

Synthesis and Antibacterial Evaluation of Novel 1,3,4-Oxadiazole Derivatives Containing Sulfonate/Carboxylate Moiety

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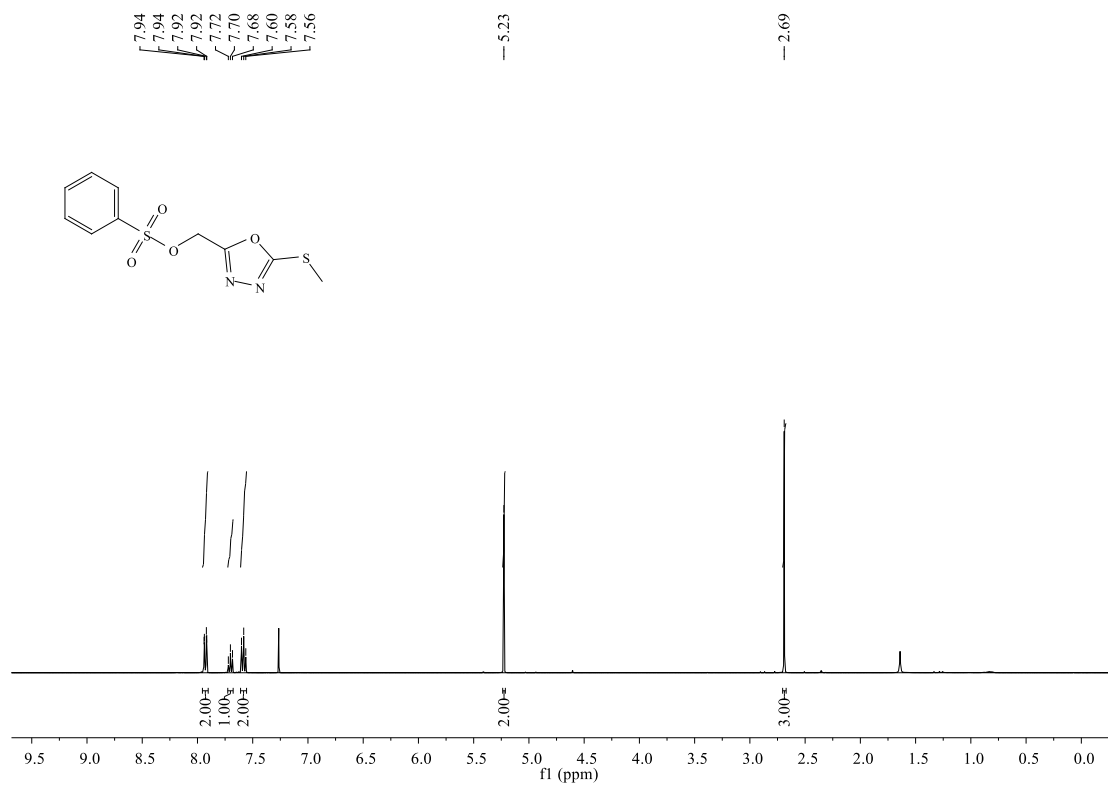
Supplemental Materials

1. *In Vitro* Antibacterial Activity

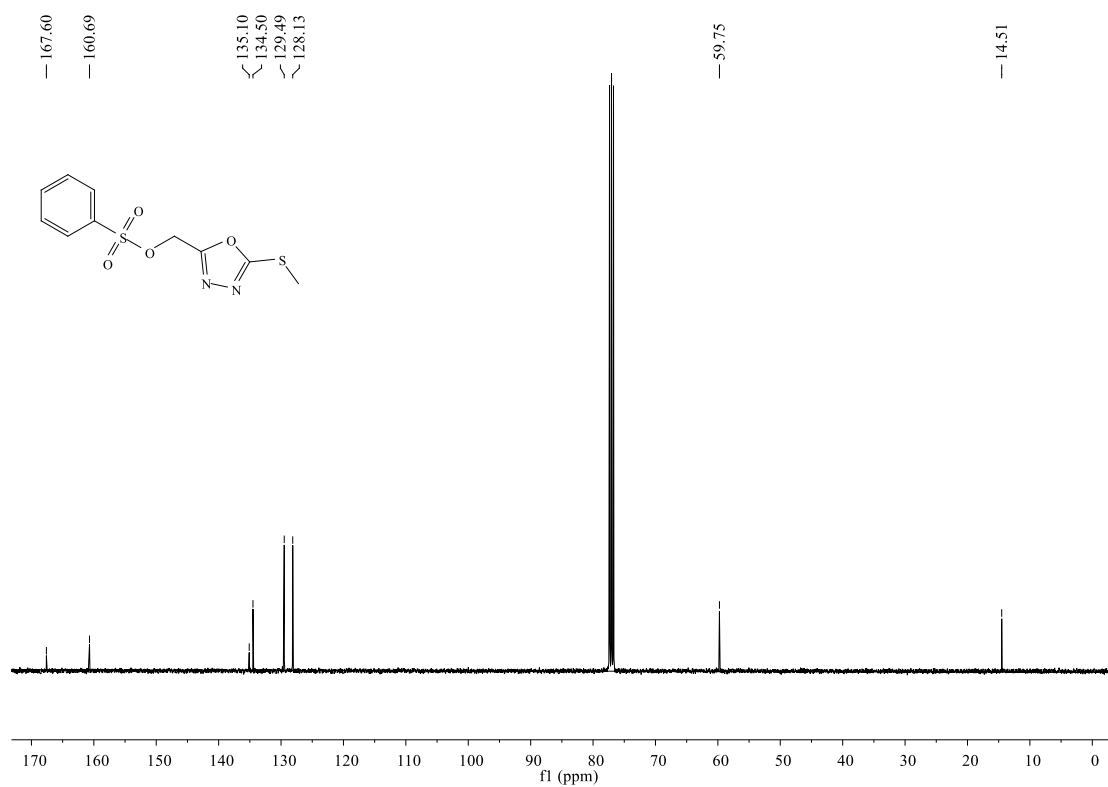
Table1. EC₅₀ (μM) of some target compounds against *Xanthomonas oryzae pv. oryzae* and *Xanthomonas axonopodis pv. citri*^a

Compd.	<i>Xanthomonas oryzae pv. oryzae</i>			<i>Xanthomonas axonopodis pv. citri</i>		
	EC ₅₀ (μM)	regression equation	r	EC ₅₀ (μM)	regression equation	r
4a-1	63.4±3.8	y = 2.70x + 0.13	0.988	114.0±6.6	y=1.85x + 1.18	0.977
4a-2	50.1±4.2	y = 3.21x - 0.45	0.988	95.8±4.6	y=2.10x + 1.04	0.984
4a-3	87.2±4.7	y = 2.87x - 0.58	0.964	132.5±7.5	y=1.56x + 1.69	0.976
4a-4	99.4±4.7	y = 3.11x - 1.22	0.966	155.2±5.8	y=1.32x + 2.10	0.979
4a-11	98.0±6.6	y = 3.22x - 1.41	0.953	/	/	/
4a-12	95.3±3.9	y = 3.15x - 1.23	0.954	/	/	/
4a-13	86.4±4.8	y = 3.22x - 1.23	0.951	/	/	/
4a-14	69.0±4.4	y = 3.52x - 1.47	0.976	/	/	/
4a-15	83.4±6.0	y = 3.32x - 1.37	0.990	/	/	/
4a-16	112.5±6.0	y = 2.60x - 0.33	0.946	/	/	/
Bismethiazol ^b	253.5±7.6	y = 2.03x + 0.12	0.969	274.3±8.6	y=1.76x + 0.70	0.978
Thiodiazole copper ^b	467.4±15.5	y = 1.78x + 0.23	0.979	406.3±13.0	y=0.92x + 2.60	0.983

^a The statistical analysis was conducted by ANOVA method at the condition of equal variances assumed ($p > 0.05$) and equal variances not assumed ($p < 0.05$); ^b The commercial agricultural antibacterial agents Bismethiazol, and Thiodiazole copper were used as positive control.

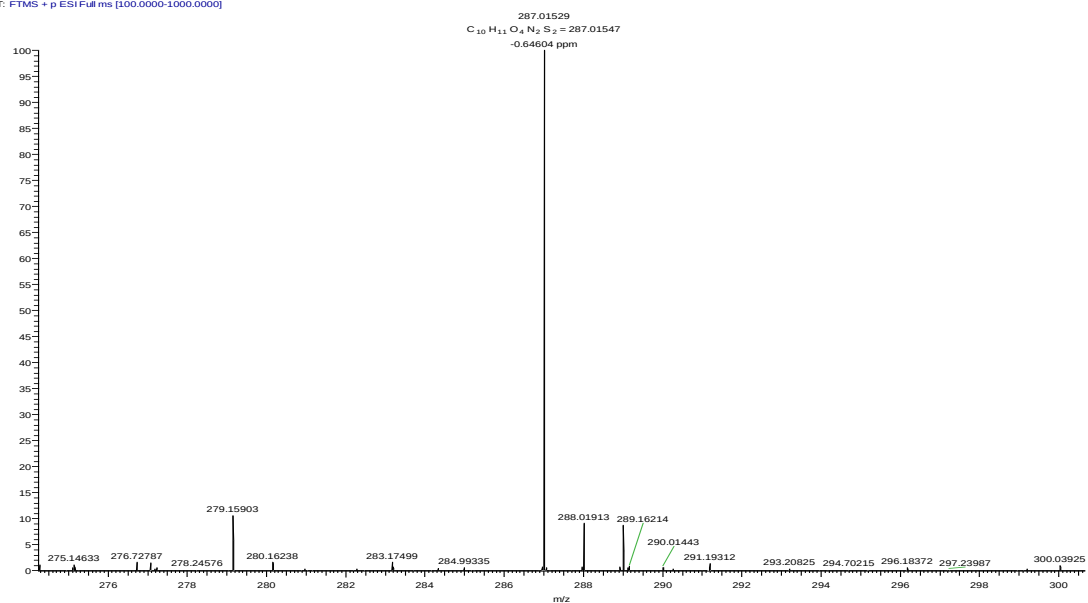


¹H NMR of compound **4a-1**

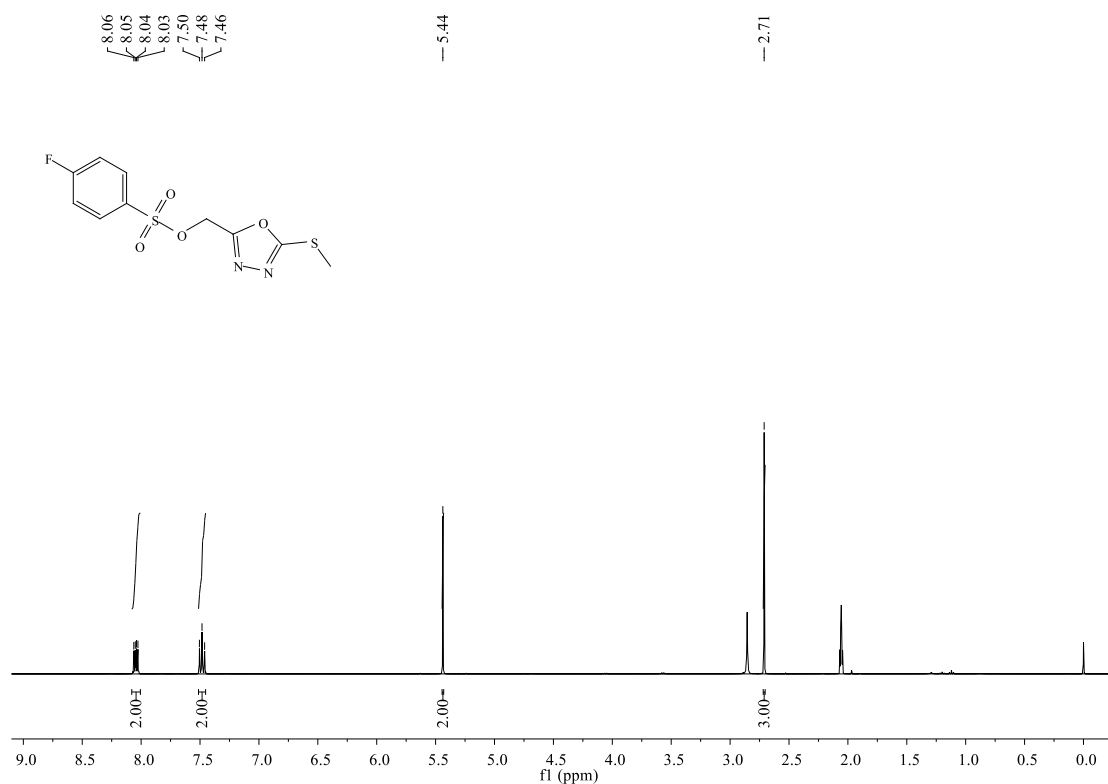


¹³C NMR of compound **4a-1**

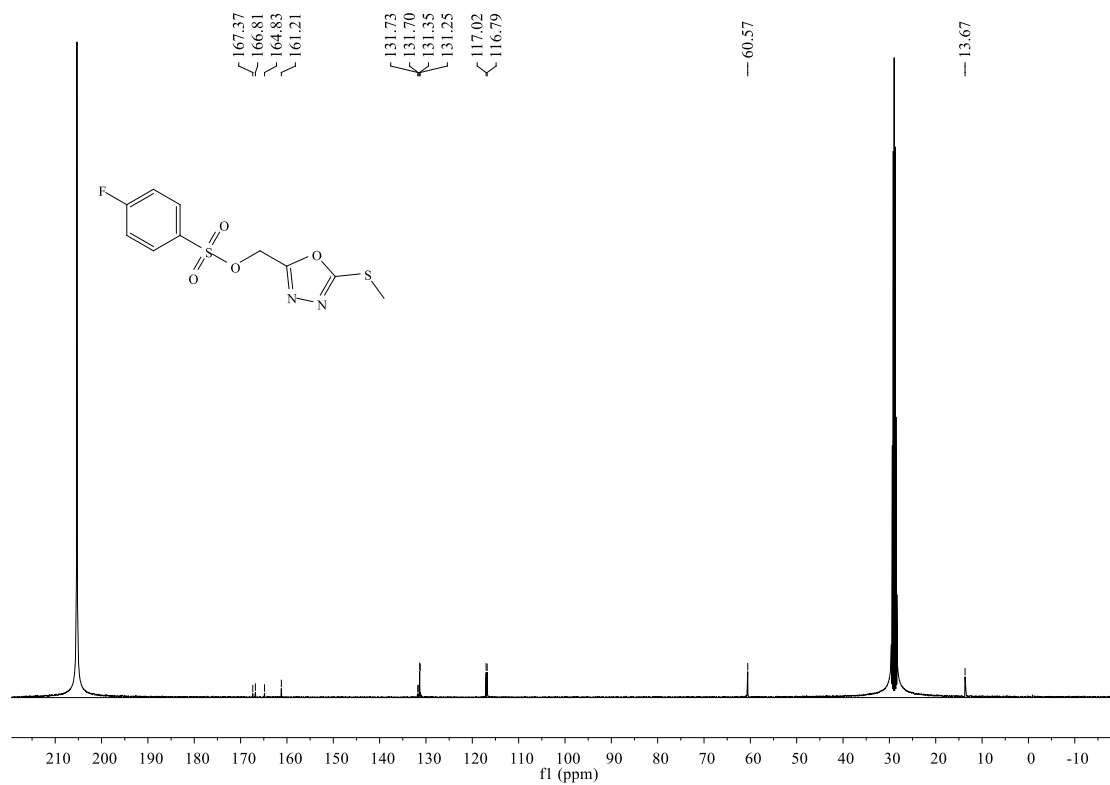
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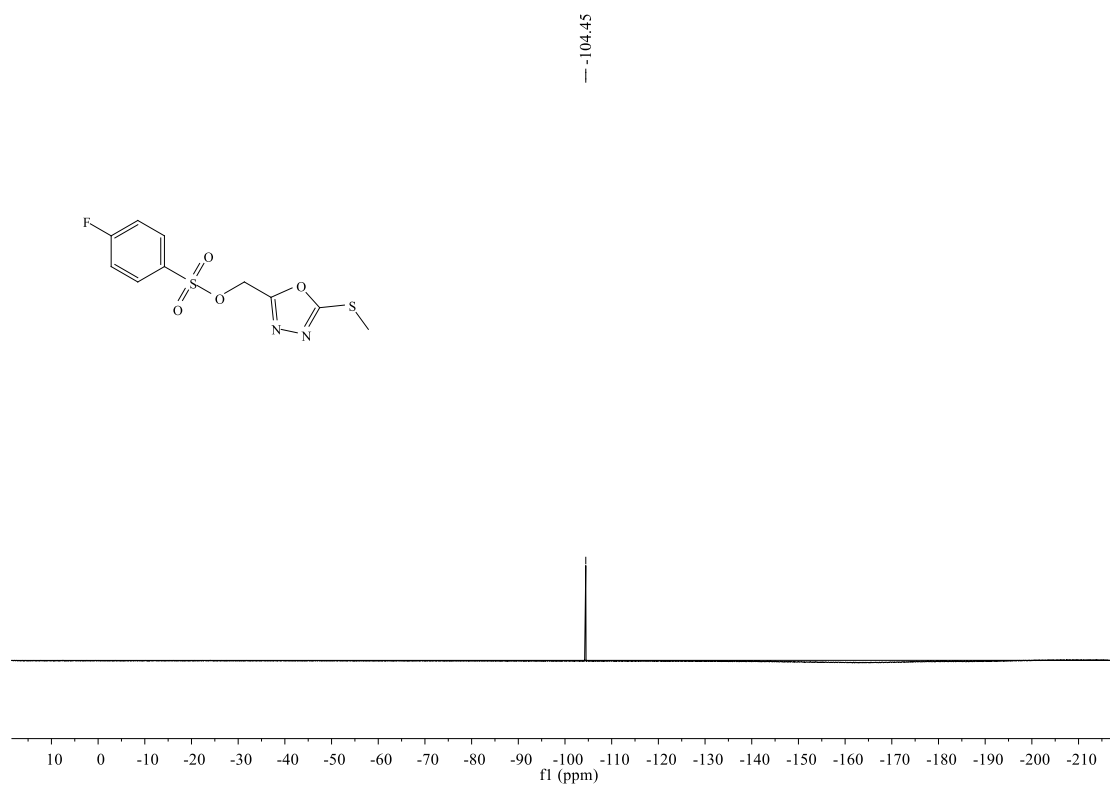
HRMS of compound 4a-1



¹H NMR of compound 4a-2

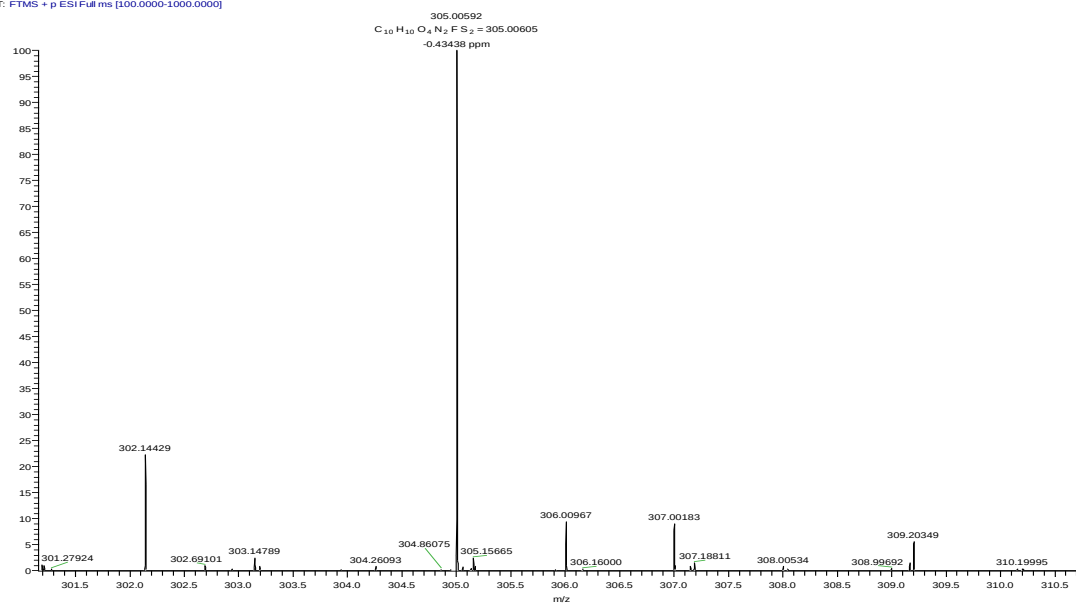


¹³C NMR of compound **4a-2**

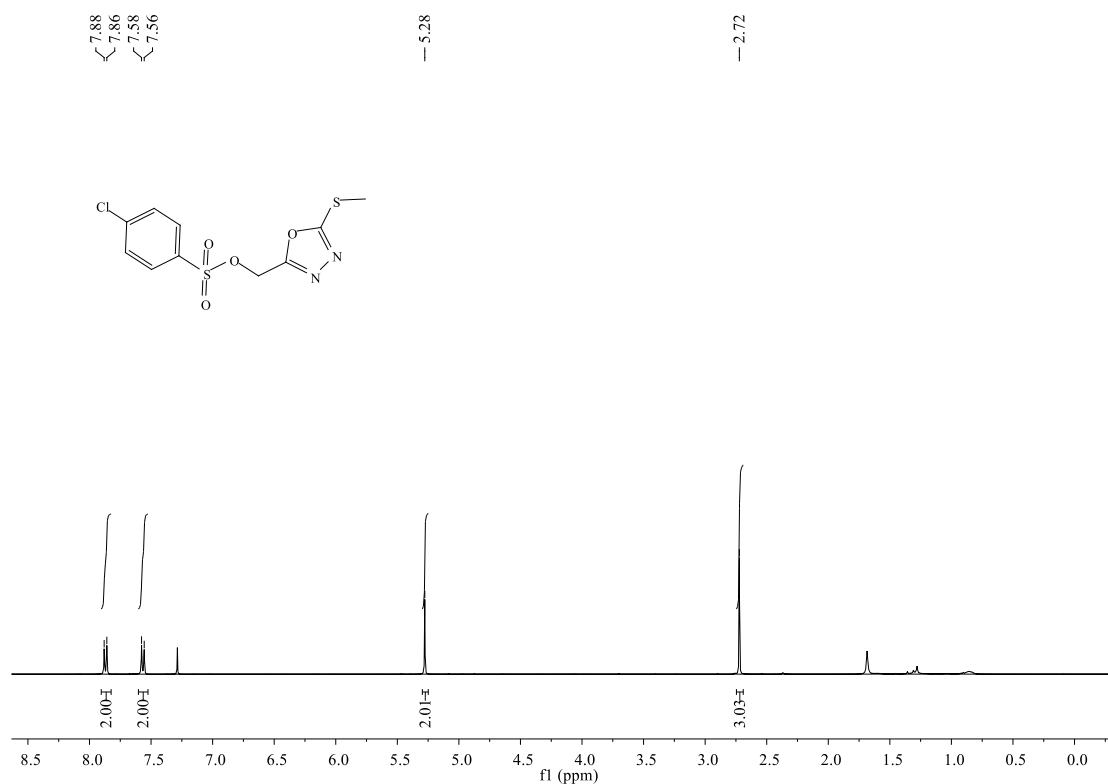


¹⁹F NMR of compound **4a-2**

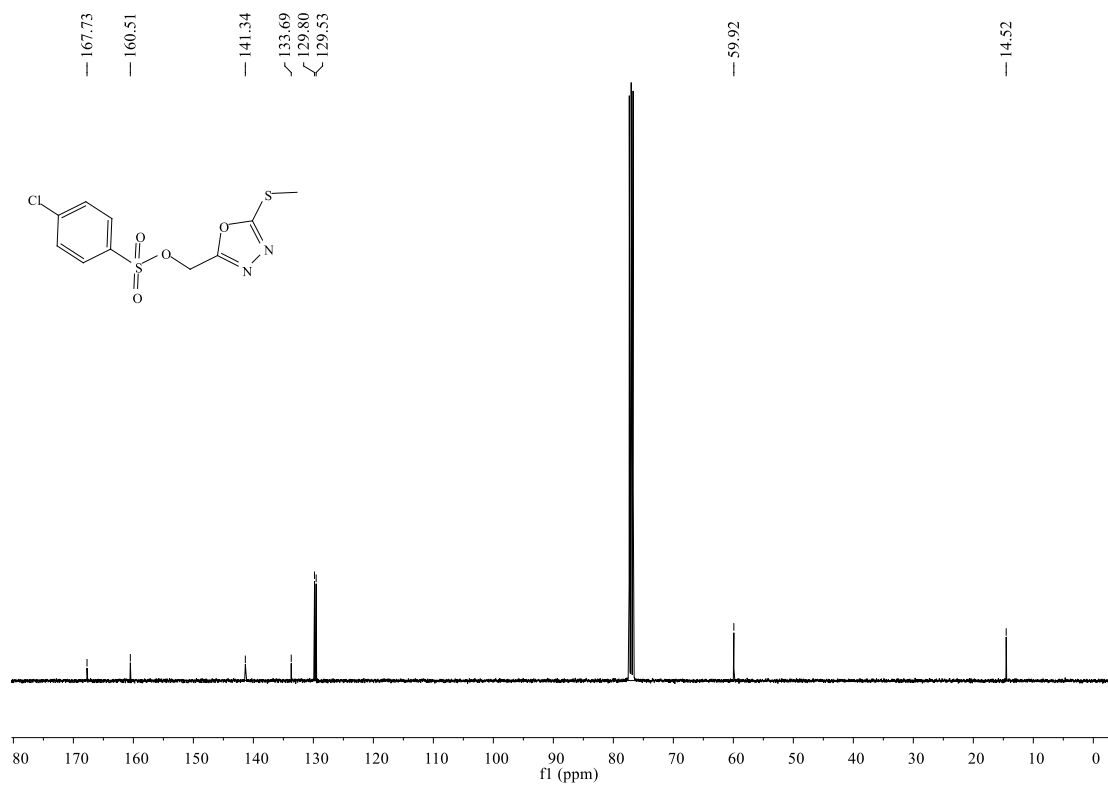
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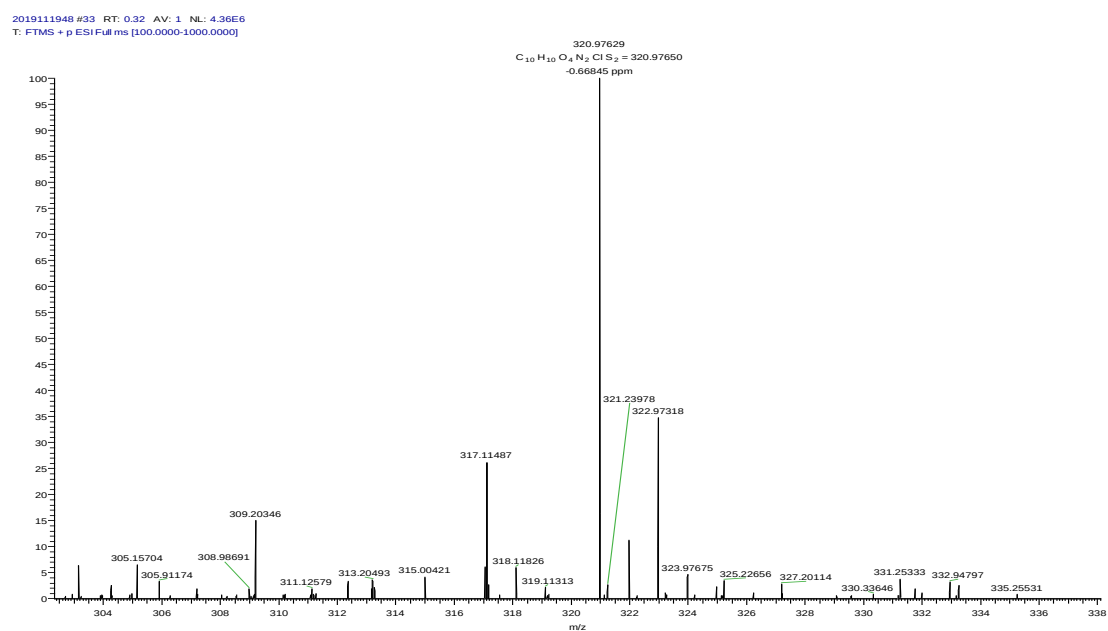
HRMS of compound **4a-2**



