

Discovery of 1,5-diaryl-1,2,4-triazole derivatives as MYOF inhibitors and its antitumor effects in pancreatic cancer

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Table S1: The optimal range of drug-likeness parameters followed by 95% of approved drugs [1]

Molecular descriptor	Molecular weight	cLogP	n HBA	n HBD	n rotatable bounds
Optimum range	130 to 725	-2.0 to 6.5	2 to 20	0 to 6	0 to 15

cLogP: the calculated octanol/water partition coefficient; HBA: Hydrogen bond acceptor; HBD: Hydrogen bond donor

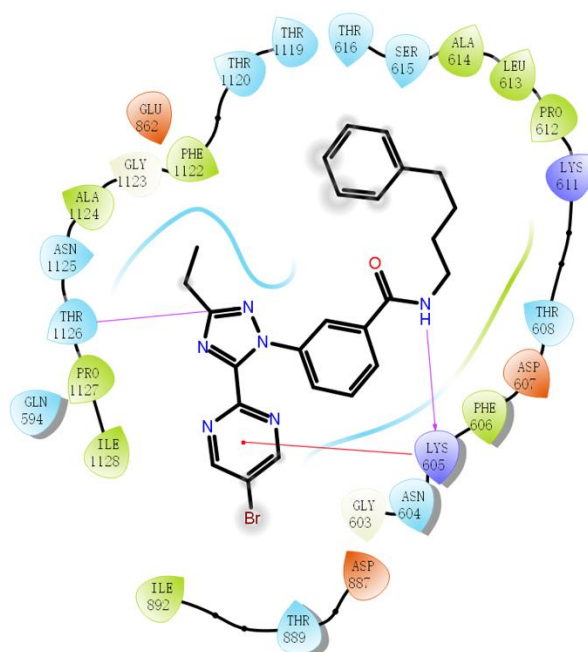
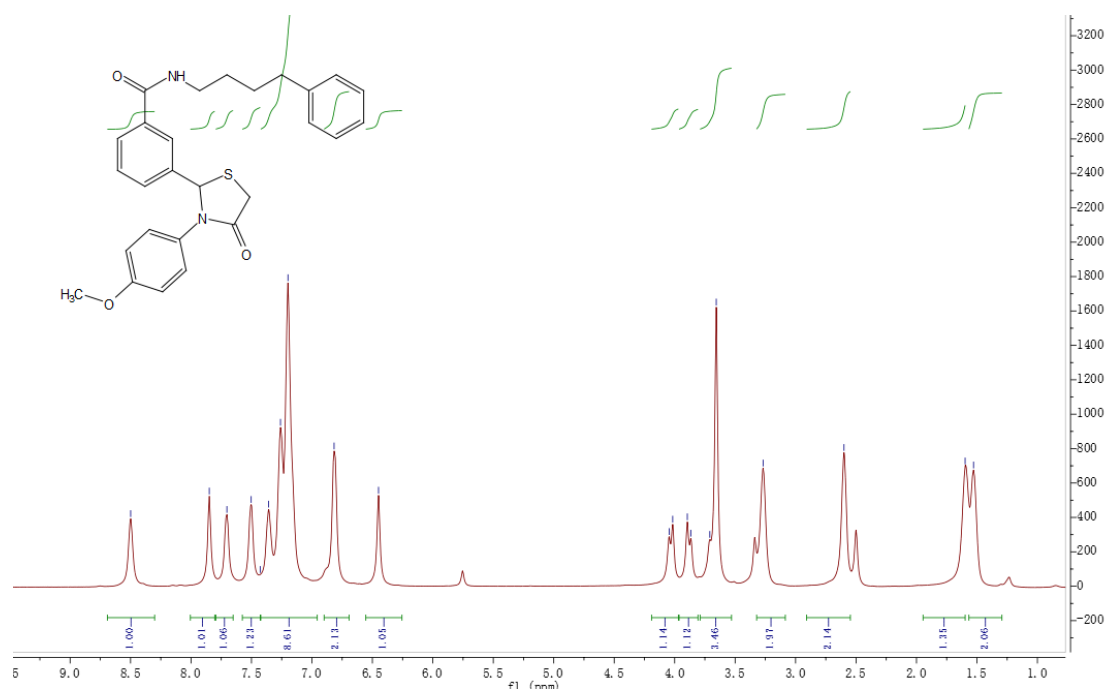
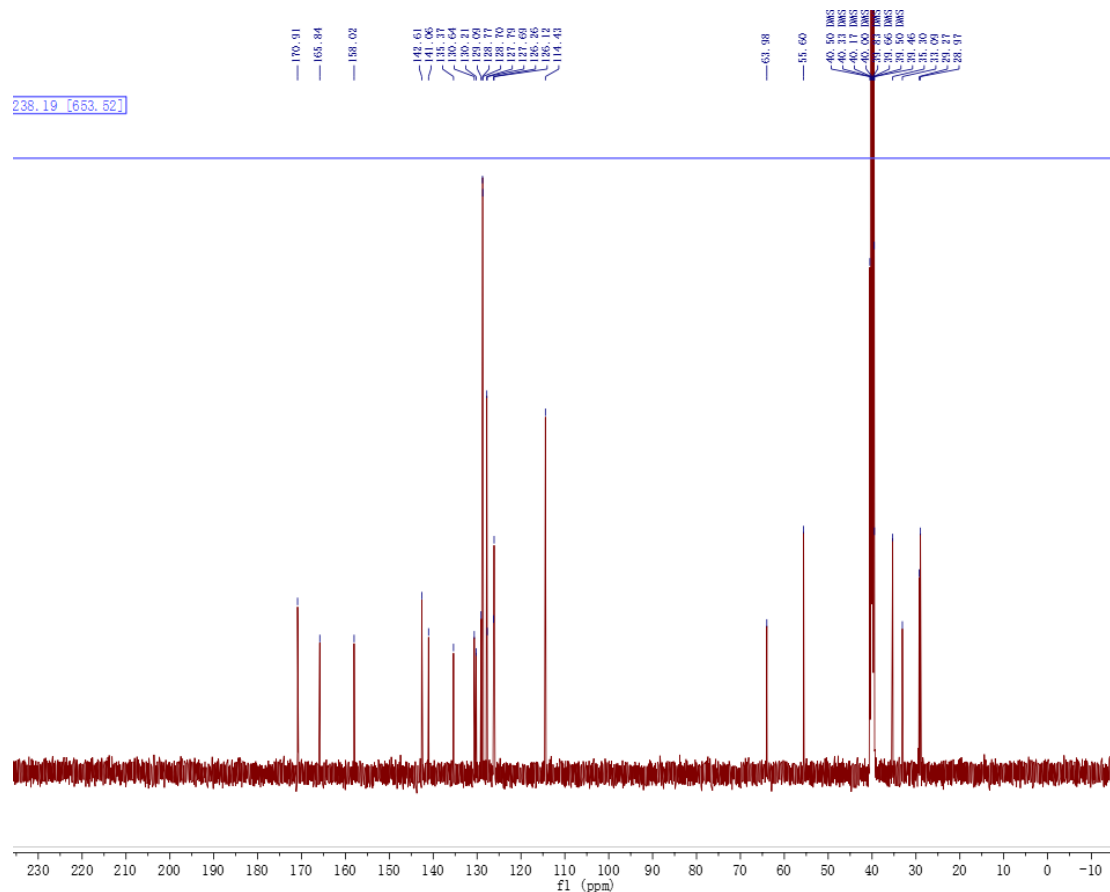


Figure S1: 2D visualization of binding postures of E4 inhibitor with MYOF

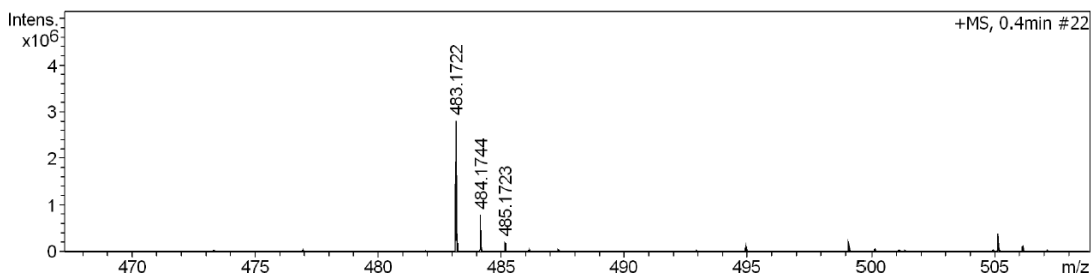
^1H -NMR spectrum of **A1**.



^{13}C NMR spectrum of **A1**.



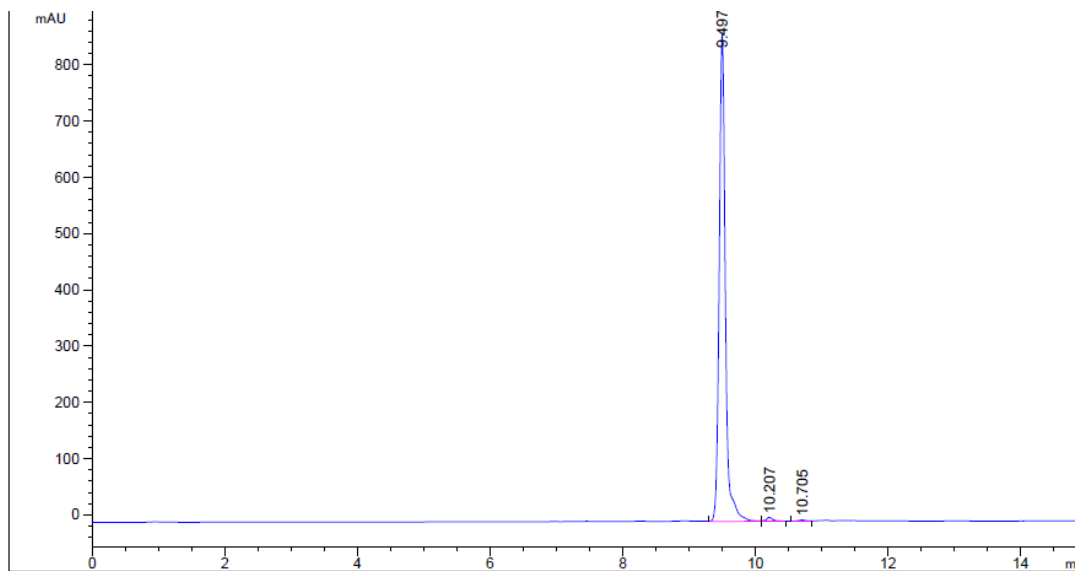
HR MS spectrum of A1.



