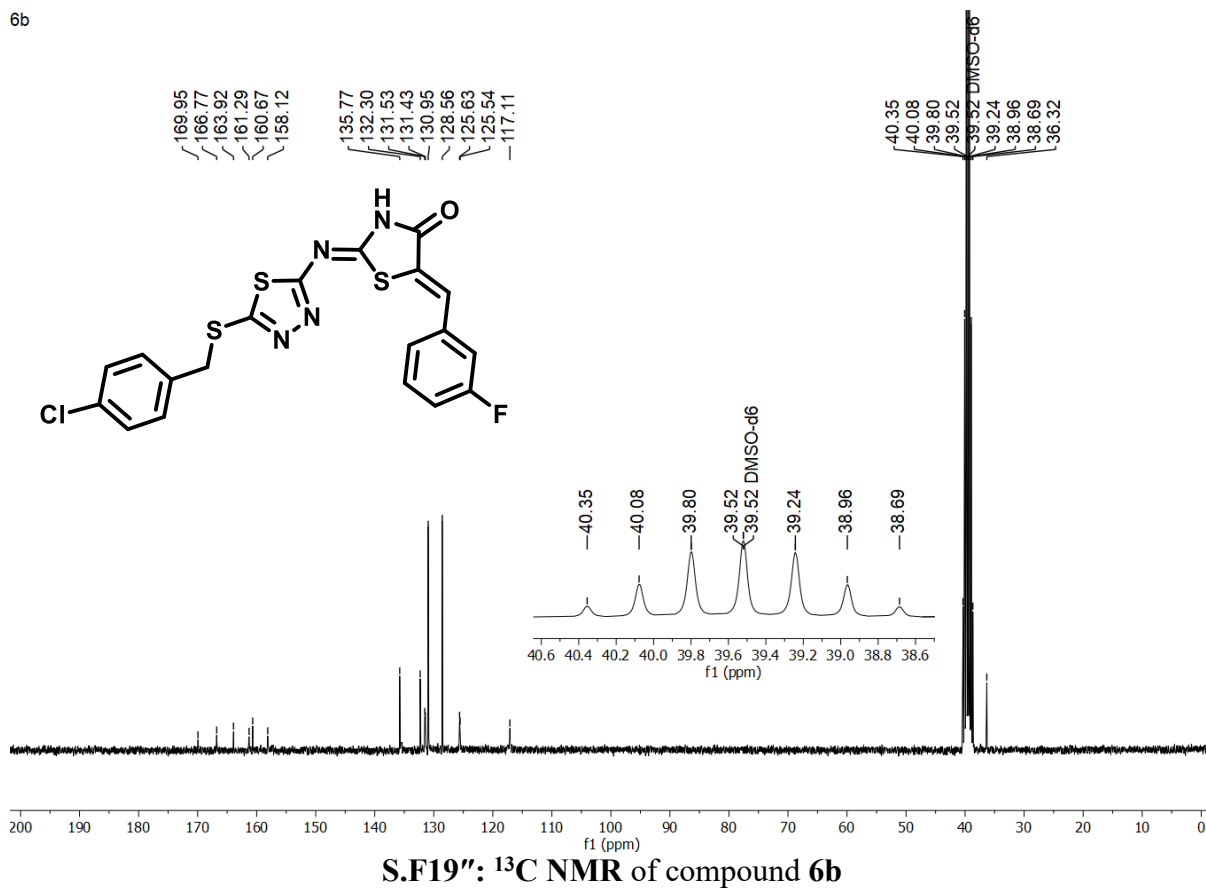
6A

S.F18'': ¹³C NMR of compound 6a

6b

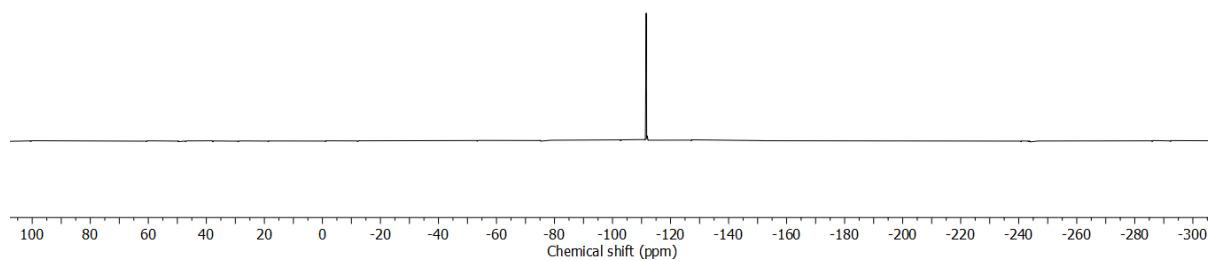
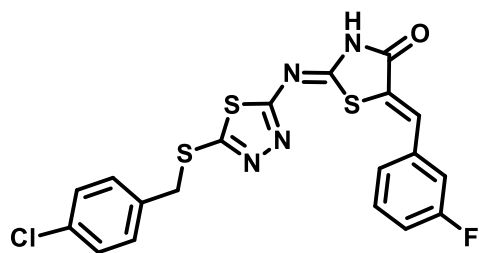


6b



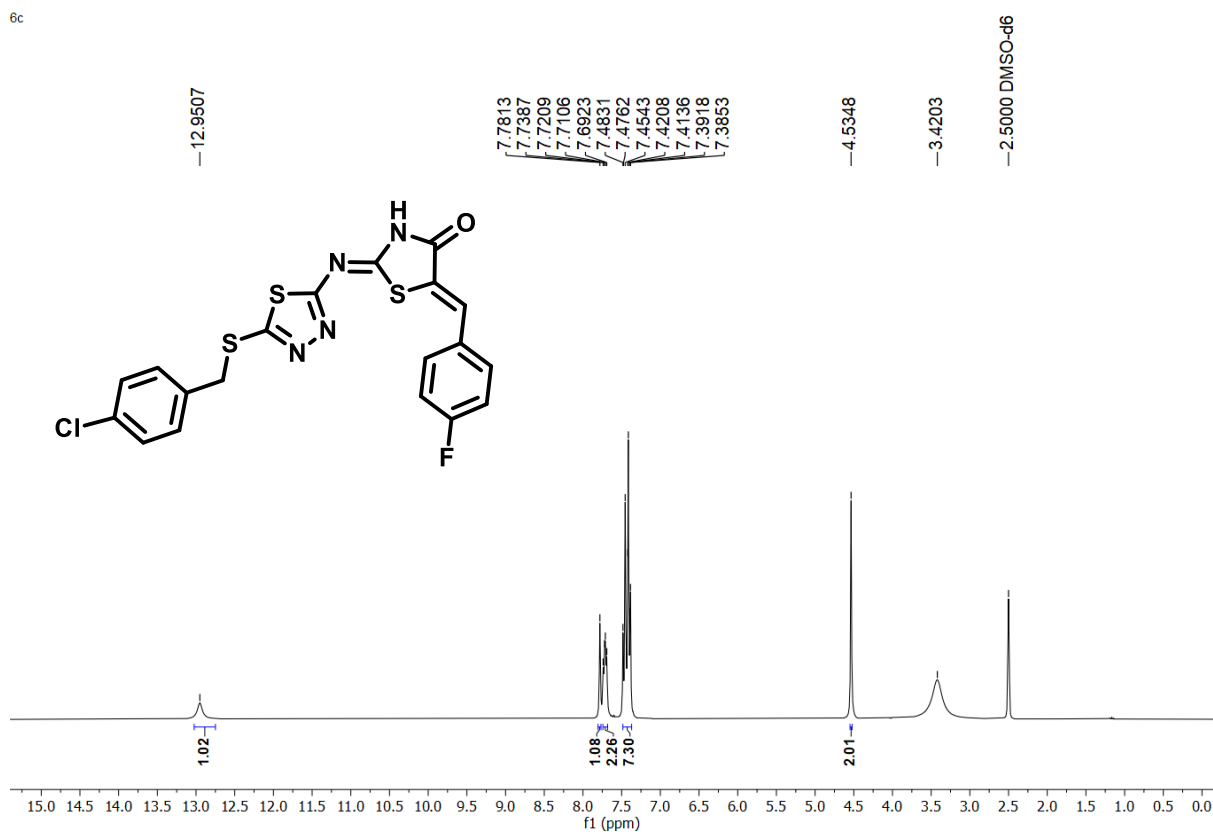
6B

--111.603

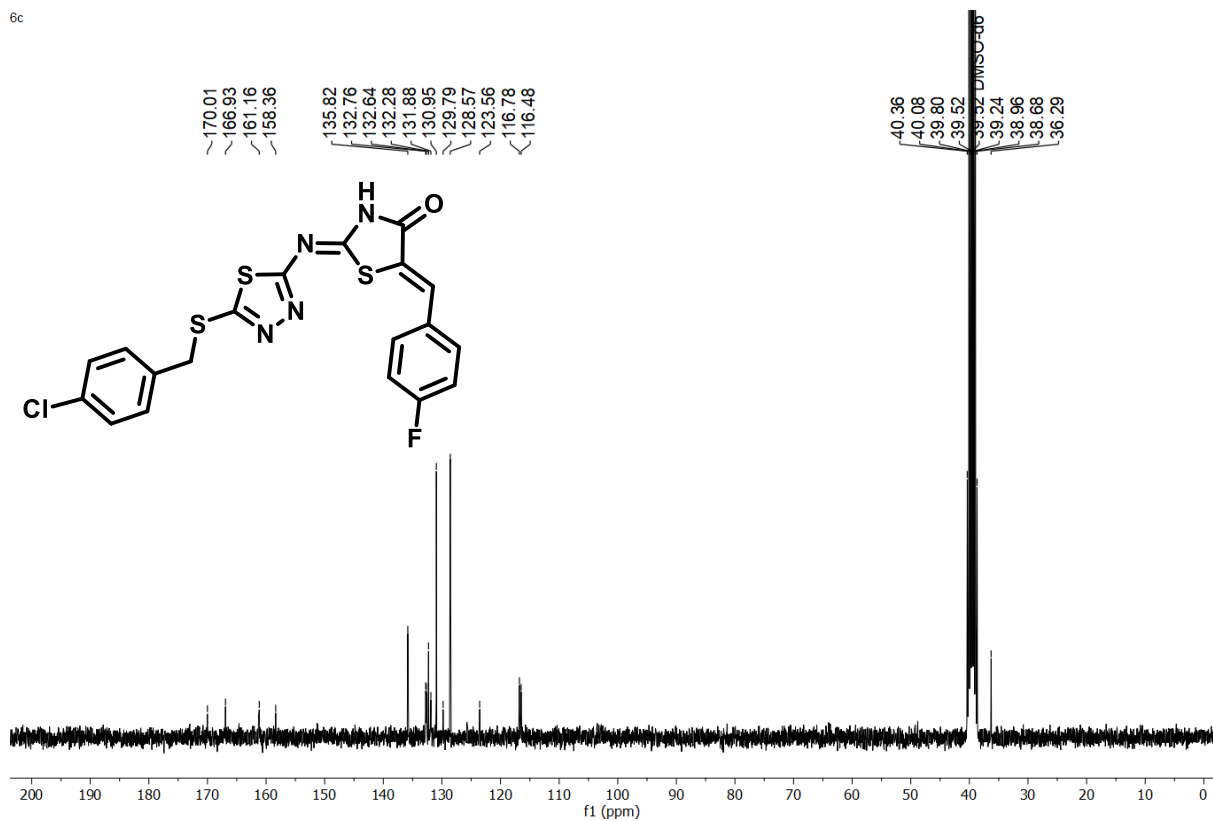


S.F19''': ¹⁹F NMR of compound 6b

6c

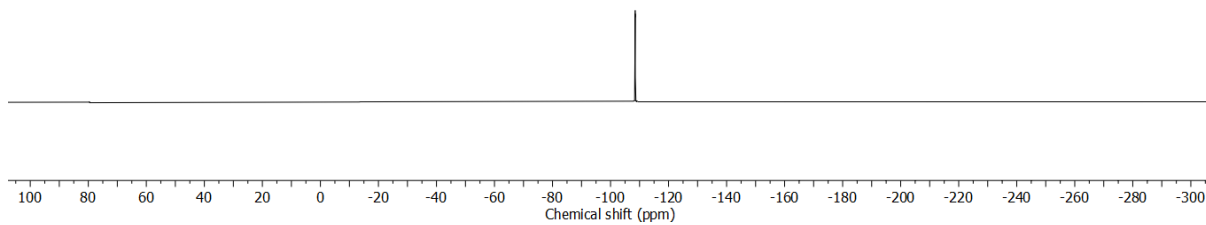
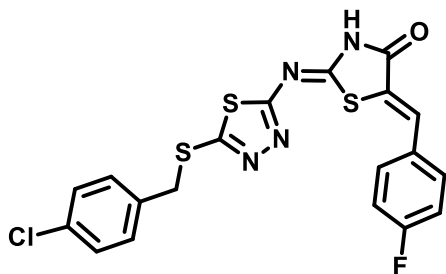
S.F20': $^1\text{H NMR}$ of compound 6c

