

HPLC and LC–MS/MS-Based Quantitative Characterization of Related Substances Associated with Sotalol Hydrochloride

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Supporting information

Figure S1 The purity of **RS1**, **RS2** and **RS3** was detected by HPLC

Figure S2 Linear relationships of **STHCL**, **RS1**, **RS2**, **RS3**

Figure S3 HRESIMS spectrum of **STHCL**

Figure S4.1 ^1H NMR spectrum of **RS1** in CD_3OD

Figure S4.2 ^{13}C NMR and dept spectrum of **RS1** in CD_3OD

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Figure S5.1 ^1H NMR spectrum of **RS2** in CD_3OD

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Figure S5.3 HRESIMS spectrum of **RS2**

Figure S6.1 ^1H NMR spectrum of **RS3** in CDCl_3

Figure S6.2 ^{13}C NMR and dept spectrum of **RS3** in CDCl_3

Figure S6.3 HRESIMS spectrum of **RS3**

Figure S1. The purity of RS1, RS2 and RS3 was detected by HPLC

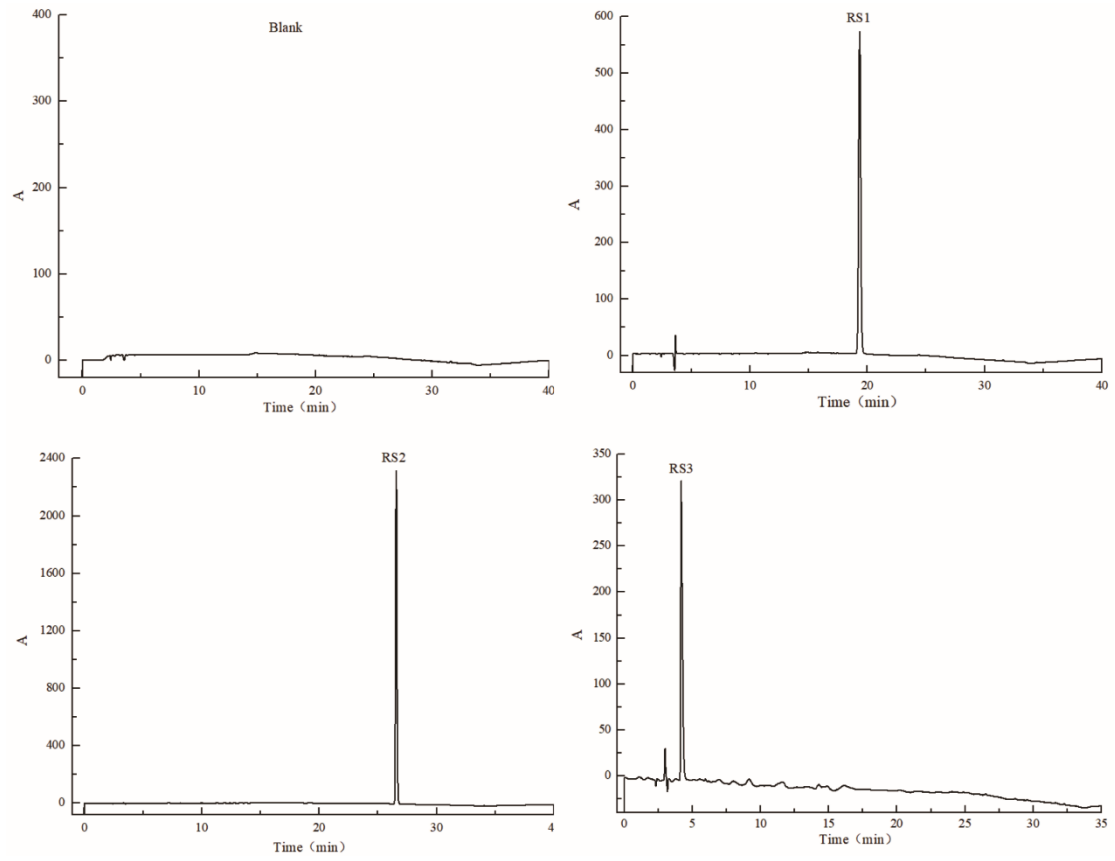


