



Supplementary Materials

# Triterpenoids from *Kochiae Fructus*: Glucose Uptake in 3T3-L1 Adipocytes and $\alpha$ -Glucosidase Inhibition, in Silico Molecular Docking

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**Figure S1.** <sup>1</sup>H NMR spectrum of compound 1 (methanol-*d*<sub>4</sub>, 500MHz).

**Figure S2.** <sup>13</sup>C NMR spectrum of compound 1 (methanol-*d*<sub>4</sub>, 125MHz).

**Figure S3.** HSQC spectrum of compound 1.

**Figure S4.** HMBC spectrum of compound 1.

**Figure S5.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 1.

**Figure S6.** ROESY spectrum of compound 1.

**Figure S7.** HSQC-TOCSY spectrum of compound 1.

**Figure S8.** HRESI-MS spectra of compound 1.

**Figure S9.** Optical rotations spectrum of compound 1.

**Figure S10.** UV spectrum of compound 1.

**Figure S11.** IR spectrum of compound 1.

**Figure S12.** <sup>1</sup>H NMR spectrum of compound 2 (methanol-*d*<sub>4</sub>, 500MHz).

**Figure S13.** <sup>13</sup>C NMR spectrum of compound 2 (methanol-*d*<sub>4</sub>, 125MHz).

**Figure S14.** HSQC spectrum of compound 2.

**Figure S15.** HMBC spectrum of compound 2.

**Figure S16.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 2.

**Figure S17.** ROESY spectrum of compound 2.

**Figure S18.** HSQC-TOCSY spectrum of compound 2.

**Figure S19.** HRESI-MS spectra of compound 2.

**Figure S20.** Optical rotations spectrum of compound 2.

**Figure S21.** UV spectrum of compound 2.

**Figure S22.** IR spectrum of compound 2.

**Figure S23.** <sup>1</sup>H NMR spectrum of compound 3 (methanol-*d*<sub>4</sub>, 500MHz).

**Figure S24.** <sup>13</sup>C NMR spectrum of compound 3 (methanol-*d*<sub>4</sub>, 125MHz).

**Figure S25.** HSQC spectrum of compound 3.

**Figure S26.** HMBC spectrum of compound 3.

**Figure S27.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 3.

**Figure S28.** ROESY spectrum of compound 3.

**Figure S29.** HRESI-MS spectra of compound 3.

**Figure S30.** Optical rotations spectrum of compound 3.

**Figure S31.** UV spectrum of compound 3.

**Figure S32.** IR spectrum of compound 3.

**Figure S33.** The CD spectra of compounds 1, 2, and 3 in MeOH.

**Figure S34.** <sup>1</sup>H NMR spectrum of compound 4 (methanol-*d*<sub>4</sub>, 500MHz).

**Figure S35.** <sup>1</sup>H NMR spectrum of compound 5 (methanol-*d*<sub>4</sub>, 500MHz).

**Figure S36.**  $^1\text{H}$  NMR spectrum of compound **6** (methanol- $d_4$ , 500MHz).

**Figure S37.**  $^1\text{H}$  NMR spectrum of compound **7** (methanol- $d_4$ , 500MHz).

**Figure S38.**  $^1\text{H}$  NMR spectrum of compound **8** (methanol- $d_4$ , 500MHz).

**Figure S39.**  $^1\text{H}$  NMR spectrum of compound **9** (methanol- $d_4$ , 500MHz).

**Figure S40.**  $^1\text{H}$  NMR spectrum of compound **10** (methanol- $d_4$ , 600MHz).

**Figure S41.**  $^1\text{H}$  NMR spectrum of compound **11** (methanol- $d_4$ , 500MHz).

**Figure S42.**  $^1\text{H}$  NMR spectrum of compound **12** (methanol- $d_4$ , 500MHz).

**Figure S43.**  $^1\text{H}$  NMR spectrum of compound **13** (methanol- $d_4$ , 600MHz).

**Figure S44.**  $^1\text{H}$  NMR spectrum of compound **14** (methanol- $d_4$ , 600MHz).

**Figure S45.**  $^1\text{H}$  NMR spectrum of compound **15** (methanol- $d_4$ , 600MHz).

**Figure S46.**  $^1\text{H}$  NMR spectrum of compound **16** (methanol- $d_4$ , 600MHz).

**Figure S47.**  $^1\text{H}$  NMR spectrum of compound **17** (methanol- $d_4$ , 600MHz).

**Table S1.** The data that was used to calculate the  $\text{IC}_{50}$  value for compound **3**.

**Table S2.** The data that was used to calculate the  $\text{IC}_{50}$  value for compound **9**.

**Table S3.** The data that was used to calculate the  $\text{IC}_{50}$  value for compound **13**.

**Table S4.** The data that was used to calculate the  $\text{IC}_{50}$  value for acarbose.

**Table S5.** The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound **3**.

**Table S6.** The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound **9**.

**Table S7.** The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound **13**.

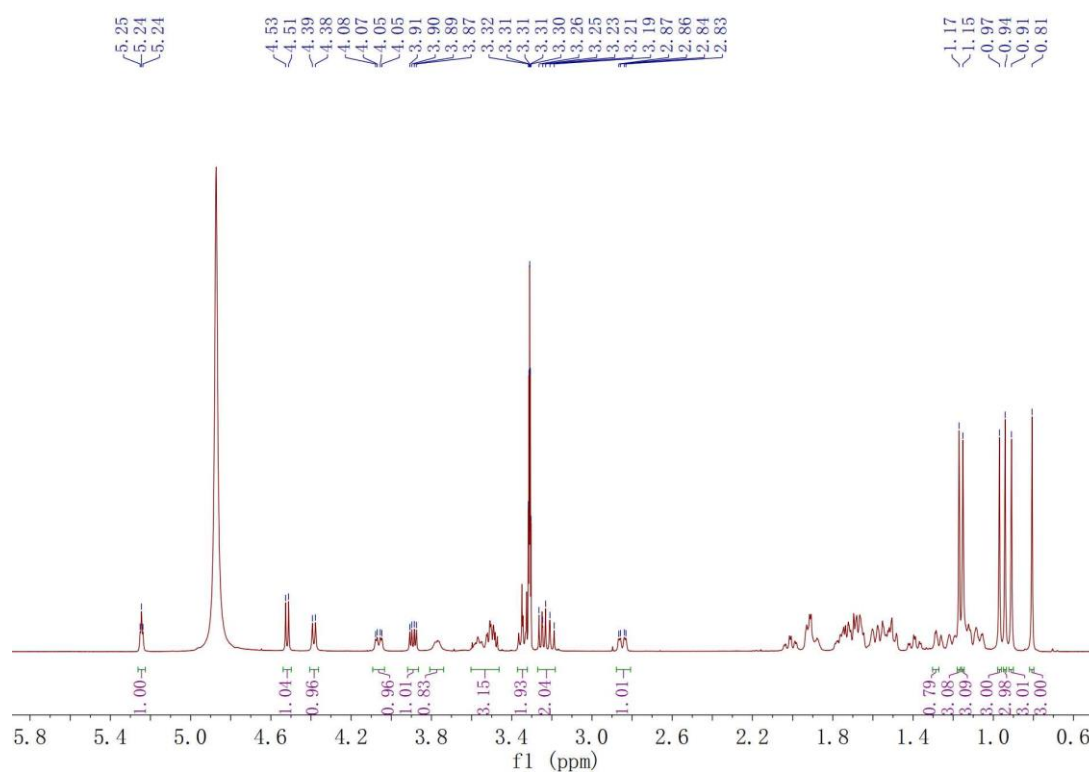


Figure S1. <sup>1</sup>H NMR spectrum of compound 1 (methanol-*d*<sub>4</sub>, 500 MHz).

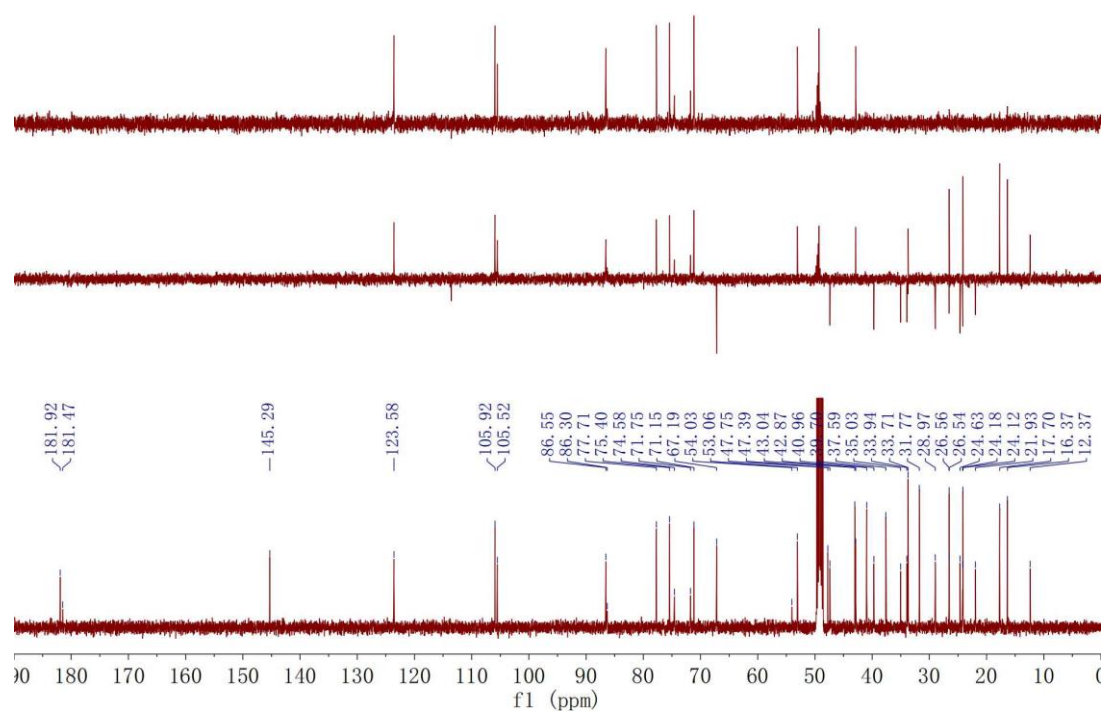


Figure S2. <sup>13</sup>C NMR spectrum of compound 1 (methanol-*d*<sub>4</sub>, 125 MHz).

