Supporting Information

Design, synthesis and evaluation of quinolinone derivatives containing dithiocarbamate moiety as multifunctional AChE inhibitors for the treatment of Alzheimer's disease

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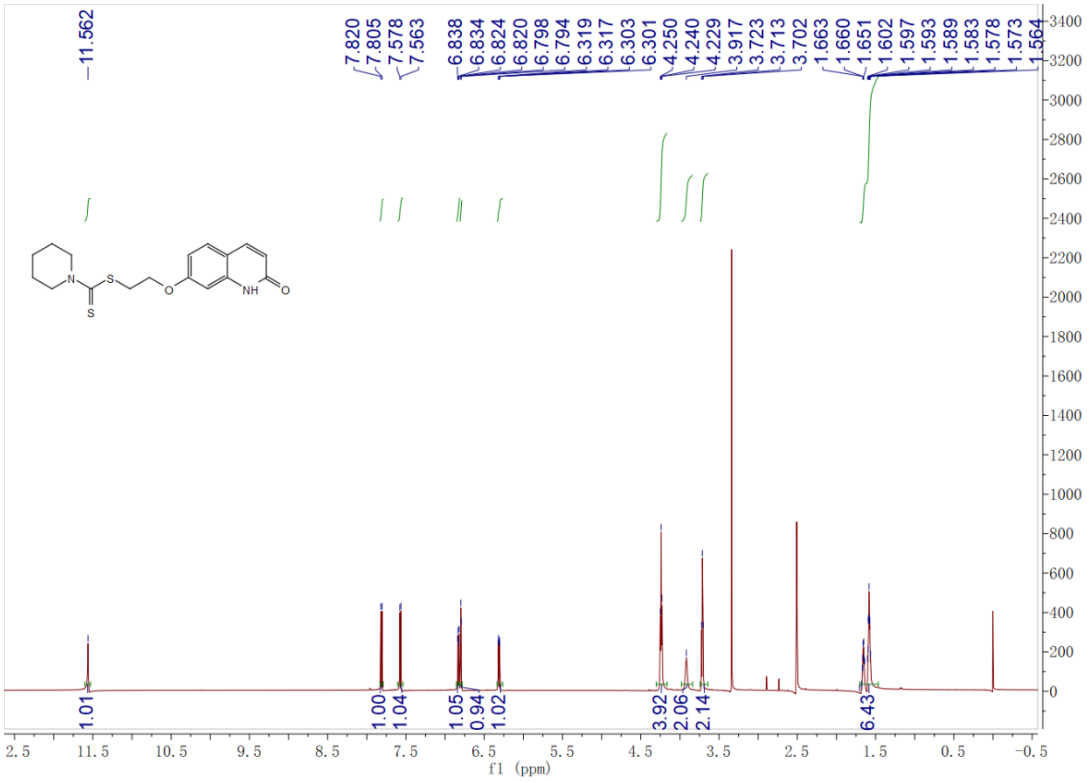
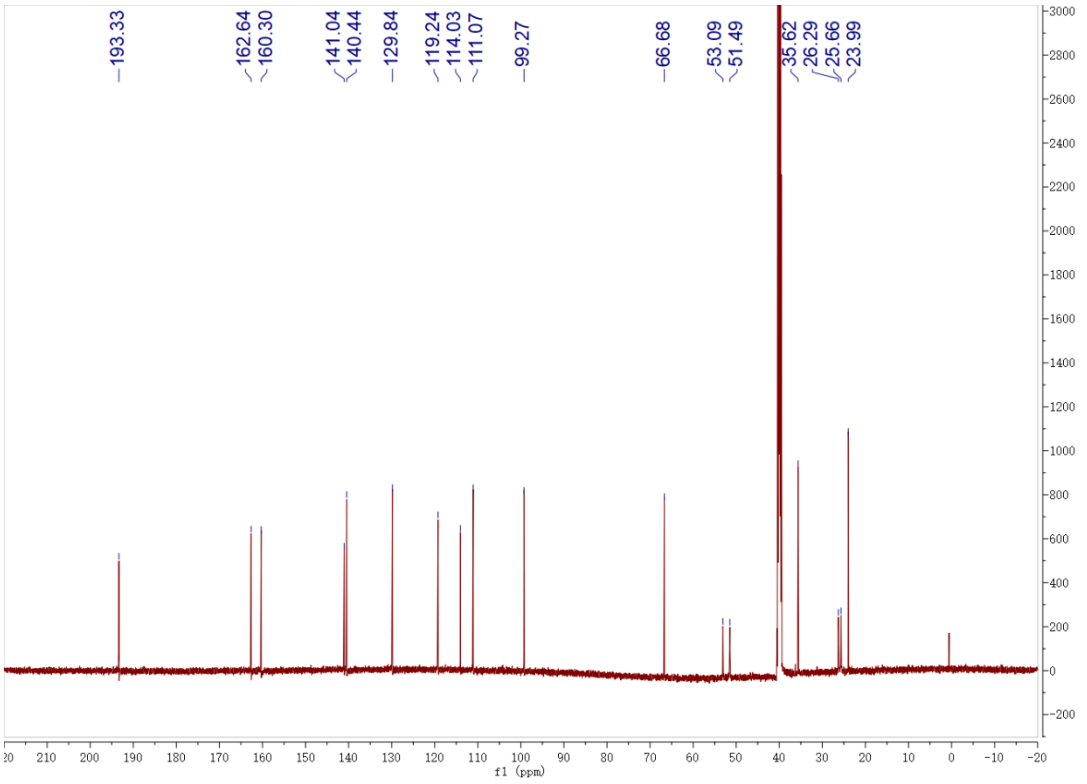
[1] H NMR spectrum of compound **4a**



[13] C NMR spectrum of compound **4a**



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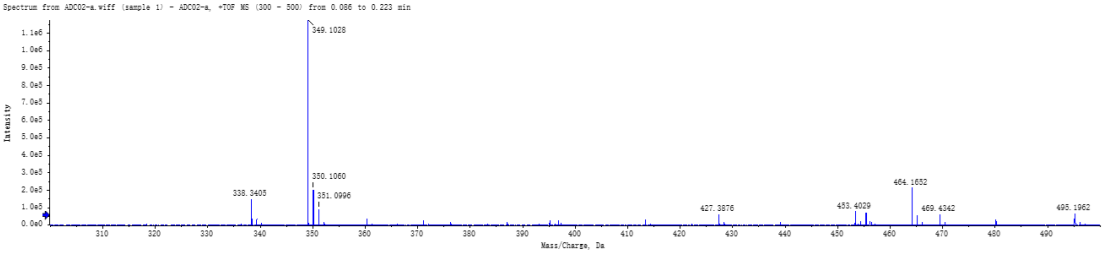

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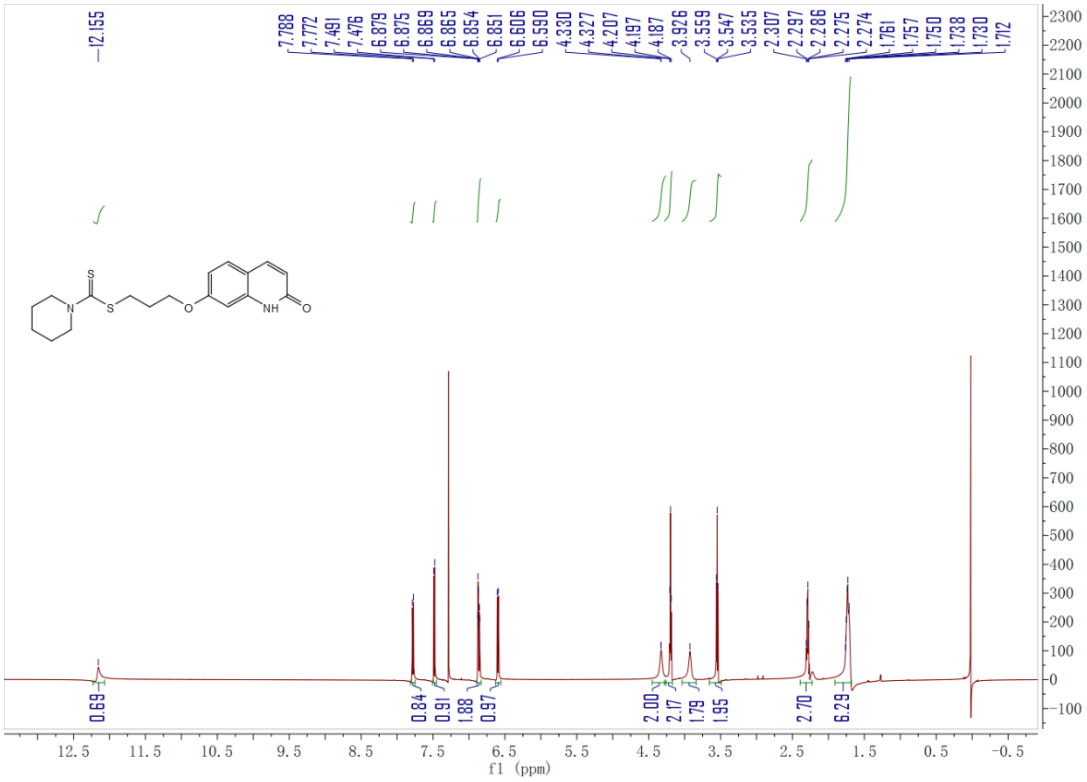

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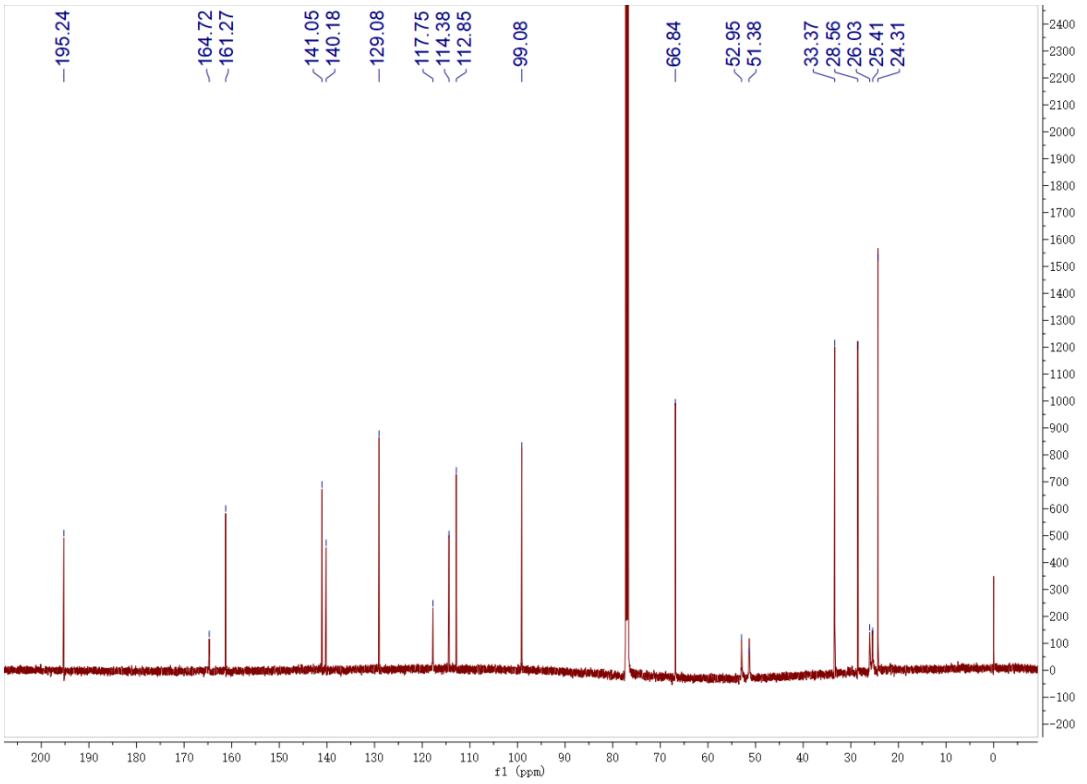

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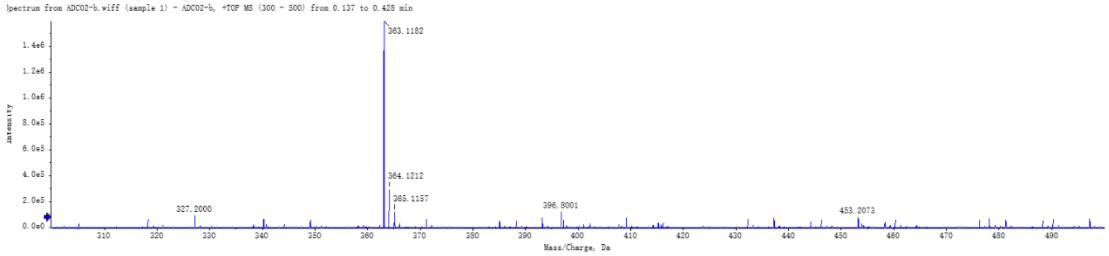