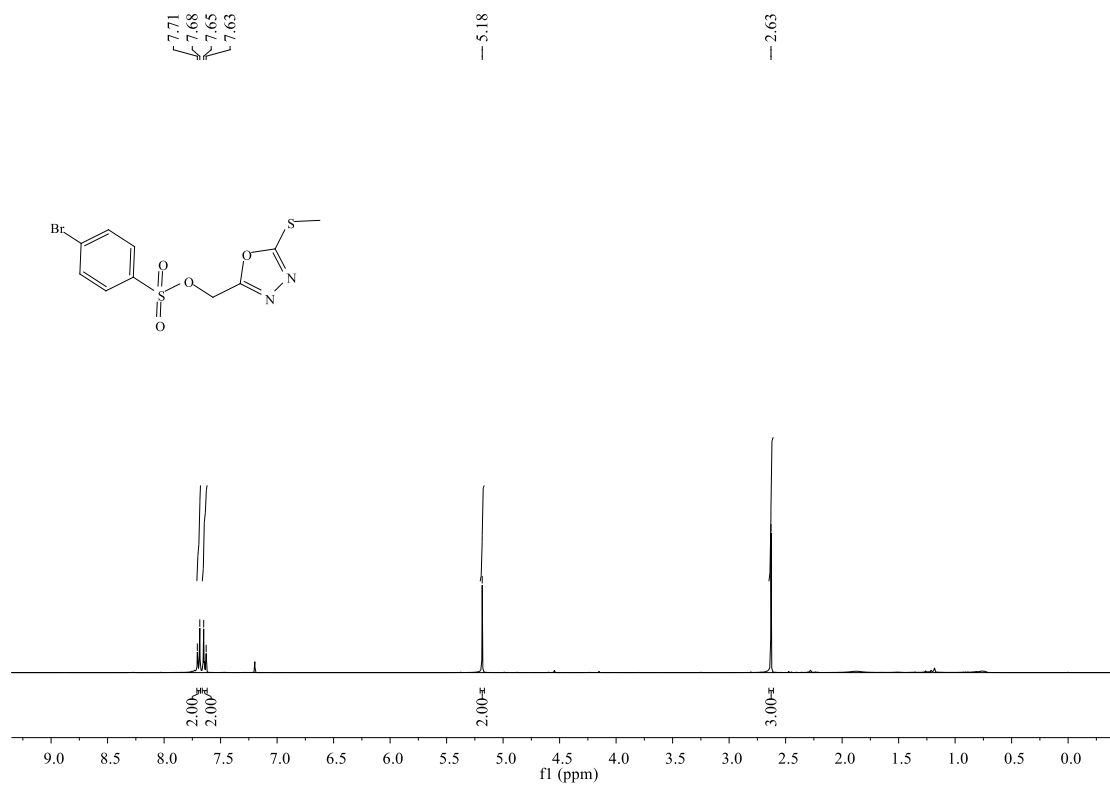
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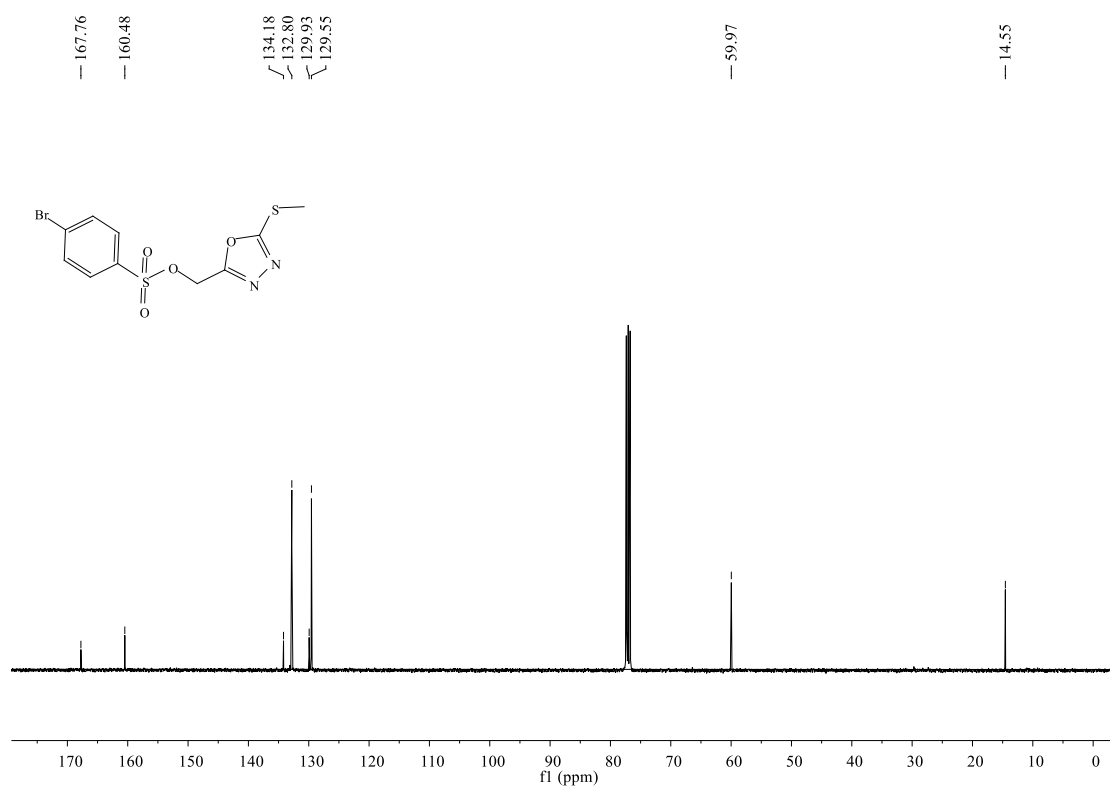
¹³C NMR of compound 4a-3



HRMS of compound 4a-3

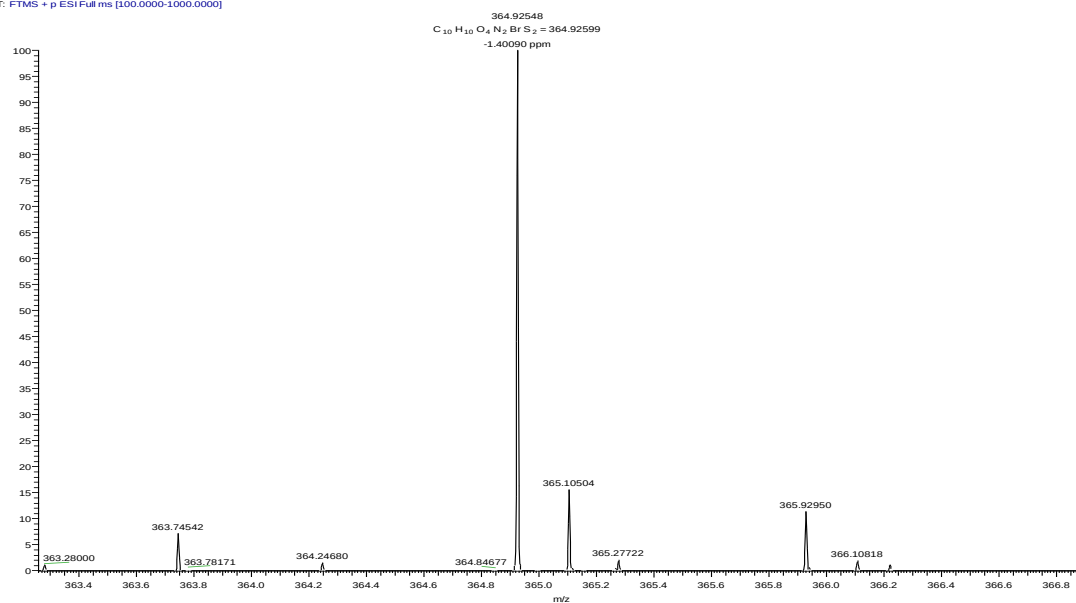


^1H NMR of compound **4a-4**

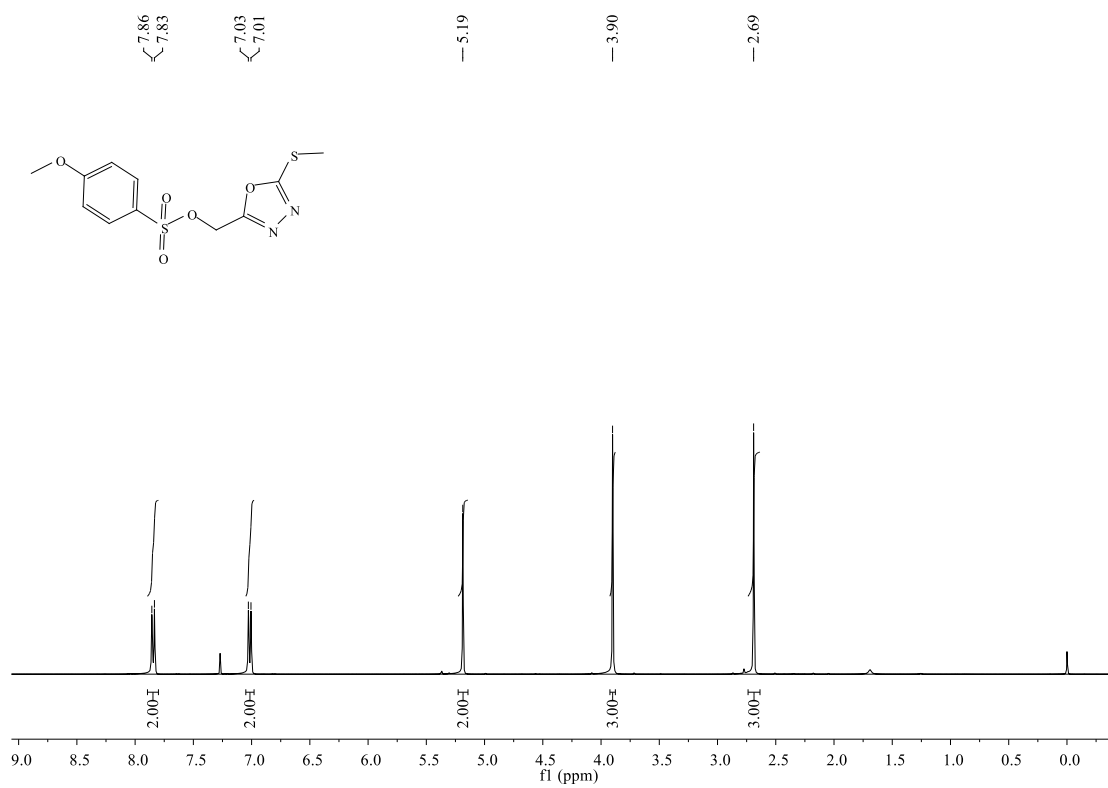


^{13}C NMR of compound **4a-4**

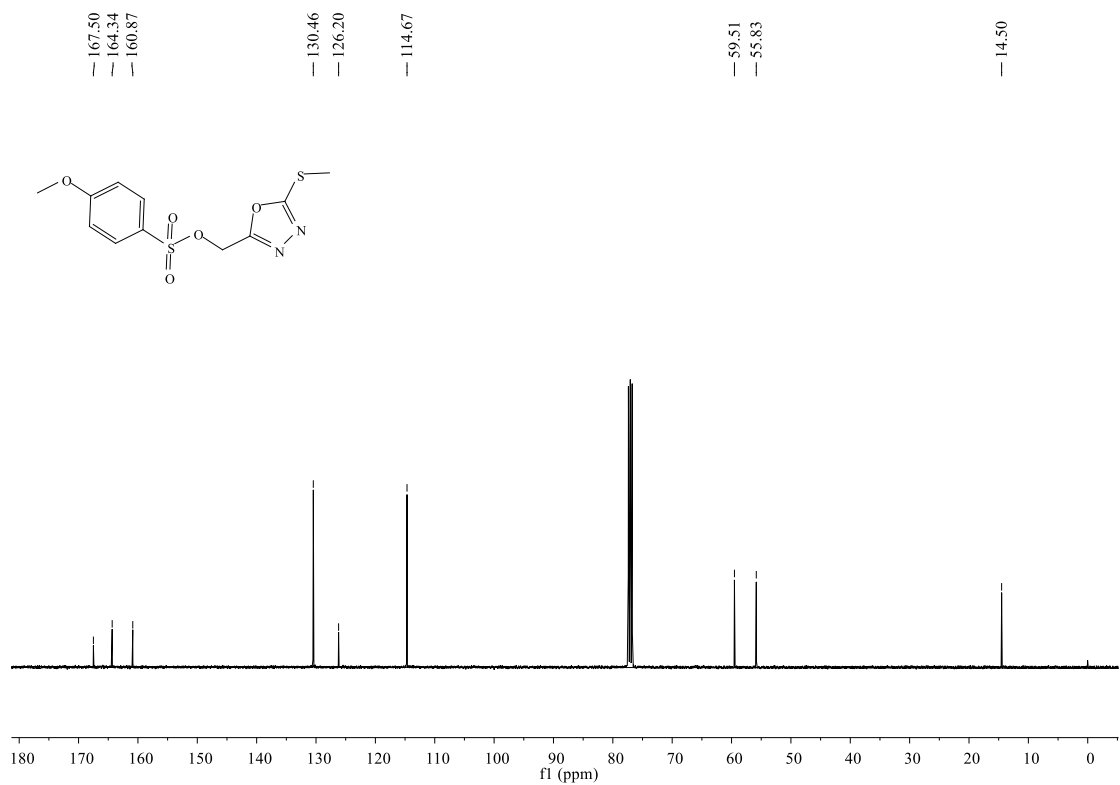
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HRMS of compound **4a-4**

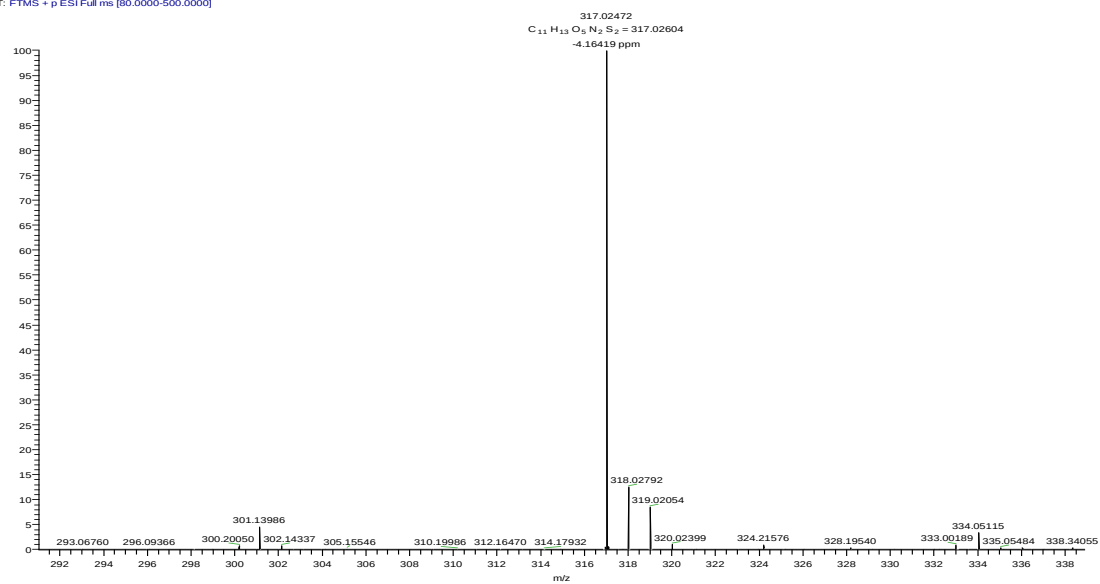


¹H NMR of compound **4a-5**

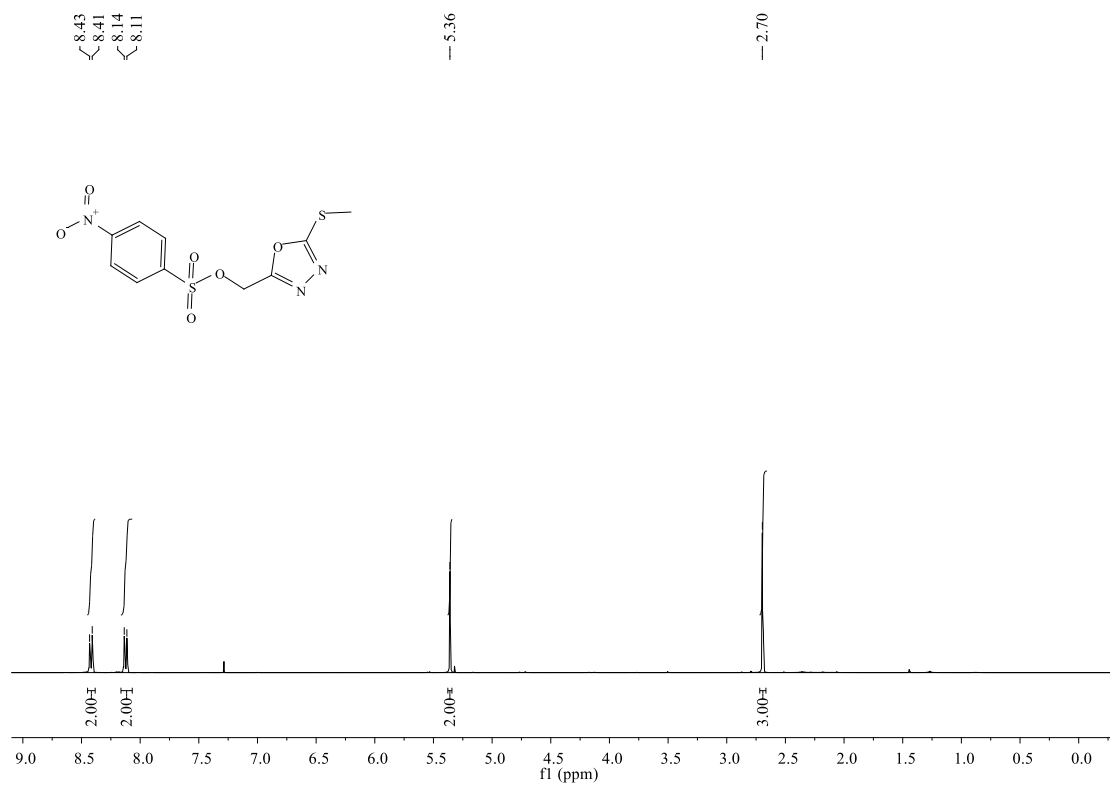


¹³C NMR of compound 4a-5

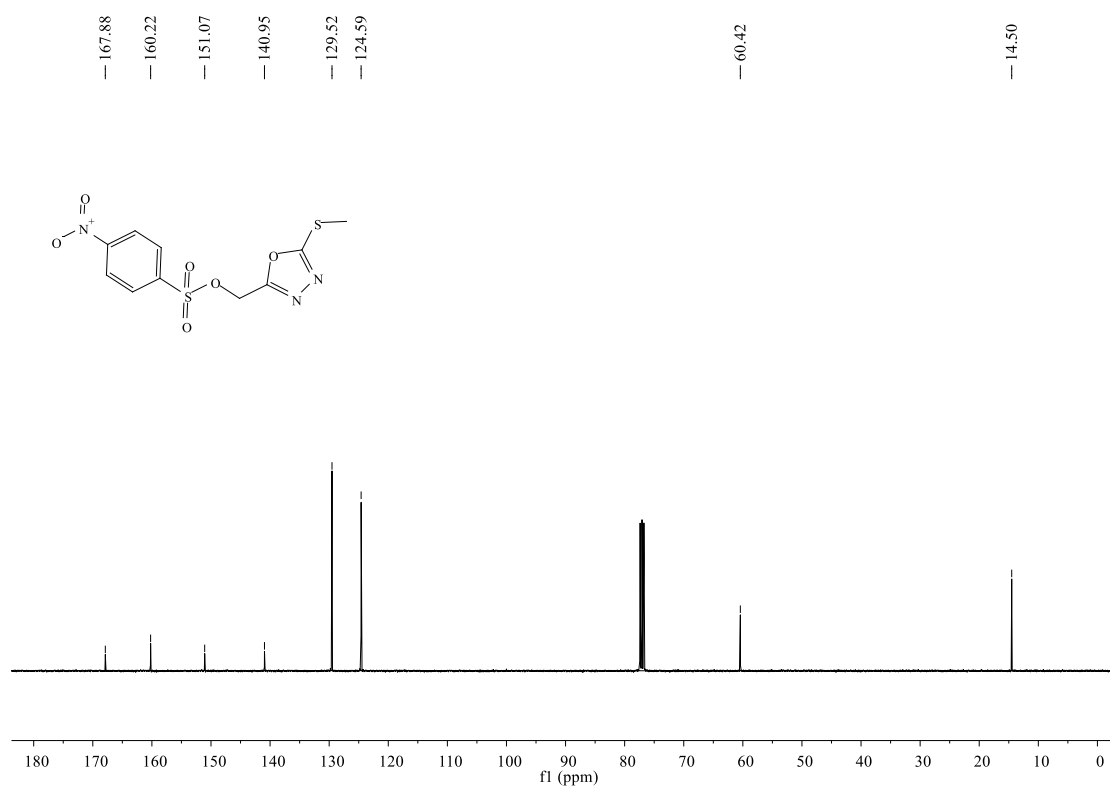
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HRMS of compound 4a-5