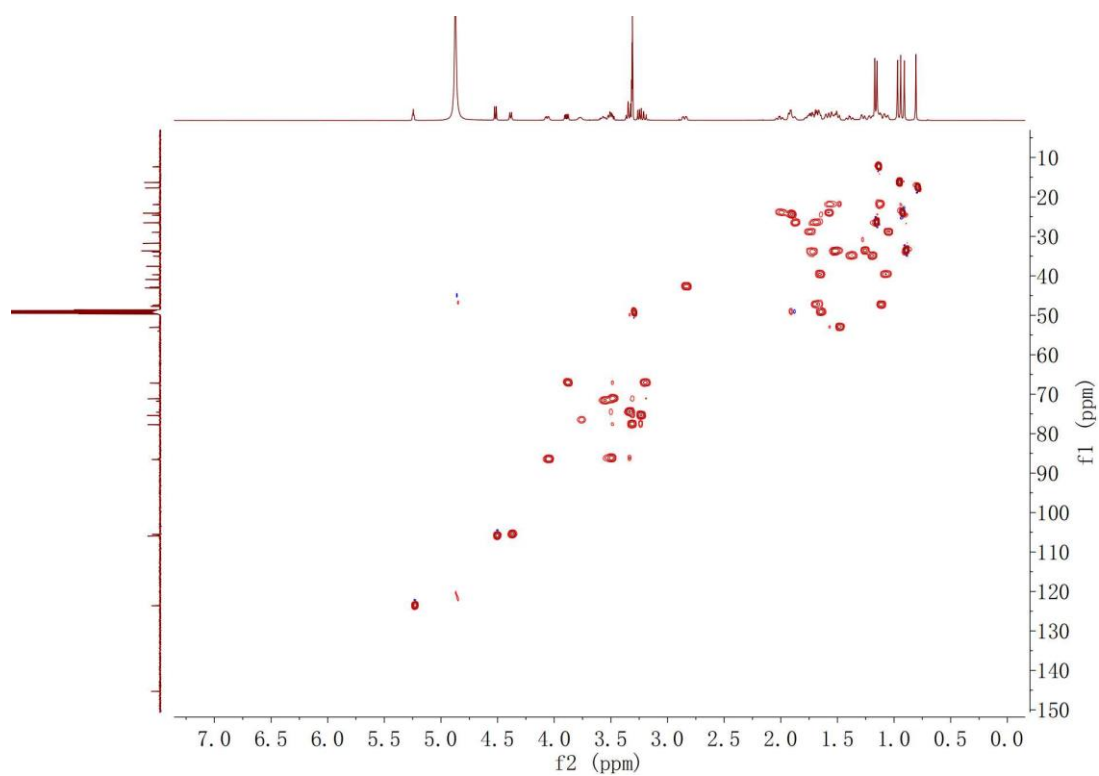


Figure S3. HSQC spectrum of compound 1.

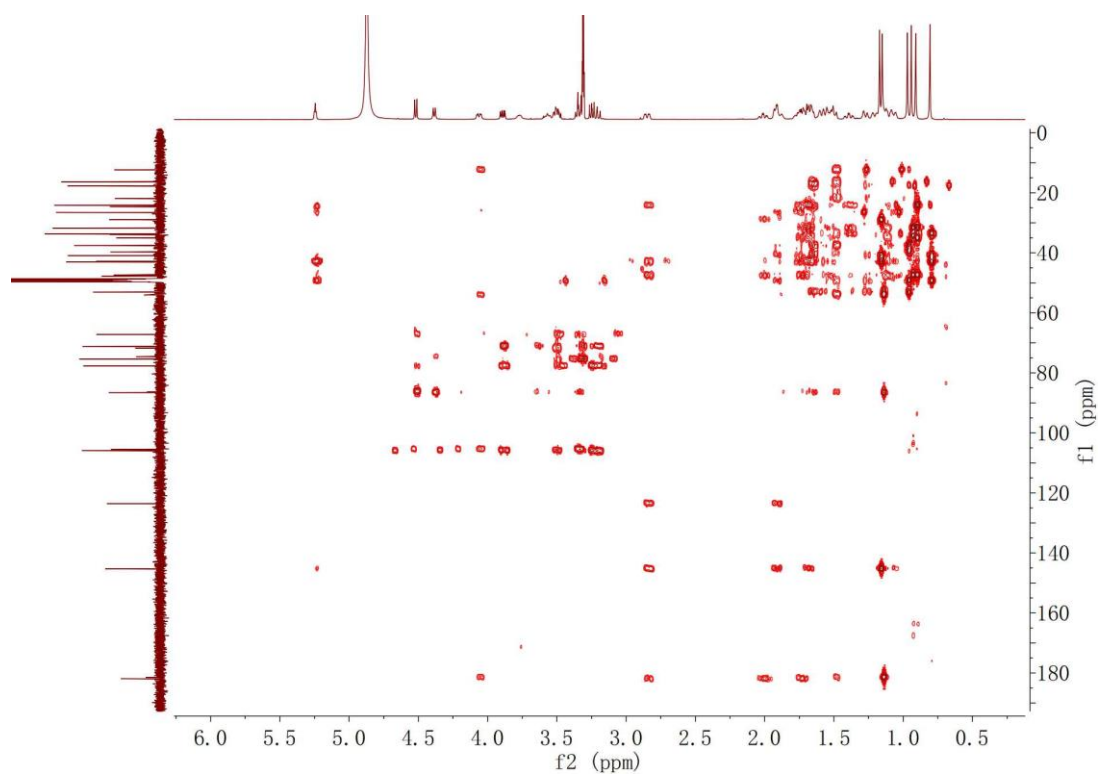


Figure S4. HMBC spectrum of compound 1.

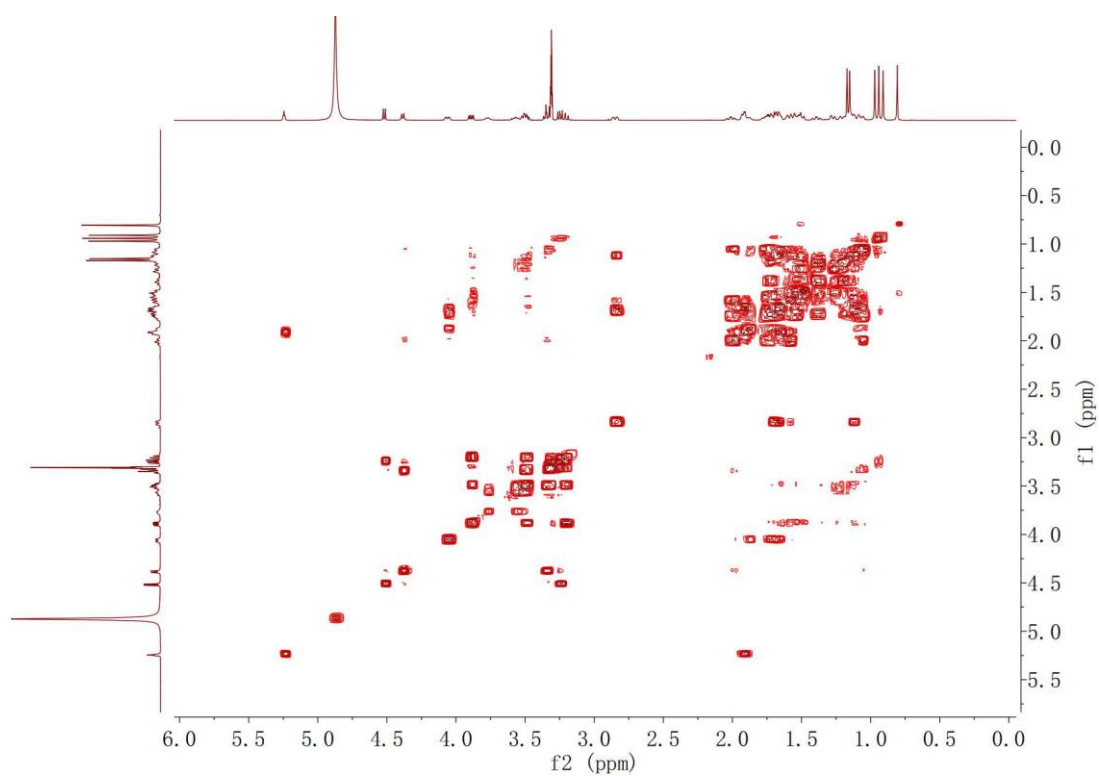


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**.