#	m/z	Res.	S/N	I	I %	FWHM
1	483.1722	25840	2591.7	2795396	100.0	0.0187
2	484.1744	27368	729.0	786140	28.1	0.0177
3	485.1723	20443	188.0	202816	7.3	0.0237

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻	Conf	N-Rule
483.1722	1	C27H28N2NaO3S	483.1713	-2.0	19.9	1	63.79	14.5	even	ok

HPLC spectrum of A1.



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面积百分比报告
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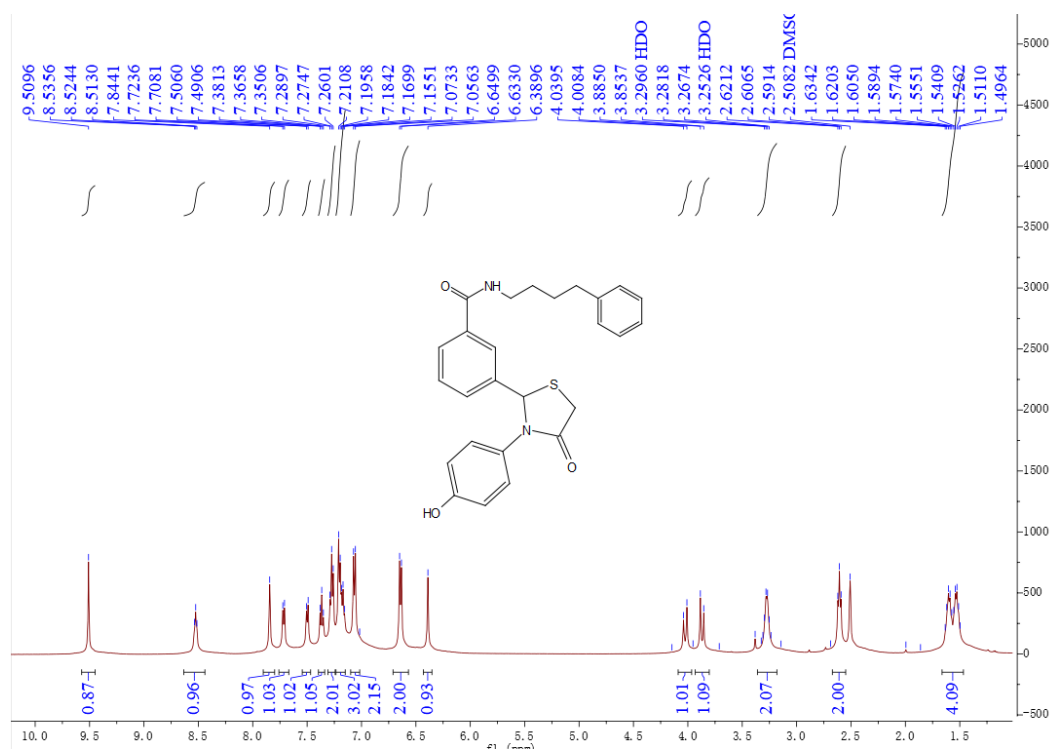
排序 : 信号
乘积因子: 1.0000
稀释因子: 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

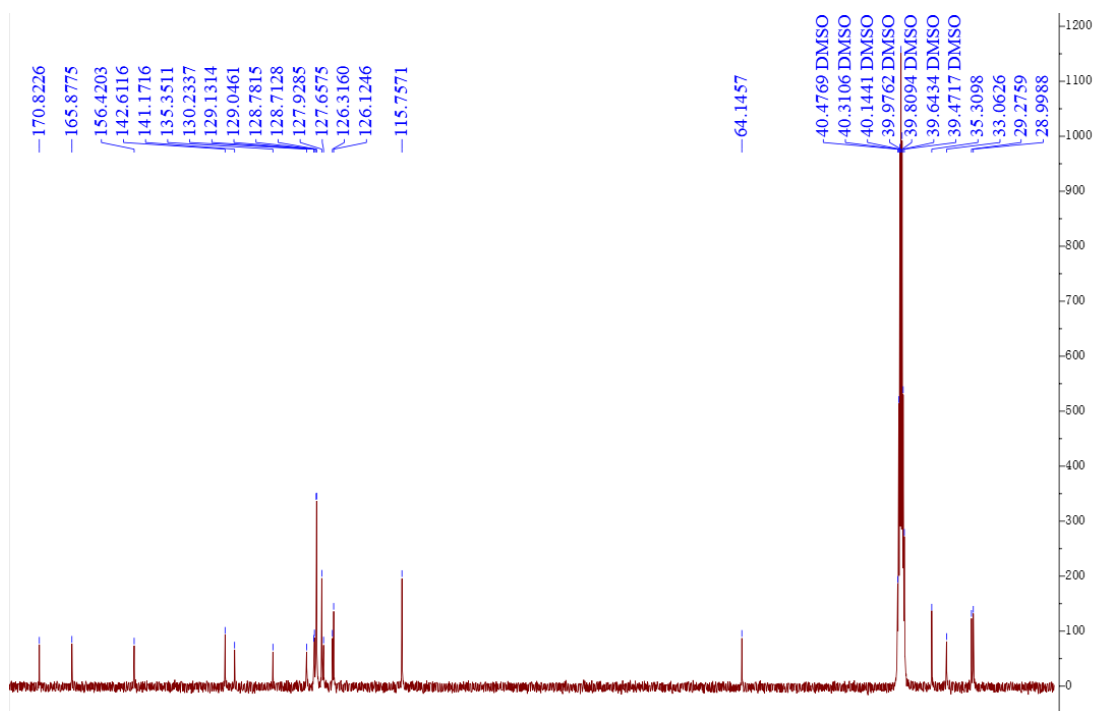
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	9.497	VV	0.0973	5594.47119	865.38190	98.8131
2	10.207	VB	0.1039	48.27137	6.86585	0.8526
3	10.705	BV	0.1197	18.92720	2.29036	0.3343

总量 : 5661.66976 874.53811

¹H-NMR spectrum of A2.



¹³C NMR spectrum of A2.



HR MS spectrum of A2.

Analysis Info

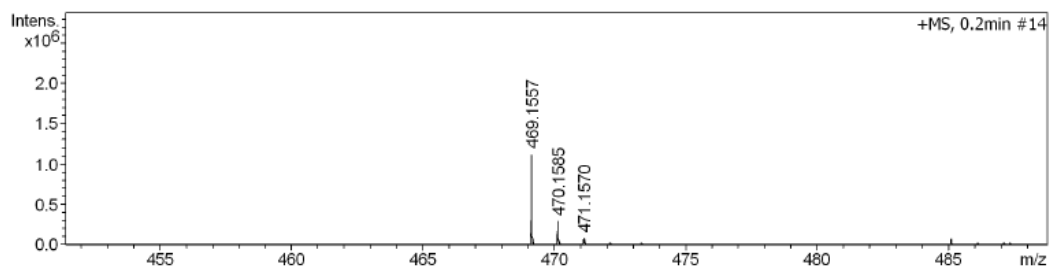
Analysis Name D:\Data\waixi\chenyihua\HJ-0128-446_P1-B-9_01_23540.d
Method Tune_pos_wide_LC with calibration-20190508-1.m
Sample Name HJ-0128-446
Comment

Acquisition Date 1/29/2021 2:25:34 PM

Operator ECNU-Chem
Instrument maXis impact 282001.00122

Acquisition Parameter

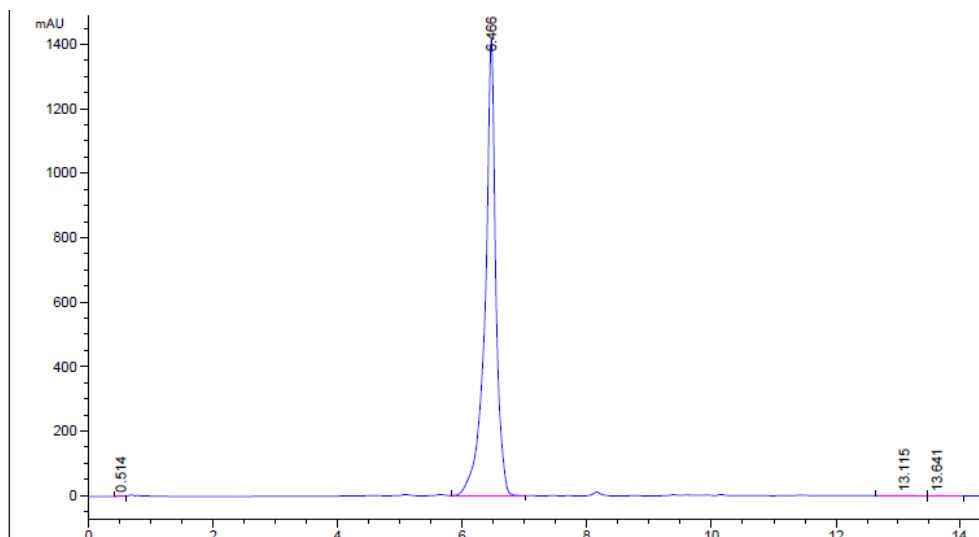
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	469.1557	26853	1853.7	1128584	100.0	0.0175
2	470.1585	20559	486.4	296620	26.3	0.0229
3	471.1570	15146	133.0	81184	7.2	0.0311

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
469.1557	1	C ₂₆ H ₂₆ N ₂ NaO ₃ S	469.1556	-0.1	22.1	1	100.00	14.5 even	ok

HPLC spectrum of A2.