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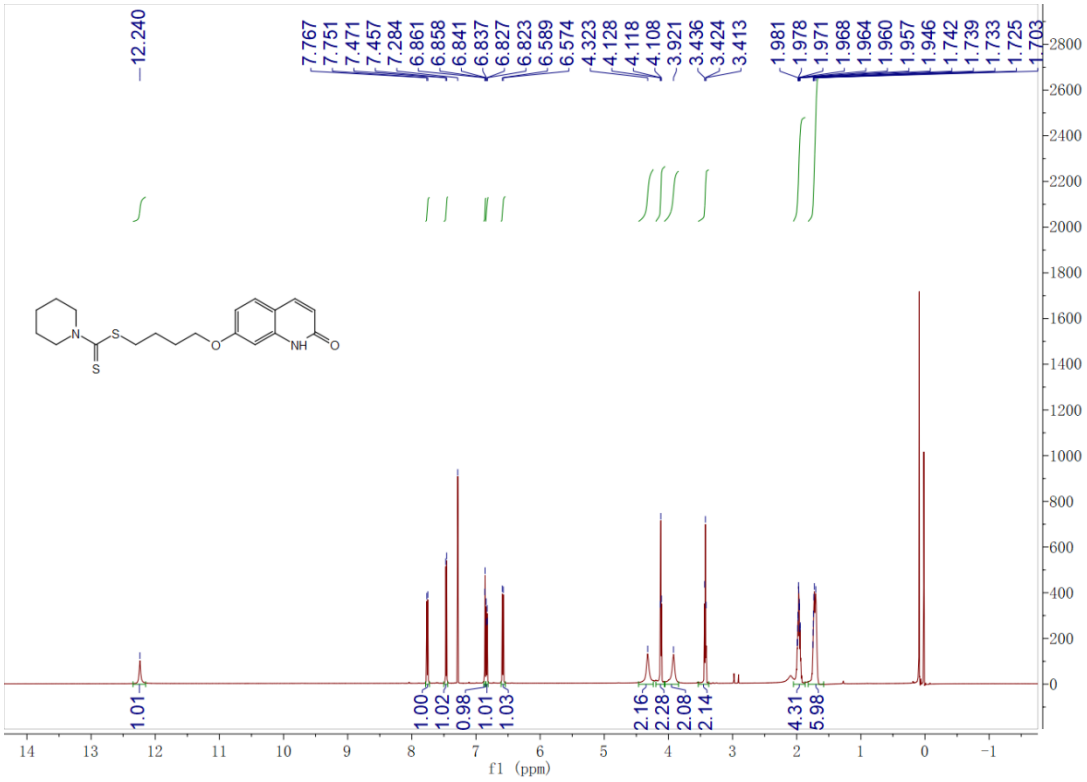

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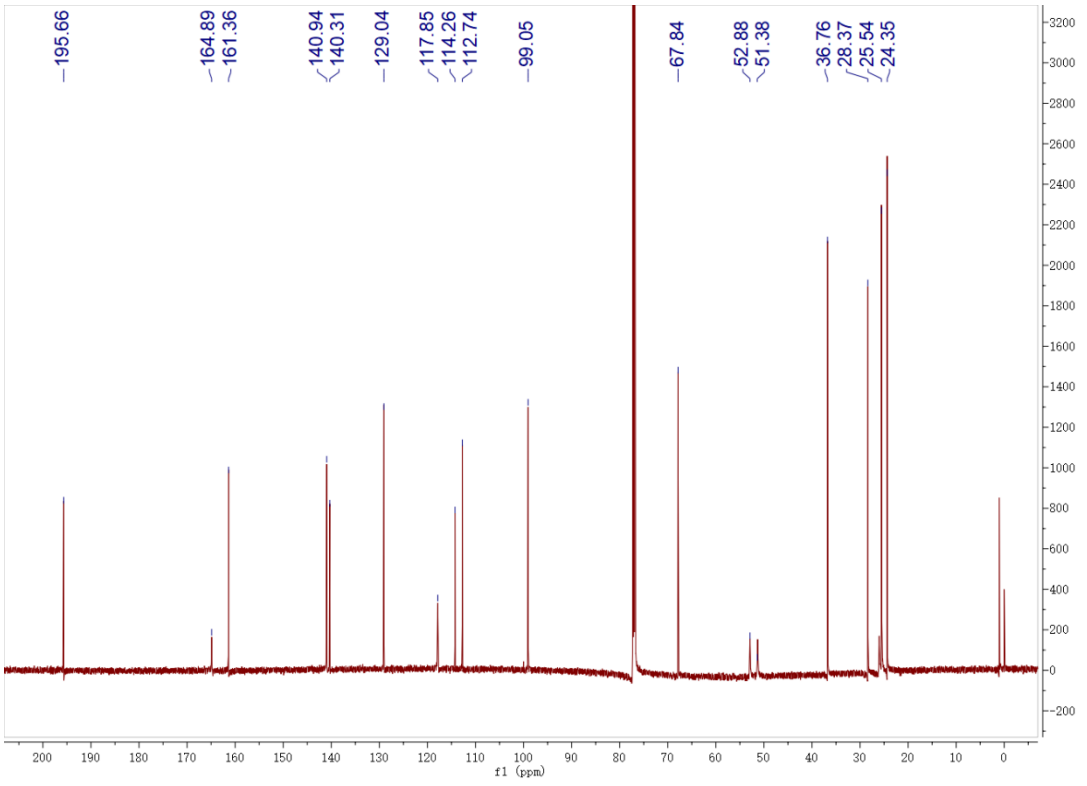

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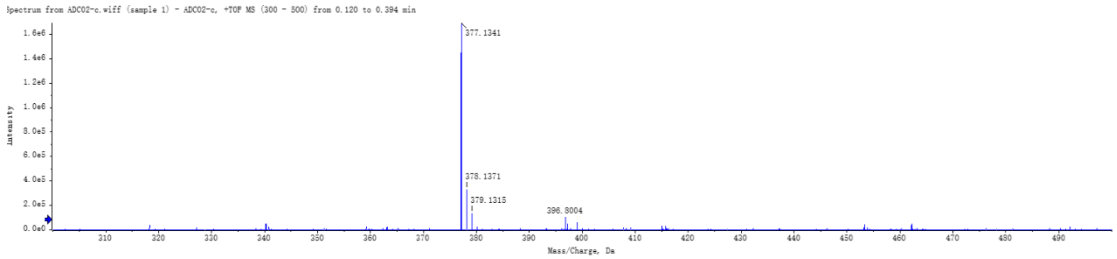

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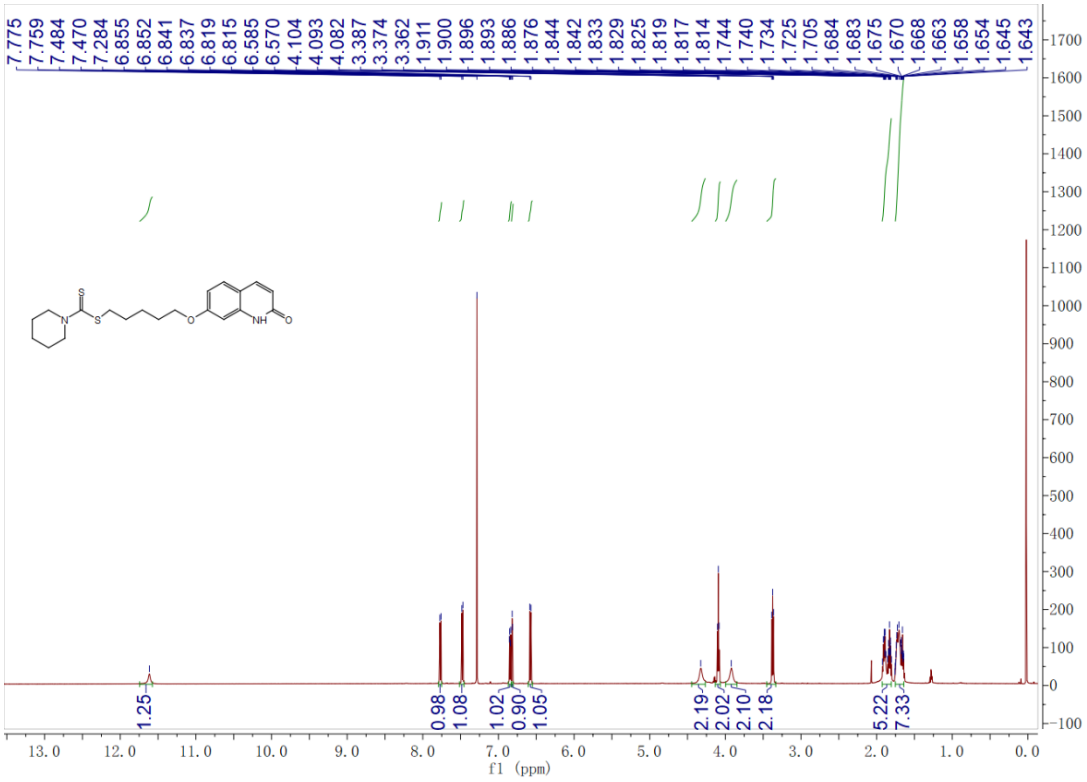

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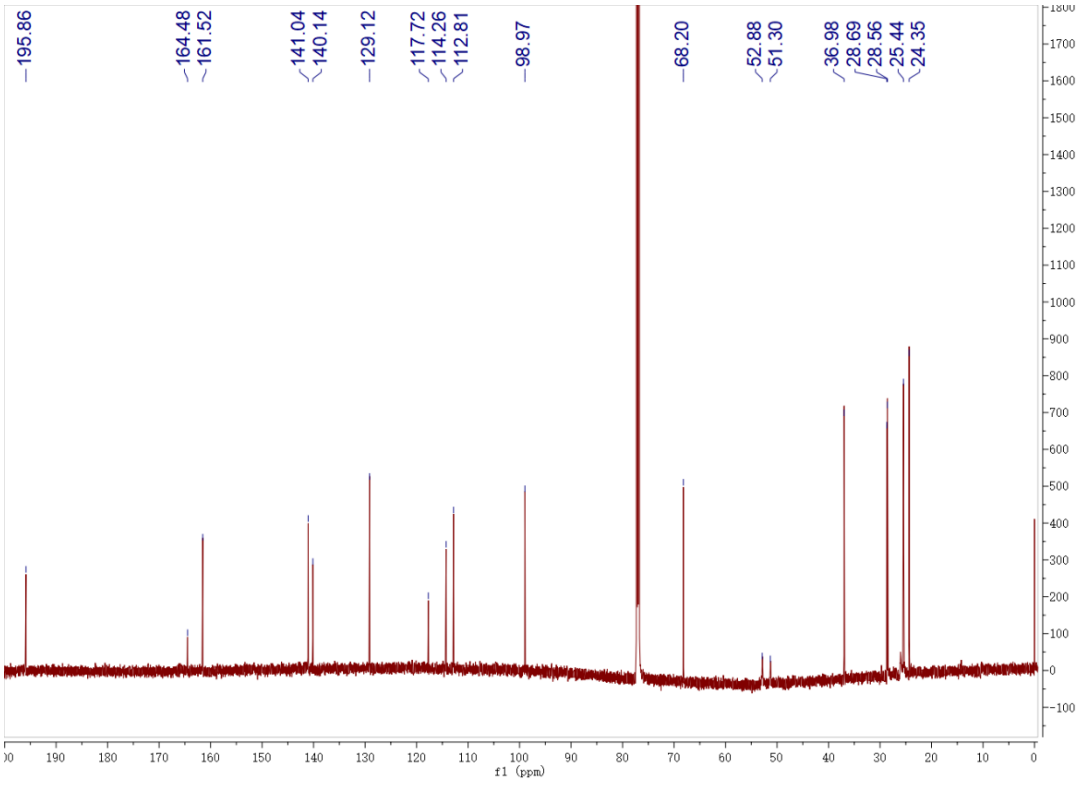

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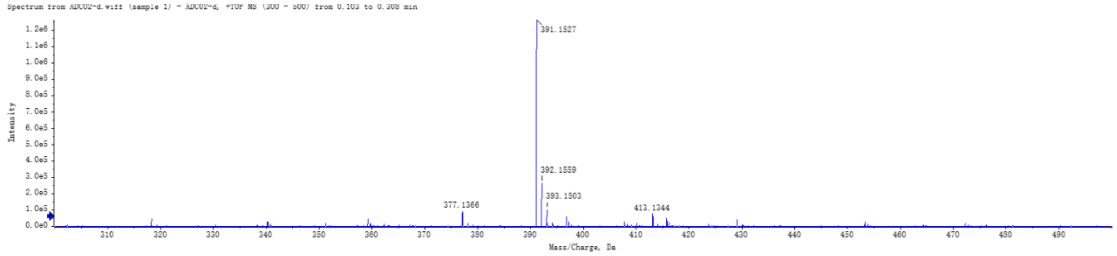

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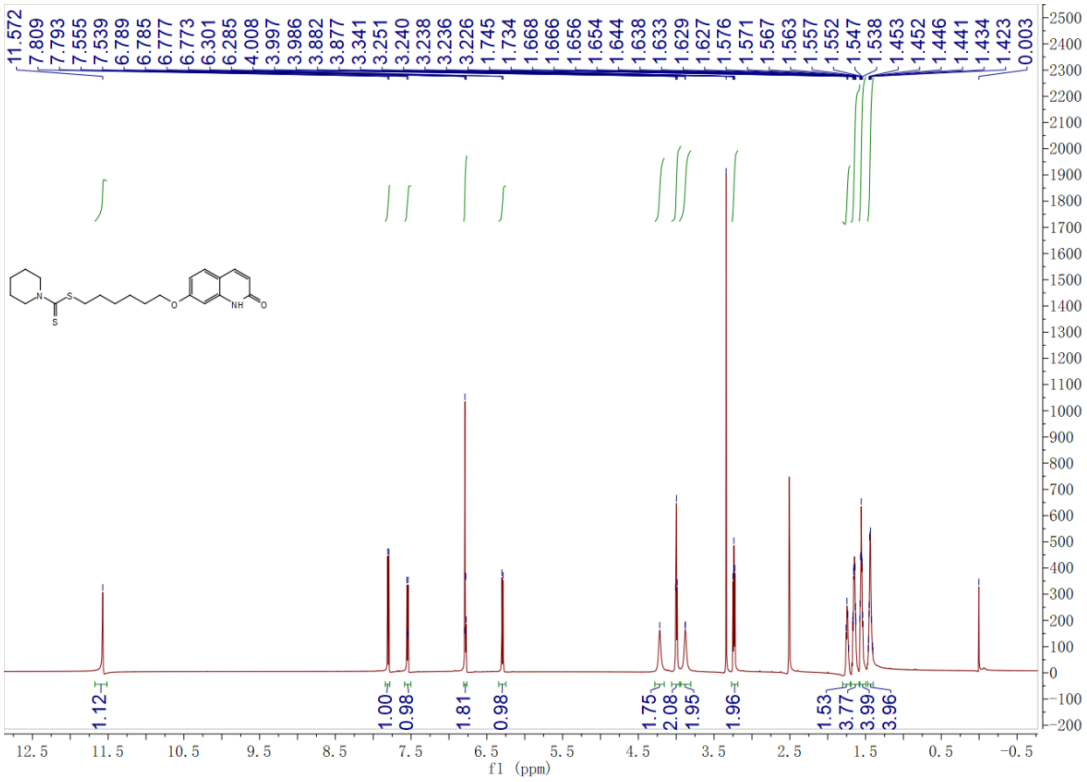