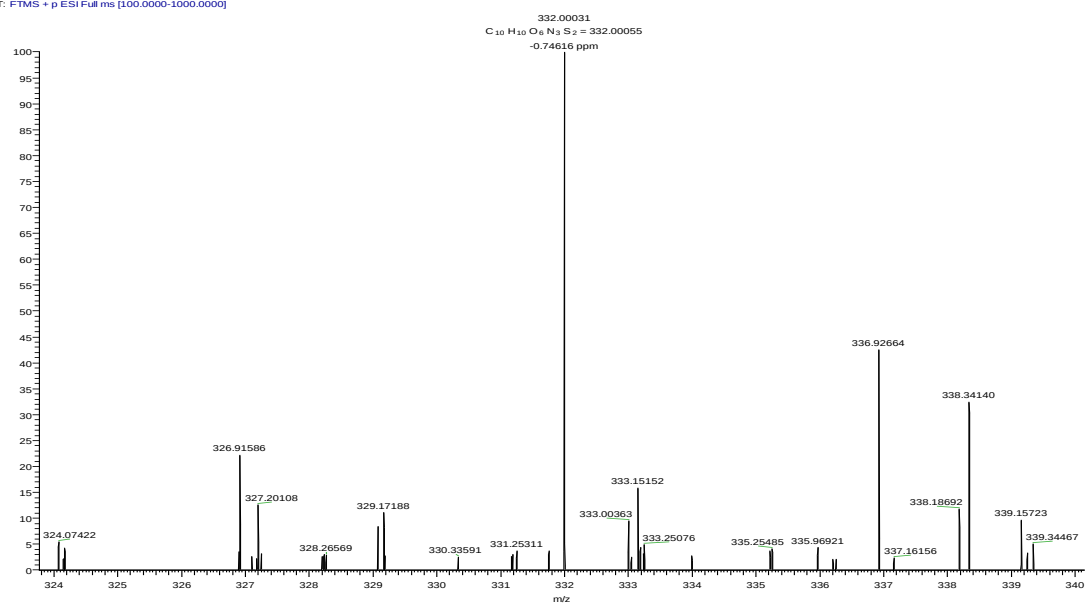


¹H NMR of compound **4a-6**

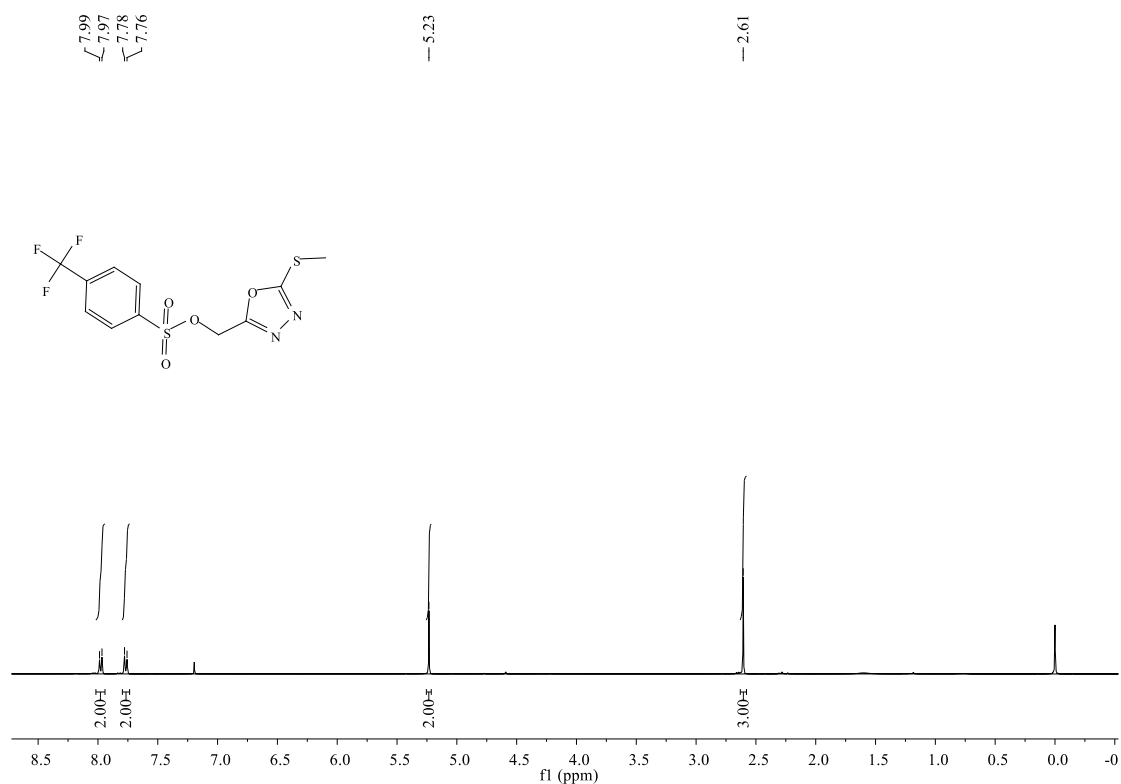


¹³C NMR of compound **4a-6**

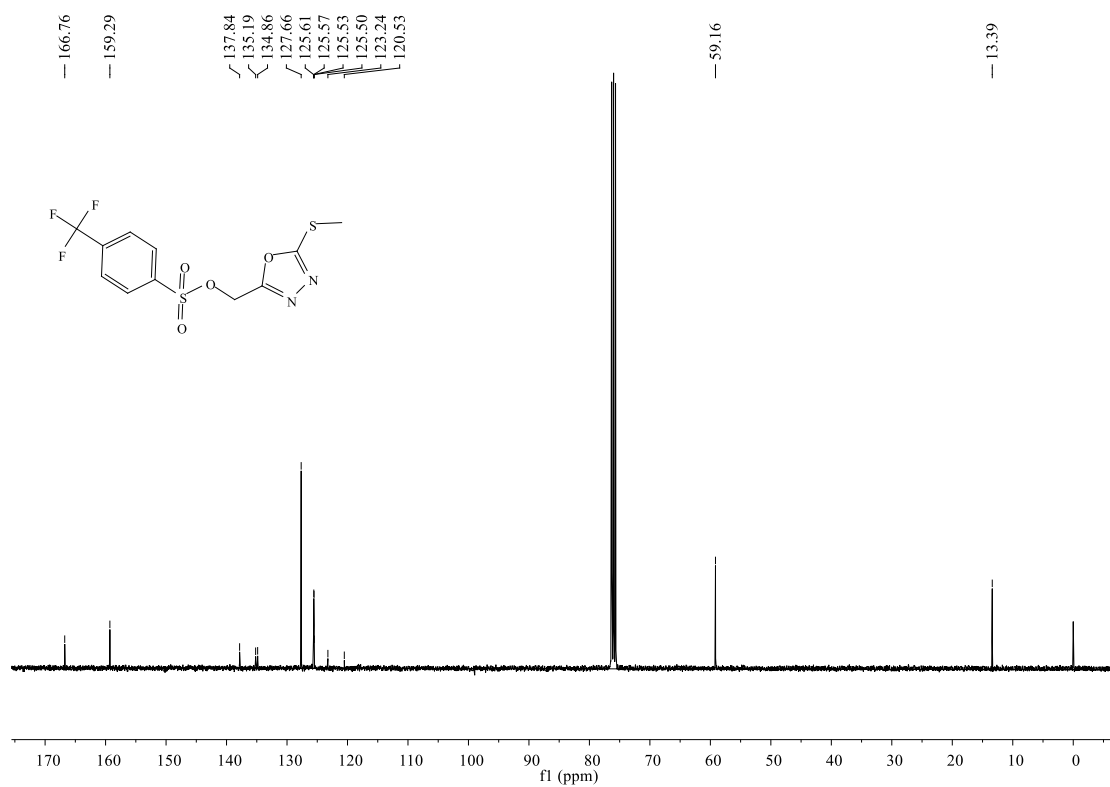
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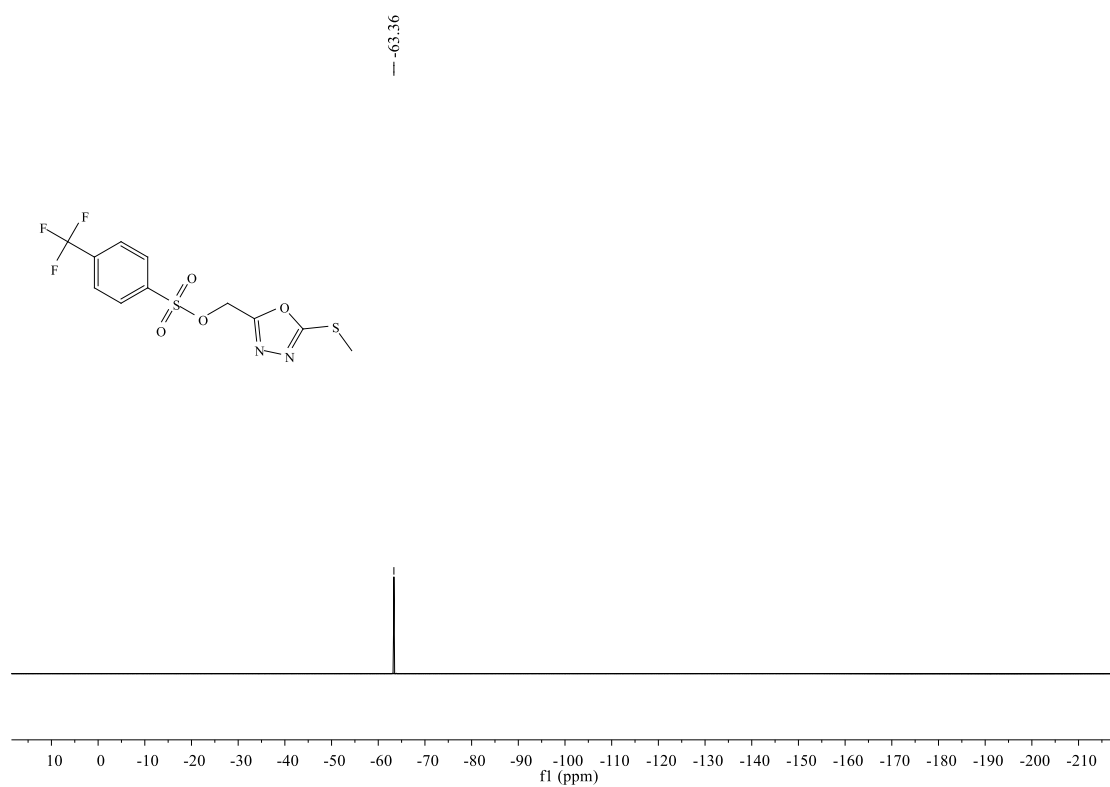
HRMS of compound 4a-6



¹H NMR of compound 4a-7

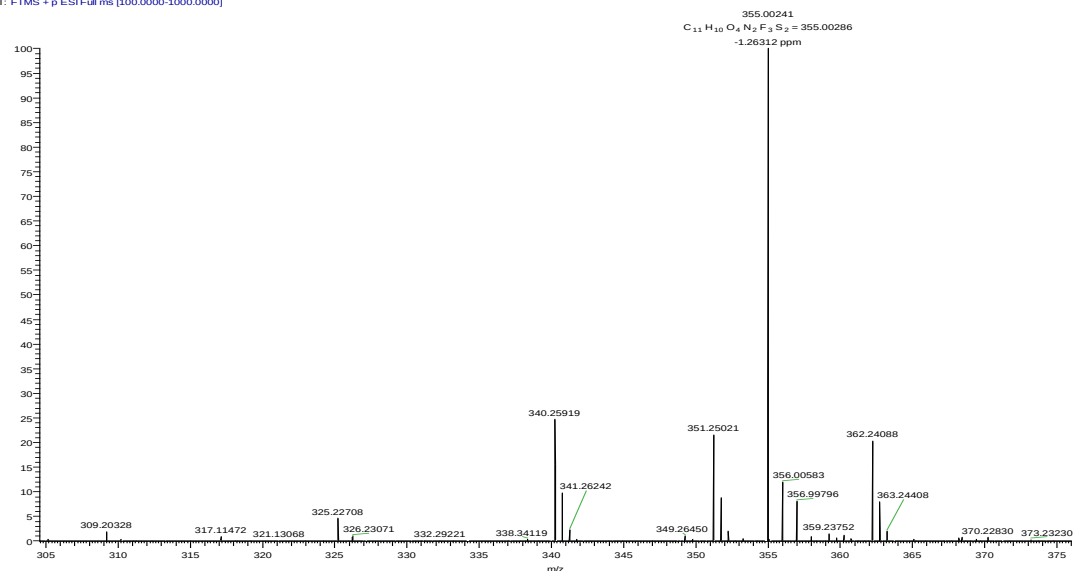


¹³C NMR of compound **4a-7**

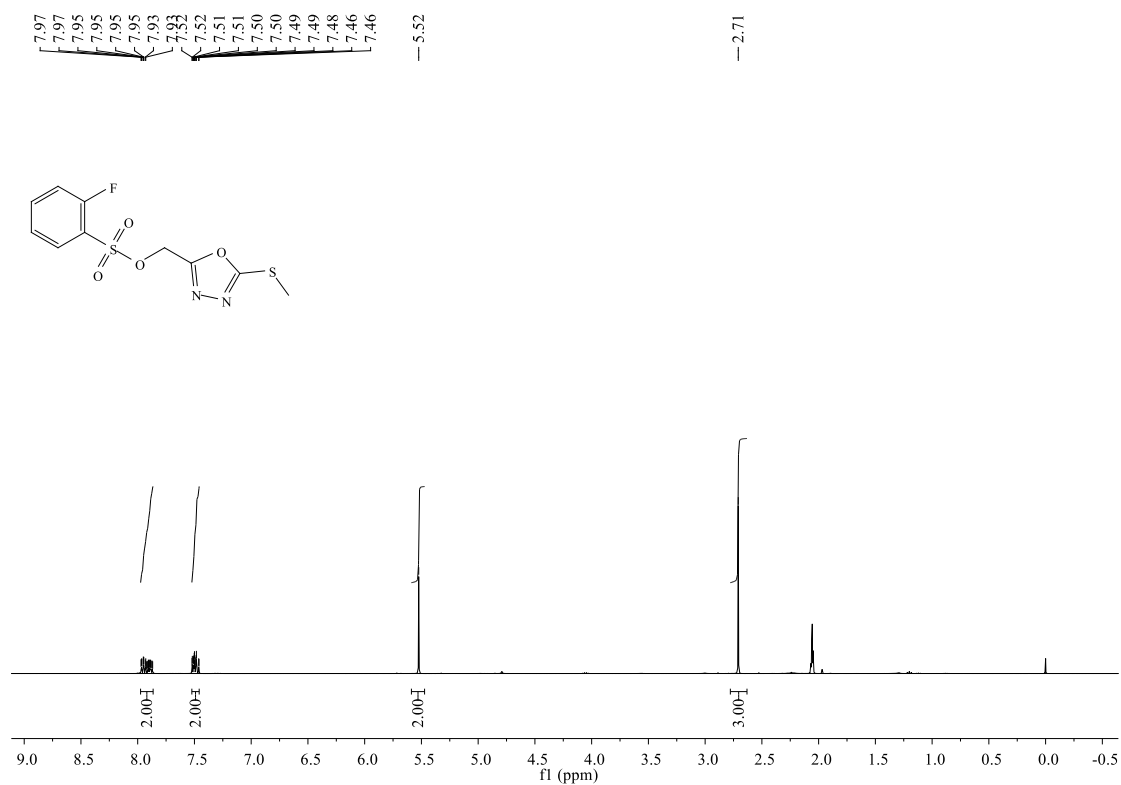


¹⁹F NMR of compound **4a-7**

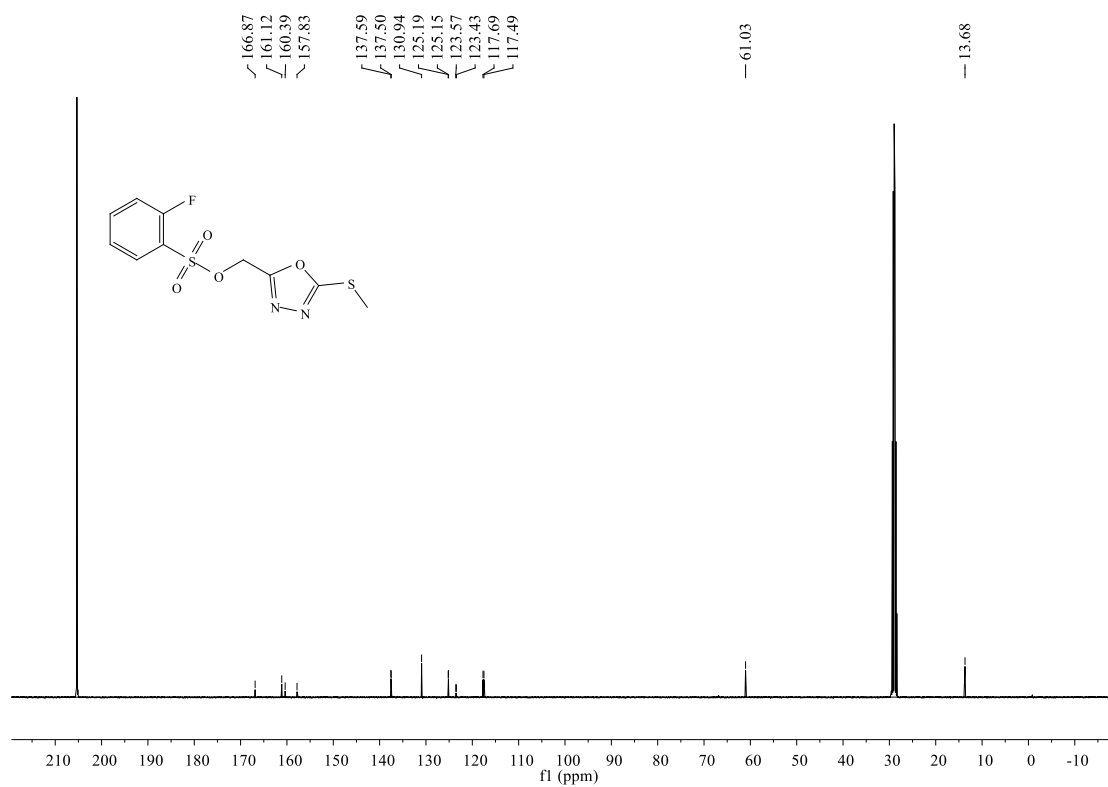
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HRMS of compound 4a-7



¹H NMR of compound 4a-8

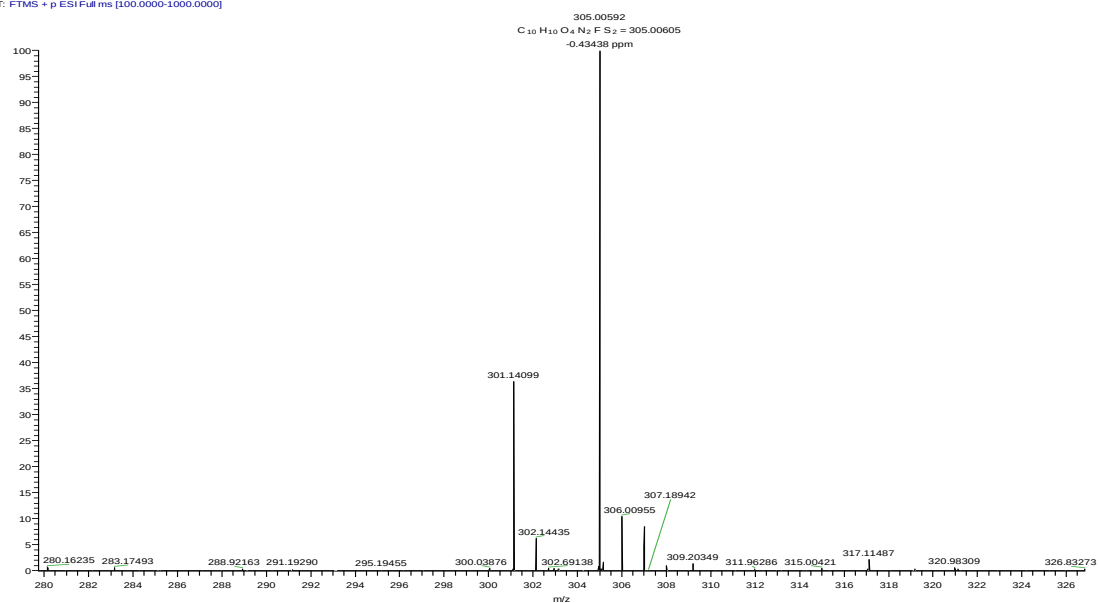


¹³C NMR of compound 4a-8

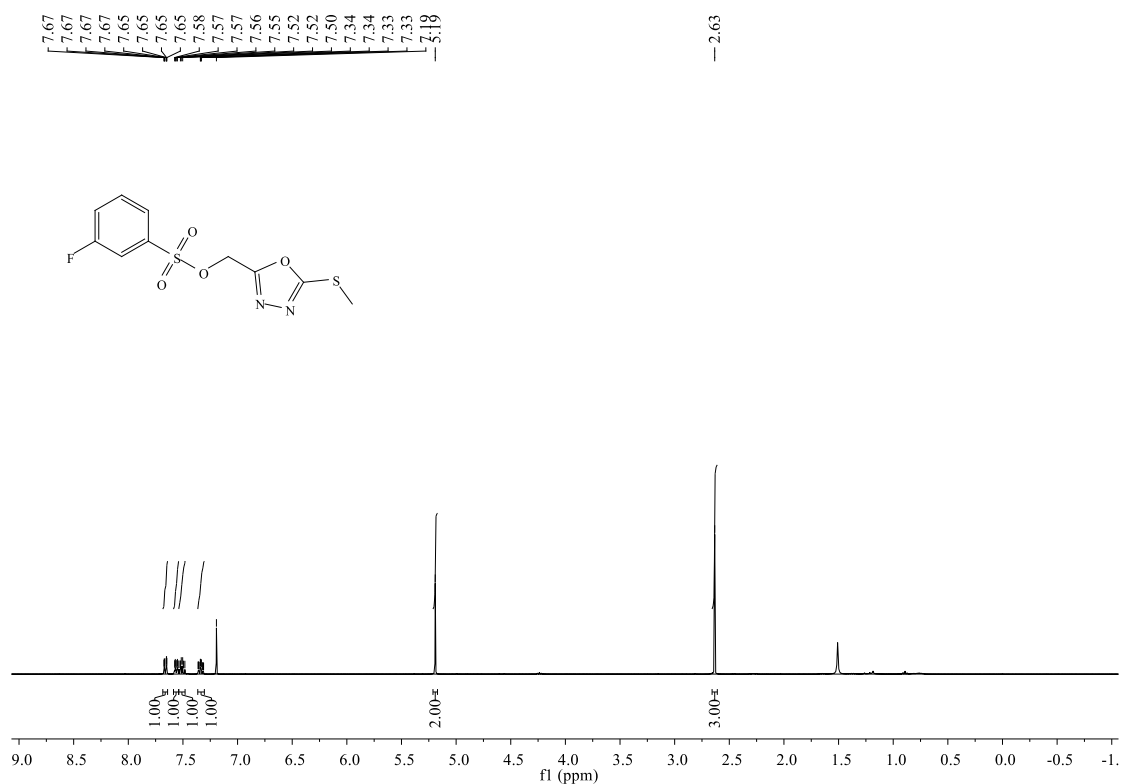


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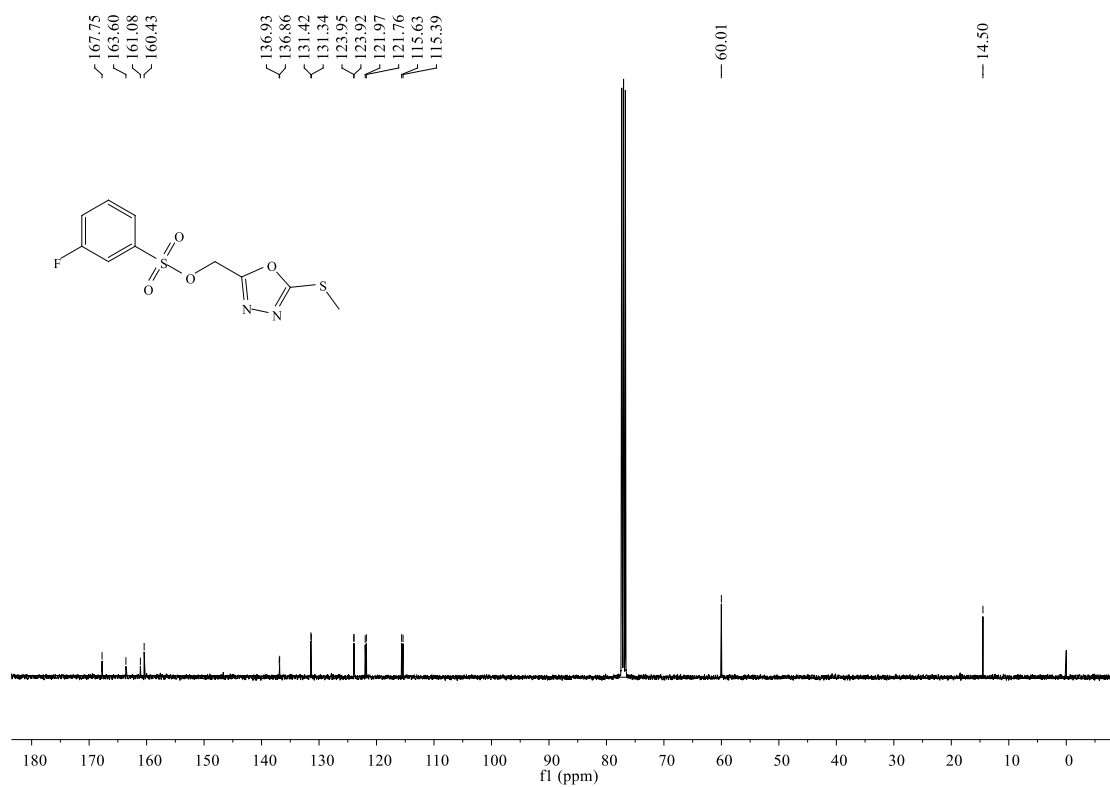
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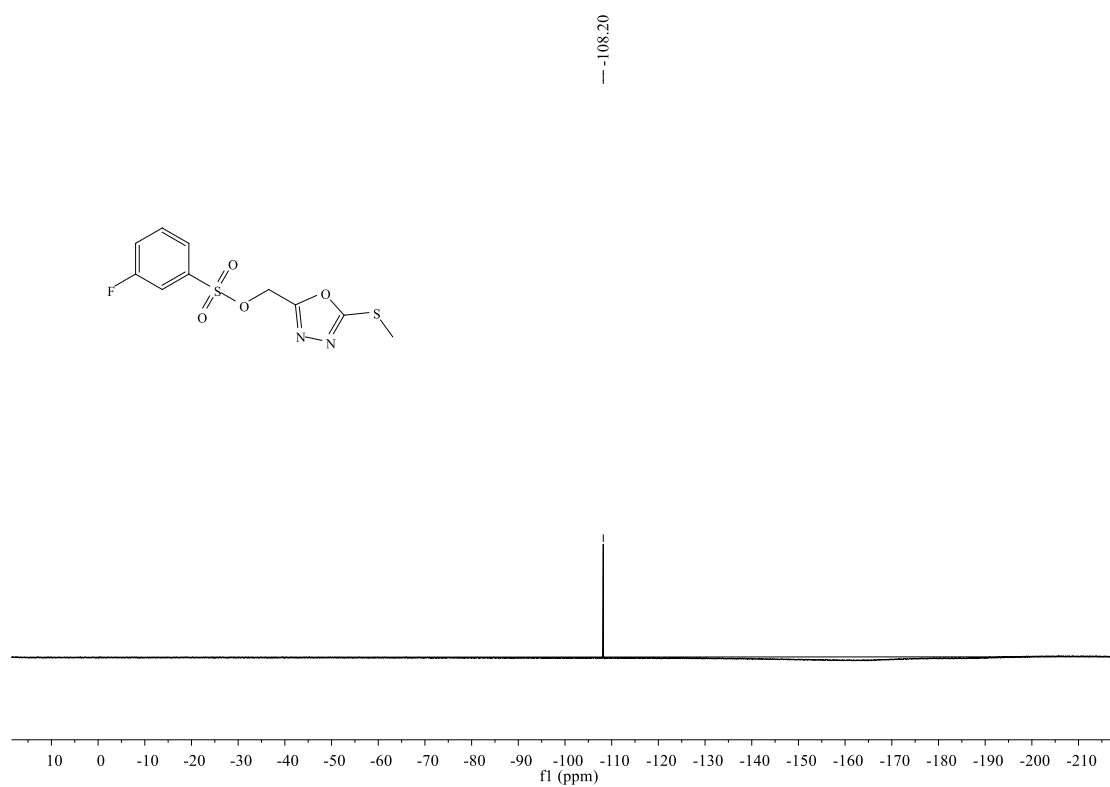
HRMS of compound 4a-8



