

Supporting information

Stereocontrolled Synthesis of Rosuvastatin Calcium via Iodine Chloride-induced Intramolecular Cyclization

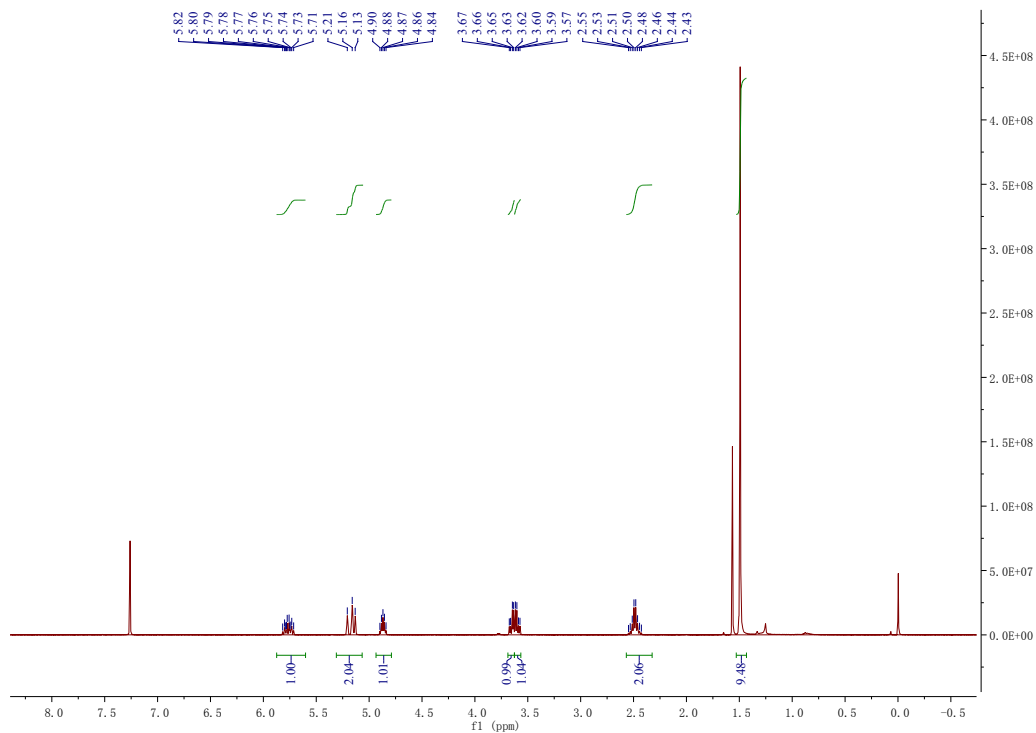
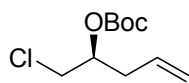
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Fener Chen*

Department of Chemistry, Fudan University, 220 Handan Road, Shanghai, 200433, People's Republic
of China

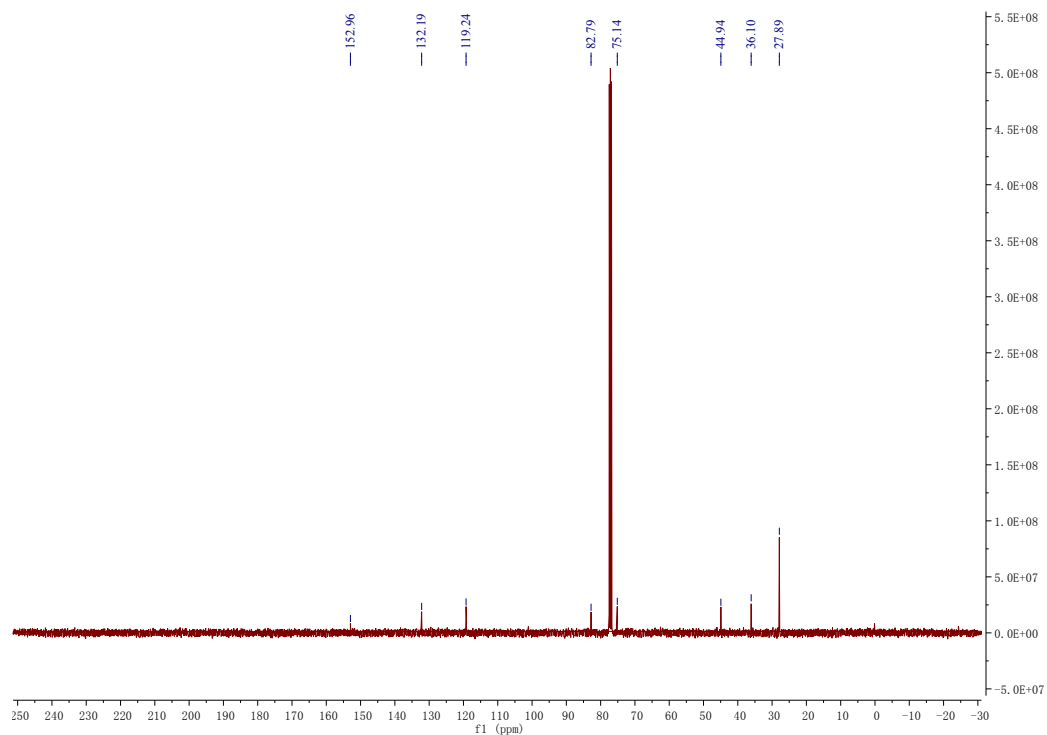
* E-mail: rfchen@fudan.edu.cn (Fener Chen)

* E-mail: wywin8@163.com (Yan Wu)

Spectral Data



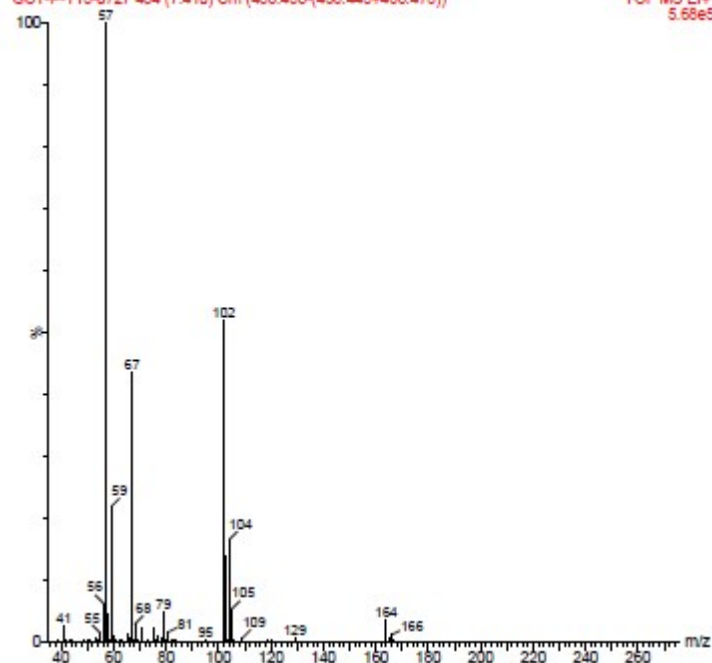
¹H NMR



¹³C NMR

GCT-P-T15-0727 454 (7.410) Cm (453:455-(438:445+458:478))

TOF MS EI+
5.68e5



Monoisotopic Mass, Odd and Even Electron Ions

382 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-45 H: 0-80 N: 0-2 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1 I: 0-1

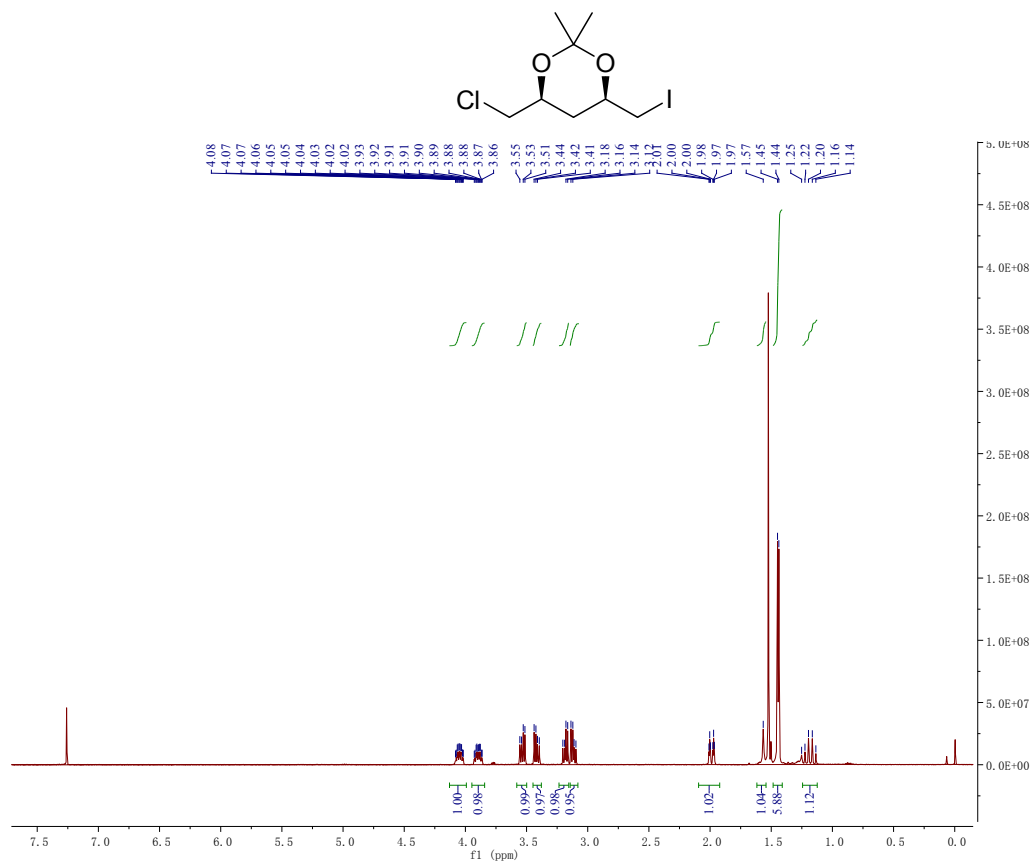
Minimum:

Maximum: -1.5

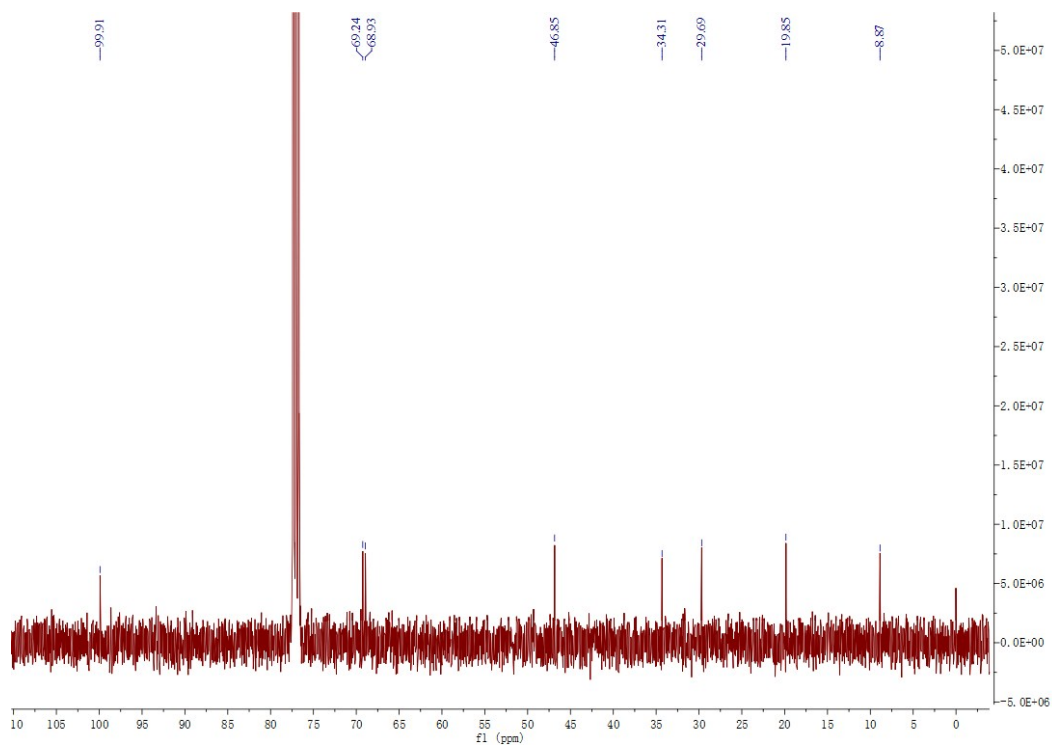
Mass Calc. Mass mDa PPM DBE i-FIT Formula

164.0243 164.0240 0.3 1.8 2.0 493.1 C6 H9 O3 Cl

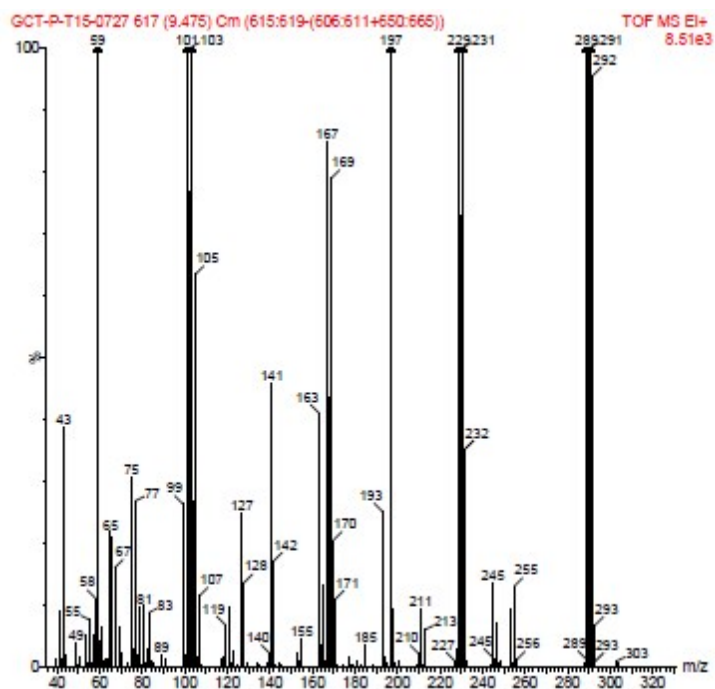
HRMS(EI)



^1H NMR



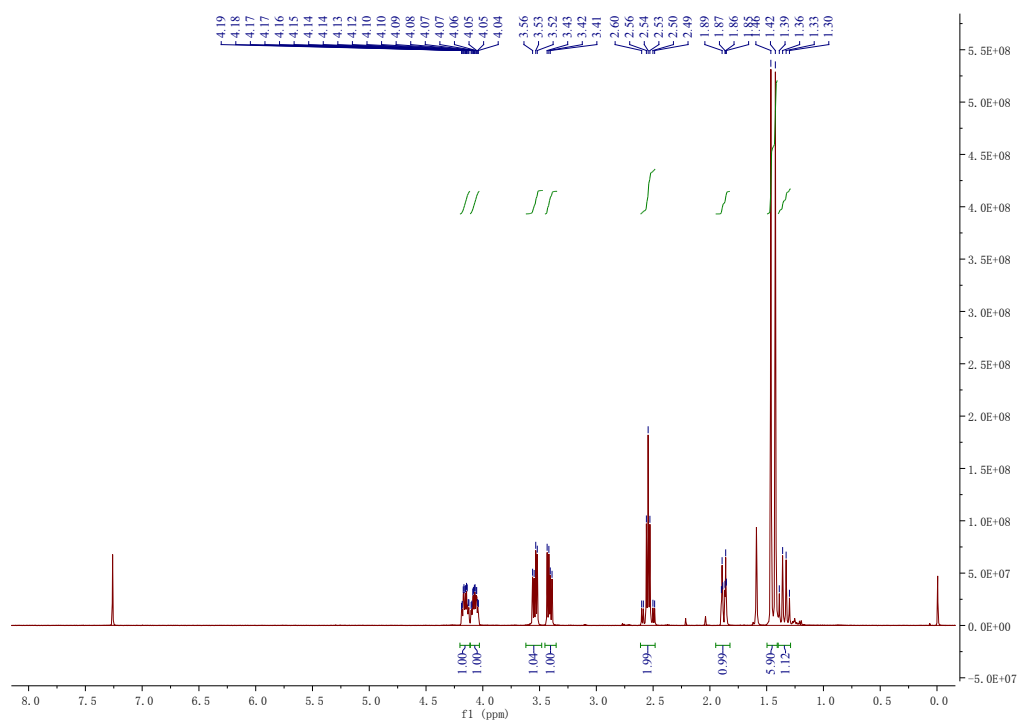
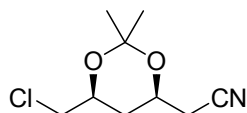
^{13}C NMR



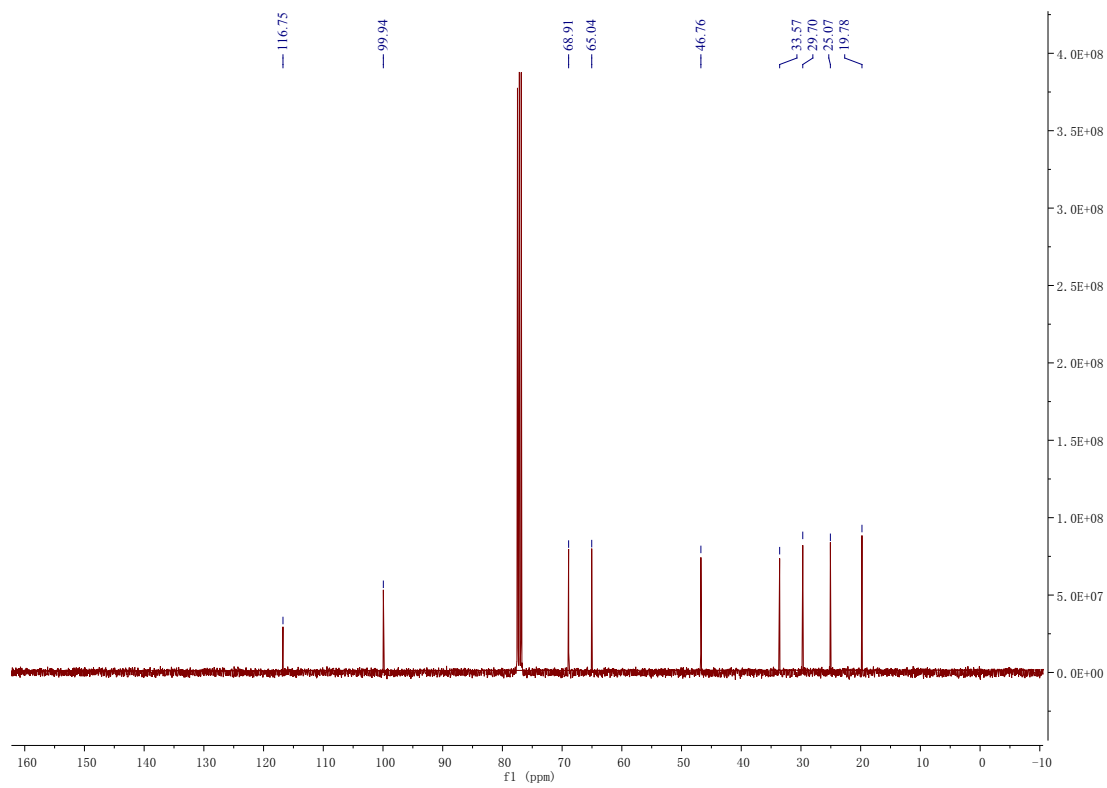
Monoisotopic Mass, Odd and Even Electron Ions
 350 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
 Elements Used:
 C: 0-45 H: 0-80 N: 0-2 O: 0-4 S: 0-1 Cl: 0-1 I: 0-1

Minimum:	Maximum:	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.9733	303.9731	0.2	0.7	21.0	1.4		C19 N2 O S
303.9727	0.6	2.0	1.0	4.7			C8 H14 O2 Cl I
303.9743	-1.0	-3.3	1.0	4.1			C6 H13 N2 O2 S I

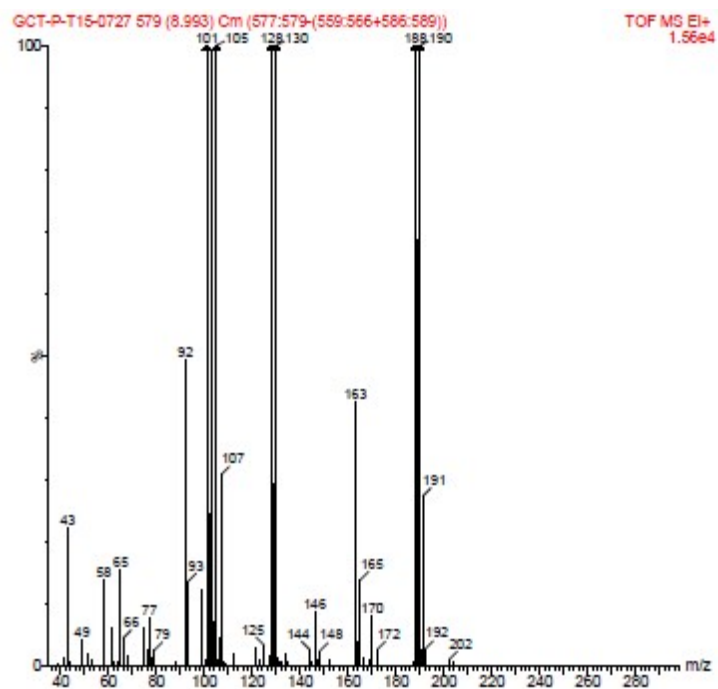
HRMS(EI)