Figure S2. Linear relationships of STHCL, RS1, RS2, RS3

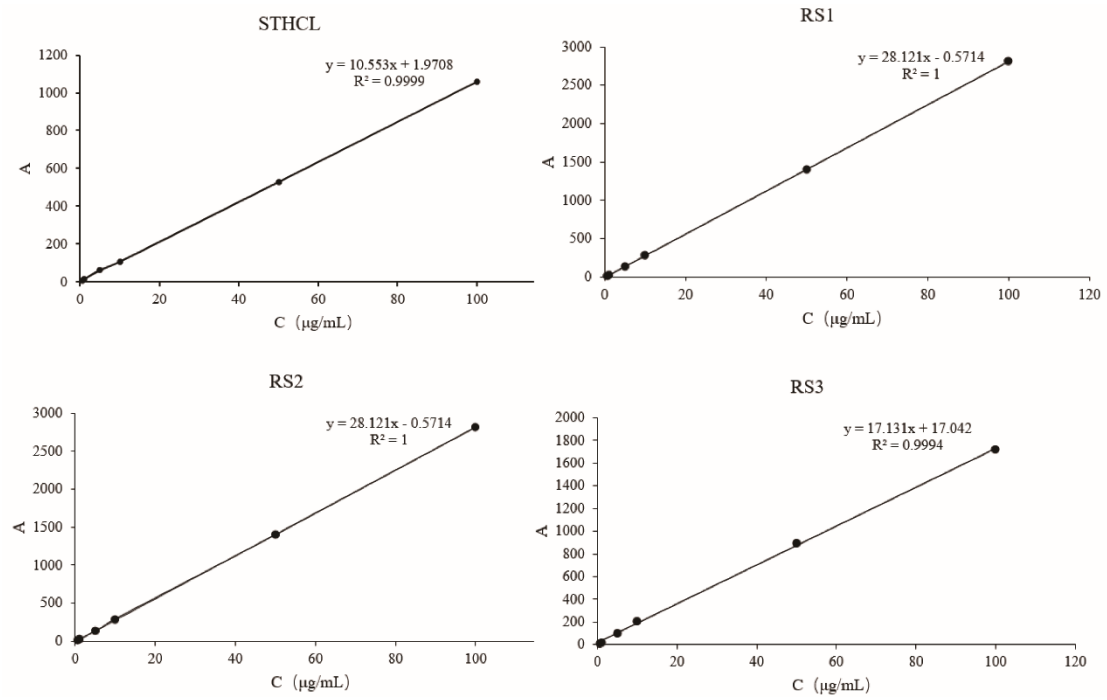
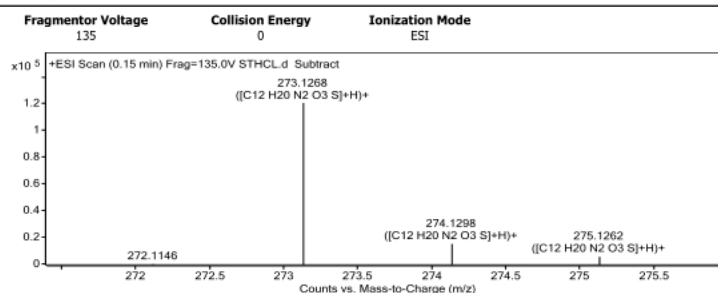


Figure S3 HRESIMS spectrum of STHCL

Qualitative Analysis Report

Data Filename	STHCL.d	Sample Name	STHCL
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	8/22/2022 4:42:21 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			
Sample Group	Info.		
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
255.1161	1	51613.22		
256.1186	1	5509.75		
271.1111	1	8149.53		
273.1268	1	120986.8	C ₁₂ H ₂₀ N ₂ O ₃ S	(M+H) ⁺
274.1298	1	15877.07	C ₁₂ H ₂₀ N ₂ O ₃ S	(M+H) ⁺
275.1262	1	6431.93	C ₁₂ H ₂₀ N ₂ O ₃ S	(M+H) ⁺
701.4951	1	18975.58		
702.4977	1	6812.53		
814.5796	1	13586.98		
815.5827	1	6741.11		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₁₂ H ₂₀ N ₂ O ₃ S	272.1195	273.1267	273.1268	-0.10	-0.37	4.0000

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Figure S4.1 ^1H NMR spectrum of RS1 in CD_3OD