¹H NMR of compound 4a-9

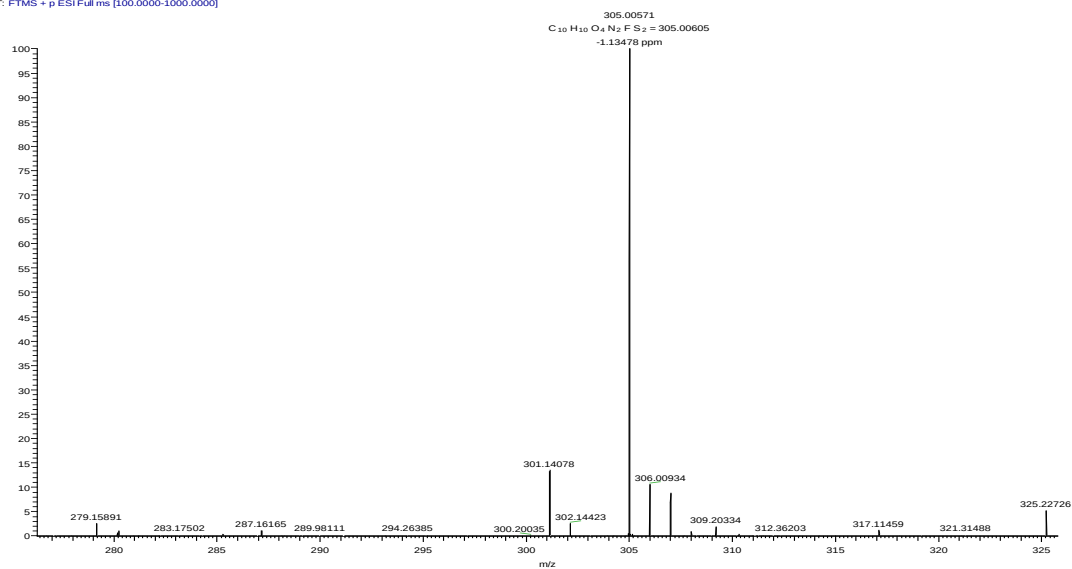


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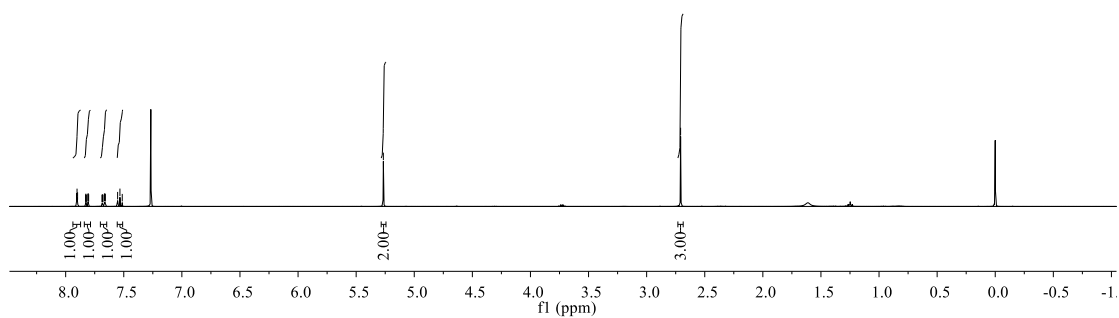
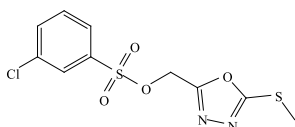
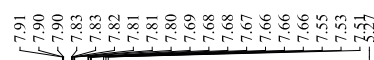


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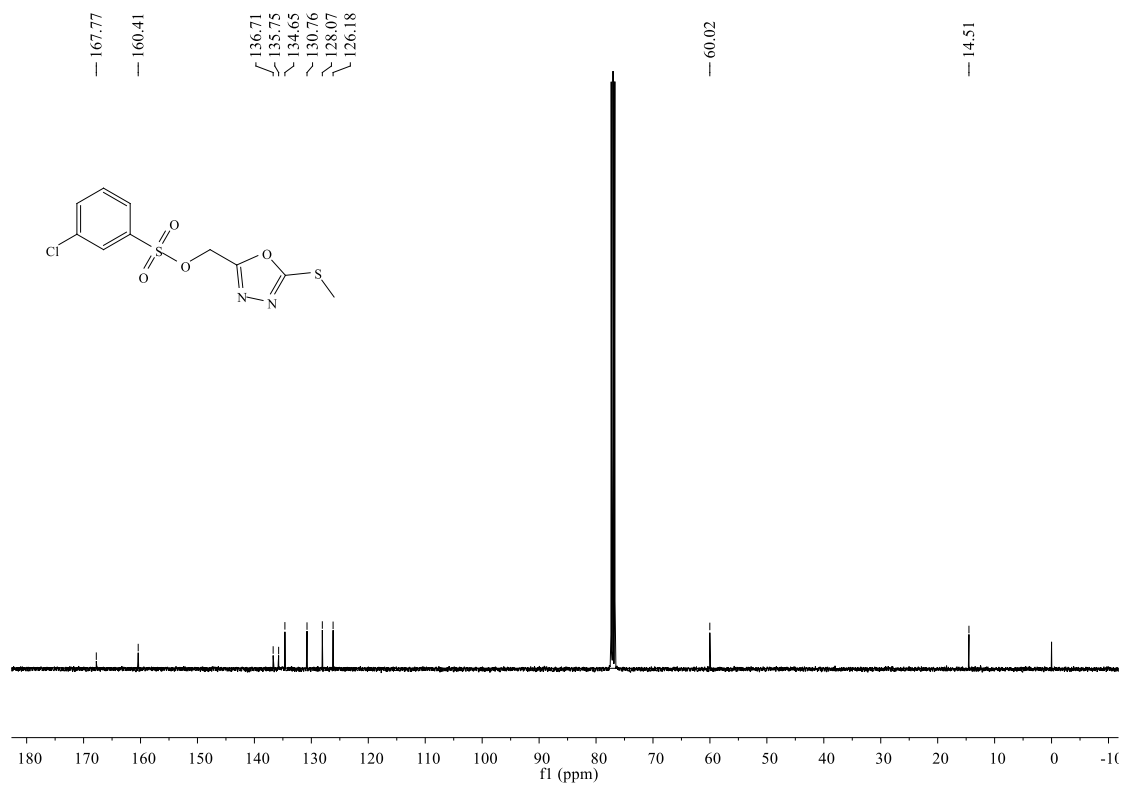
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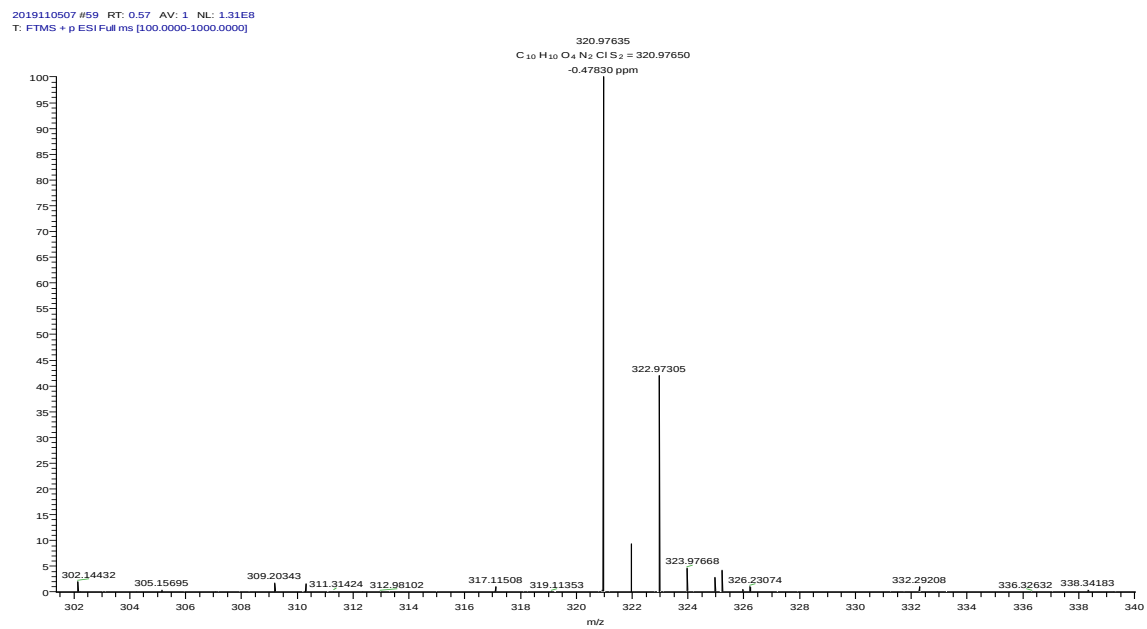
HRMS of compound 4a-9



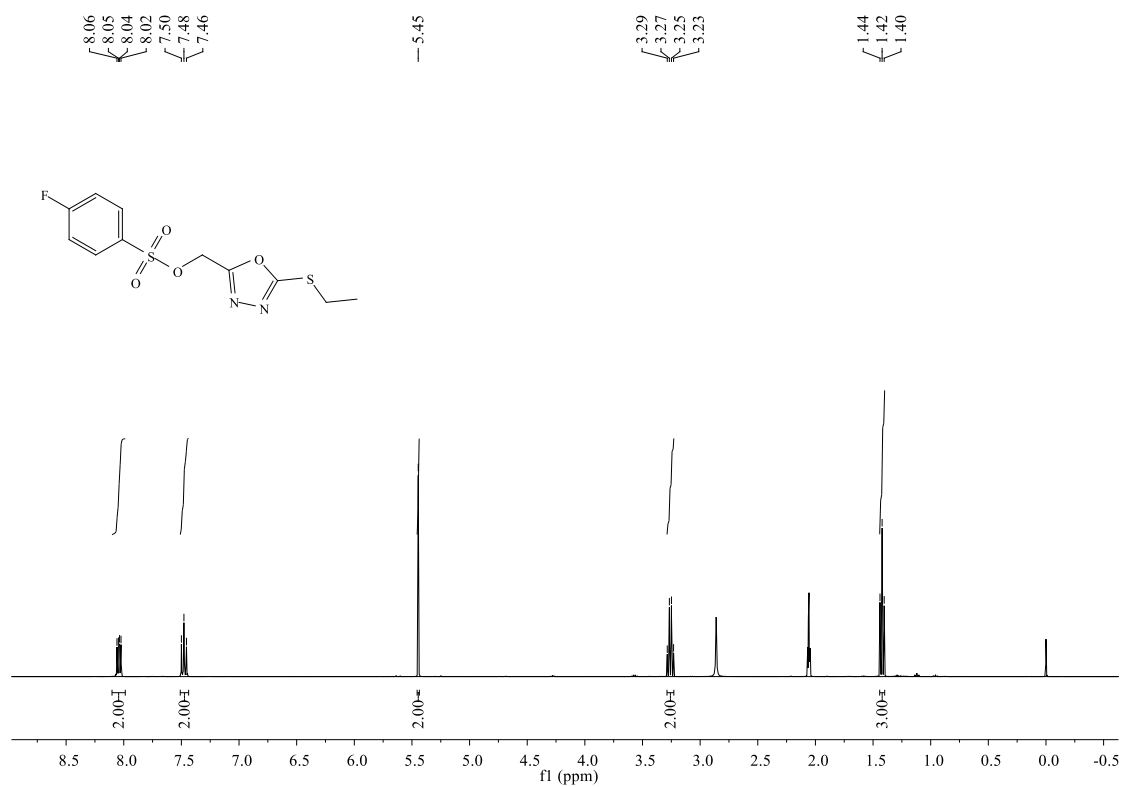
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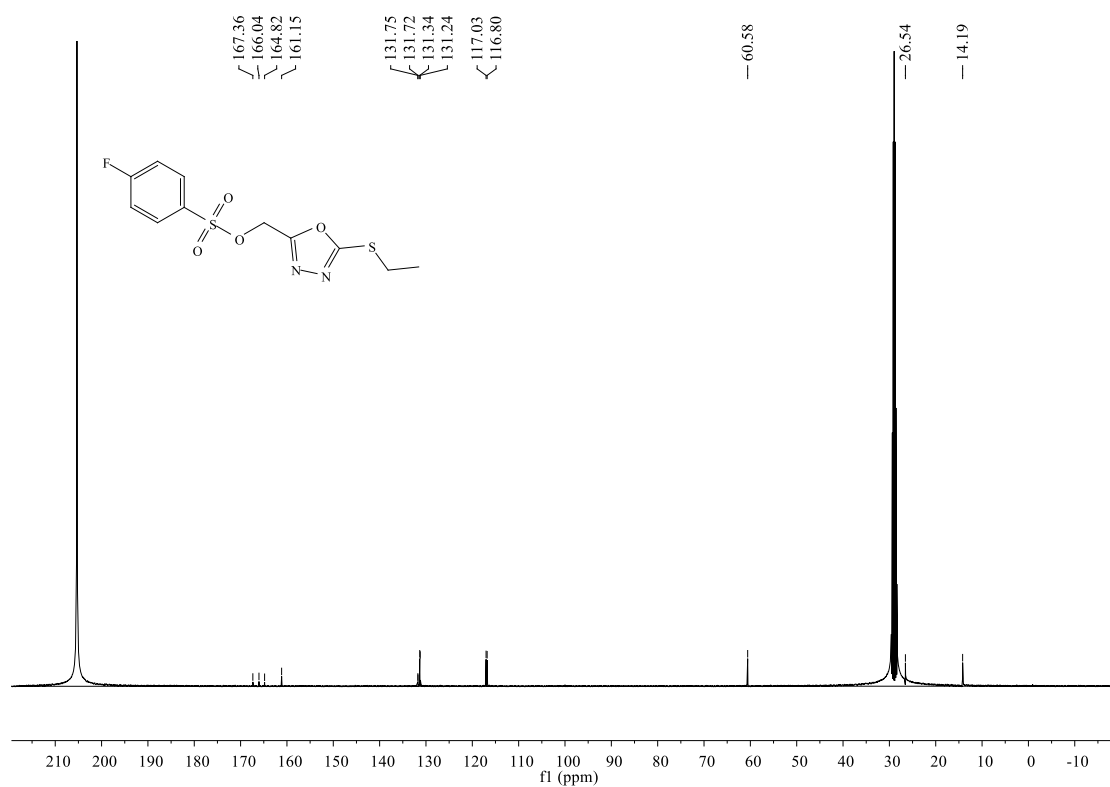
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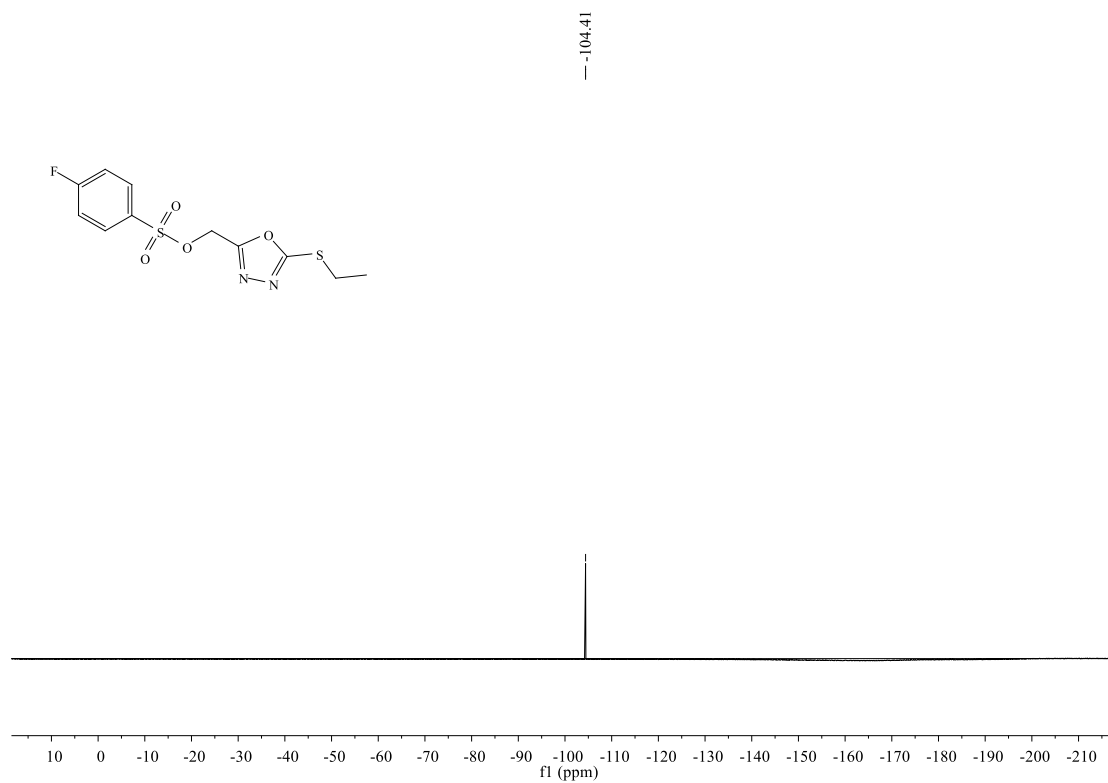
HRMS of compound 4a-10



^1H NMR of compound **4a-11**

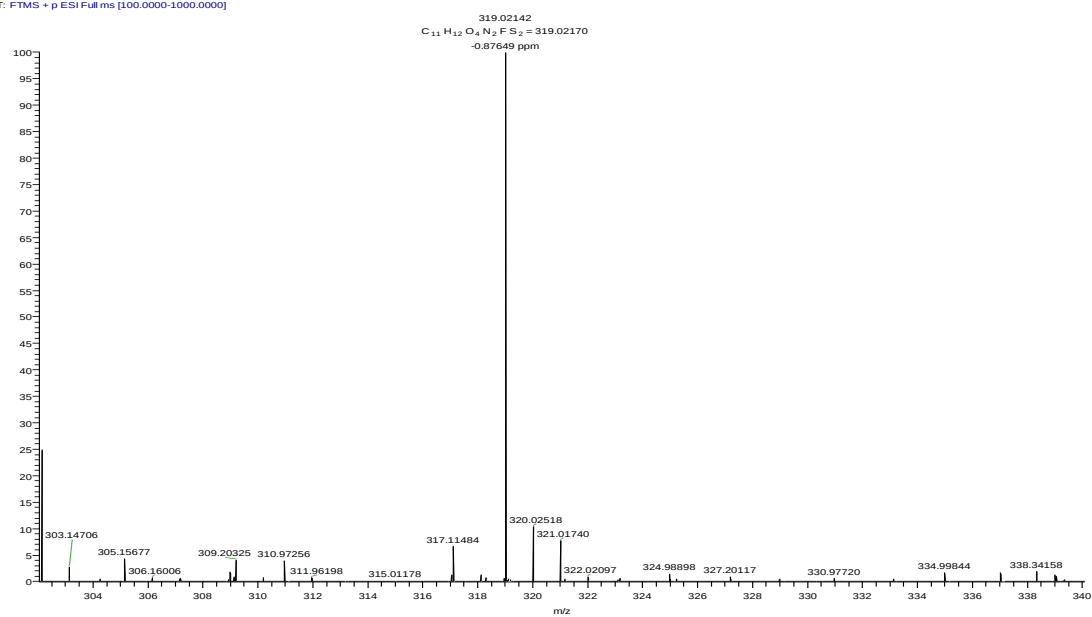


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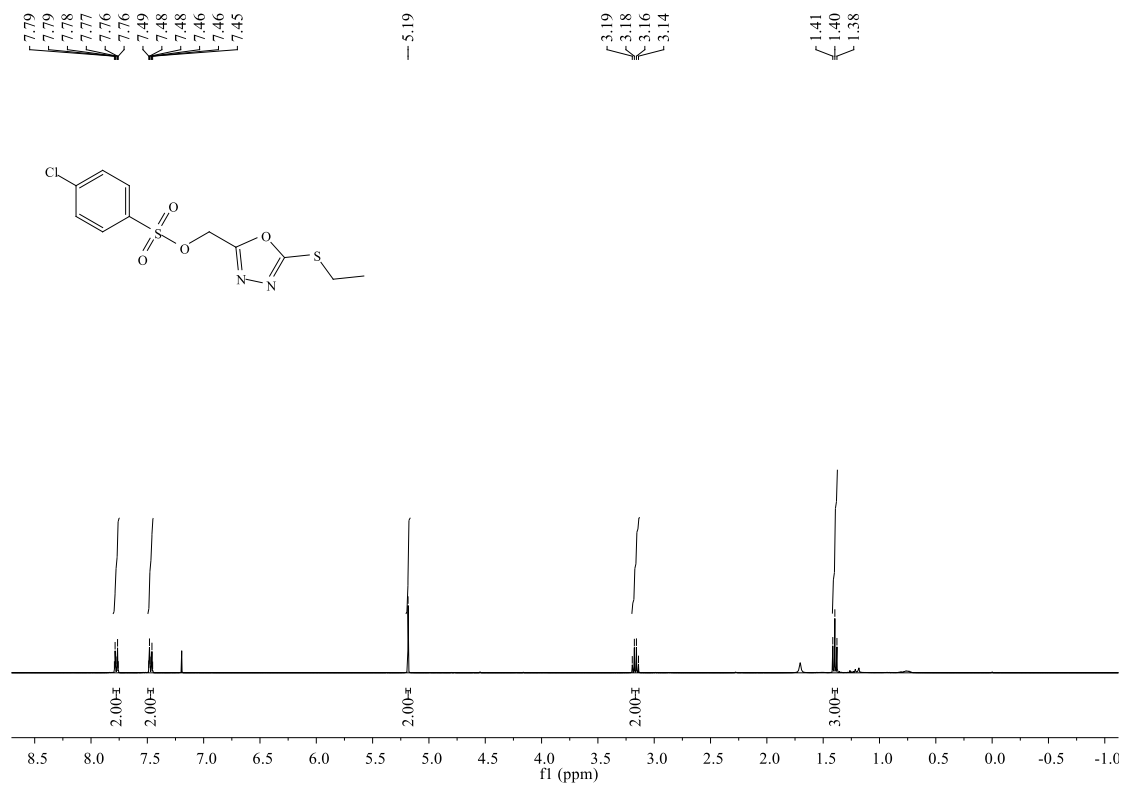


^{19}F NMR of compound **4a-11**

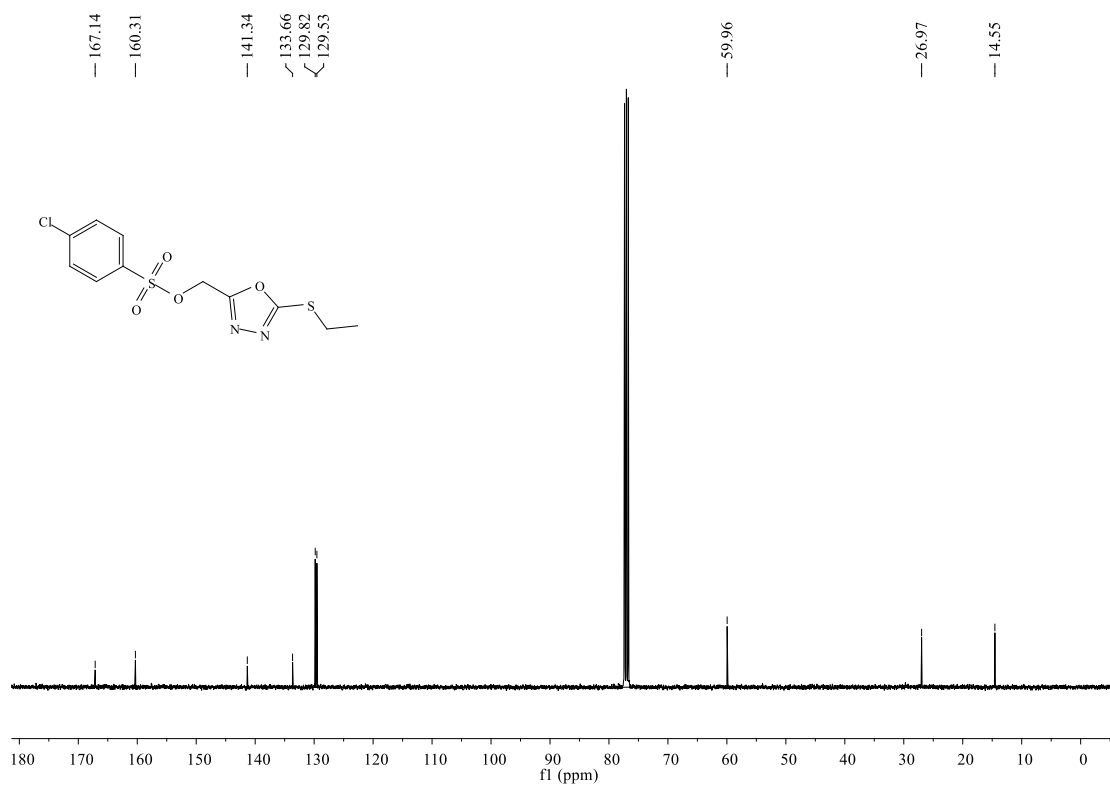
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HRMS of compound **4a-11**