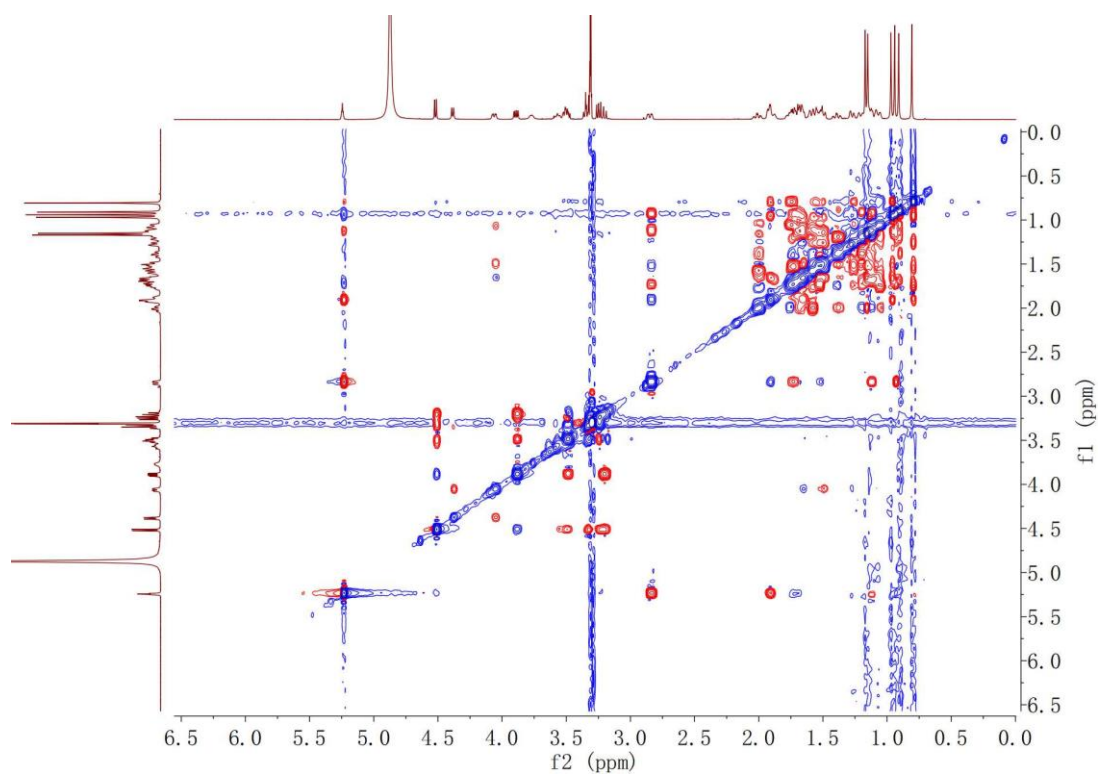
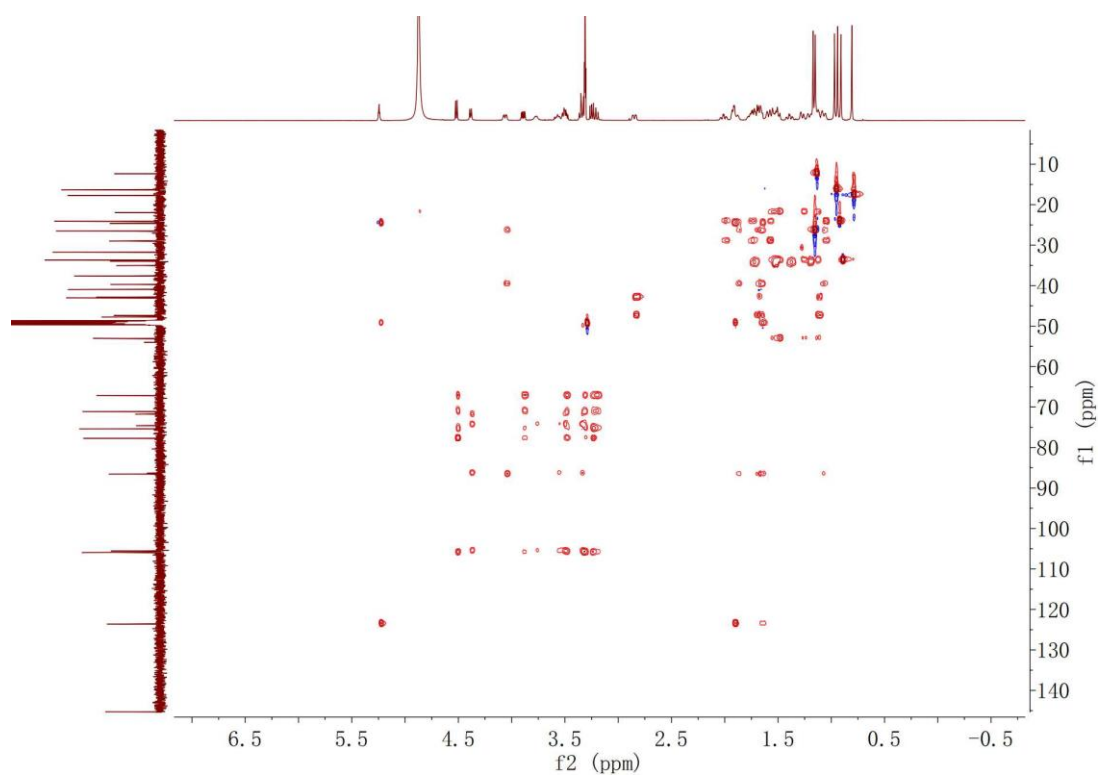


Figure S6. ROESY spectrum of compound **1**.



**Figure S7.** HSQC-TOCSY spectrum of compound 1.

Formula Predictor Report - ZKF22.lcd

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Data File: E:\DATA\2022\0518\ZKF22.lcd

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2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	10	50	Si	4	0	0	Se	2	0	0					
N	3	0	0	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5

DBE Range: not fixed

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: no

Use MSn Info: yes

Max Isotopes: all

Isotope RI (%): 1.00

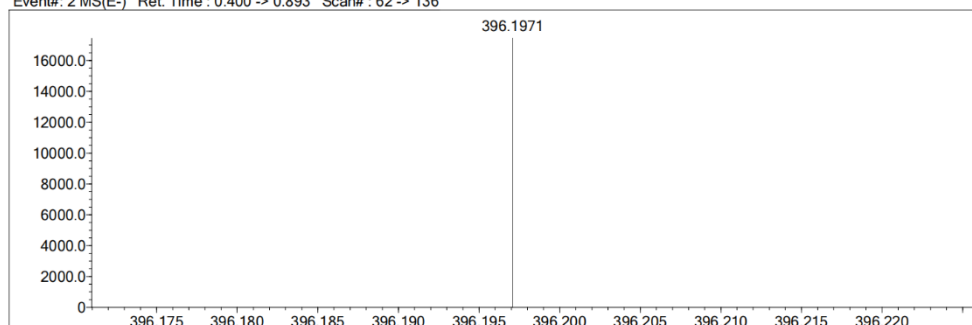
Isotope Res: 10000

MSn Iso RI (%): 75.00

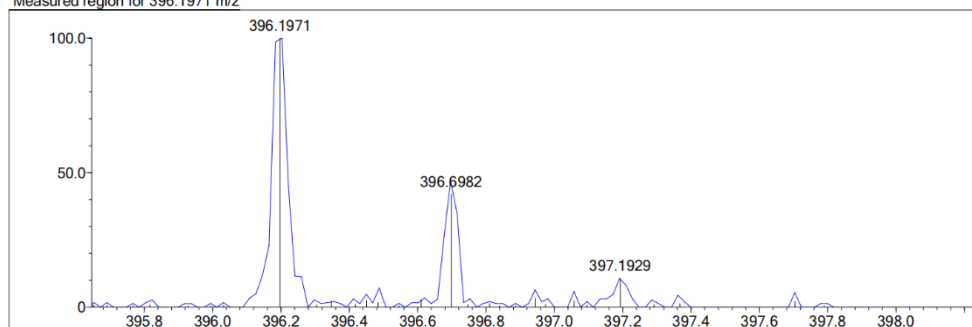
MSn Logic Mode: OR

Max Results: 30

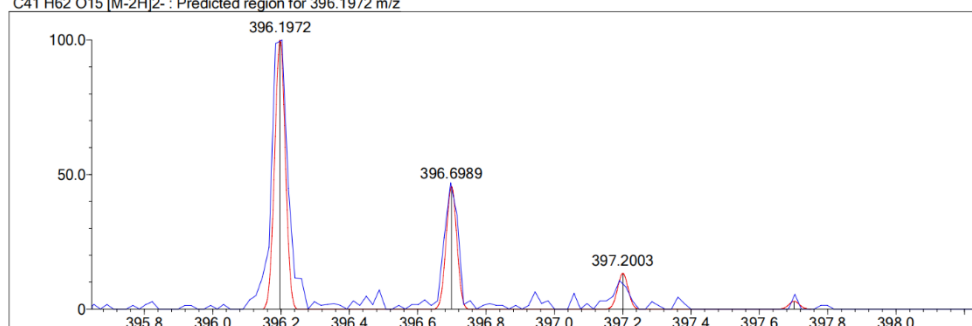
Event#: 2 MS(E-) Ret. Time : 0.400 -&gt; 0.893 Scan#: 62 -&gt; 136



Measured region for 396.1971 m/z



C41 H62 O15 [M-2H]2- : Predicted region for 396.1972 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C41 H62 O15	[M-2H]2-	396.1971	396.1972	-0.1	-0.25	11.0

Figure S8. HRESI-MS spectra of compound 1.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058  
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 31-MAY-2022