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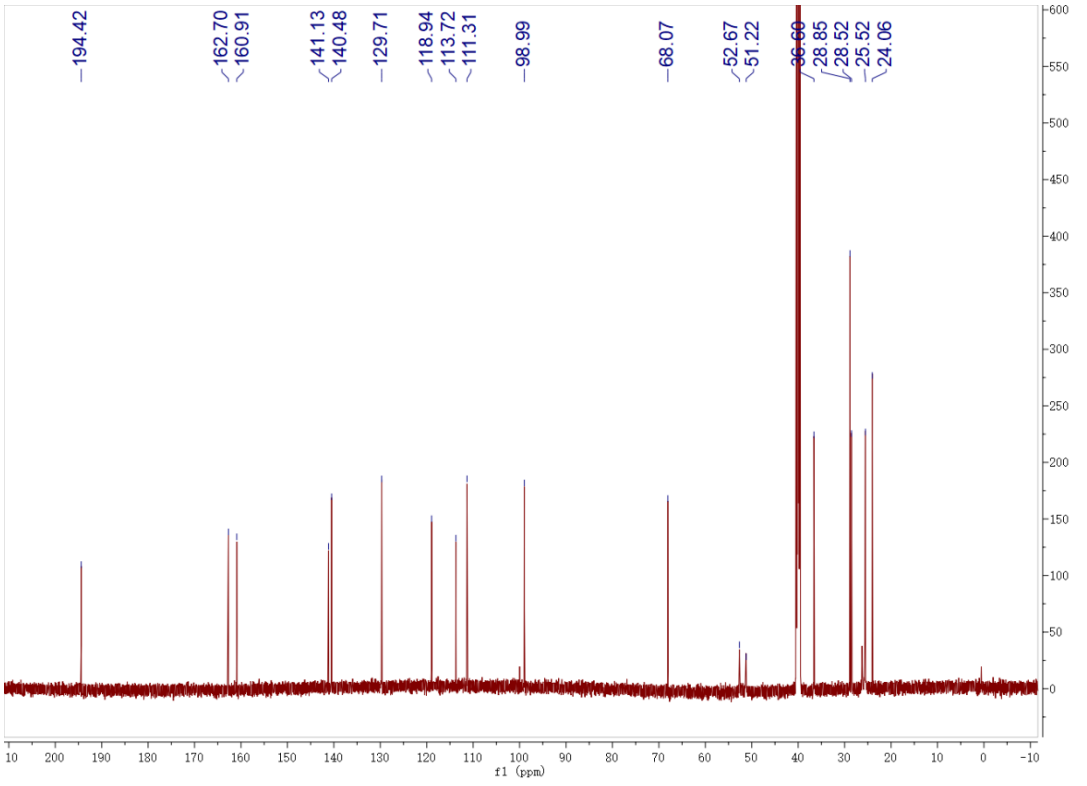

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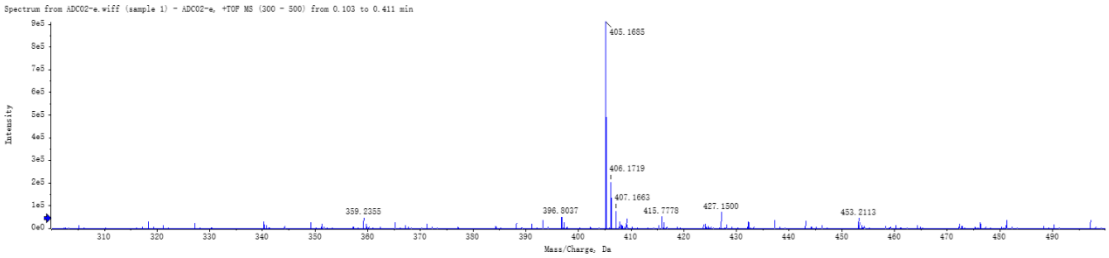

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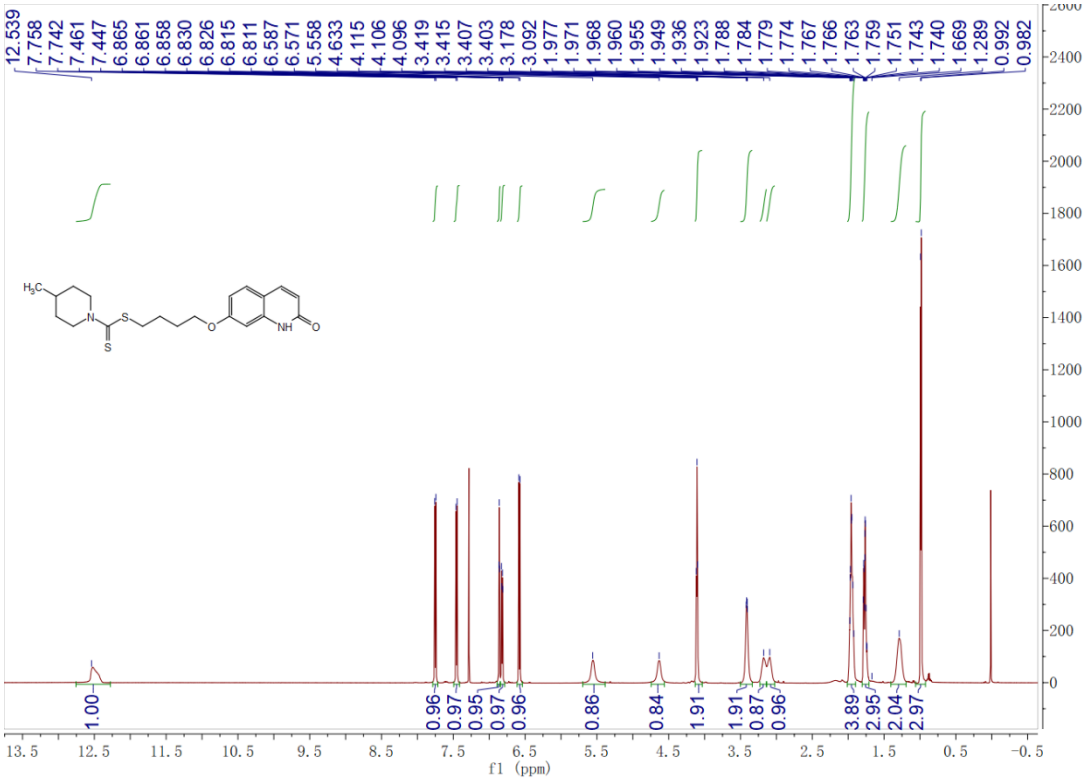

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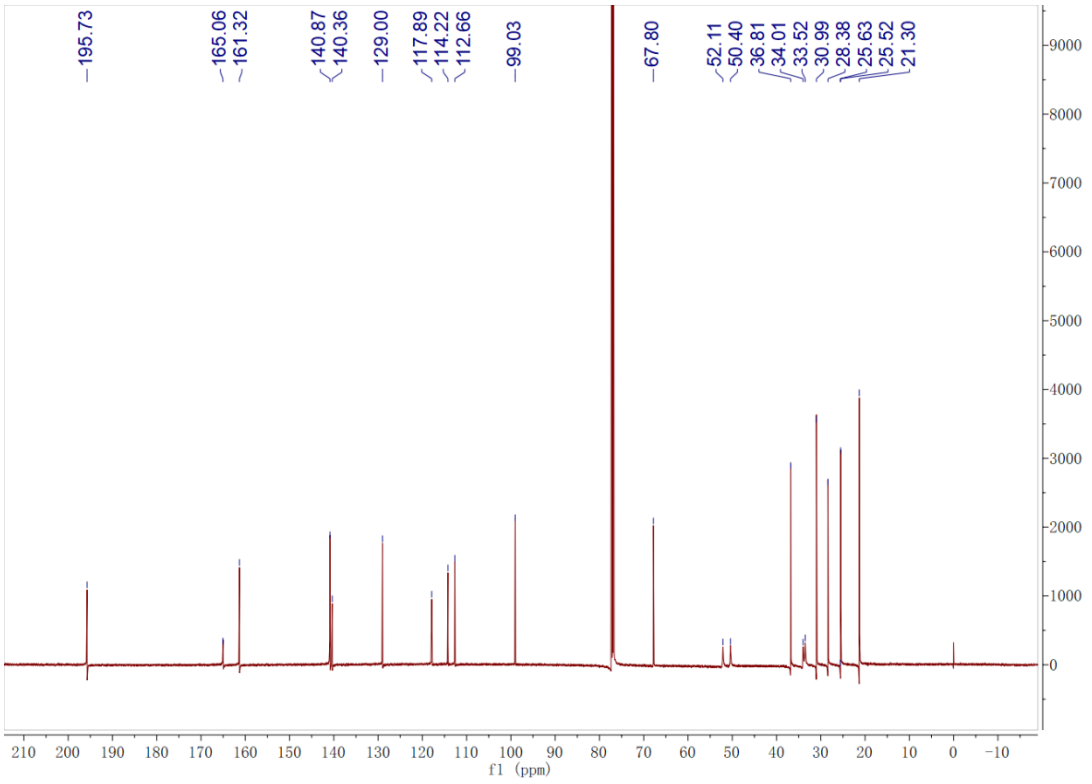

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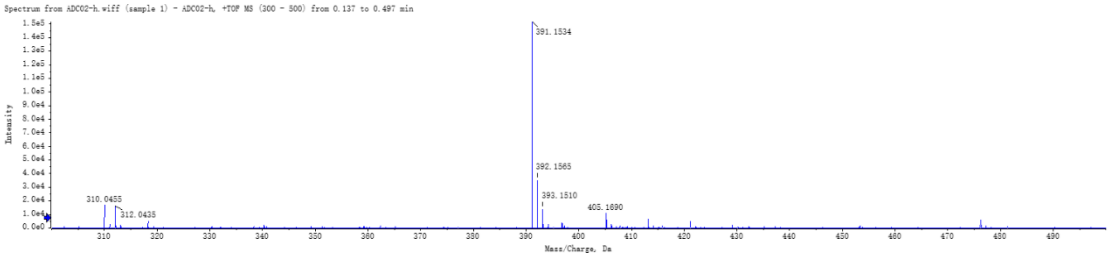

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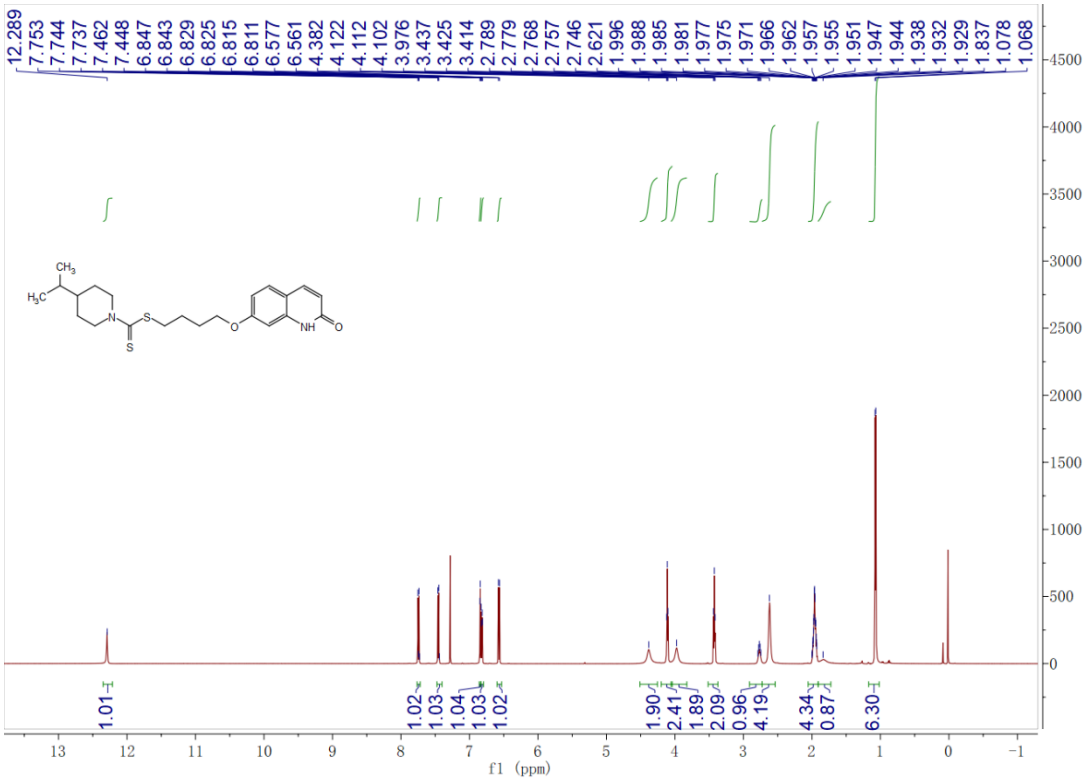