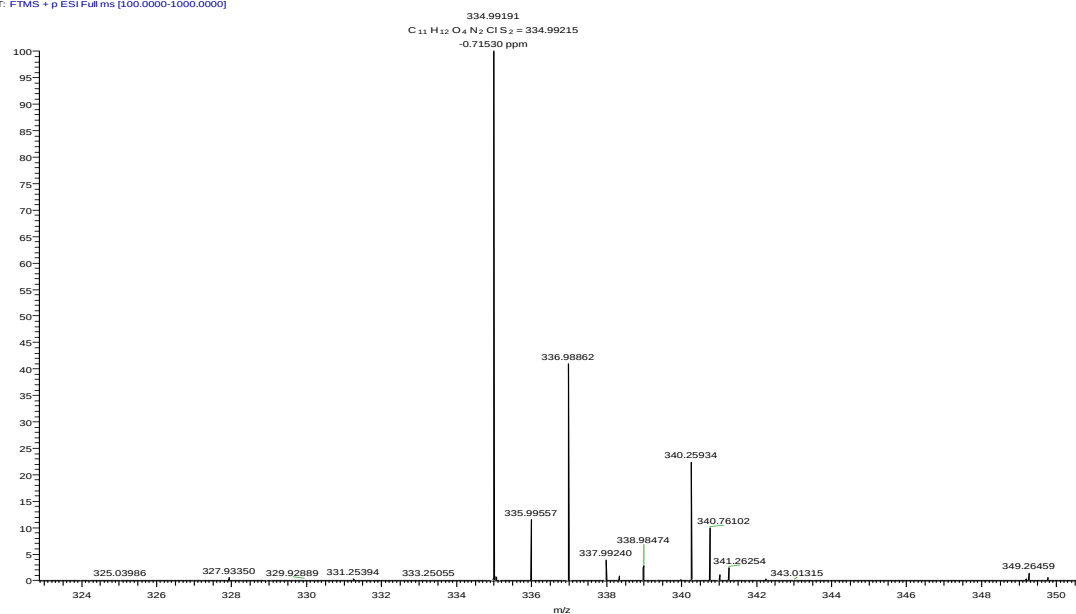


¹H NMR of compound **4a-12**

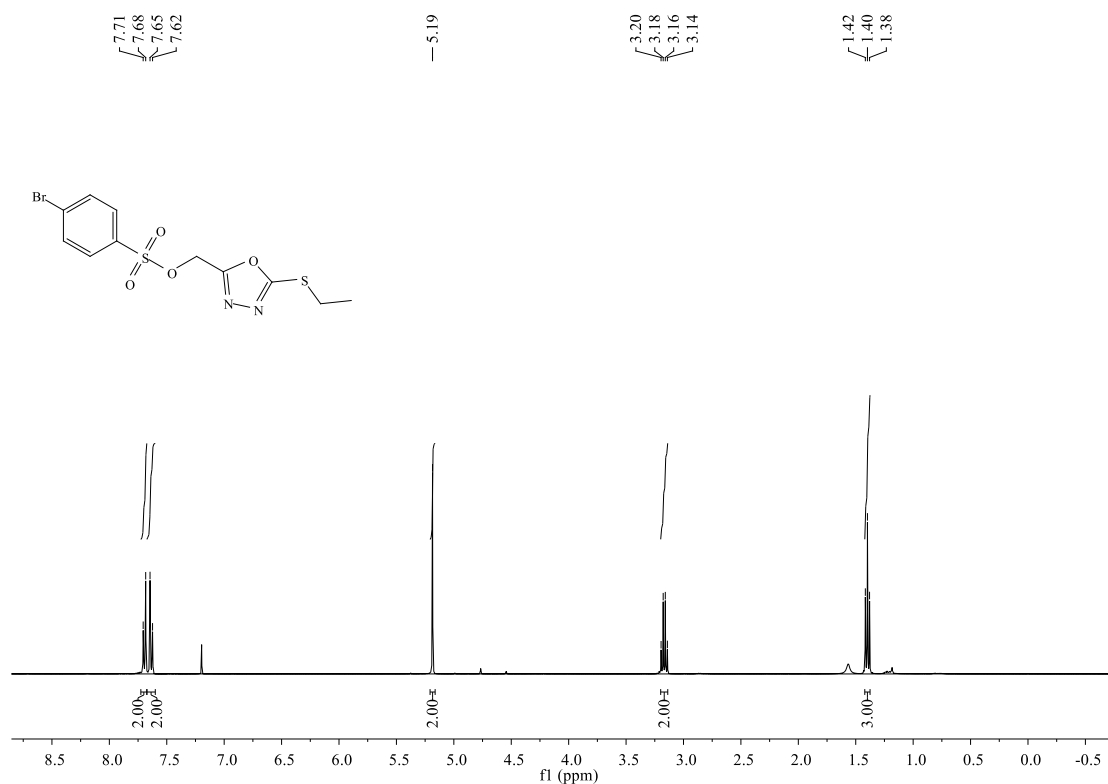


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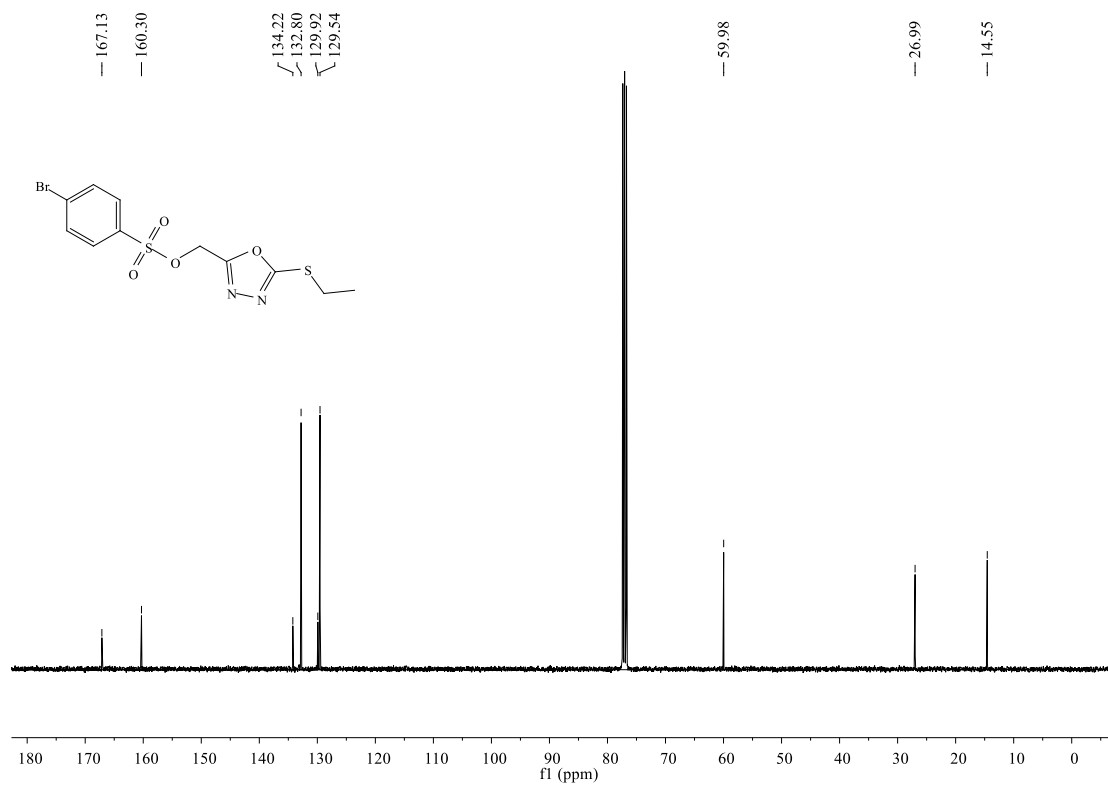
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HRMS of compound 4a-12

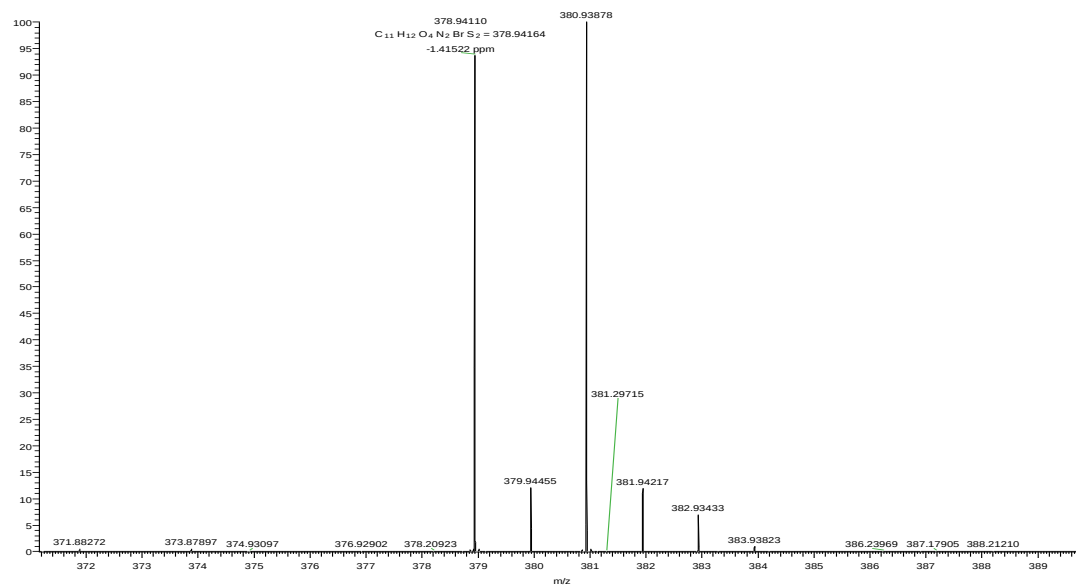


¹H NMR of compound 4a-13

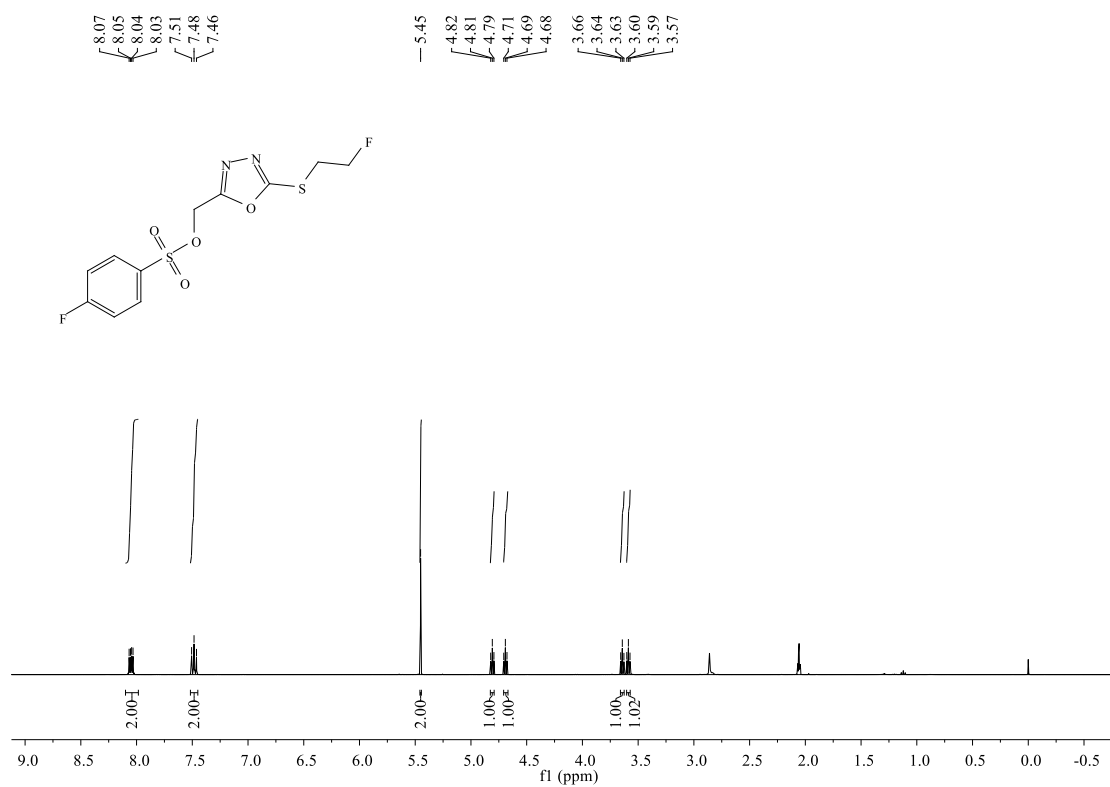


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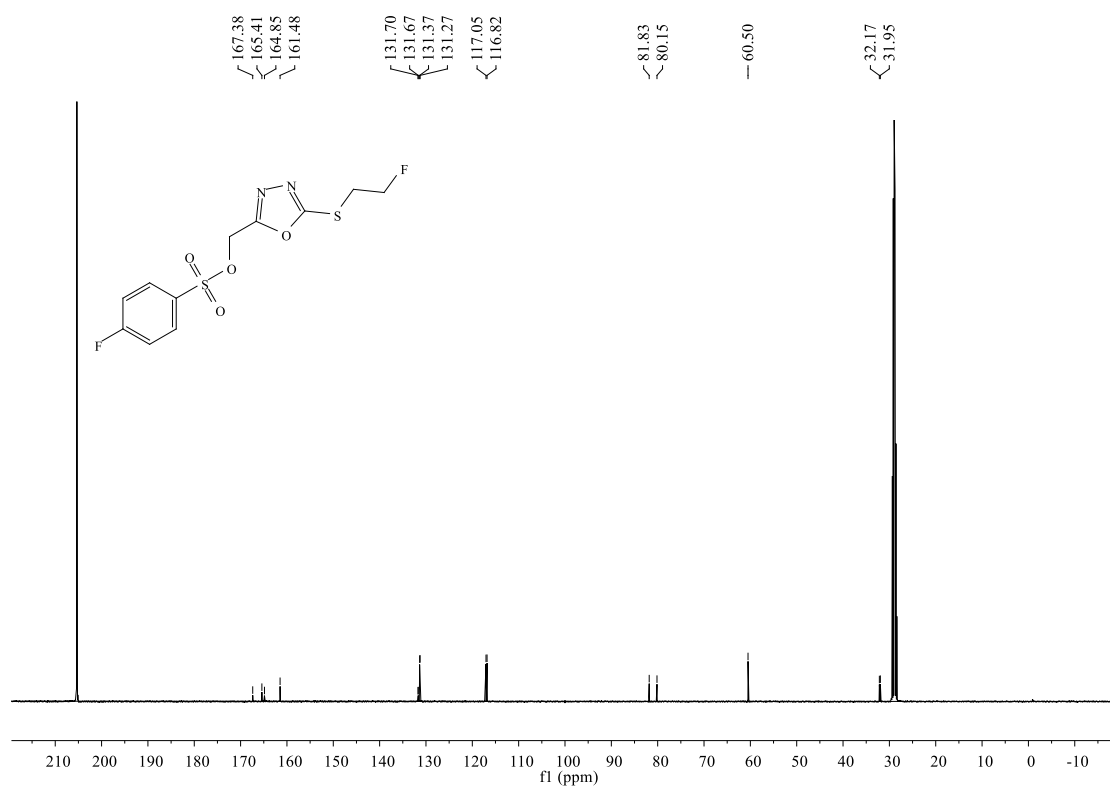
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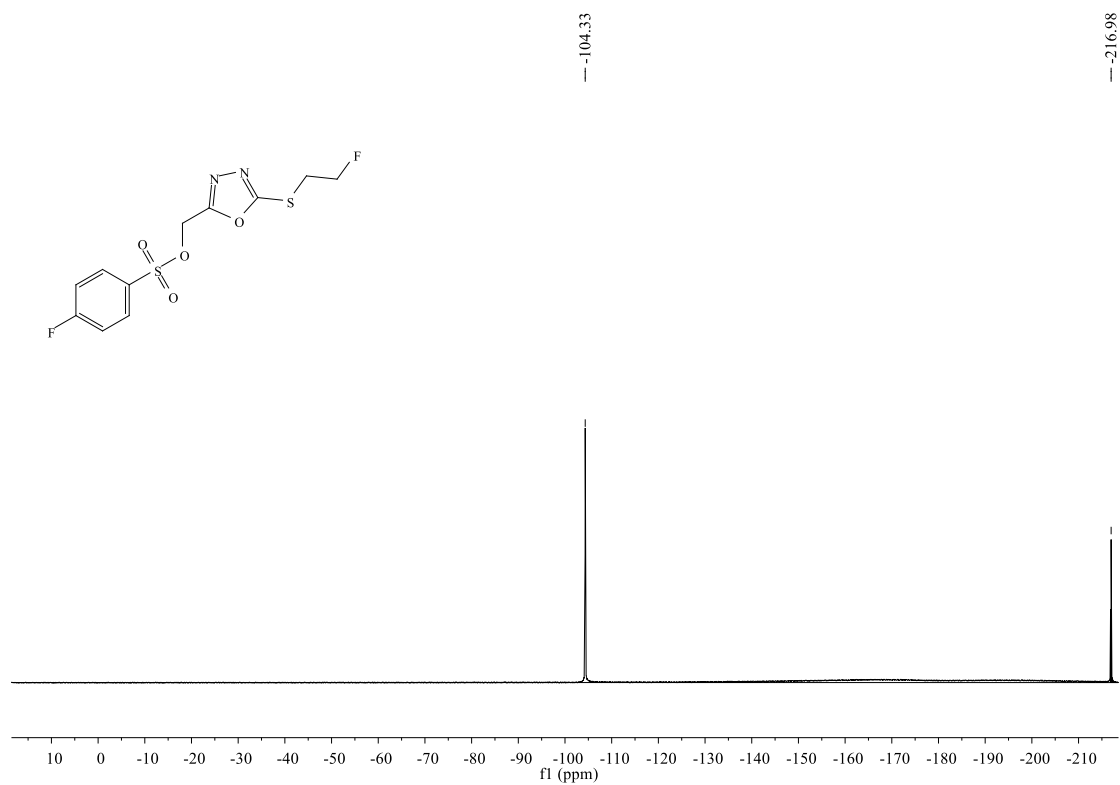
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^1H NMR of compound **4a-14**

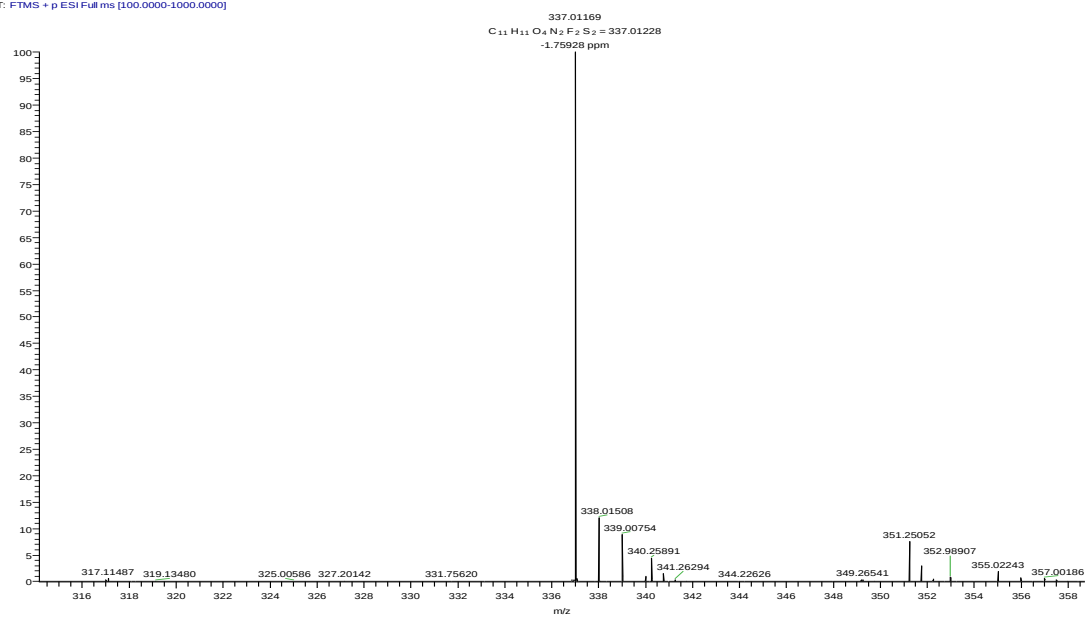


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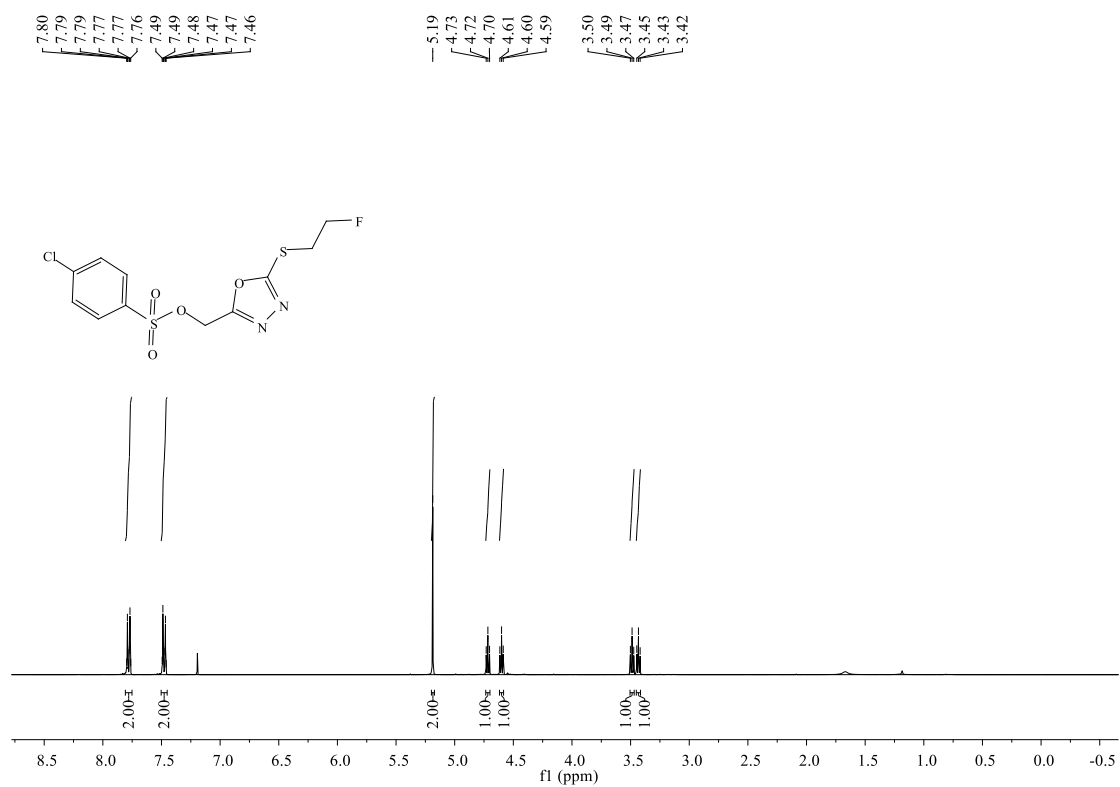


^{19}F NMR of compound **4a-14**

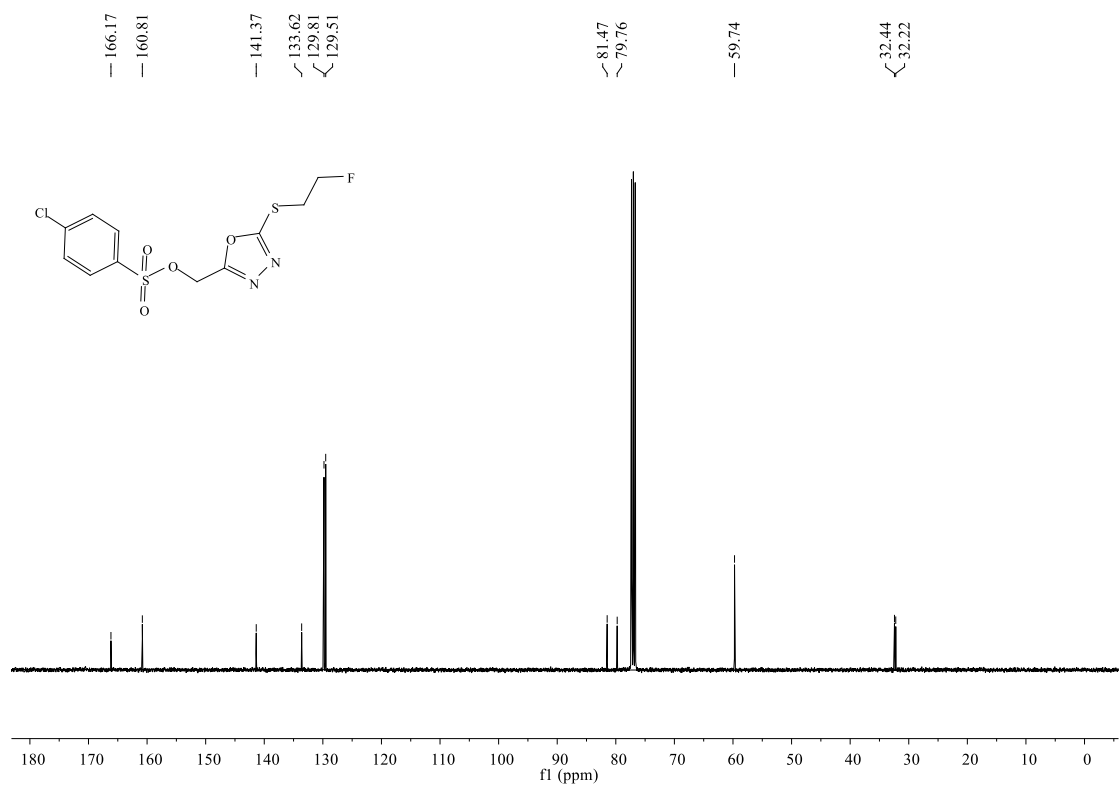
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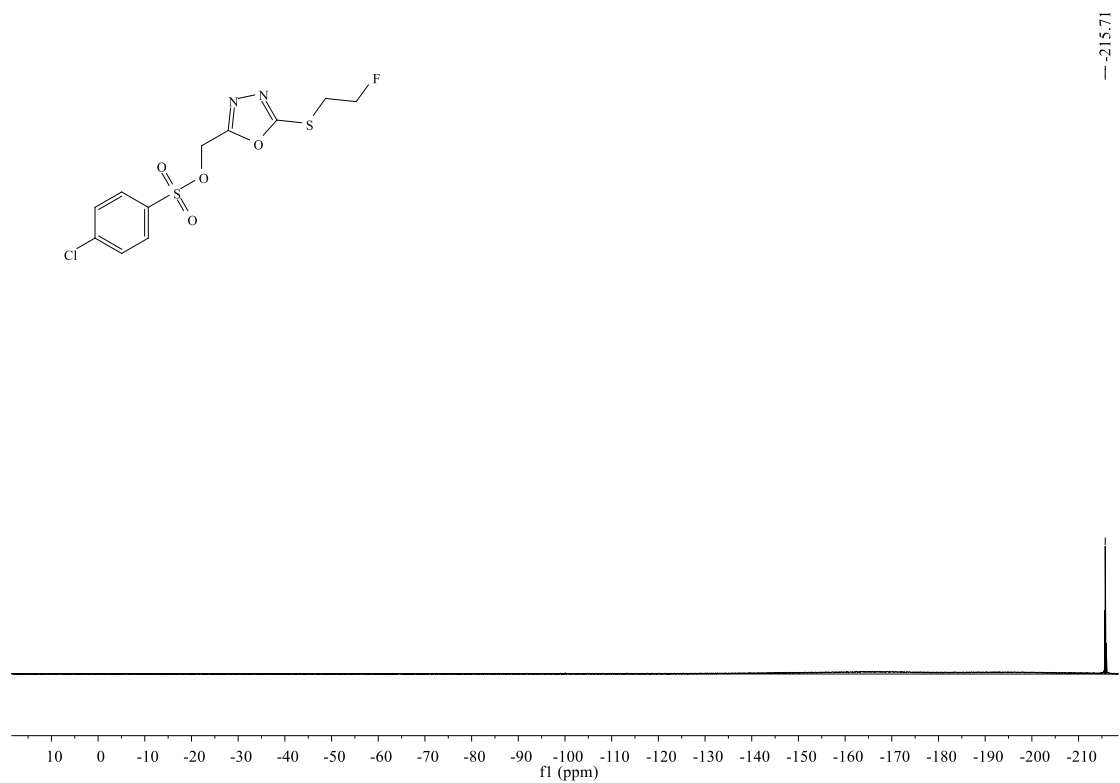
HRMS of compound **4a-14**