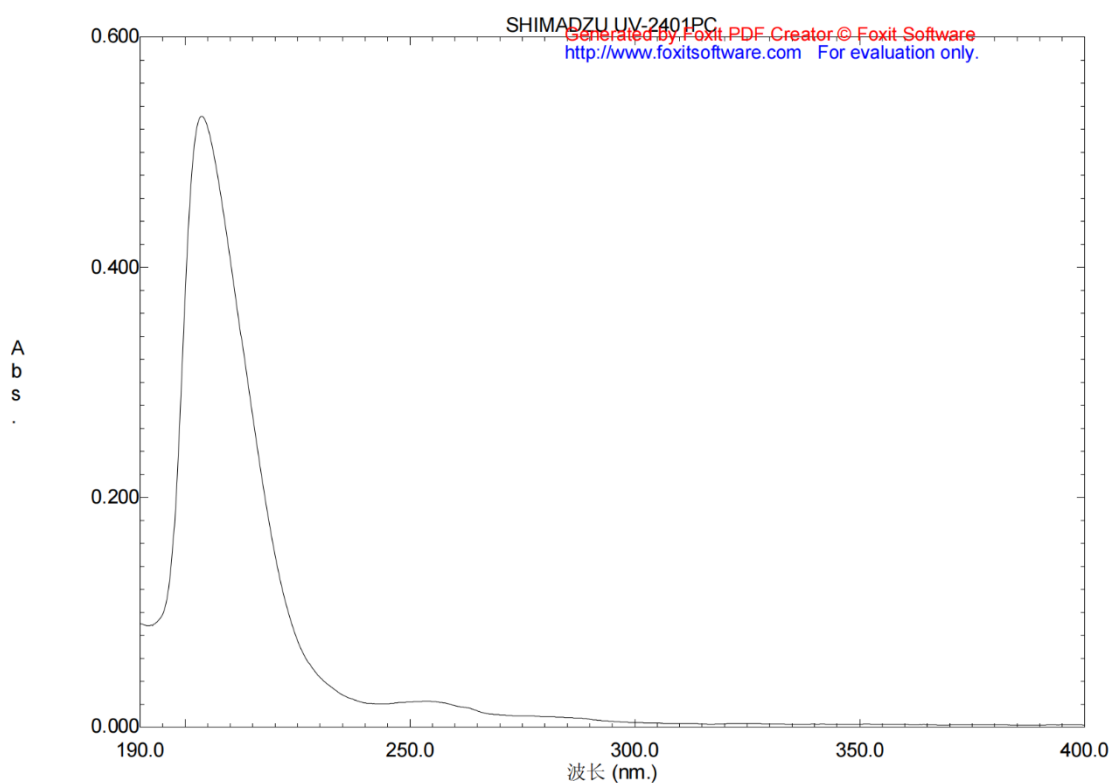
Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum				
5	17.22	0.58	3.36	18.18	16.58				
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	ZKF-22	06:55:35 PM	17.11	SR	0.032	589	100.00	0.187	25.1
2	ZKF-22	06:55:42 PM	16.58	SR	0.031	589	100.00	0.187	25.1
3	ZKF-22	06:55:48 PM	17.11	SR	0.032	589	100.00	0.187	25.1
4	ZKF-22	06:55:54 PM	17.11	SR	0.032	589	100.00	0.187	25.0
5	ZKF-22	06:56:01 PM	18.18	SR	0.034	589	100.00	0.187	25.0

Figure S9. Optical rotations spectrum of compound 1.



文件名: ZKF-22

ZKF-22

创建于: 20:17 22-06-01

数据: 原始

样品浓度: 0.0748毫克/毫升

溶剂: 甲醇

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	253.20	0.0224
2	203.60	0.5311

Figure S10. UV spectrum of compound 1.



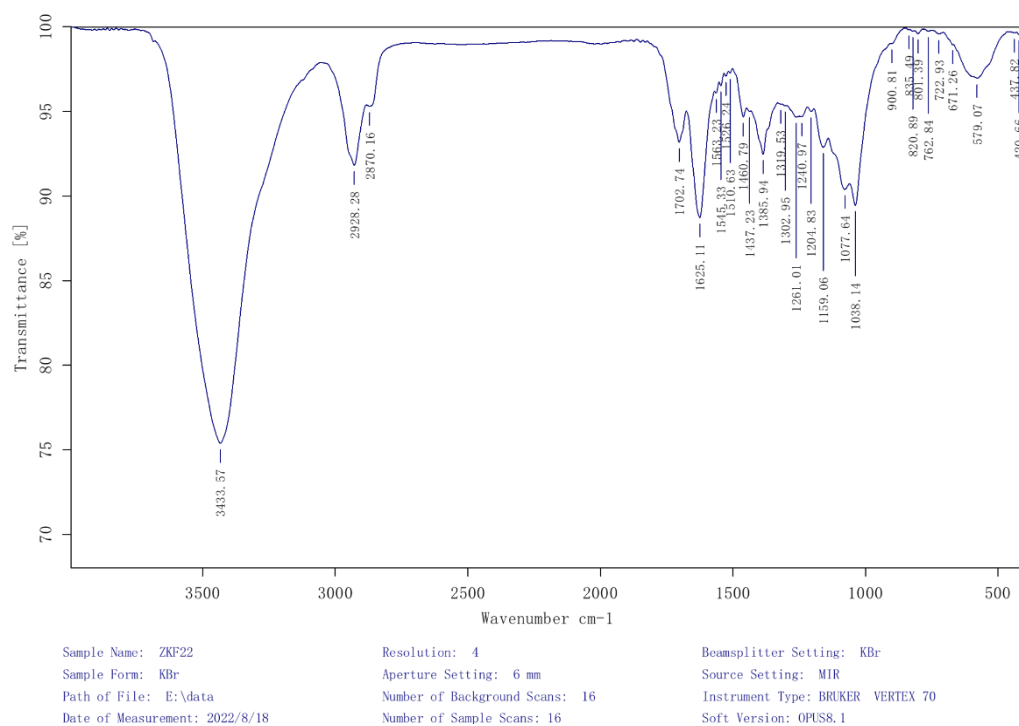
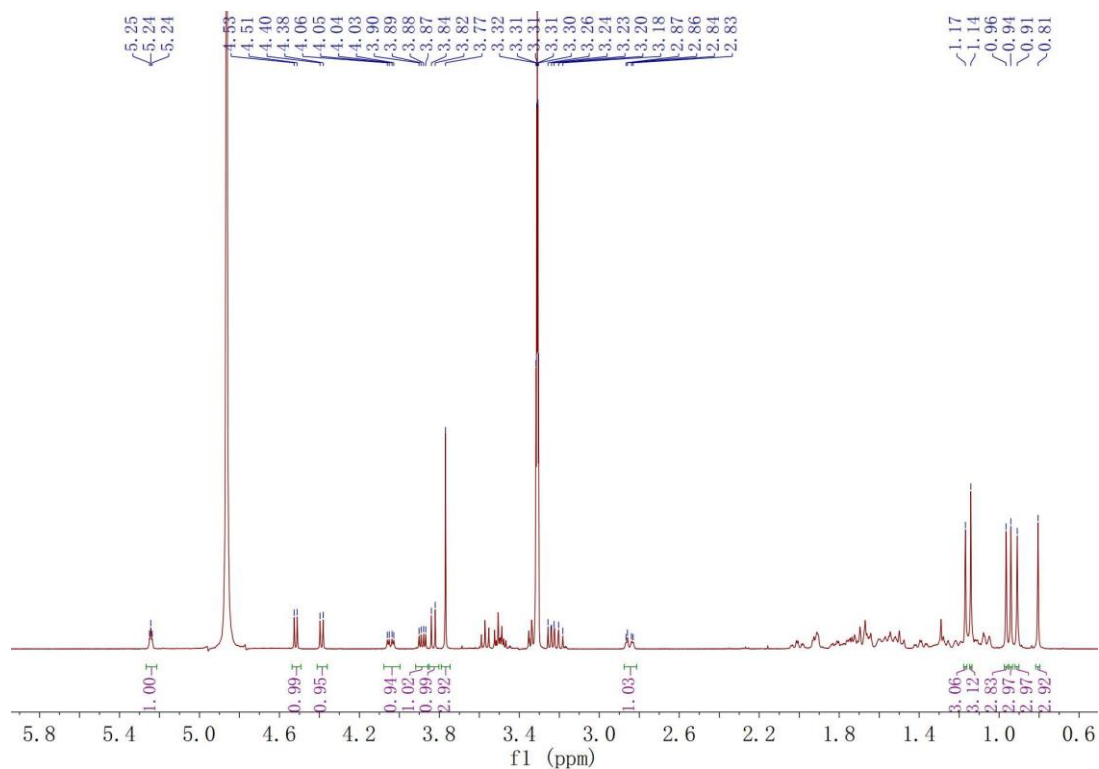


Figure S11. IR spectrum of compound 1.

Figure S12. <sup>1</sup>H NMR spectrum of compound 2 (methanol-*d*<sub>4</sub>, 500MHz).