6c

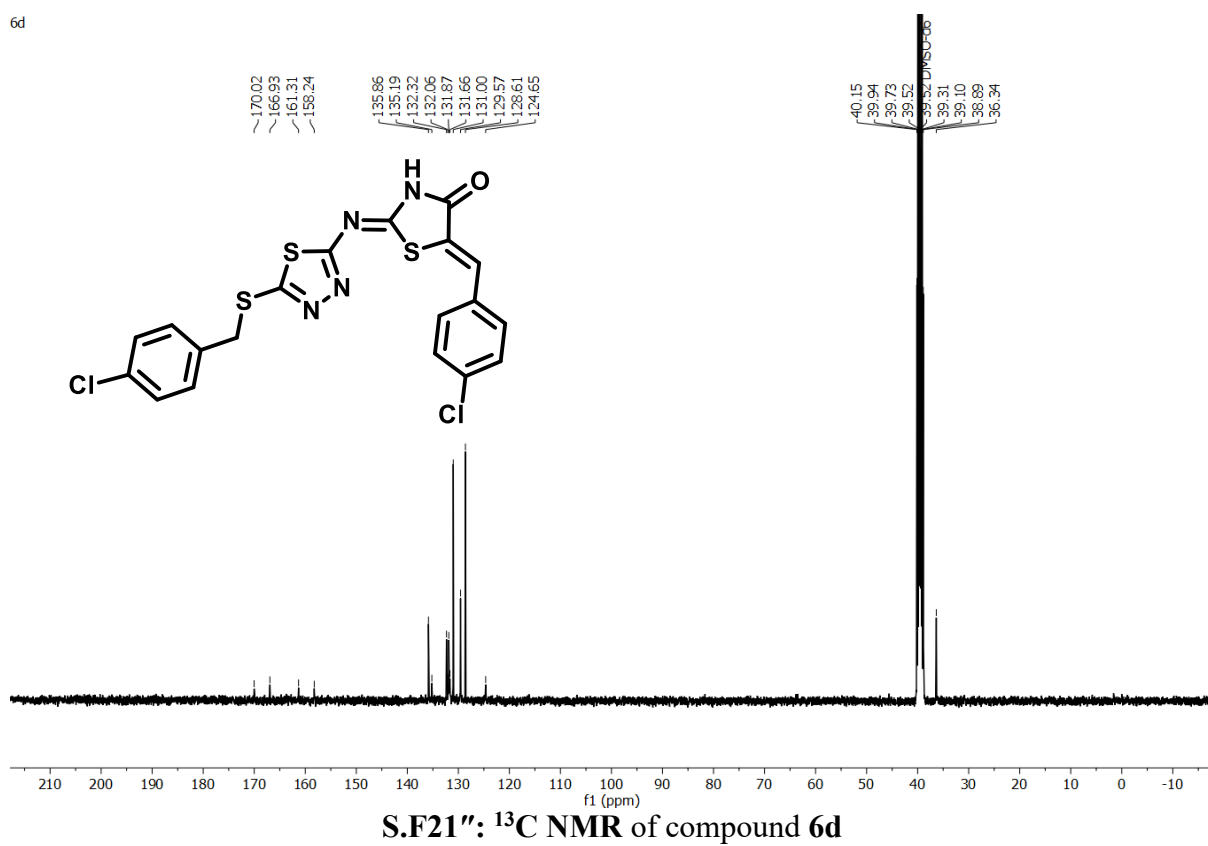
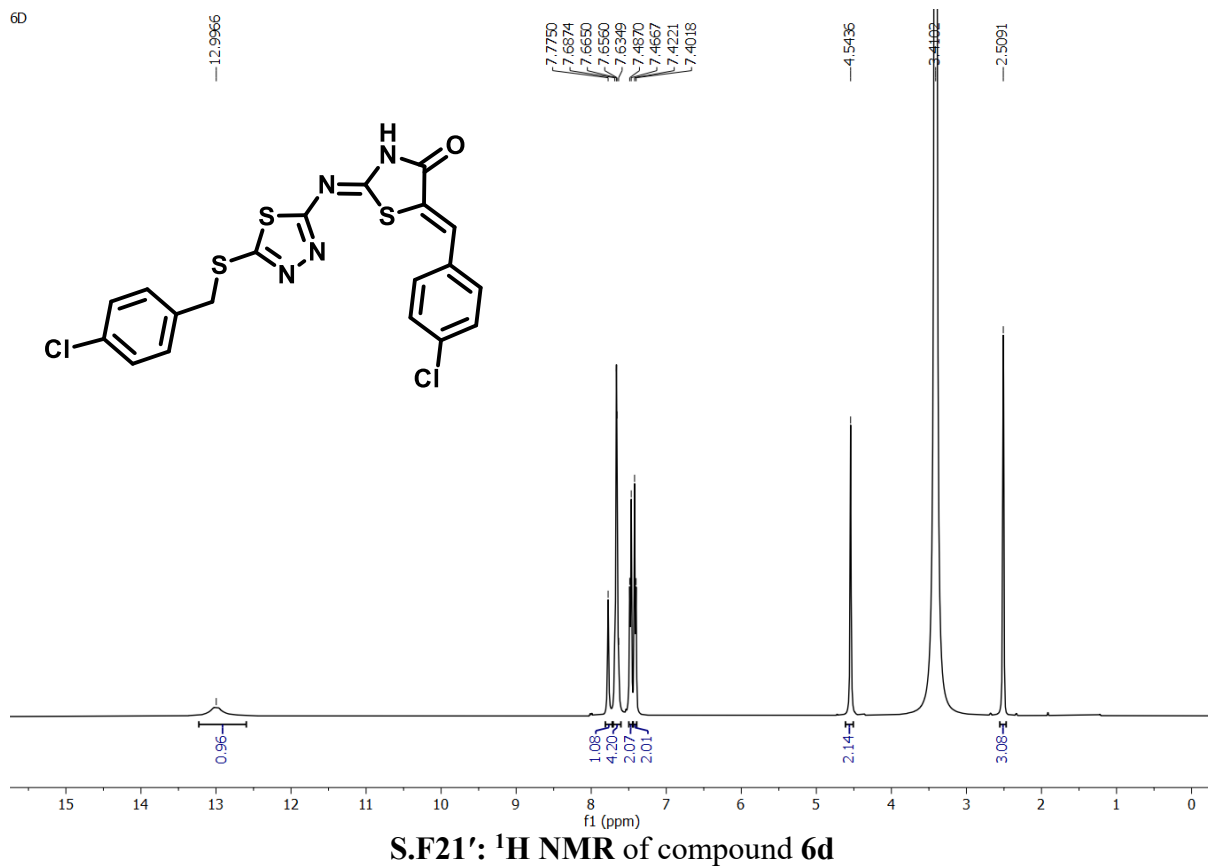
S.F20'': $^{13}\text{C NMR}$ of compound 6c

6c

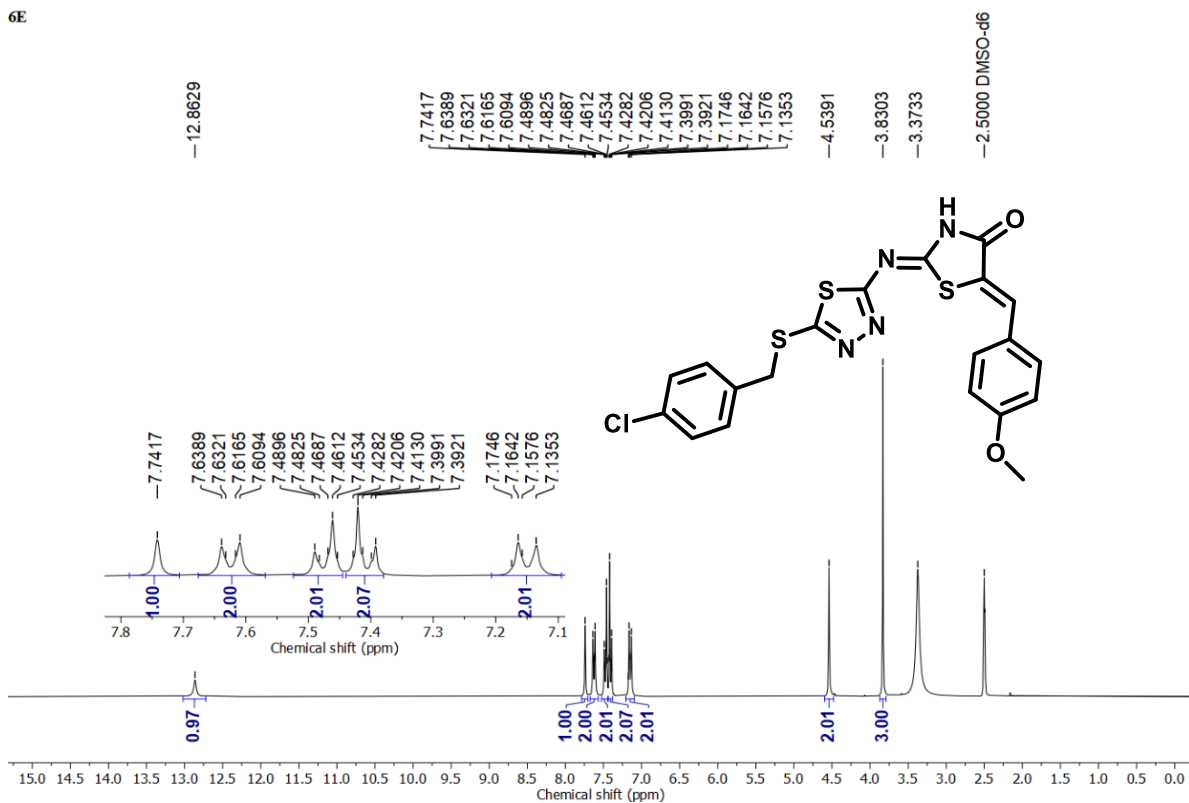
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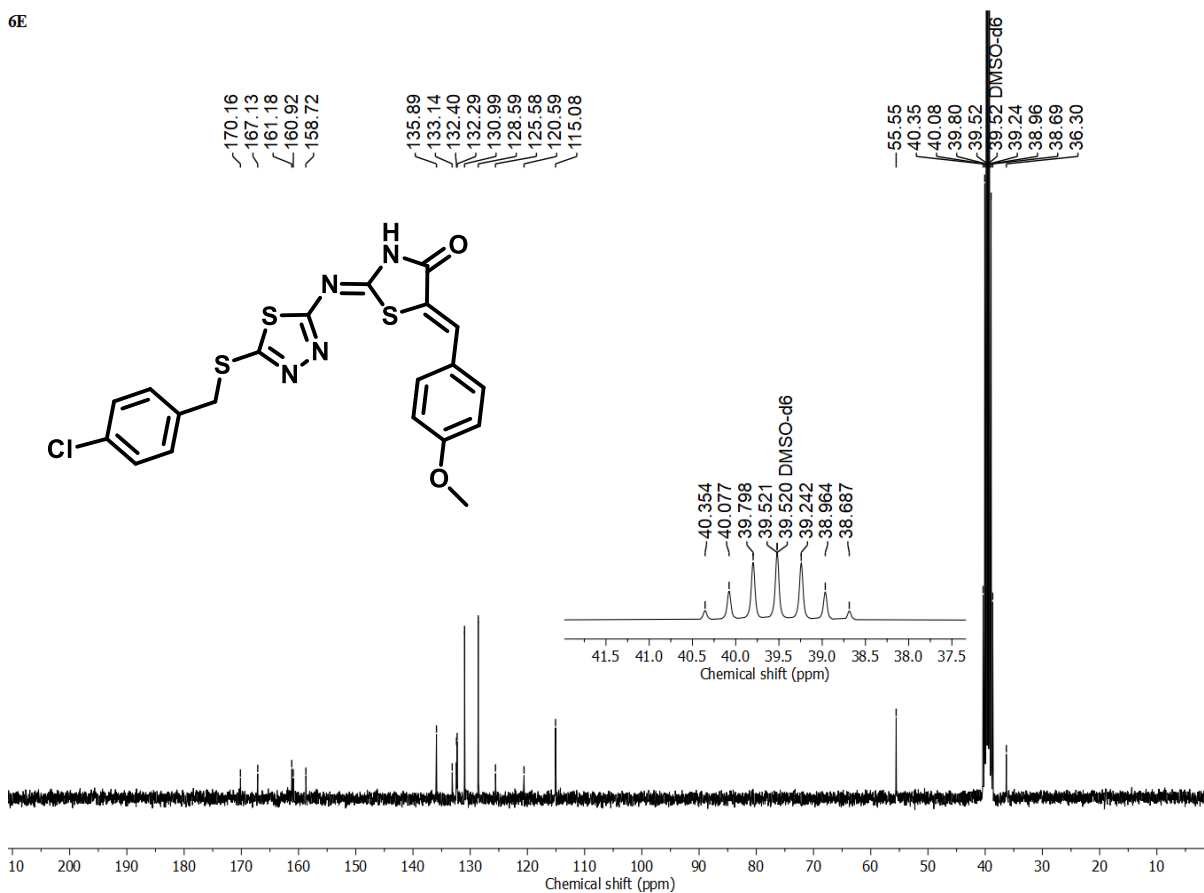
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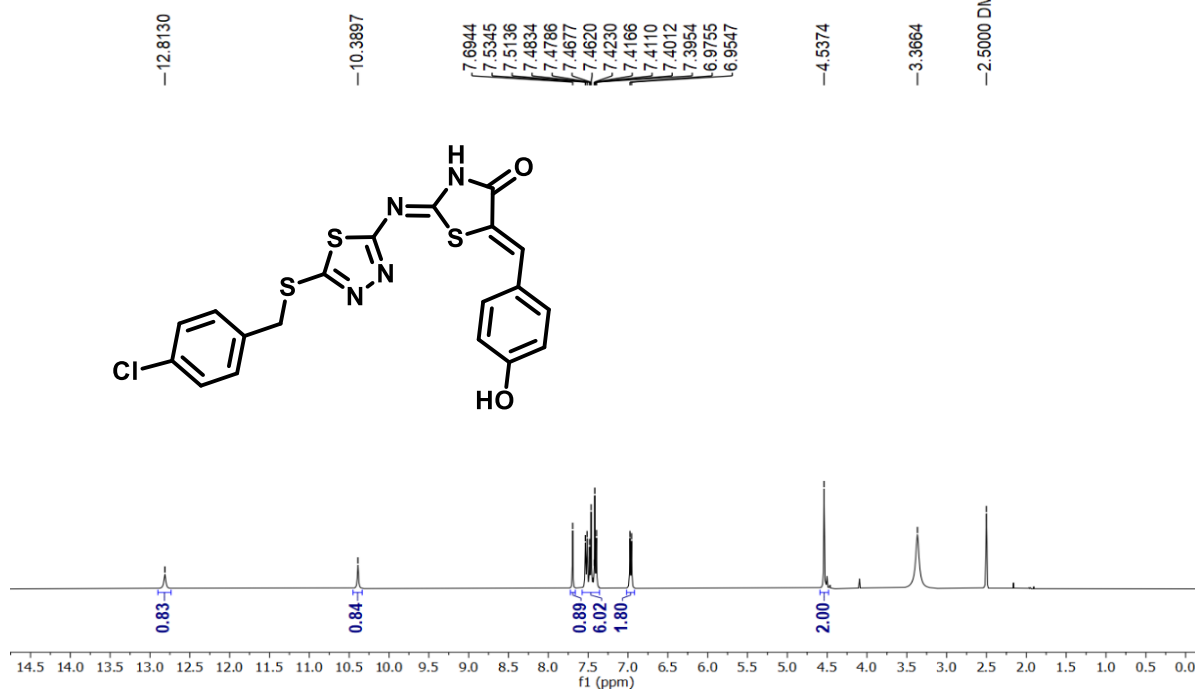
6E