面积百分比报告

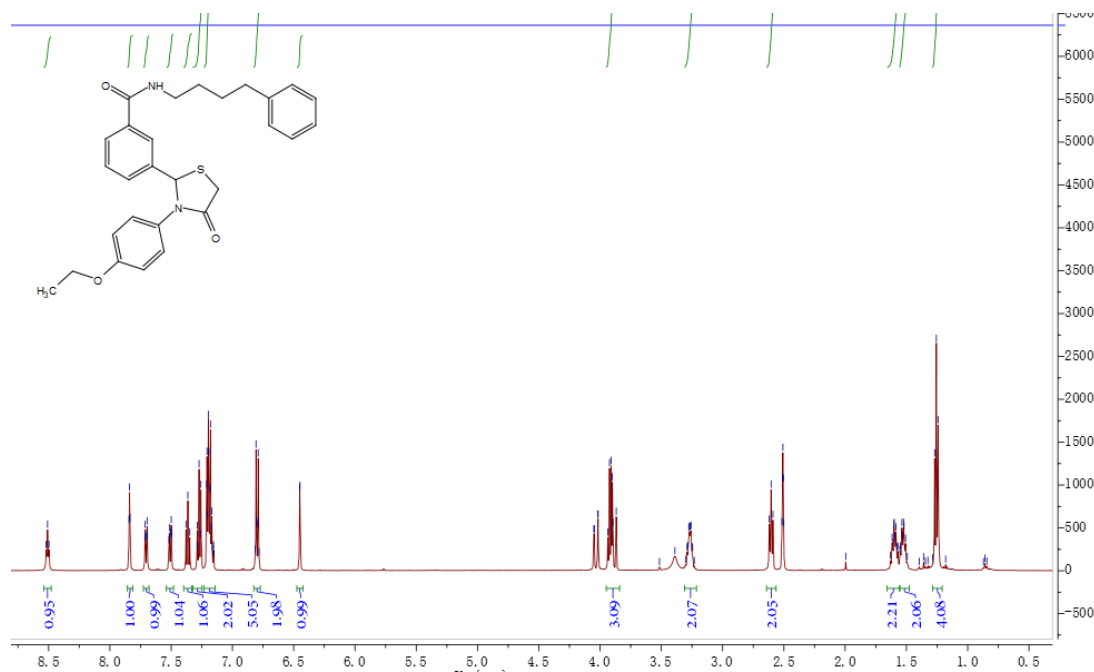
排序 : 信号
 乘积因子: 1.0000
 稀释因子: 1.0000
 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

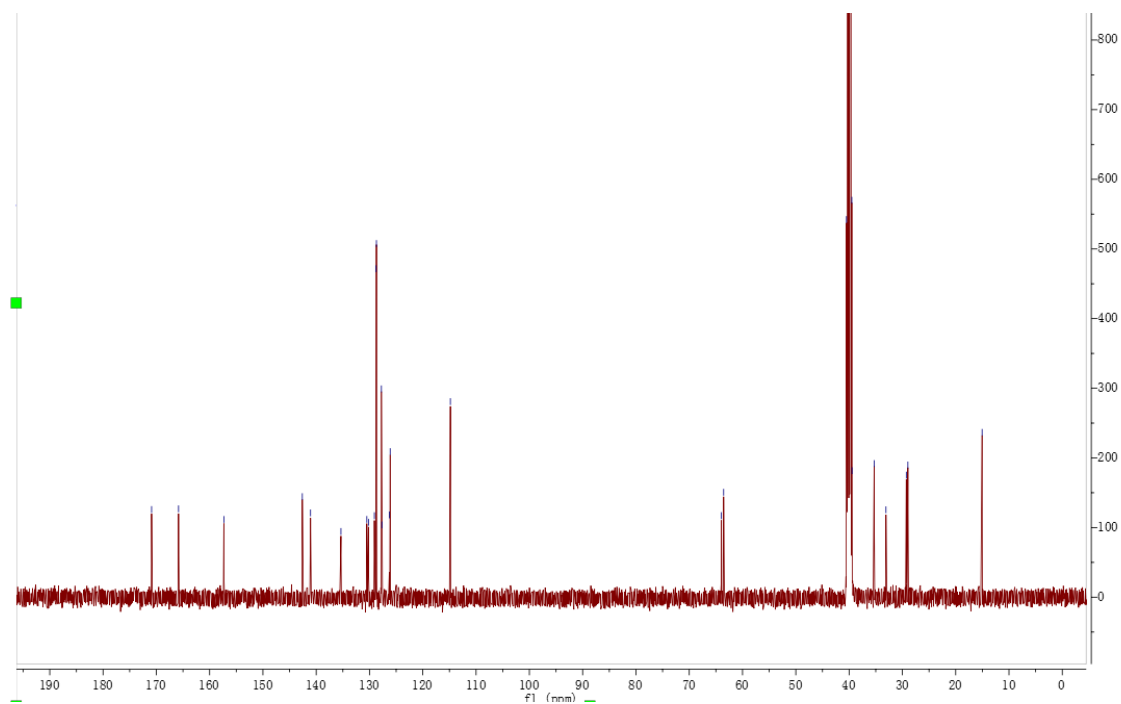
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	0.514	BV	0.0818	8.54324	1.58631	0.0498
2	6.466	VV	0.1667	1.71087e4	1420.37097	99.7761
3	13.115	VV	0.5201	22.37261	5.39653e-1	0.1305
4	13.641	VB	0.2993	7.48490	3.41651e-1	0.0437

总量 : 1.71471e4 1422.83858

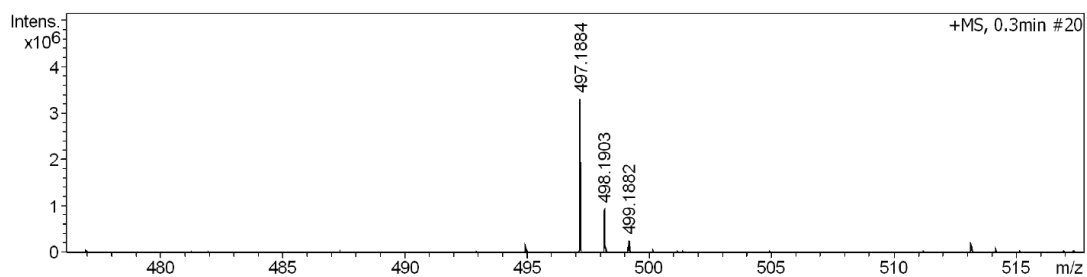
¹H-NMR spectrum of A3.



^{13}C NMR spectrum of **A3**.



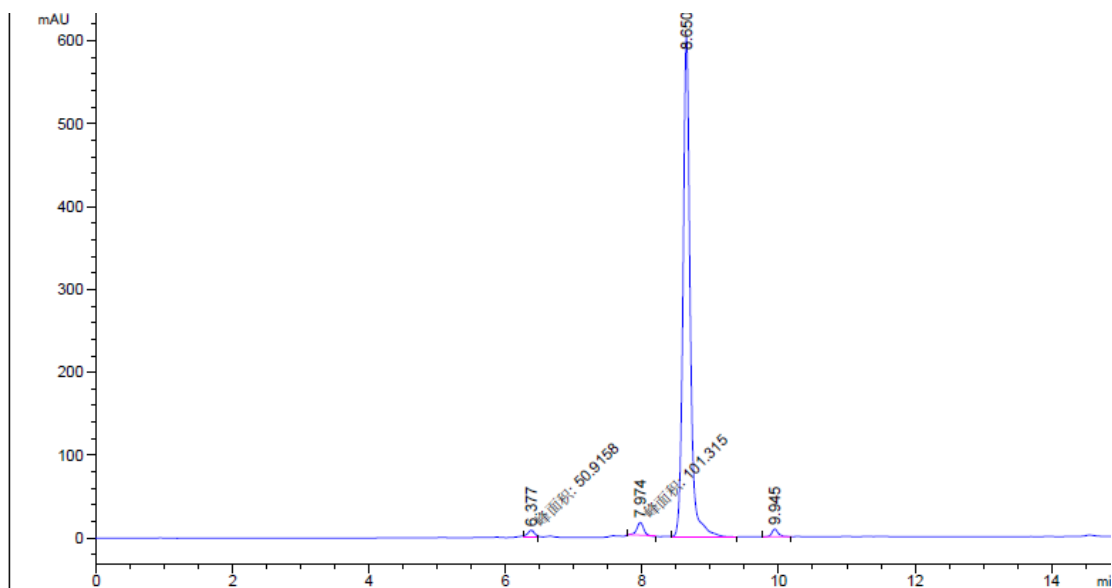
HR MS spectrum of **A3**.



#	m/z	Res.	S/N	I	I %	FWHM
1	497.1884	23375	2968.1	3297960	100.0	0.0213
2	498.1903	27842	853.1	947492	28.7	0.0179
3	499.1882	20662	231.2	256504	7.8	0.0242

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻	Conf	N-Rule
497.1884	1	C ₂₈ H ₃₀ N ₂ NaO ₃ S	497.1869	-2.9	21.4	1	56.41	14.5	even	ok

HPLC spectrum of **A3**.



面积百分比报告

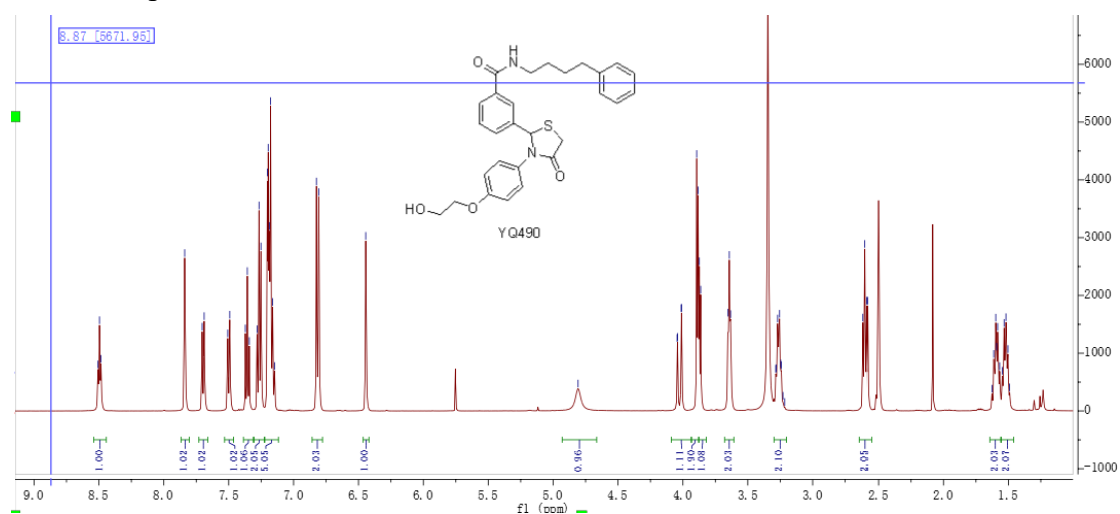
排序 : 信号
 乘积因子: : 1.0000
 稀释因子: : 1.0000
 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