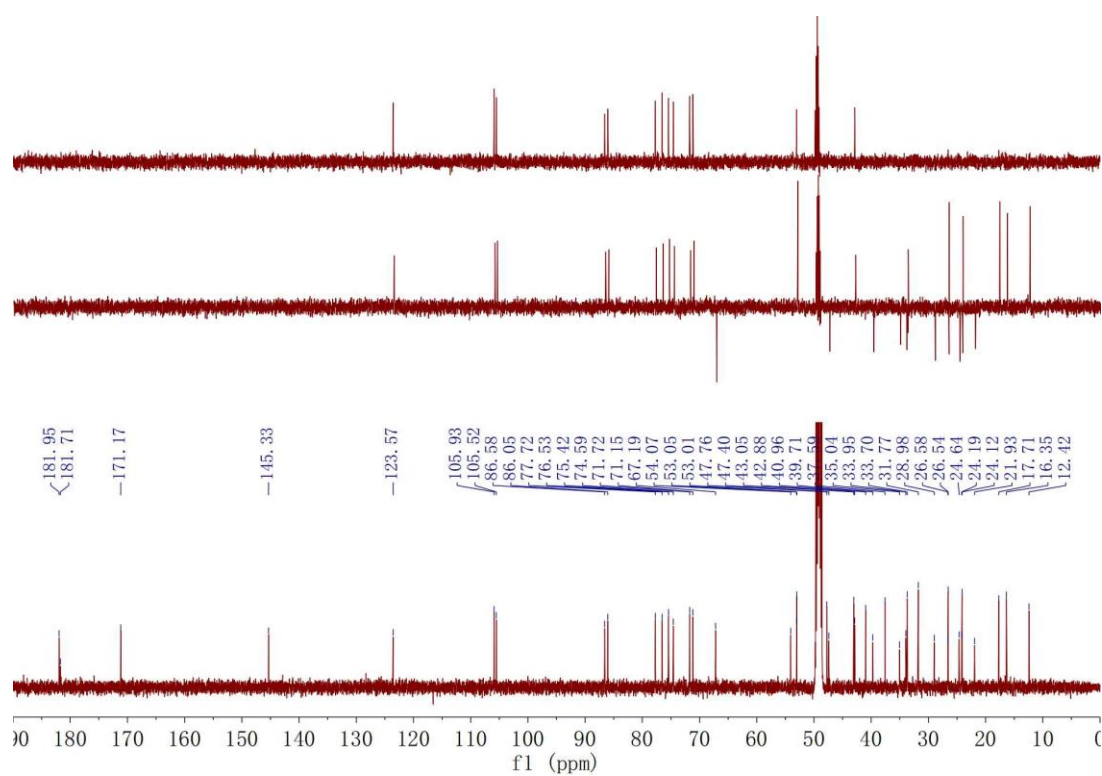


Figure S13. <sup>13</sup>C NMR spectrum of compound 2 (methanol-*d*<sub>4</sub>, 125MHz).

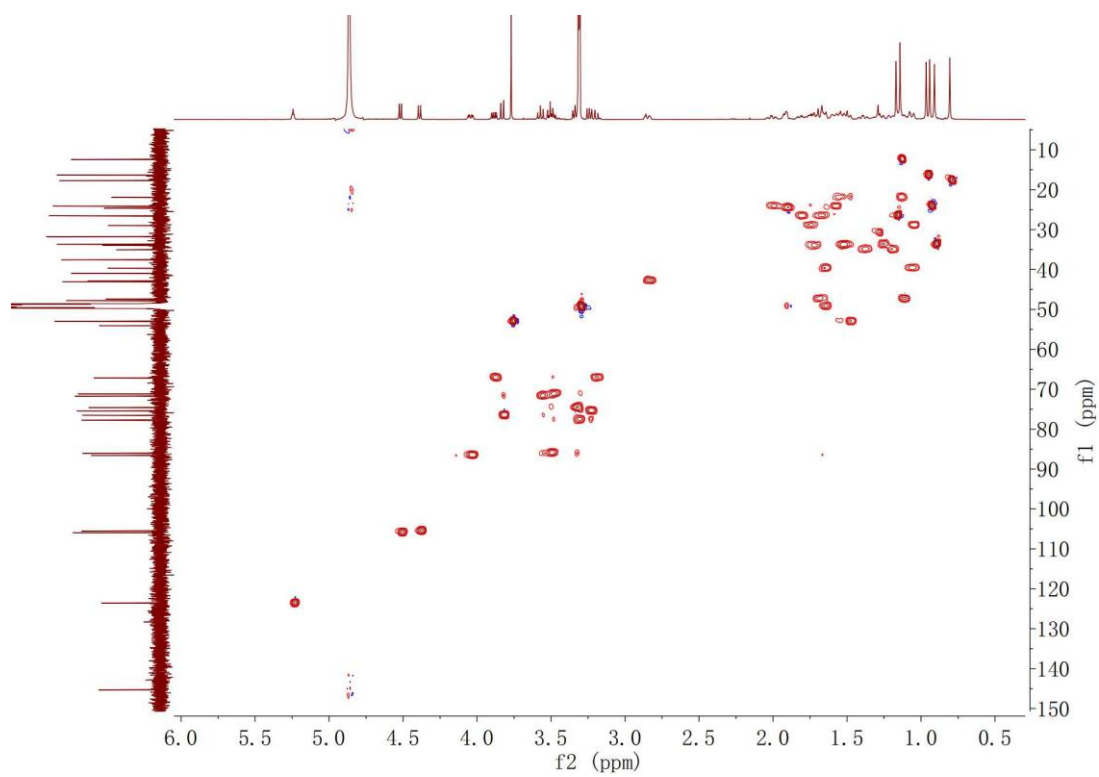


Figure S14. HSQC spectrum of compound 2.

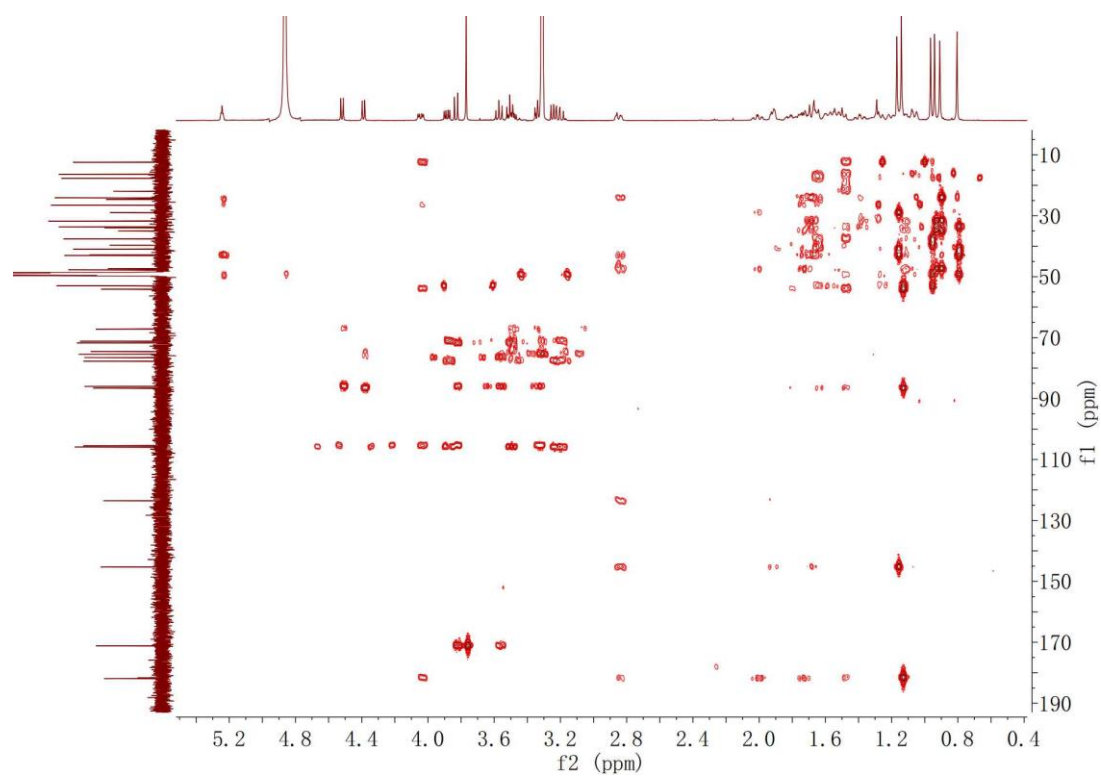


Figure S15. HMBC spectrum of compound 2.

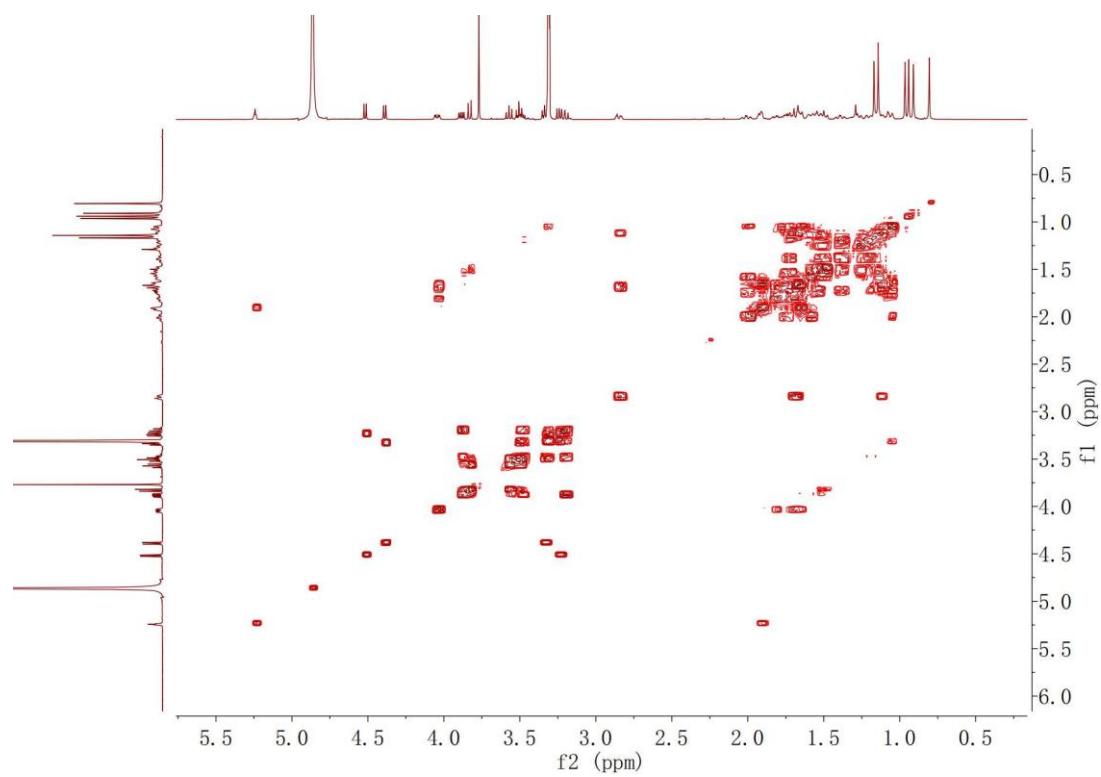


Figure S16.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2.