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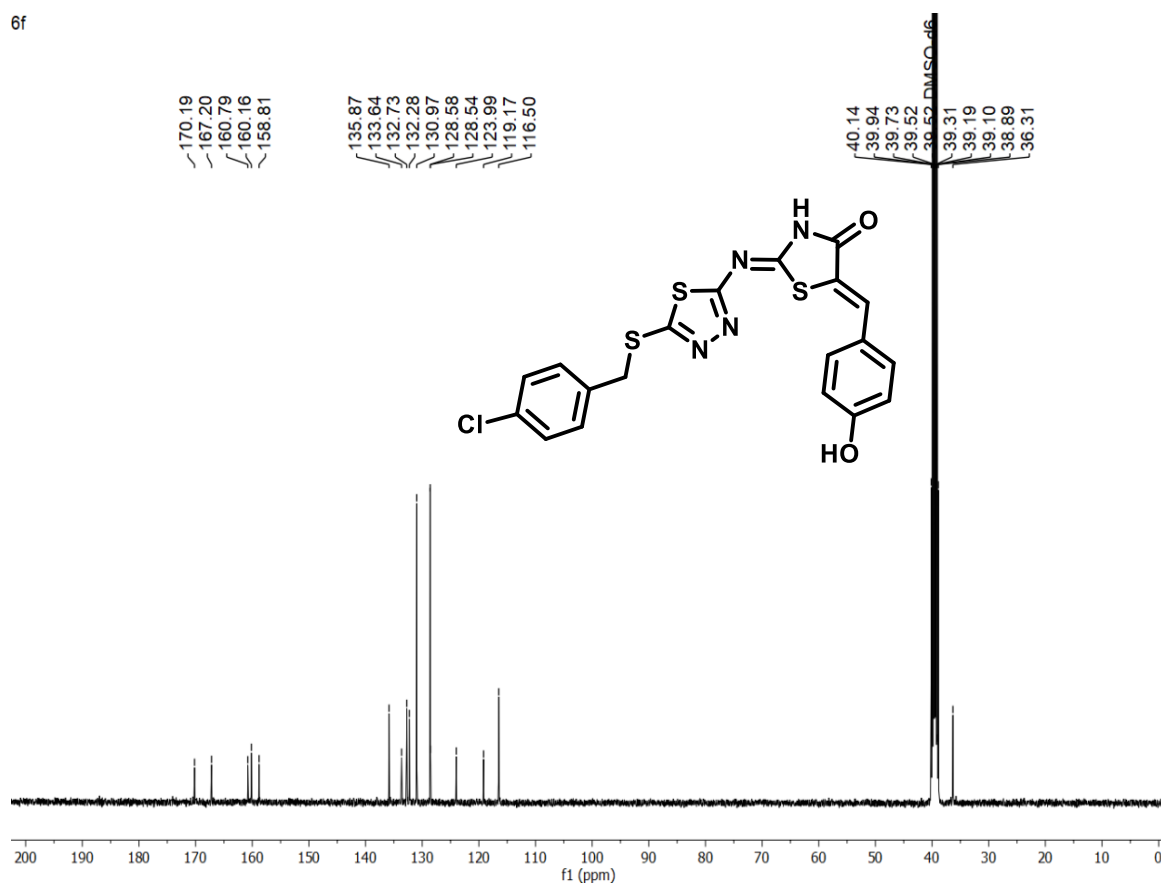
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S.F22'': ¹³C NMR of compound 6e

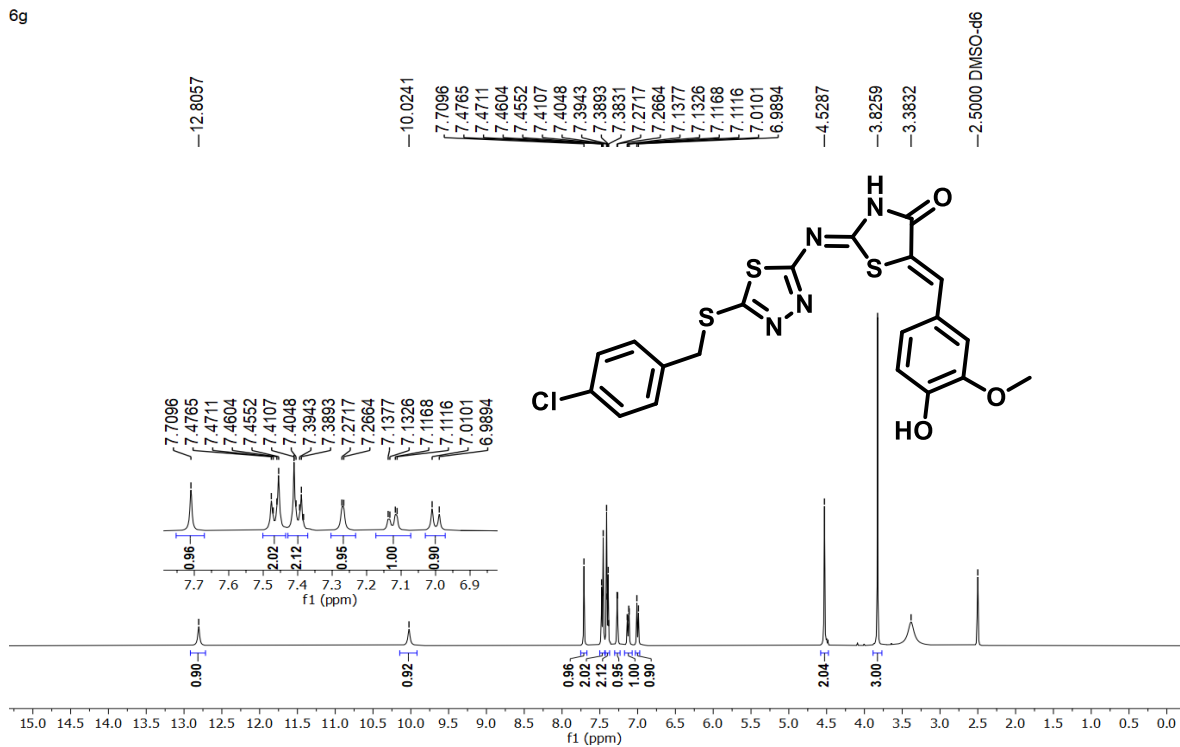
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S.F23': $^1\text{H NMR}$ of compound 6f

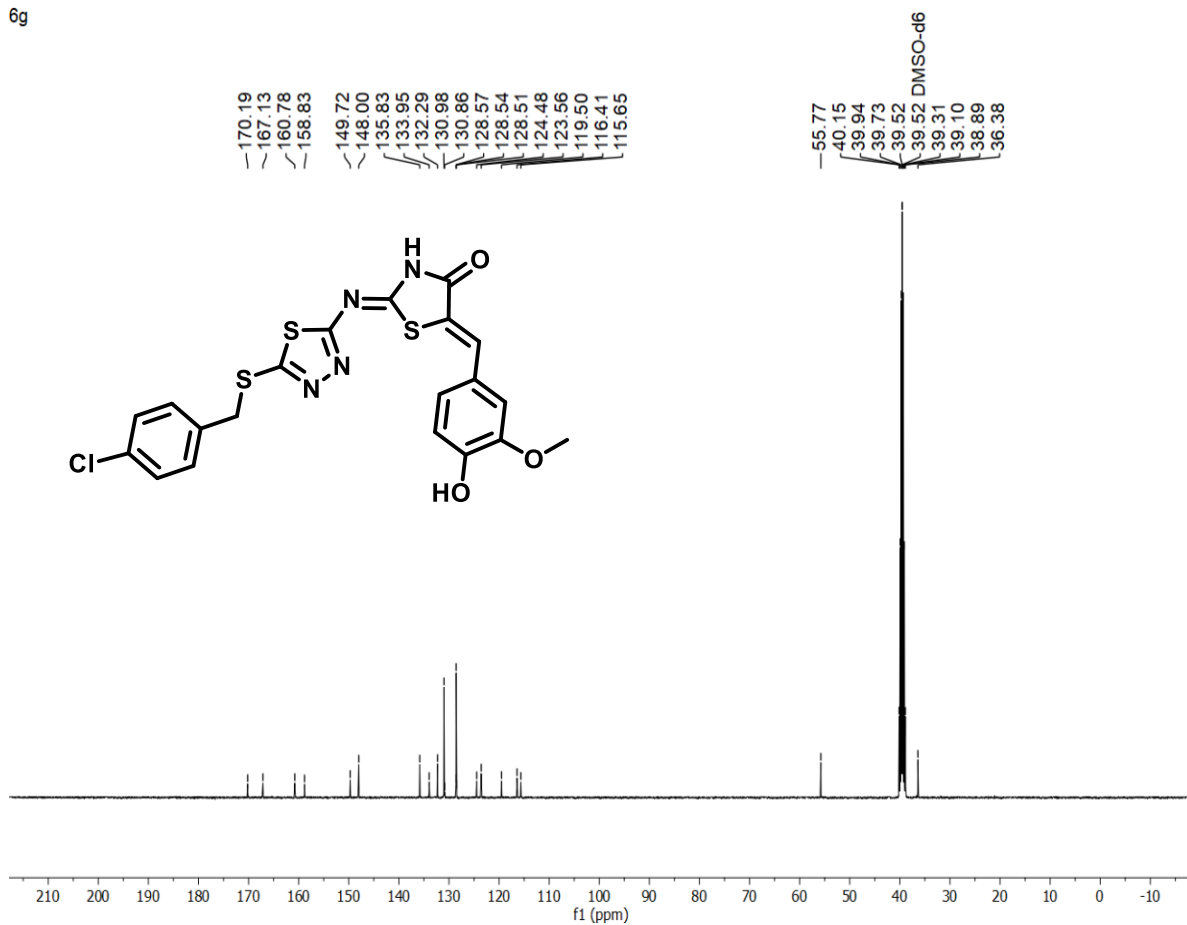
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S.F23'': $^{13}\text{C NMR}$ of compound 6f

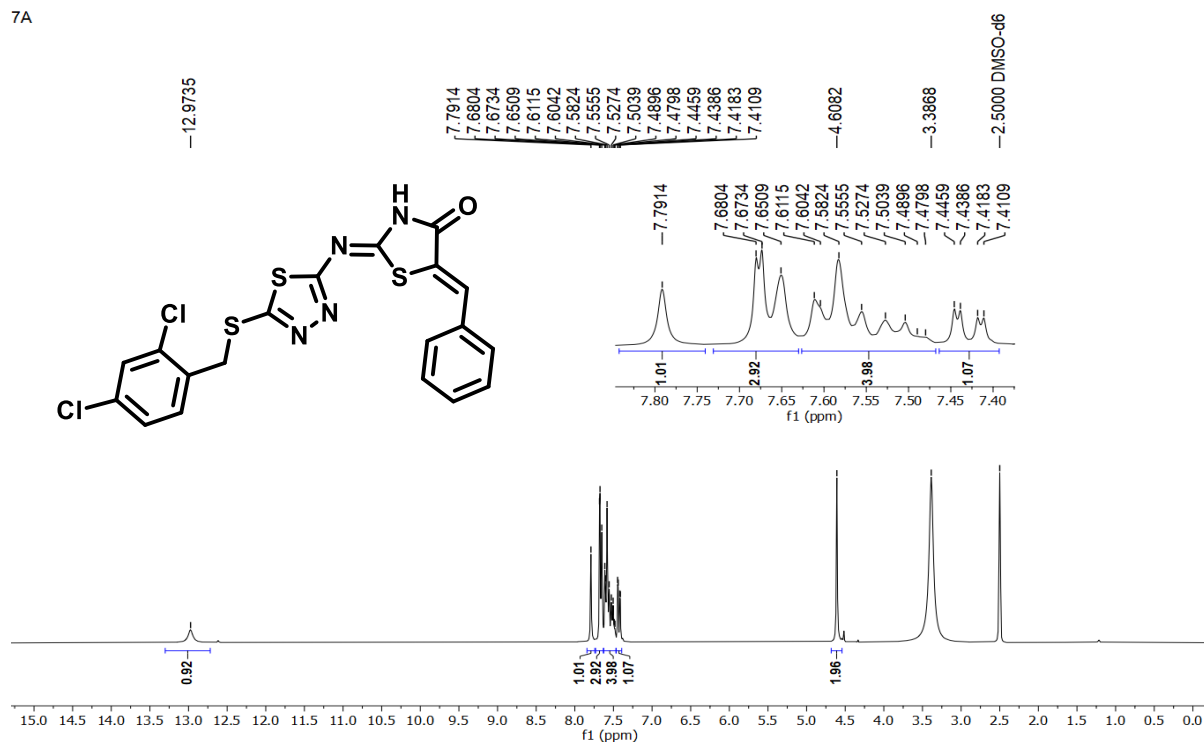
6g

S.F24': $^1\text{H NMR}$ of compound 6g

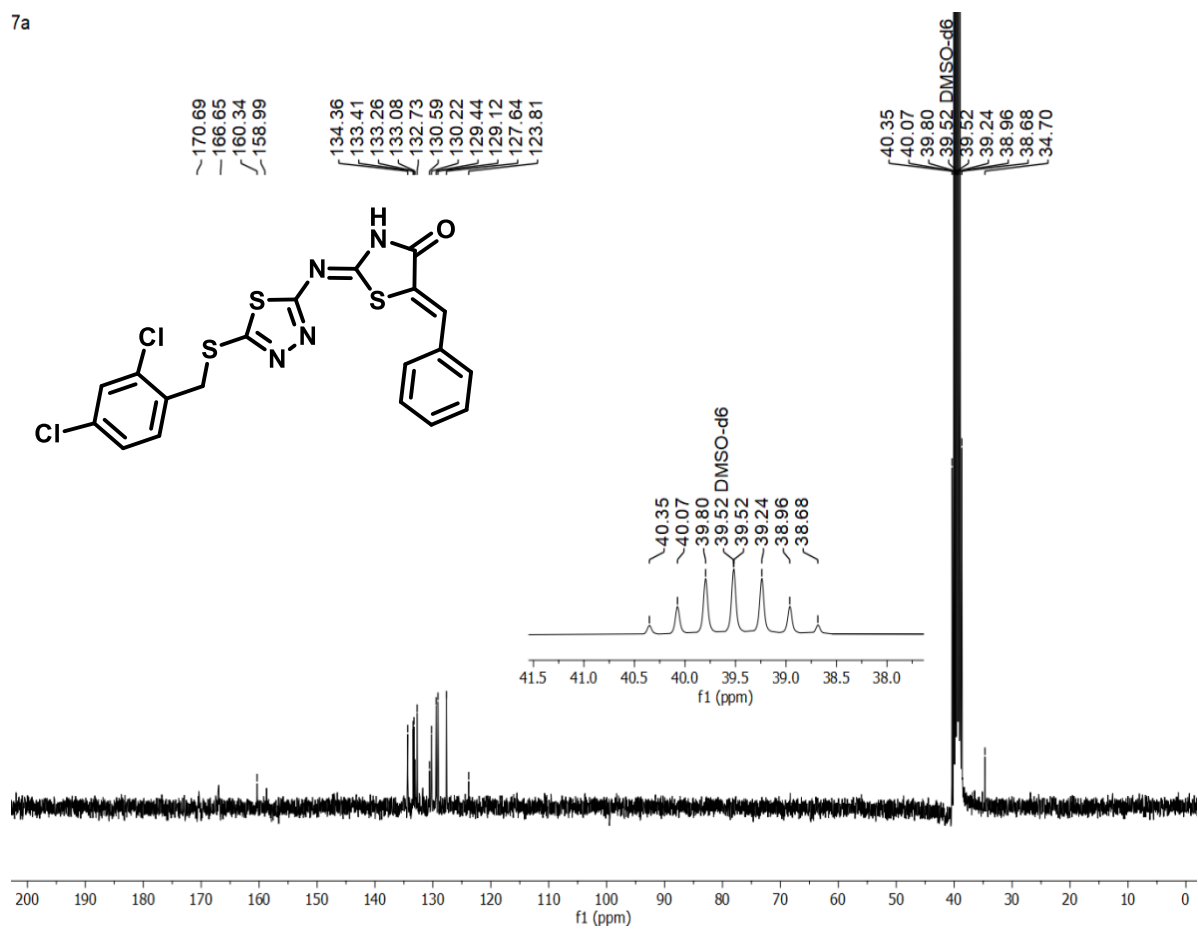
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S.F24'': $^{13}\text{C NMR}$ of compound 6g