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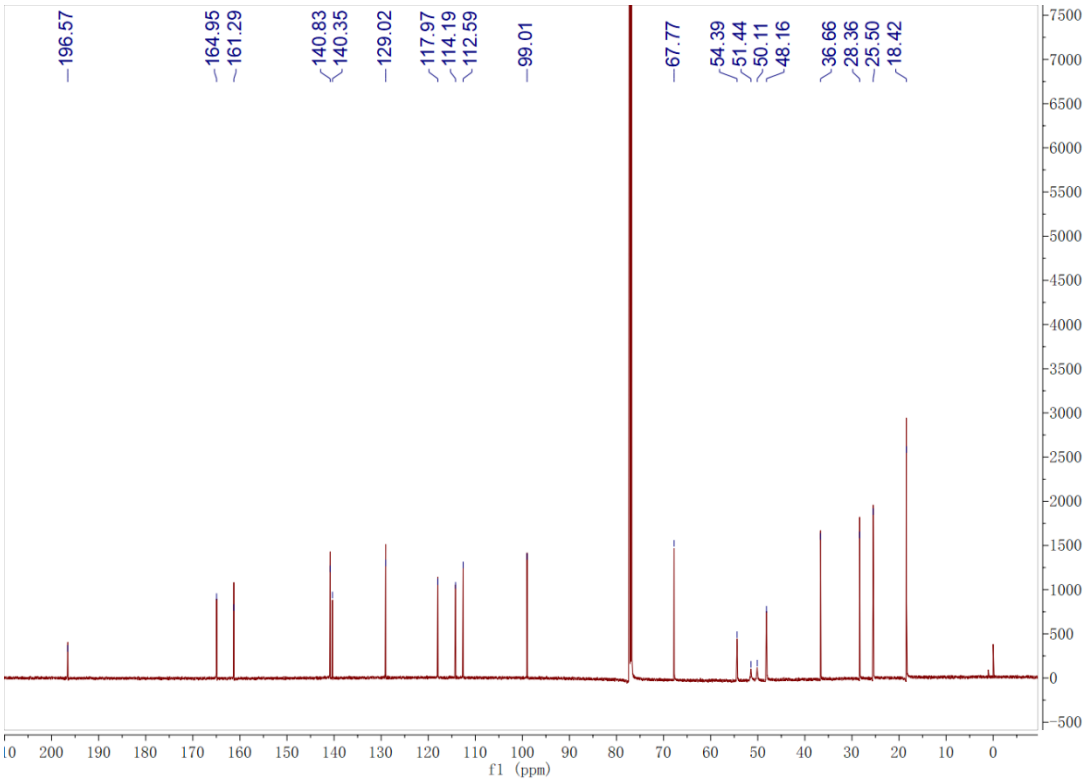

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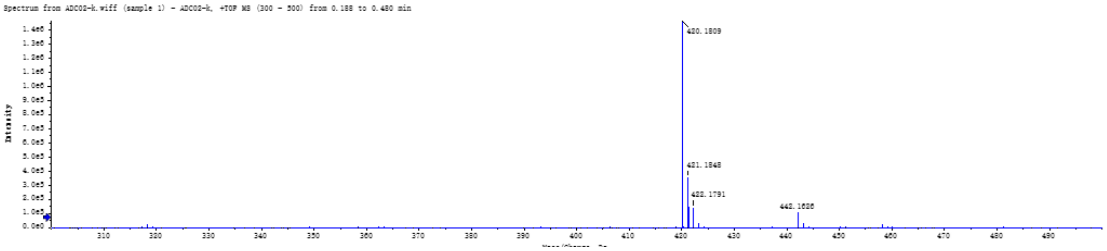

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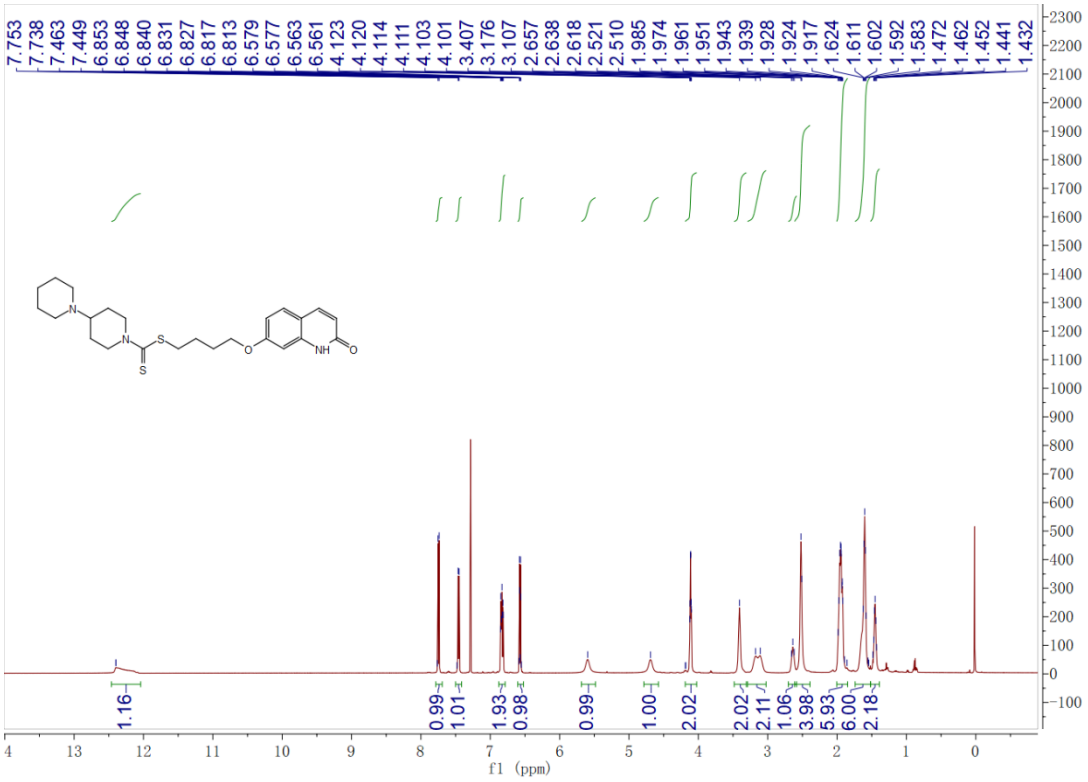

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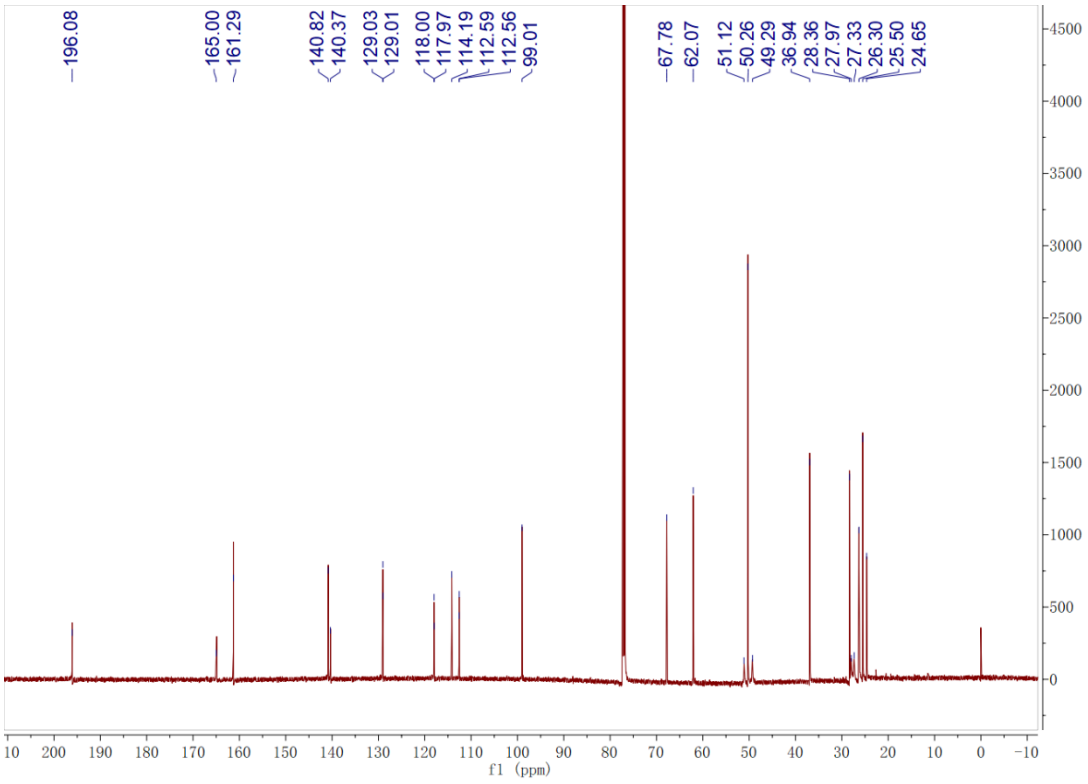

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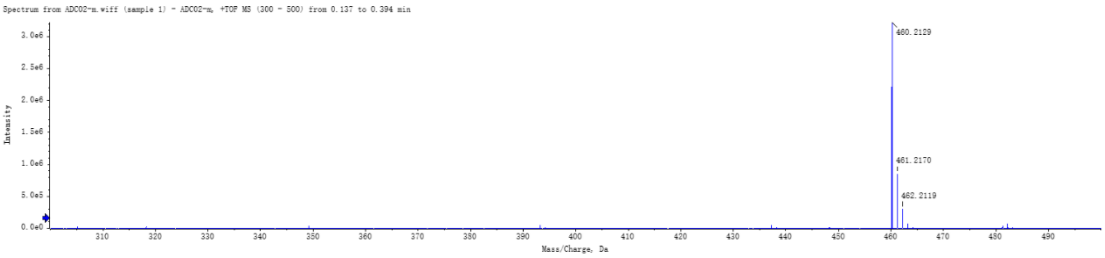

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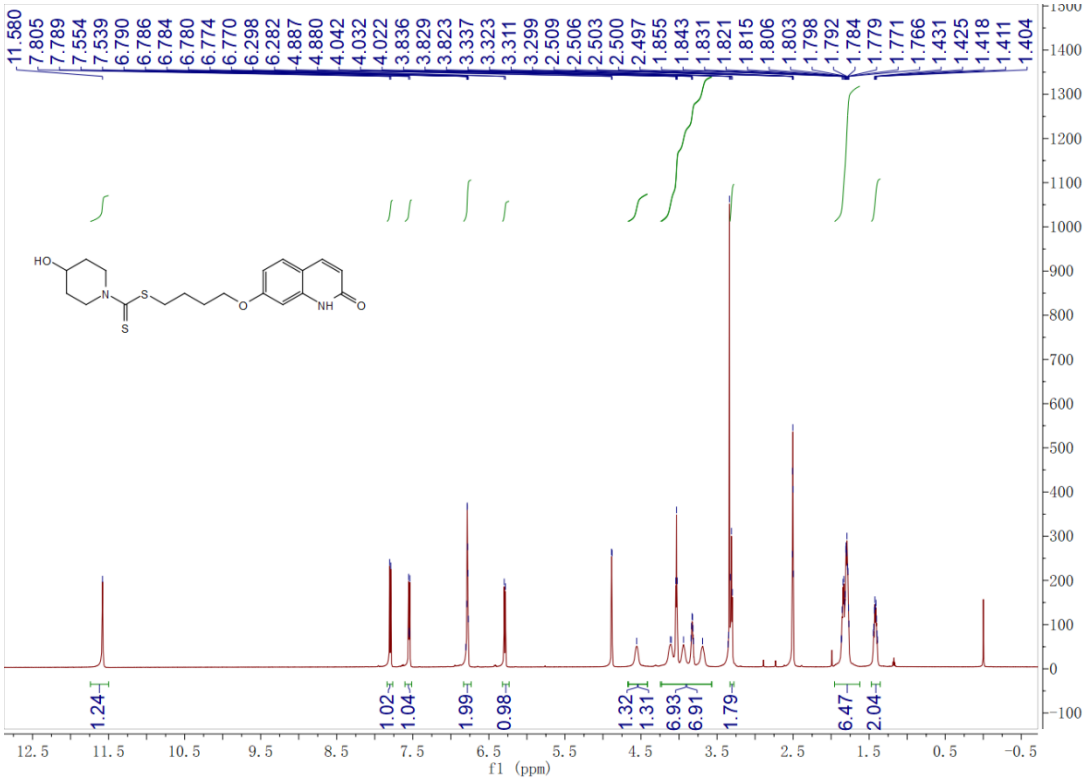