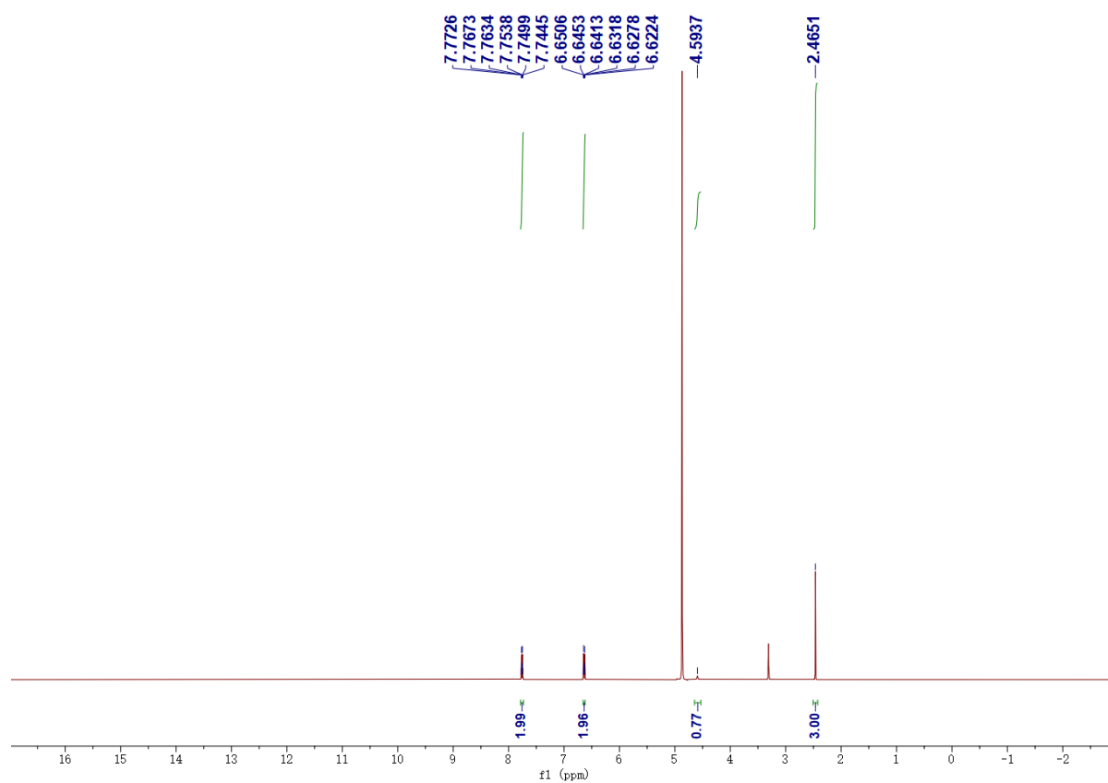


Figure S4.2 ^{13}C NMR spectrum of RS1 in CD_3OD

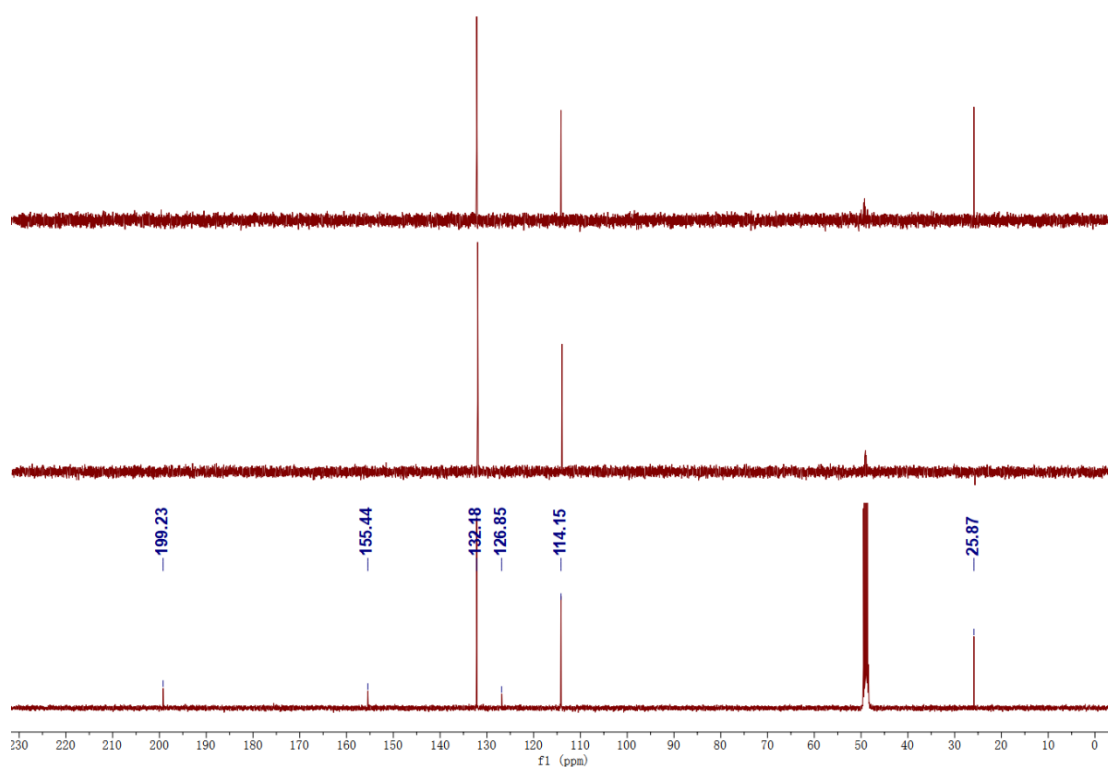


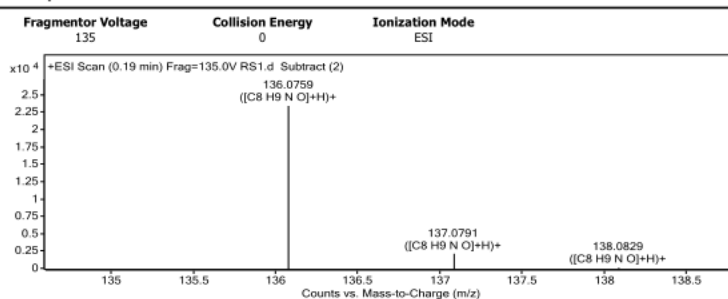
Figure S4.3 HRESIMS spectrum of RS1

Qualitative Analysis Report

Data Filename	RS1.d	Sample Name	RS1
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	8/22/2022 4:43:32 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
136.0759	1	23525.47	C8 H9 N O	(M+H)+
158.0578	1	8511.72		
349.184	1	3729.81		
393.2096	1	3115.03		
437.2353	1	2878.5		
588.41	1	3202.58		
701.495	1	9609.03		
702.5003	1	4550.32		
814.5789	1	7417.28		
815.5824	1	4182.02		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C8 H9 N O	135.0684	136.0757	136.0759	-0.20	-1.47	5.0000

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Figure S5.1 ^1H NMR spectrum of RS2 in CD_3OD

