Design, Synthesis, and Activity Evaluation of Arctigenin Derivatives with HDAC Inhibition Activity

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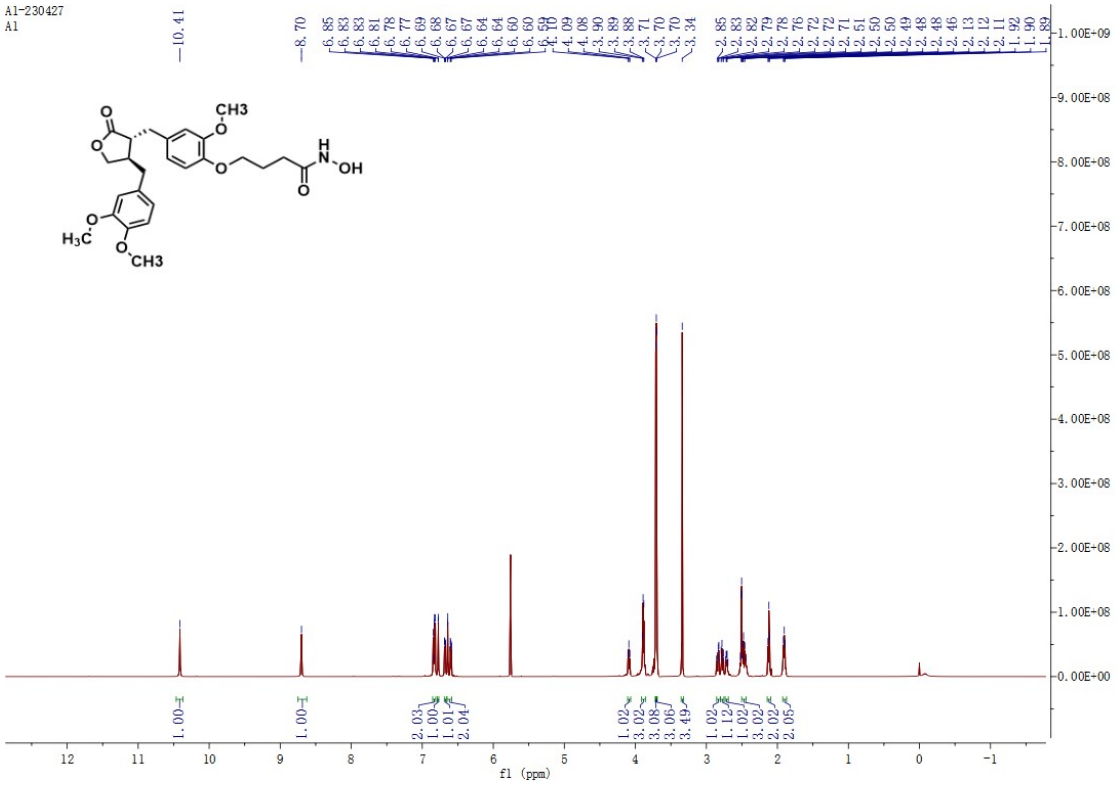
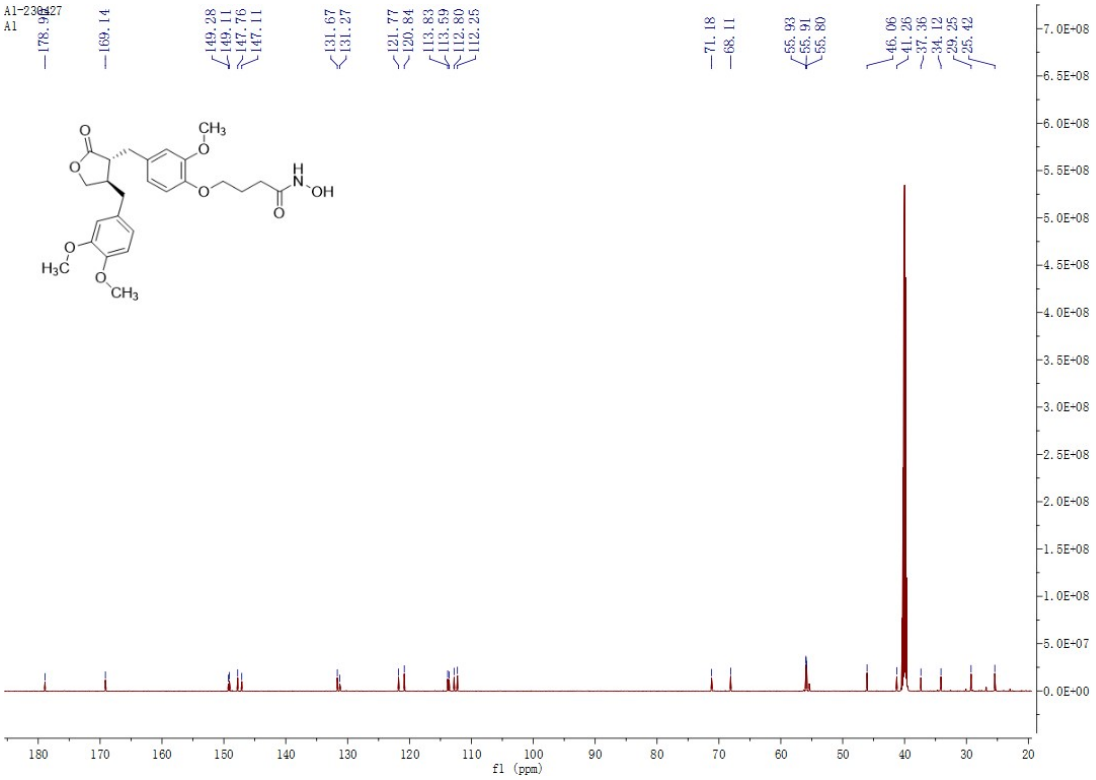
1. The ^{1}H and ^{13}C spectra of the compounds (A1 - A10，B1 - B8)

Figure S1. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A1





Mass Spectrum SmartFormula Report

Analysis Info

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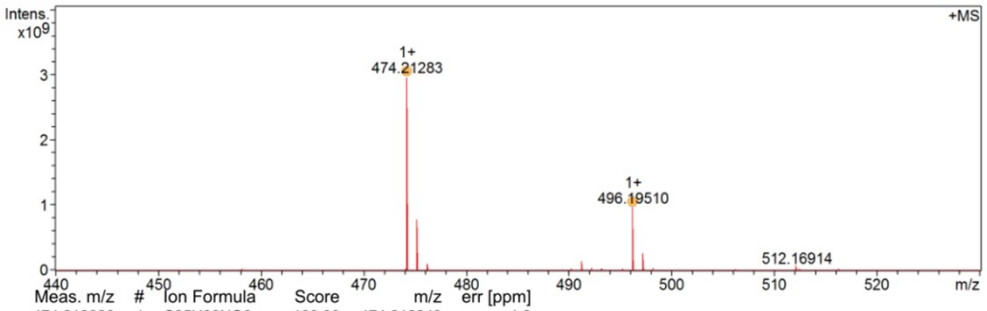
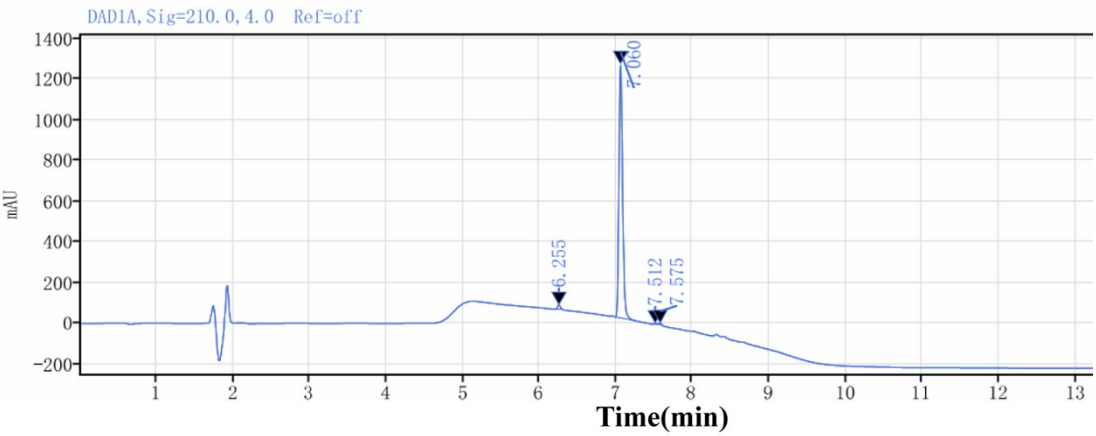
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

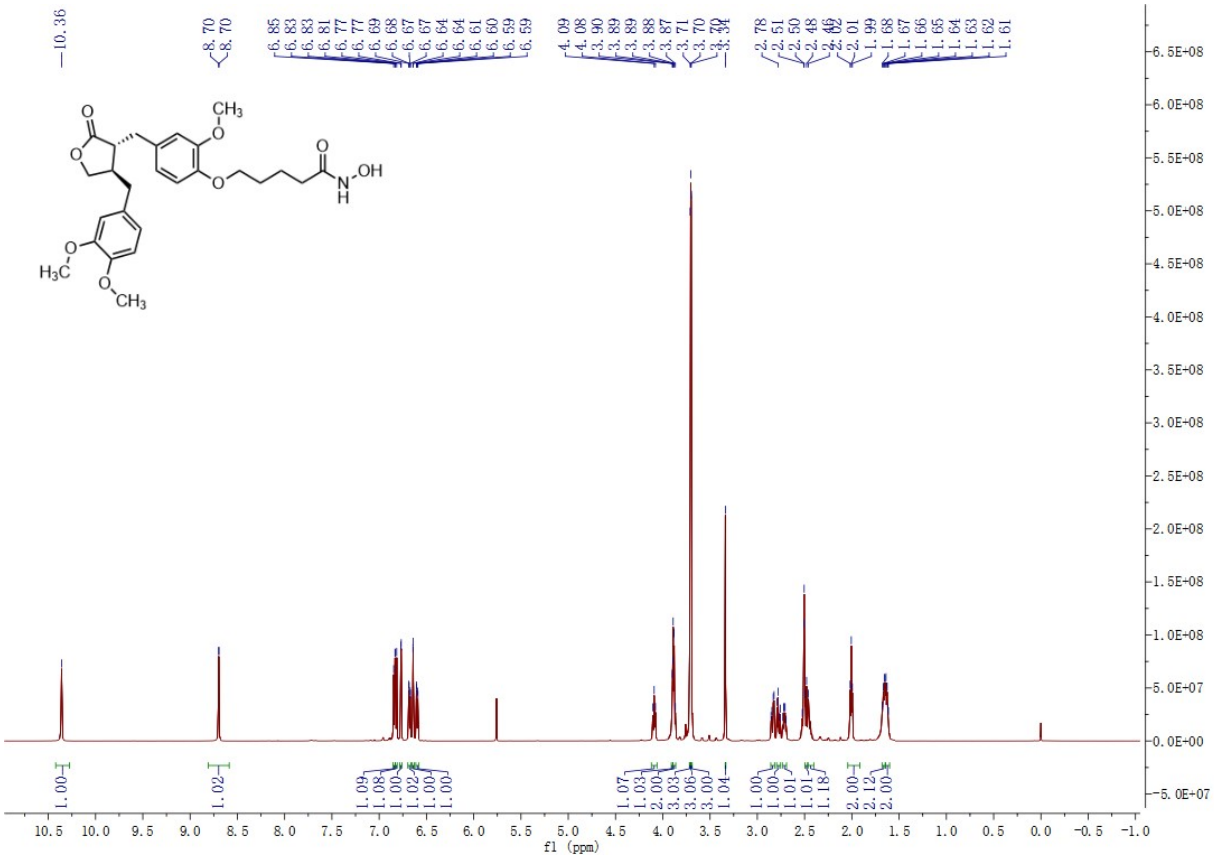


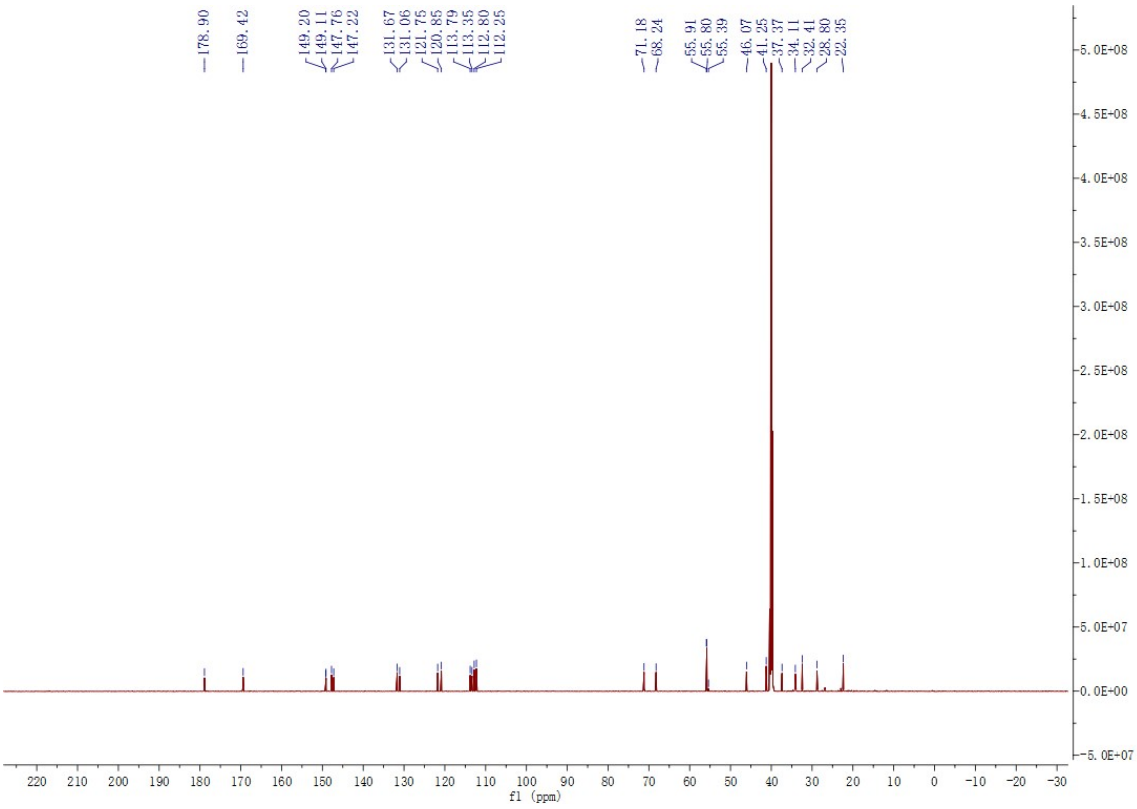
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
474.212826	1	C25H32NO8	100.00	474.212243	-1.2
496.195098	1	C25H31NNaO8	100.00	496.194188	-1.8



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.255	MM m	0.09	54.86	20.92	1.27
7.060	MM m	0.26	4236.57	1250.03	98.24
7.512	MM m	0.06	5.35	2.87	0.12
7.575	MM m	0.07	15.85	7.18	0.37

Figure S2. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A2





Mass Spectrum SmartFormula Report

Analysis Info

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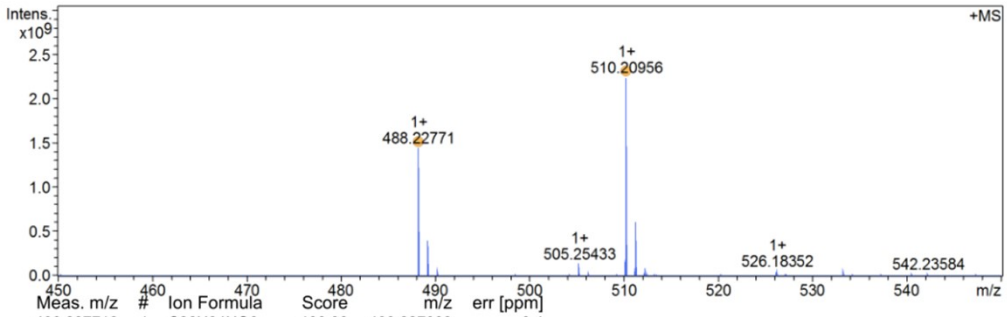
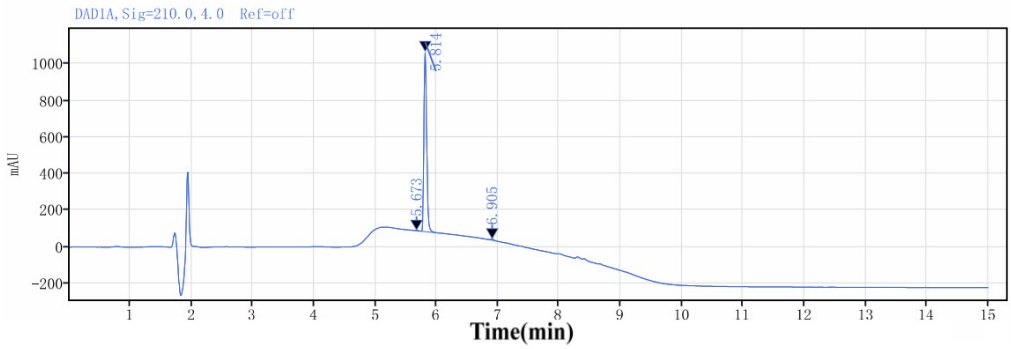
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

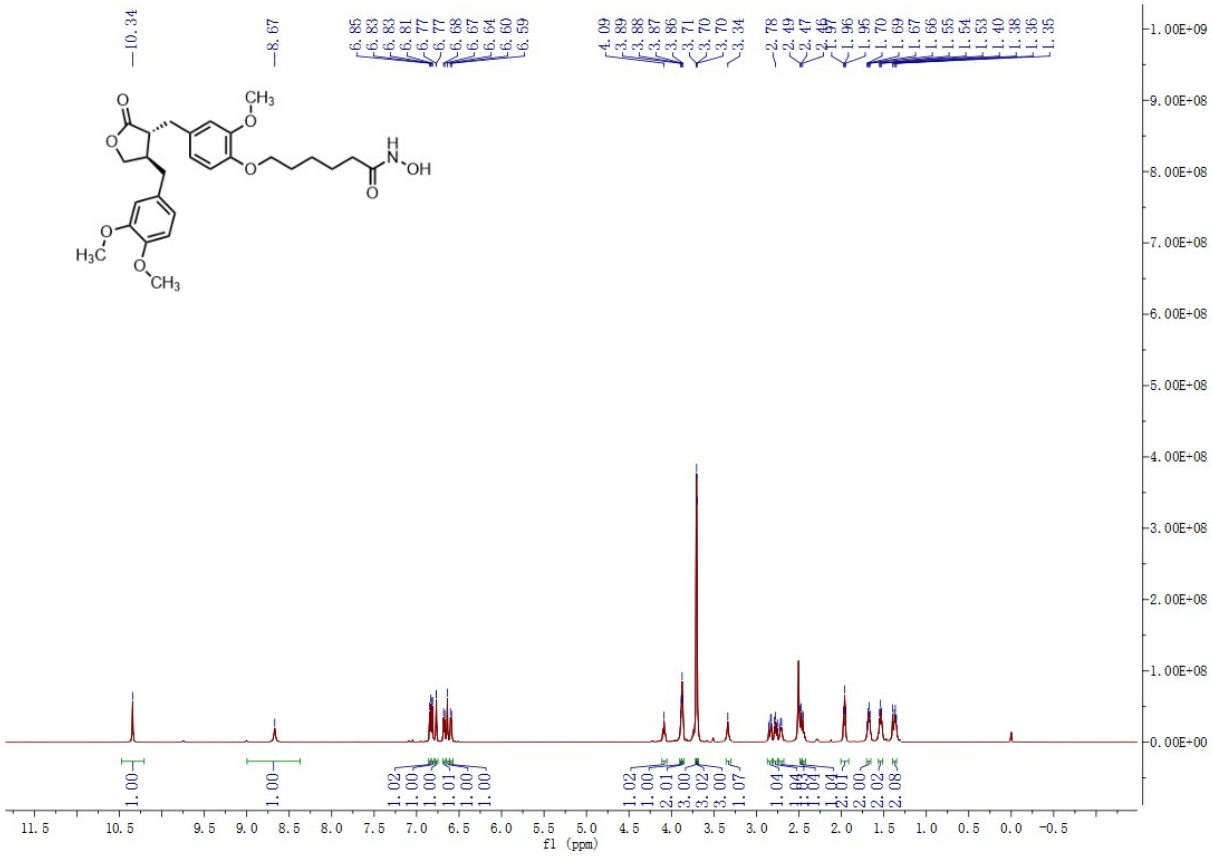


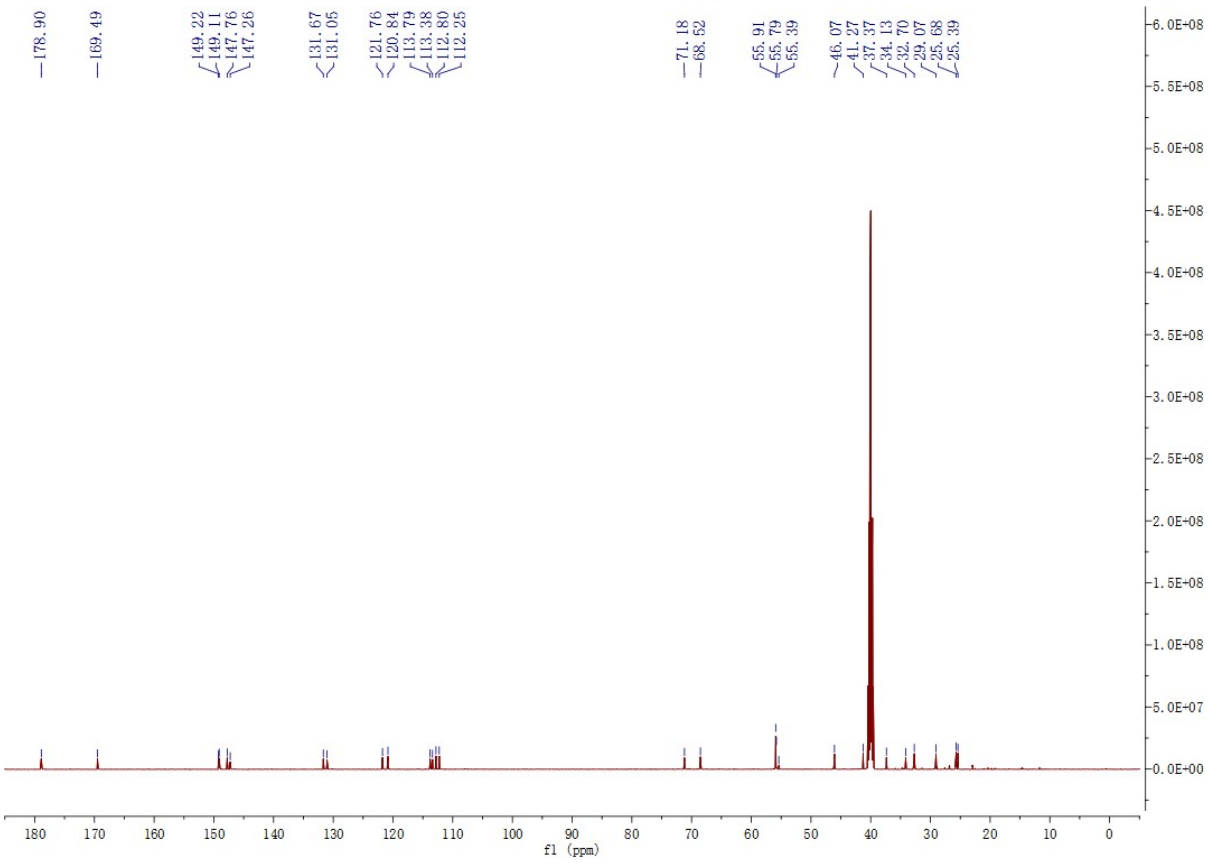
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
488.227712	1	C26H34NO8	100.00	488.227893	0.4
510.209564	1	C26H33NNaO8	100.00	510.209838	0.5