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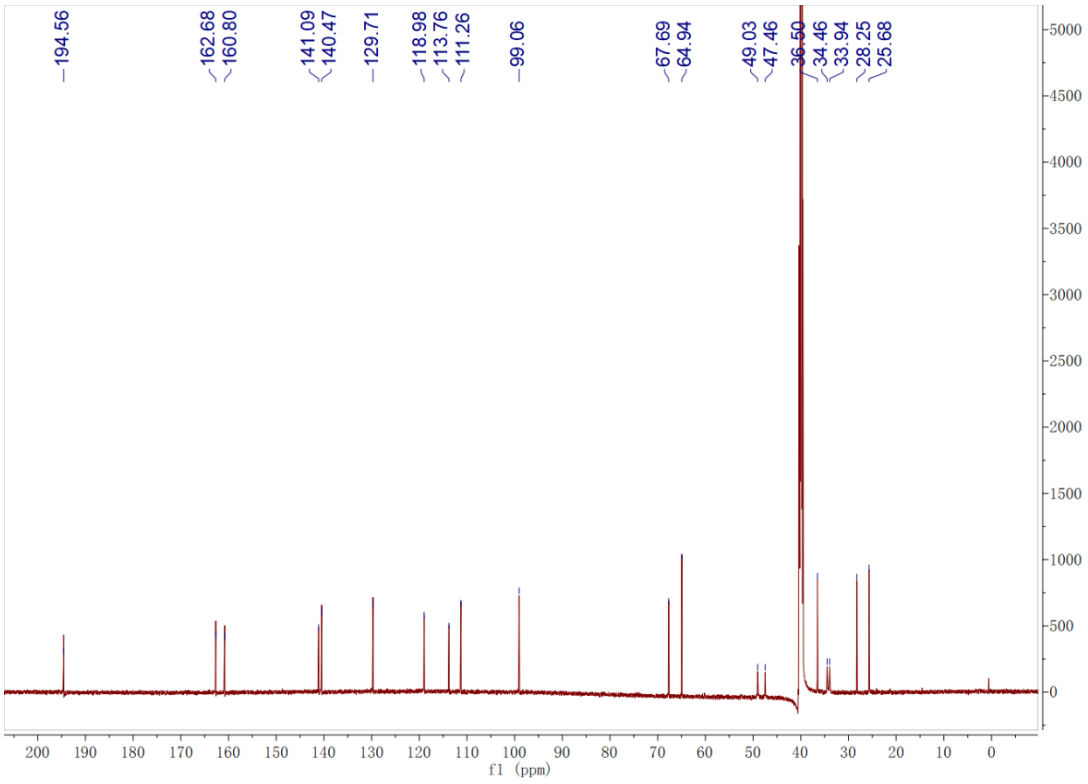

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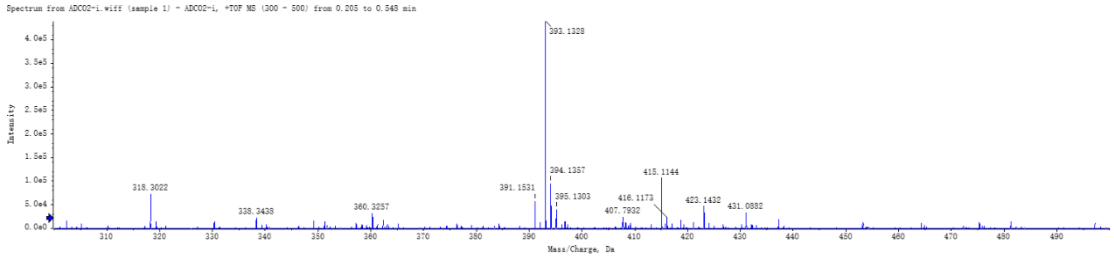

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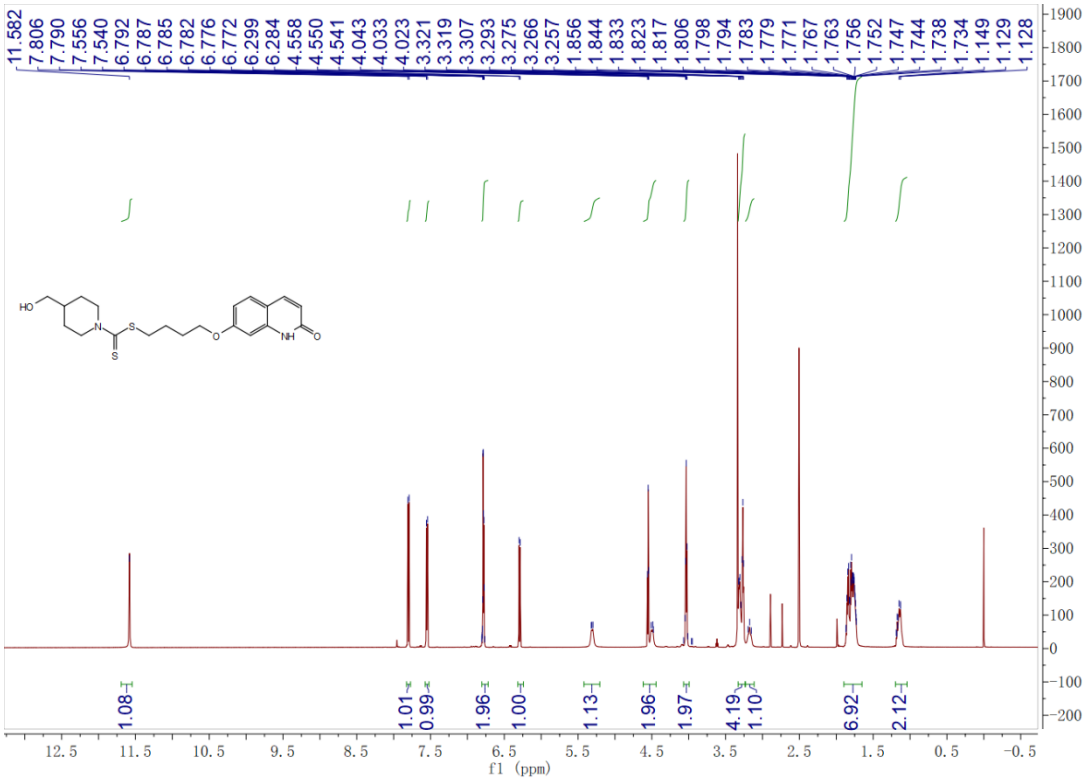

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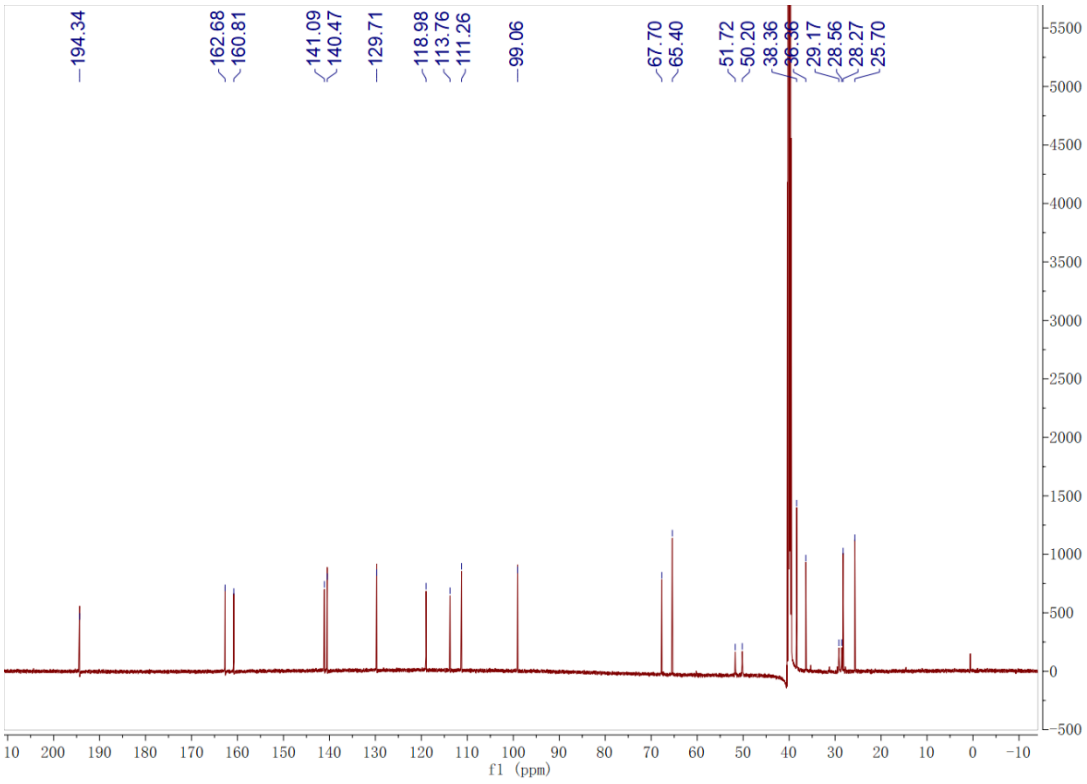

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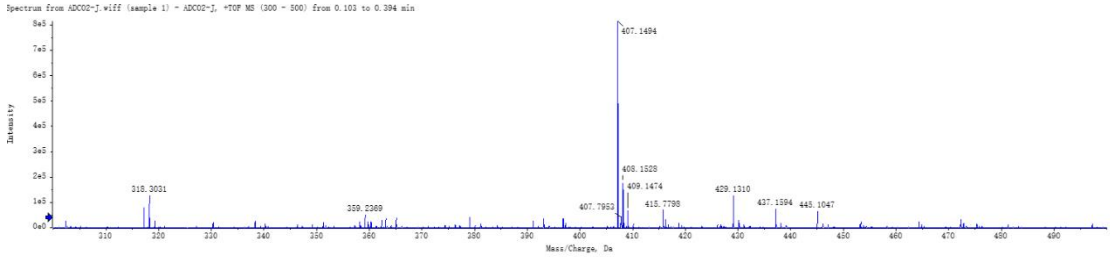

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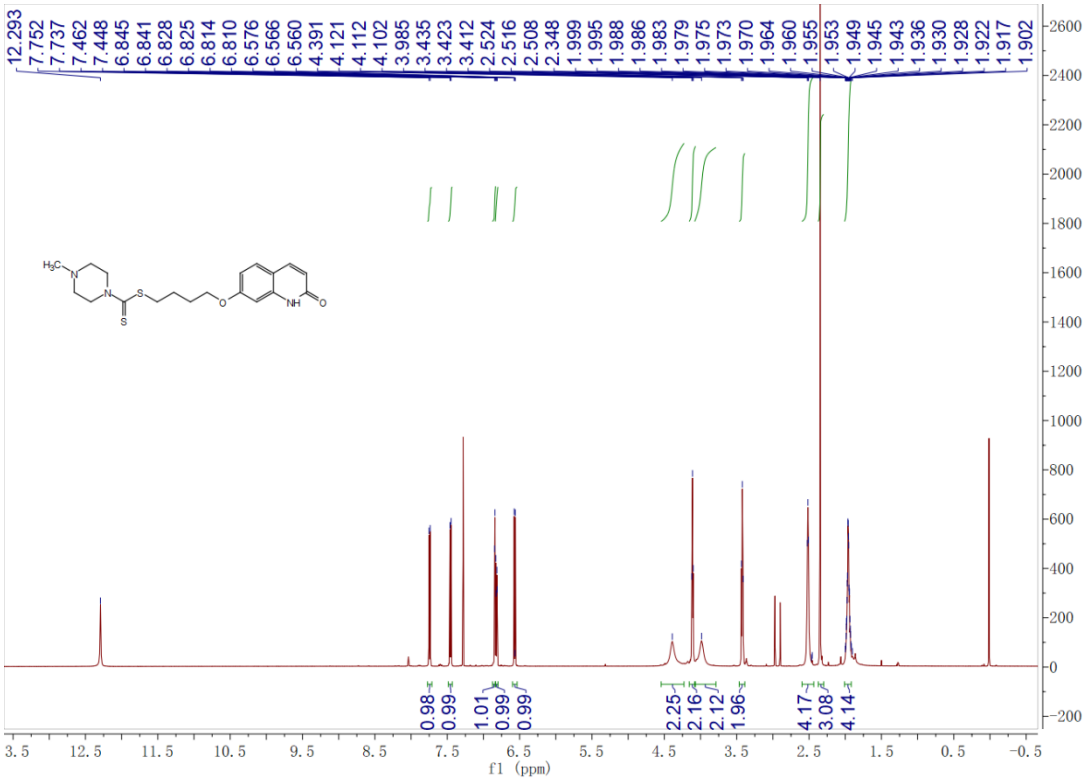

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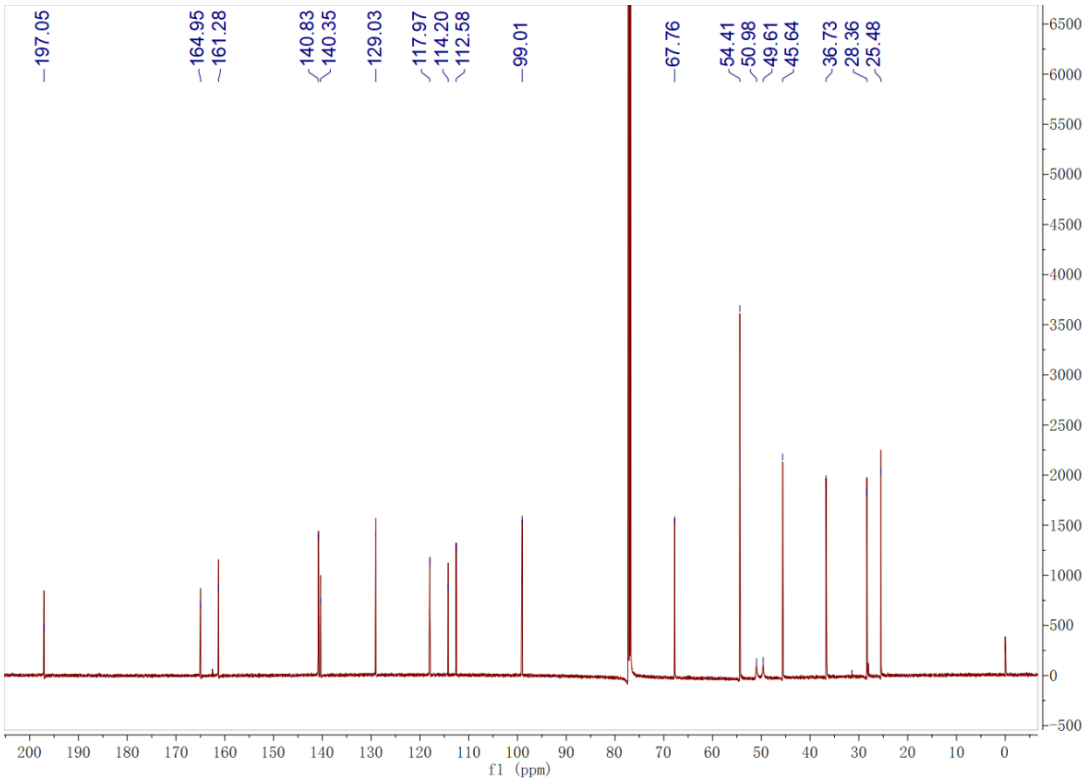
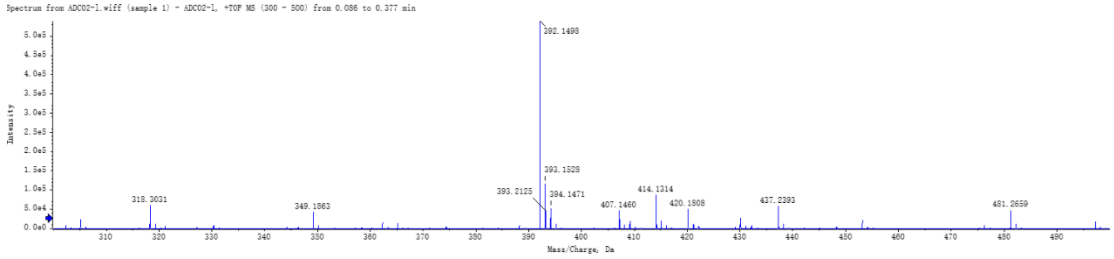


HRMS (ESI) spectrum of compound **4k**.