¹H NMR



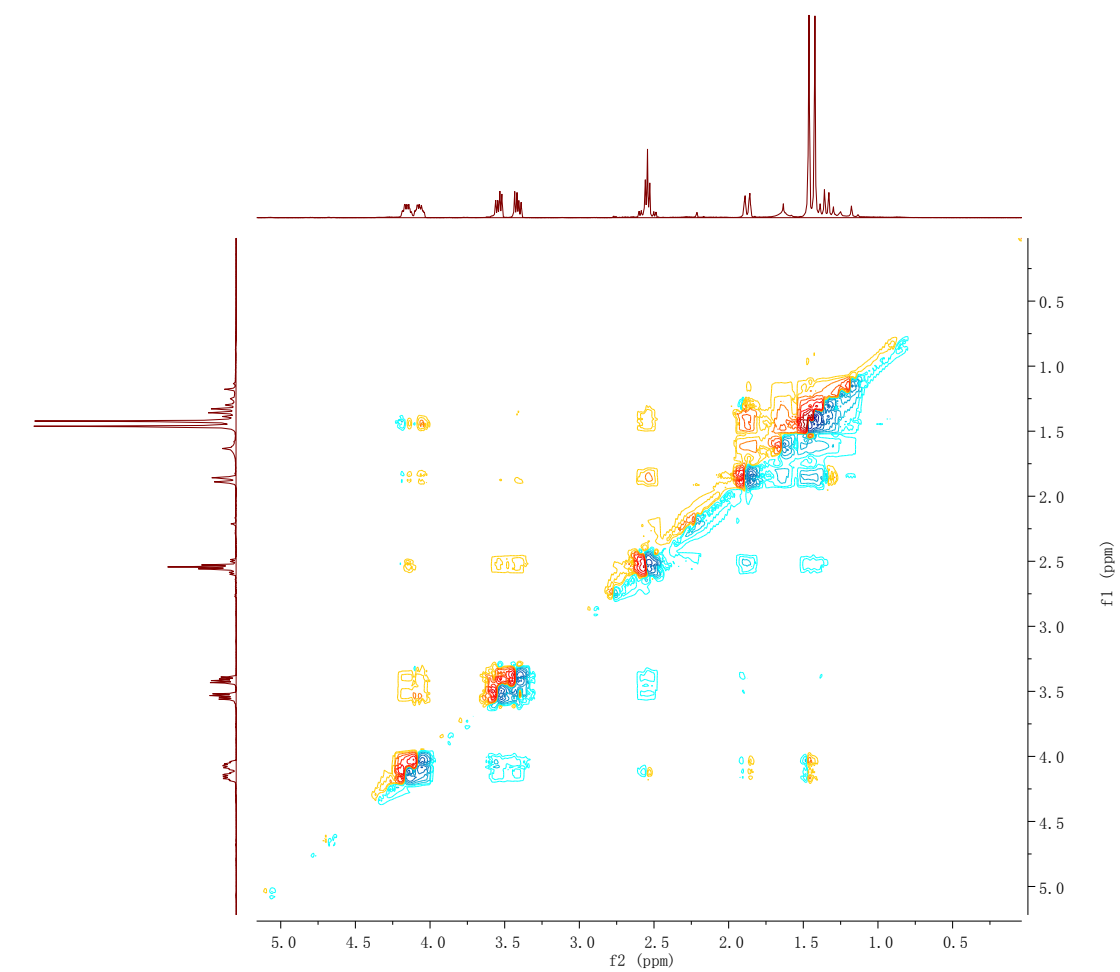
¹³C NMR



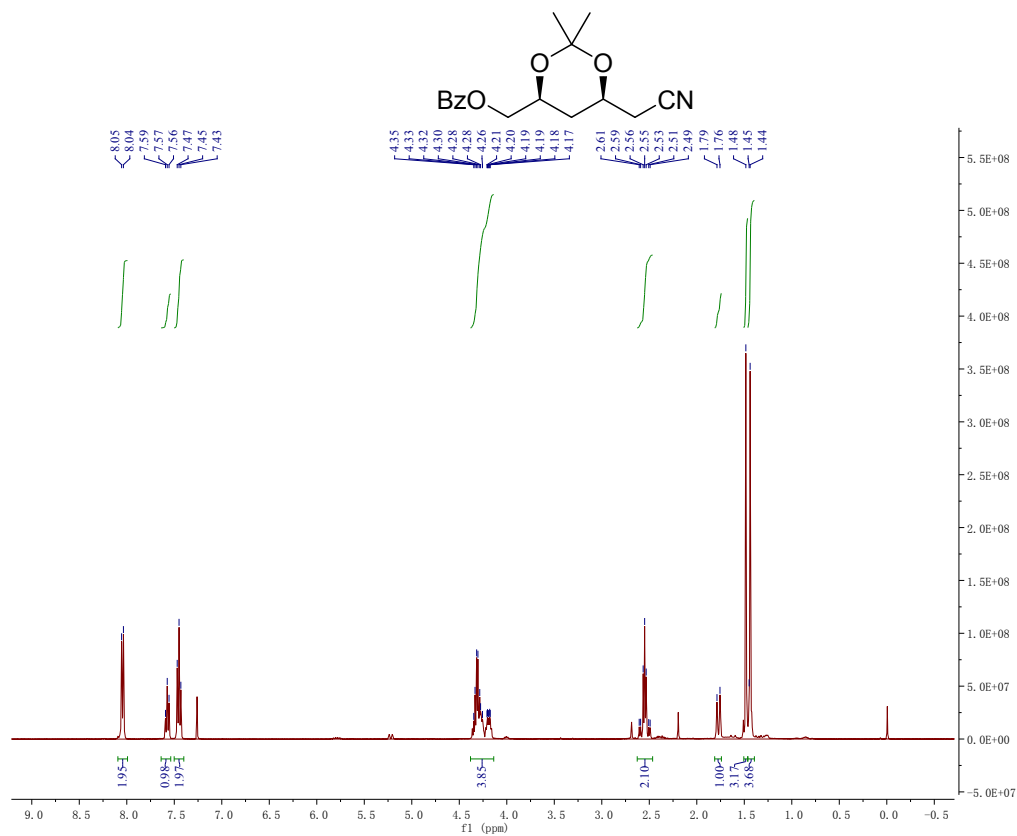
Monoisotopic Mass, Odd and Even Electron Ions
 543 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
 Elements Used:
 C: 0-48 H: 0-80 N: 0-2 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1 I: 0-1

Minimum:	Maximum:	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
202.0691	202.0690	0.1	0.5	5.0	2779132.3	C12 H10 O2	
	202.0628	0.3	1.5	4.0	2779126.5	C10 H12 F2 S	
	202.0635	-0.4	-2.0	3.5	2779103.0	C9 H12 N O2 Cl	
	202.0639	-0.8	-4.0	0.0	2779112.5	C7 H12 O F3 S	

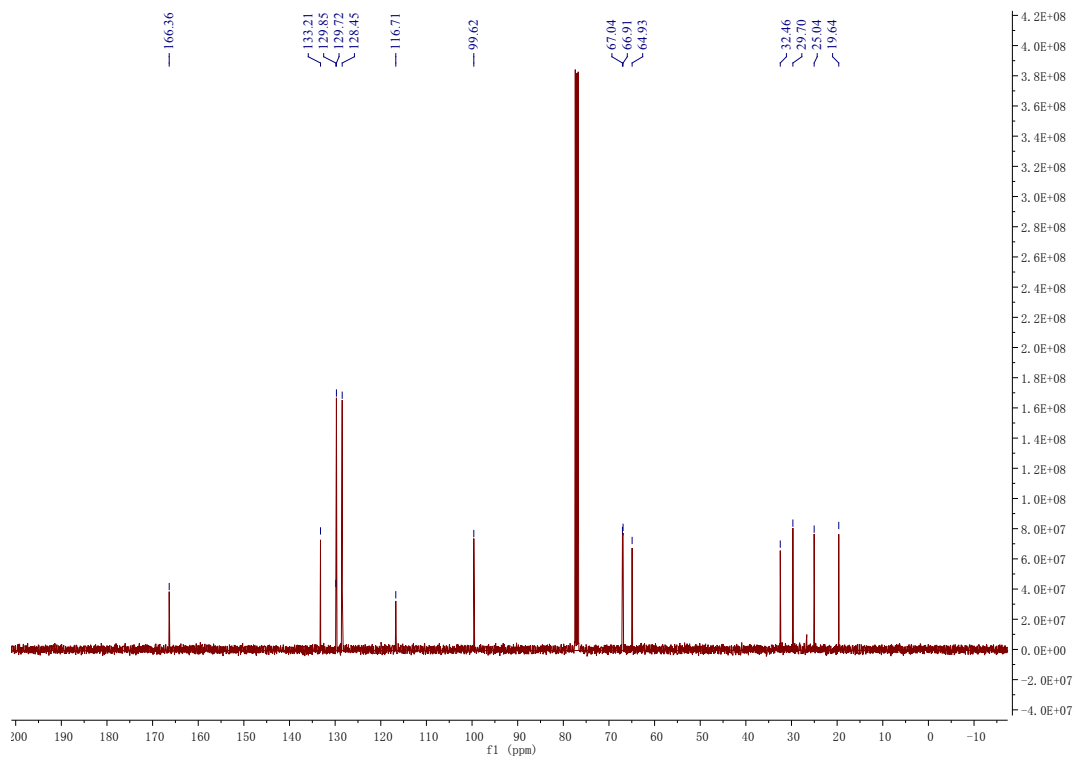
HRMS(EI)