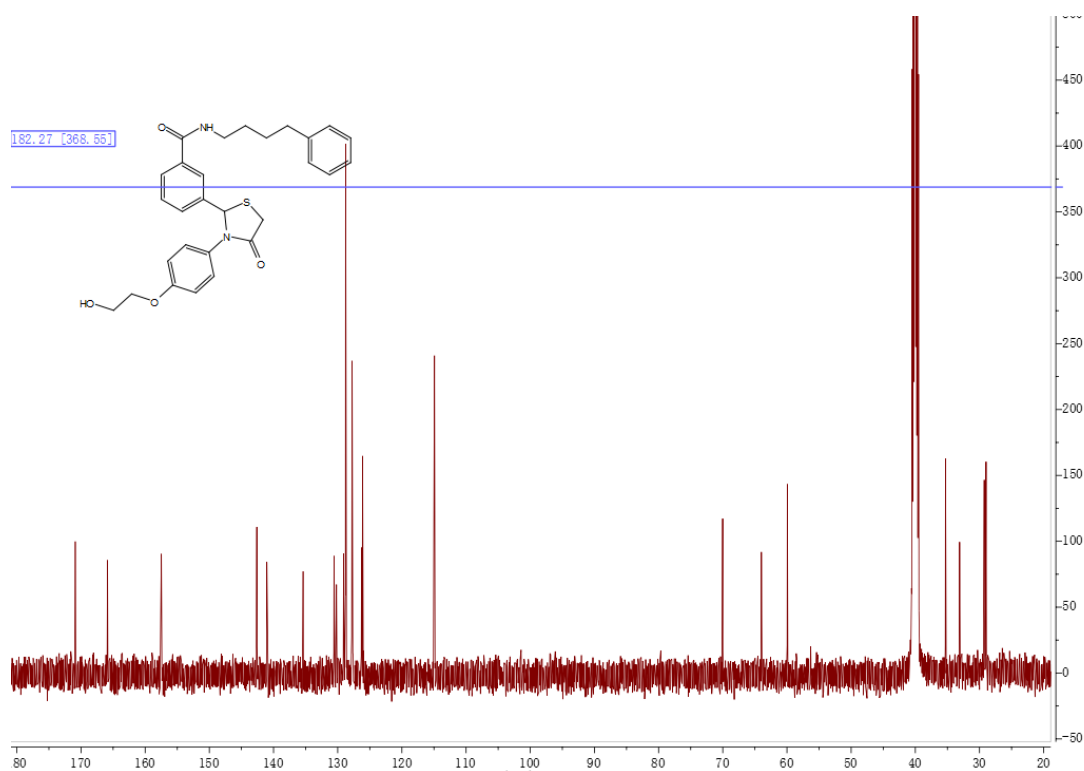
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	6.377	MM	0.1099	50.91585	7.71920	1.0944
2	7.974	MM	0.1092	101.31451	15.45693	2.1776
3	8.650	VV	0.1090	4437.38672	604.40155	95.3759
4	9.945	VB	0.0998	62.90944	9.41531	1.3522

总量 : 4652.52651 636.99299

¹H-NMR spectrum of A4.



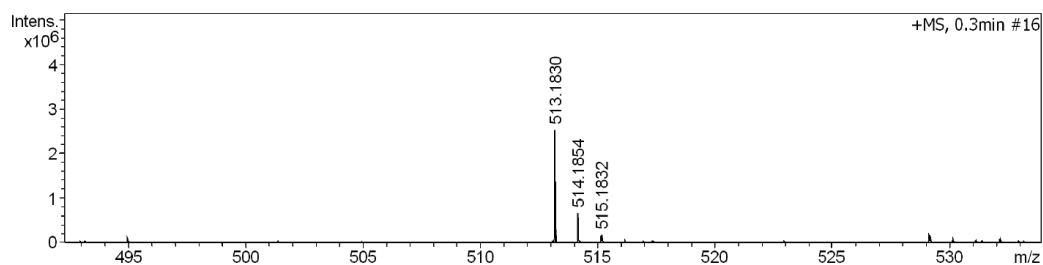
¹³C NMR spectrum of A4.



HR MS spectrum of A4.

Acquisition Parameter

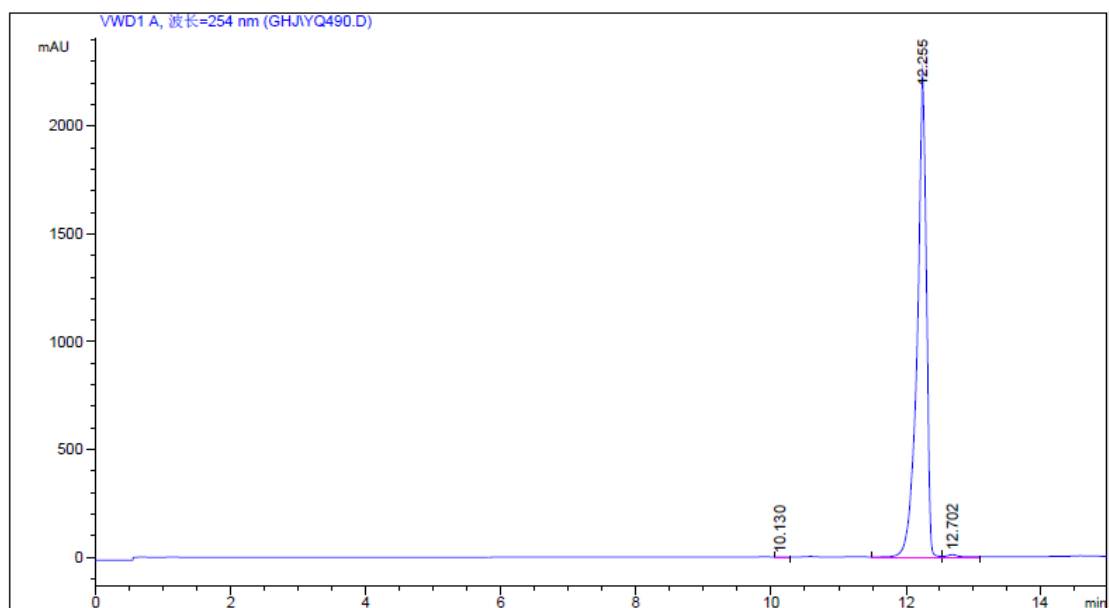
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	513.1830	27382	2208.8	2531572	100.0	0.0187
2	514.1854	25660	603.0	690792	27.3	0.0200
3	515.1832	19316	163.3	187032	7.4	0.0267

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
513.1830	1	C28H30N2NaO4S	513.1818	-2.3	29.2	3	50.95	14.5	even ok

HPLC spectrum of A4.



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 面积百分比报告
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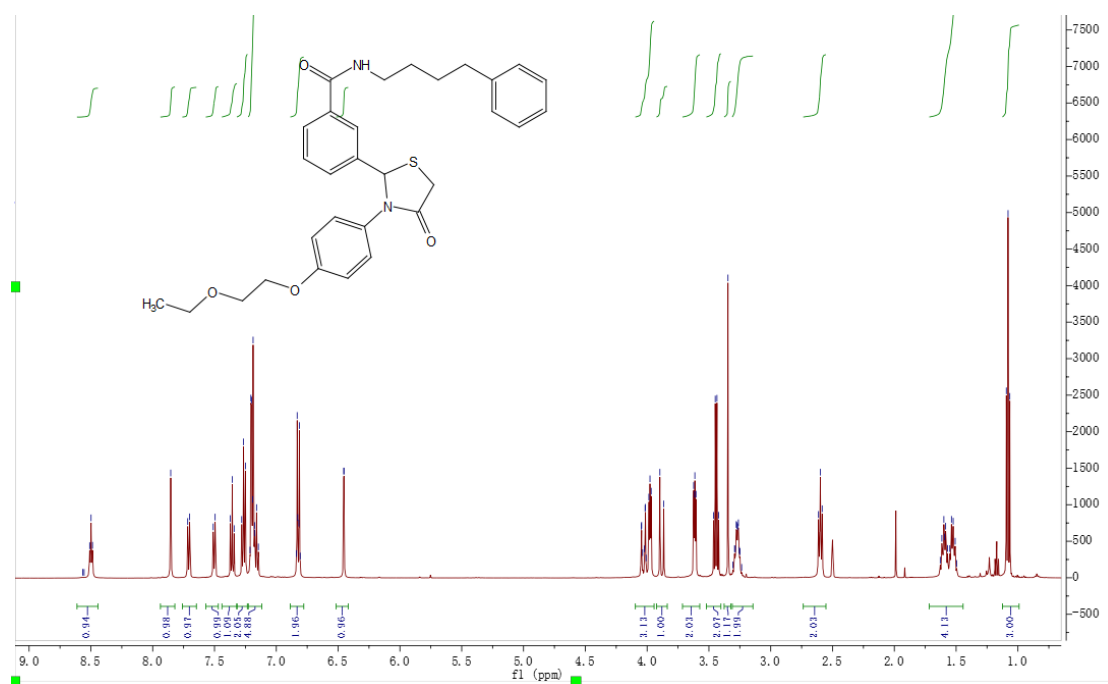
排序 : 信号
 乘积因子: : 1.0000
 稀释因子: : 1.0000
 内标使用乘积因子和稀释因子

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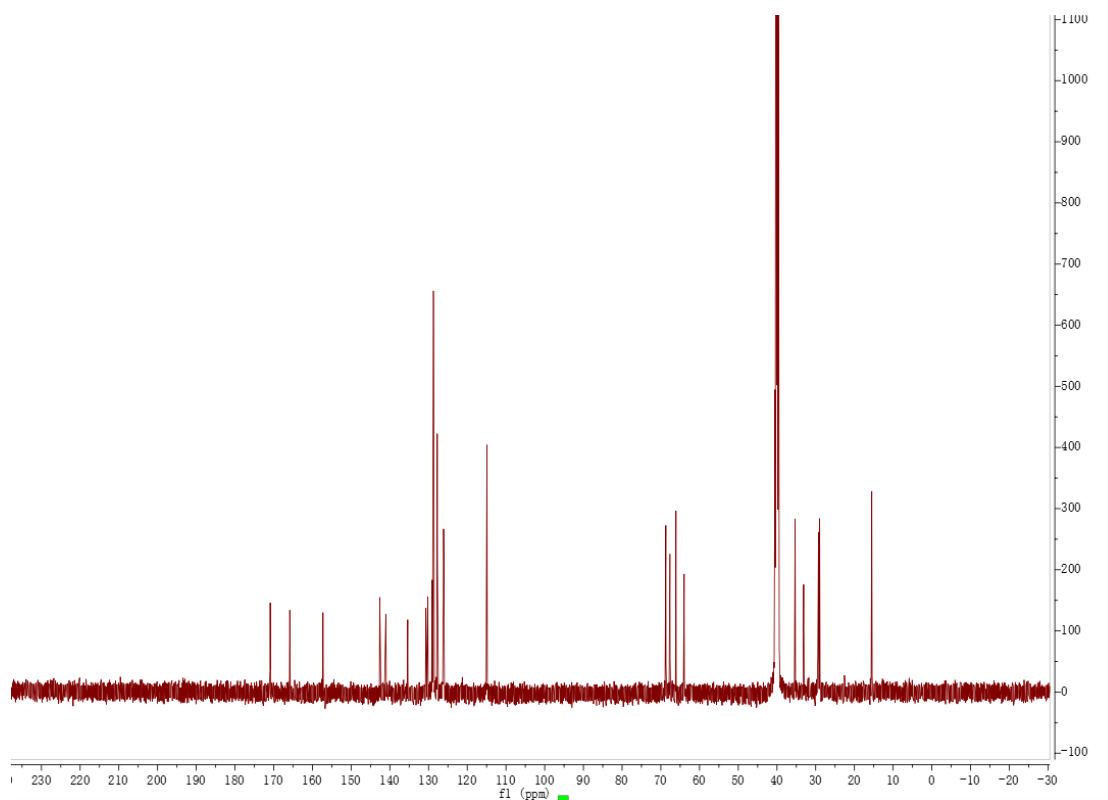
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	10.130	VV	0.1602	12.00046	1.06780	0.0498
2	12.255	VV	0.1614	2.39487e4	2288.95288	99.3432
3	12.702	VB	0.1772	146.33272	11.53133	0.6070