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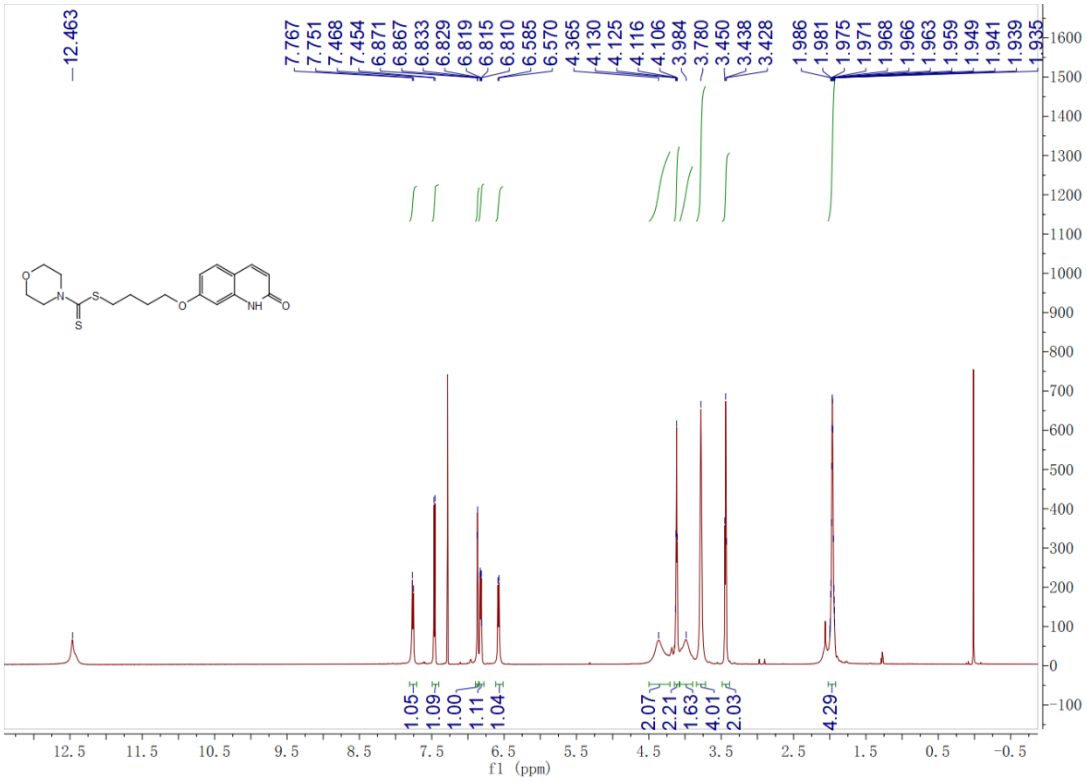
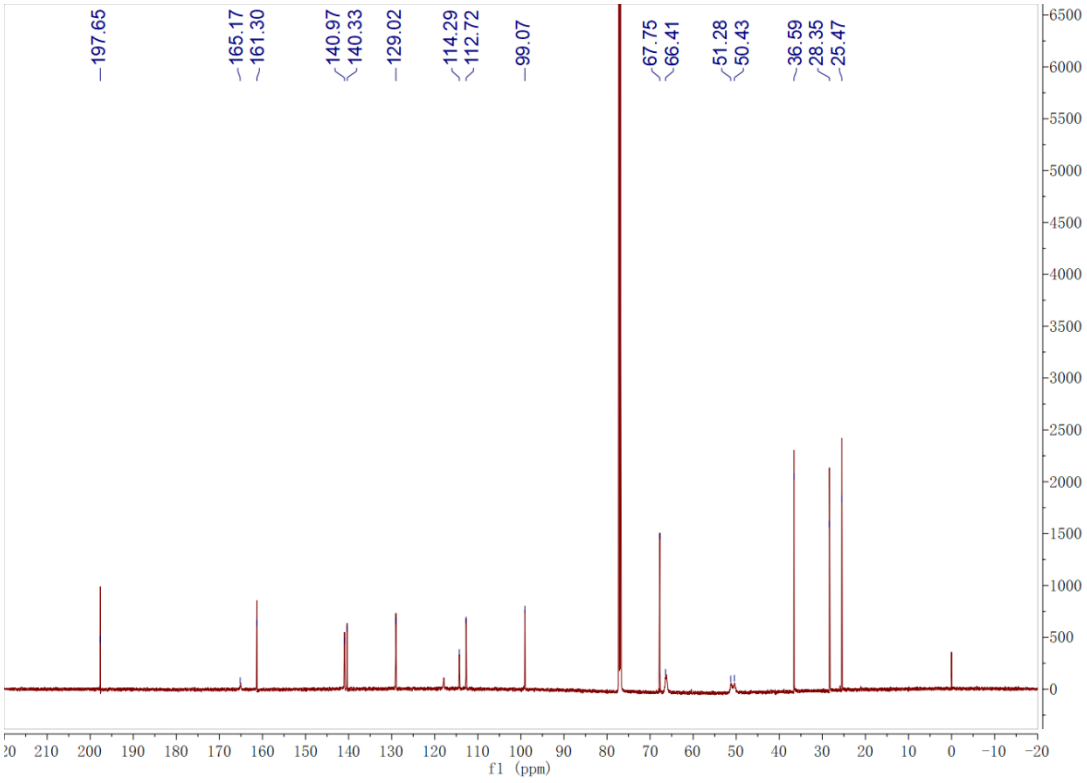


[13]C NMR spectrum of compound **4l**



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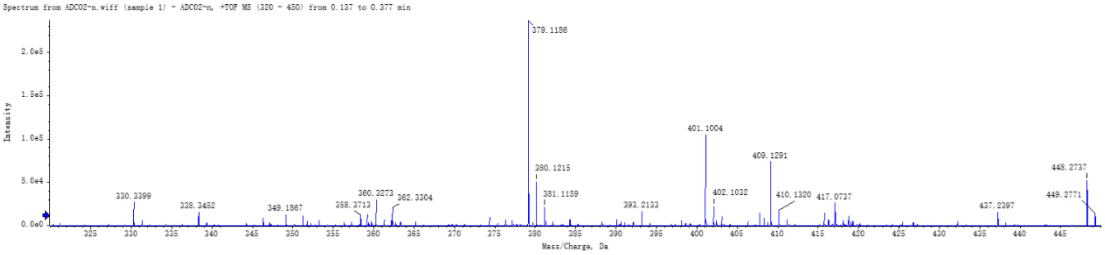

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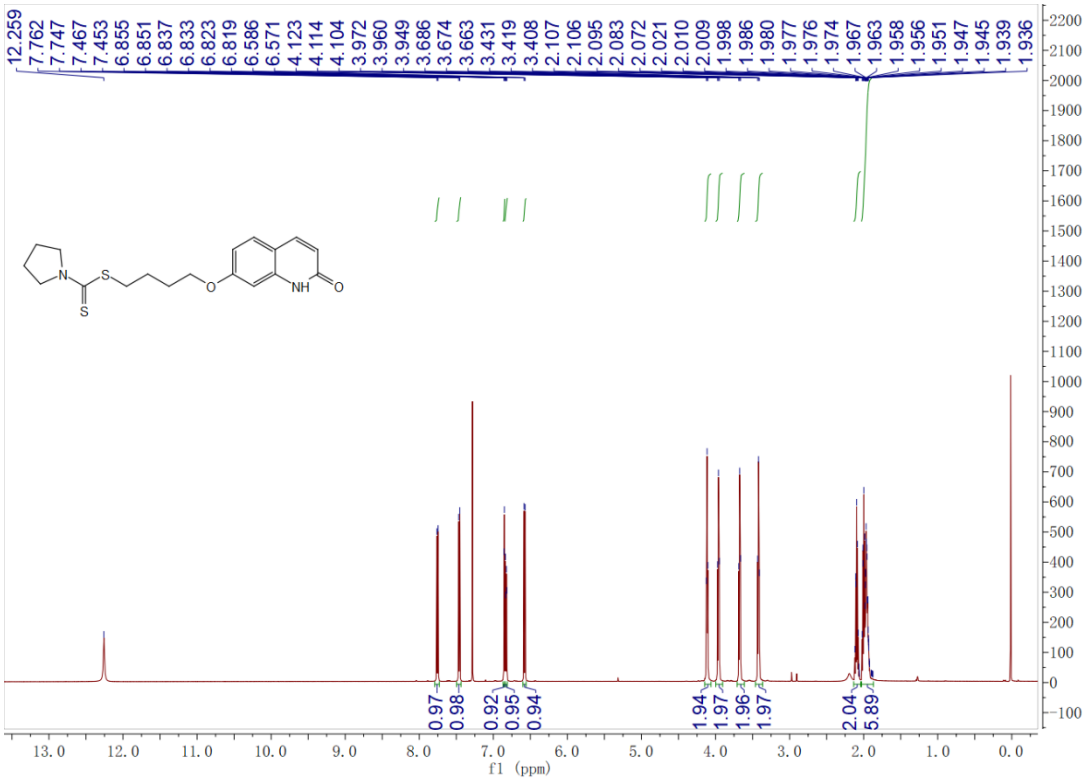

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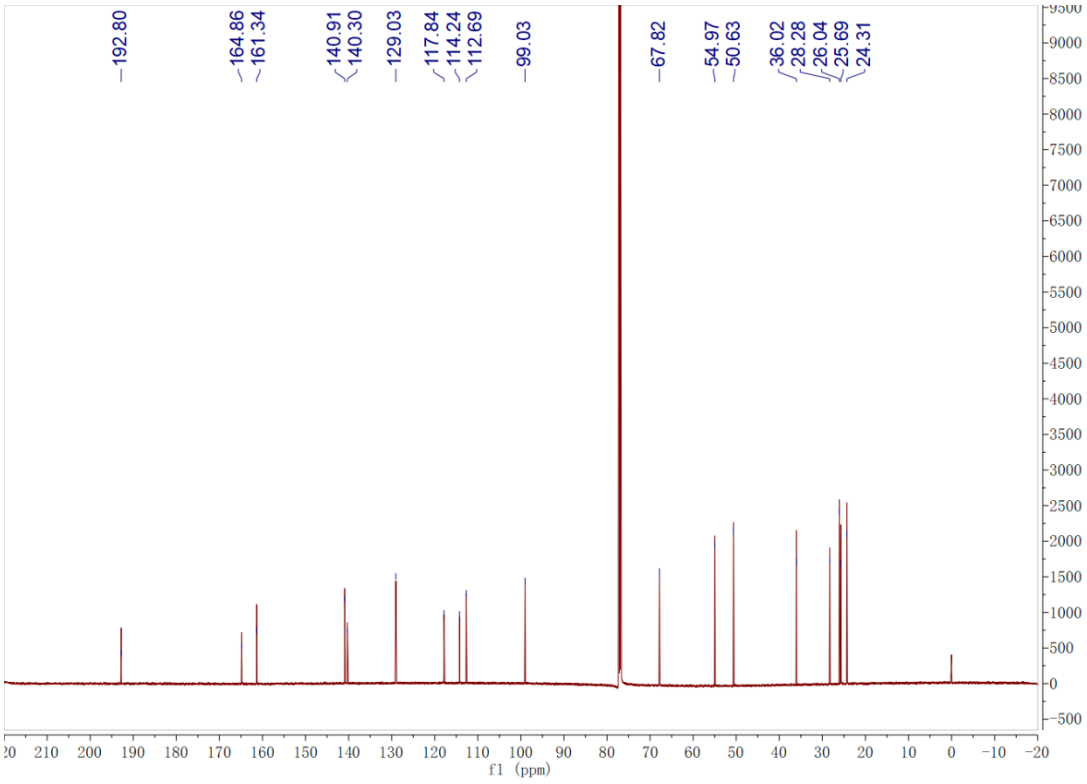