¹H NMR of compound **4a-15**

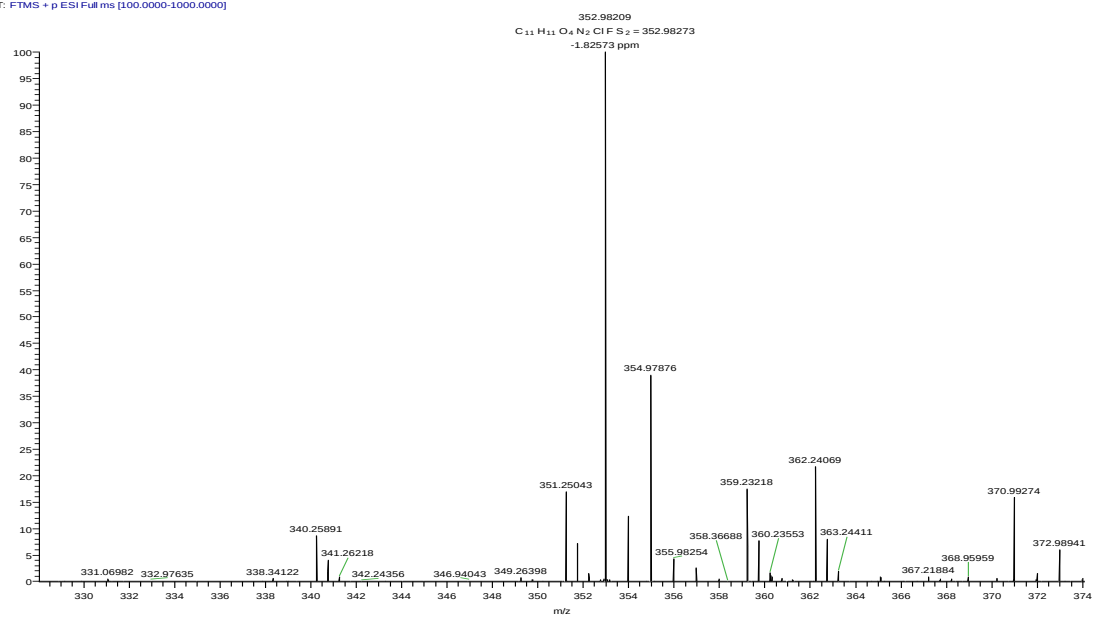


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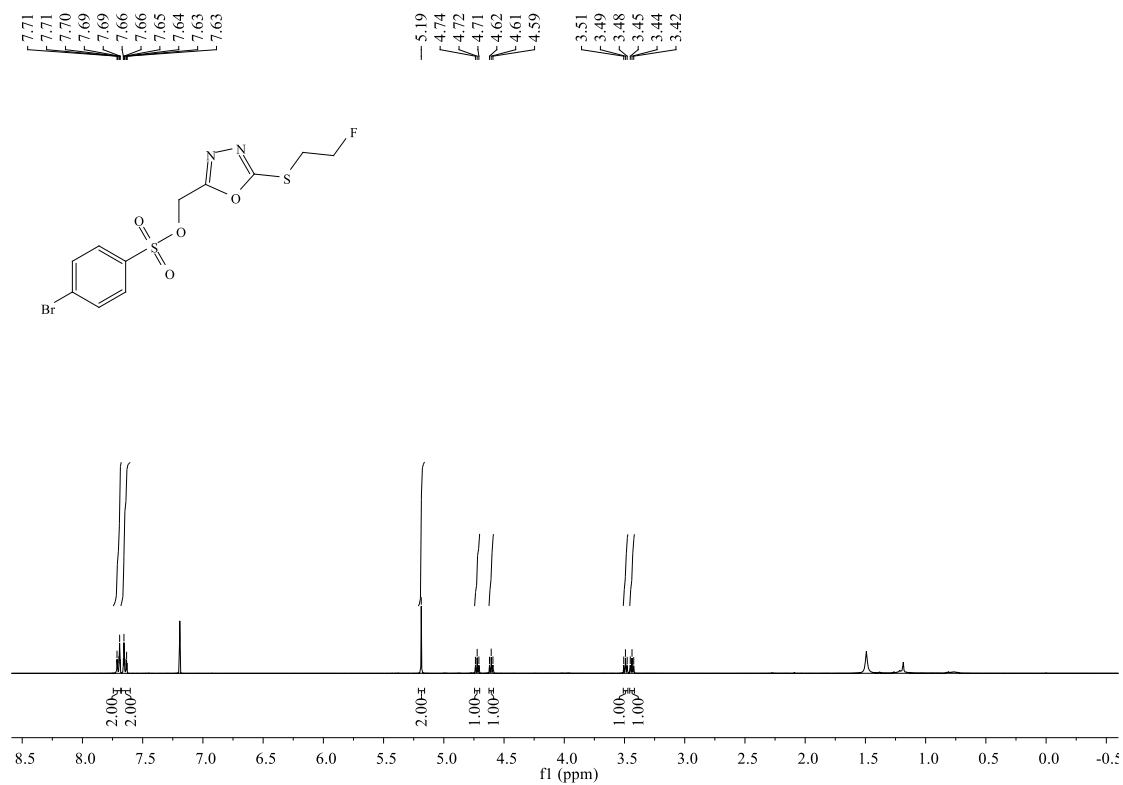


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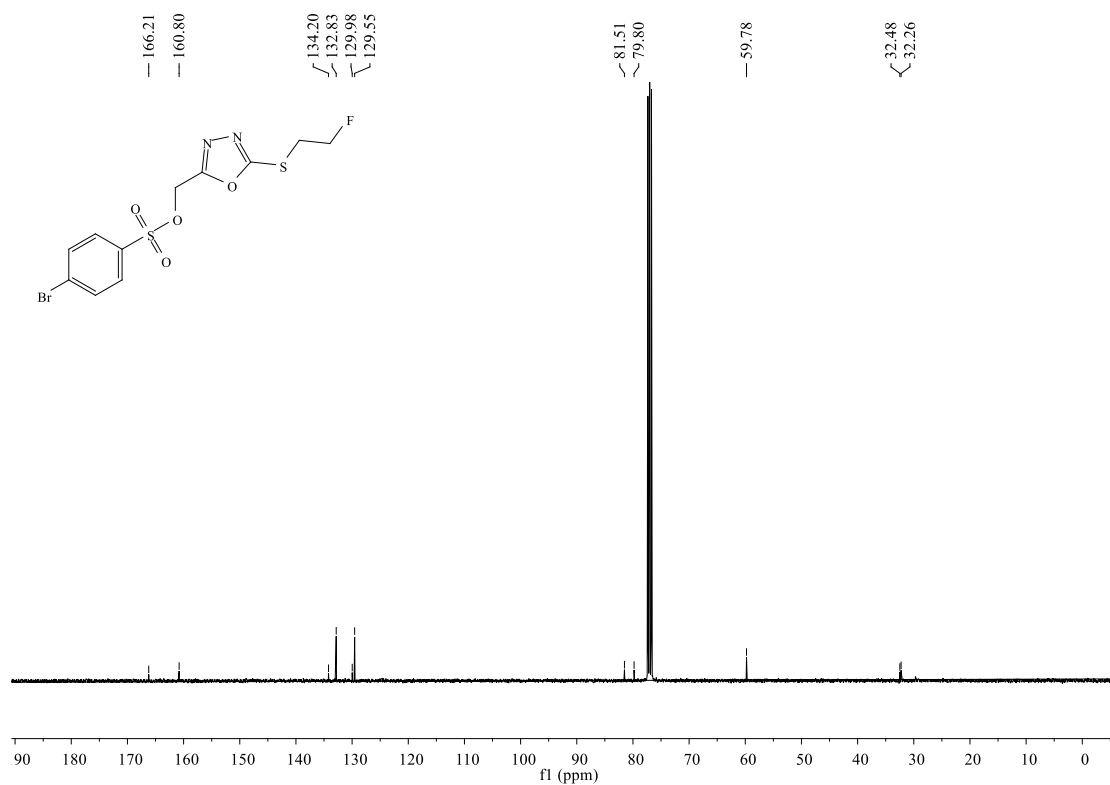
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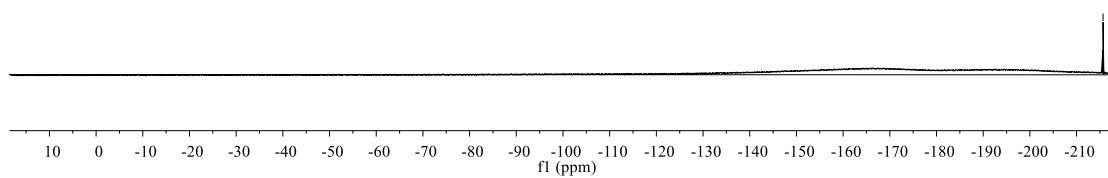
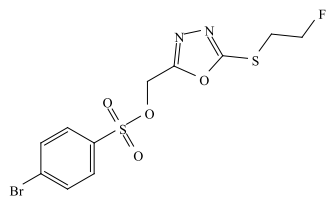
HRMS of compound 4a-15



¹H NMR of compound **4a-16**

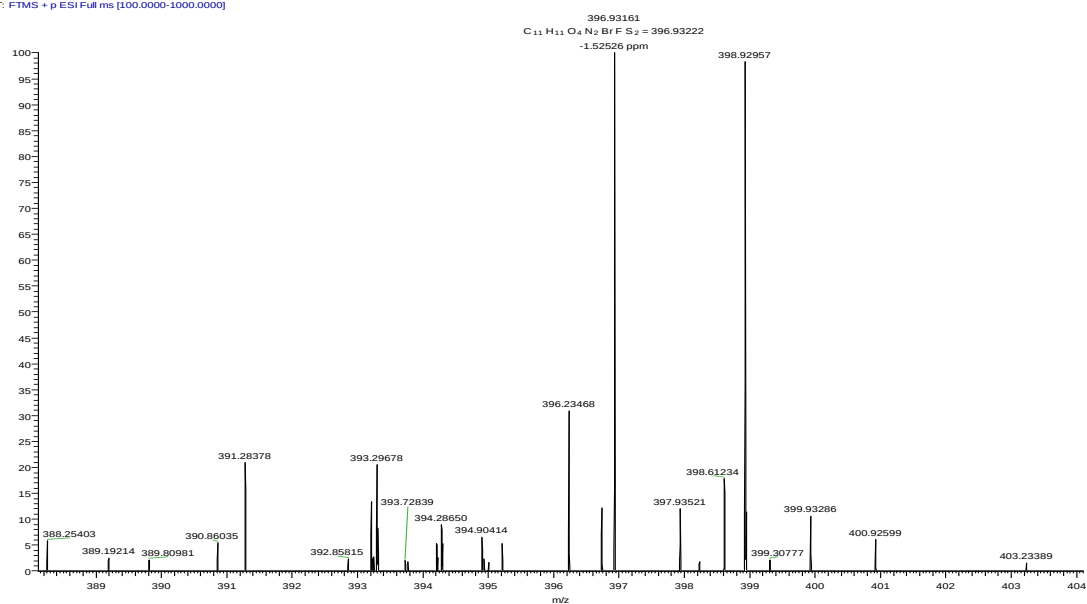


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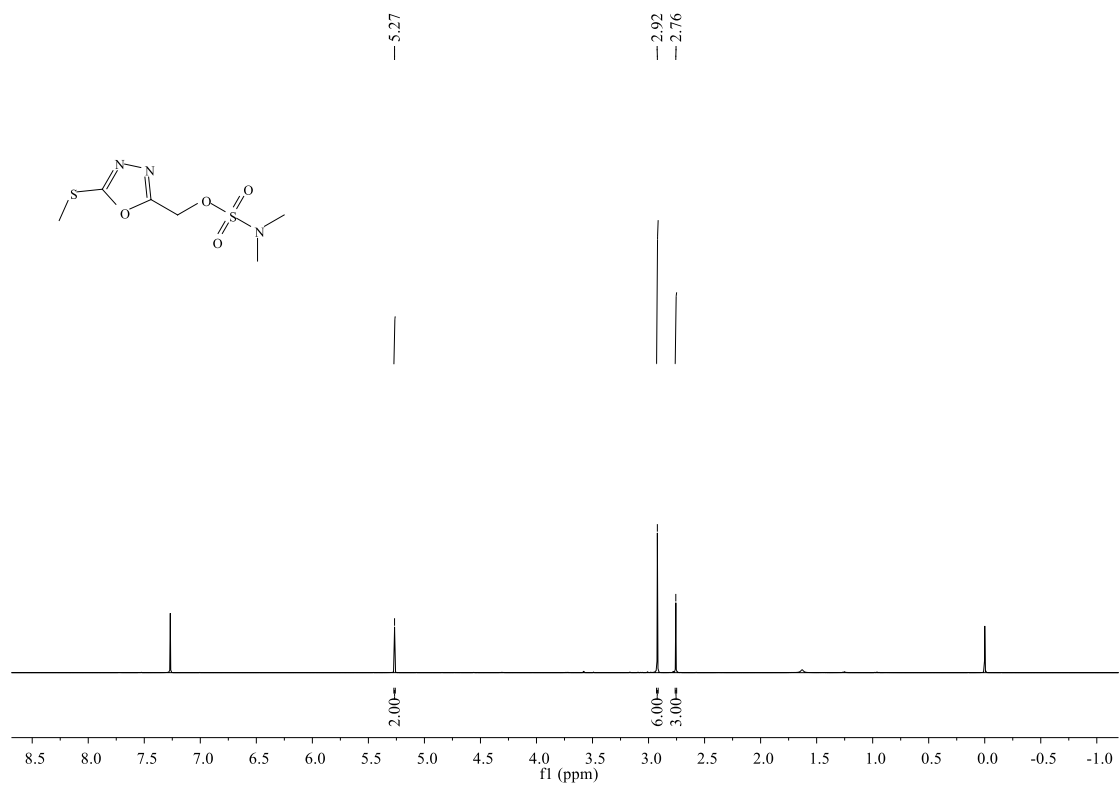


¹⁹F NMR of compound **4a-16**

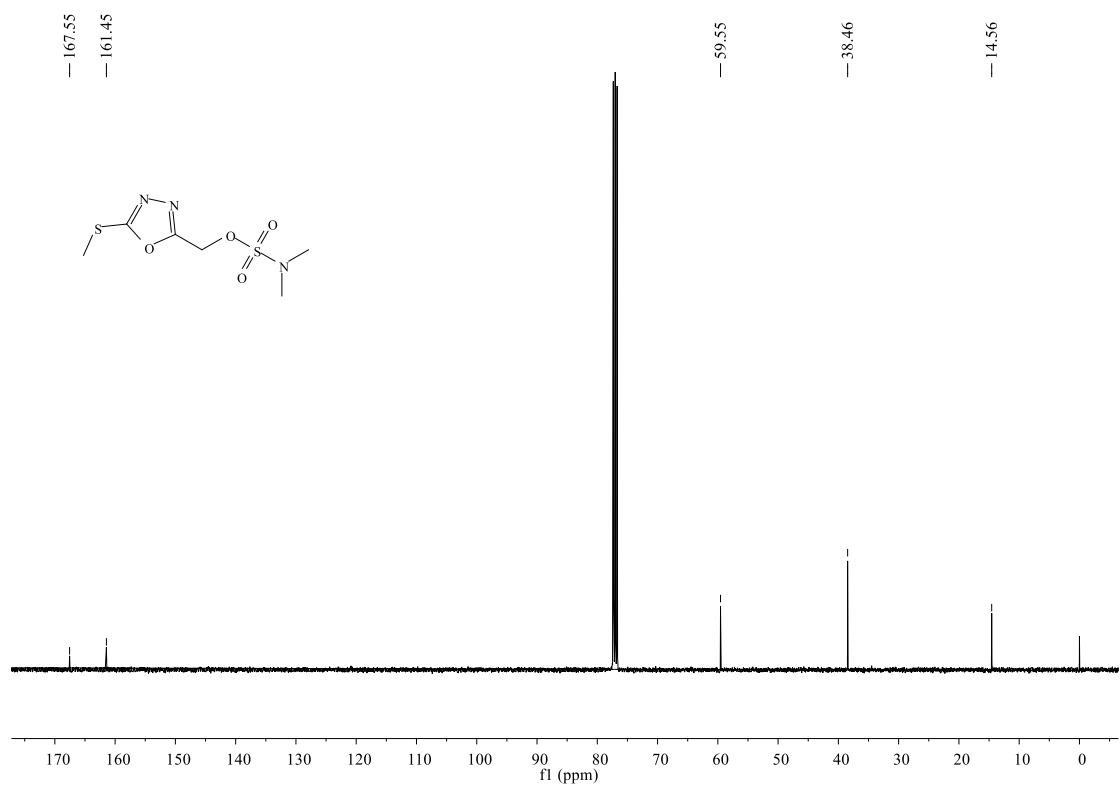
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HRMS of compound **4a-16**

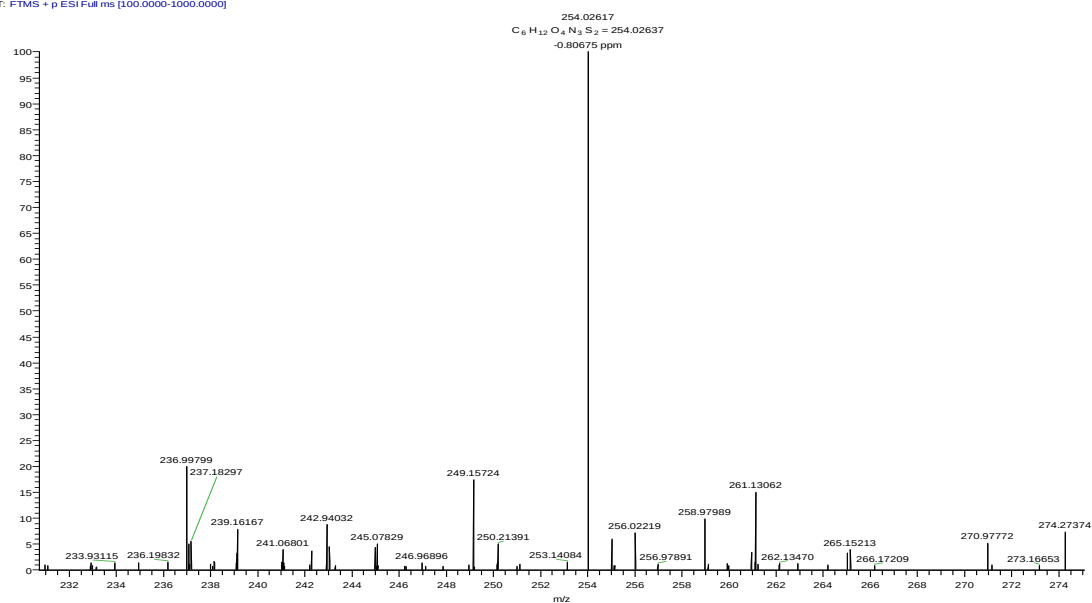


^1H NMR of compound **4a-17**

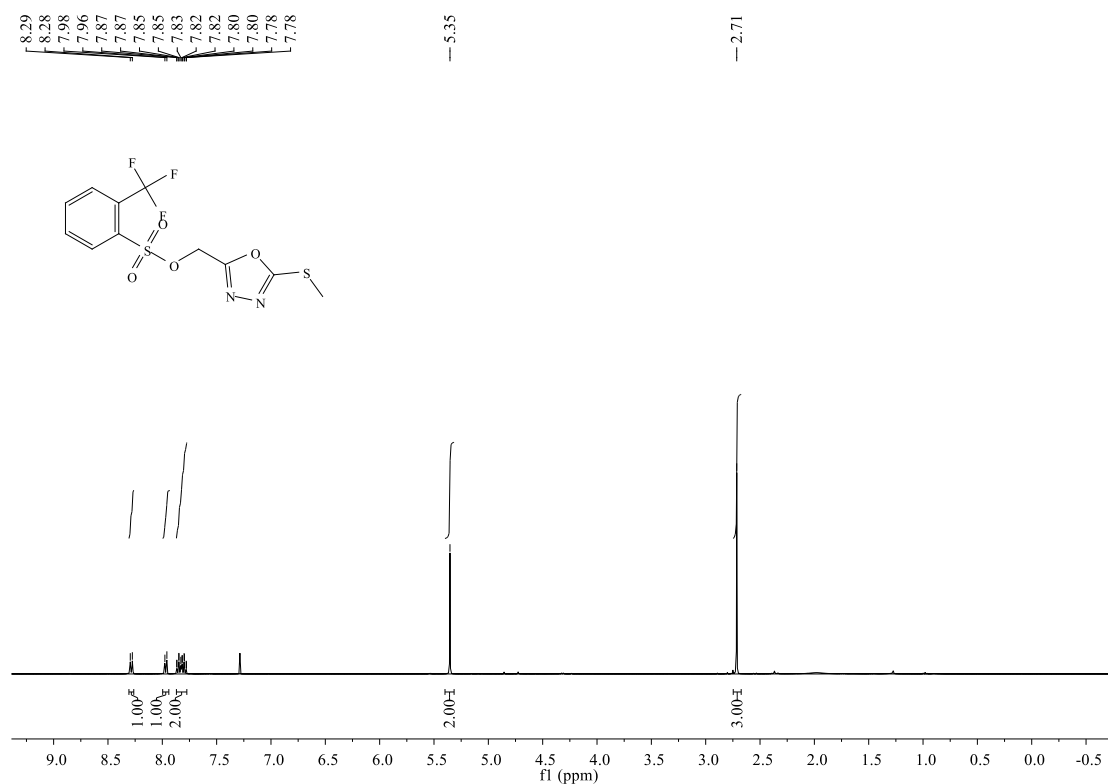


^{13}C NMR of compound **4a-17**

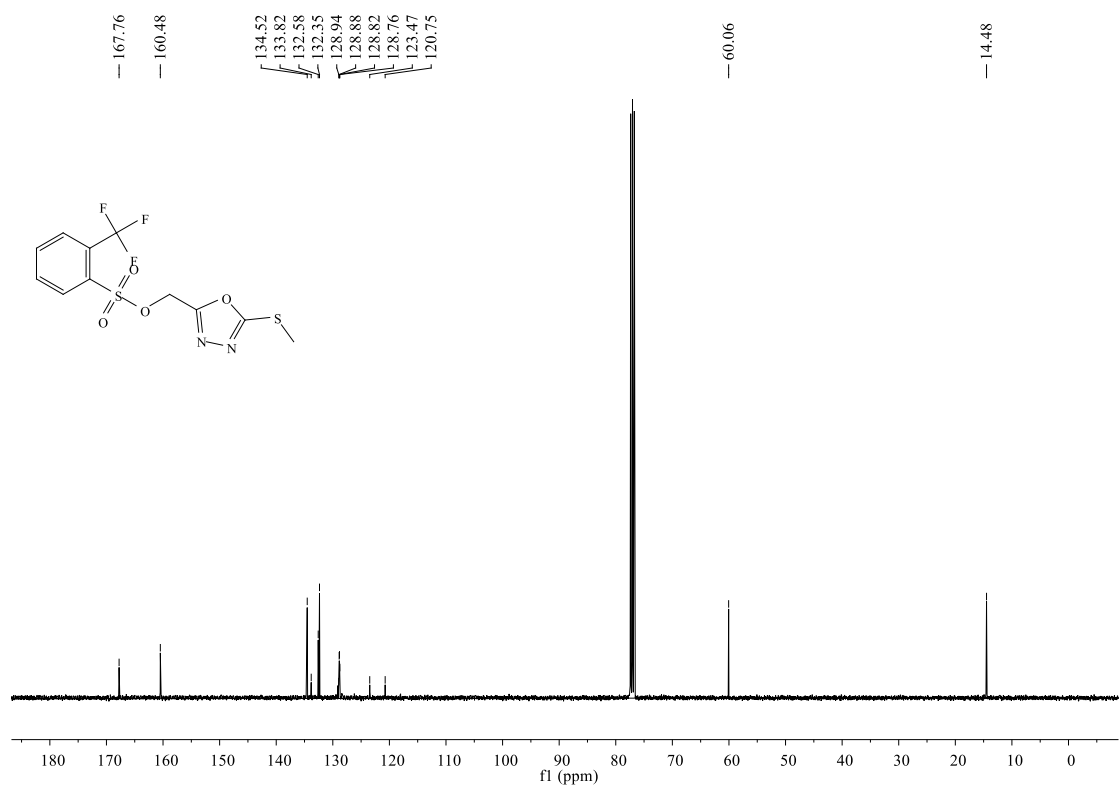
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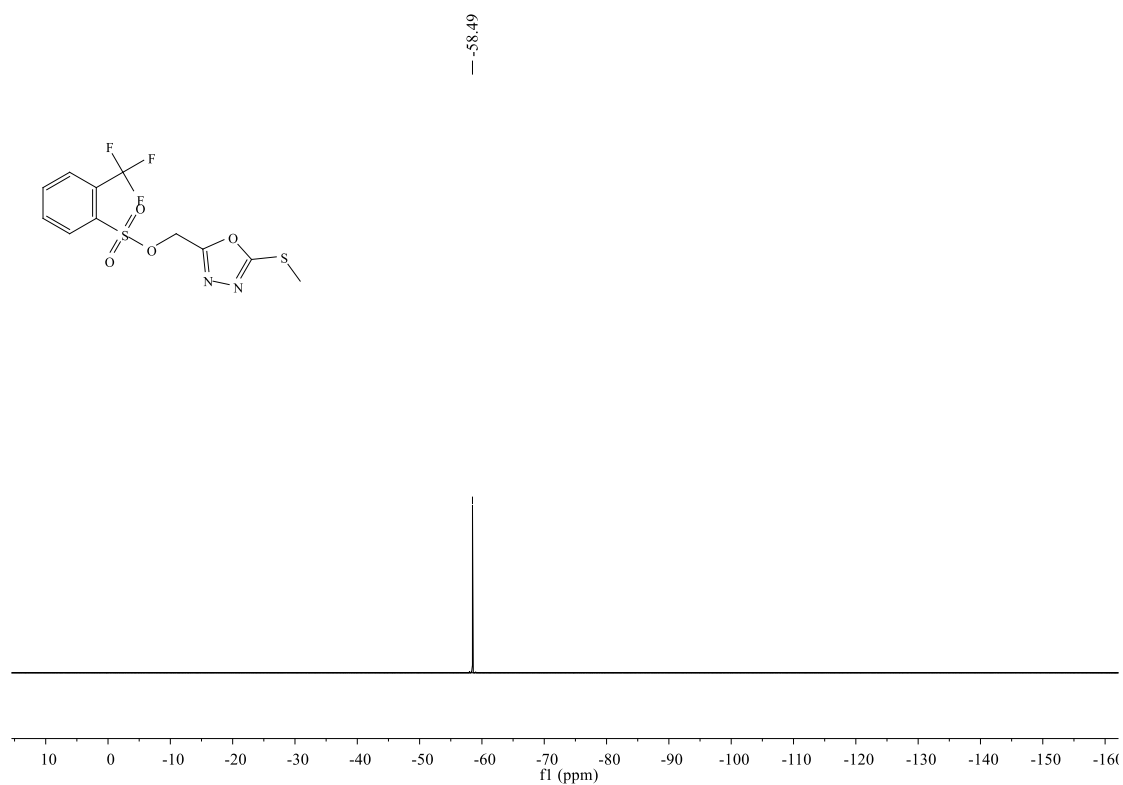
HRMS of compound 4a-17