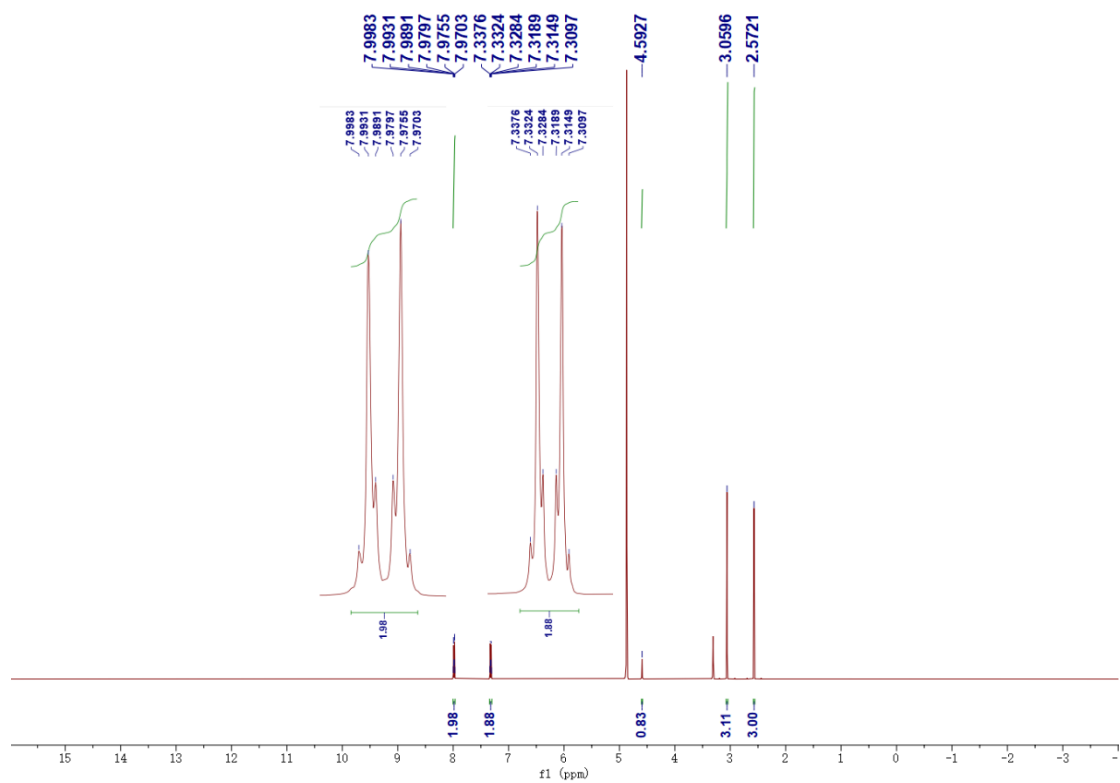


Figure S5.2 ^{13}C NMR spectrum of RS2 in CD_3OD

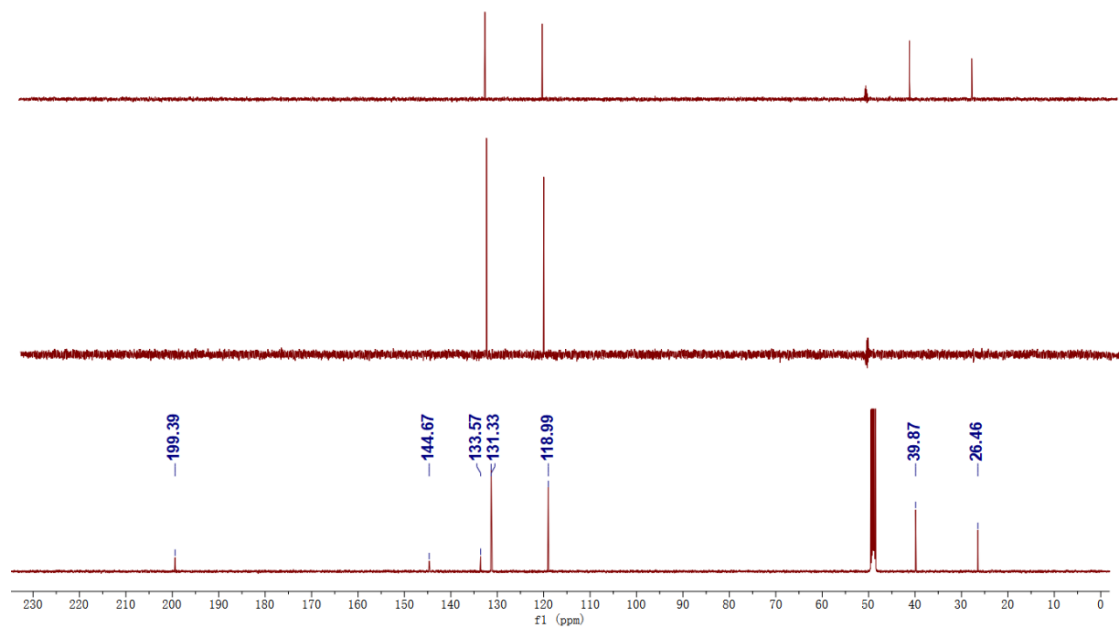
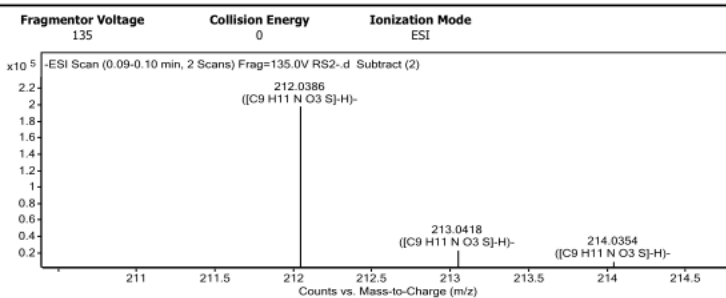