总量 : 2.41070e4 2301.55201

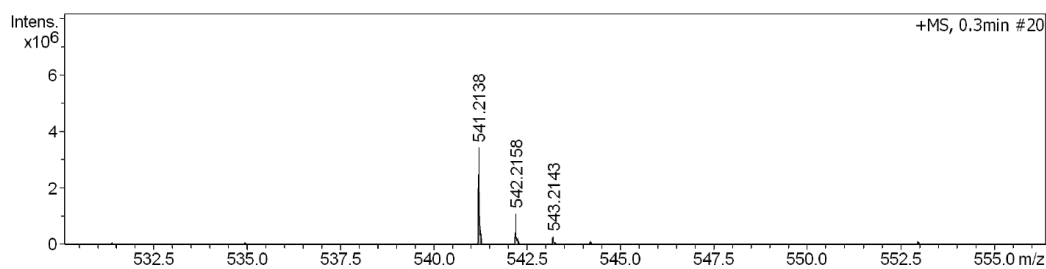
¹H-NMR spectrum of **A5**.



¹³C NMR spectrum of A5.



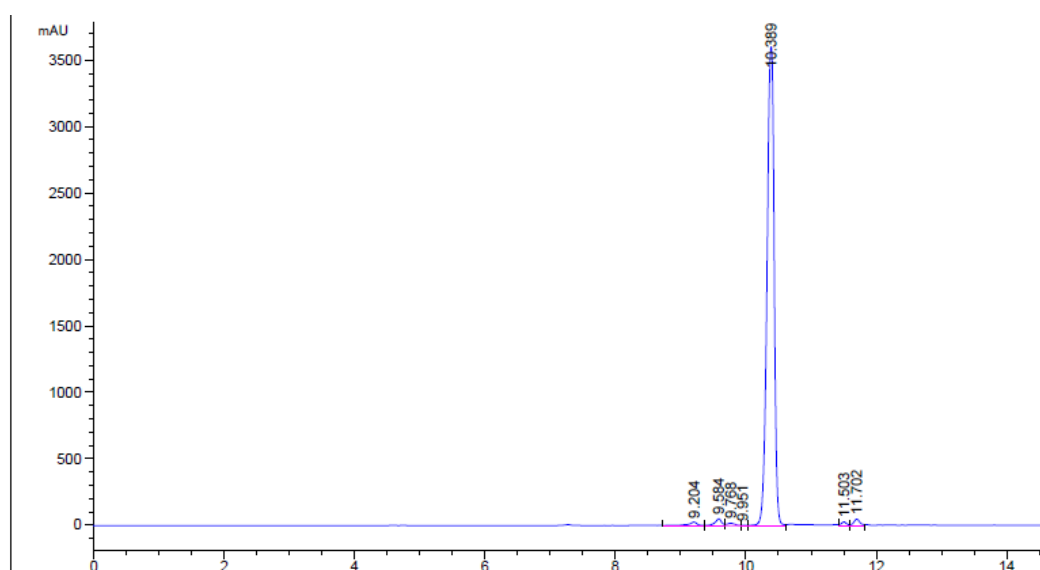
HR MS spectrum of A5.



#	m/z	Res.	S/N	I	I %	FWHM
1	541.2138	21888	3240.1	3426364	100.0	0.0247
2	542.2158	30103	1061.2	1121368	32.7	0.0180
3	543.2143	22122	290.9	307236	9.0	0.0246
4	544.2142	17773	56.7	59888	1.7	0.0306

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdB	e ⁻ Conf	N-Rule
541.2138	1	C30H34N2NaO4S	541.2131	-1.2	12.7	1	98.89	14.5	even ok

HPLC spectrum of A5.



面积百分比报告

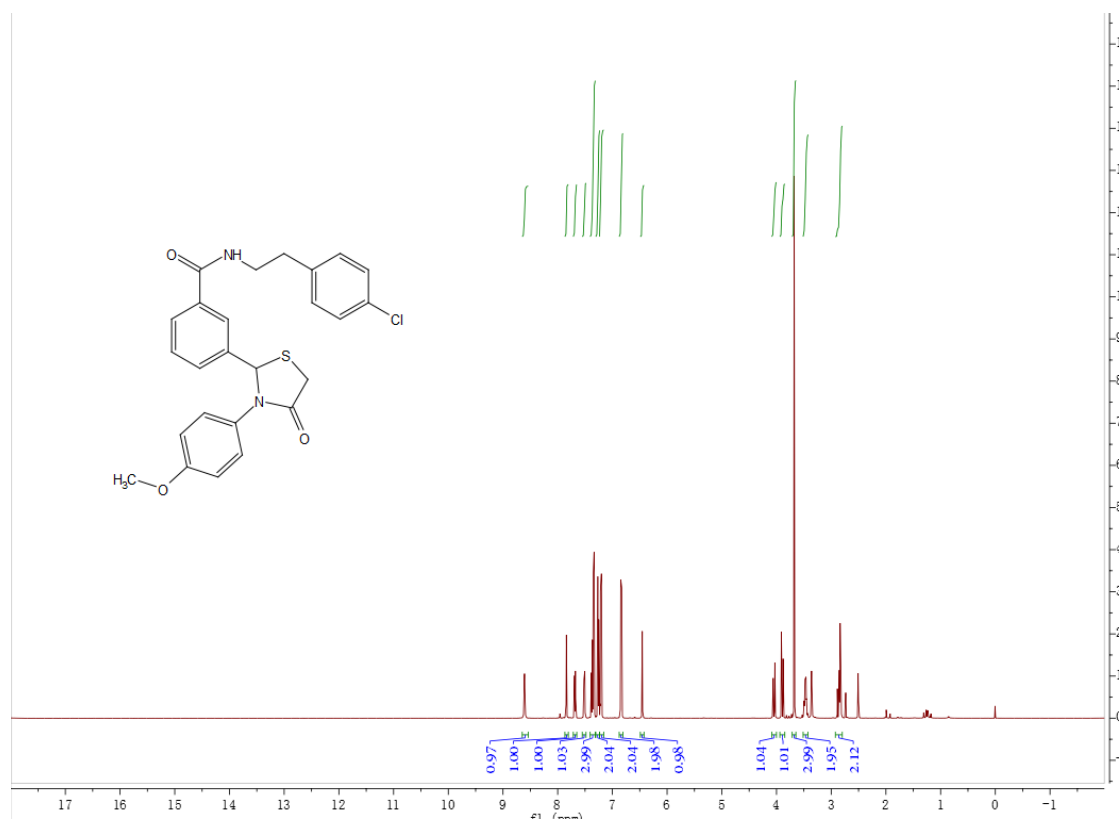
排序 : 信号
 乘积因子: 1.0000
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 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

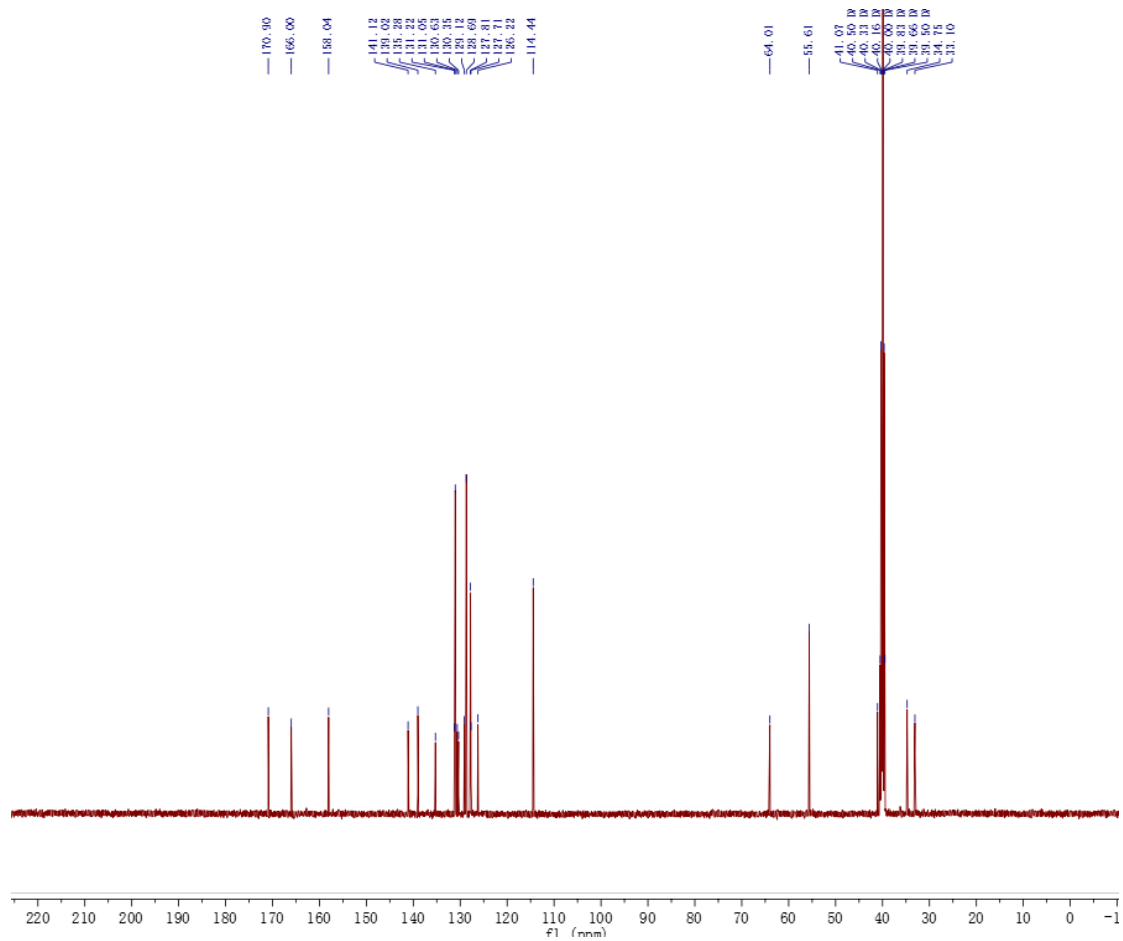
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	9.204	VV	0.1302	246.96506	26.58918	0.8670
2	9.584	VV	0.0999	351.91422	50.69724	1.2354
3	9.768	VV	0.1256	147.11328	17.79389	0.5165
4	9.951	VV	0.0773	11.03711	2.05198	0.0387
5	10.389	VV	0.1174	2.72813e4	3606.45508	95.7726
6	11.503	VV	0.0800	144.62350	27.00417	0.5077
7	11.702	VV	0.0959	302.53372	47.62869	1.0621