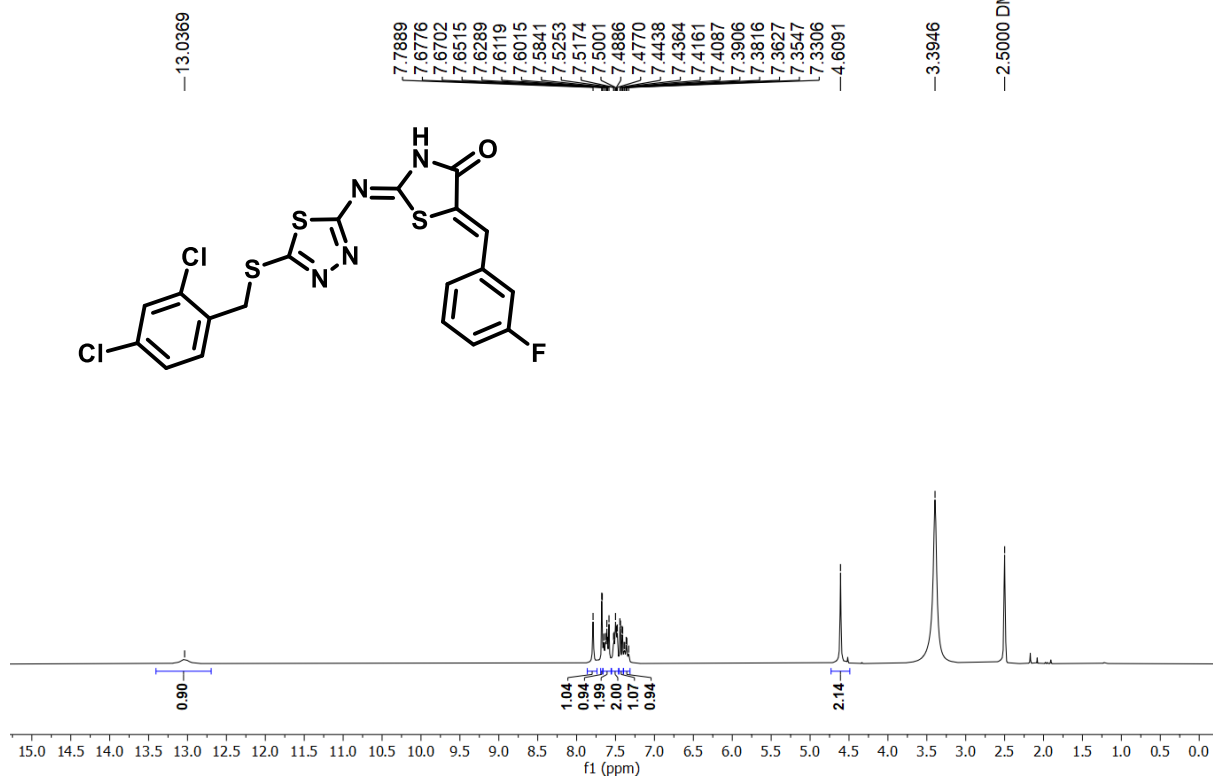
7A

S.F25': $^1\text{H NMR}$ of compound 7a

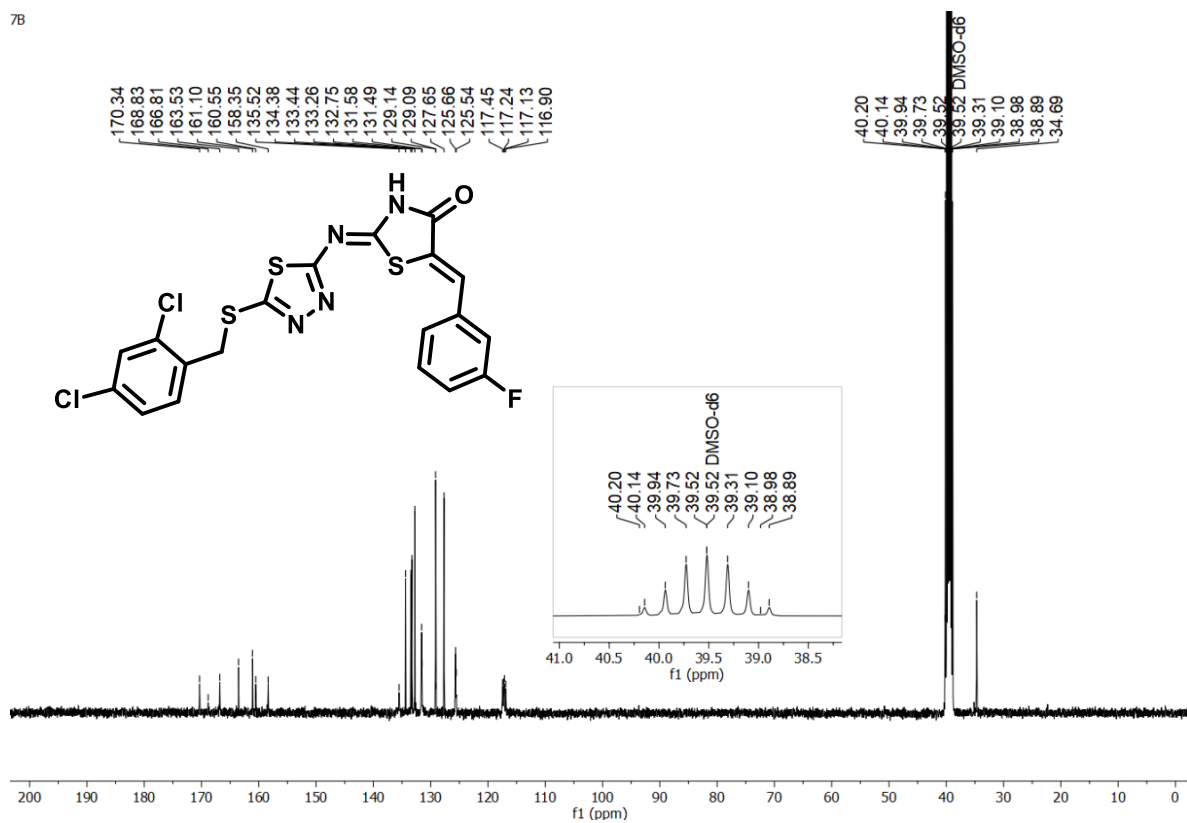
7a

S.F25'': $^{13}\text{C NMR}$ of compound 7a

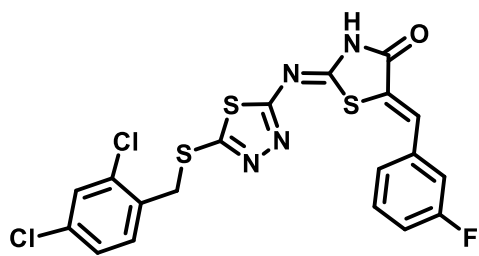
7b

S.F26': ¹H NMR of compound 7b

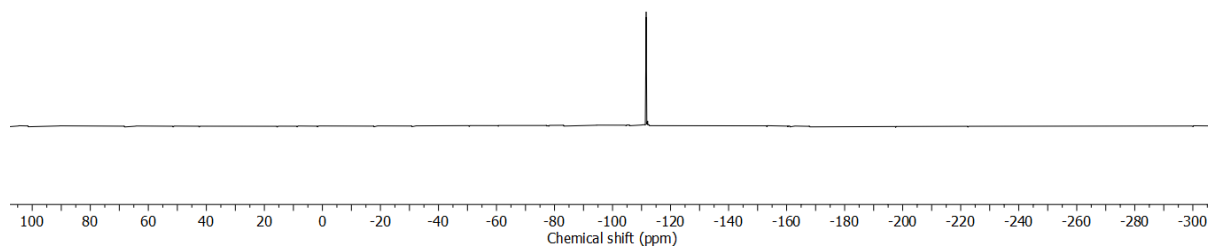
7b

S.F26'': ¹³C NMR of compound 7b

7B

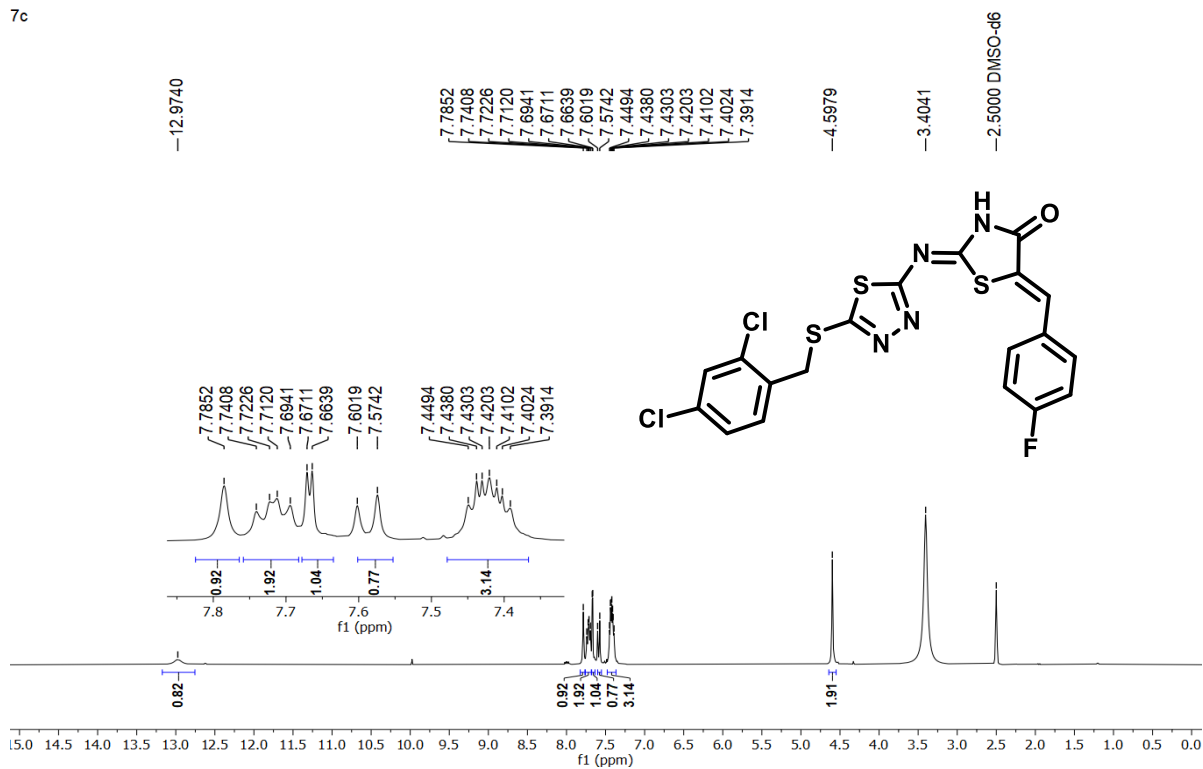


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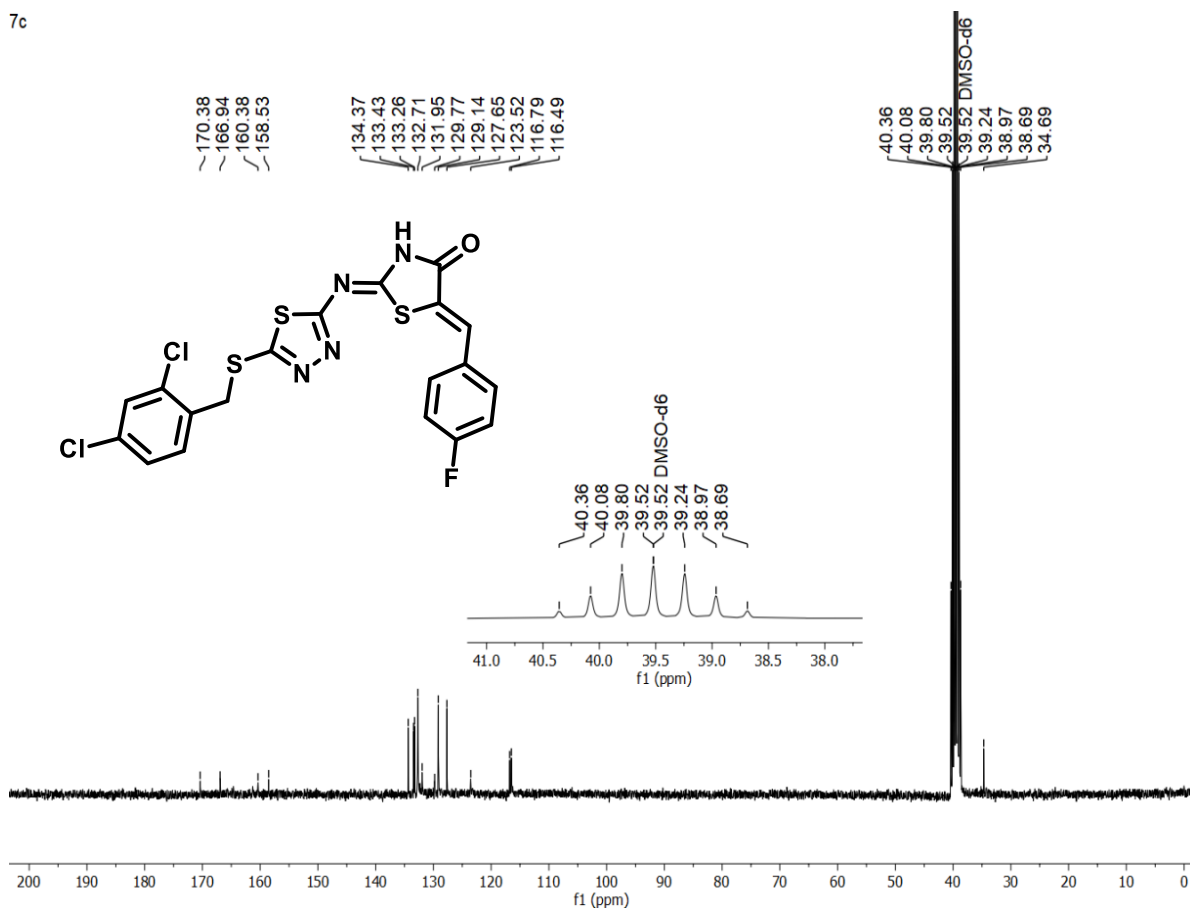