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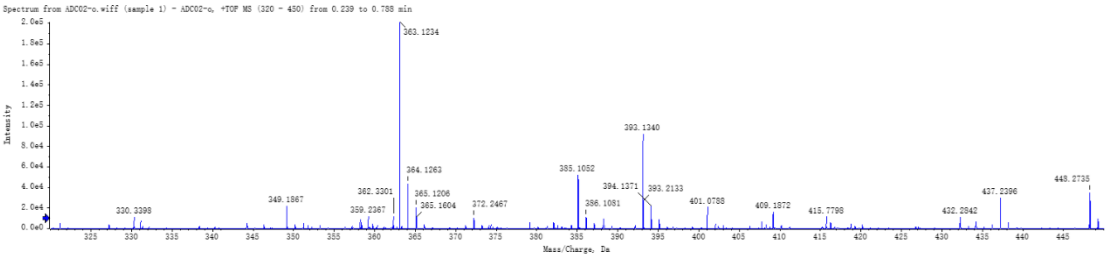
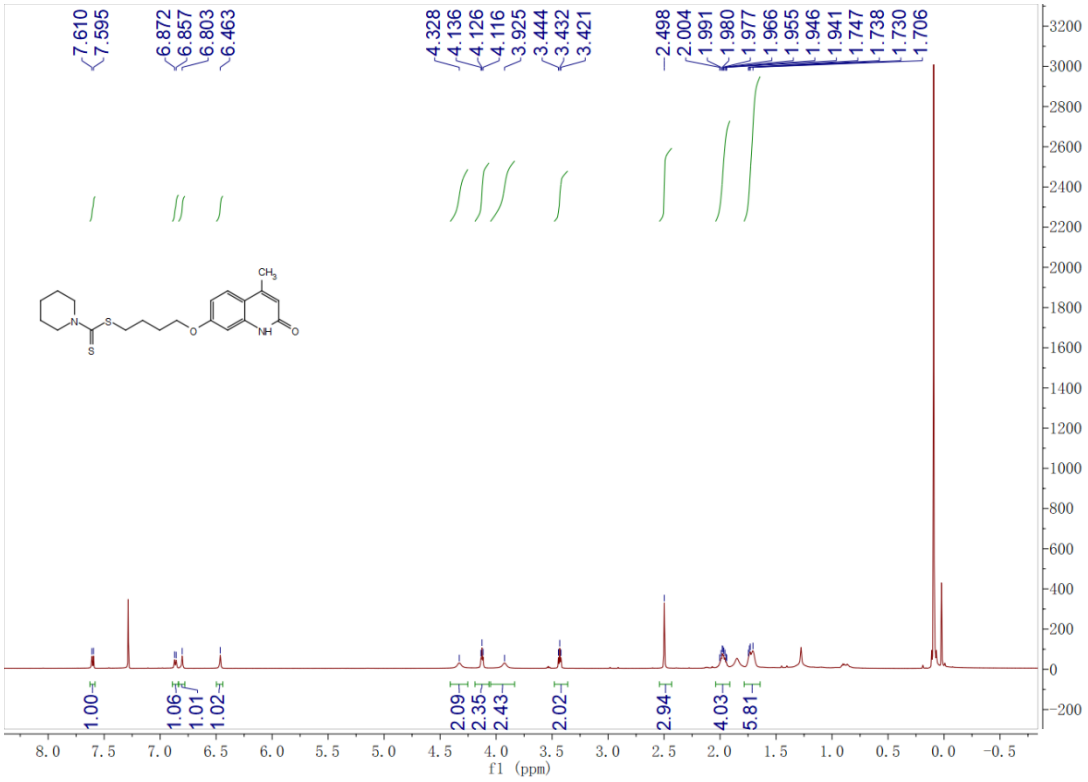


[1] H NMR spectrum of compound **9a**



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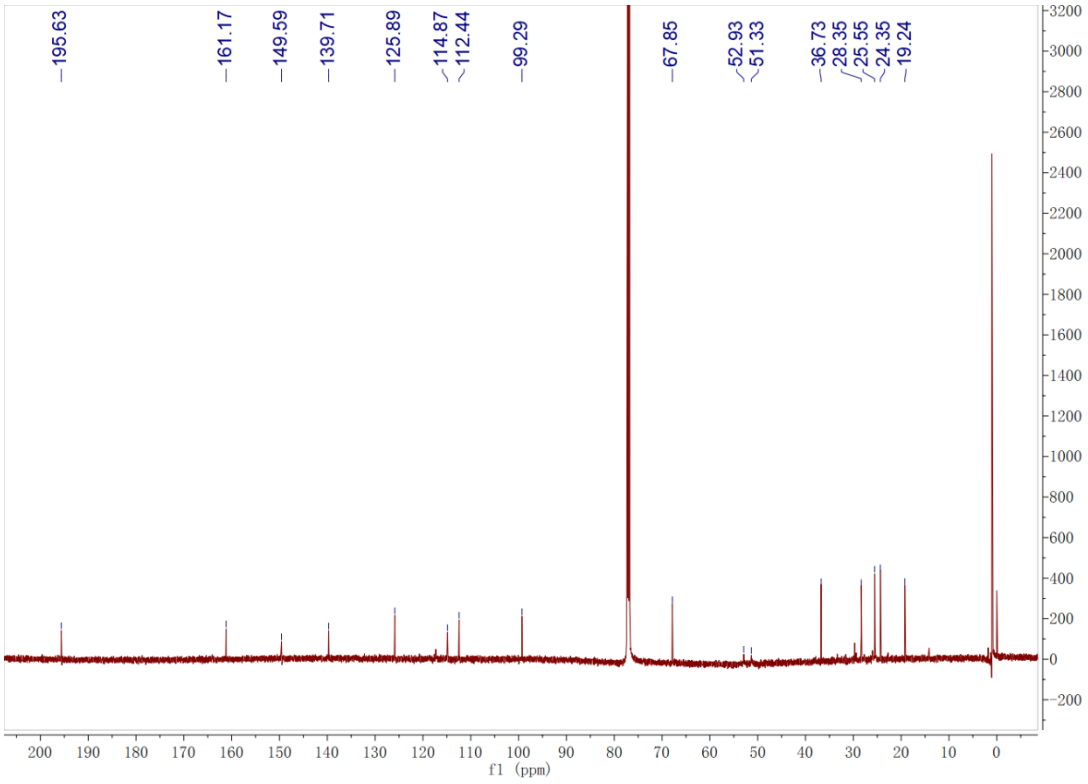

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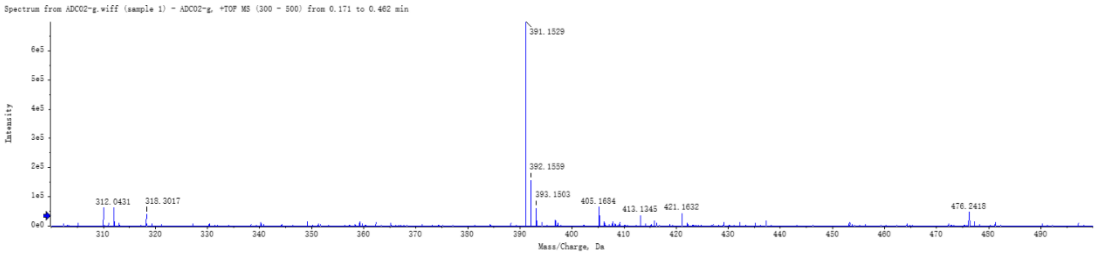

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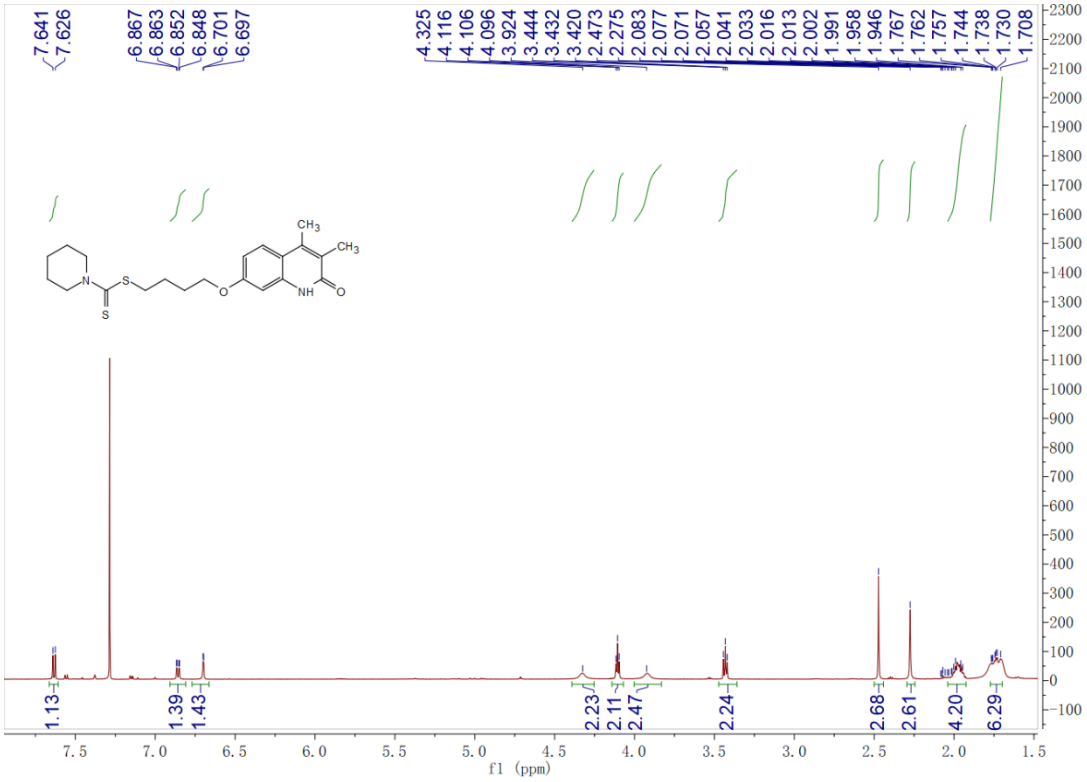

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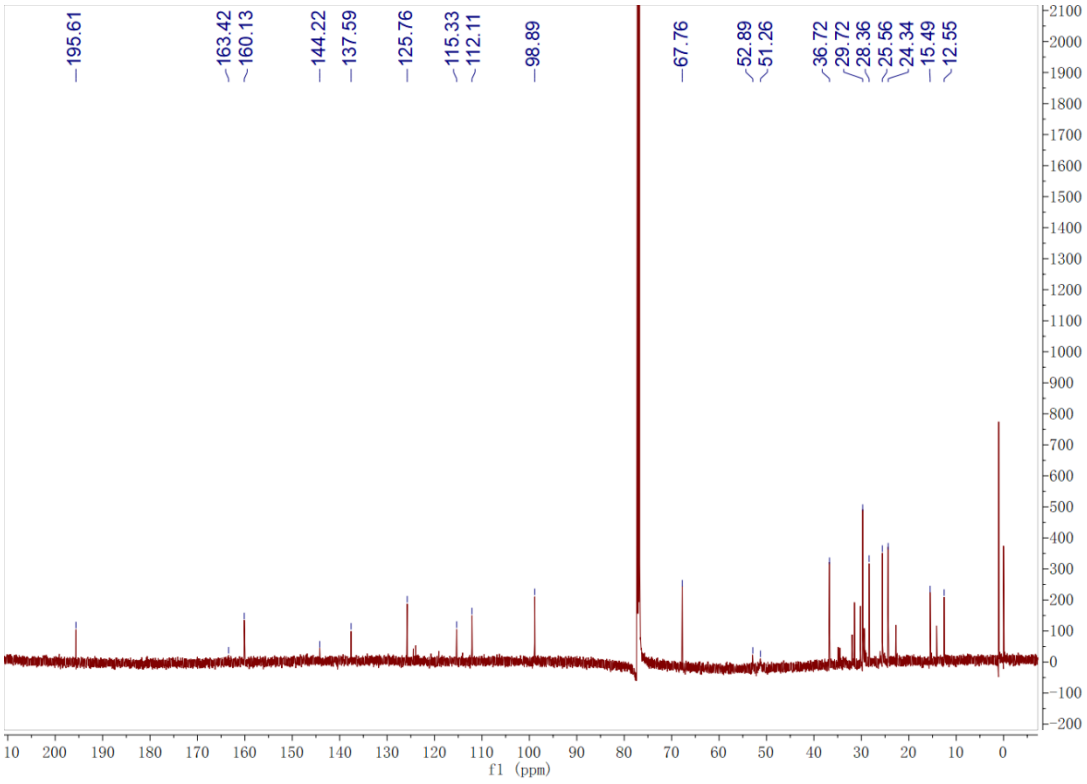