总量 : 2.84854e4 3778.22022

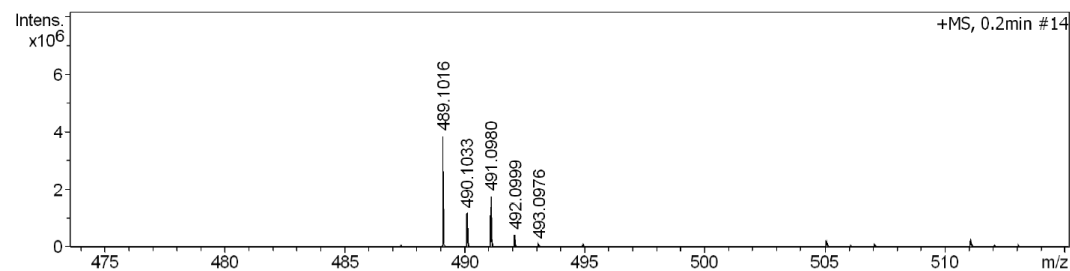
¹H-NMR spectrum of A6.



¹³C NMR spectrum of A6.



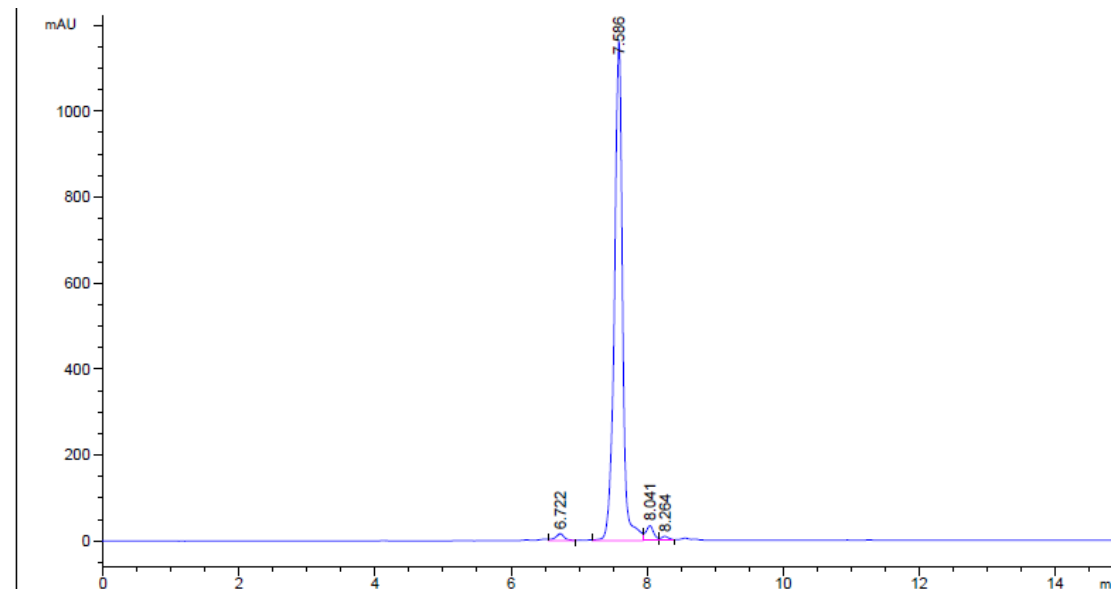
HR MS spectrum of A6.



#	m/z	Res.	S/N	I	I %	FWHM
1	489.1016	18360	2934.8	3839992	100.0	0.0266
2	490.1033	29695	902.0	1180048	30.7	0.0165
3	491.0980	31137	1355.0	1772620	46.2	0.0158
4	492.0999	24996	325.1	425164	11.1	0.0197
5	493.0976	17386	81.6	106628	2.8	0.0284

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
489.1016	1	C25H23ClN2NaO3S	489.1010	-1.2	21.9	1	100.00	14.5	even ok

HPLC spectrum of A6.



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面积百分比报告
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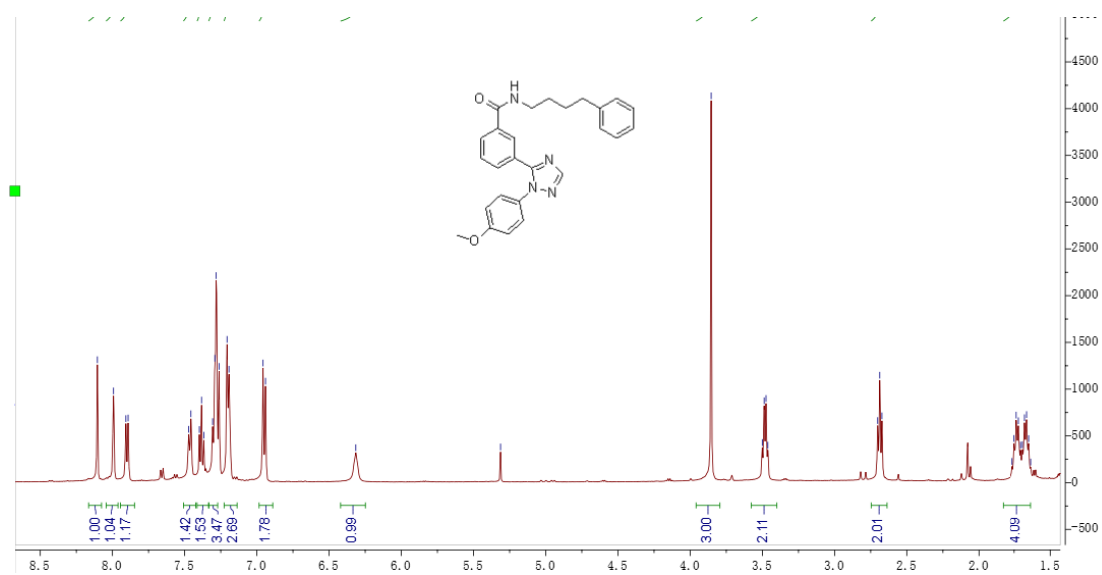
排序 : 信号
乘积因子: 1.0000
稀释因子: 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

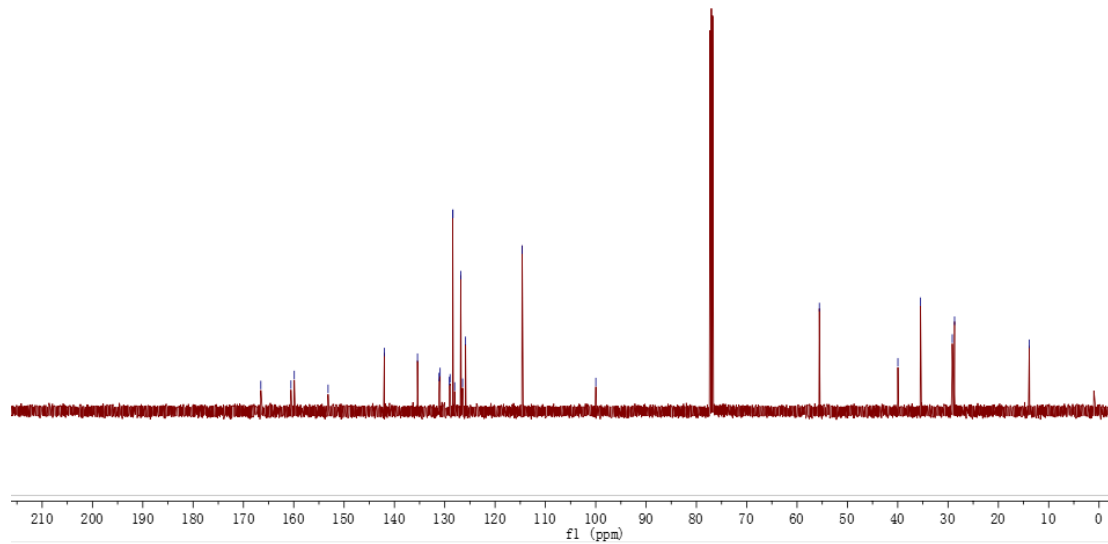
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1	6.722	VV	0.1353	150.89954	16.13788	1.4784
2	7.586	VV	0.1265	9699.25391	1161.45764	95.0291
3	8.041	VV	0.1178	280.19705	34.58686	2.7452
4	8.264	VV	0.1138	76.26358	9.82962	0.7472

总量 : 1.02066e4 1222.01200

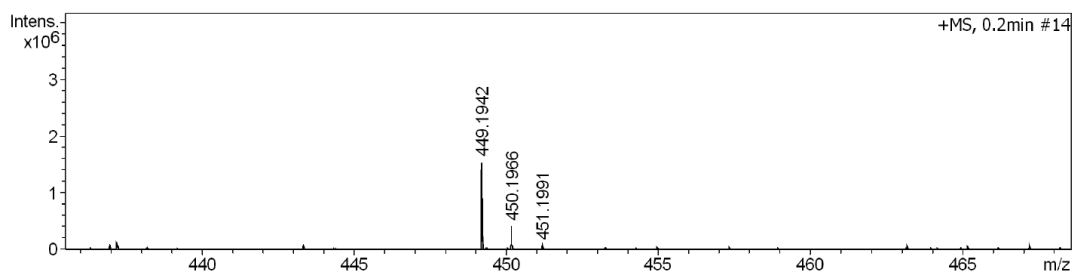
^1H -NMR spectrum of **D1**.