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
5.673	MM m	0.06	3.70	1.49	0.12
5.814	MM m	0.27	3110.79	985.38	99.27
6.905	MM m	0.10	19.08	6.76	0.61

Figure S3. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A3





Mass Spectrum SmartFormula Report

Analysis Info

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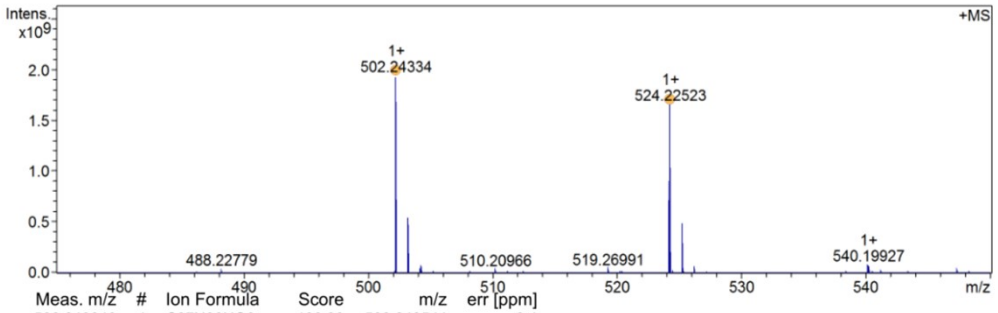
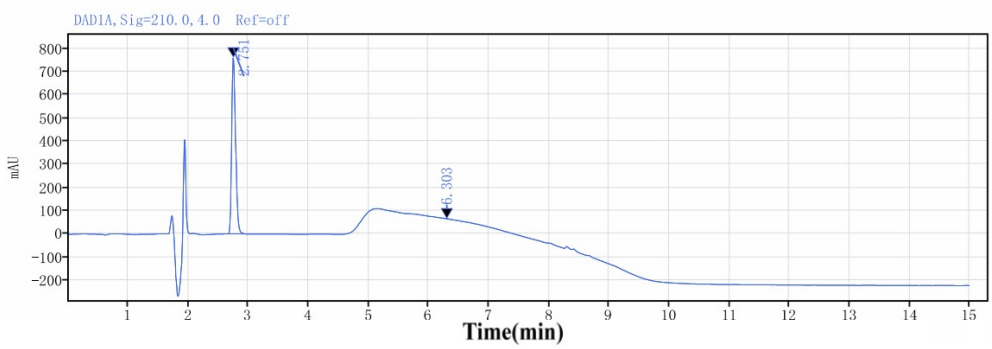
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

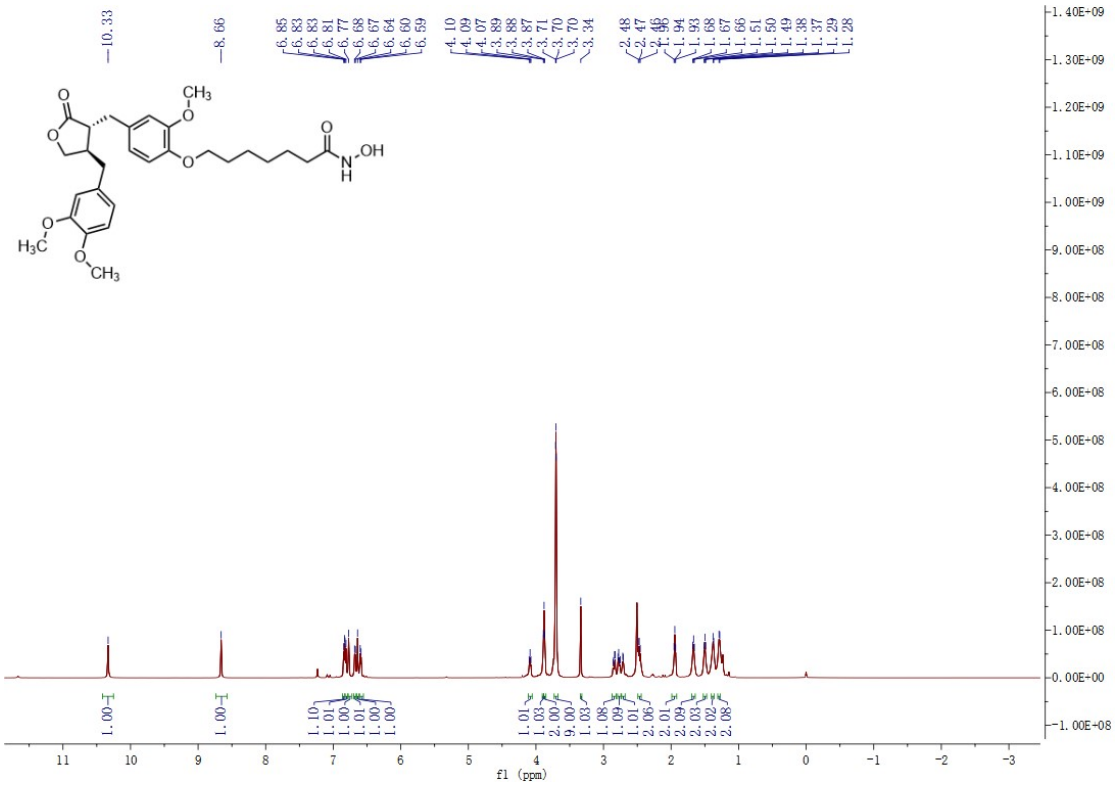


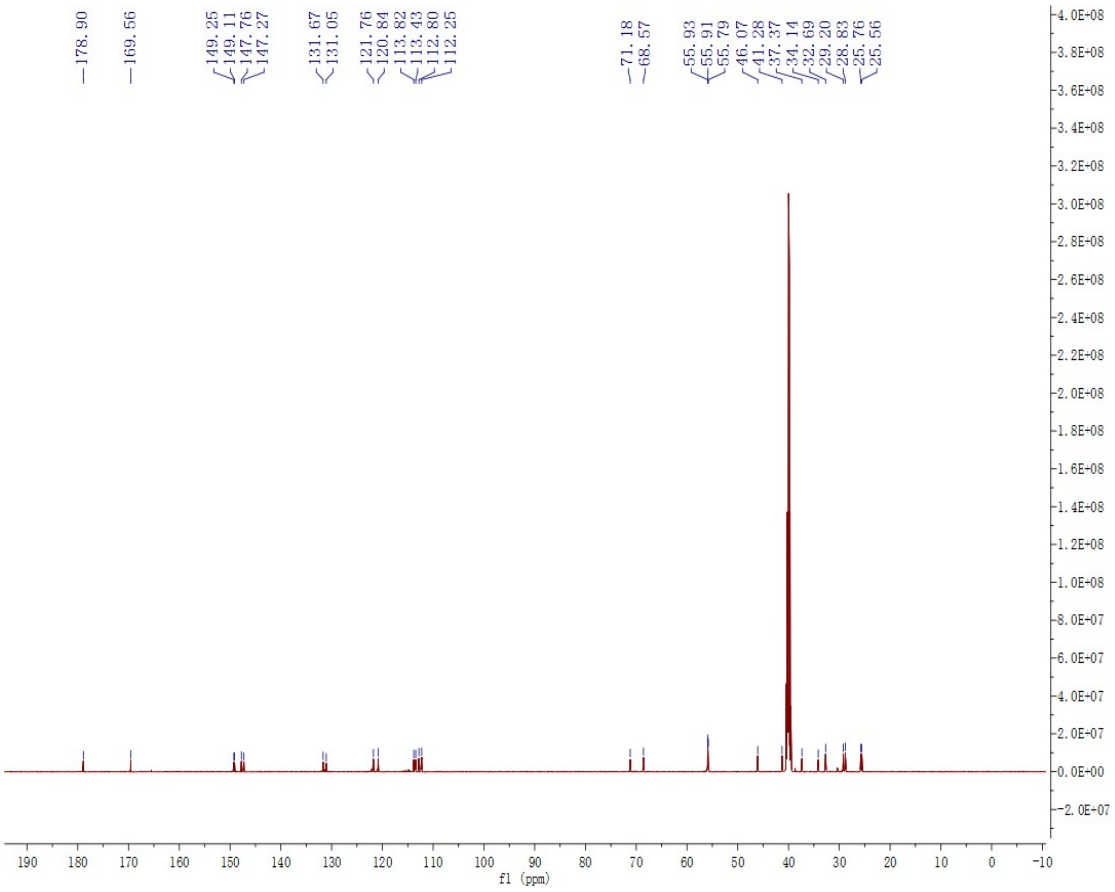
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
502.243340	1	C27H36NO8	100.00	502.243544	0.4
524.225229	1	C27H35NNaO8	100.00	524.225488	0.5



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
2.751	MM m	0.29	3464.83	760.99	99.87
6.303	MM m	0.13	4.49	0.98	0.13

Figure S4. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A4





Mass Spectrum SmartFormula Report

Analysis Info

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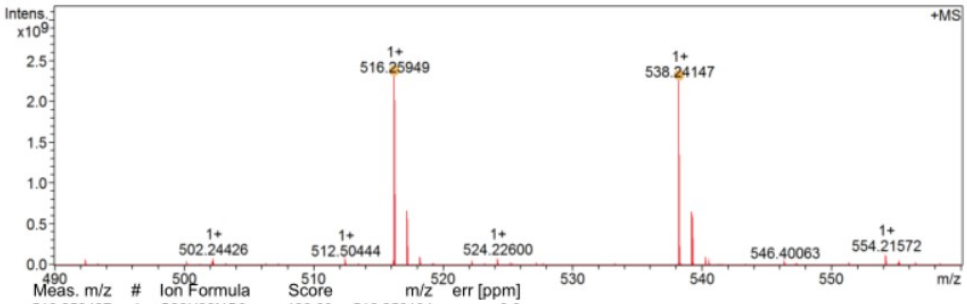
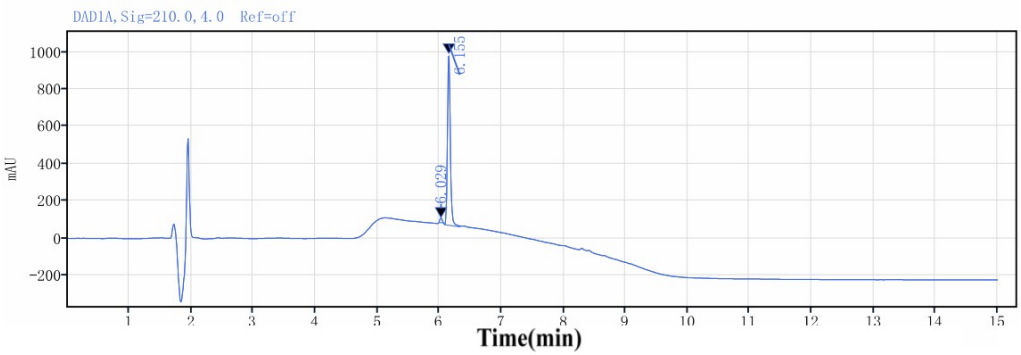
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

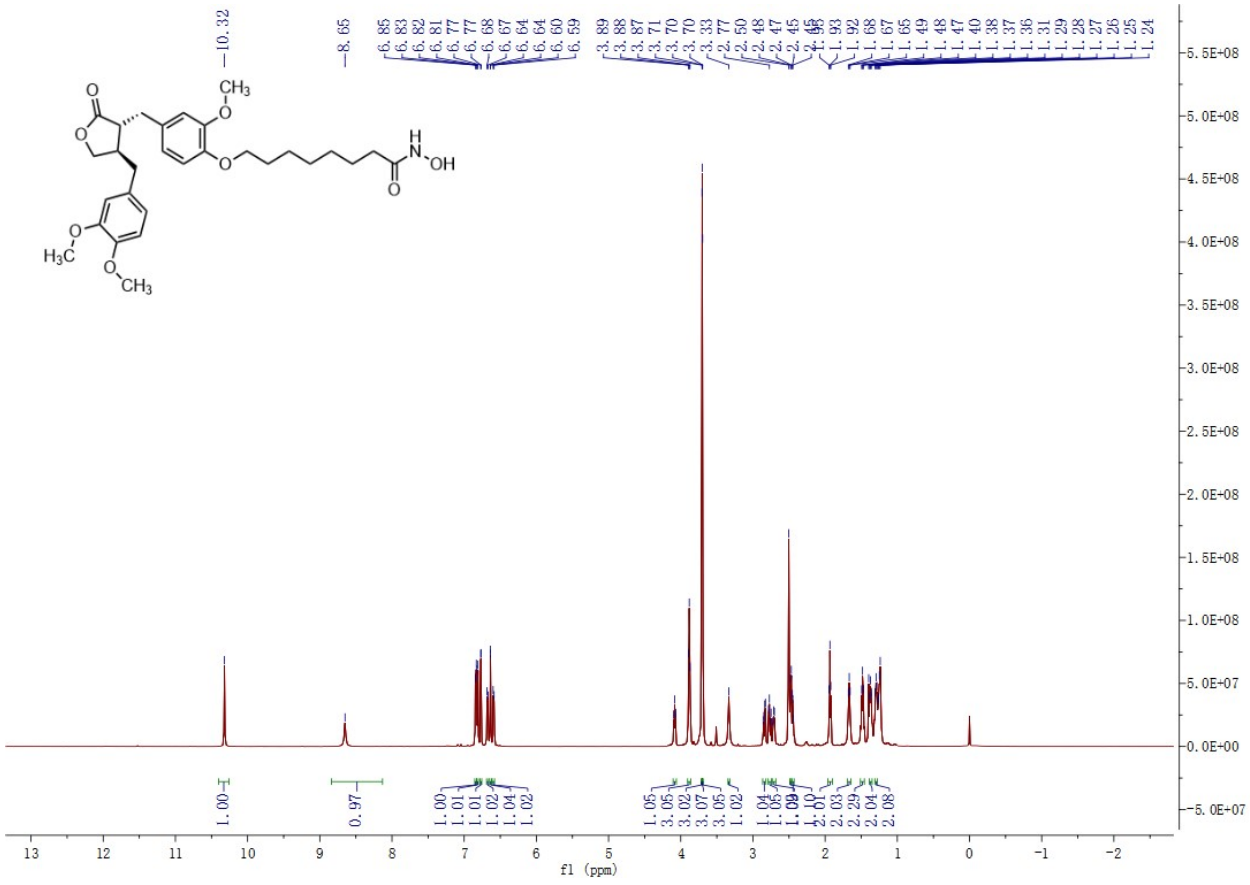


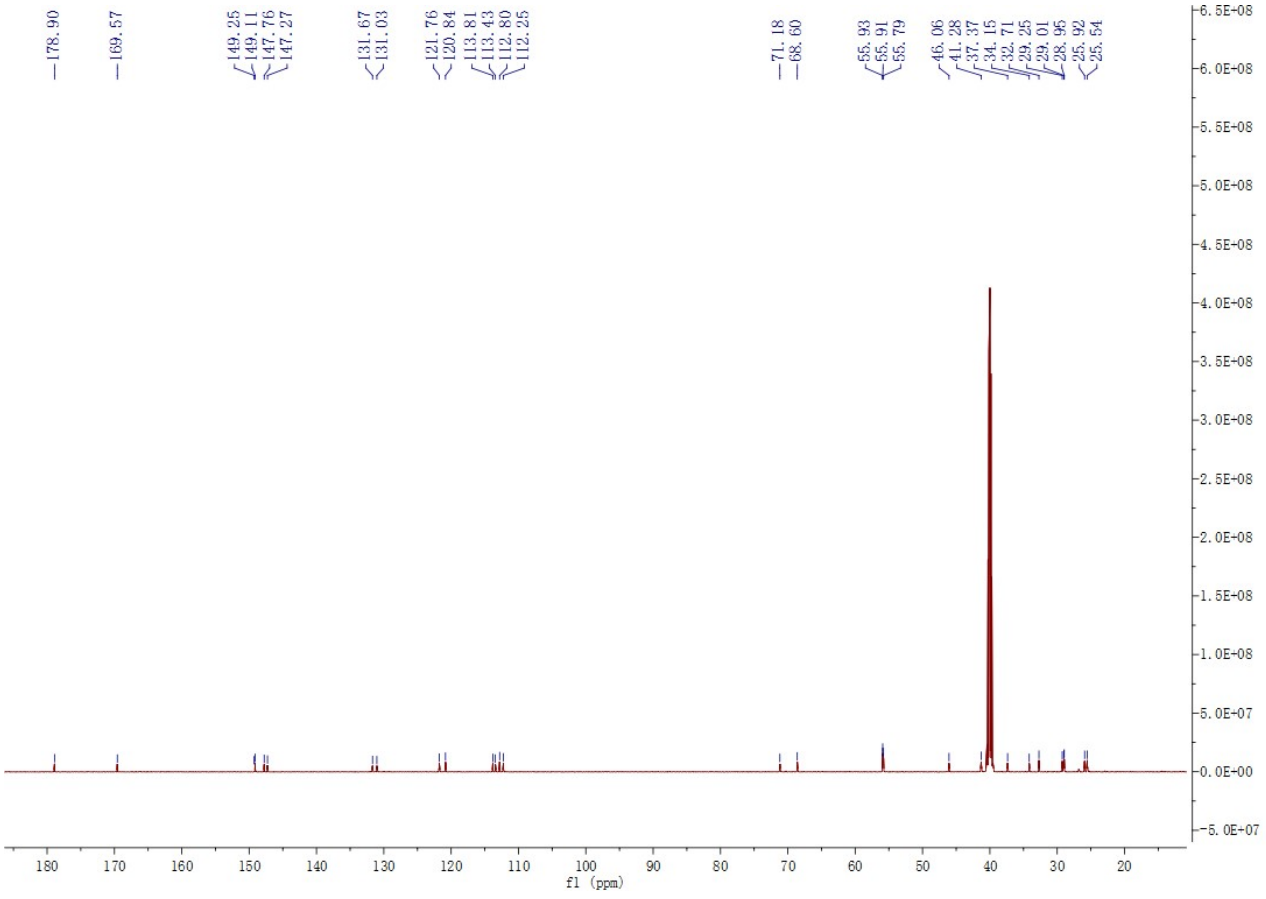
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
516.259487	1	C28H38NO8	100.00	516.259194	-0.6
538.241465	1	C28H37NNaO8	100.00	538.241138	-0.6



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.029	MM m	0.07	60.83	25.44	1.99
6.155	MM m	0.25	2993.56	917.62	98.01

Figure S5. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A5





Mass Spectrum SmartFormula Report

Analysis Info

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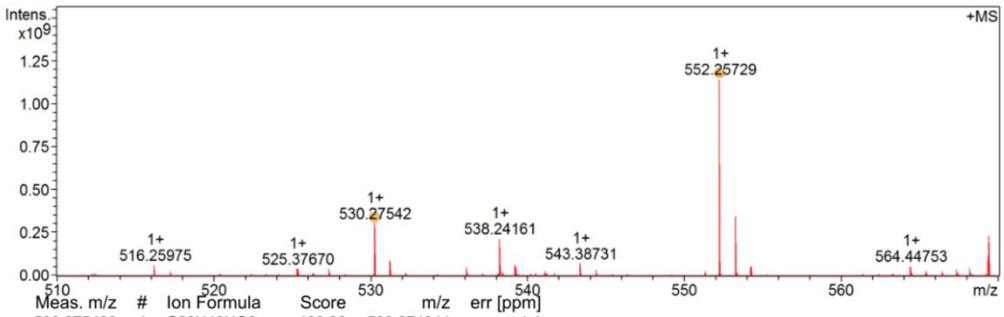
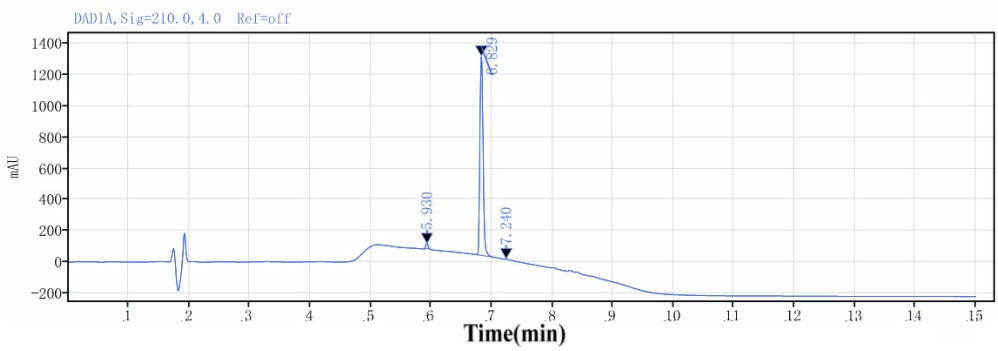
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