¹H NMR of compound 4a-18

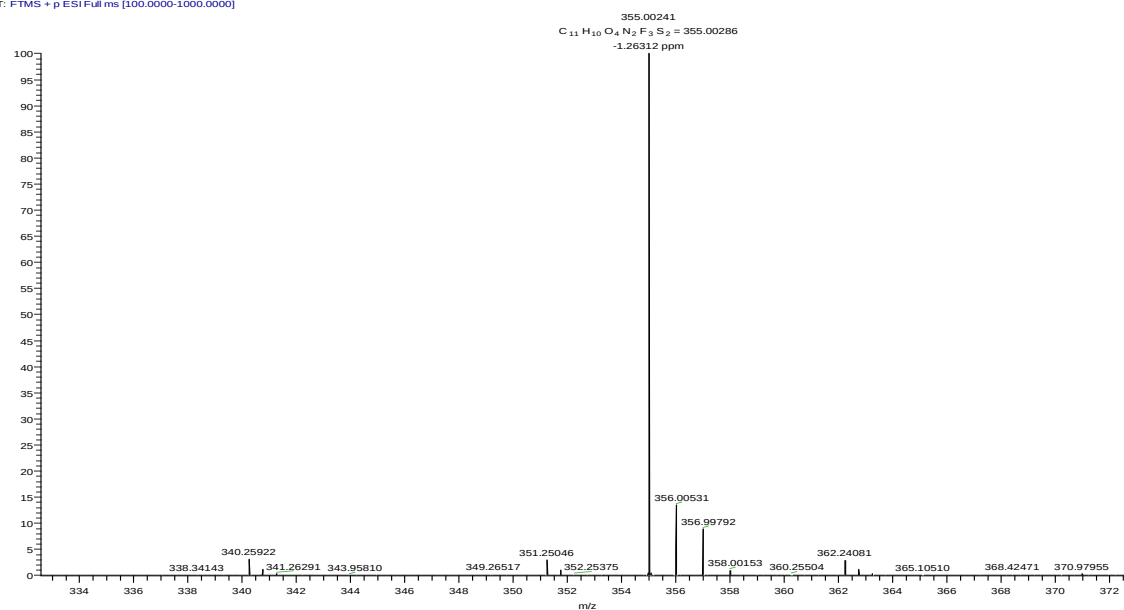


¹³C NMR of compound **4a-18**

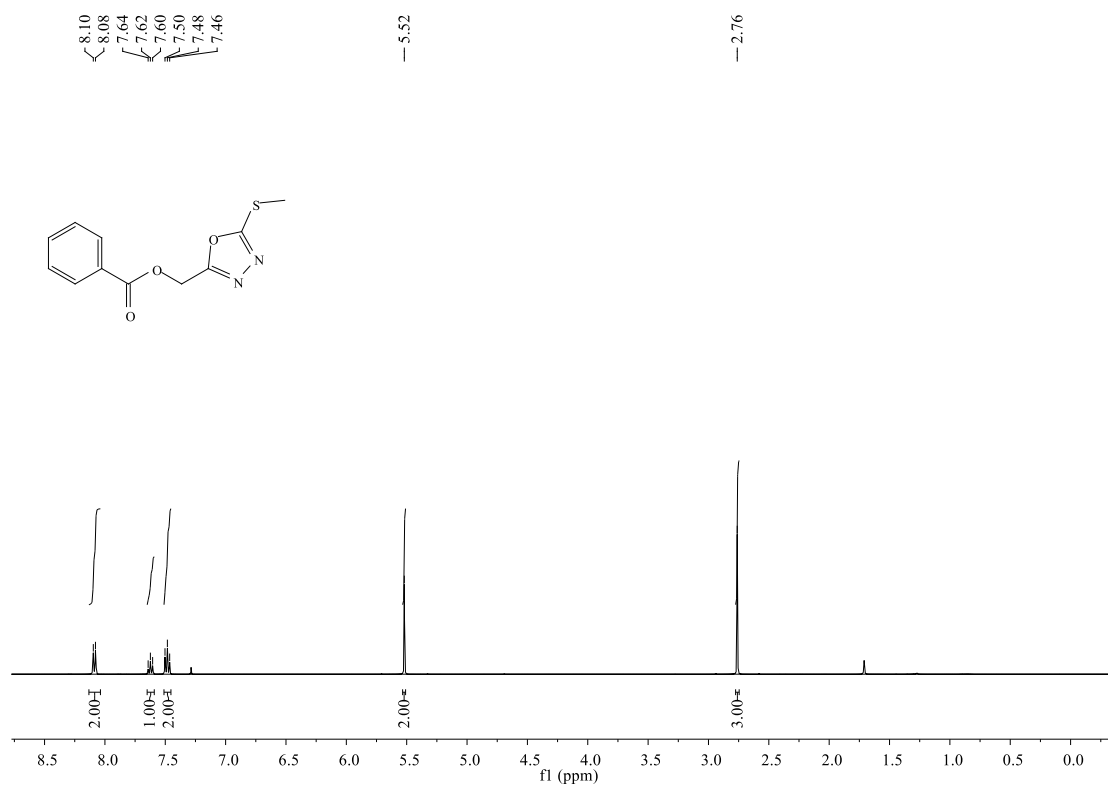


¹⁹F NMR of compound **4a-18**

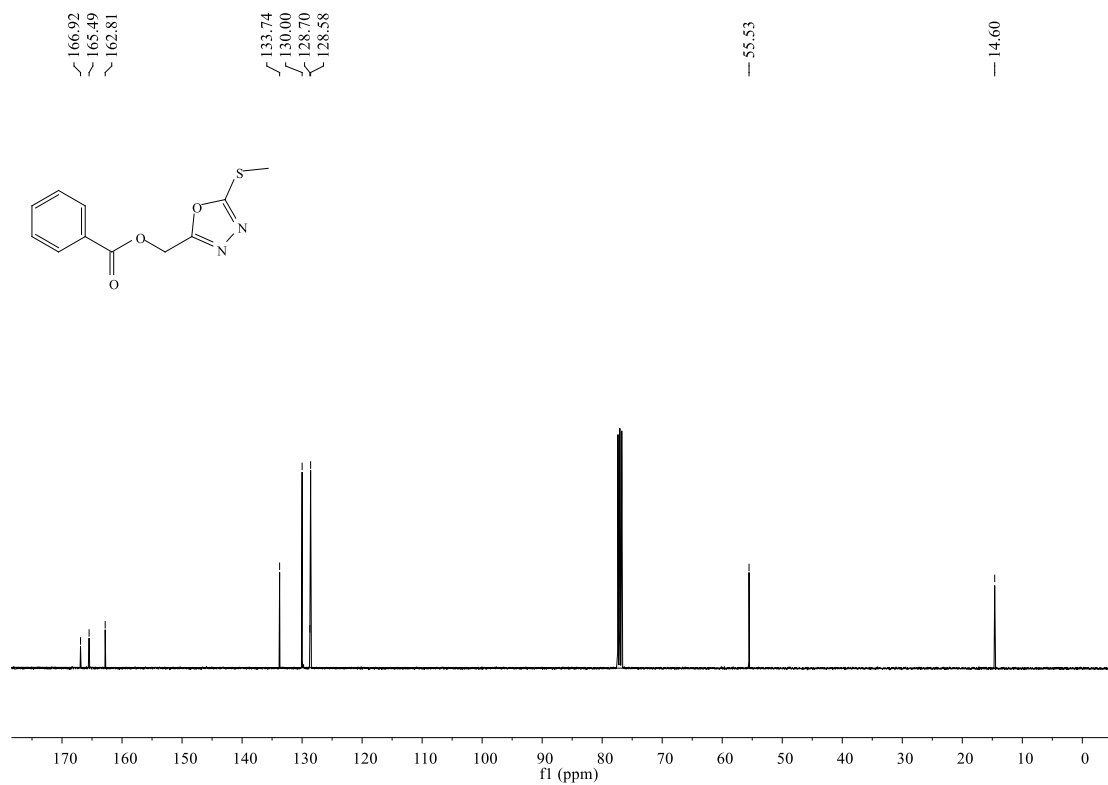
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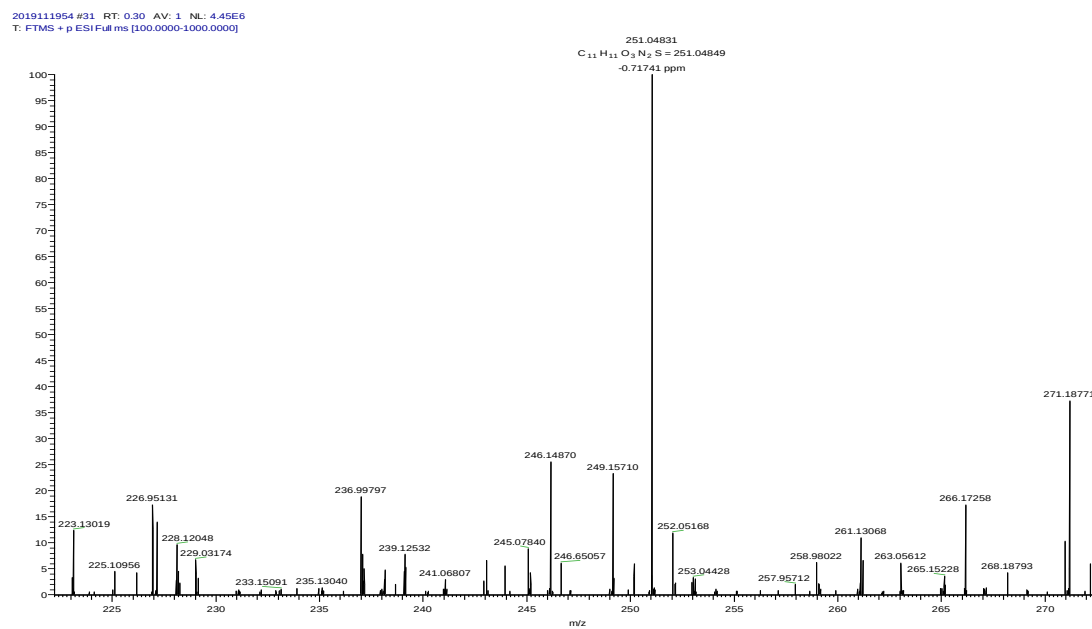
HRMS of compound 4a-18



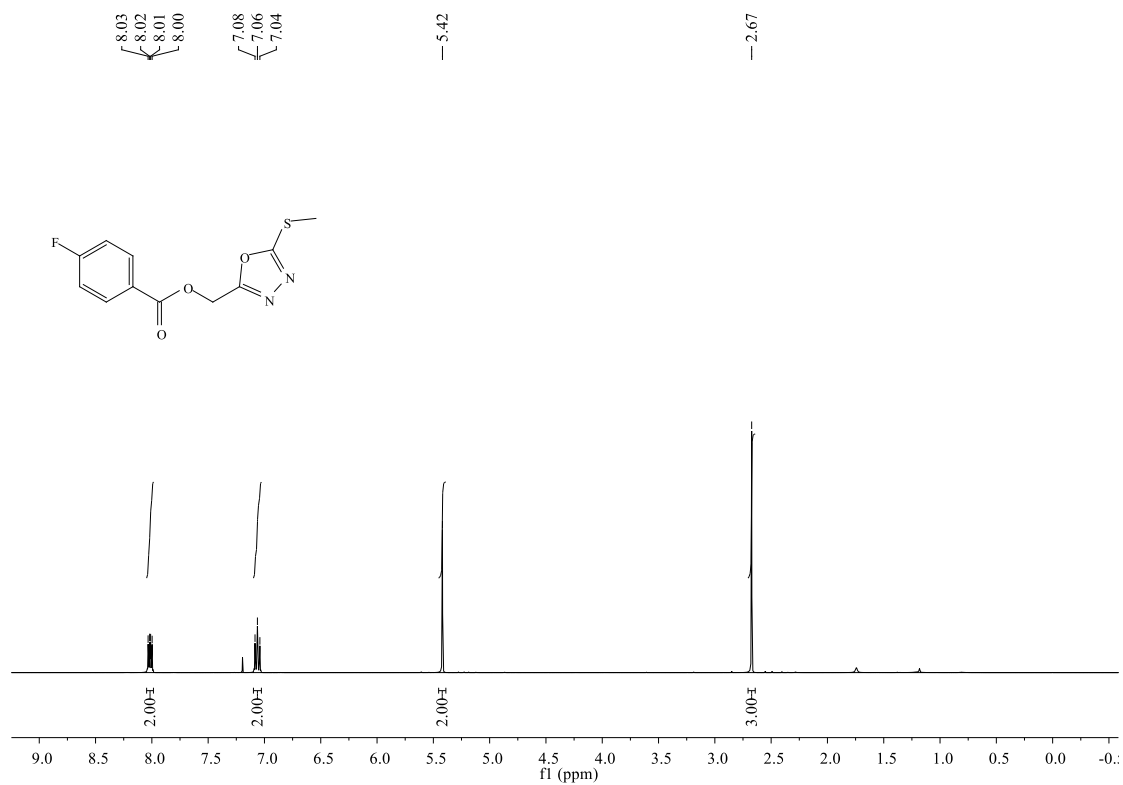
¹H NMR of compound 5a-1



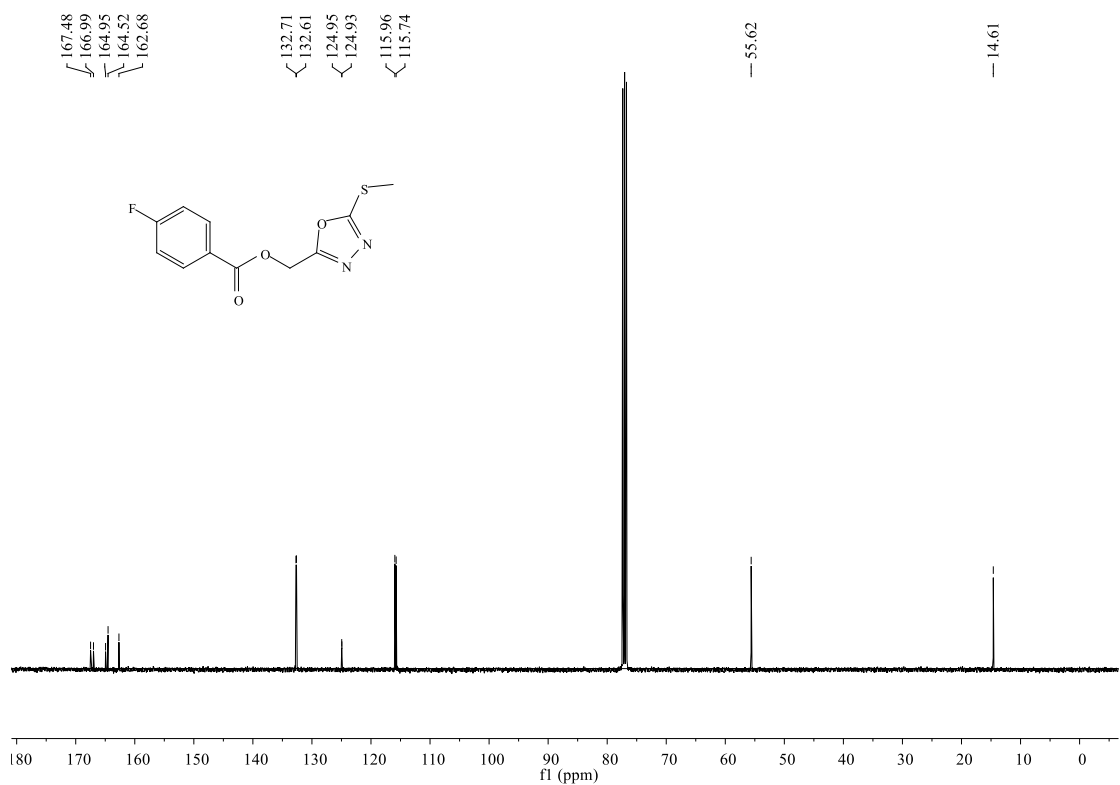
¹³C NMR of compound **5a-1**



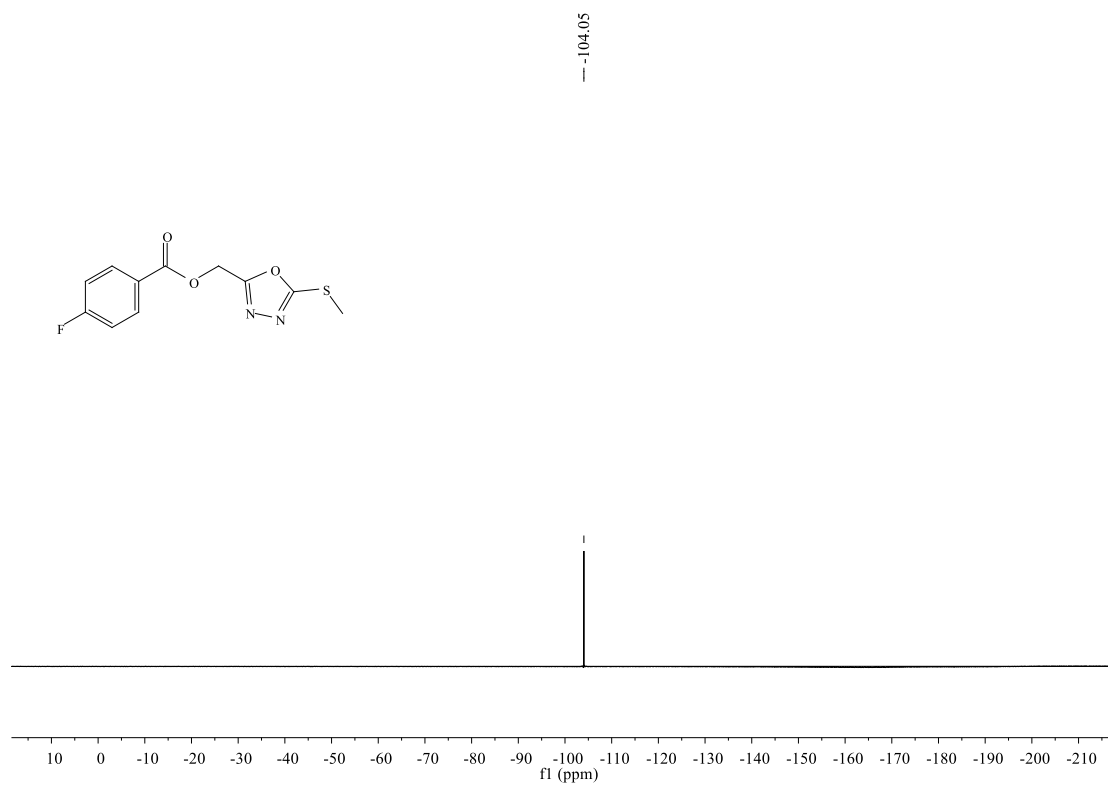
HRMS of compound **5a-1**



¹H NMR of compound **5a-2**

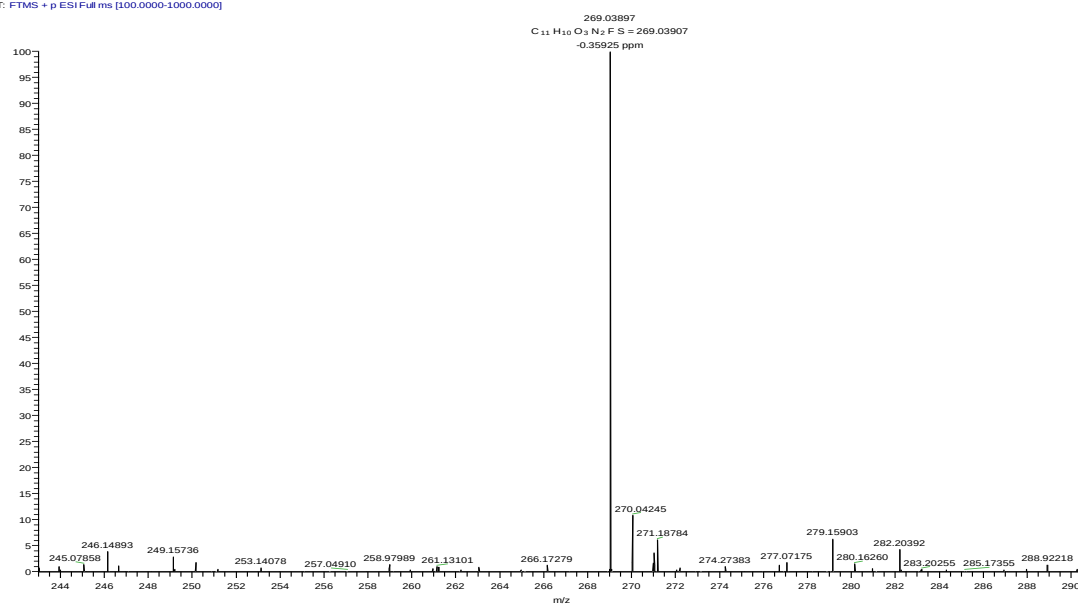


¹³C NMR of compound **5a-2**

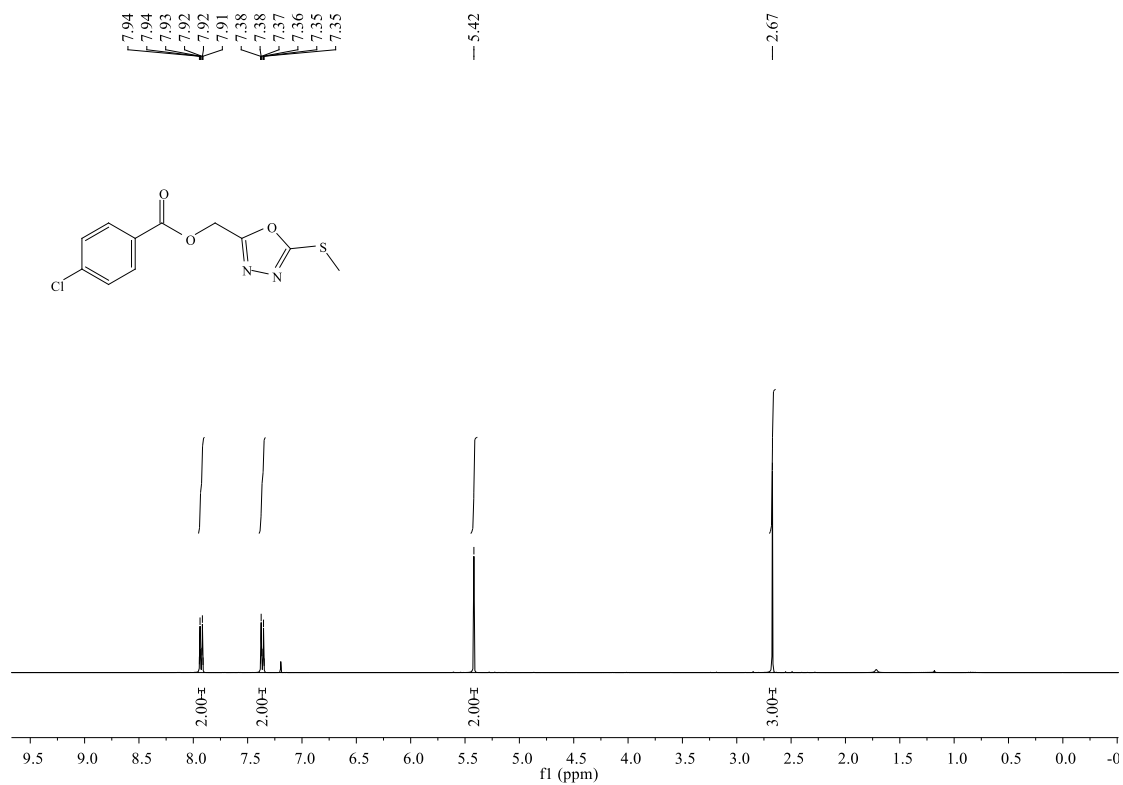


^{19}F NMR of compound **5a-2**

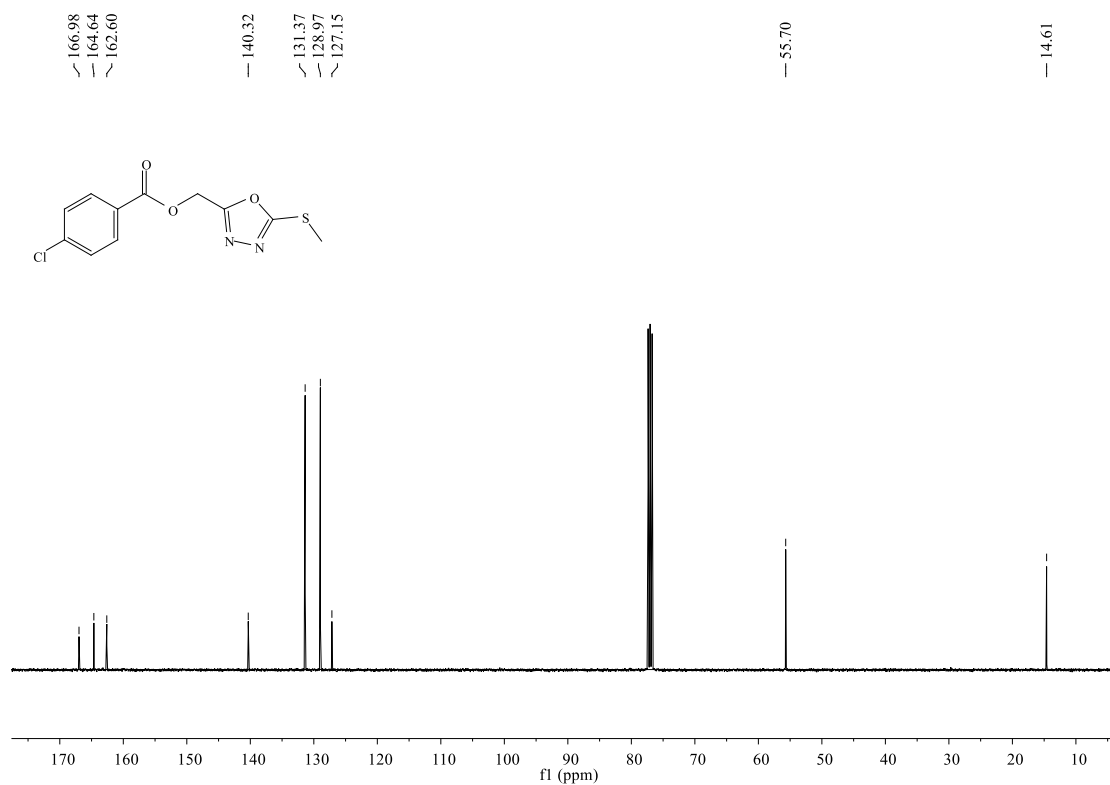
2019111955 #33 RT: 0.32 AV: 1 NL: 2.77E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]