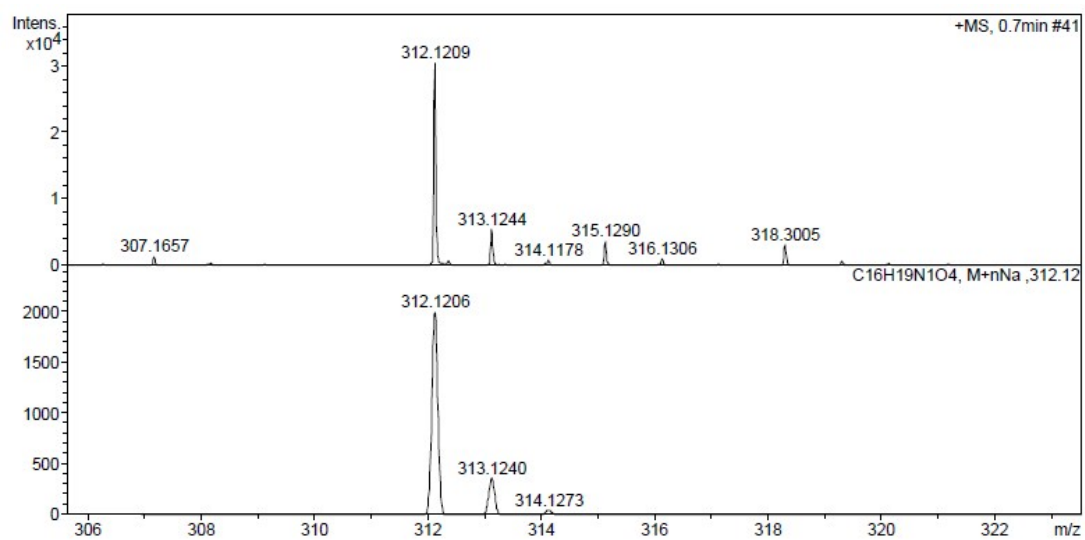
NOESY



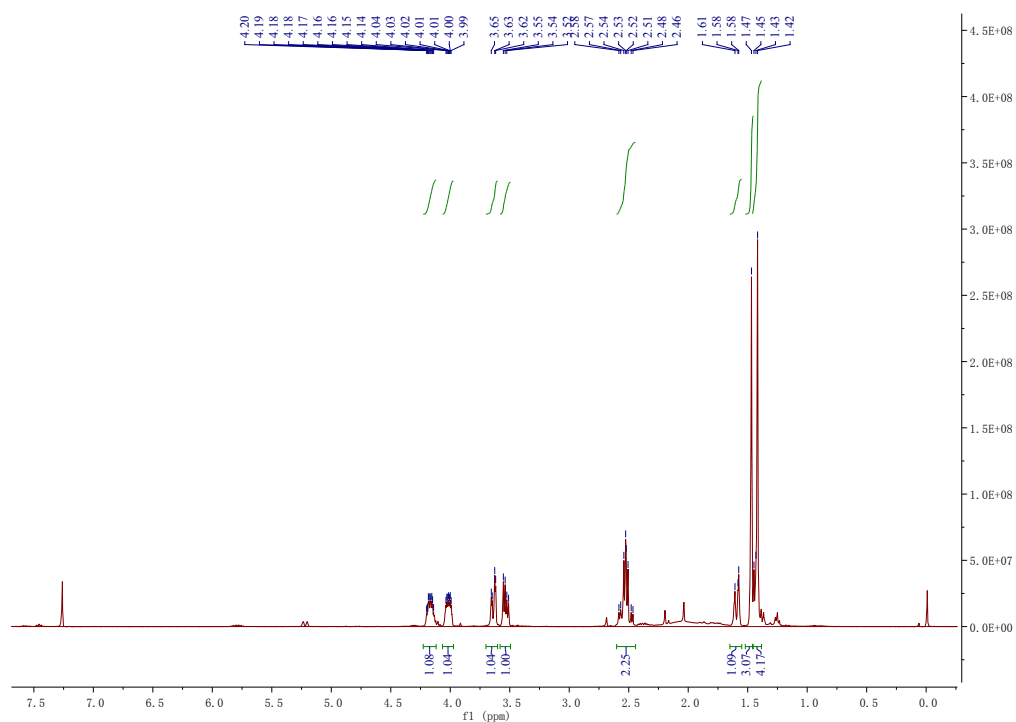
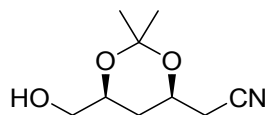
¹H NMR



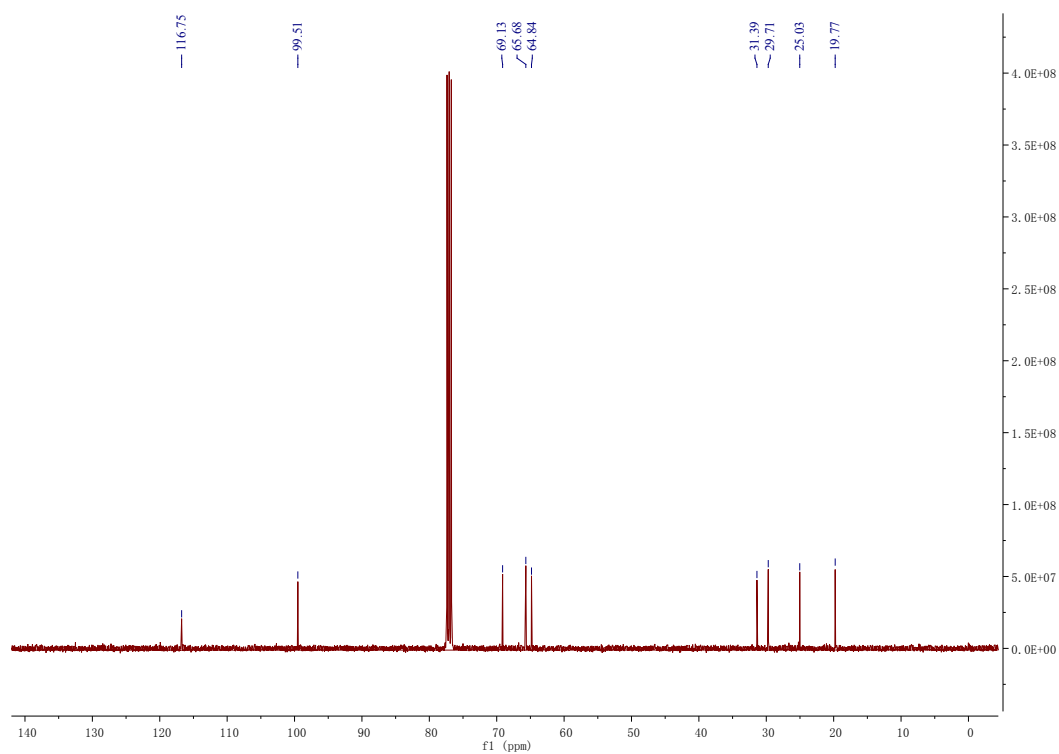
¹³C NMR



HRMS(ESI)



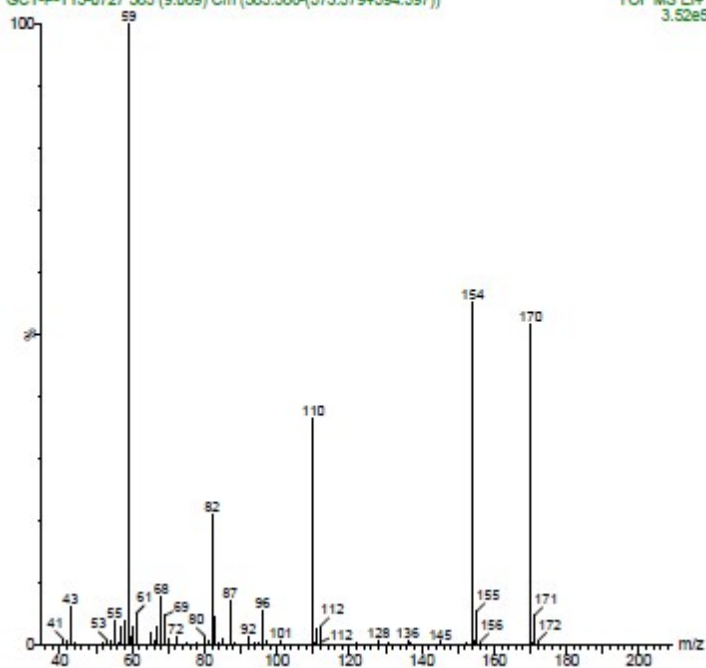
¹H NMR



¹³C NMR

GCT-P-T15-0727 585 (9.069) Cm (585:586-(573:579+594:597))

TOF MS EI+
3.52e5



Monoisotopic Mass, Odd and Even Electron Ions

998 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-48 H: 0-80 N: 0-2 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1 I: 0-1

Minimum:

Maximum:

Mass Calc. Mass

170.0816

170.0817

170.0818

170.0822

mDa

-0.1

0.1

-0.6

PPM

-0.6

0.6

-3.5

-1.5

50.0

3.5

-0.5

-1.0

i-FIT

87.8

7846.7

81709.5

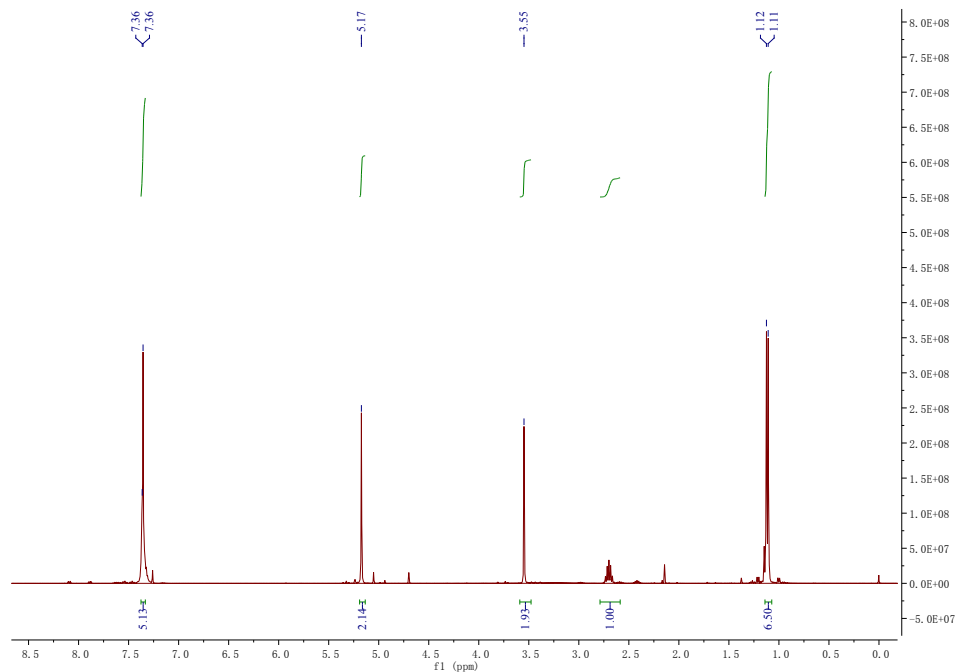
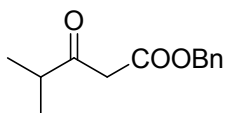
Formula