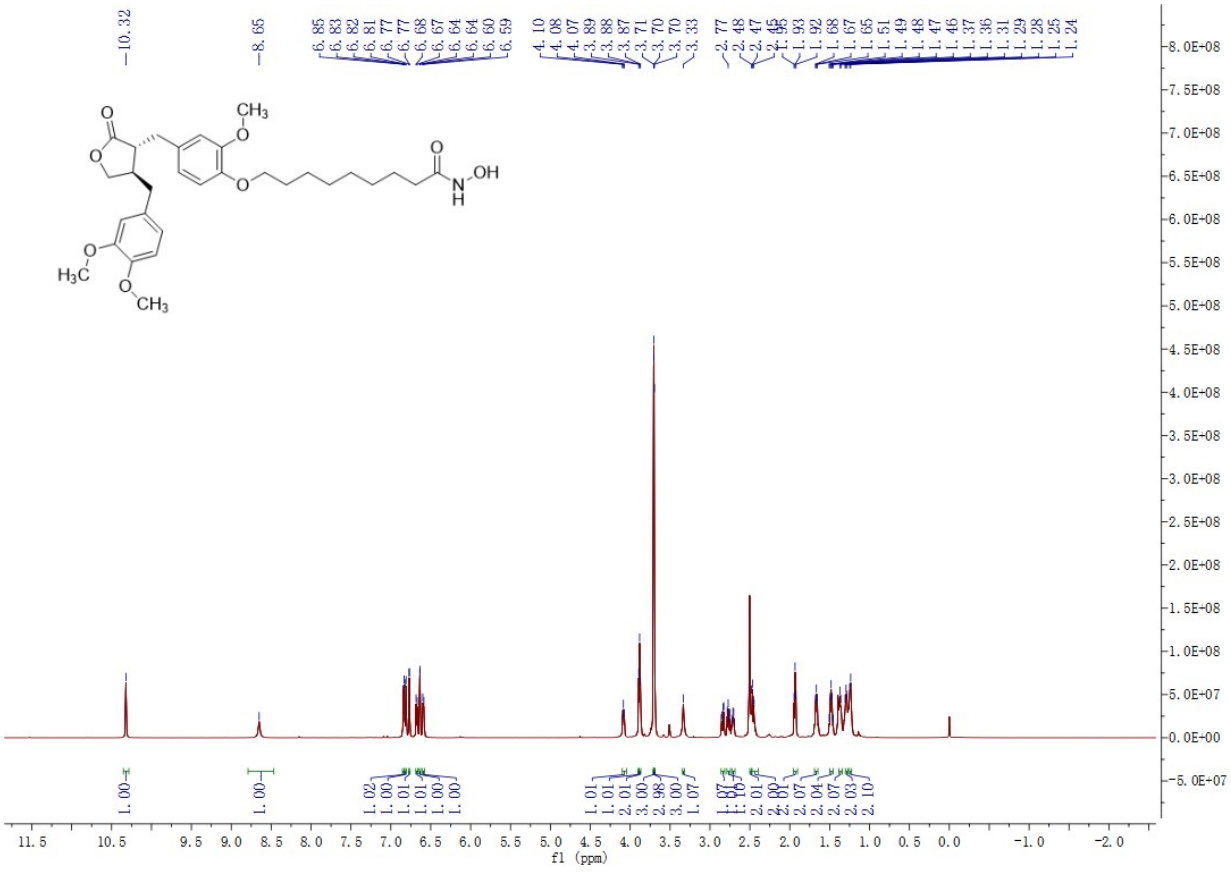


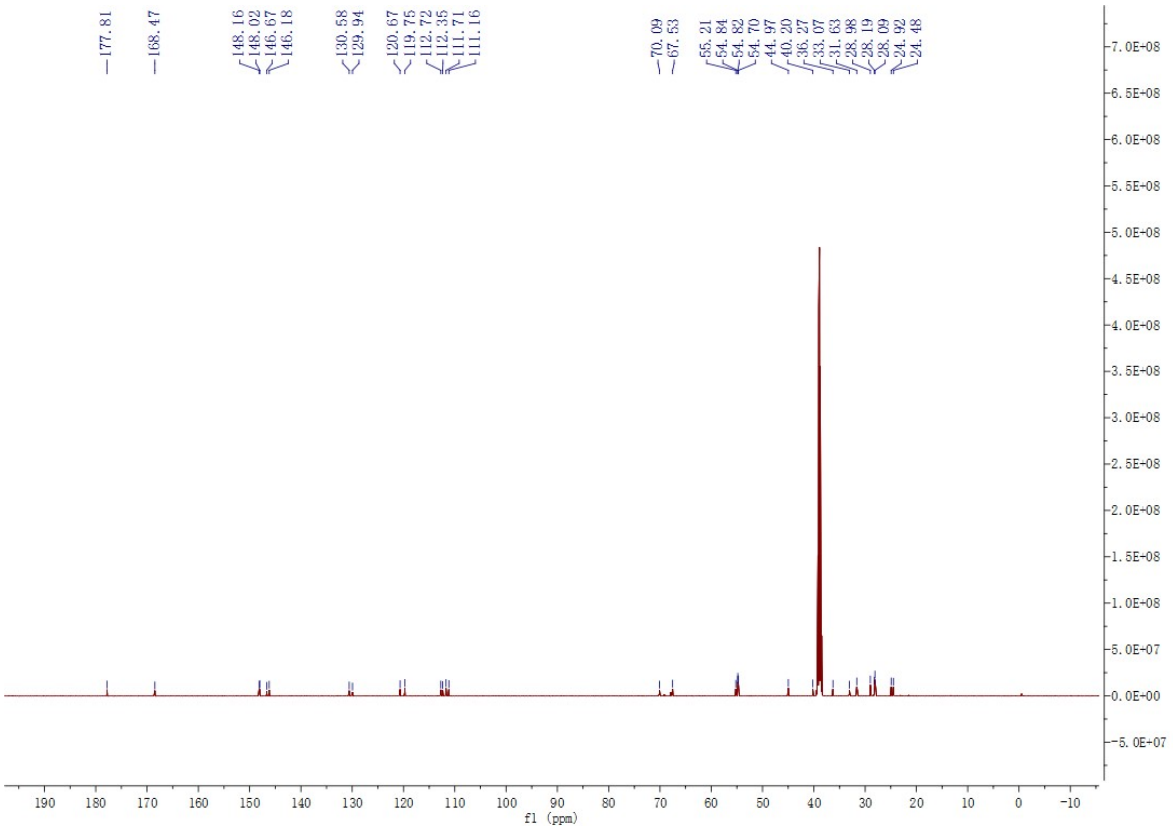
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
530.275420	1	C29H40NO8	100.00	530.274844	-1.1
552.257289	1	C29H39NNaO8	100.00	552.256788	-0.9



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
5.930	MM m	0.08	87.32	33.39	1.86
6.829	MM m	0.26	4608.87	1278.94	98.04
7.240	MM m	0.05	4.67	2.70	0.10

Figure S6. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A6





Mass Spectrum SmartFormula Report

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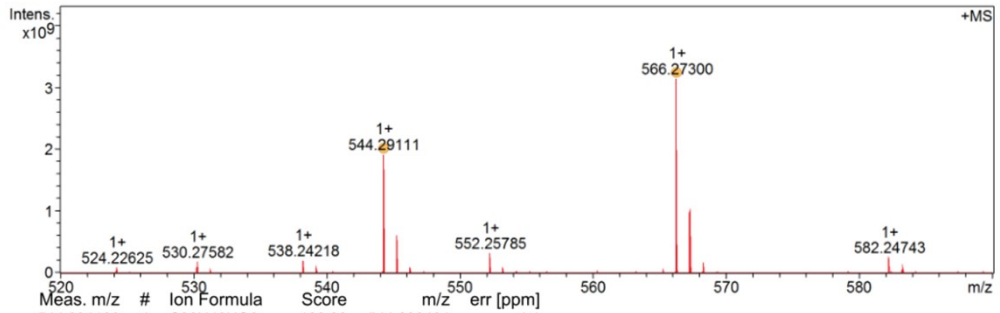
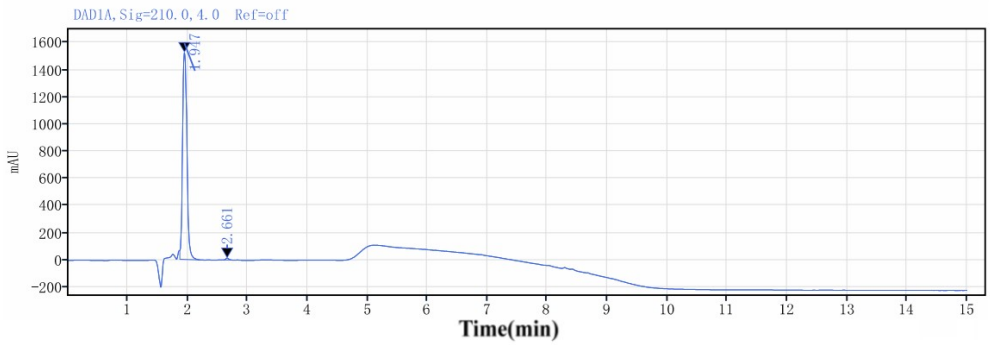
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

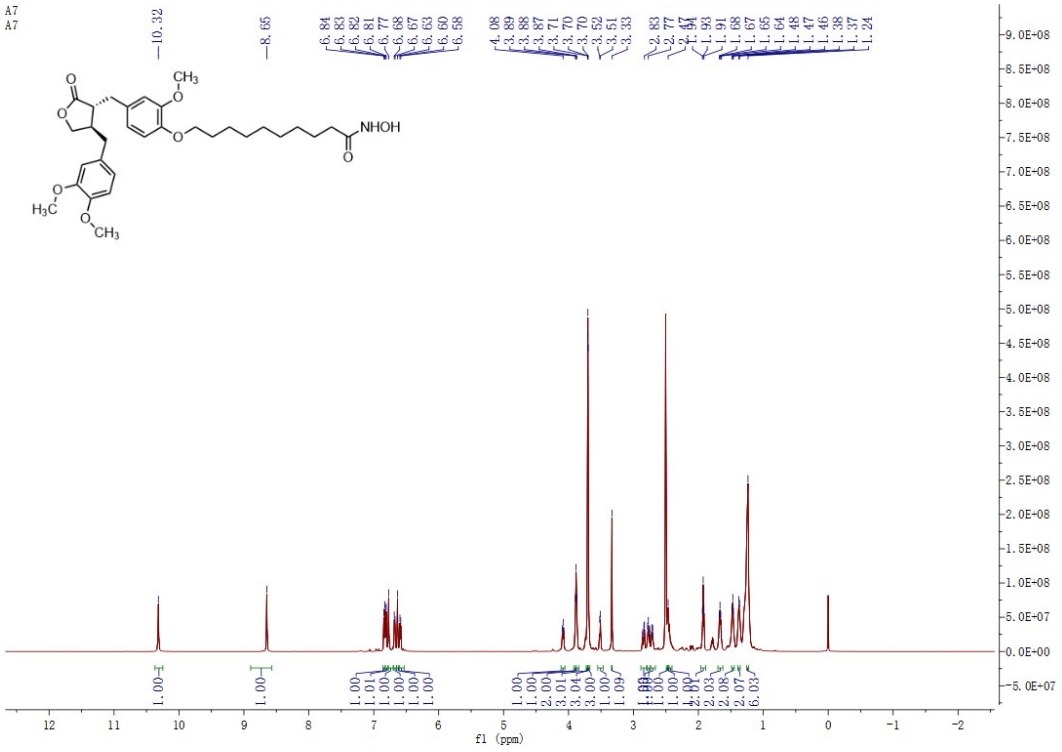


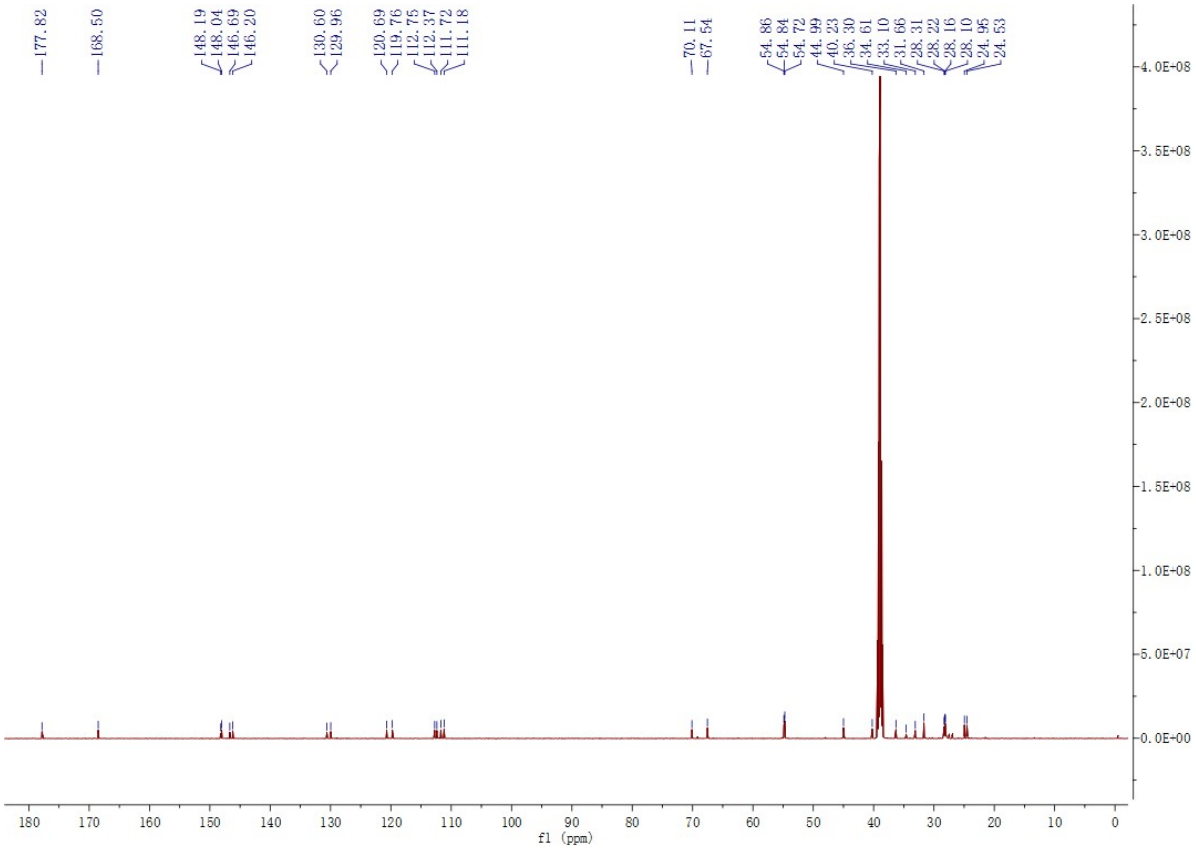
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
544.291108	1	C30H42NO8	100.00	544.290494	-1.1
566.272999	1	C30H41NNaO8	100.00	566.272438	-1.0



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
1.947	MM m	0.34	7795.63	1523.80	99.45
2.661	MM m	0.11	43.48	12.86	0.55

Figure S7. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A7





Mass Spectrum SmartFormula Report

Analysis Info

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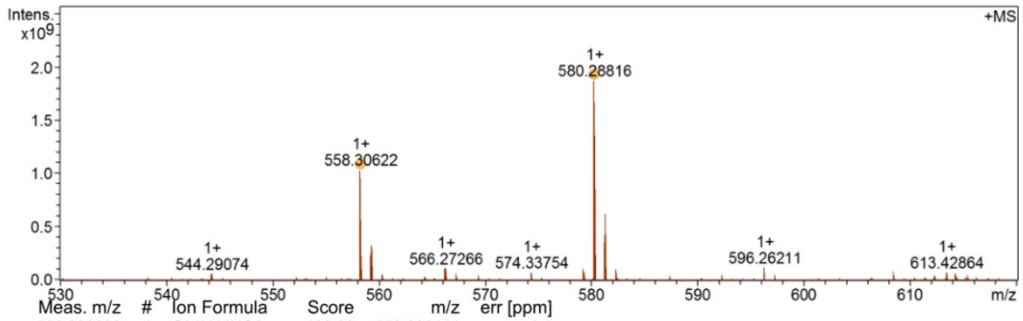
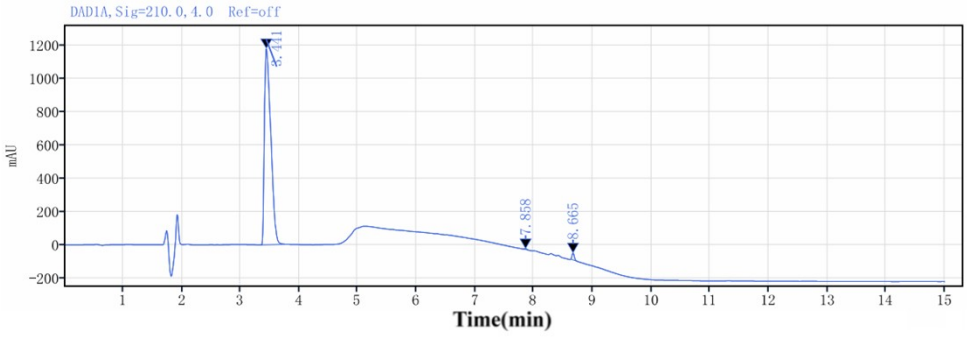
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

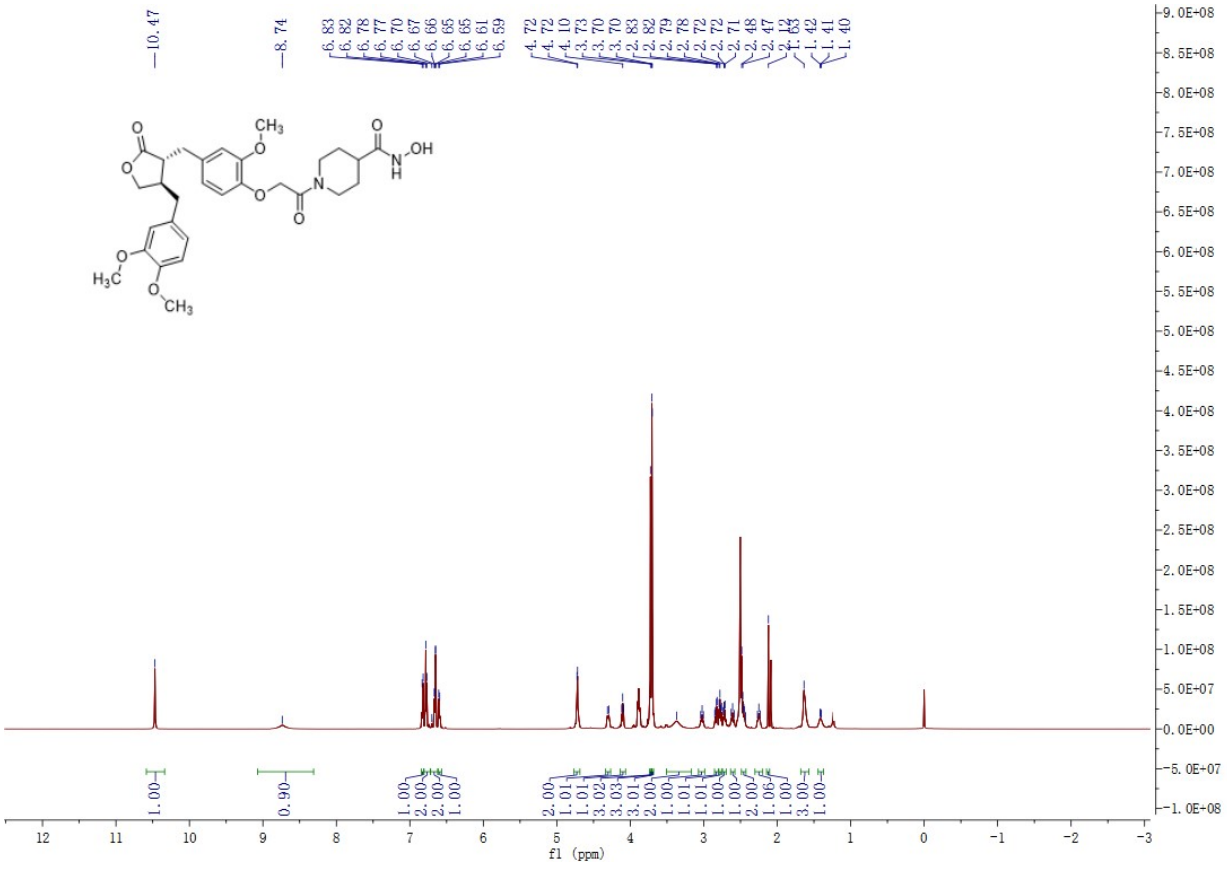


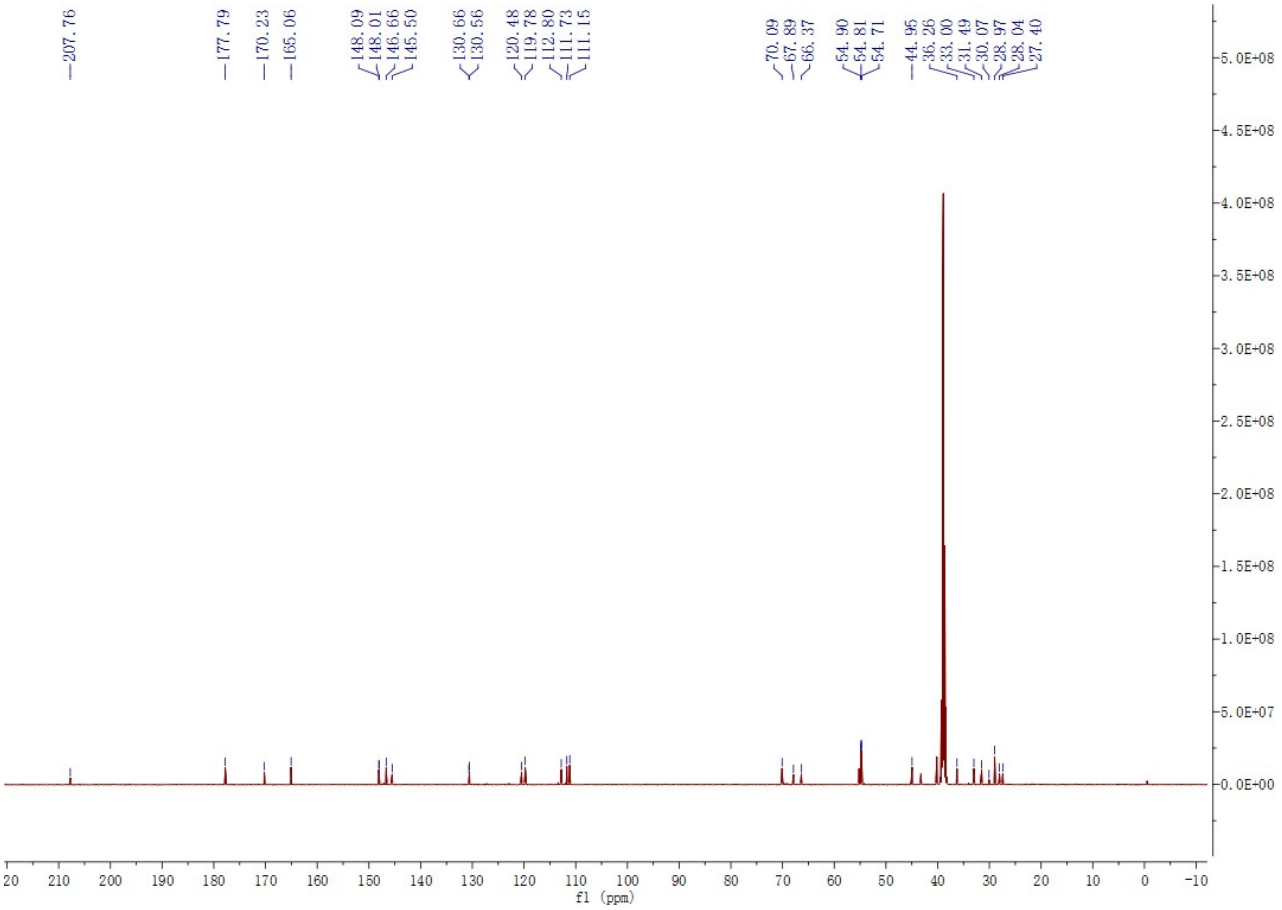
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
558.306223	1	C31H44NO8	100.00	558.306144	-0.1
580.288157	1	C31H43NNaO8	100.00	580.288088	-0.1