HRMS of compound **5a-2**

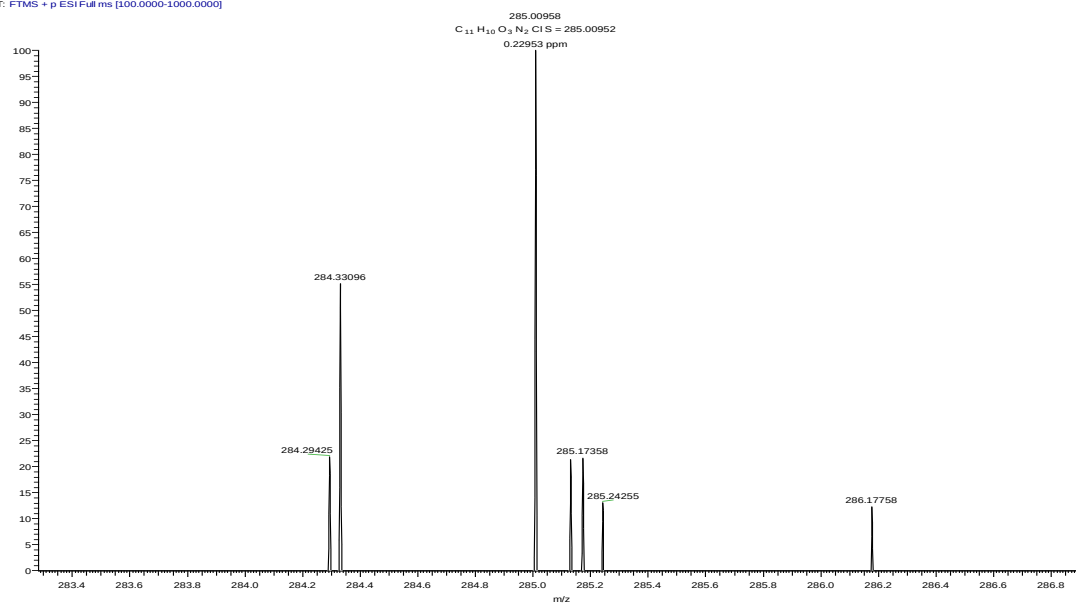


¹H NMR of compound **5a-3**

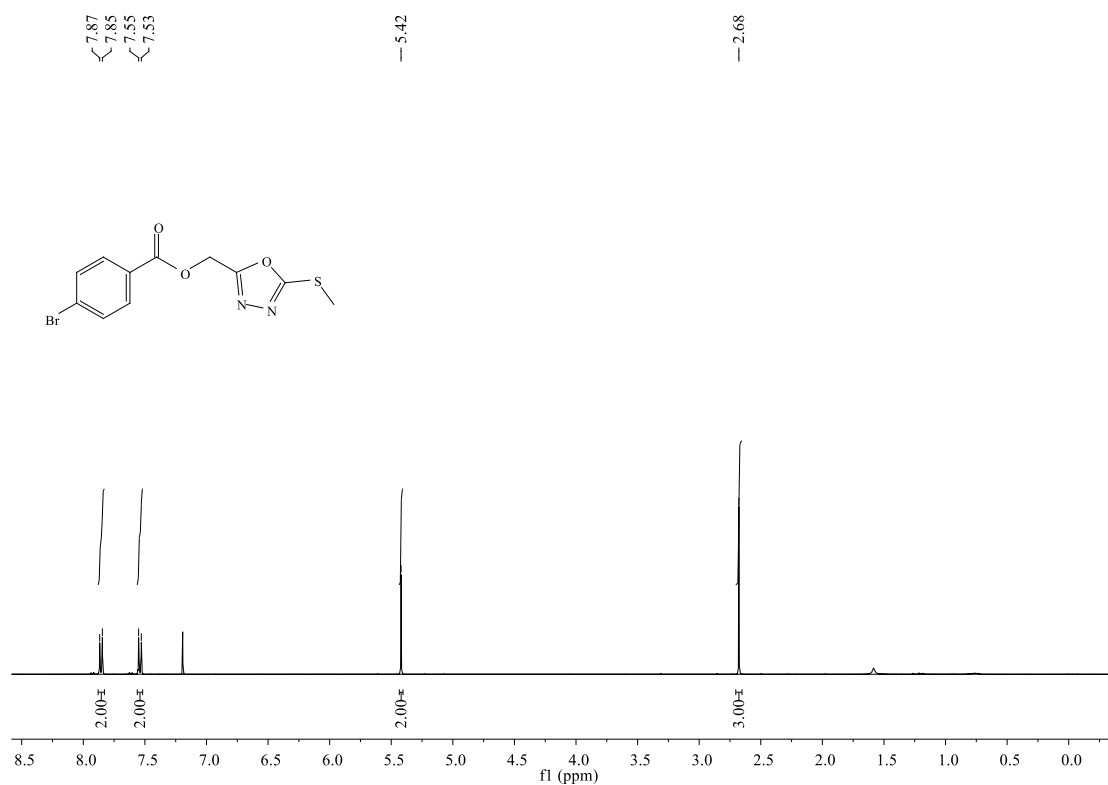


¹³C NMR of compound **5a-3**

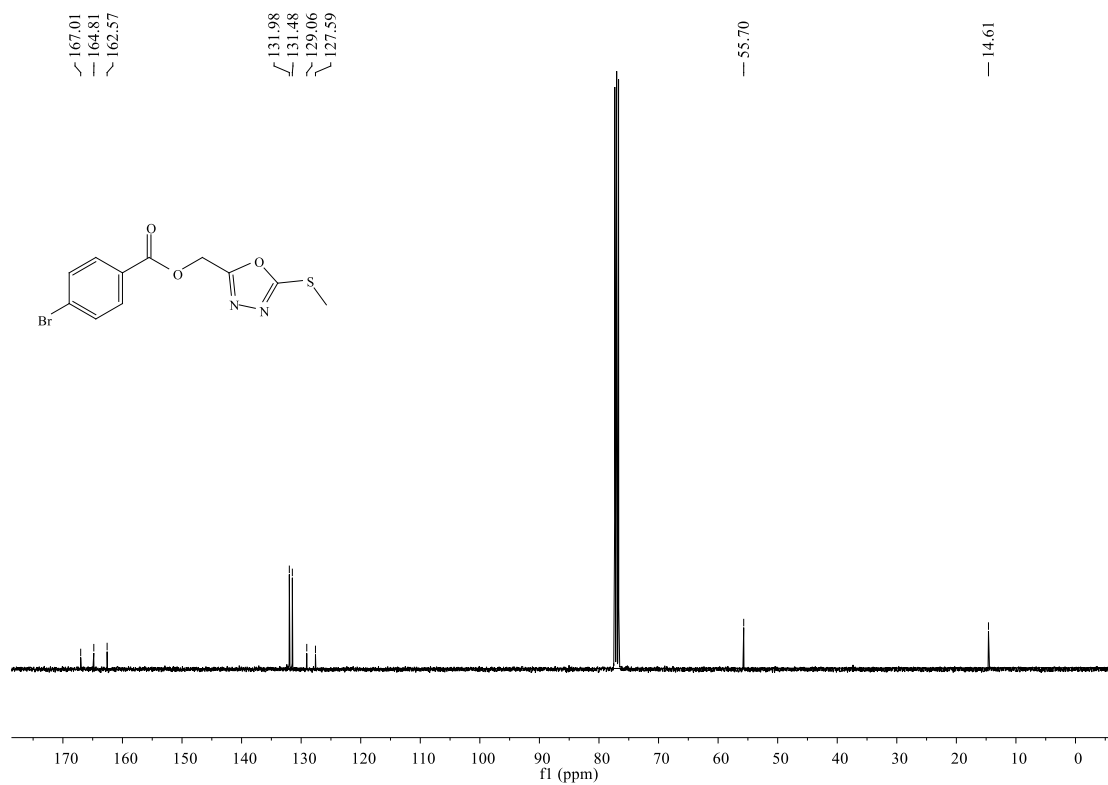
2019111956 #37 RT: 0.36 AV: 1 NL: 2.03E5
T: FTMS + p ESI Full ms [100.0000-1000.0000]



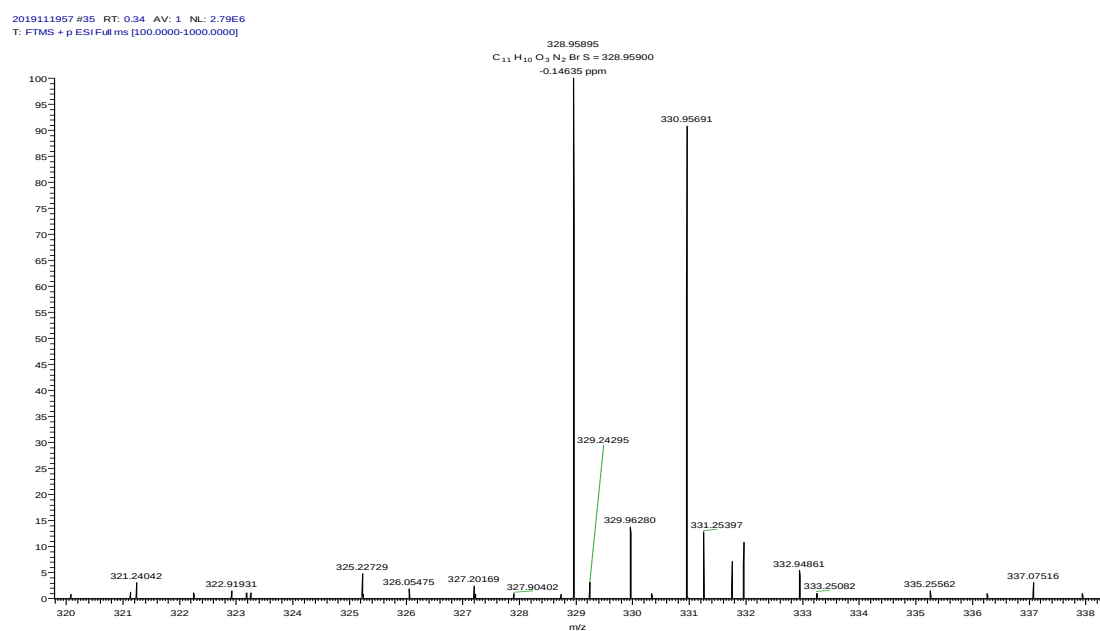
HRMS of compound **5a-3**



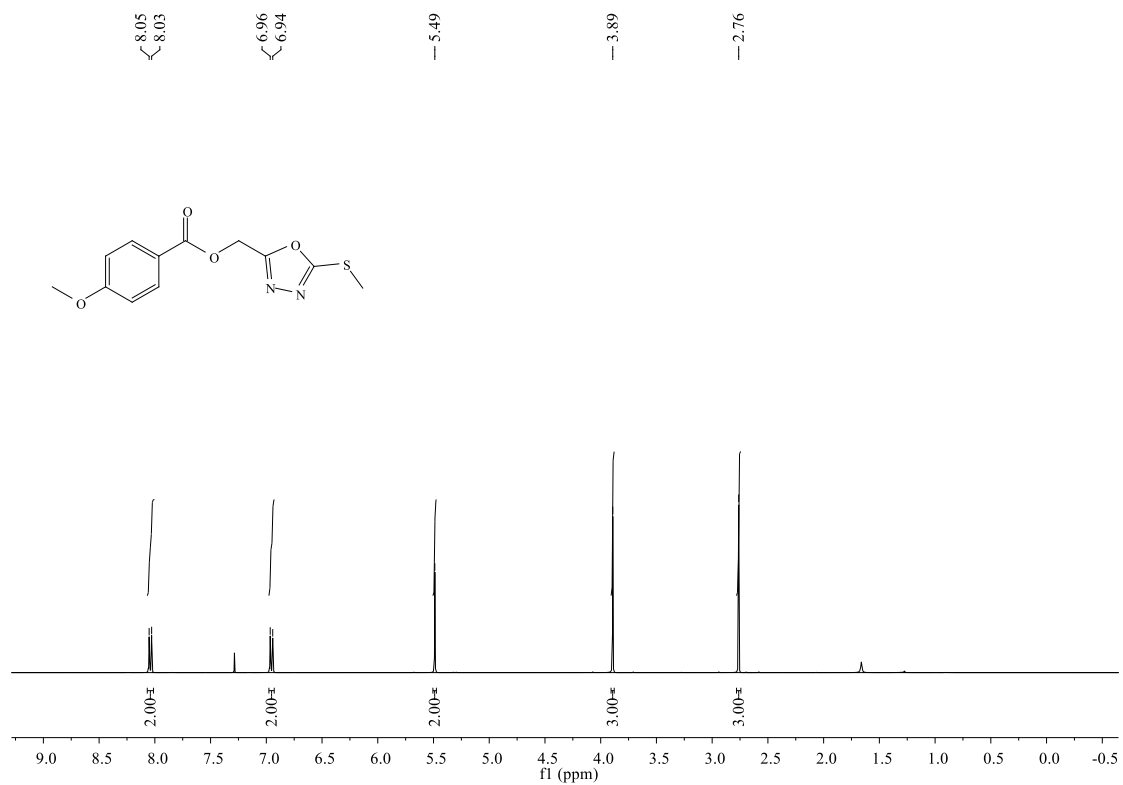
¹H NMR of compound **5a-4**



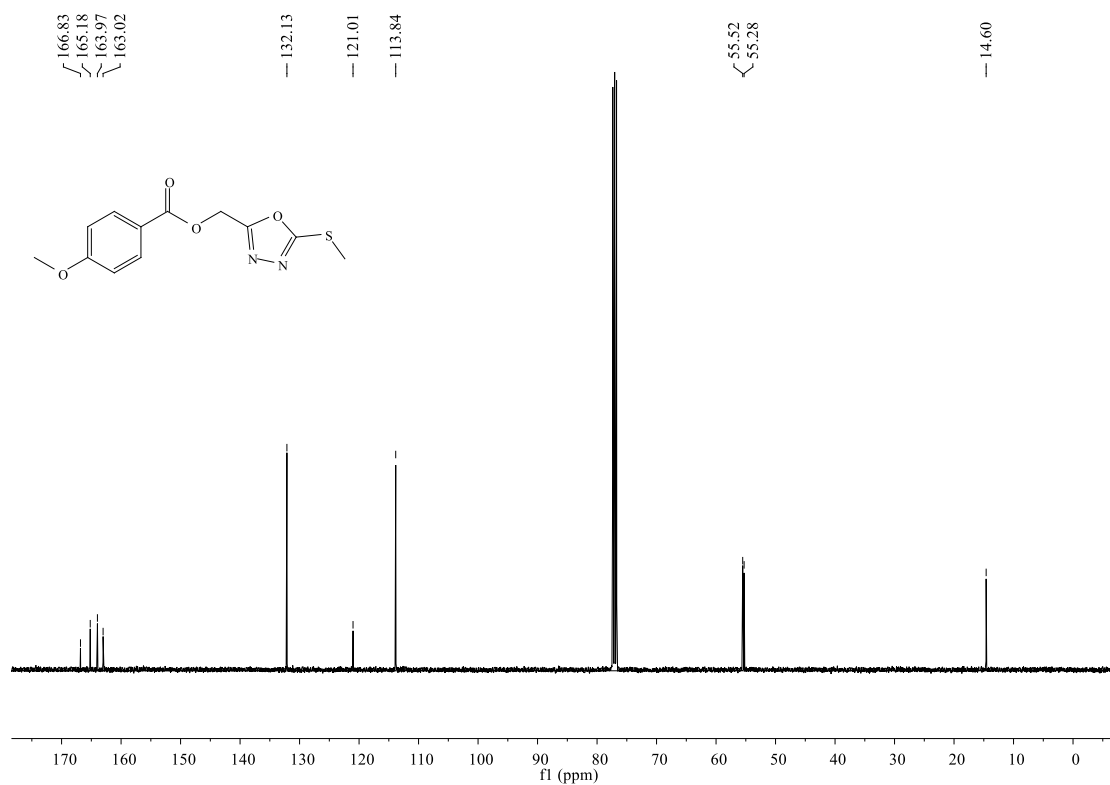
¹³C NMR of compound 5a-4



HRMS of compound 5a-4

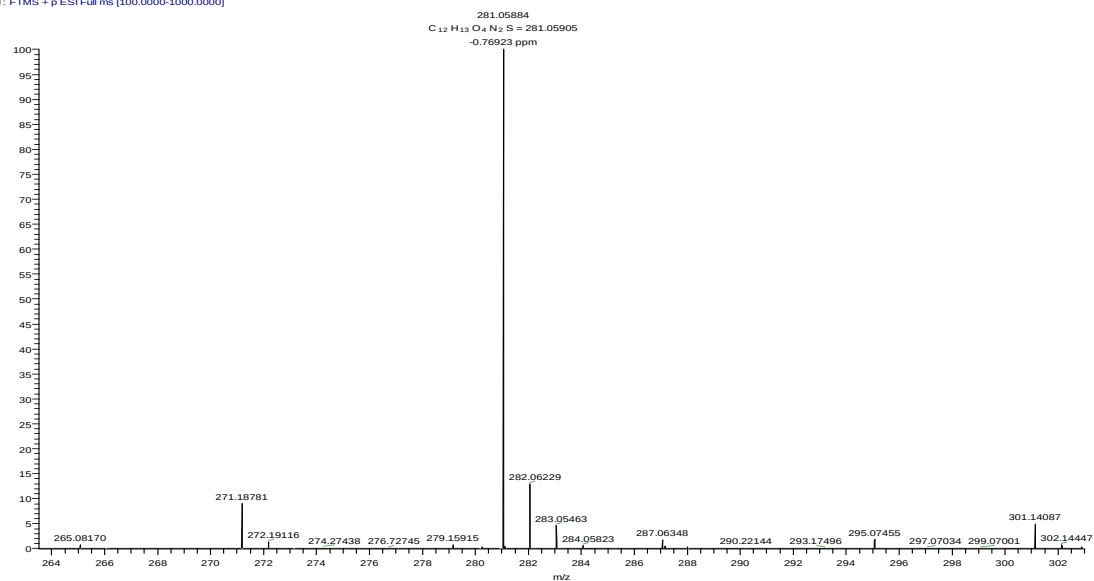


¹H NMR of compound **5a-5**

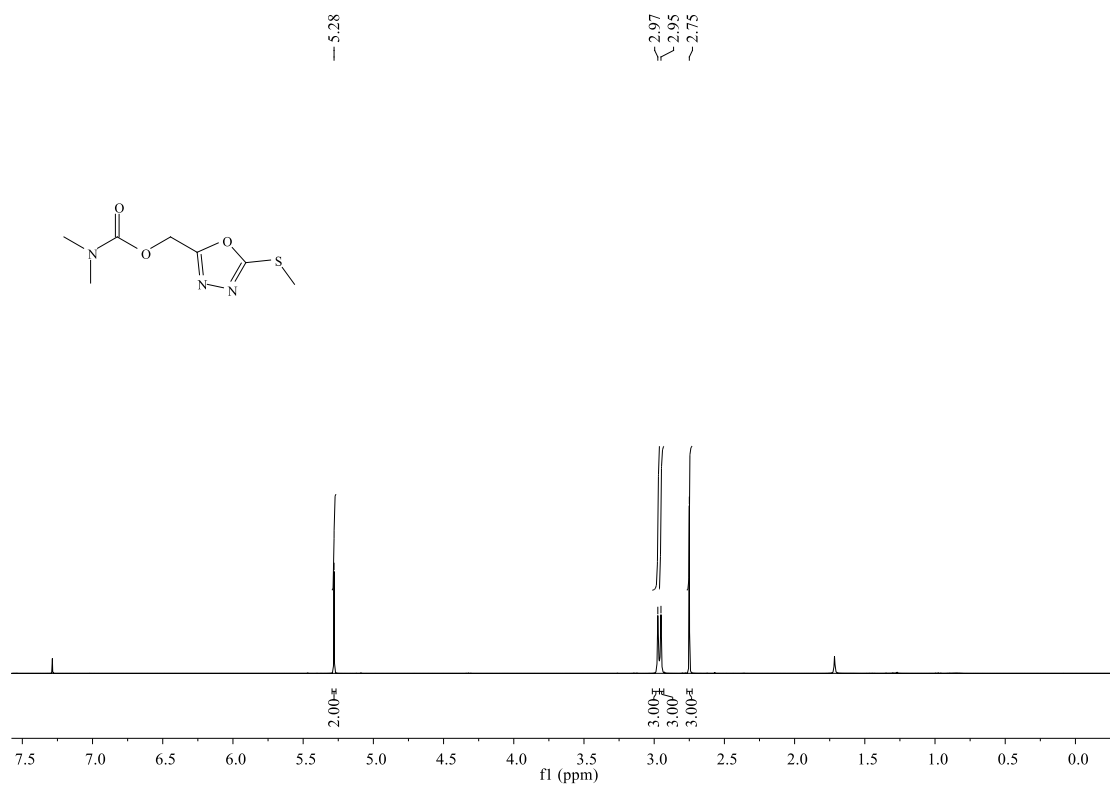


¹³C NMR of compound **5a-5**

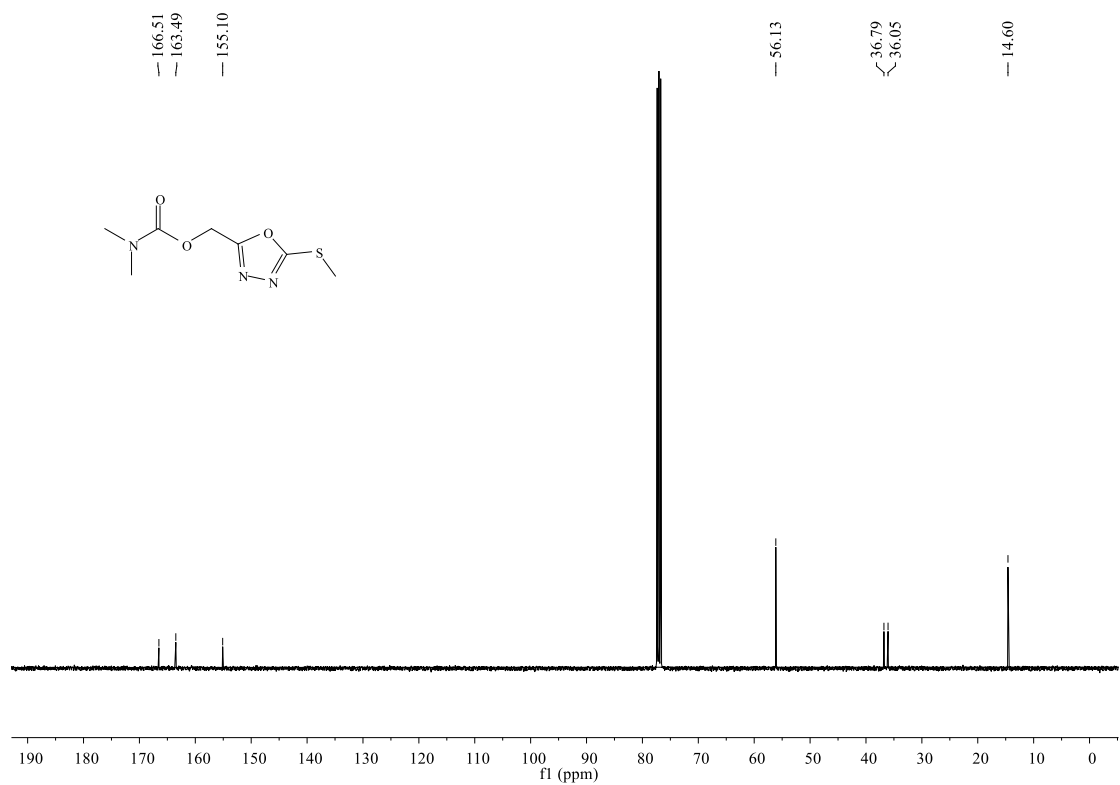
2019110505 #57 RT: 0.55 AV: 1 NL: 2.99E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]



HRMS of compound 5a-5

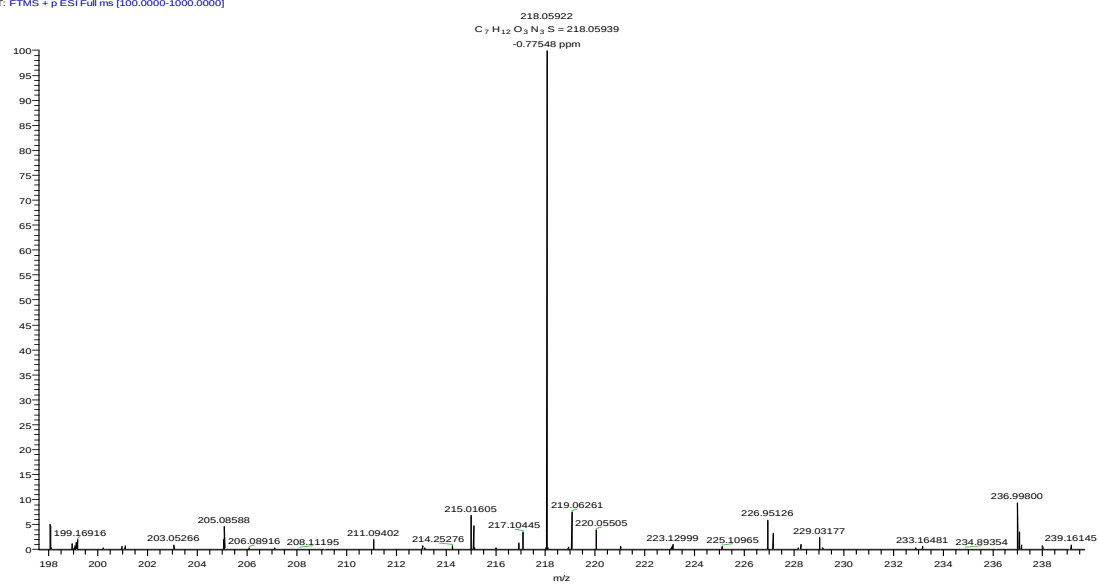


¹H NMR of compound 5a-6



¹³C NMR of compound 5a-6

2019110509 #73 RT: 0.70 AV: 1 NL: 2.32E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]



HRMS of compound 5a-6