C8 H12 N O3

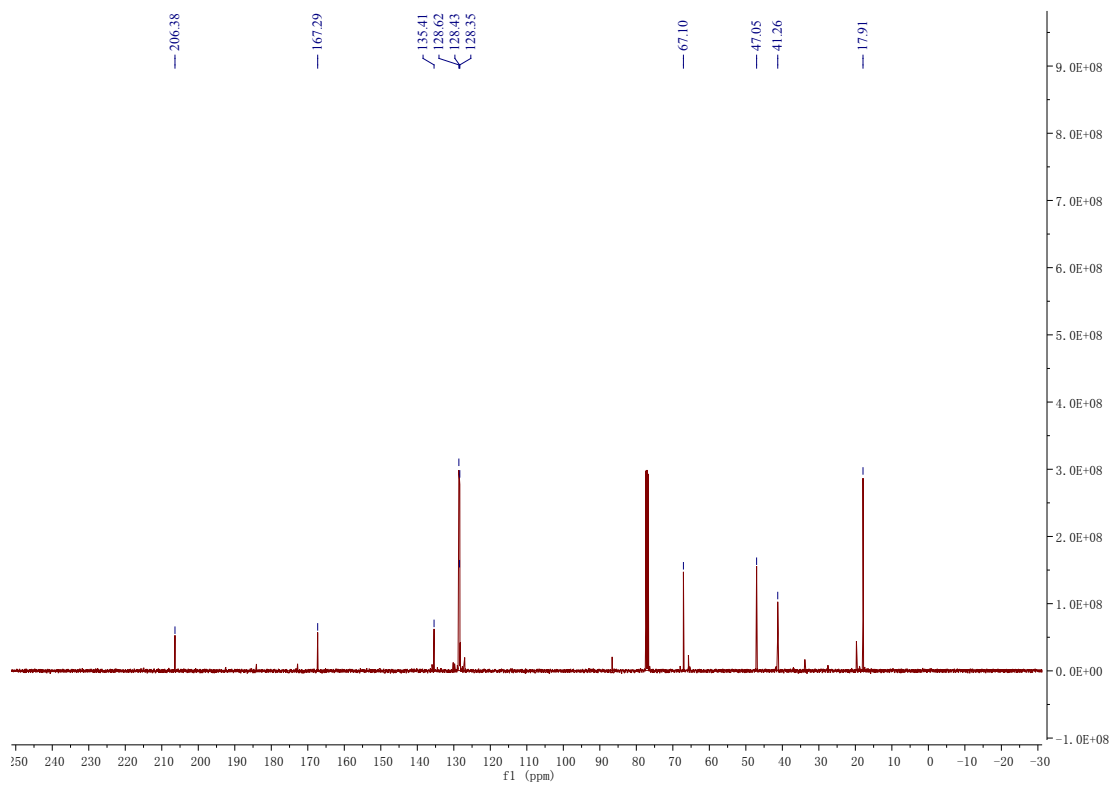
C6 H14 N F2 S

C8 H15 N2 O2 Cl

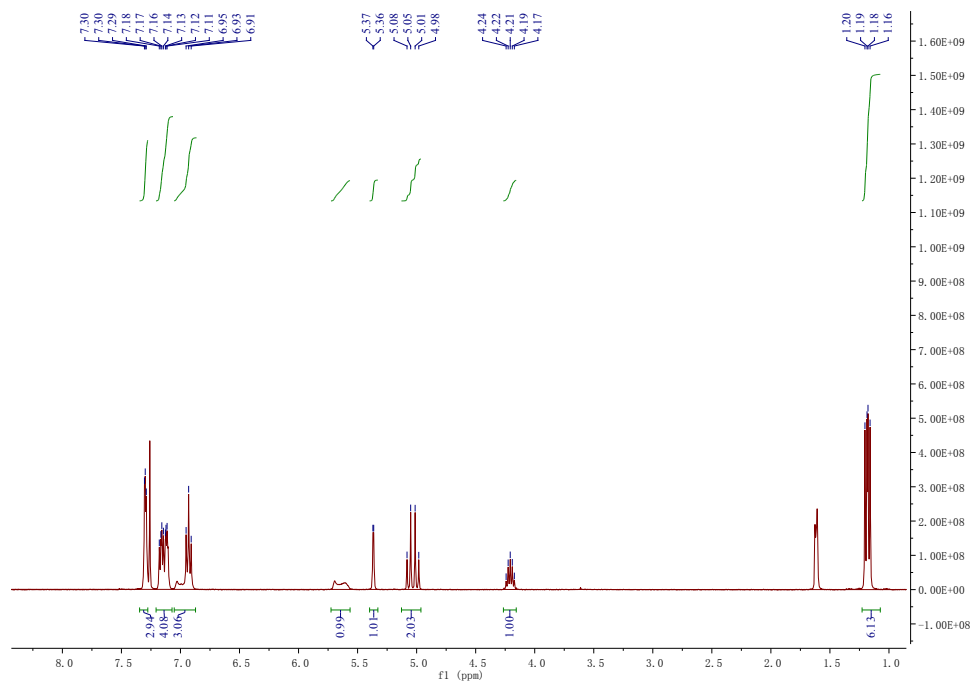
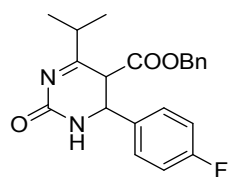
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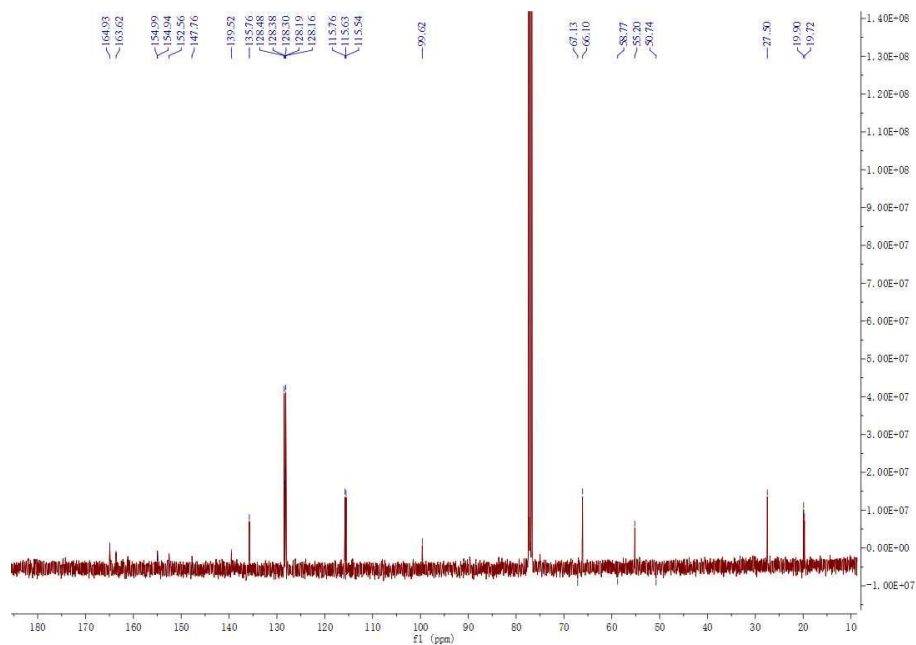
¹H NMR



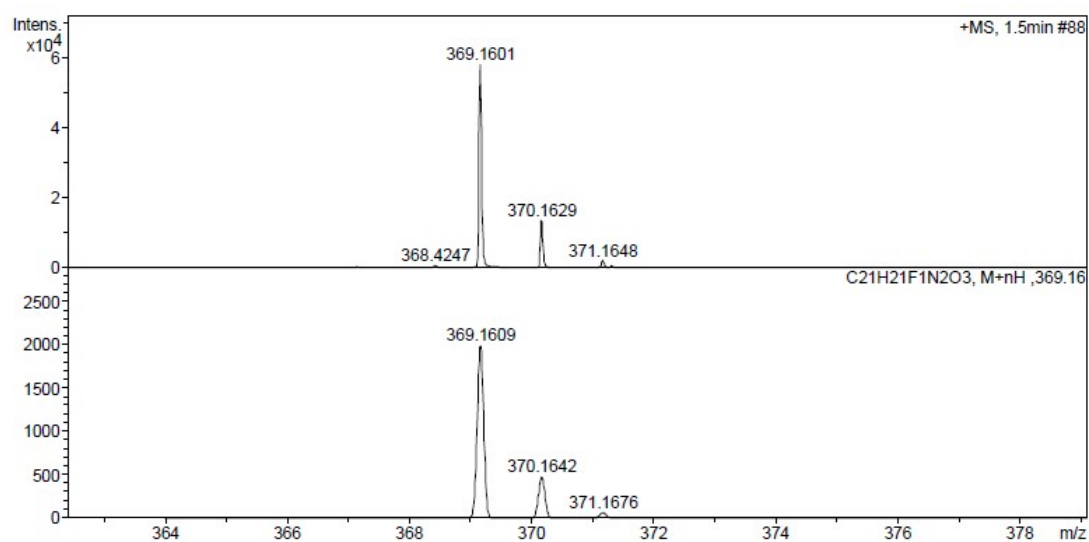
¹³C NMR



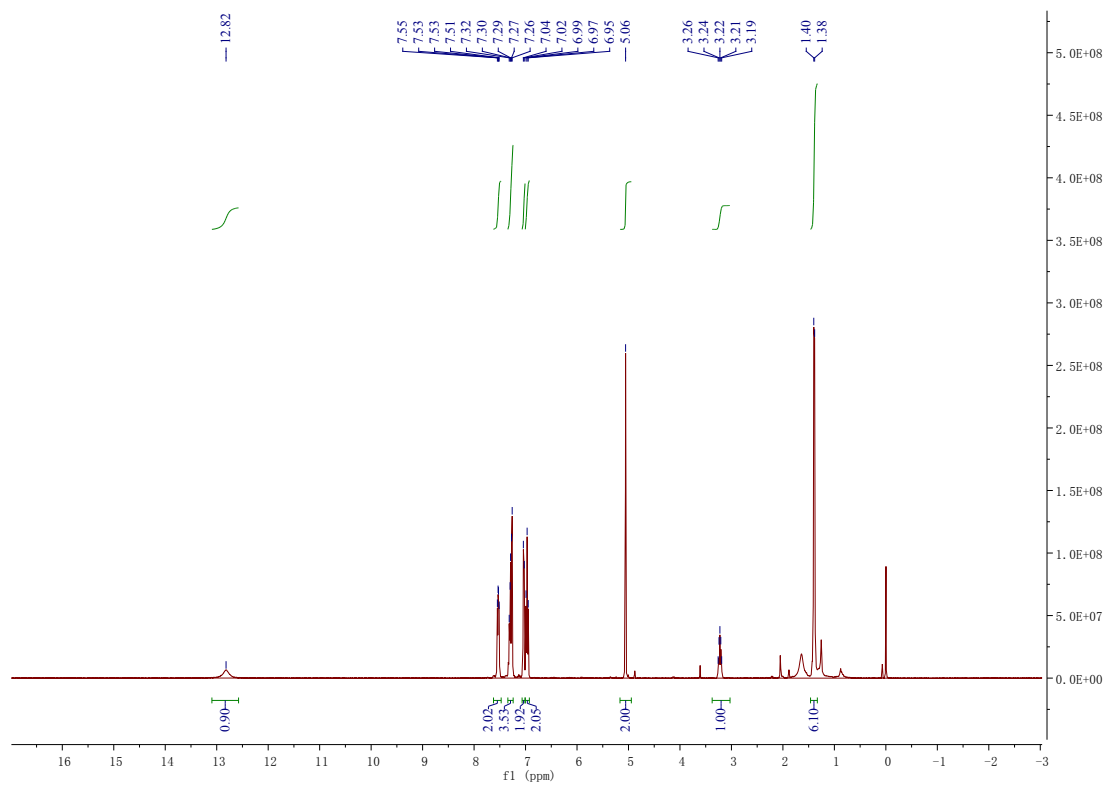
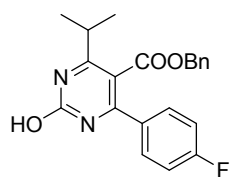
¹H NMR