S.F26''': ^{19}F NMR compound 7b

7c

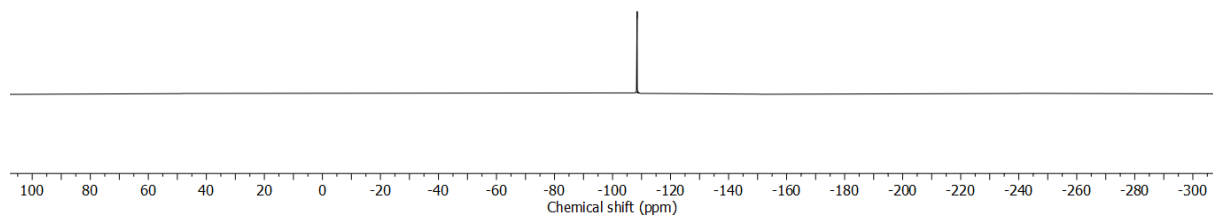
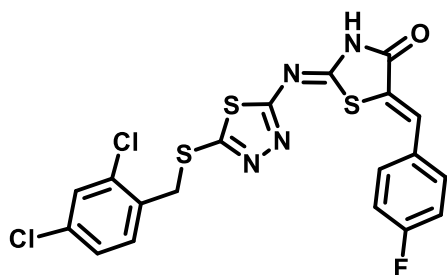
S.F27': ¹H NMR of compound 7c