Figure S5.3 HRESIMS spectrum of RS2

Qualitative Analysis Report

Data Filename	RS2-.d	Sample Name	RS2
Sample Type	Sample	Position	P1-B3
Instrument Name	Instrument 1	User Name	
Acq Method	s-.m	Acquired Time	8/22/2022 4:49:48 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			
Sample Group	Info.		
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
133.0529	1	5192.46		
134.0605	1	6864.87		
212.0386	1	198340.78	C9 H11 N O3 S	(M-H)-
213.0418	1	24395.58	C9 H11 N O3 S	(M-H)-
214.0354	1	10774.88	C9 H11 N O3 S	(M-H)-
297.0161	1	5272.23		
348.0136	1	4083.97		
447.0662	1	11666.21		
471.2747	1	12397.93		
472.2783	1	3433.79		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C9 H11 N O3 S	213.0460	212.0387	212.0386	0.10	0.47	5.0000

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Figure S6.1 ^1H NMR spectrum of RS3 in CDCl_3

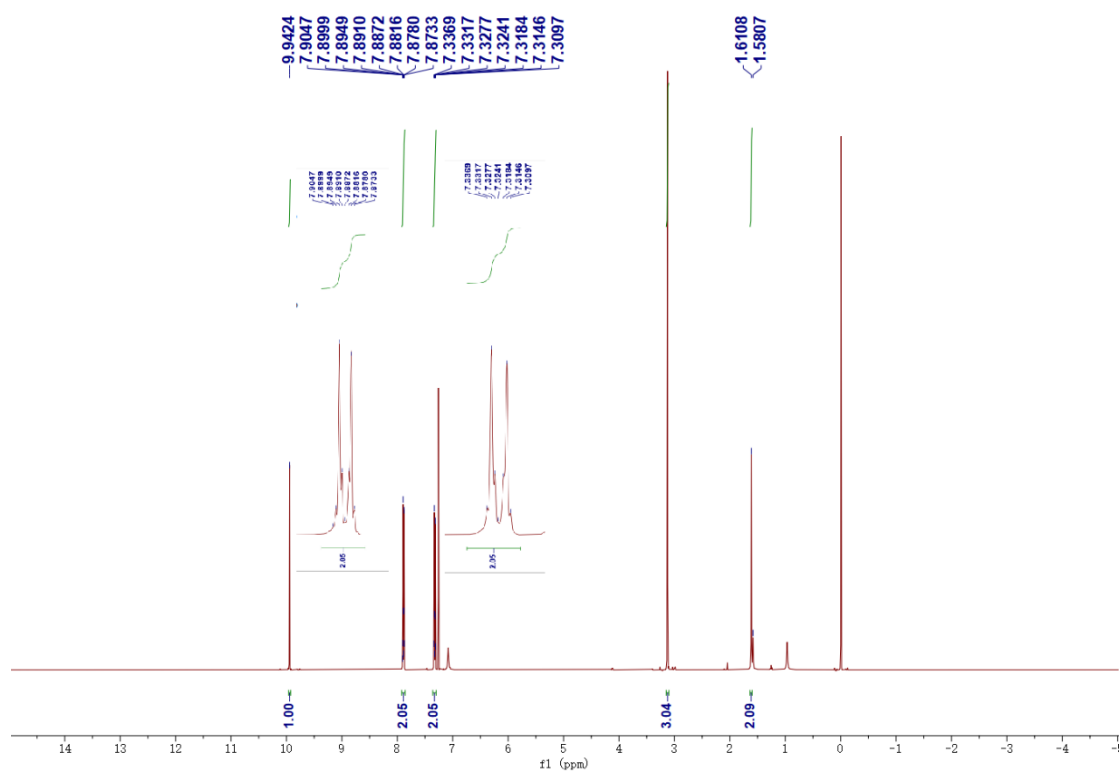