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
3.441	MM m	0.49	8923.24	1181.04	98.53
7.858	MM m	0.10	14.02	4.89	0.15
8.665	MM m	0.11	118.76	41.80	1.31

Figure S8. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A8





Mass Spectrum SmartFormula Report

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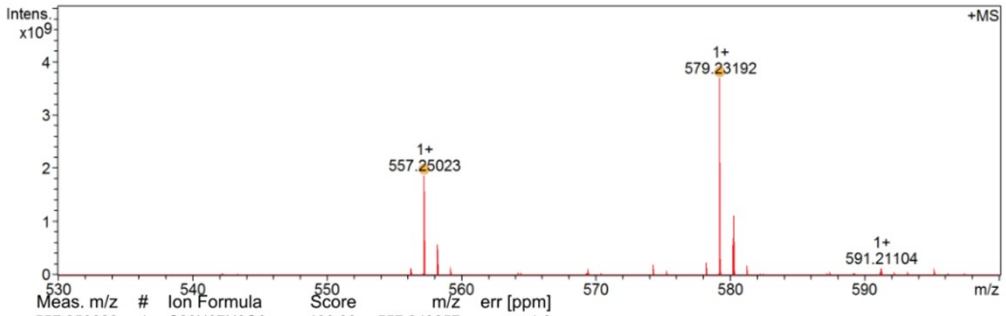
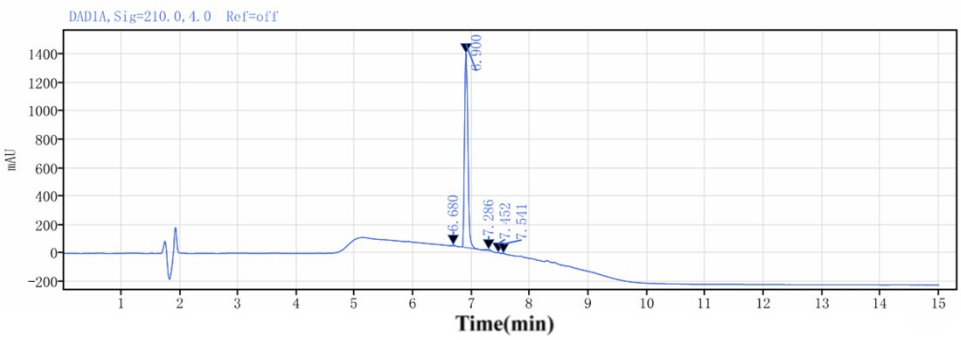
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

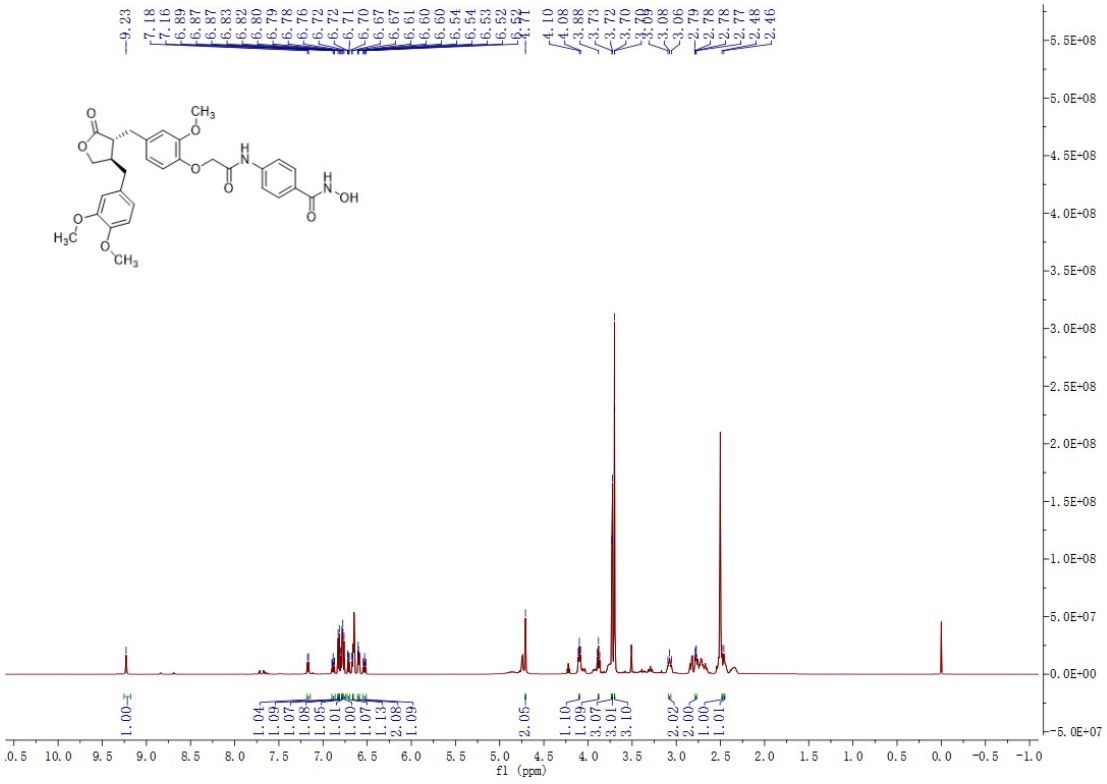


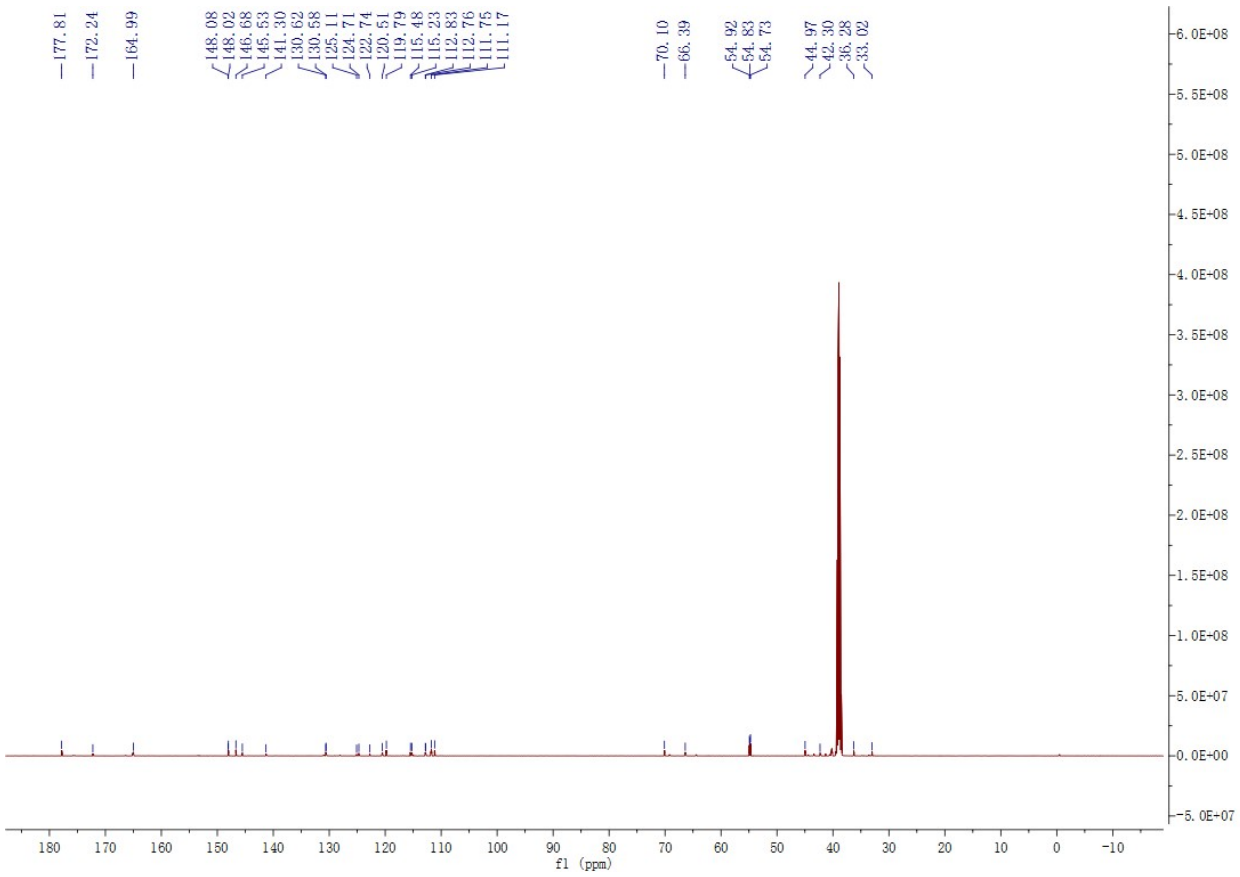
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
557.250228	1	C29H37N2O9	100.00	557.249357	-1.6
579.231925	1	C29H36N2NaO9	100.00	579.231301	-1.1



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.680	MM m	0.08	18.46	7.08	0.33
6.900	MM m	0.28	5435.31	1367.21	98.39
7.286	MM m	0.18	55.07	9.71	1.00
7.452	MM m	0.09	5.90	1.96	0.11
7.541	MM m	0.06	9.31	3.95	0.17

Figure S9. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A9





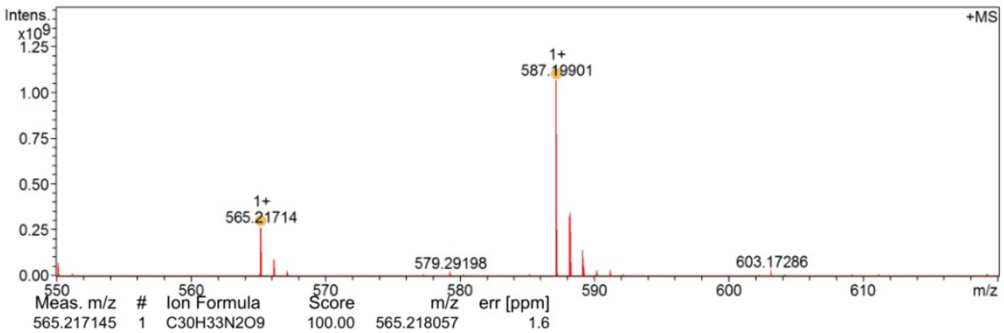
Mass Spectrum SmartFormula Report

Analysis Info

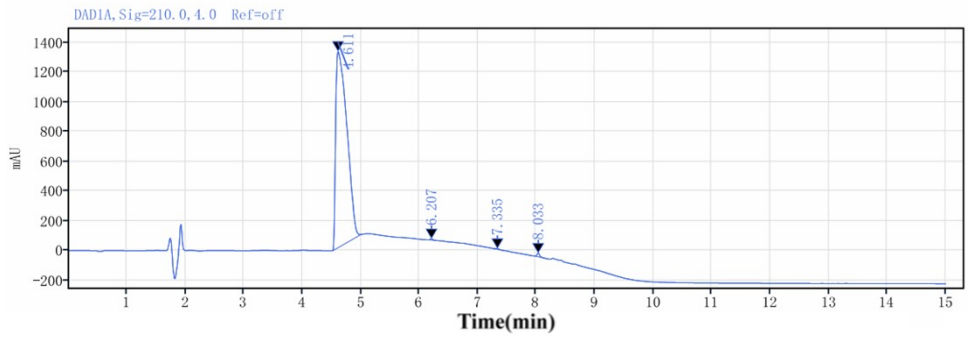
Analysis Name	D:\data\Sample Detection\20230524\BEN-NHOH pos_000004.d	Acquisition Date	5/24/2023 11:54:54 AM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

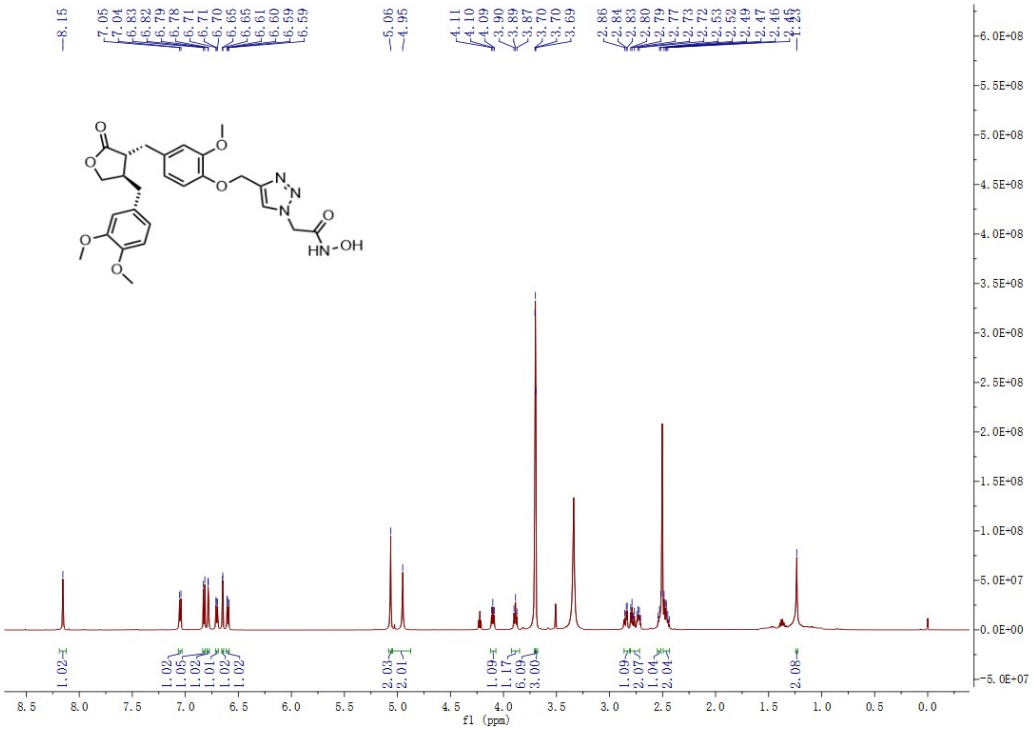


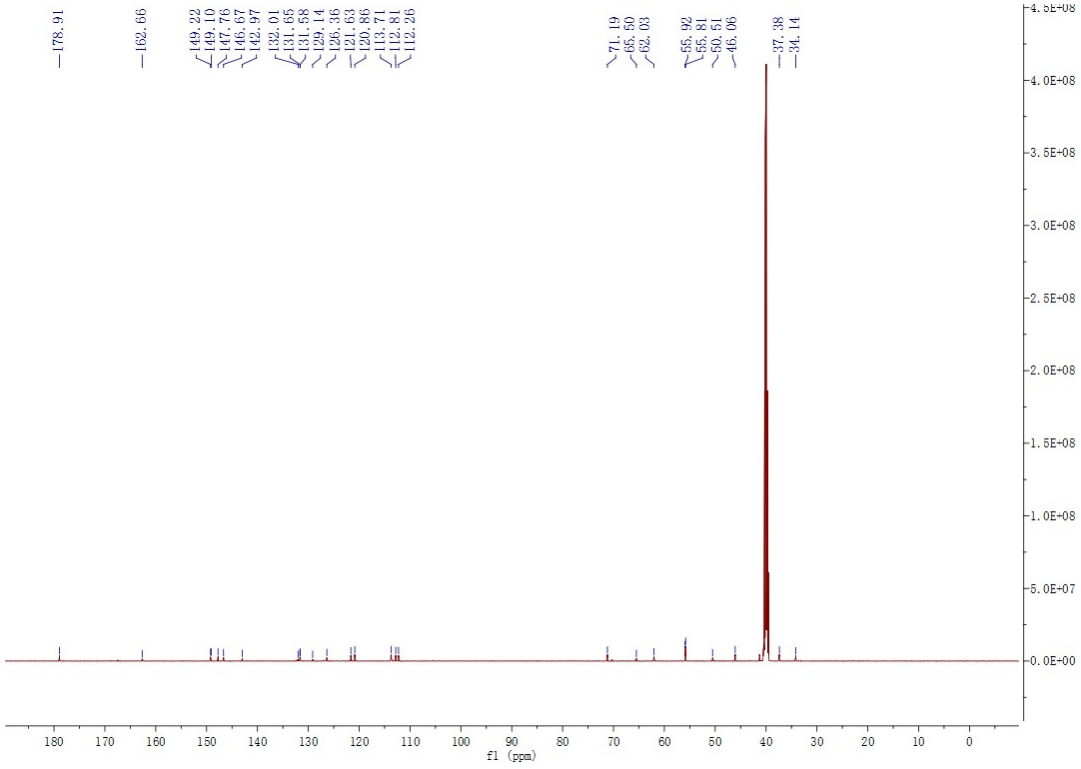
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
565.217145	1	C30H33N2O9	100.00	565.218057	1.6



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
4.611	MM m	0.49	17270.62	1316.90	99.32
6.207	MM m	0.12	24.90	8.68	0.14
7.335	MM m	0.17	14.00	4.68	0.08
8.033	MM m	0.20	79.61	24.50	0.46

Figure S10. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of A10





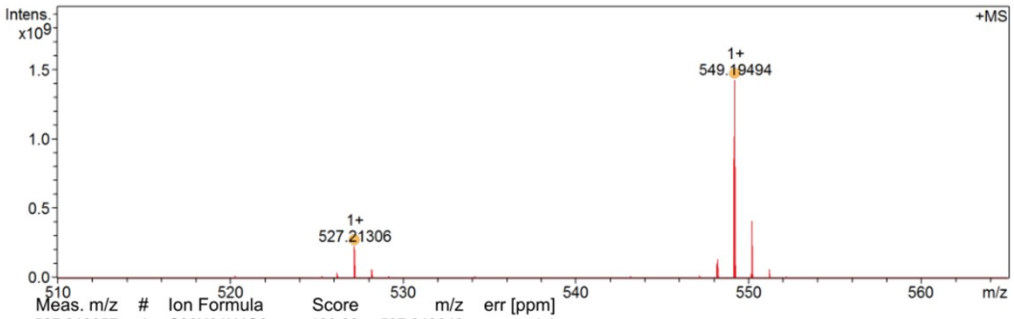
Mass Spectrum SmartFormula Report

Analysis Info

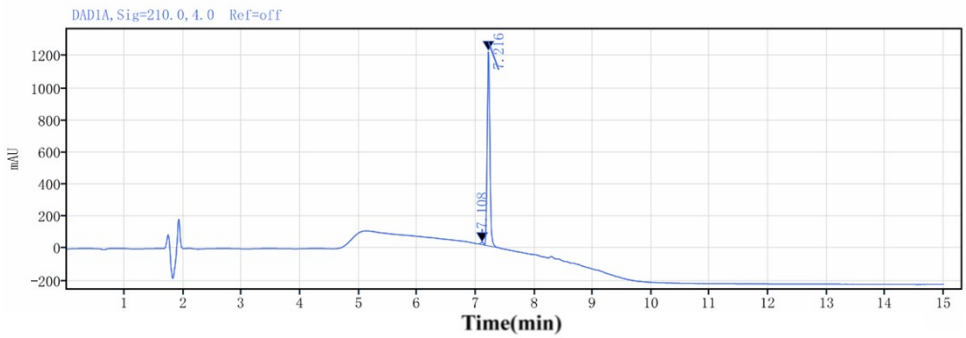
Analysis Name	D:\data\Sample Detection\20230524\TRI-NHOH pos_000004.d	Acquisition Date	5/24/2023 11:42:45 AM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