7c

S.F27'': ¹³C NMR of compound 7c

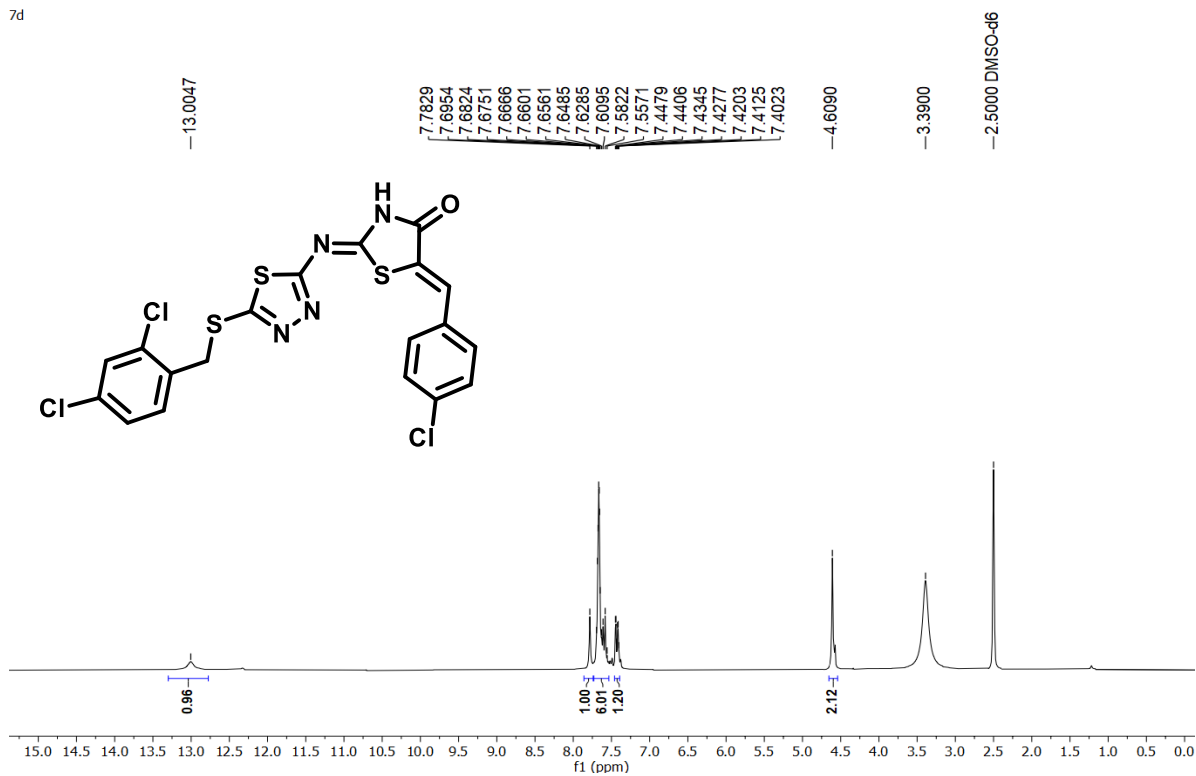
7c

-108.458

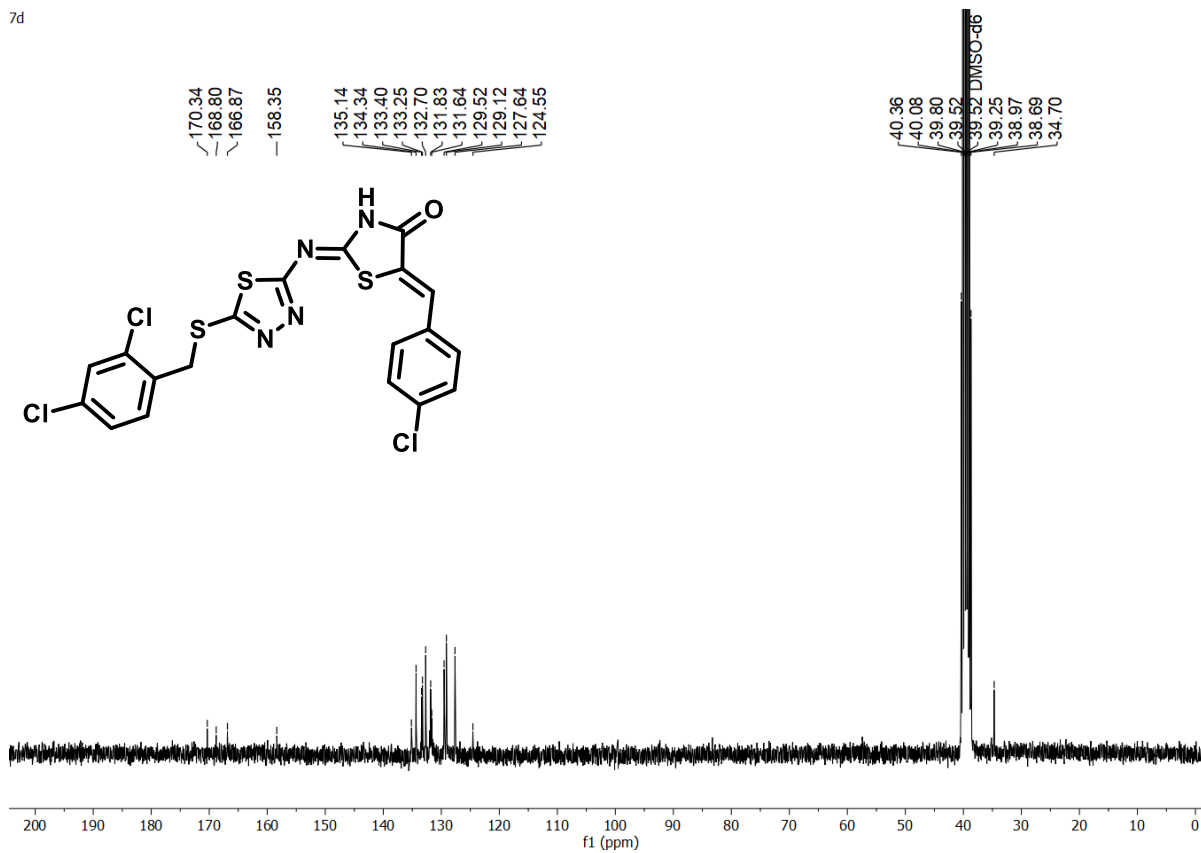


S.F27''': ^{19}F NMR of compound 7c

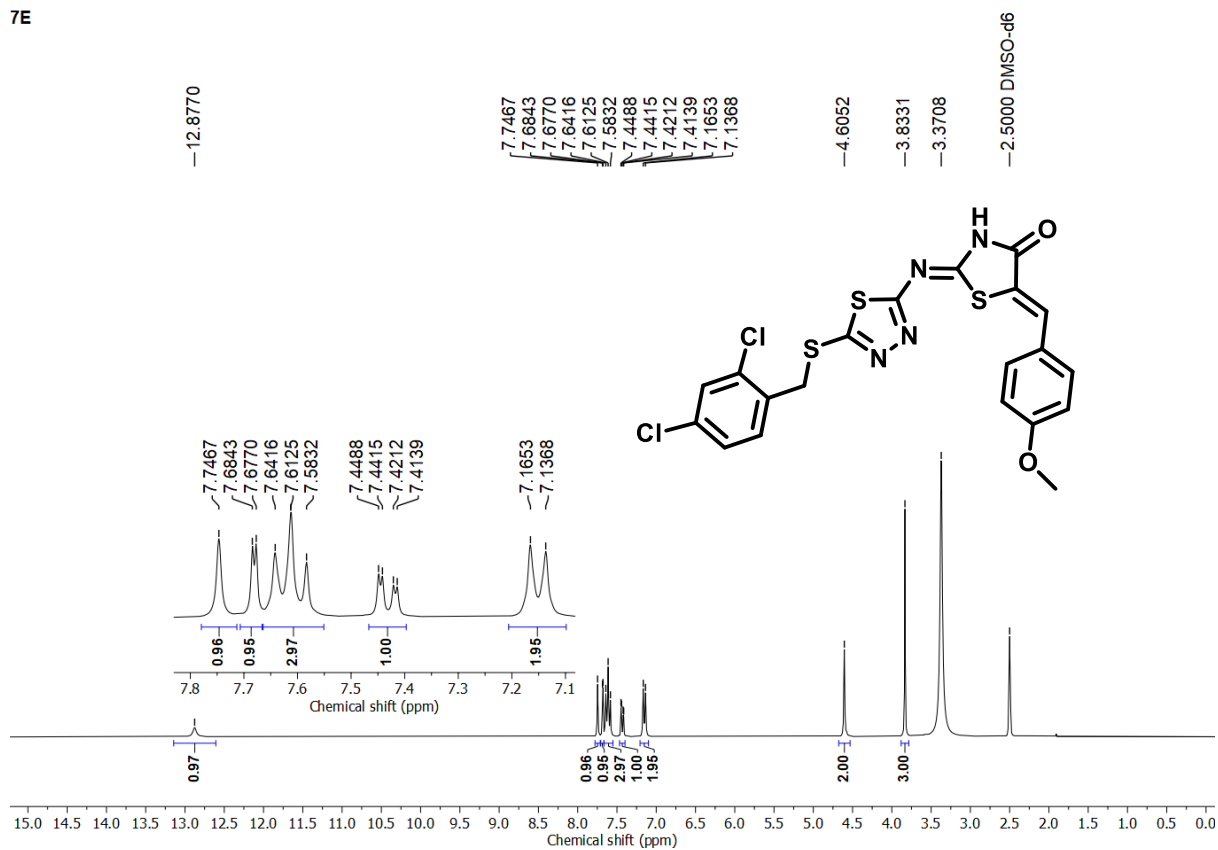
7d

S.F28': ¹H NMR of compound 7d

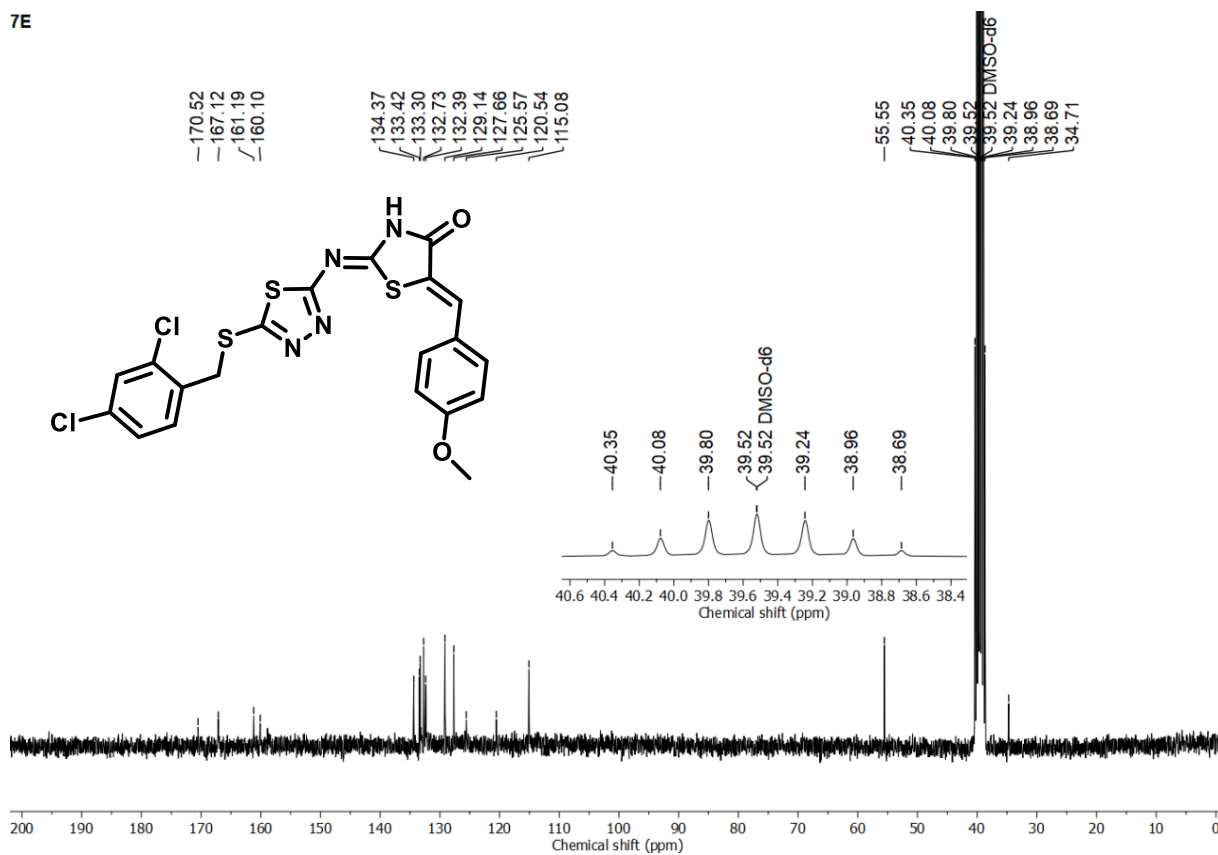
7d

S.F28'': ¹³C NMR of compound 7d

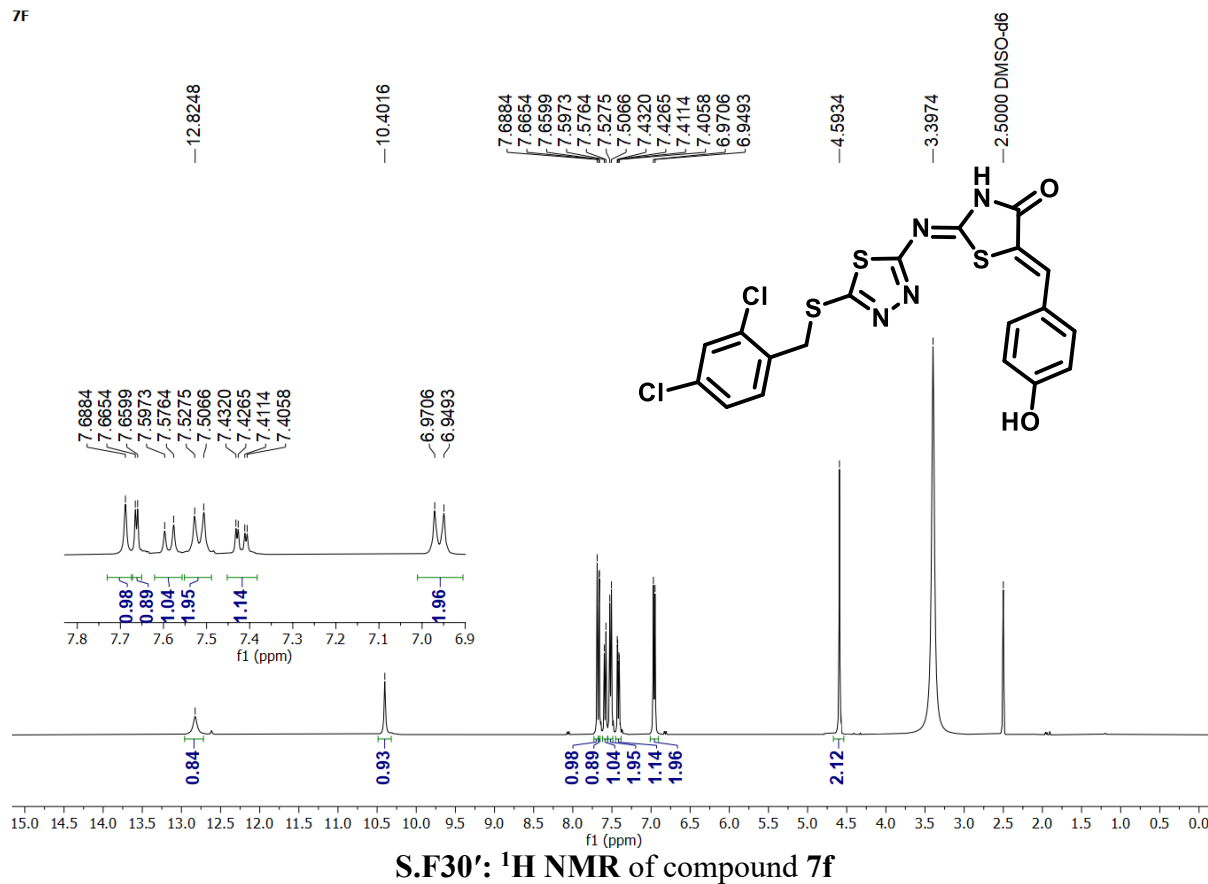
7E

S.F29': ¹H NMR of compound 7e

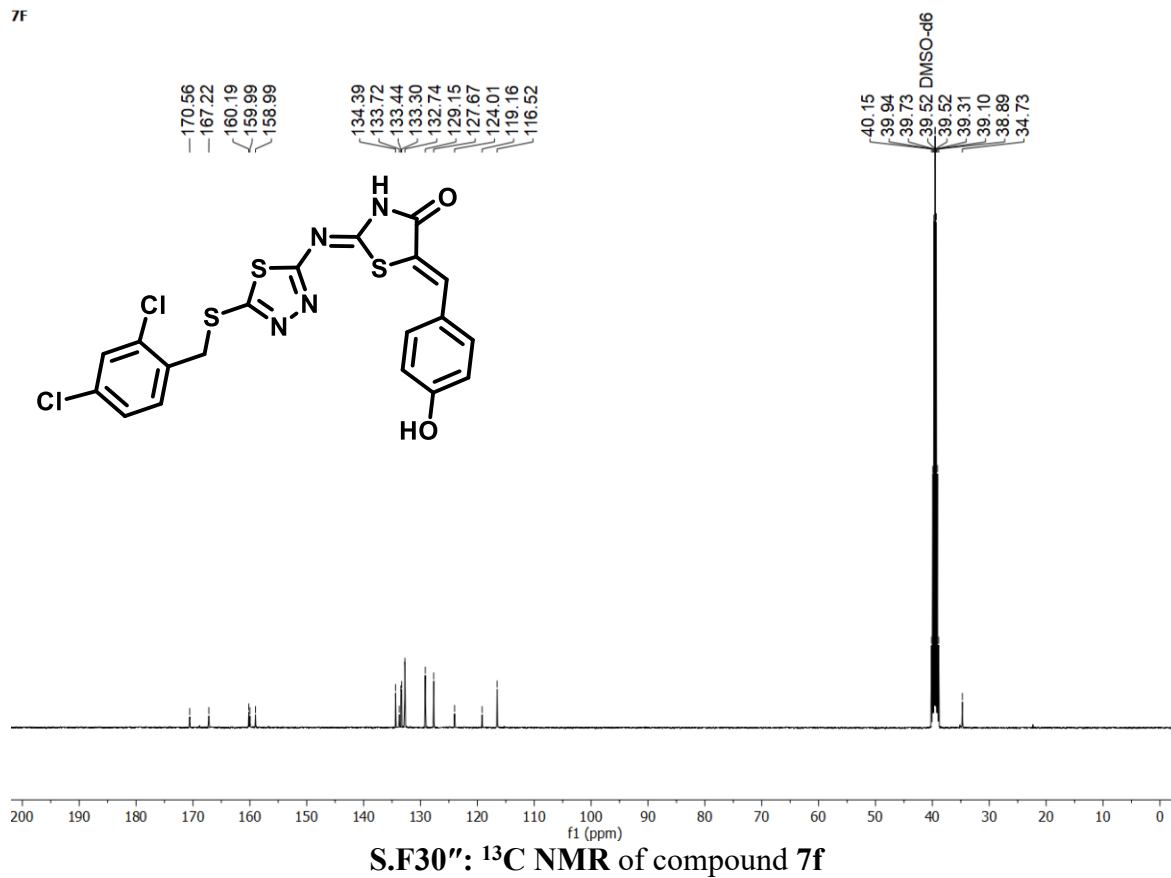
7E

S.F29'': ¹³C NMR of compound 7e

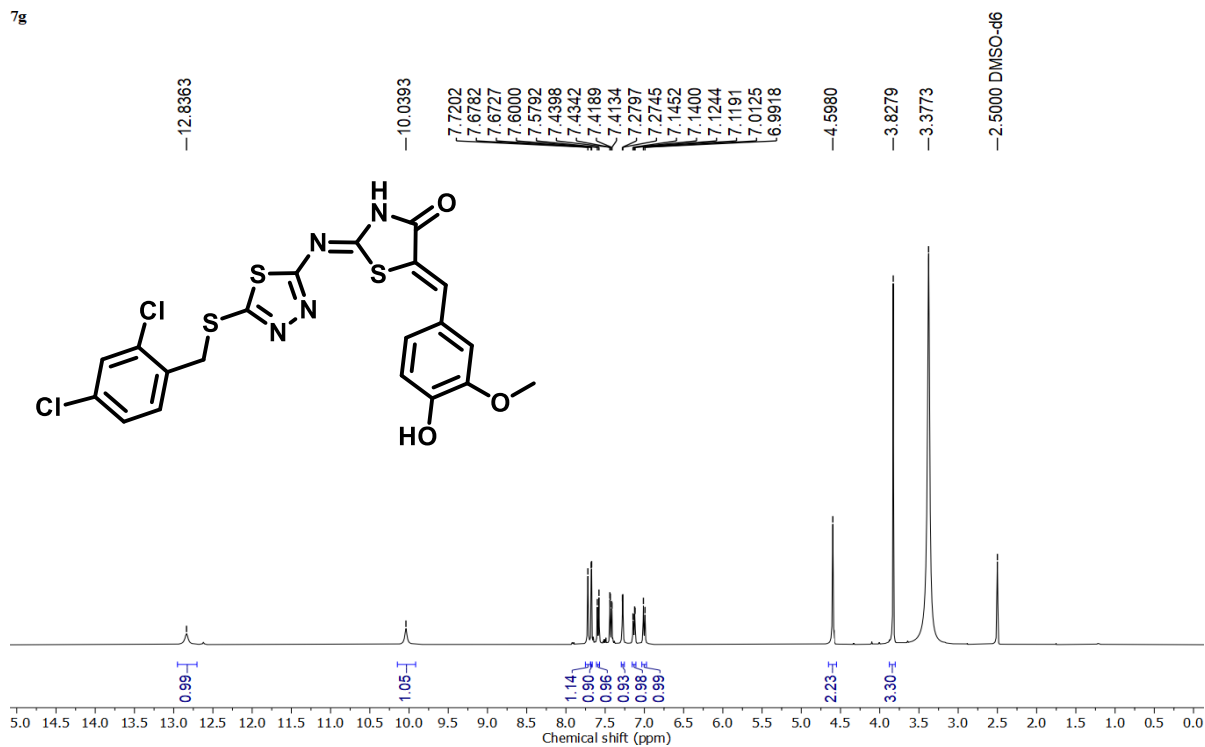
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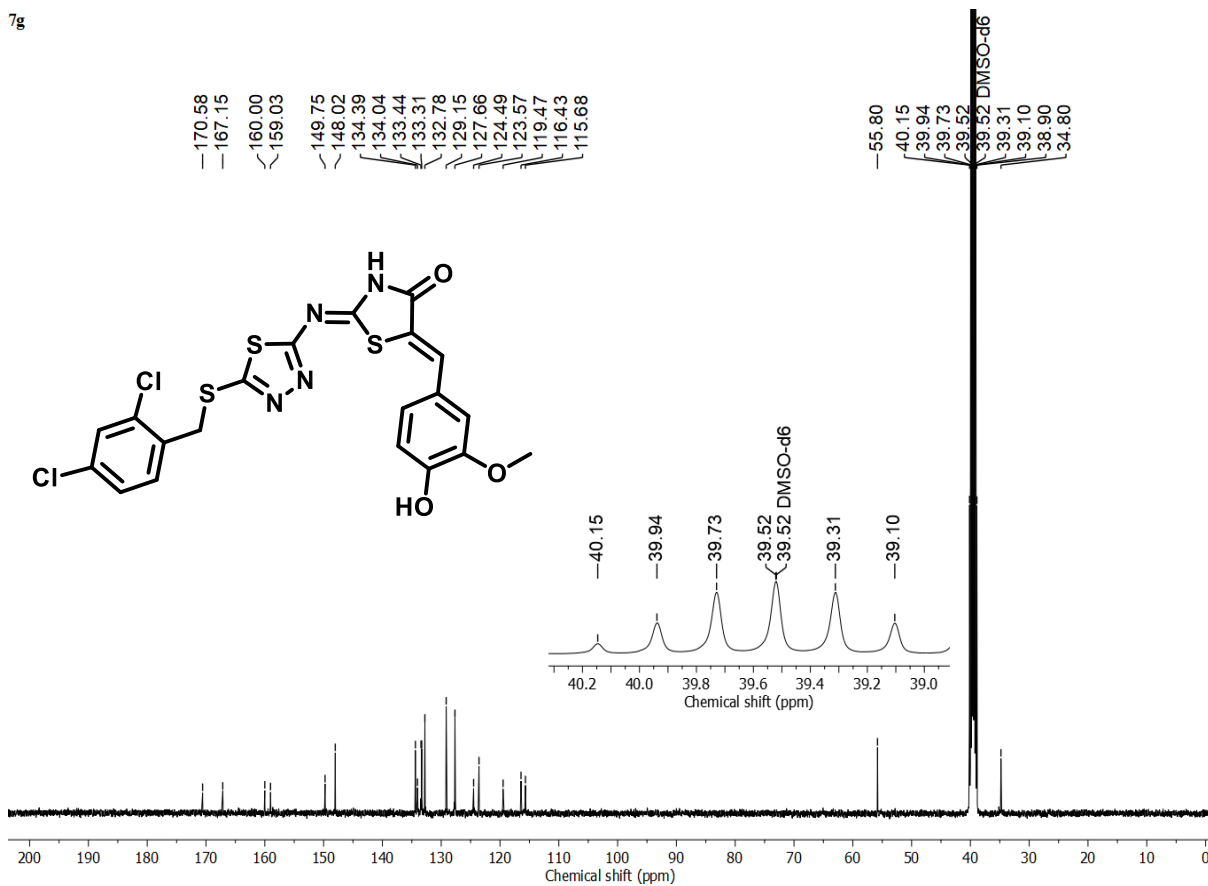
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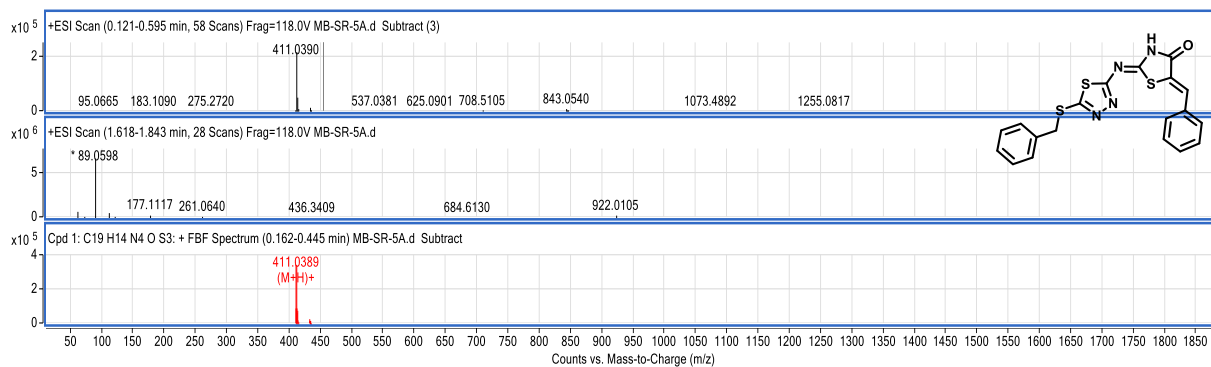
7g