Figure S6.2 ^{13}C NMR spectrum of RS3 in CDCl_3

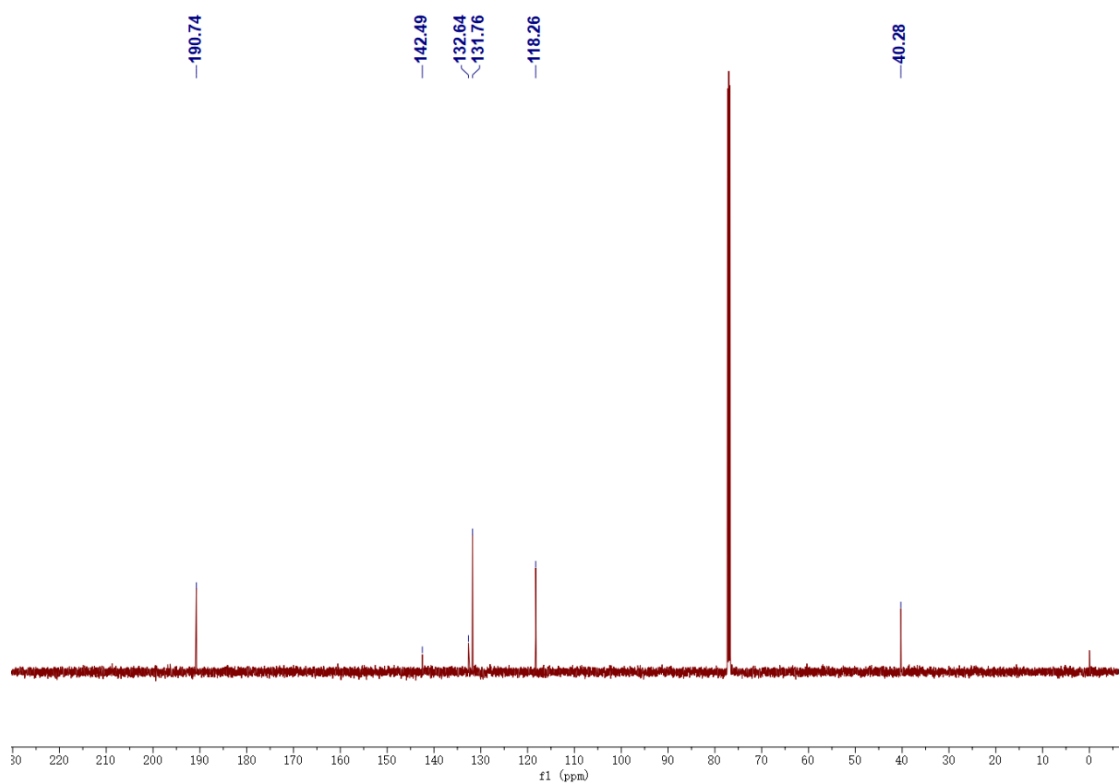


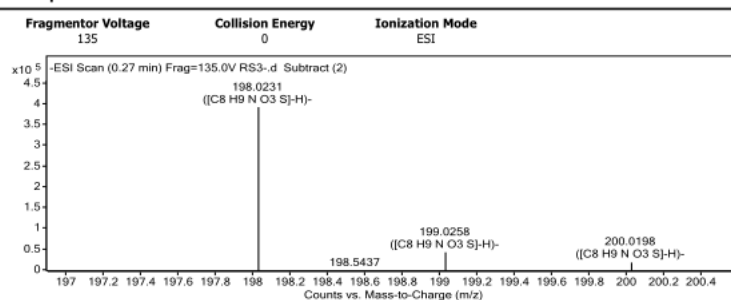
Figure S6.3 HRESIMS spectrum of RS3

Qualitative Analysis Report

Data Filename	RS3-.d	Sample Name	RS3
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	s-.m	Acquired Time	8/22/2022 4:50:46 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			

Sample Group		Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
120.043	1	13732.47		
121.0486	1	3846.79		
198.0231	1	392664.34	C8 H9 N O3 S	(M-H)-
199.0258	1	43927.92	C8 H9 N O3 S	(M-H)-
200.0198	1	20884.49	C8 H9 N O3 S	(M-H)-
283.0003	1	5716.74		
333.9976	1	5367.96		
419.0345	1	16222.55		
420.0386	1	3568.73		
471.2738	1	10529.69		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C8 H9 N O3 S	199.0303	198.0230	198.0231	-0.10	-0.50	5.0000

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