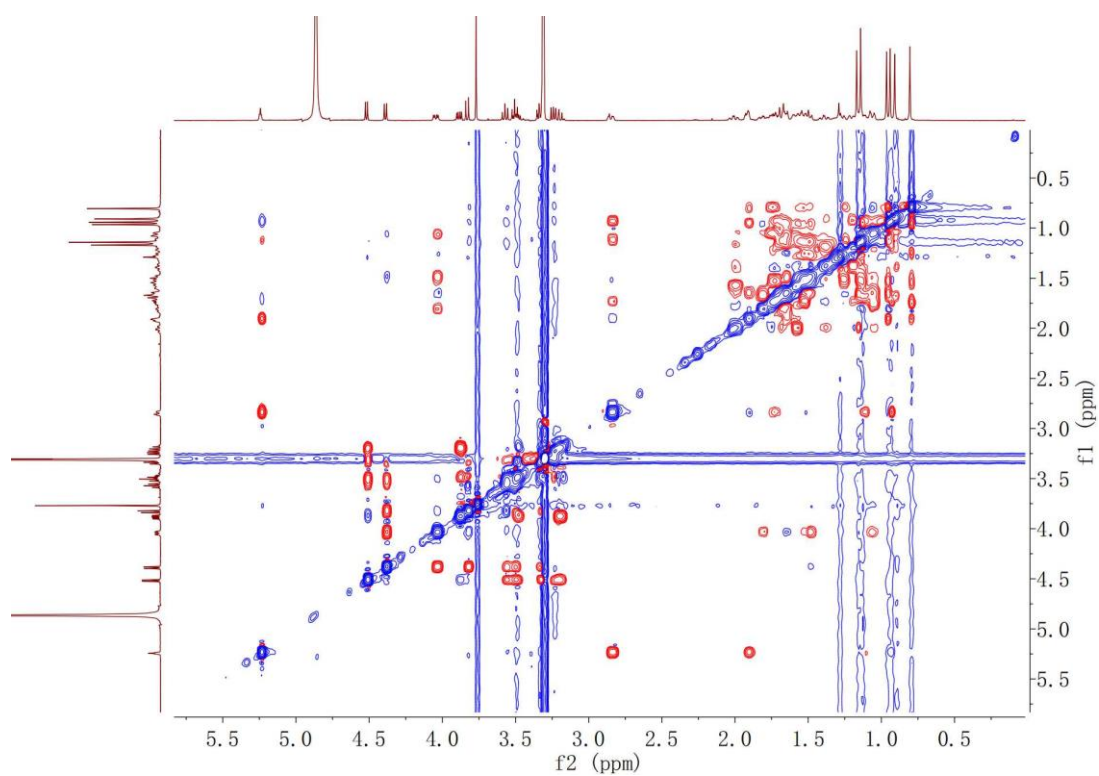


Figure S17. ROESY spectrum of compound 2.

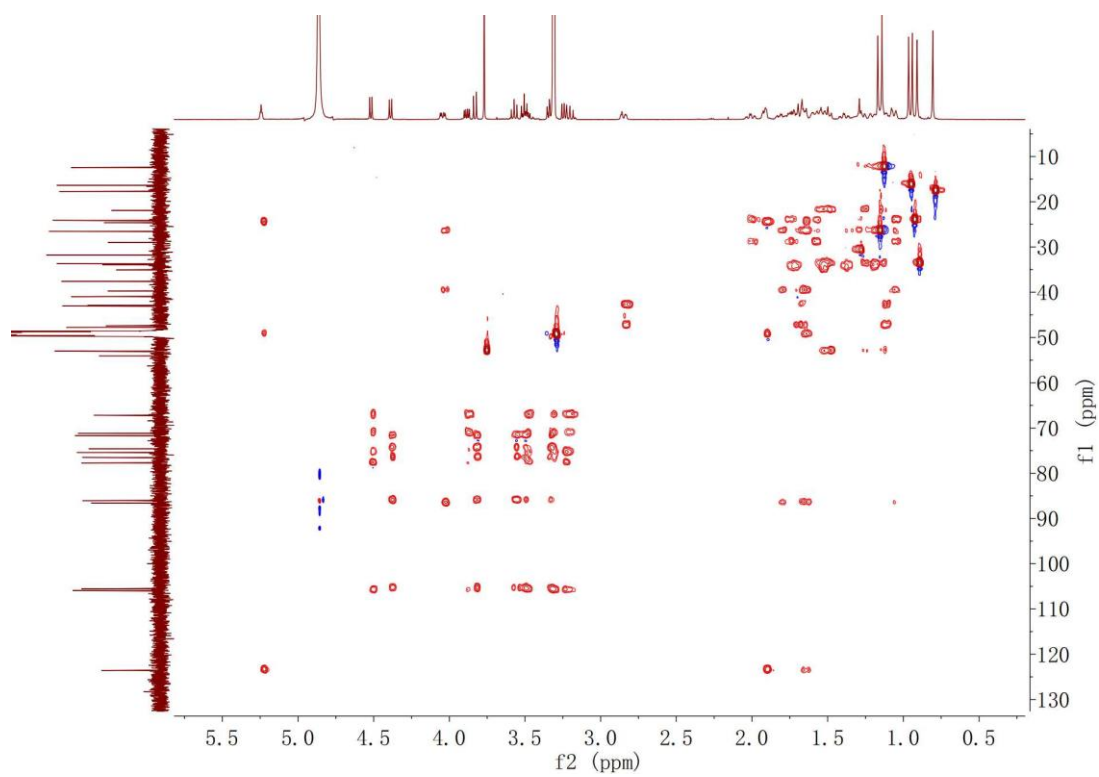


Figure S18. HSQC-TOCSY spectrum of compound 2.

Formula Predictor Report - ZKF31.lcd

Page 1 of 1

Data File: E:\DATA\2022\0518\ZKF31.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	10	50	Si	4	0	0	Se	2	0	0					
N	3	0	20	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 58

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: OR

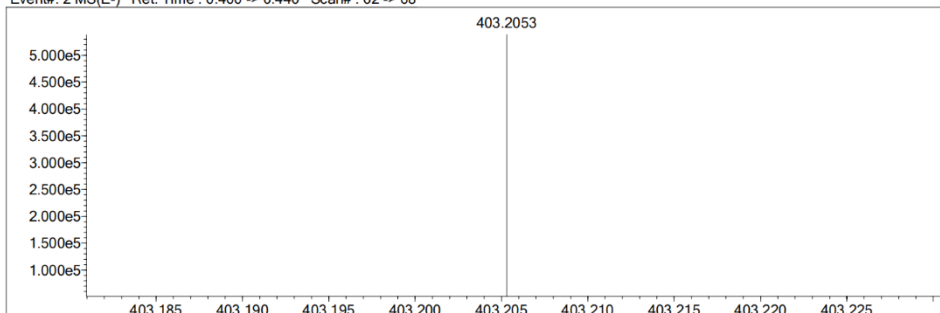
Electron Ions: both

Use MSn Info: yes

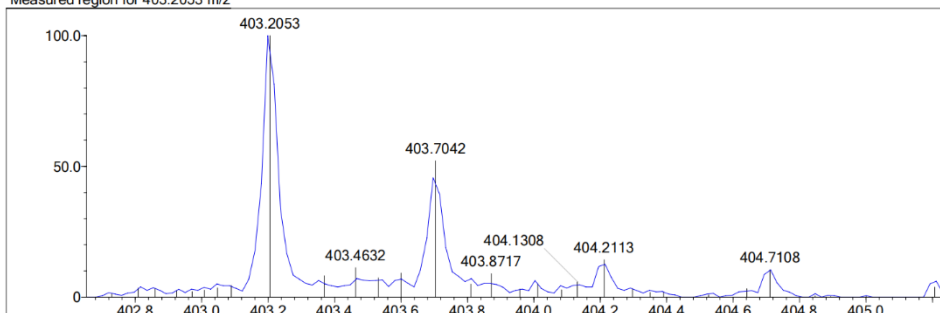
Isotope Res: 10000

Max Results: 30

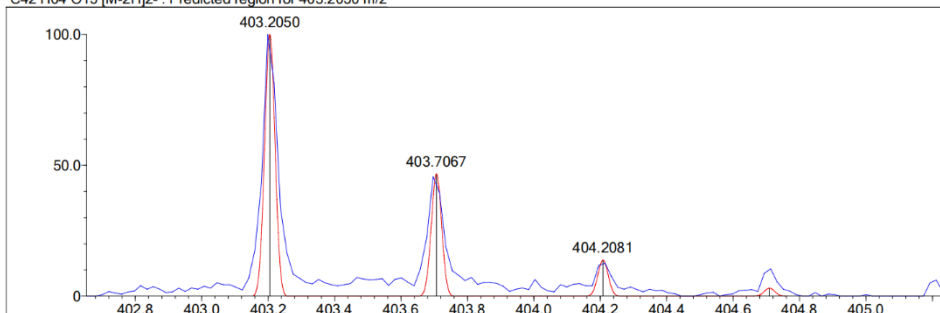
Event#: 2 MS(E-) Ret. Time : 0.400 -&gt; 0.440 Scan#: 62 -&gt; 68