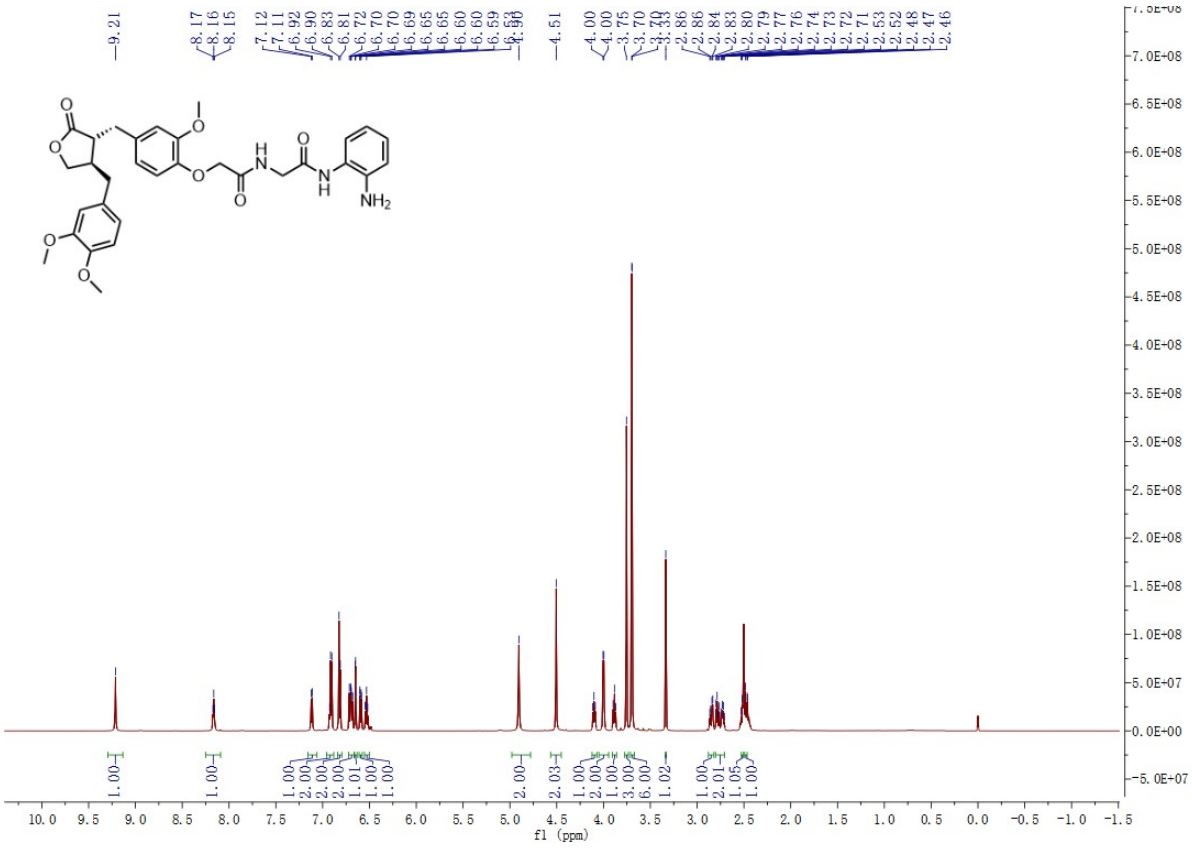


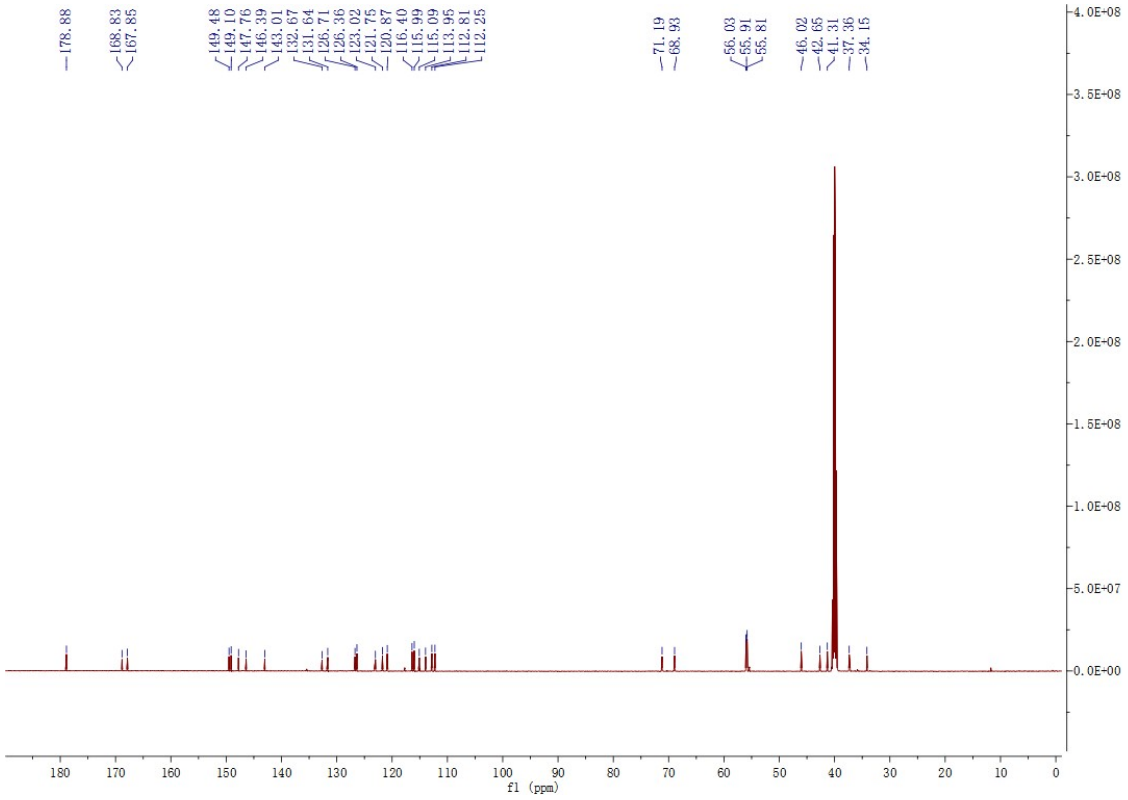
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
527.213057	1	C26H31N4O8	100.00	527.213640	1.1
549.194935	1	C26H30N4NaO8	100.00	549.195585	1.2



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
7.108	MM m	0.12	52.88	14.66	1.31
7.216	MM m	0.23	3968.63	1215.97	98.69

Figure S11. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B1





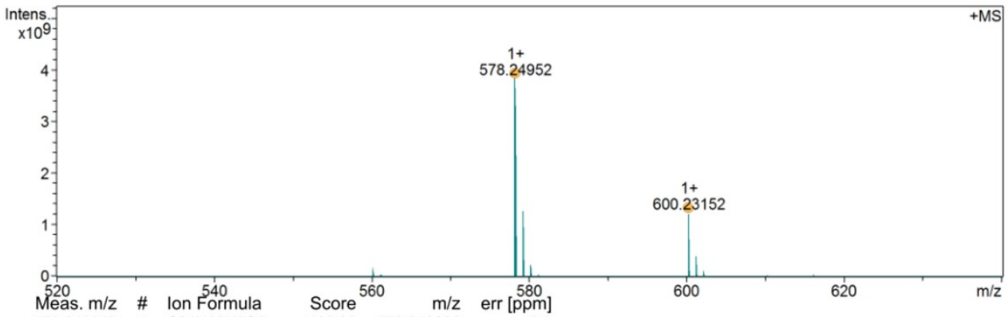
Mass Spectrum SmartFormula Report

Analysis Info

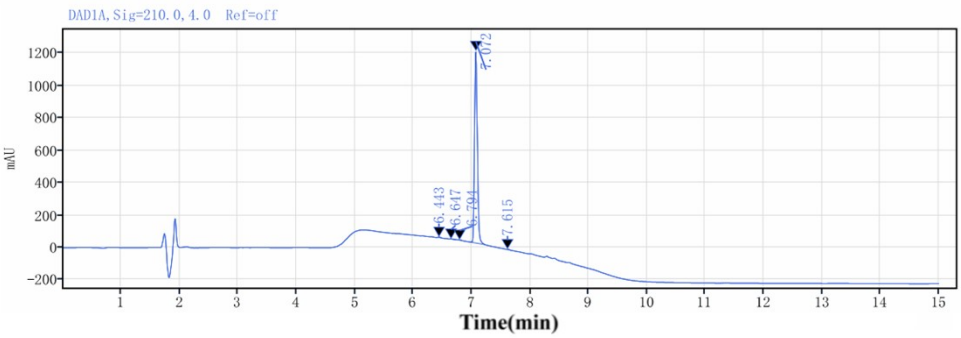
Analysis Name	D:\data\Sample Detection\20230511\1C-Ben pos_000008.d	Acquisition Date	5/11/2023 2:18:42 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

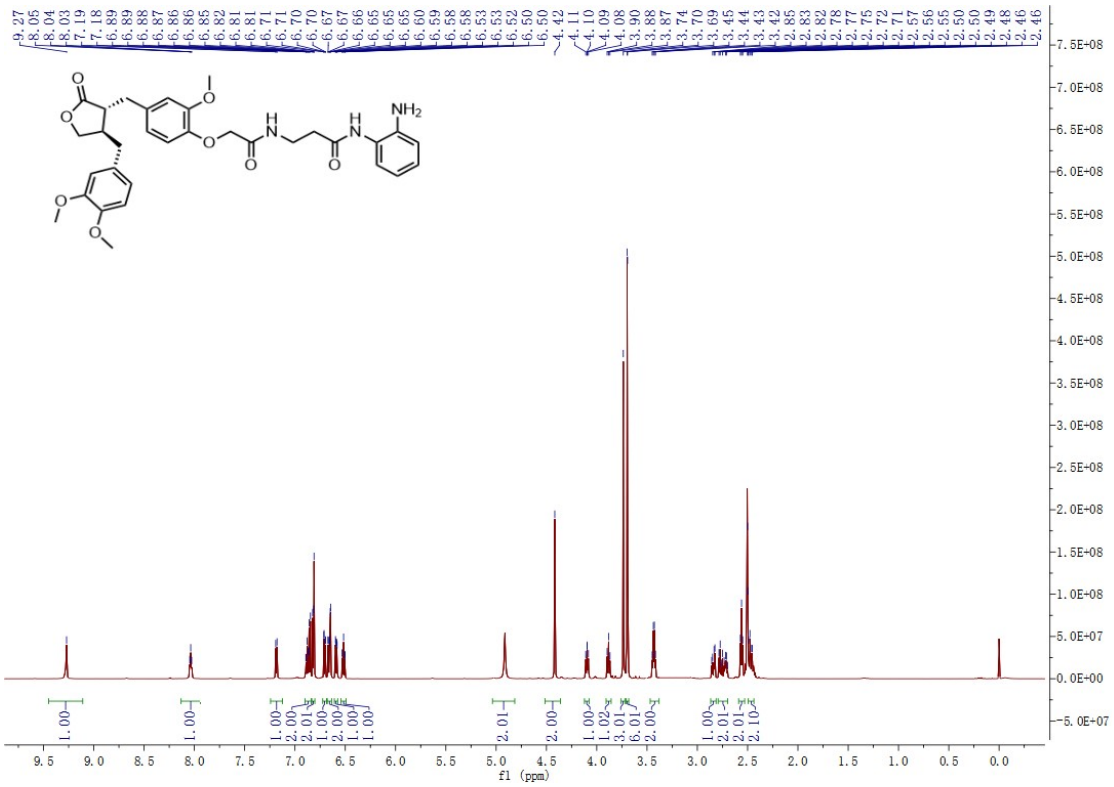


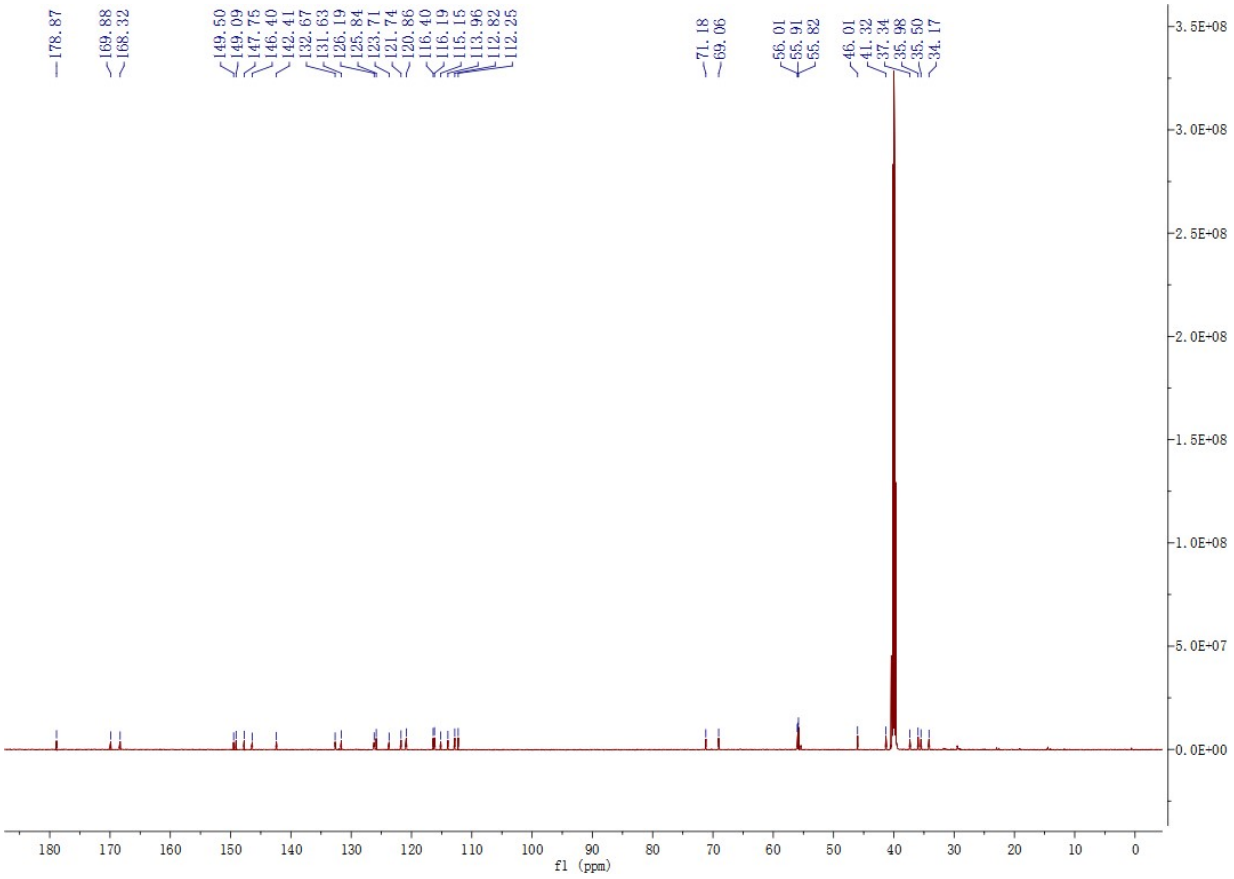
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
578.249517	1	C31H36N3O8	100.00	578.249692	0.3
600.231524	1	C31H35N3NaO8	100.00	600.231636	0.2



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.443	MM m	0.07	12.97	5.27	0.32
6.647	MM m	0.10	4.77	1.56	0.12
6.794	MM m	0.11	8.75	2.86	0.22
7.072	MM m	0.25	4035.96	1184.11	99.22
7.615	MM m	0.07	5.19	1.65	0.13

Figure S12. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B2





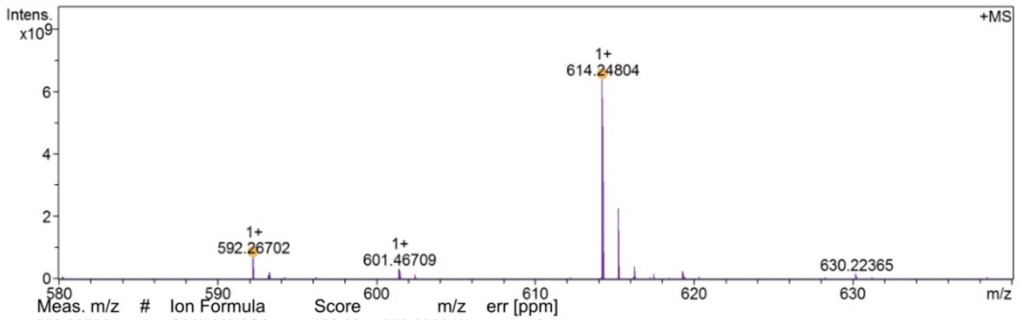
Mass Spectrum SmartFormula Report

Analysis Info

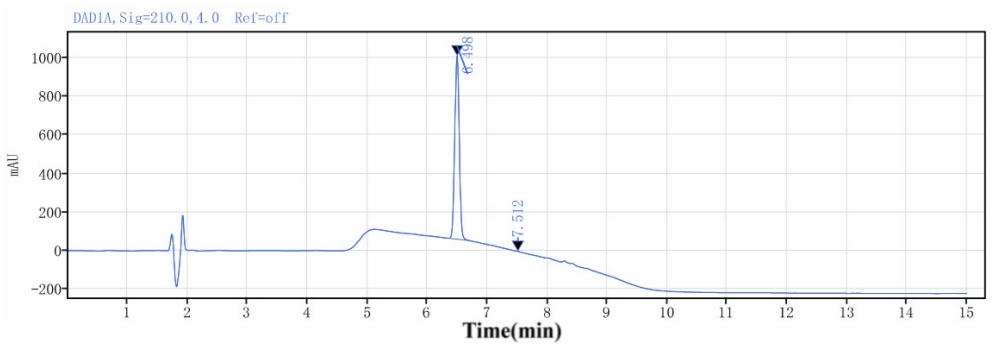
Analysis Name	D:\data\Sample Detection\20230524\2C-Ben pos_000002.d	Acquisition Date	5/24/2023 1:31:14 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

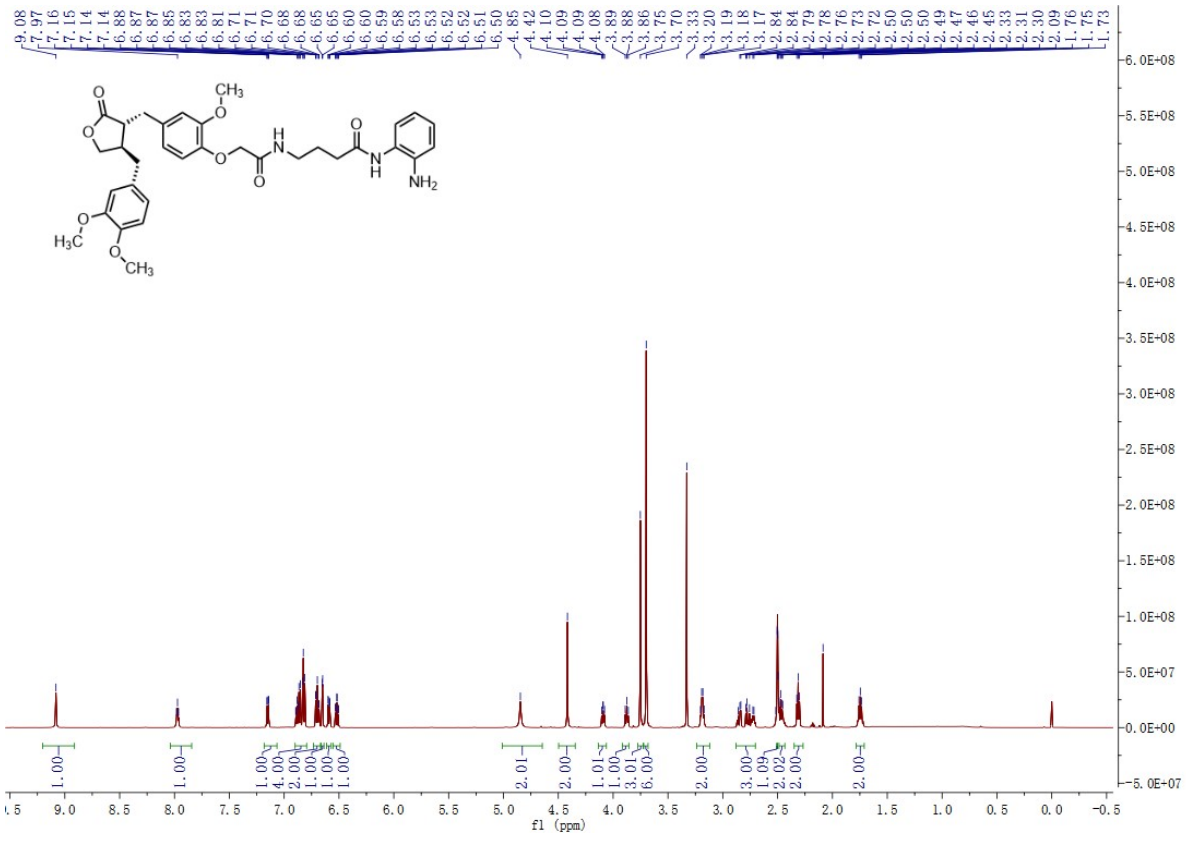


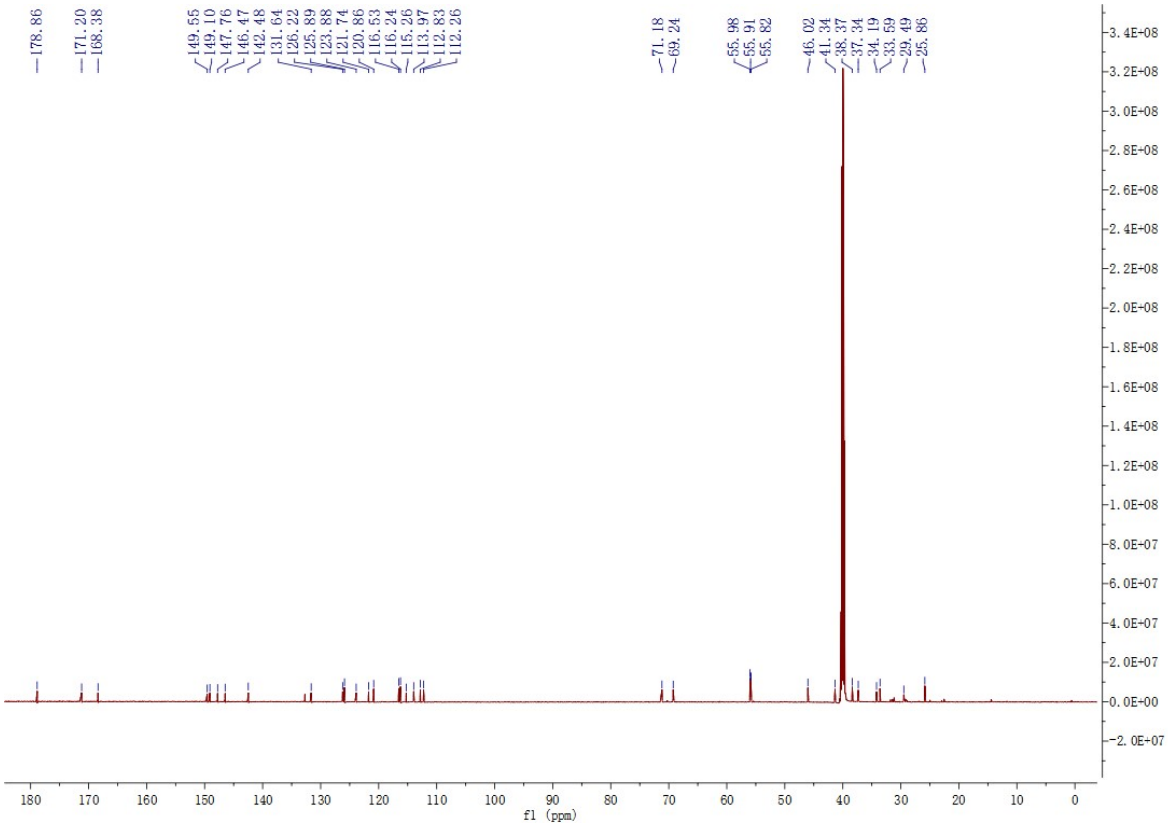
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
592.267021	1	C32H38N3O8	100.00	592.265342	-2.8
614.248045	1	C32H37N3NaO8	100.00	614.247286	-1.2