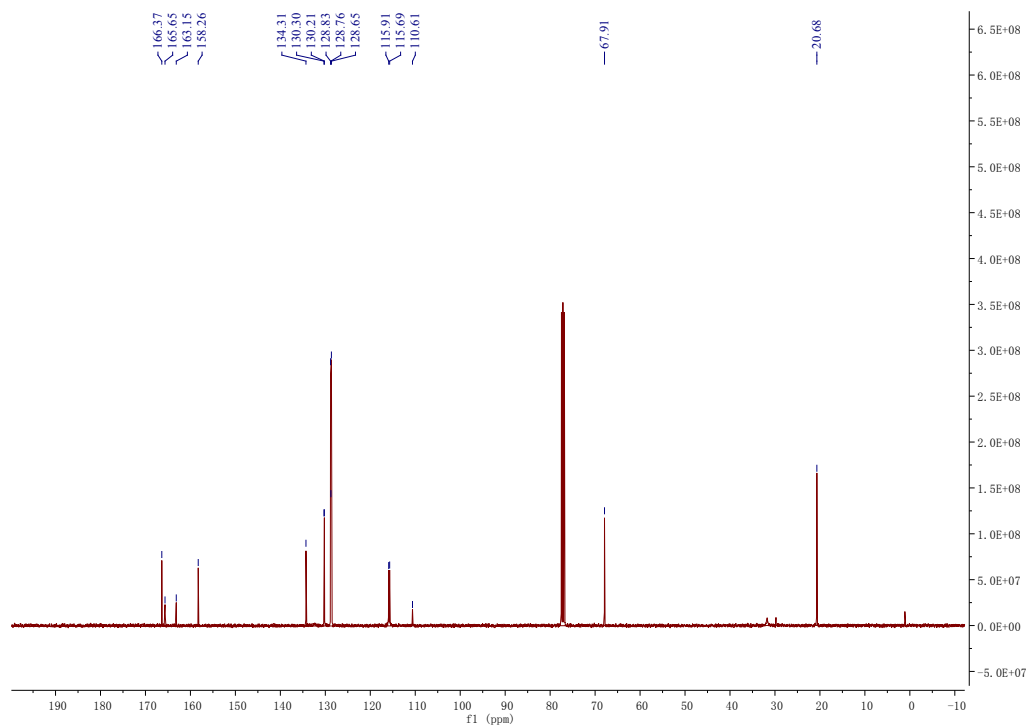
¹³C NMR



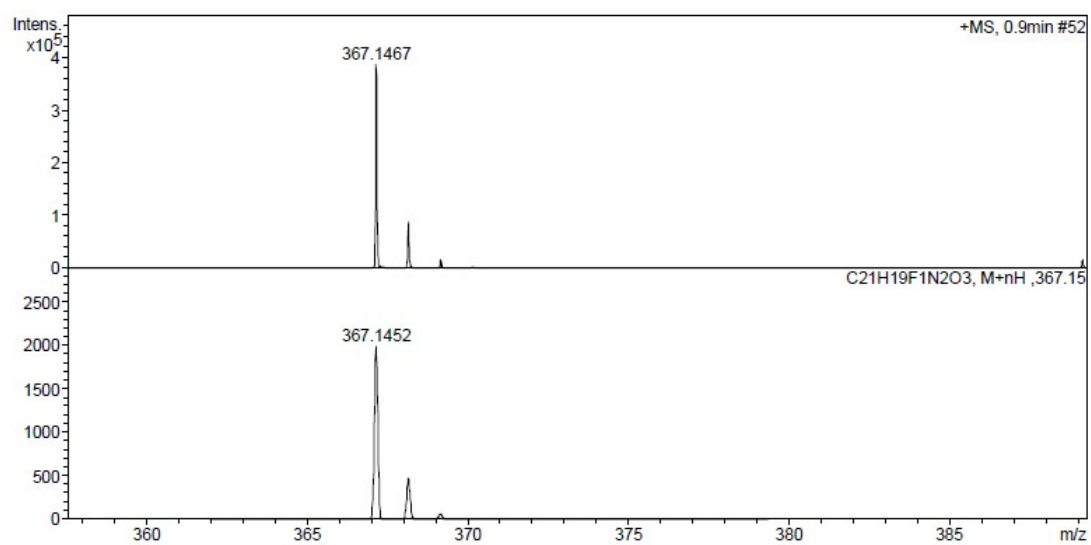
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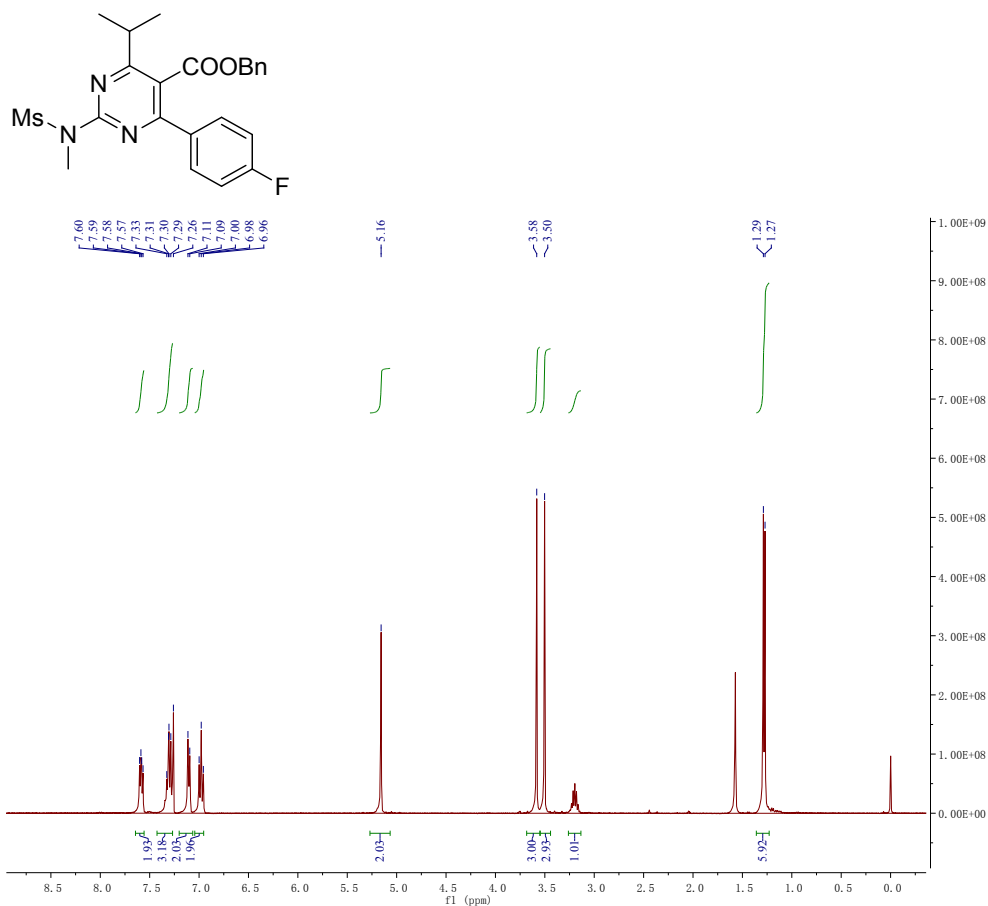
¹H NMR



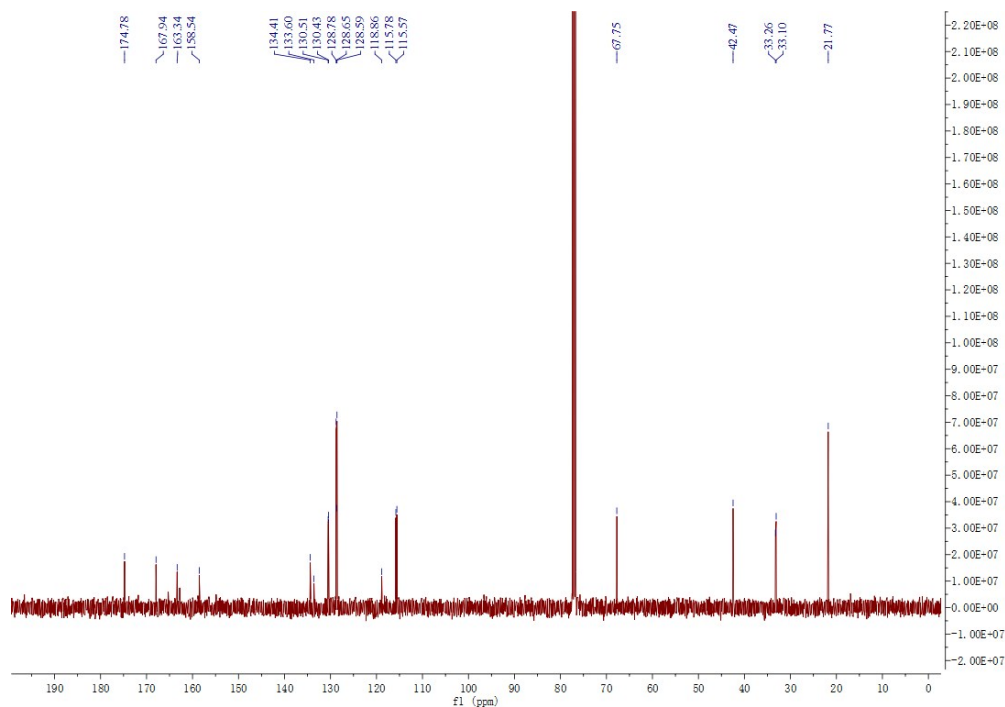
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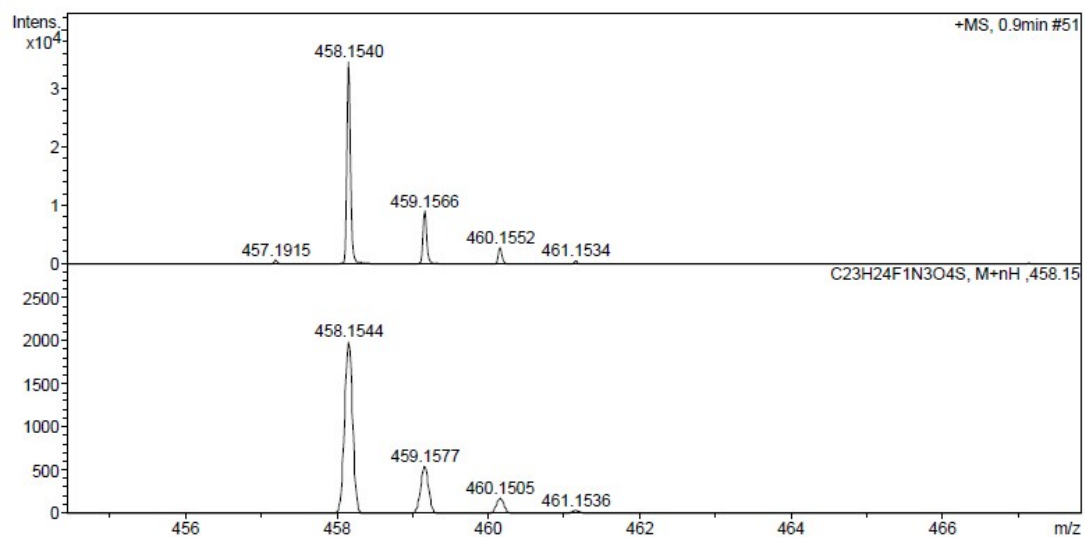
HRMS(ESI)