Measured region for 403.2053 m/z



C42 H64 O15 [M-2H]2- : Predicted region for 403.2050 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H64 O15	[M-2H]2-	403.2053	403.2050	0.3	0.74	11.0

Figure S19. HRESI-MS spectra of compound 2.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058  
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 31-MAY-2022

Set Temperature : OFF

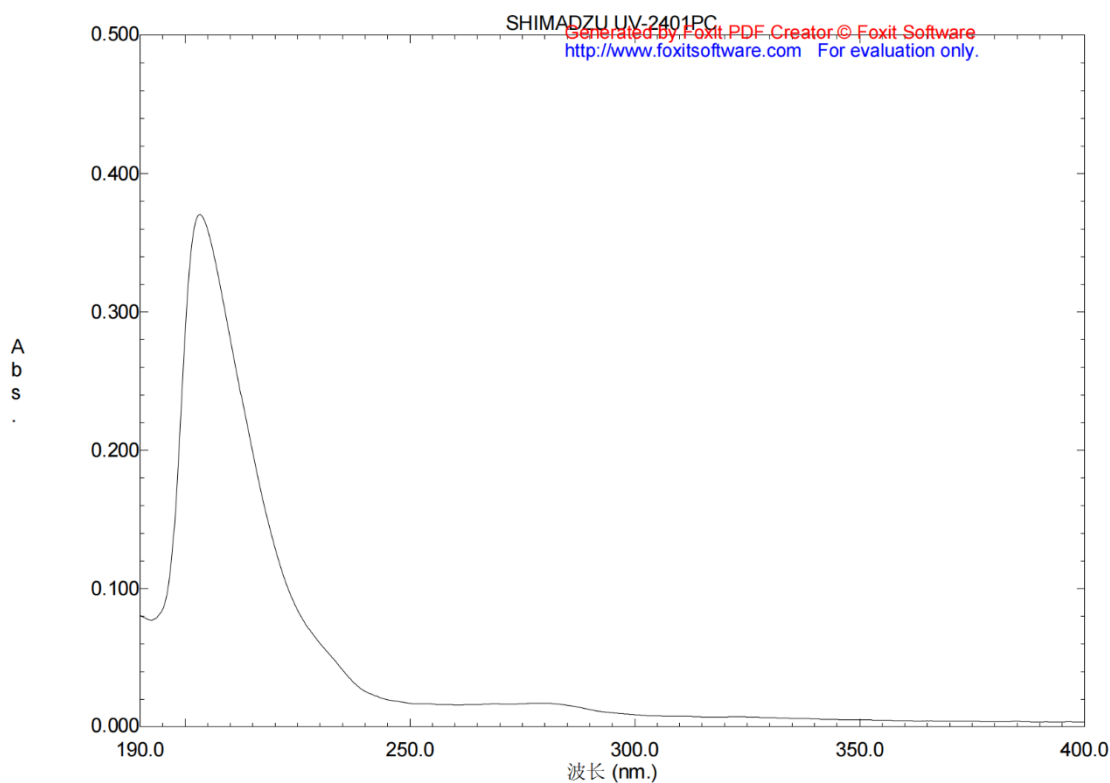
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Delay between Measurement : Disabled

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5	4.31	0.59	13.68	5.06	3.48

<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	ZKF-31	07:03:52 PM	5.06	SR	0.0045	589	100.00	0.089	25.2
2	ZKF-31	07:04:01 PM	4.04	SR	0.0036	589	100.00	0.089	25.2
3	ZKF-31	07:04:09 PM	4.49	SR	0.0040	589	100.00	0.089	25.2
4	ZKF-31	07:04:17 PM	4.49	SR	0.0040	589	100.00	0.089	25.1
5	ZKF-31	07:04:25 PM	3.48	SR	0.0031	589	100.00	0.089	25.1

**Figure S20.** Optical rotations spectrum of compound 2.



文件名: ZKF-31

ZKF-31

创建于: 20:23 22-06-01

数据: 原始

样品浓度: 0.0356毫克/毫升  
溶剂: 甲醇

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	279.40	0.0169
2	203.20	0.3704

**Figure S21.** UV spectrum of compound 2.

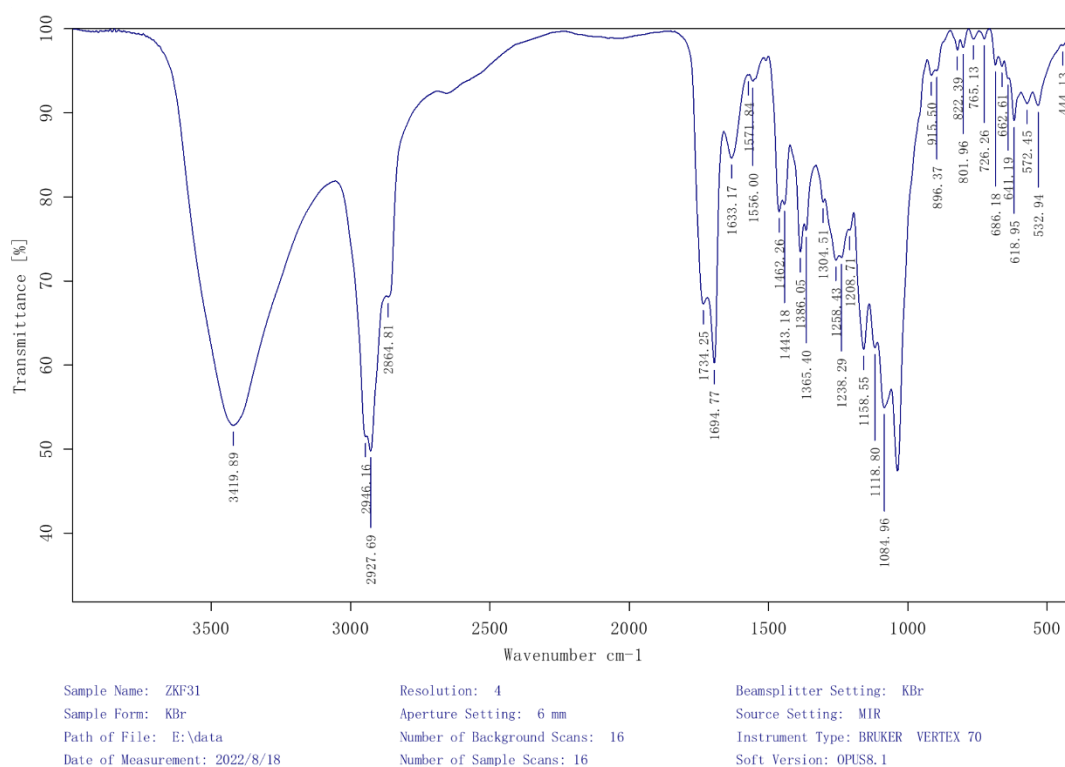
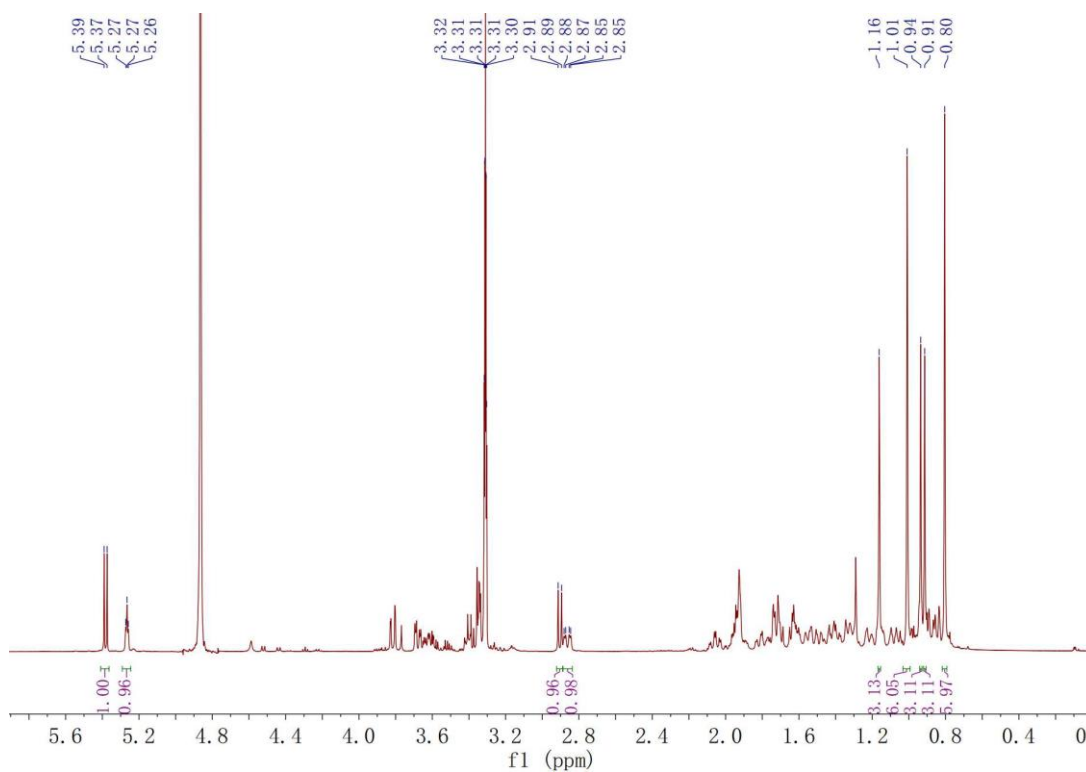


Figure S22. IR spectrum of compound 2.