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.498	MM m	0.39	5007.68	951.69	99.89
7.512	MM m	0.08	5.53	2.17	0.11

Figure S13. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B3





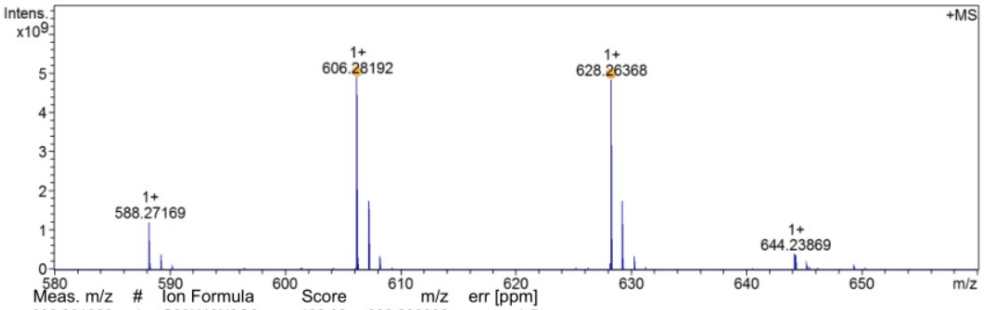
Mass Spectrum SmartFormula Report

Analysis Info

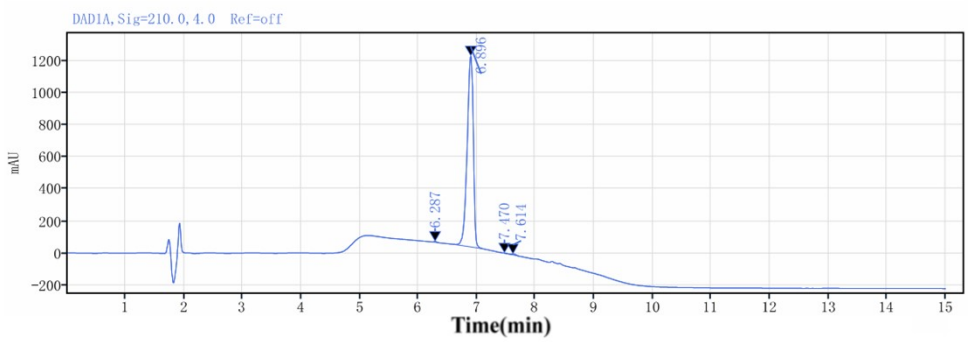
Analysis Name	D:\data\Sample Detection\20230524\3C-Ben pos_000001.d	Acquisition Date	5/24/2023 1:47:49 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	7	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

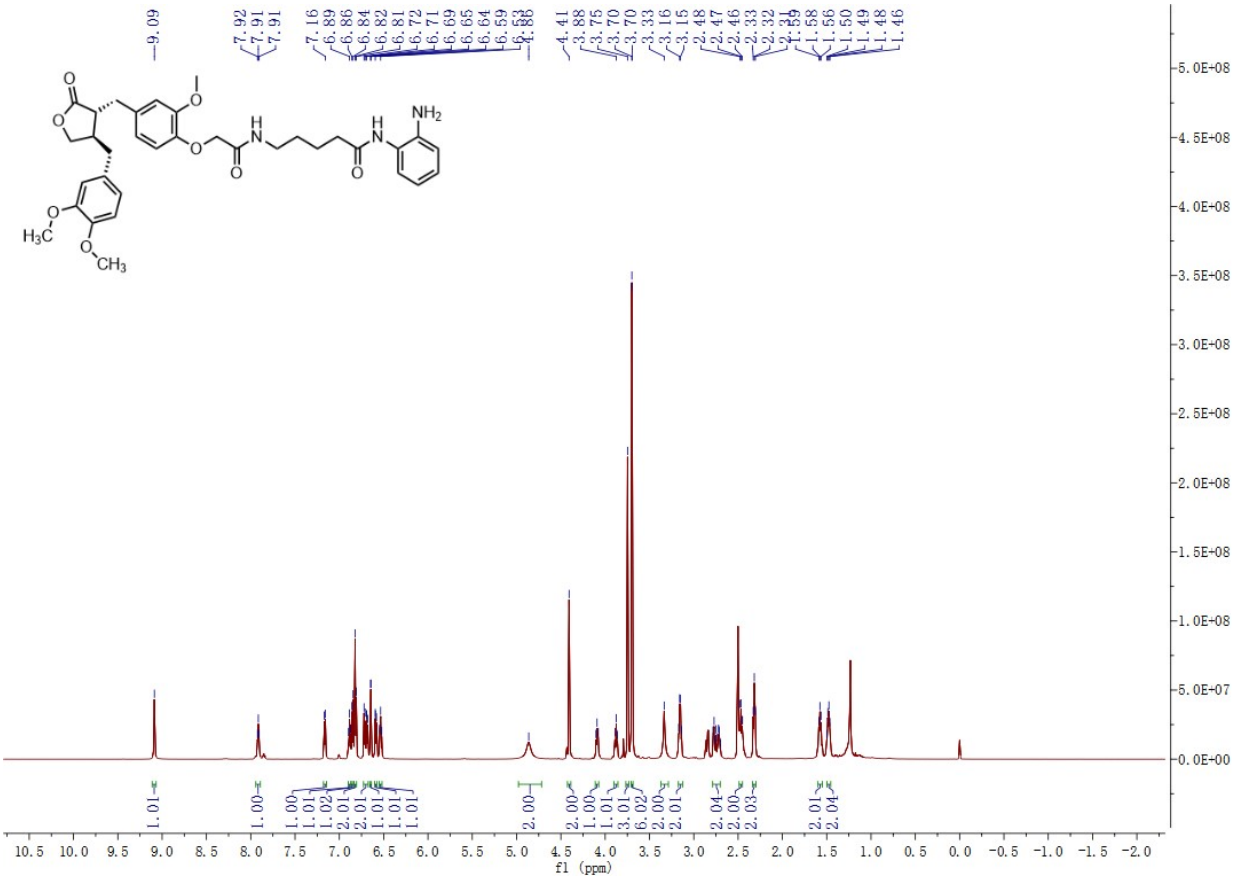


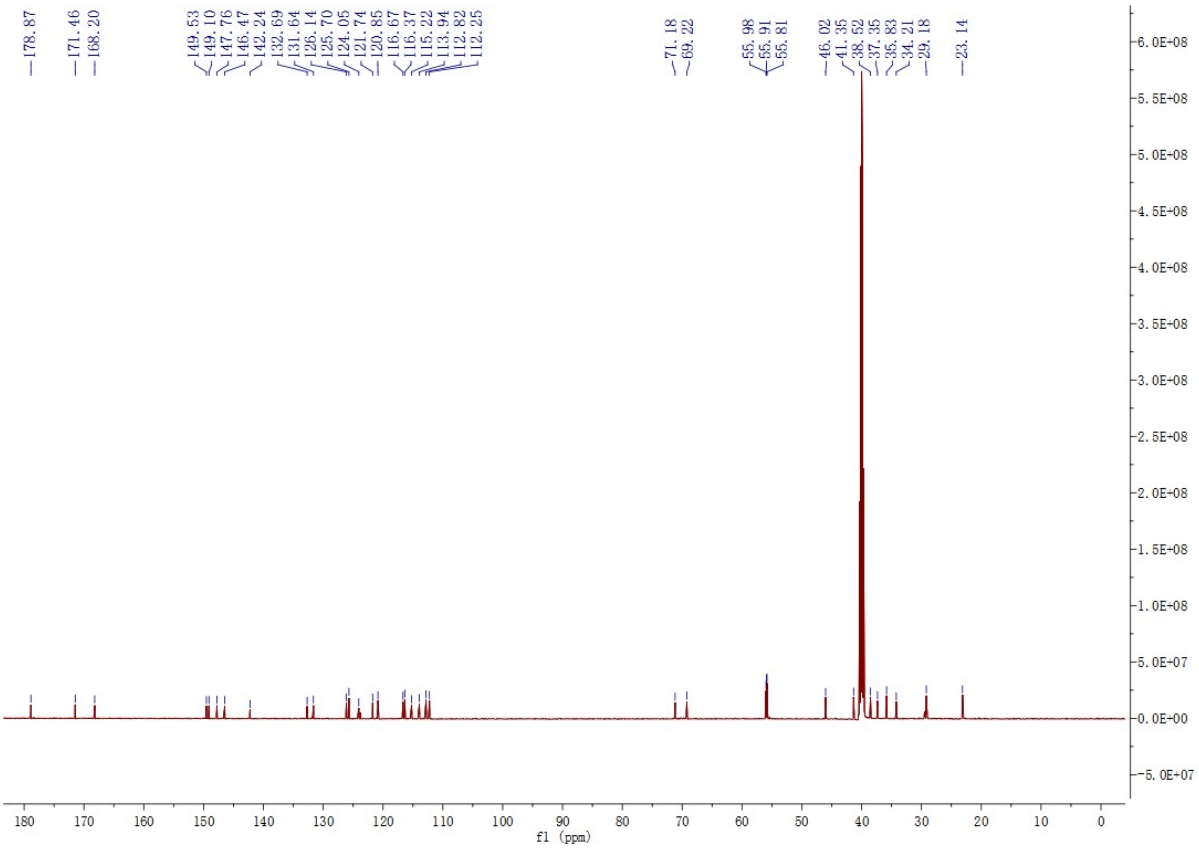
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
606.281920	1	C33H40N3O8	100.00	606.280992	-1.5
628.263677	1	C33H39N3NaO8	100.00	628.262936	-1.2



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.287	MM m	0.13	18.44	5.87	0.21
6.896	MM m	0.51	8680.96	1193.34	99.42
7.470	MM m	0.10	3.76	1.36	0.04
7.614	MM m	0.15	28.49	5.00	0.33

Figure S14. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B4





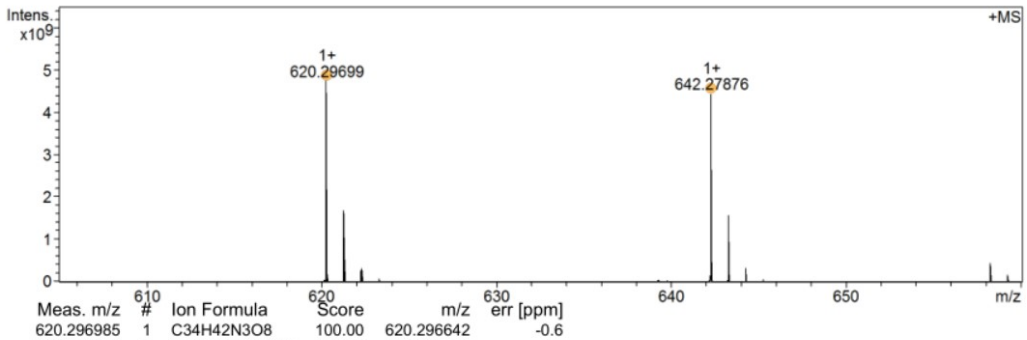
Mass Spectrum SmartFormula Report

Analysis Info

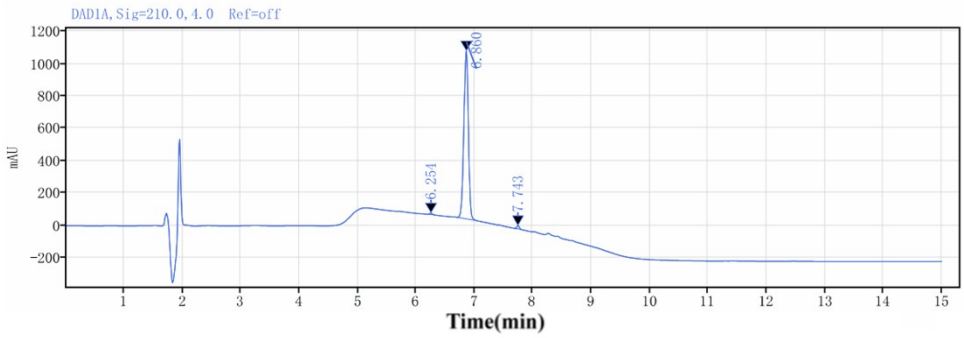
Analysis Name	D:\data\Sample Detection\20230524\4C-Ben pos_000005.d	Acquisition Date	5/24/2023 2:01:27 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

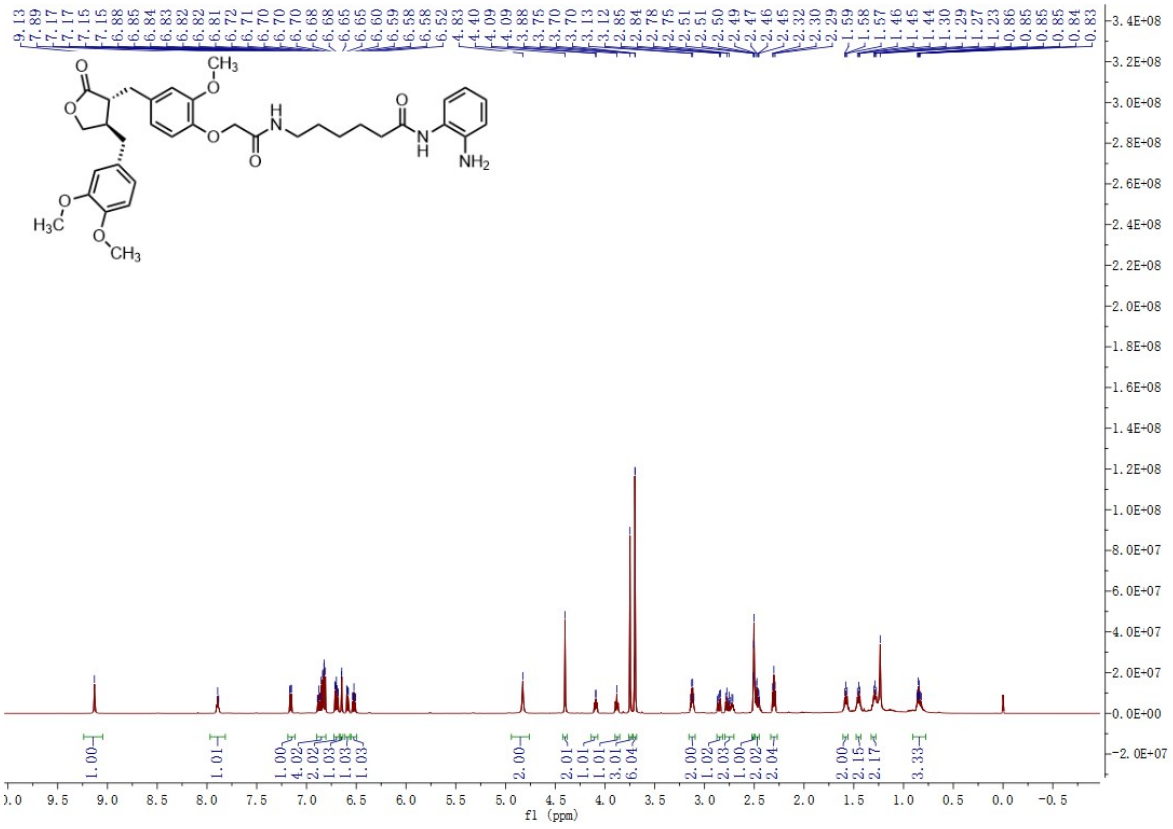


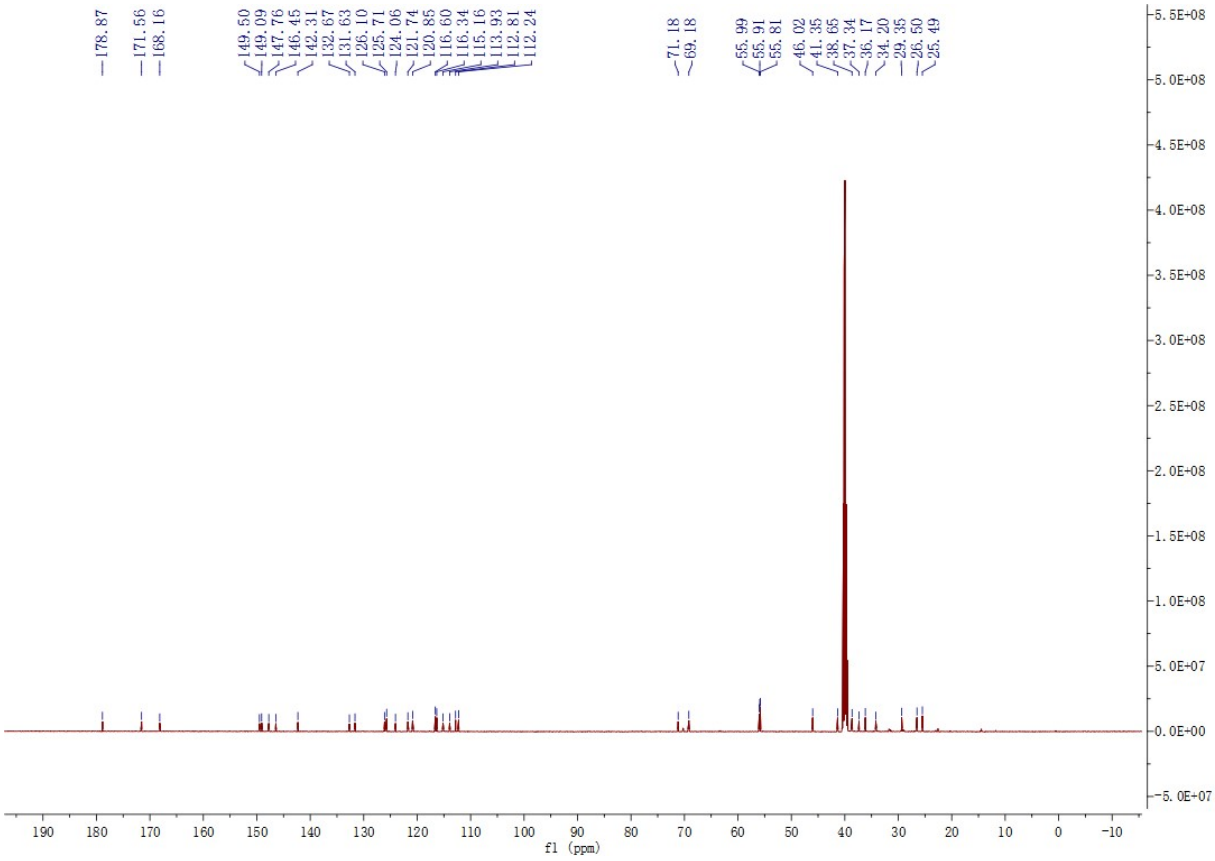
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
620.296985	1	C34H42N3O8	100.00	620.296642	-0.6
642.278765	1	C34H41N3NaO8	100.00	642.278586	-0.3



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.254	MM m	0.10	27.13	9.56	0.48
6.860	MM m	0.36	5579.25	1036.14	98.44
7.743	MM m	0.12	61.54	20.46	1.09

Figure S15. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B5





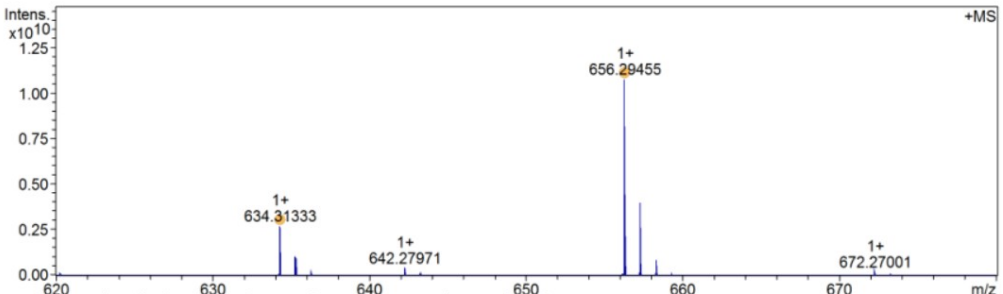
Mass Spectrum SmartFormula Report

Analysis Info

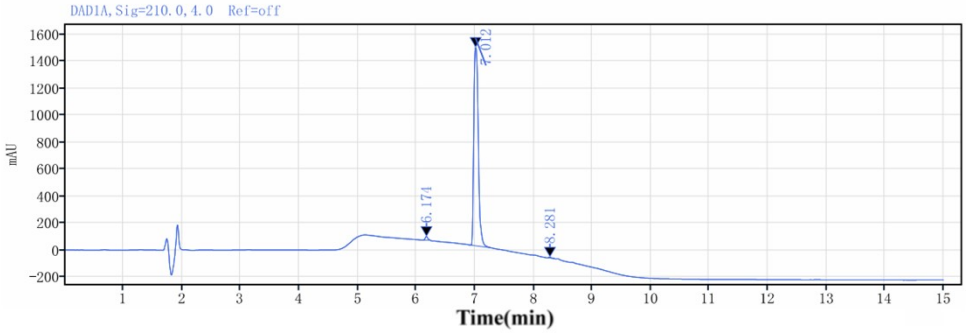
Analysis Name	D:\data\Sample Detection\20230524\5C-Ben pos_000004.d	Acquisition Date	5/24/2023 2:24:08 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