^{13}C NMR spectrum of **D1**.



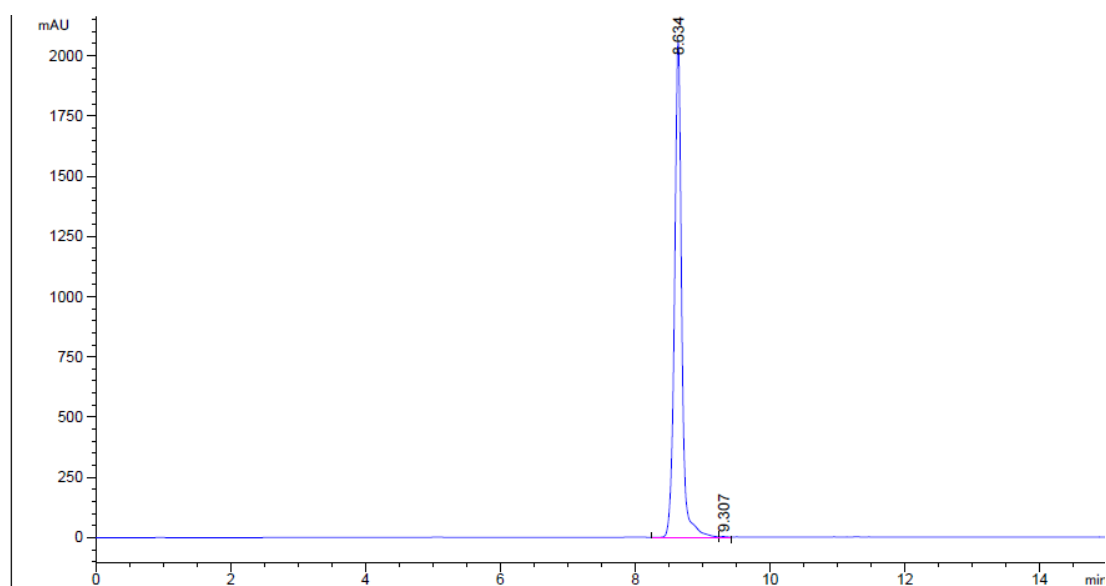
HR MS spectrum of **D1**.



#	m/z	Res.	S/N	I	I %	FWHM
1	449.1942	30222	1213.2	1543412	100.0	0.0149
2	450.1966	24543	322.5	410200	26.6	0.0183
3	451.1991	20293	51.7	65796	4.3	0.0222

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
449.1942	1	C ₂₆ H ₂₆ N ₄ NaO ₂	449.1948	1.4	17.1	2	83.96	15.5	even ok

HPLC spectrum of D1.



面积百分比报告

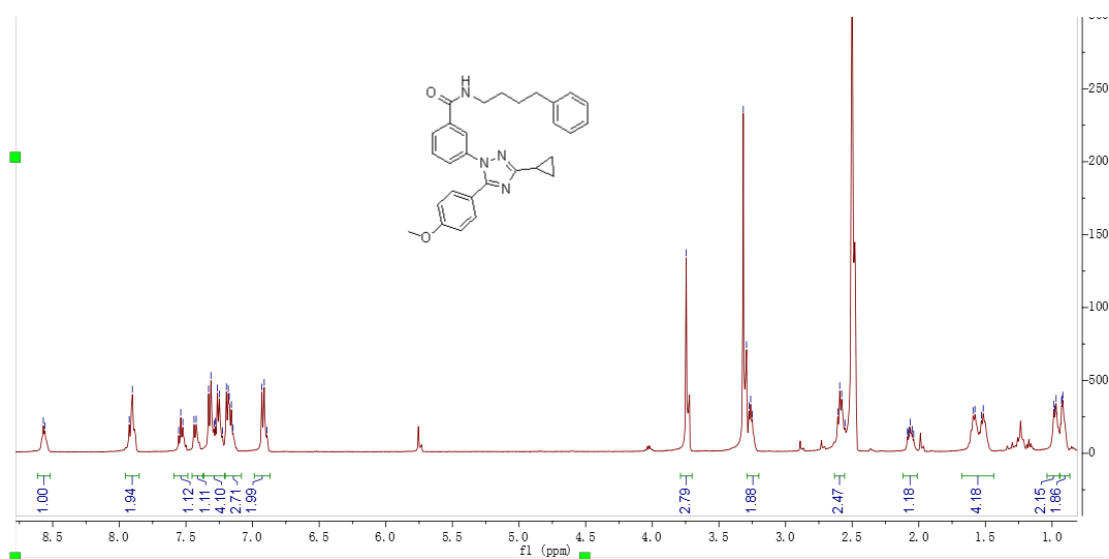
排序 : 信号
 乘积因子: 1.0000
 稀释因子: 1.0000
 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

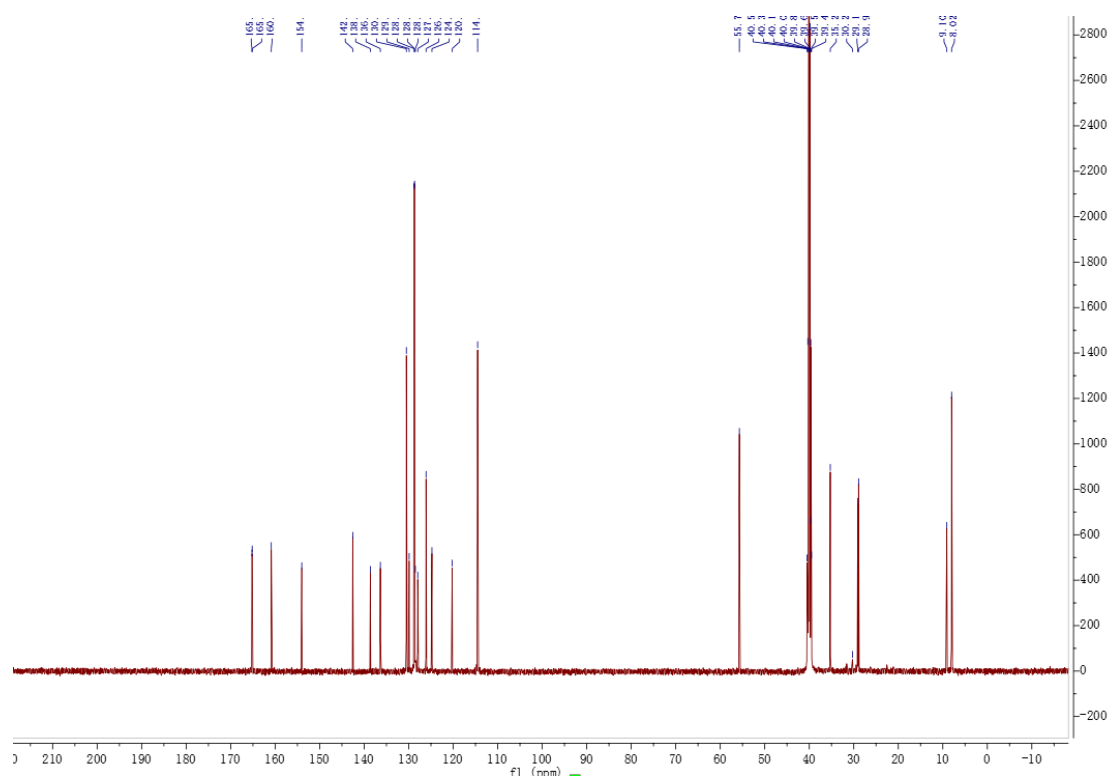
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1	8.634	VV	0.1117	1.53347e4	2057.62061	99.8582
2	9.307	VV	0.1096	21.76803	2.89327	0.1418

总量 : 1.53565e4 2060.51388

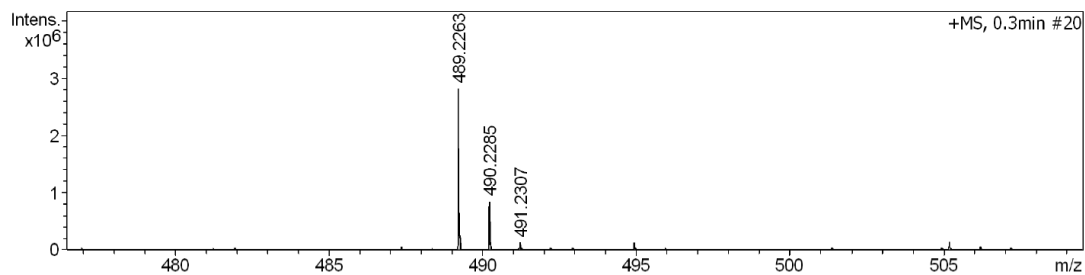
¹H-NMR spectrum of E2.



¹³C NMR spectrum of E2.



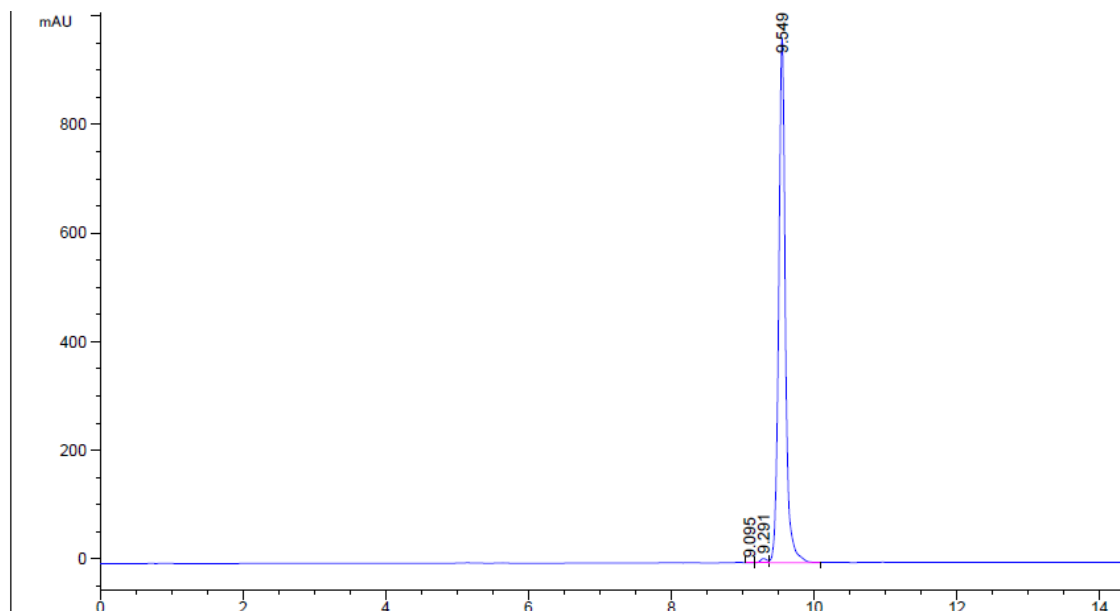
HR MS spectrum of E2.