S.F31': $^1\text{H NMR}$ of compound 7g

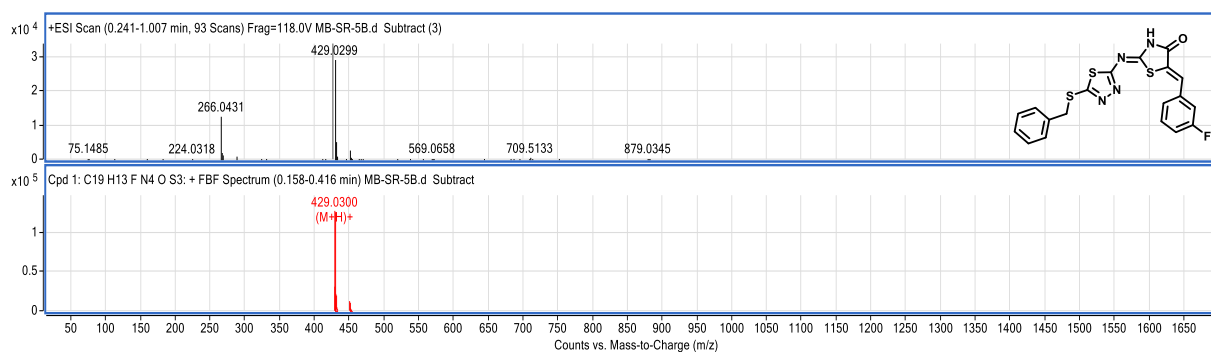
7g

S.F31'': $^{13}\text{C NMR}$ of compound 7g

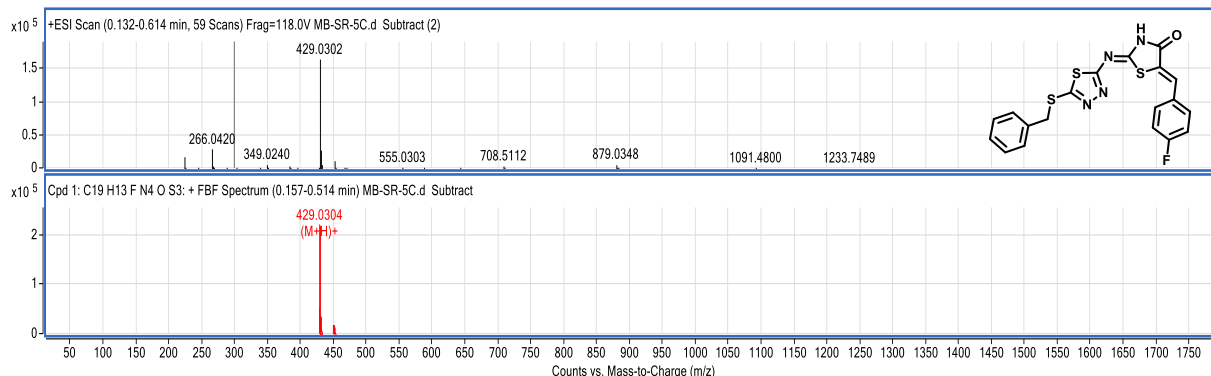
Copy of HRMS Data (Final Compounds):



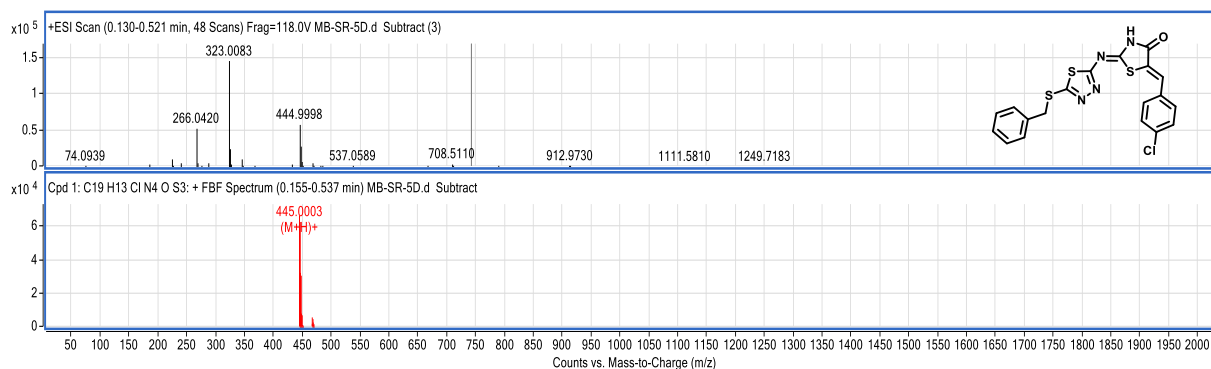
S.F32: HRMS Compound 5a



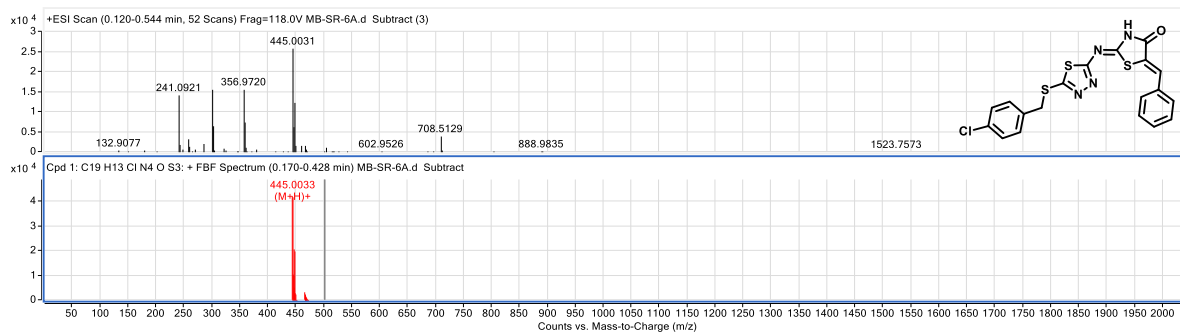
S.F33: HRMS Compound 5b



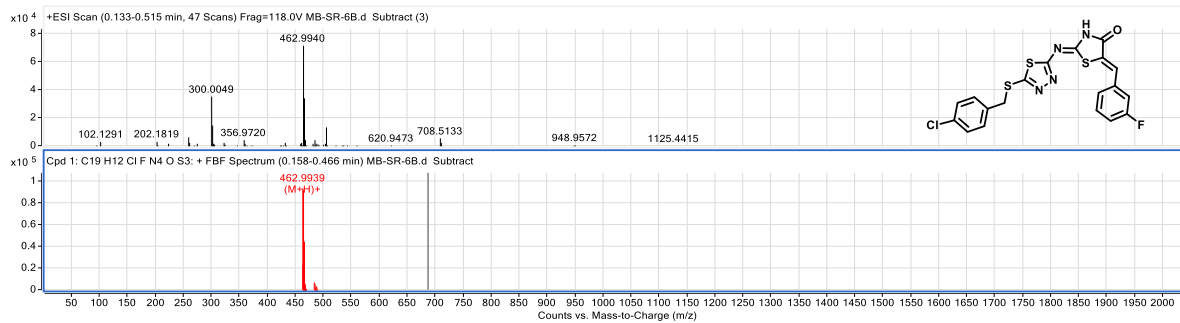
S.F34: HRMS Compound 5c



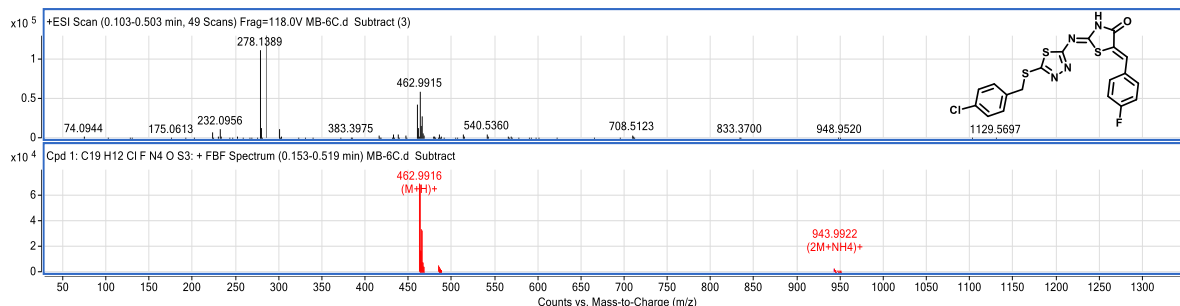
S.F35: HRMS Compound 5d



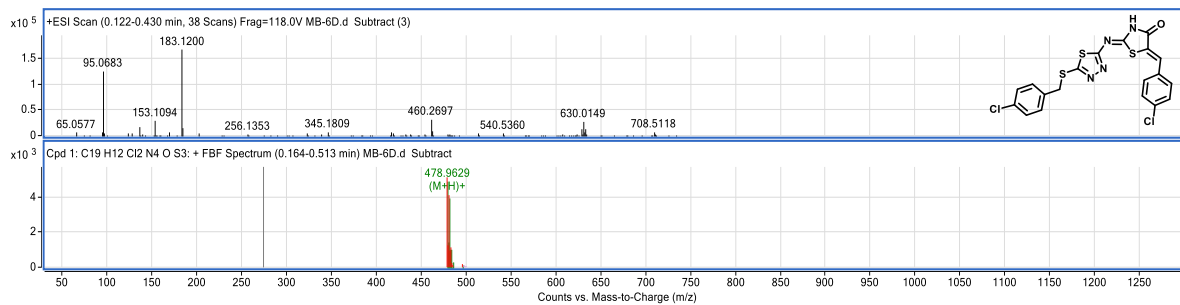
S.F36: HRMS Compound 6a



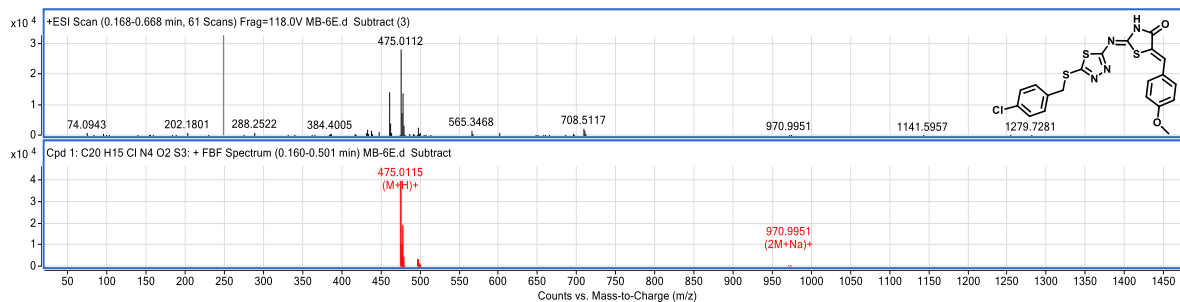
S.F37: HRMS Compound 6b



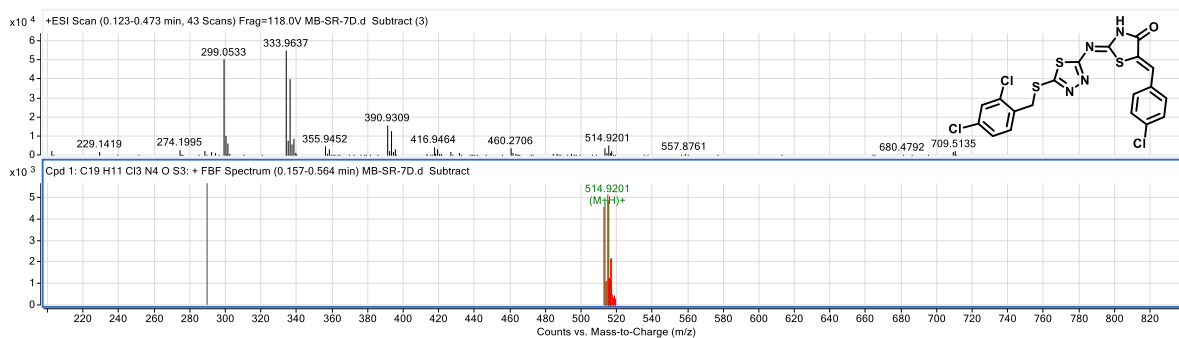
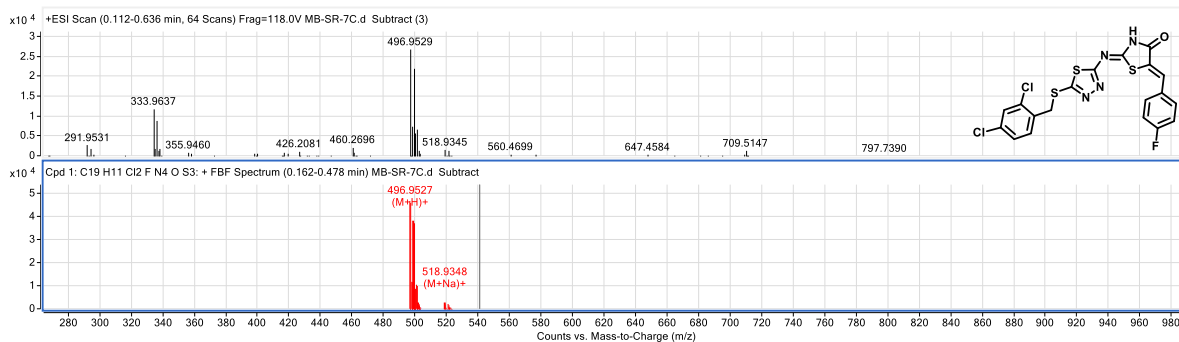
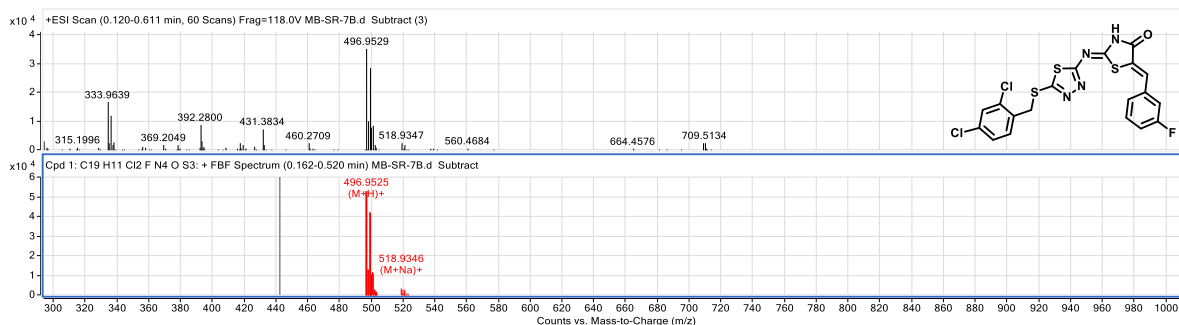
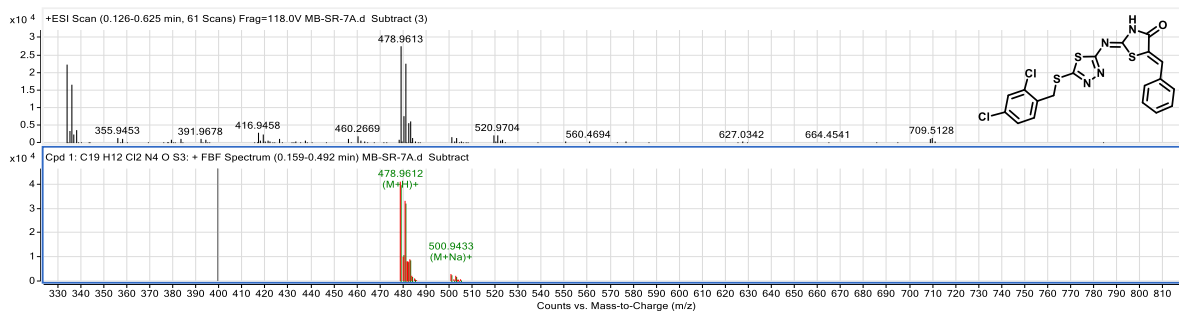
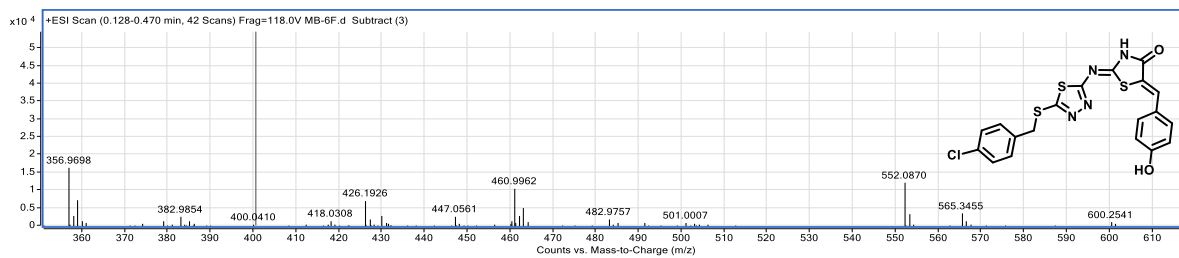
S.F38: HRMS Compound 6c