HRMS (ESI) spectrum of compound **9b**

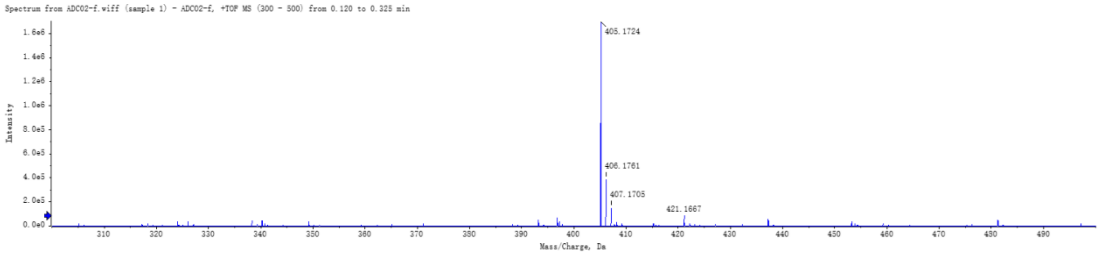
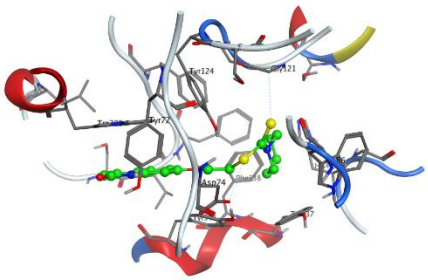
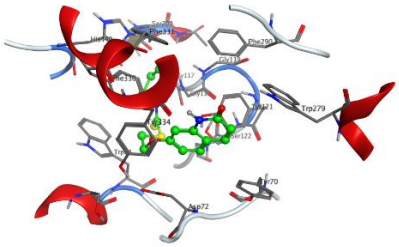
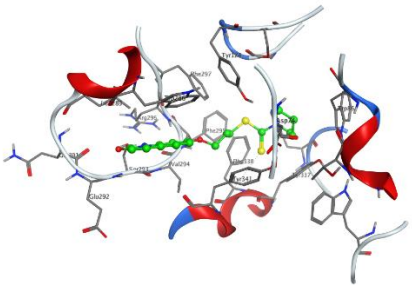
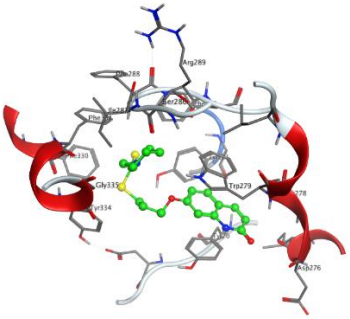
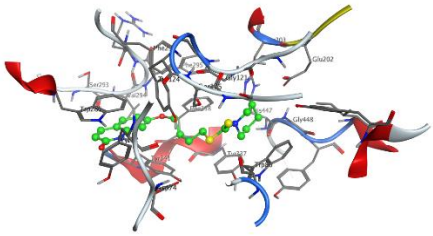
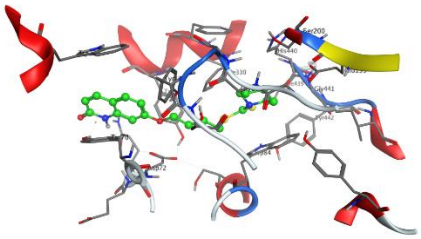
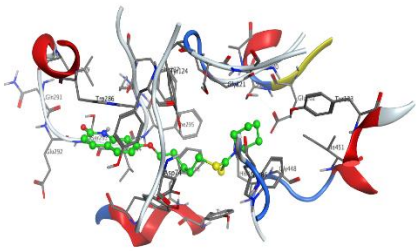
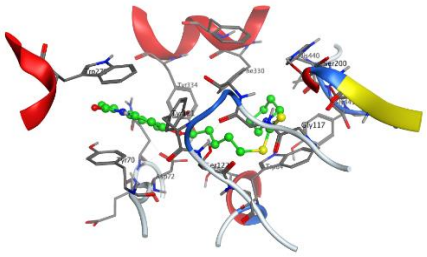
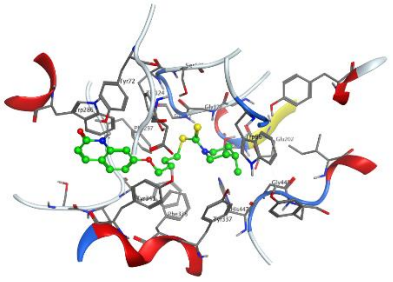
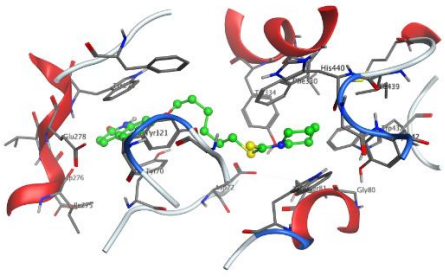
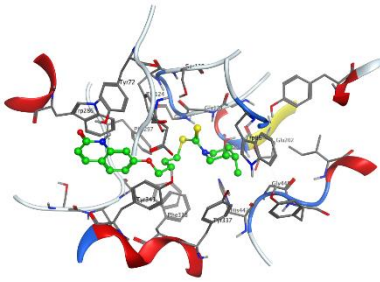
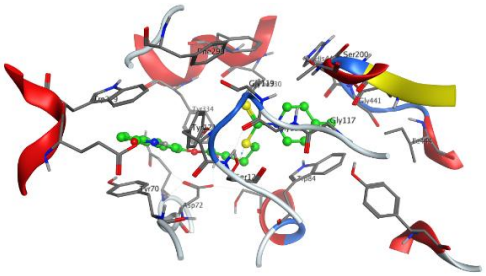
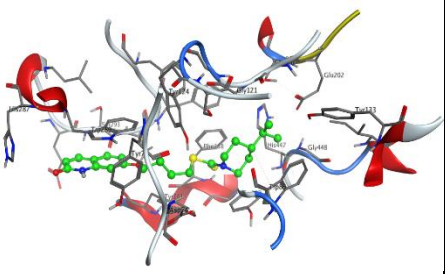
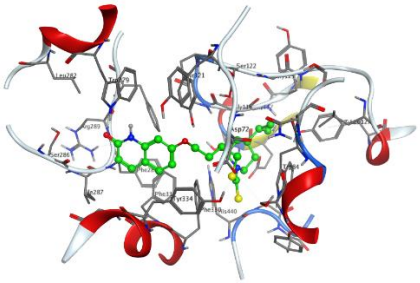
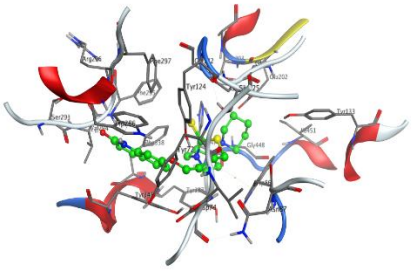
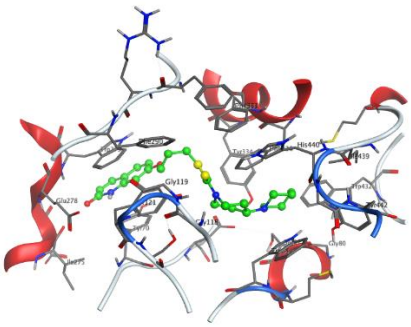
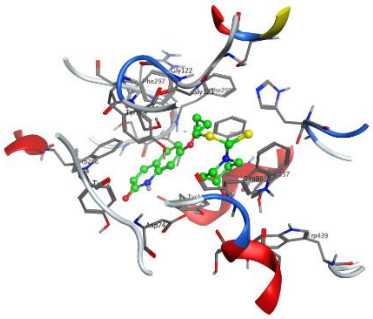
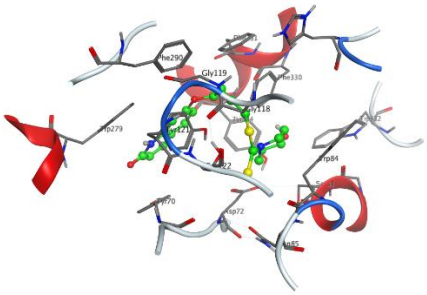
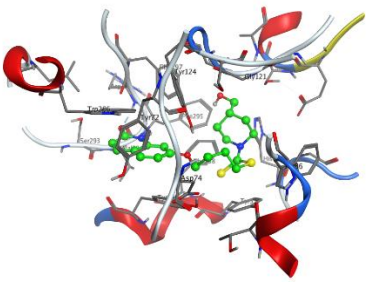
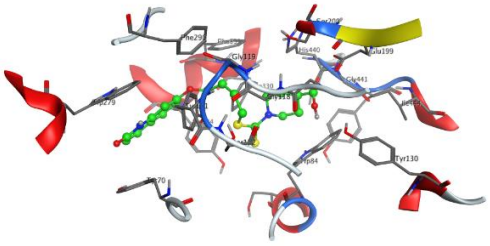


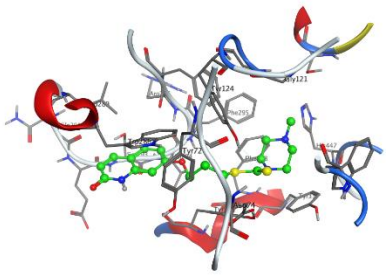
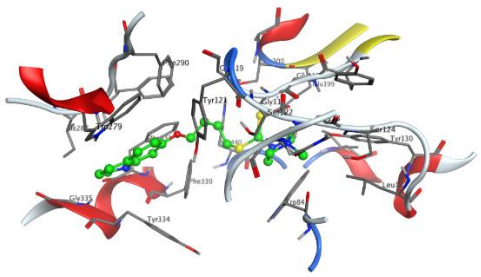
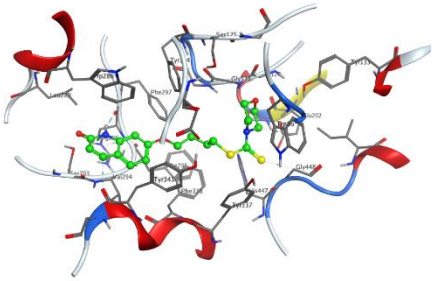
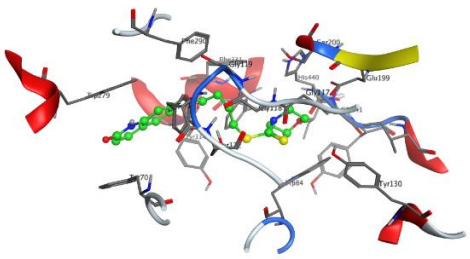
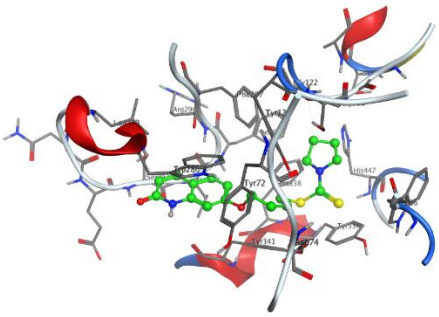
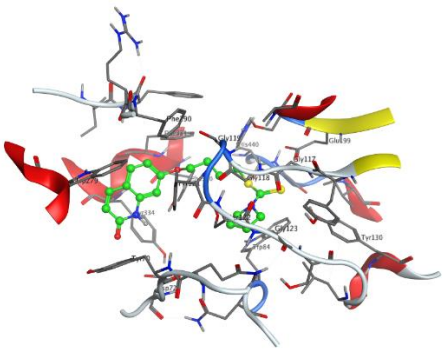
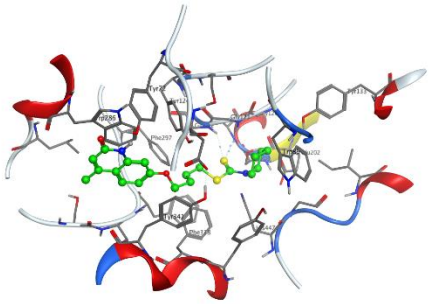
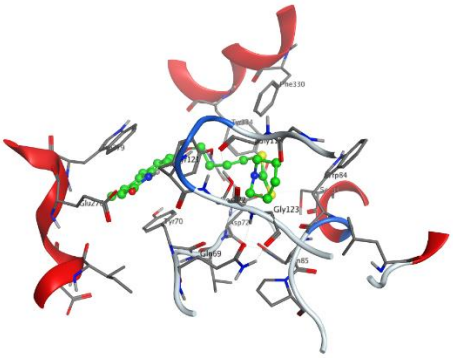
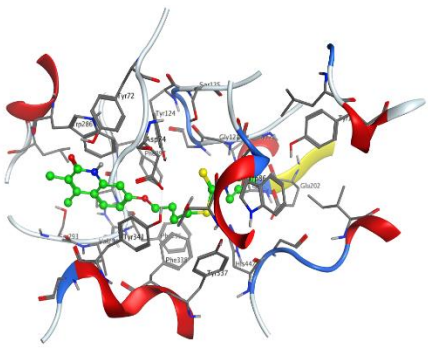
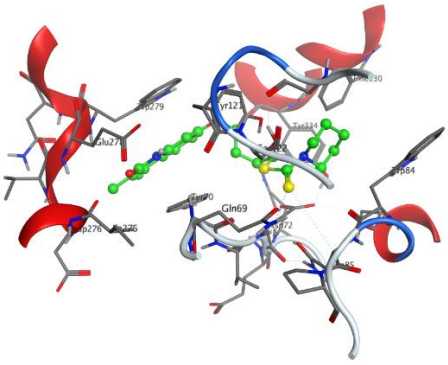
Table S1 S value of the compounds **4a-m** and **9a-b** in active site of AChE.

Compound	S value	
	*h*AChE(4EY7)	*Tc*AChE(2CKM)
4a	-6.237	-6.940
4b	-7.025	-7.061
4c	**-7.863**	**-7.540**
4d	-7.739	-7.154
4e	-7.384	-7.238
4f	-7.350	-7.119
4g	-7.027	-7.002
4h	-7.000	-7.039
4i	-6.105	-5.580
4j	-6.557	-5.719
4k	-6.399	-4.353
4l	-6.054	-6.091
4m	-6.605	-5.750
9a	-7.631	-7.155
9b	-7.851	-7.468
donepezil	-8.300	-7.472

Table S2 Docking orientations of compounds **4a-m** and **9a-b** with *h*AChE and *Tc*AChE.

Compd.	*h*AChE (4EY7)	*Tc*AChE(2CKM)
4a		
4b		
4c		
4d		
4e		

4f		
4g		
4h		
4i		
4j		

4k		
4l		
4m		
9a		
9b		

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