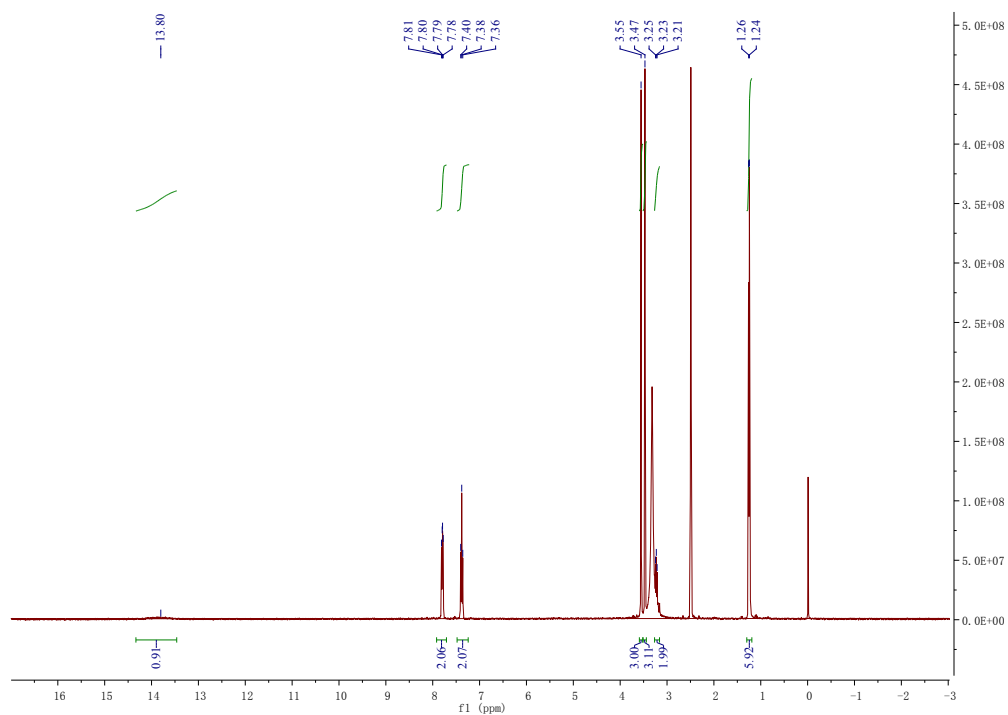
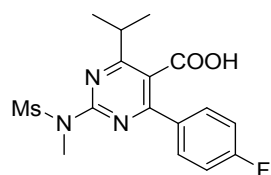
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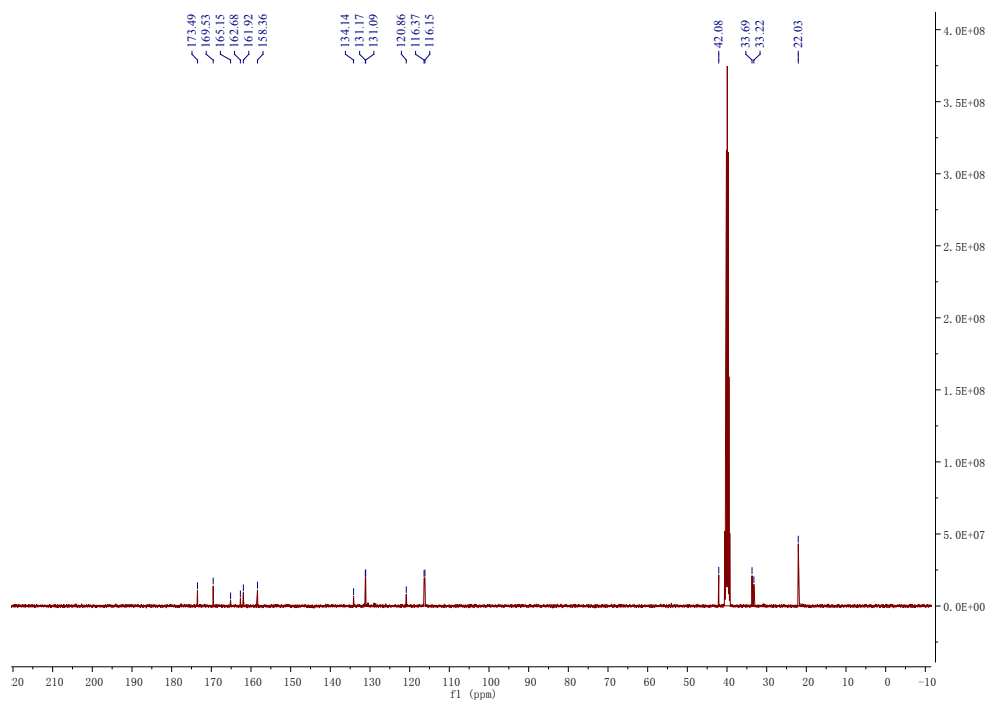
¹³C NMR



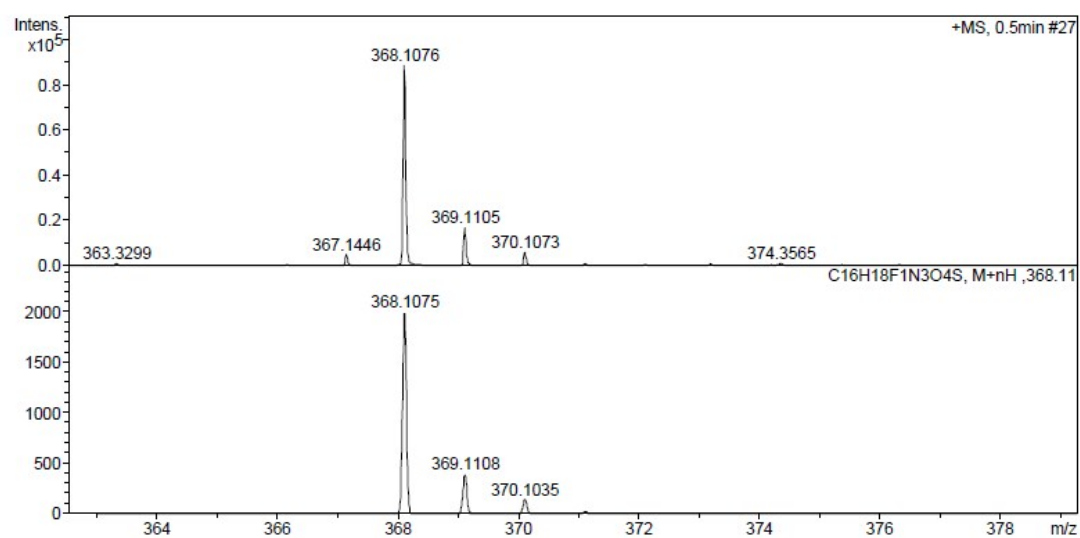
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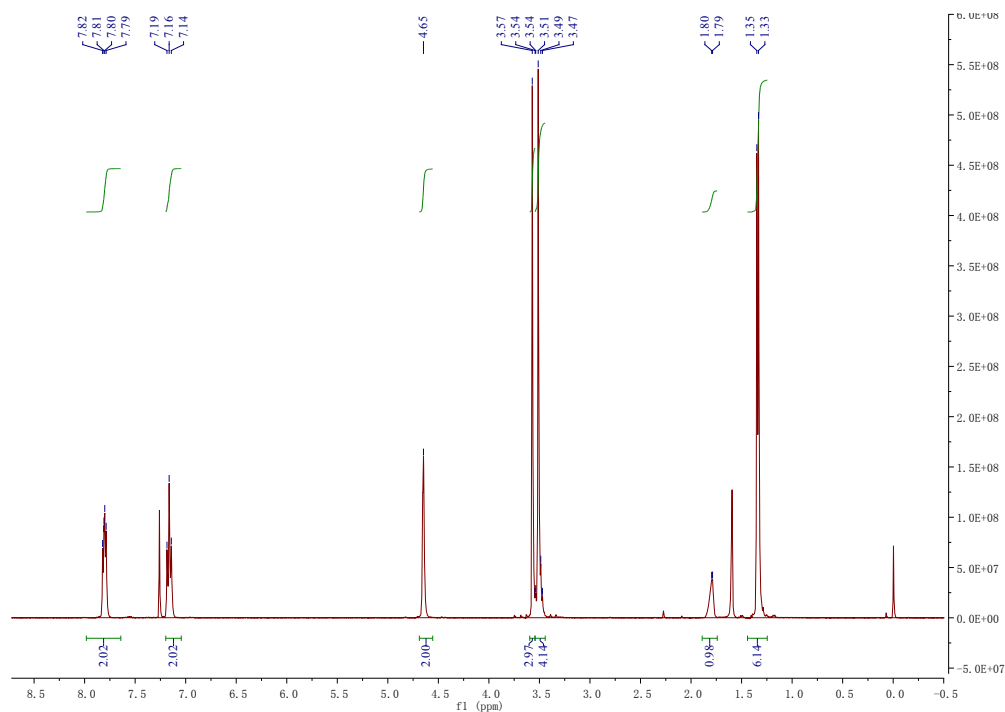
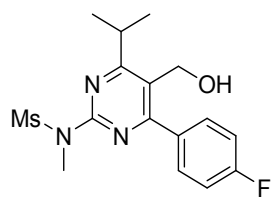
¹H NMR