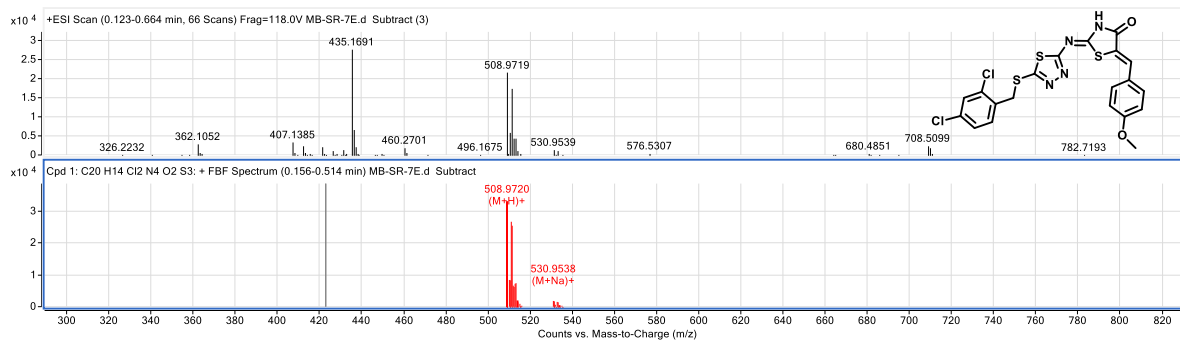


S.F39: HRMS Compound 6d

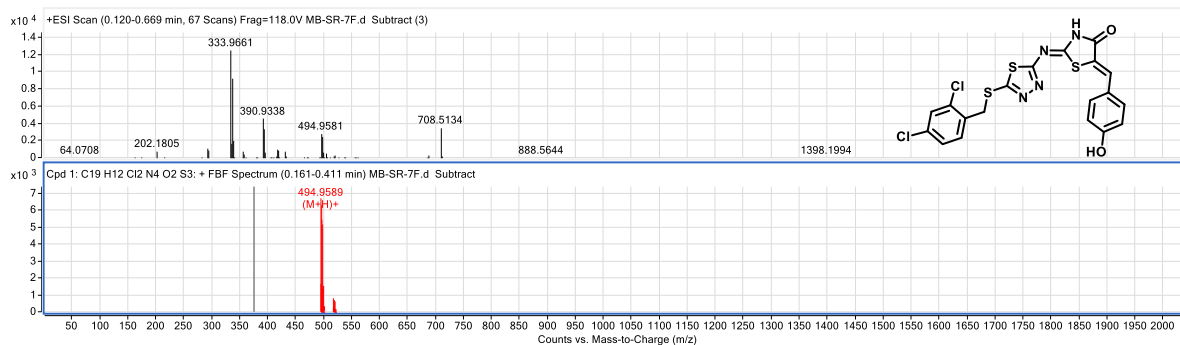


S.F40: HRMS Compound 6e

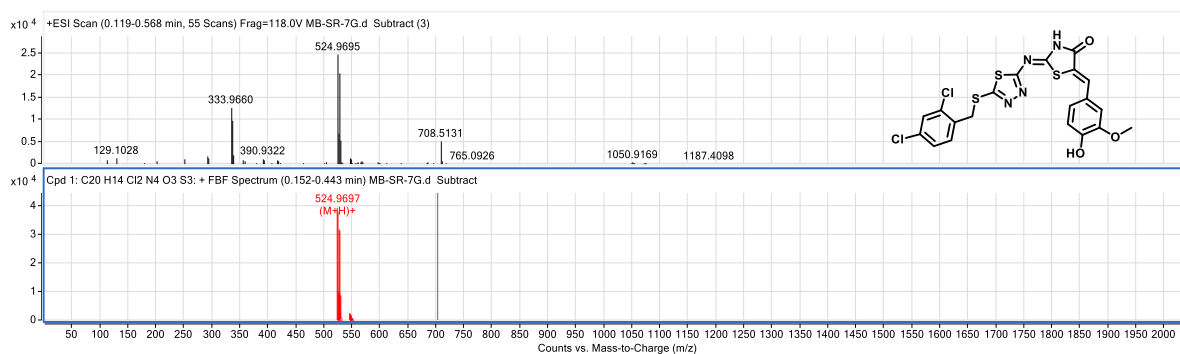




S.F46: HRMS Compound 7e

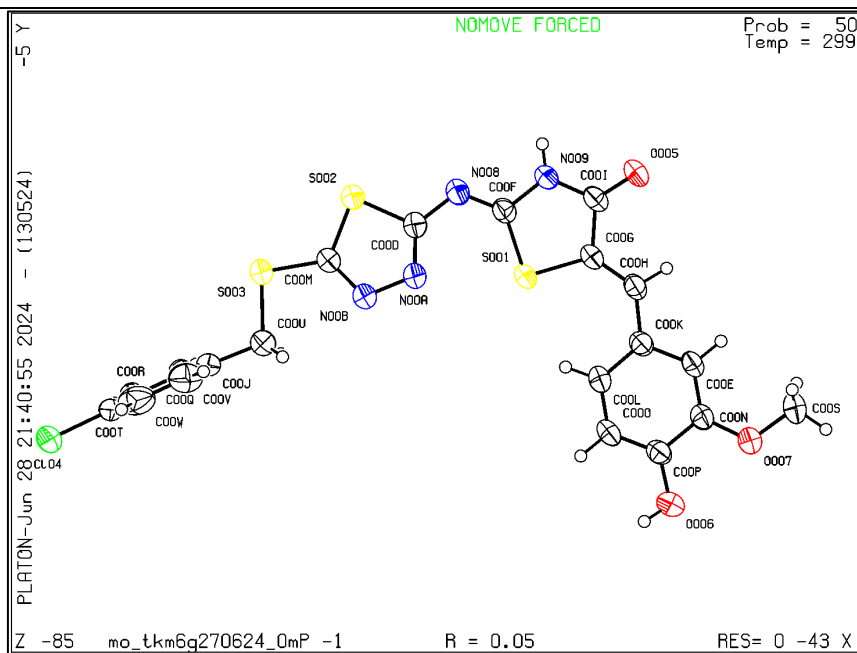


S.F47: HRMS Compound 7f

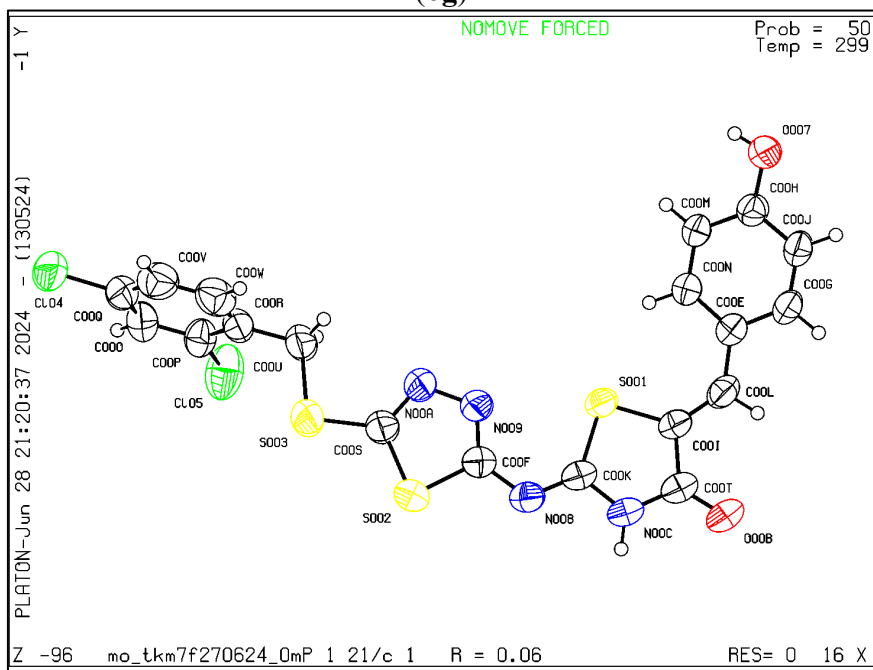


S.F48: HRMS Compound 7g

X-Ray Crystallography of compounds 6g and 7f:



(6g)



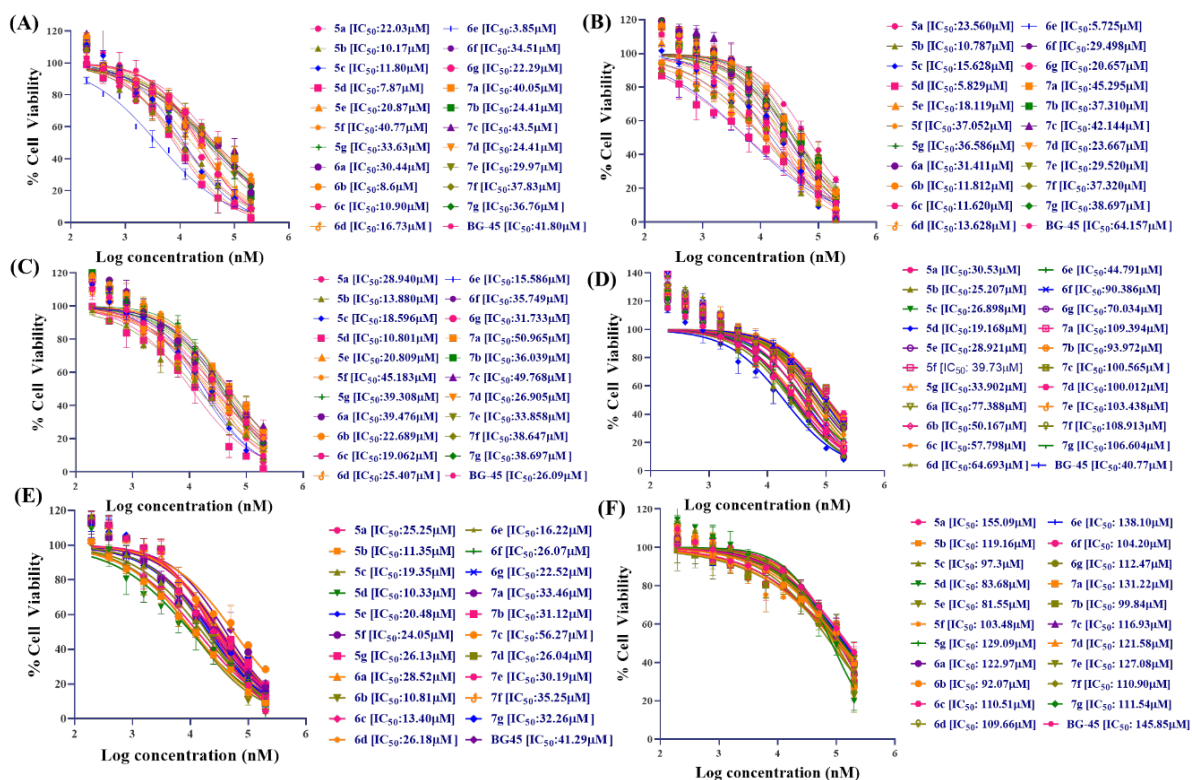
(7f)

S.F49: Molecular geometries of (a) 6g and (b) 7f in crystals.

Table S1: Crystallographic table:

Complexes	6g	7f
CCDC	2366716	2366780
formula	C ₂₀ H ₁₅ ClN ₄ O ₃ S ₃	C ₁₉ H ₁₂ Cl ₂ N ₄ O ₂ S ₃
fw	490.99	495.41
crystal system	triclinic	monoclinic
space group	P -1	P 21/c
<i>a</i> (Å)	10.270(2)	10.146(2)
<i>b</i> (Å)	10.497(2)	17.022(5)
<i>c</i> (Å)	13.887(3)	15.237(4)
α (°)	73.266(7)	90
β (°)	81.446(7)	101.398(7)
γ (°)	85.763(6)	90
<i>V</i> (Å ³)	1416.8(5)	2579.5(11)
<i>Z</i>	2	4
<i>T</i> (K)	299	299
D _x , g cm ⁻³	1.275	1.477
μ (mm ⁻¹)	0.389	0.607
R1 ^a [I>2 σ (I)]/GOF ^b	0.0514/ 1.020	0.0580/ 1.026
wR2 ^c (I>2 σ (I))	0.1689	0.1938
observation criterion: ^a R1 = $\Sigma F_o - F_c /\Sigma F_o $. ^b GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, ^c wR2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2+bP]$, $P = (F_o^2+2F_c^2)/3$.		

Biological assay data:



S.F50: Dose-response curve and IC₅₀ values of **5a-g**, **6a-g**, and **7a-g** series of compounds along with **BG45**. All compounds were tested in the concentrations range of 0.195 μM - 200 μM on (A) MCF-7, (B) PC3, (C) 4T1, (D) MOC2, (E) MDA-MB-231, and (F) HEK-293. Cells were treated with compounds for 48 h, and cell viability was measured using the *in vitro* MTT assay method. Data represents mean ± SD (n = 2) and is plotted in dose-response format. IC₅₀ was calculated using a nonlinear regression analysis method using GraphPad Prism 8.0.1.

NB. S. F: Supplementary Figure