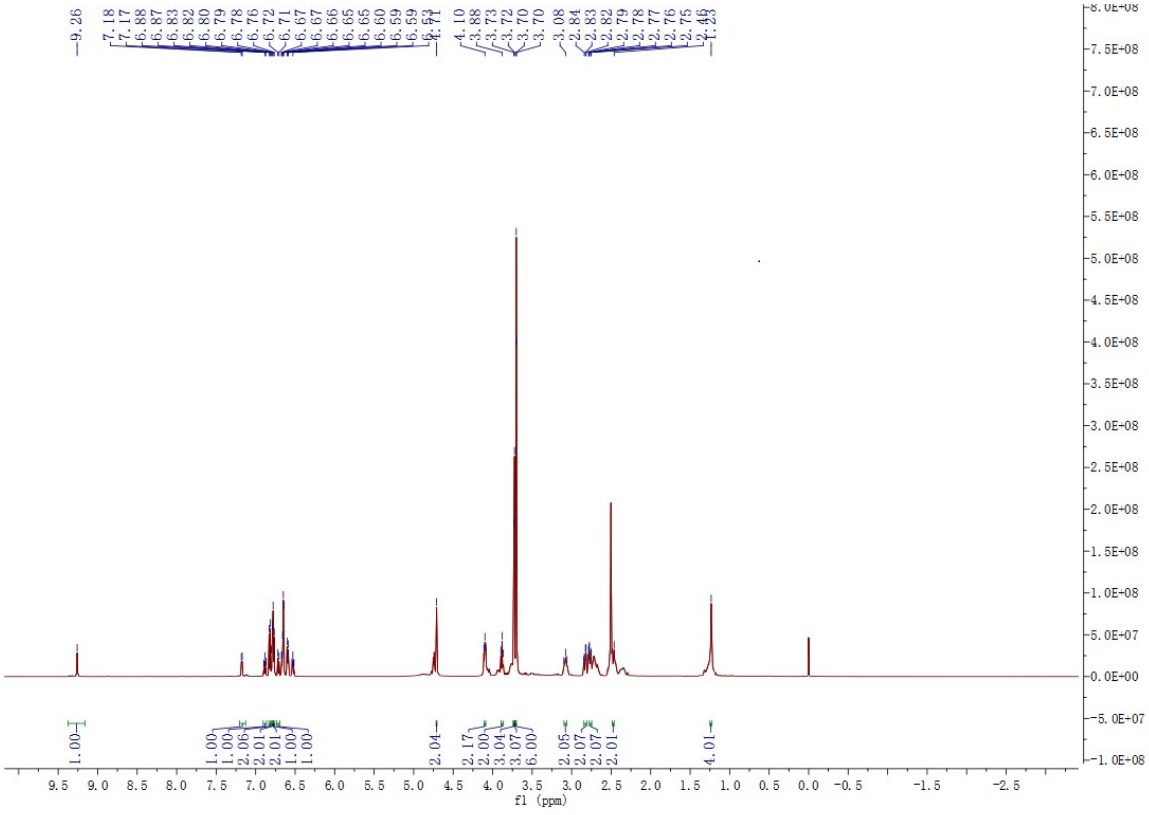


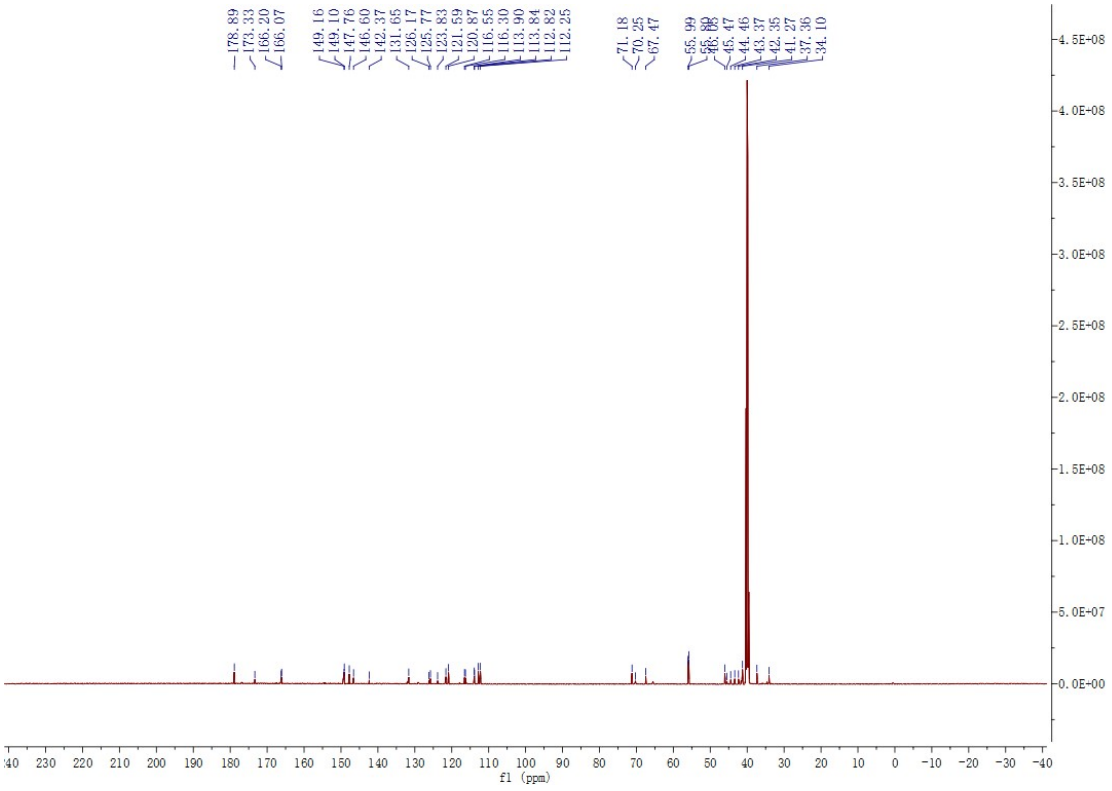
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
634.313328	1	C35H44N3O8	100.00	634.312292	-1.6
656.294545	1	C35H43N3NaO8	100.00	656.294236	-0.5



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
6.174	MM m	0.12	81.50	27.64	1.03
7.012	MM m	0.35	7837.34	1472.45	98.67
8.281	MM m	0.11	24.43	7.69	0.31

Figure S16. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B6





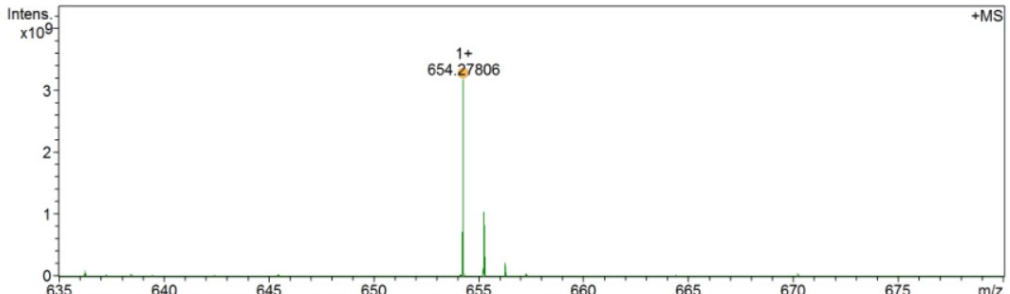
Mass Spectrum SmartFormula Report

Analysis Info

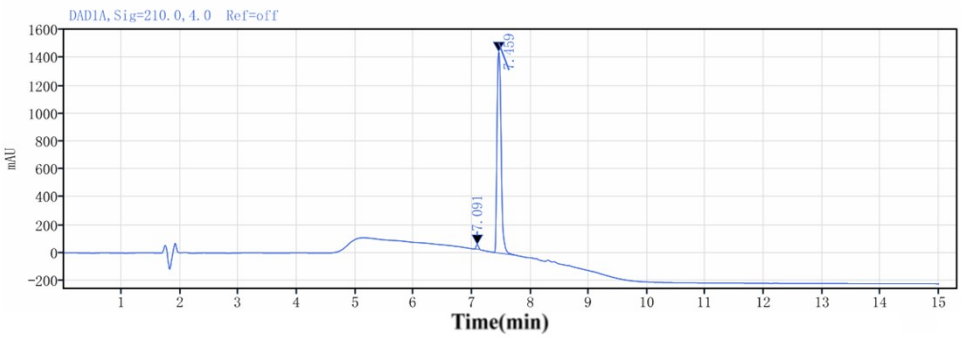
Analysis Name	D:\data\Sample Detection\20230524\Pai-Ben pos_000002.d	Acquisition Date	5/24/2023 2:47:18 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

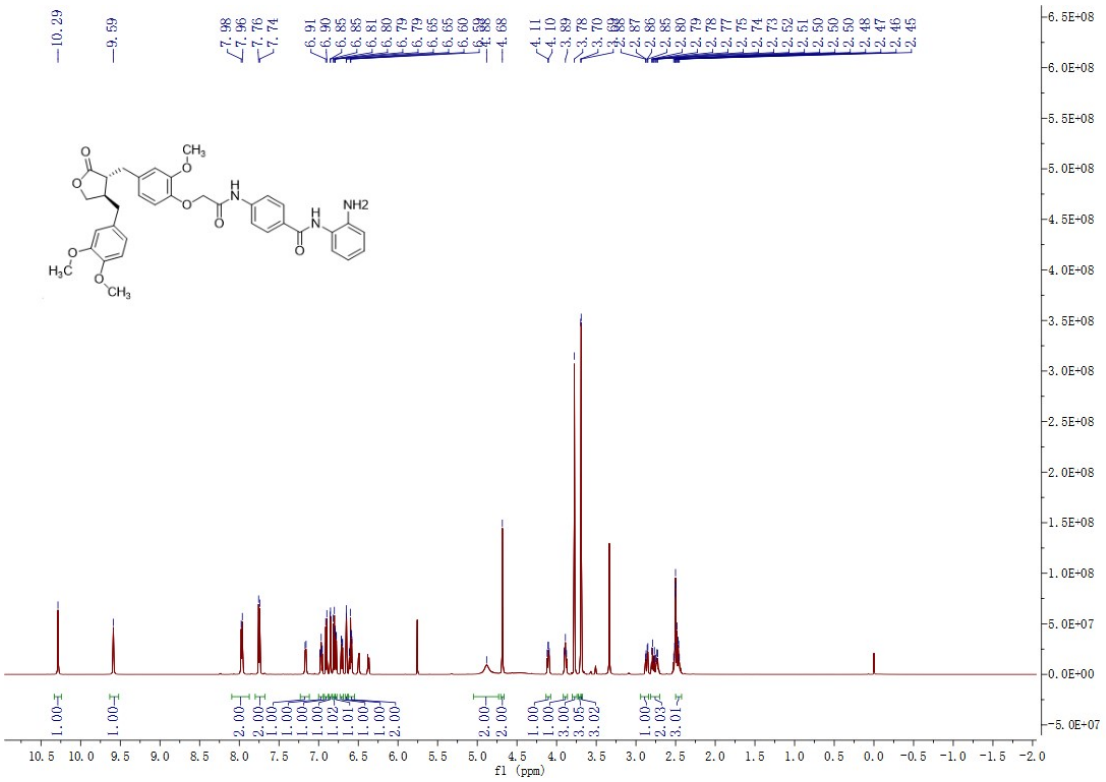


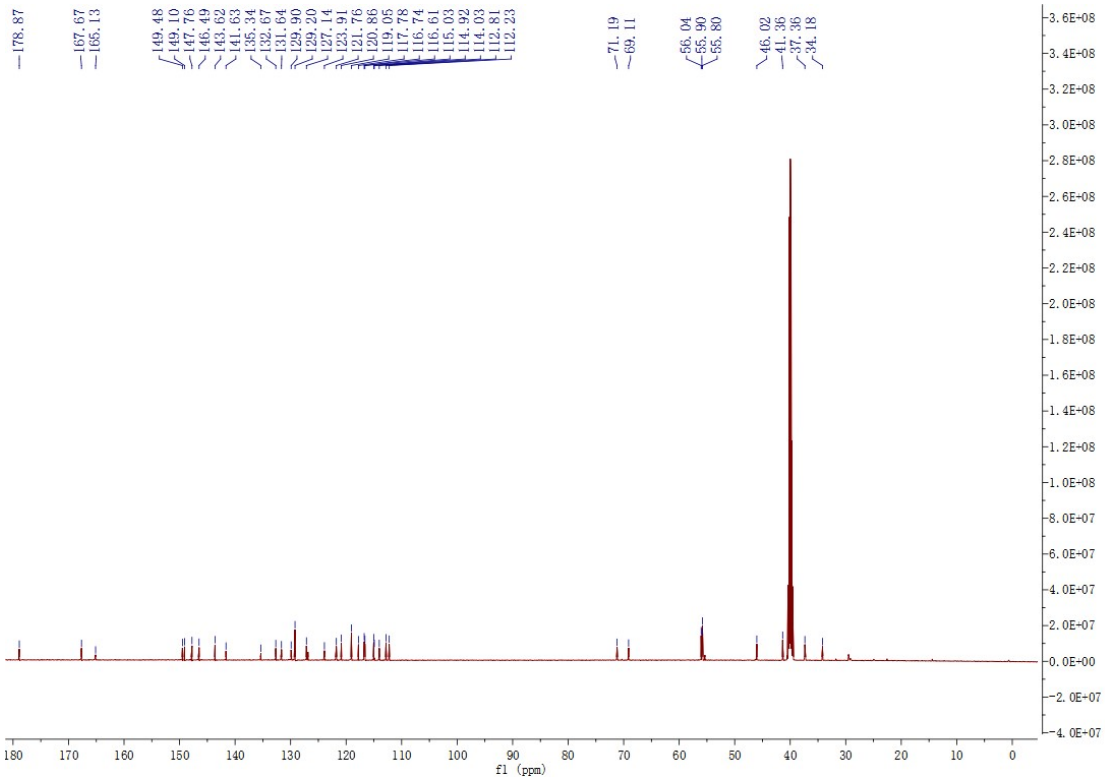
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
654.278063	1	C35H41N3NaO8	100.00	654.278586	0.8



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
7.091	MM m	0.08	80.72	30.92	1.13
7.459	MM m	0.35	7057.21	1444.55	98.87

Figure S17. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B7





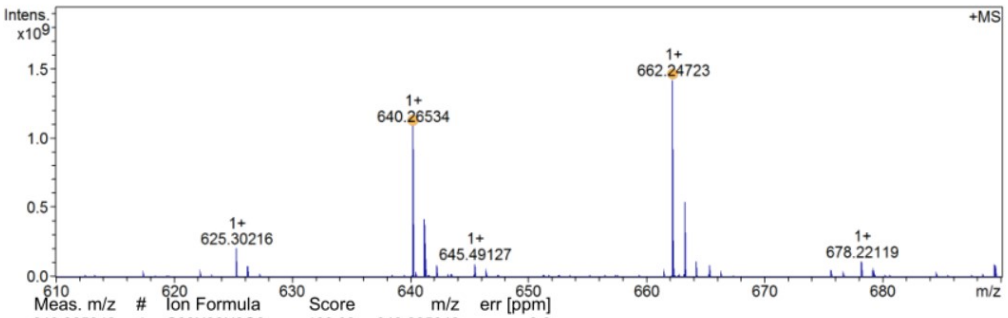
Mass Spectrum SmartFormula Report

Analysis Info

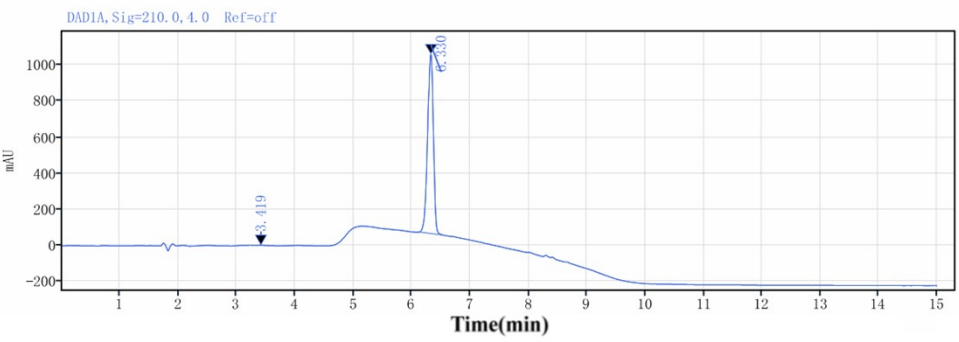
Analysis Name	D:\data\Sample Detection\20230524\Ben-Ben pos_000001.d	Acquisition Date	5/24/2023 3:04:06 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

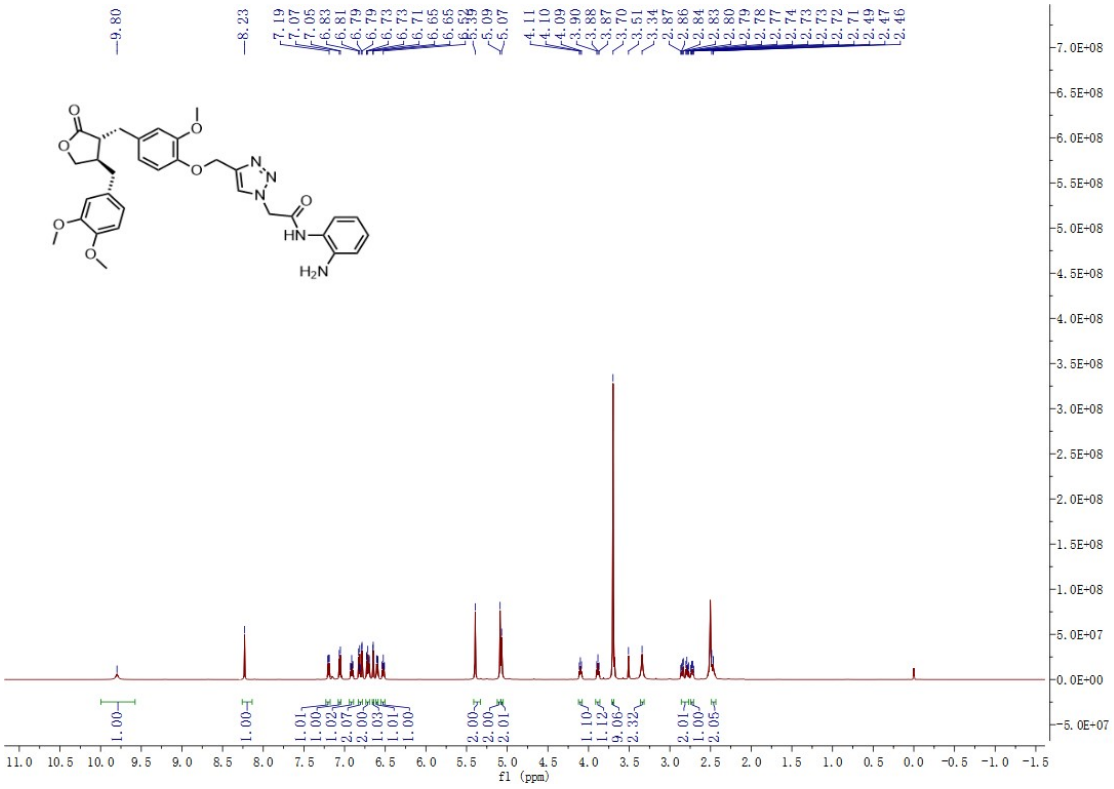


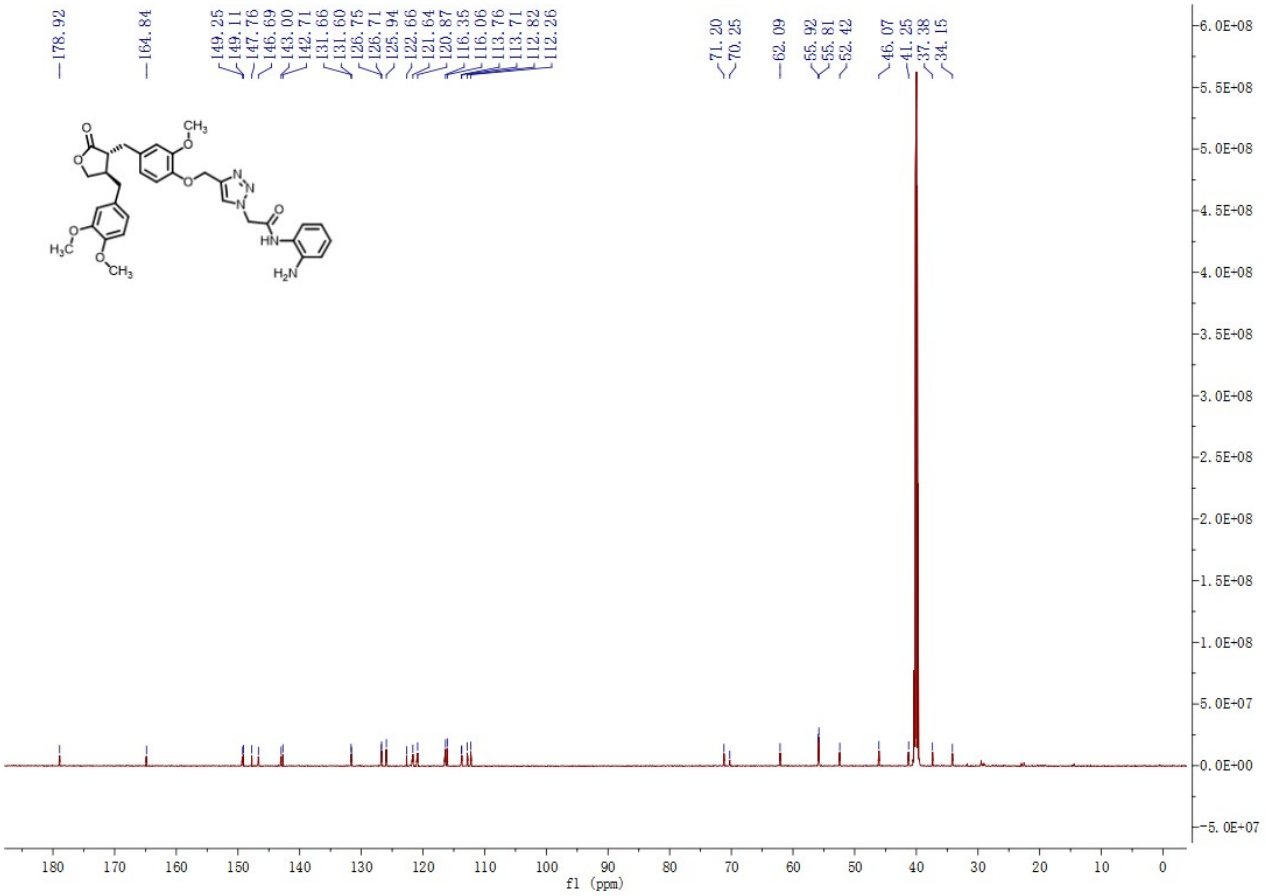
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
640.265342	1	C36H38N3O8	100.00	640.265342	0.0
662.247229	1	C36H37N3NaO8	100.00	662.247286	0.1



Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
3.419	MM m	0.14	8.95	2.21	0.13
6.330	MM m	0.41	6884.96	993.04	99.87

Figure S18. ^{1}H NMR , ^{13}C NMR, FT-MS, HPLC of B8





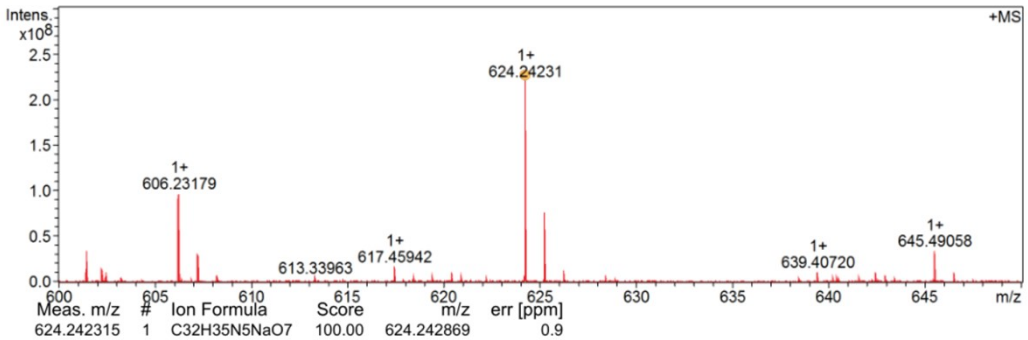
Mass Spectrum SmartFormula Report

Analysis Info

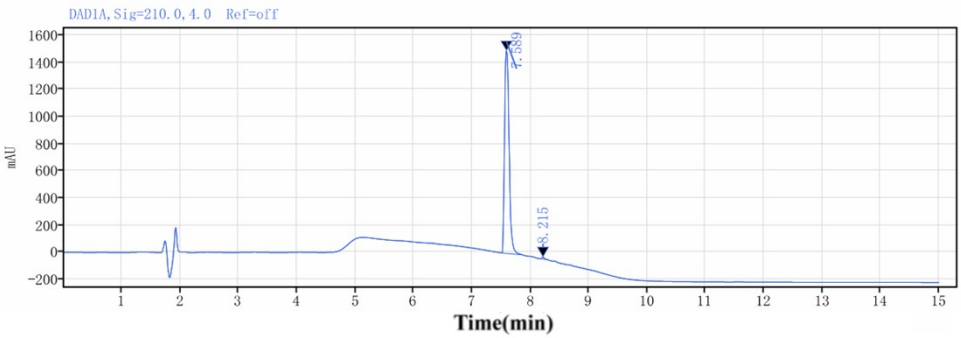
Analysis Name	D:\data\Sample Detection\20230524\Tri-Ben pos_000002.d	Acquisition Date	5/24/2023 2:39:17 PM
Method	20230410 pos 100-2000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Mon Apr 10 10:10:45 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	1048576
Broadband Low Mass	100.3 m/z	No. of Laser Shots	500	Data Processing Size (SI)	2097152
Broadband High Mass	2000.0 m/z	Laser Power	20.0 lp	Apodization	Full-Sine
Source Accumulation	0.000 sec	Laser Shot Frequency	0.001 sec		
Ion Accumulation Time	0.100 sec				

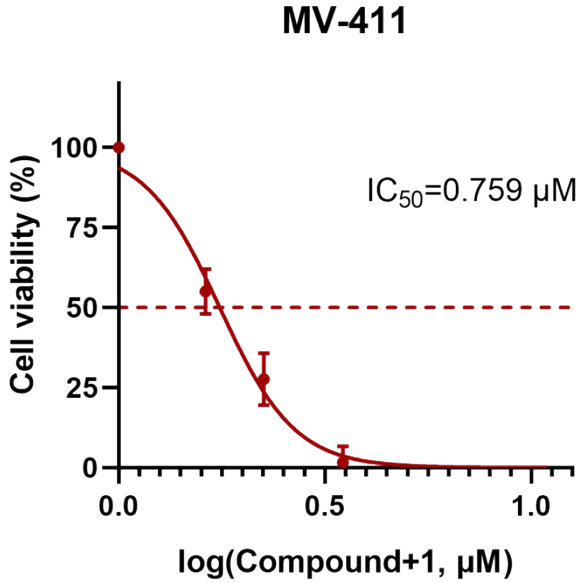


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]
624.242315	1	C32H35N5NaO7	100.00	624.242869	0.9

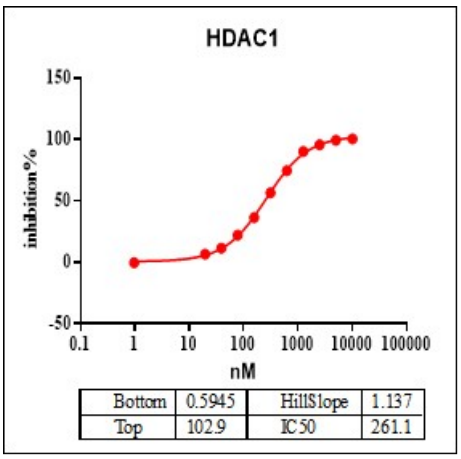


Retention Time [min]	Type	Peak Width [min]	Peak Area	Peak Height	Peak Area (%)
7.589	MM m	0.36	8193.68	1492.40	99.56
8.215	MM m	0.09	36.60	15.13	0.44

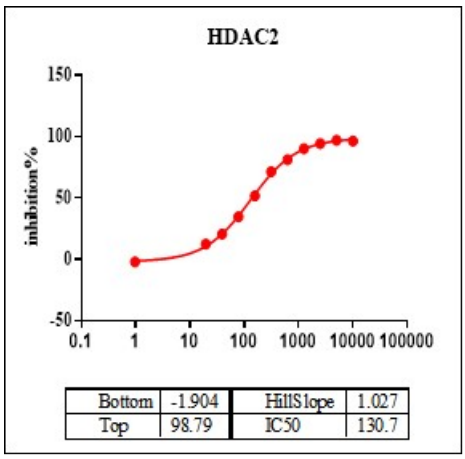
2. IC_{50} fitting curve of compound B7



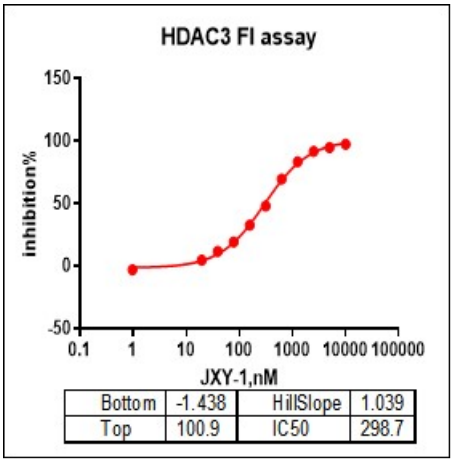
3. IC_{50} fitting curve of HDAC isomer inhibitory activity of compound B7



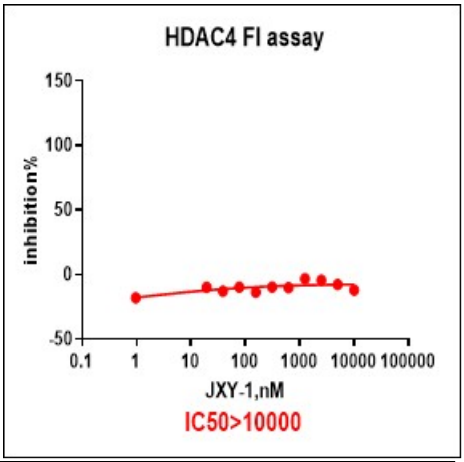
Bottom	0.5945	HillSlope	1.137
Top	102.9	IC50	261.1

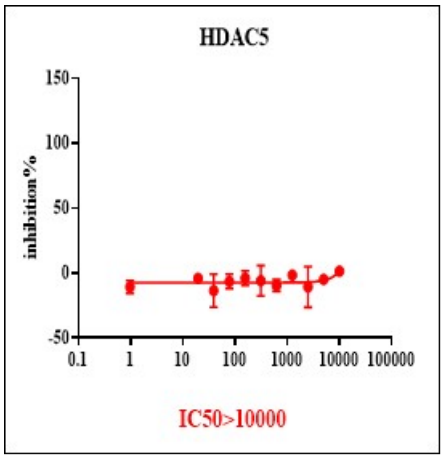


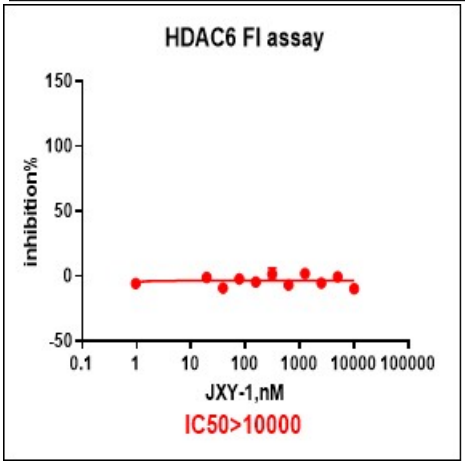
Bottom	-1.904	HillSlope	1.027
Top	98.79	IC50	130.7

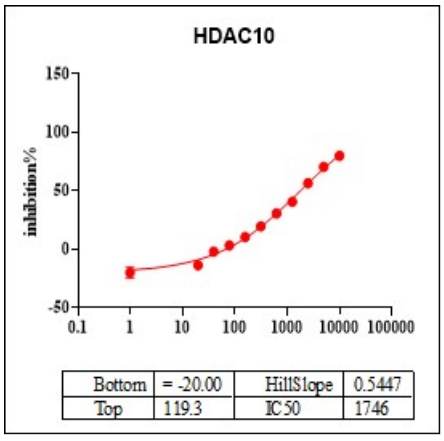


Bottom	-1.438	HillSlope	1.039
Top	100.9	IC50	298.7



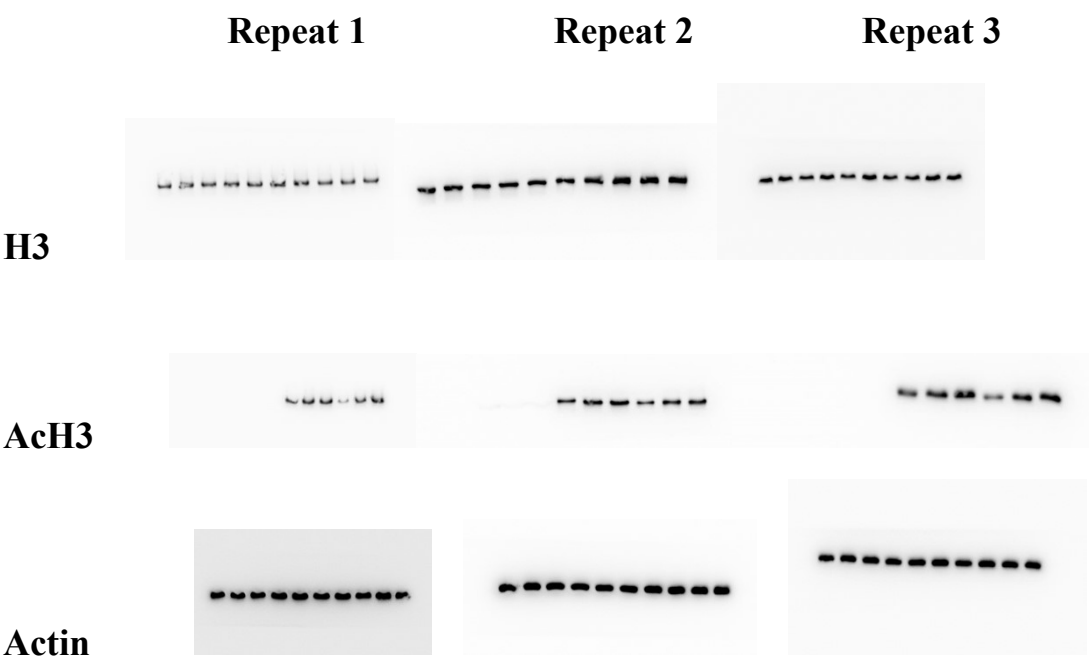




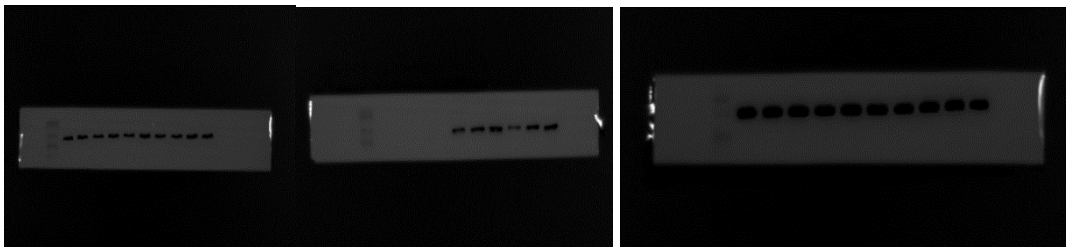


Bottom	= -20.00	HillSlope	0.5447
Top	119.3	IC50	1746

4.1 western blot experiments



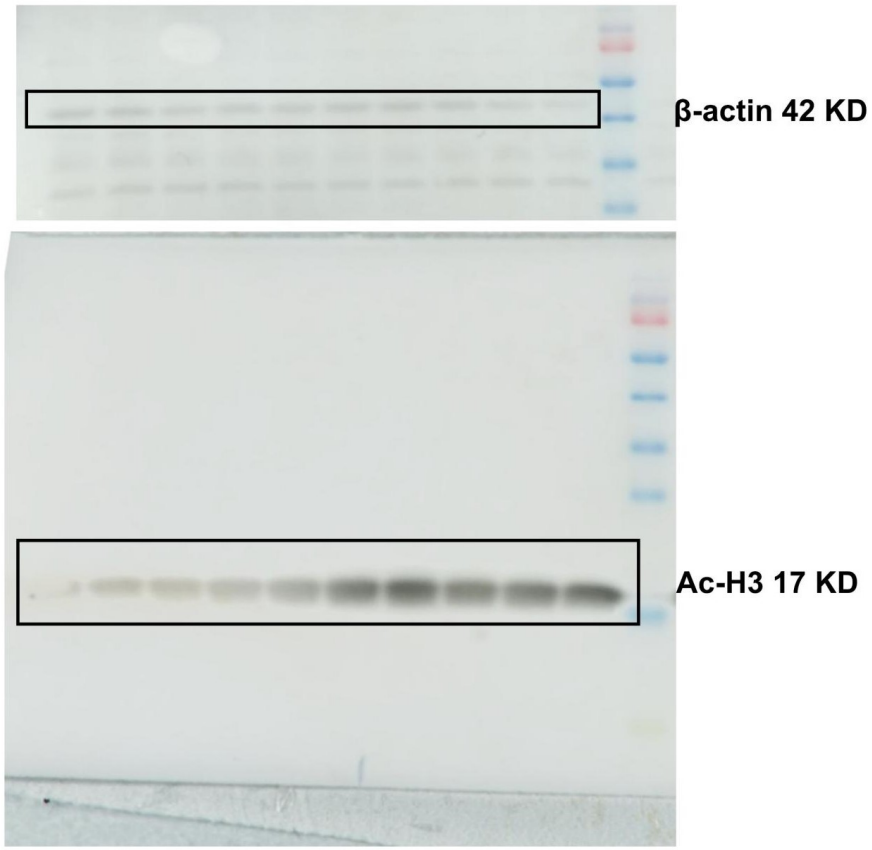
1. The Western blot membranes with markers in the previously provided supplementary data：



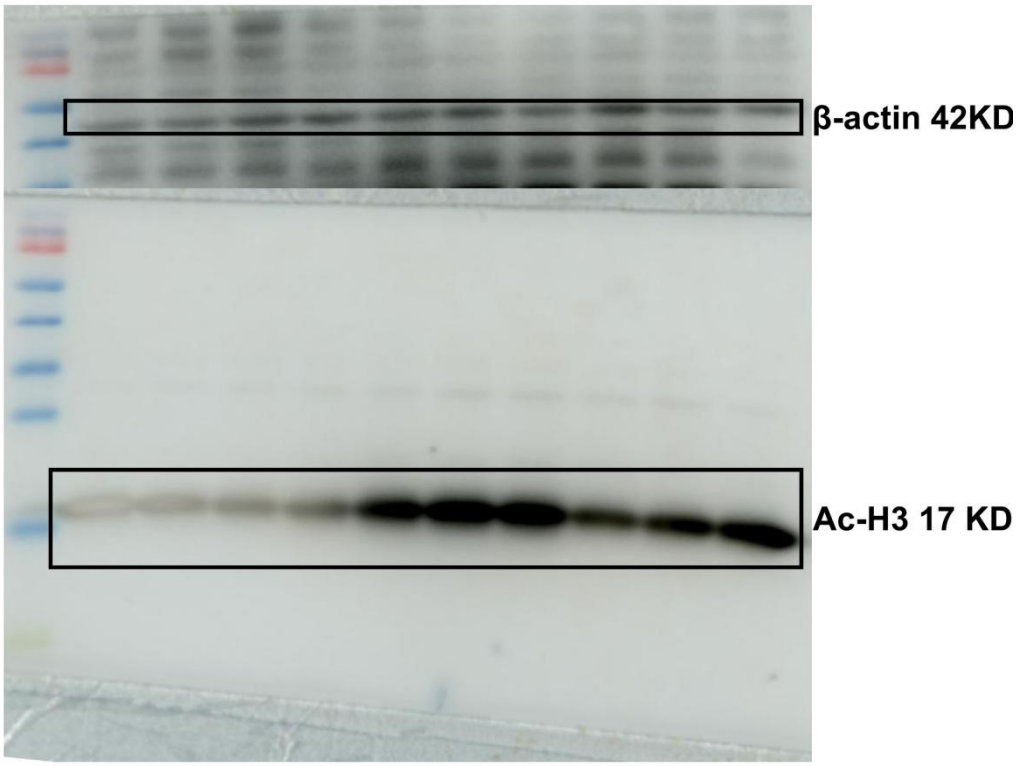
2. The supplementary full membrane Western blot:

Due to the expression of H3 and Ac-H3 affecting the luminescence of Actin, the membrane was trimmed during the Actin luminescence; however, it can be clearly identified as a full membrane through the markers.

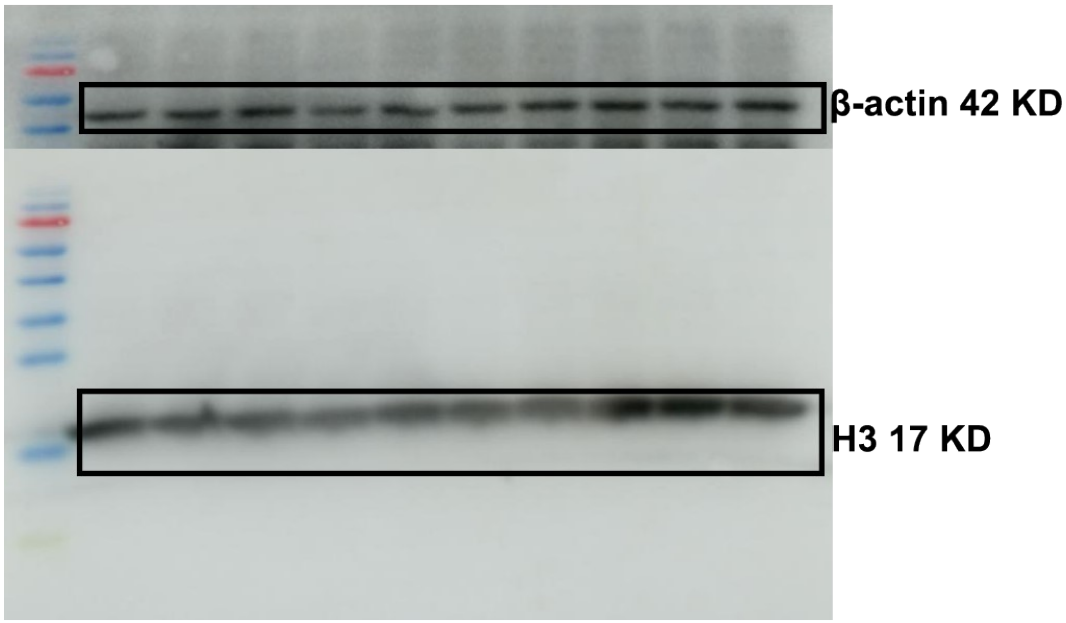
（1）Ac-H3 - repeat 1



（2）Ac-H3 - repeat 2



(3) H3 - repeat 1



（4）H3 - repeat 2