#	m/z	Res.	S/N	I	I %	FWHM
1	489.2263	24918	2542.3	2810684	100.0	0.0196
2	490.2285	27650	764.6	845256	30.1	0.0177
3	491.2307	19374	116.2	128456	4.6	0.0254

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻	Conf	N-Rule
489.2263	1	C ₂₉ H ₃₀ N ₄ NaO ₂	489.2261	-0.4	17.0	2	100.00	16.5	even	ok

HPLC spectrum of E2.



面积百分比报告

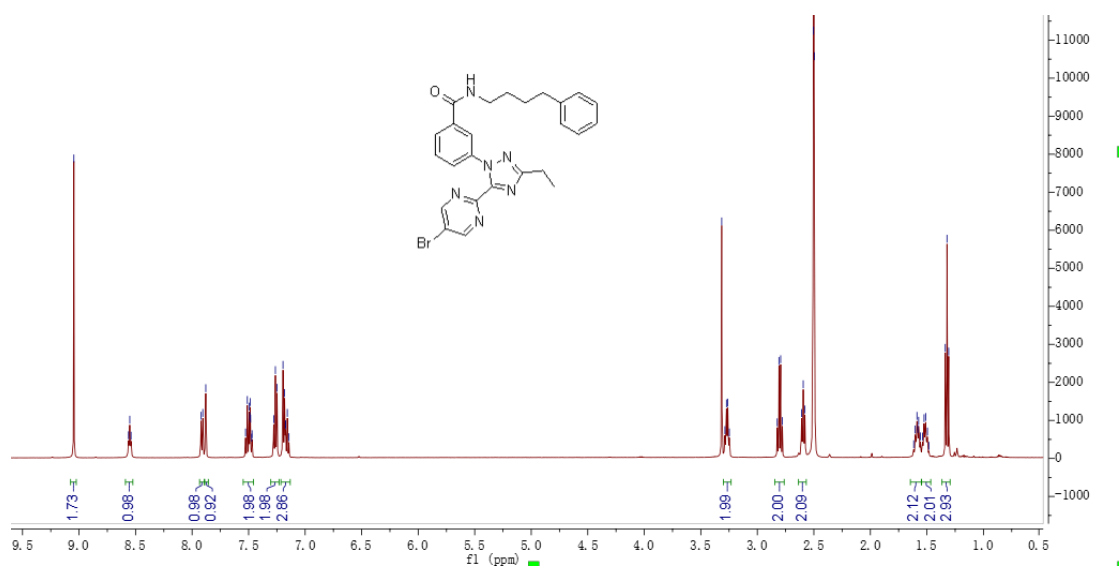
排序 : 信号
 乘积因子: 1.0000
 稀释因子: 1.0000
 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

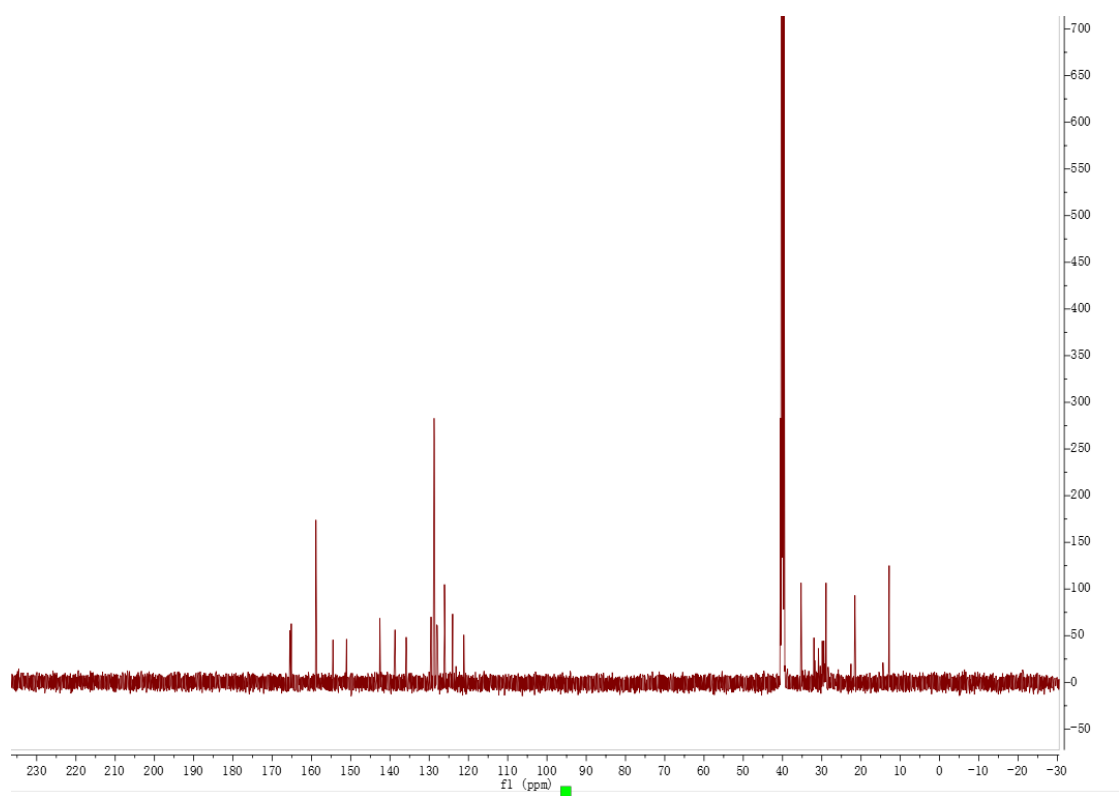
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU * s	峰高 [mAU]	峰面积 %
1	9.095	VV	0.0886	3.14392	5.26633e-1	0.0491
2	9.291	VV	0.0950	48.81165	7.78783	0.7627
3	9.549	VV	0.1000	6347.69727	966.05048	99.1882

总量 : 6399.65284 974.36494

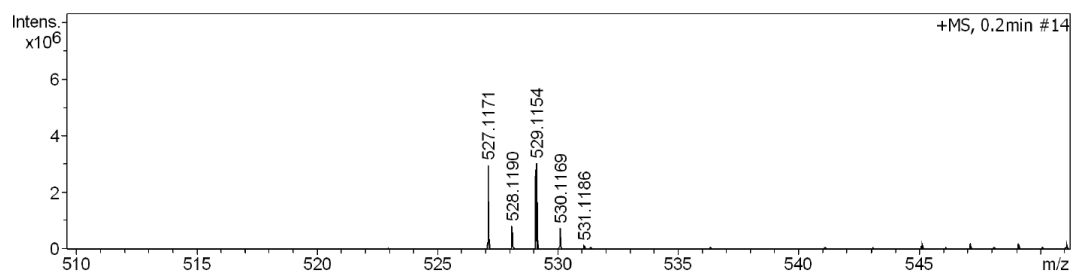
¹H-NMR spectrum of E4.



¹³C NMR spectrum of E4.



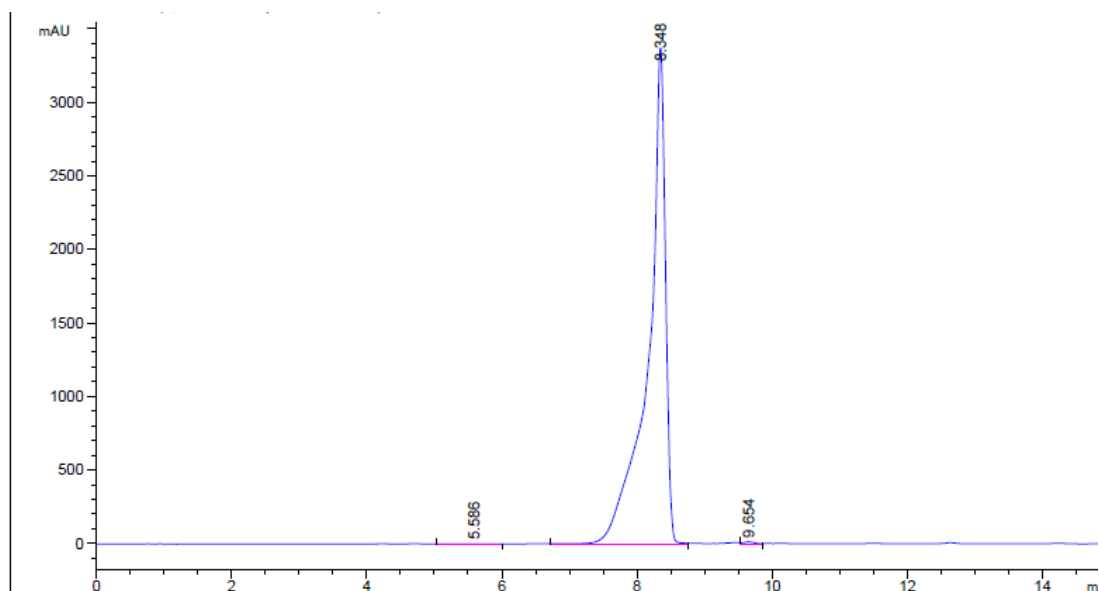
HR MS spectrum of E4.



#	m/z	Res.	S/N	I	I %	FWHM
1	527.1171	25093	2325.1	2961972	98.1	0.0210
2	528.1190	28211	624.6	794864	26.3	0.0187
3	529.1154	25349	2375.2	3019724	100.0	0.0209
4	530.1169	26900	576.3	732164	24.2	0.0197
5	531.1186	19723	86.6	109928	3.6	0.0269

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻	Conf	N-Rule
527.1171	1	C25H25BrN6NaO	527.1165	-1.0	21.6	2	100.00	15.5	even	ok

HPLC spectrum of E4.



面积百分比报告

排序 : 信号
 乘积因子: 1.0000
 稀释因子: 1.0000
 内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	5.586	VV	0.4870	68.20441	1.76011	0.1134
2	8.348	VV	0.2390	5.98826e4	3375.22192	99.5577
3	9.654	VV	0.1663	197.85706	16.65076	0.3289

总量 : 6.01487e4 3393.63280

- Adinarayana Nandikoll SS, Karan Kumar Banoth *et al.* Design, synthesis and evaluation of novel phenanthridine triazole analogs as potential antileishmanial agents. *Future Med. Chem.* 14(12), 867-880 (2022)