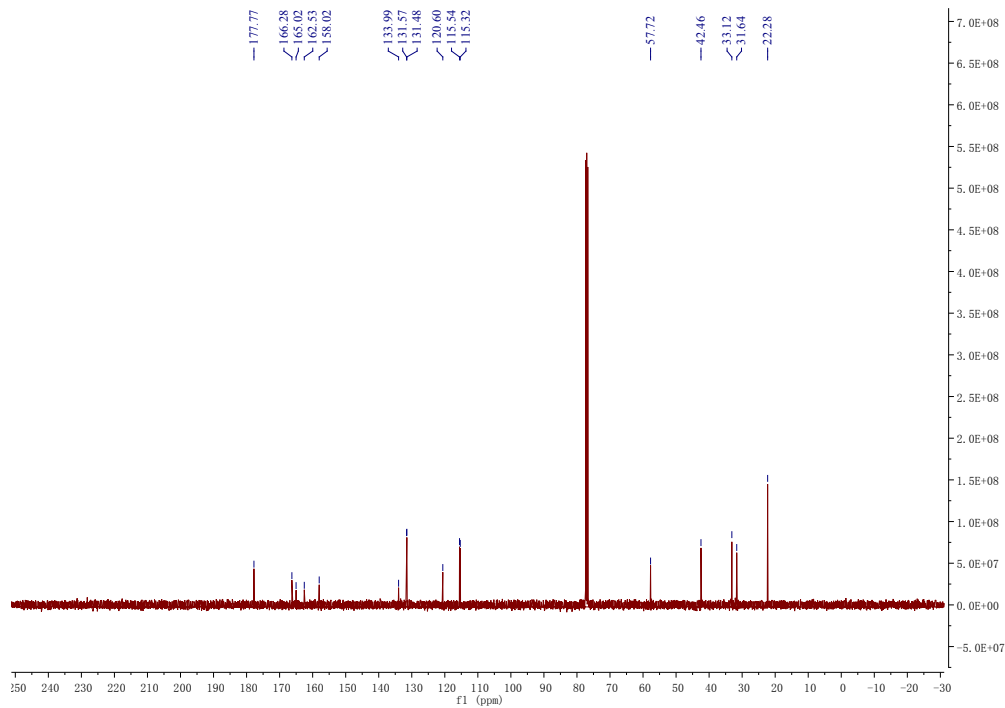
¹³C NMR



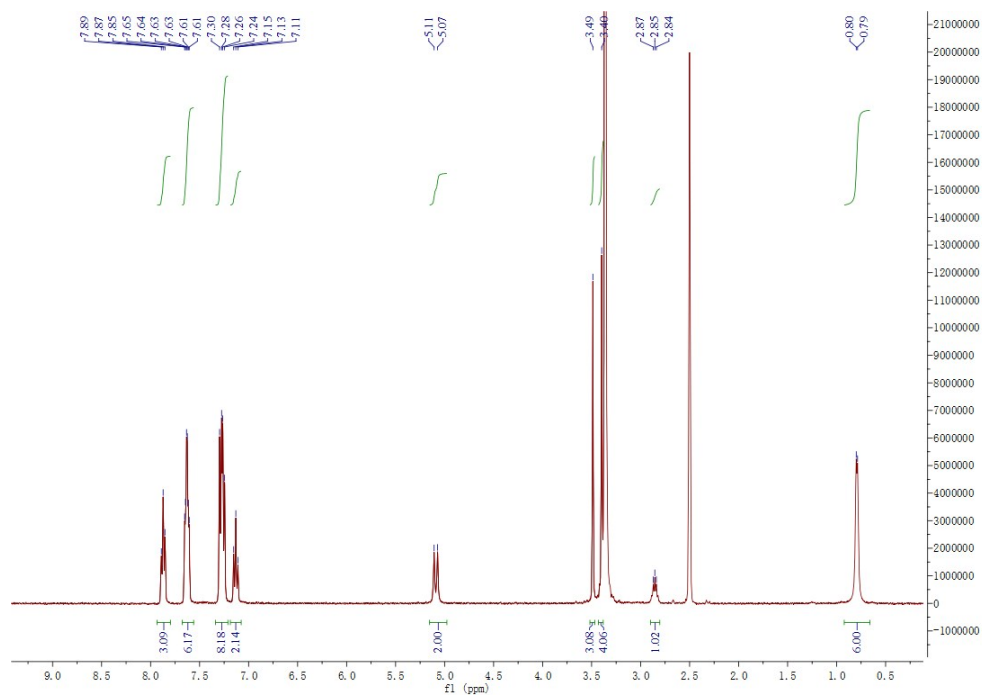
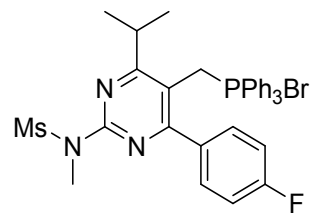
HRMS(ESI)



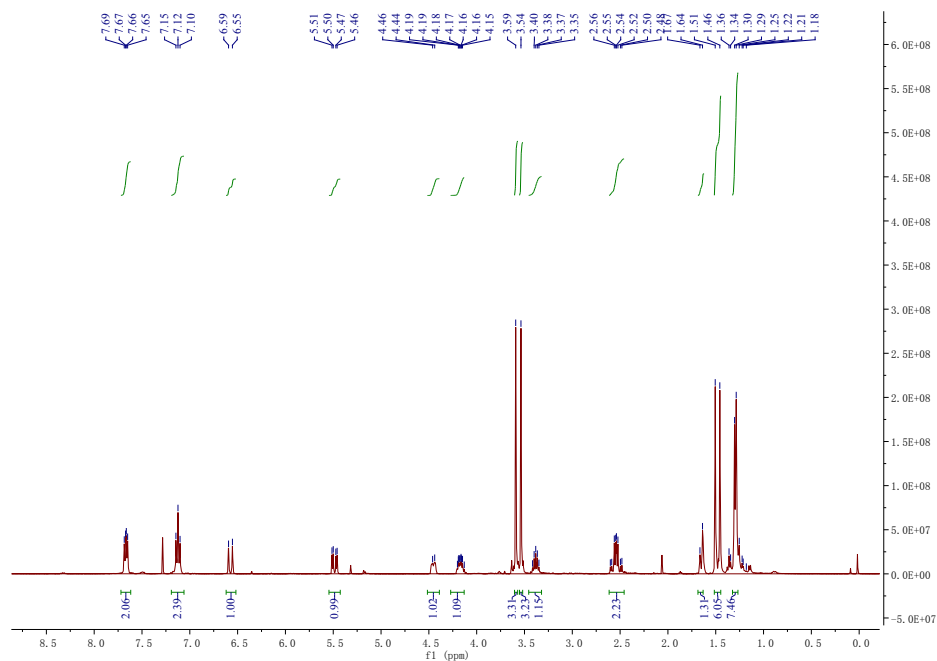
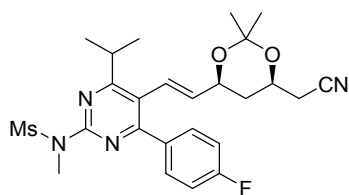
¹H NMR



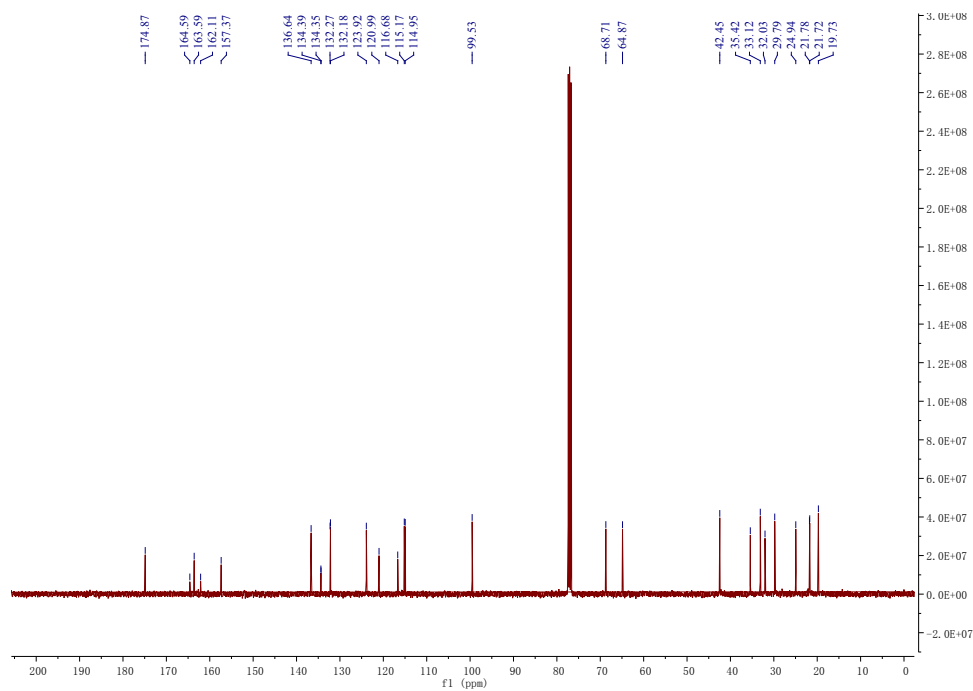
¹³C NMR



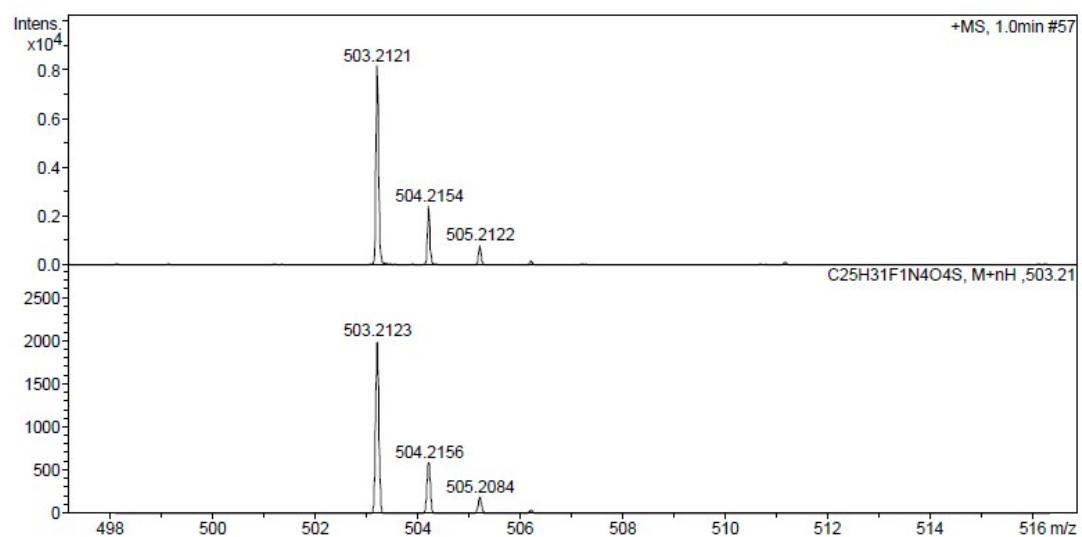
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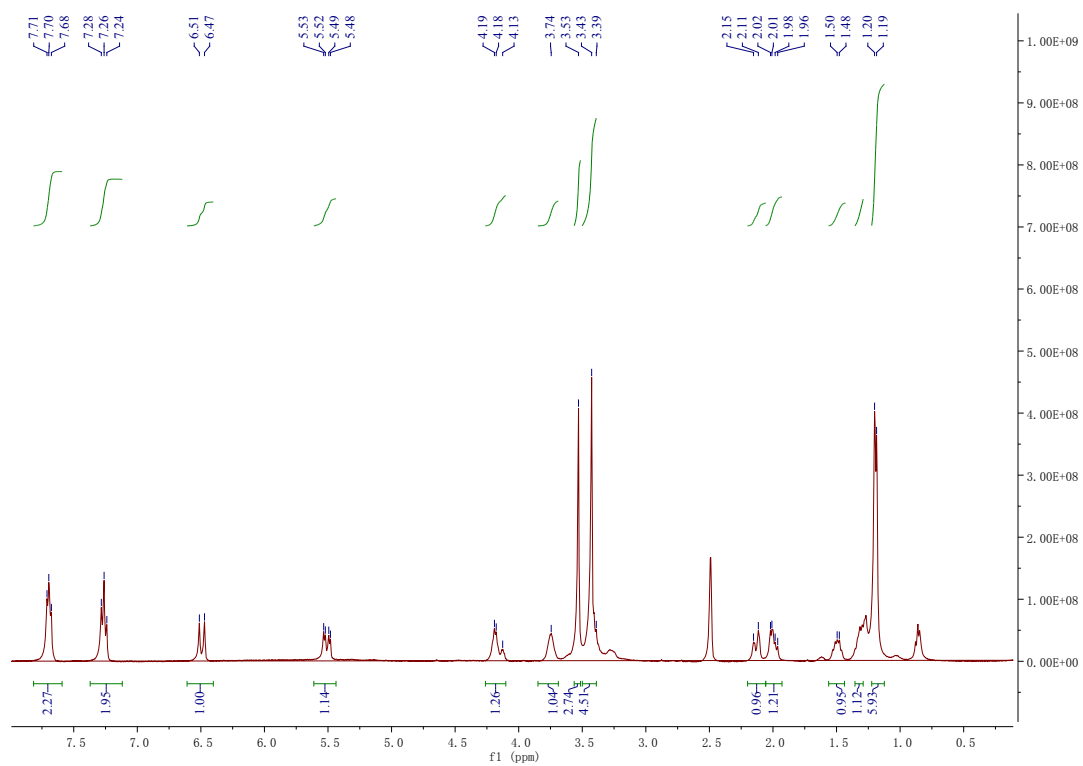
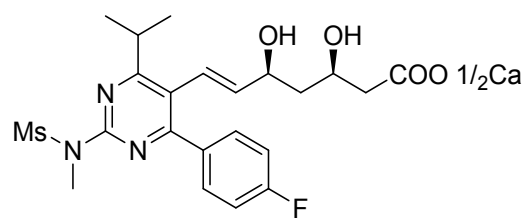
¹H NMR



¹³C NMR



HRMS(ESI)



¹H NMR