Figure S23.  $^1\text{H}$  NMR spectrum of compound 3 (methanol- $d_4$ , 500 MHz).



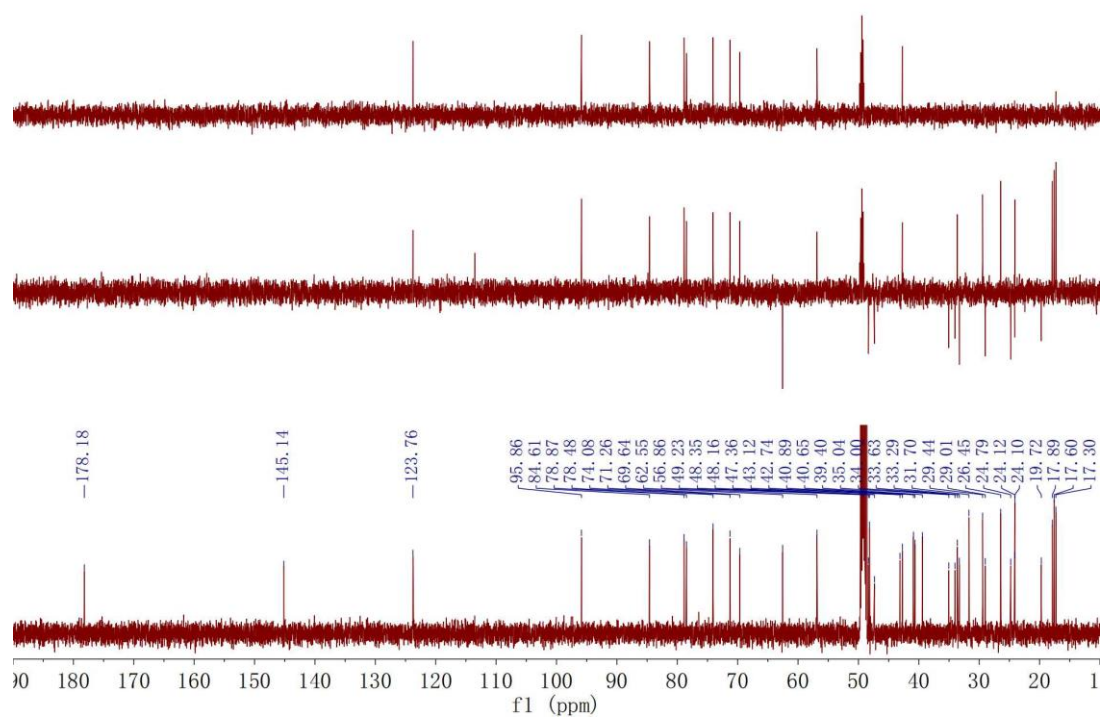


Figure S24. <sup>13</sup>C NMR spectrum of compound 3 (methanol-*d*<sub>4</sub>, 125MHz).

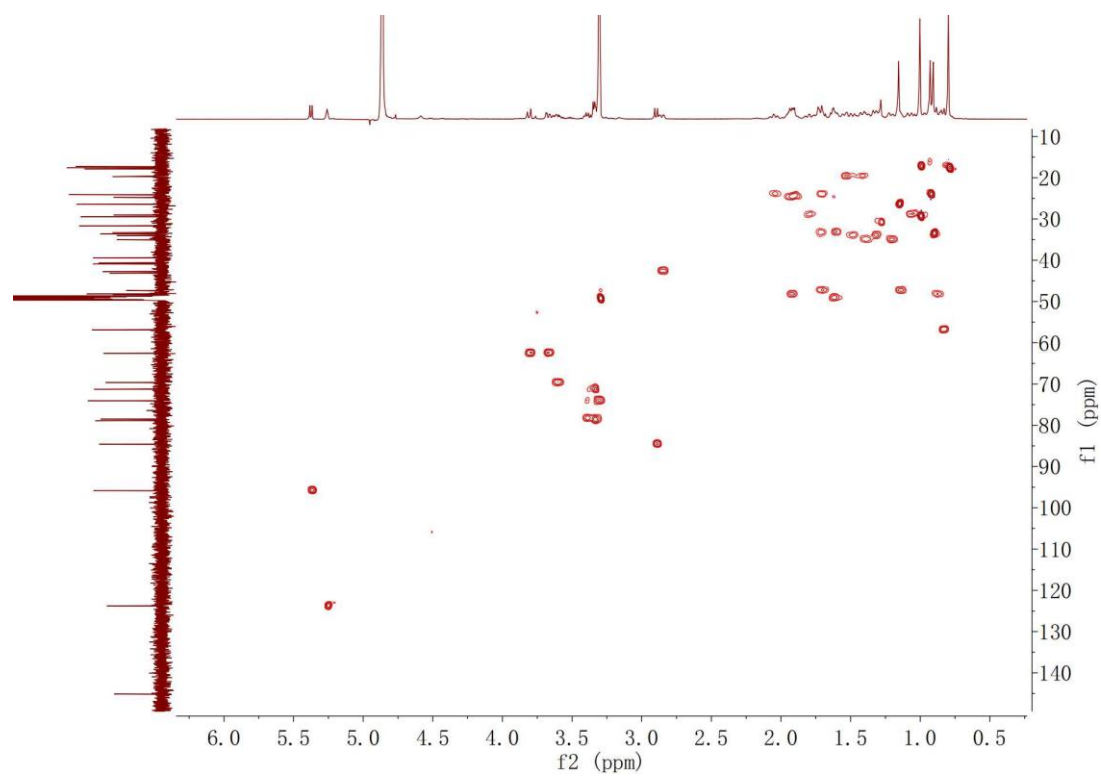


Figure S25. HSQC spectrum of compound 3.



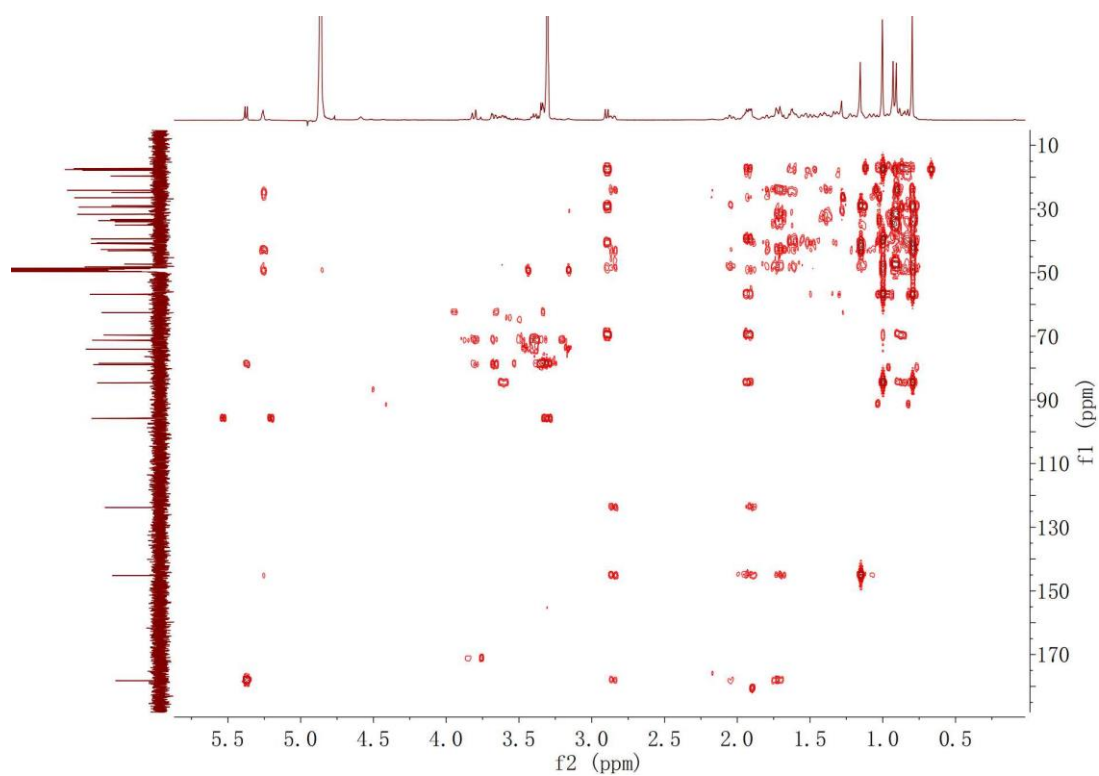


Figure S26. HMBC spectrum of compound 3.

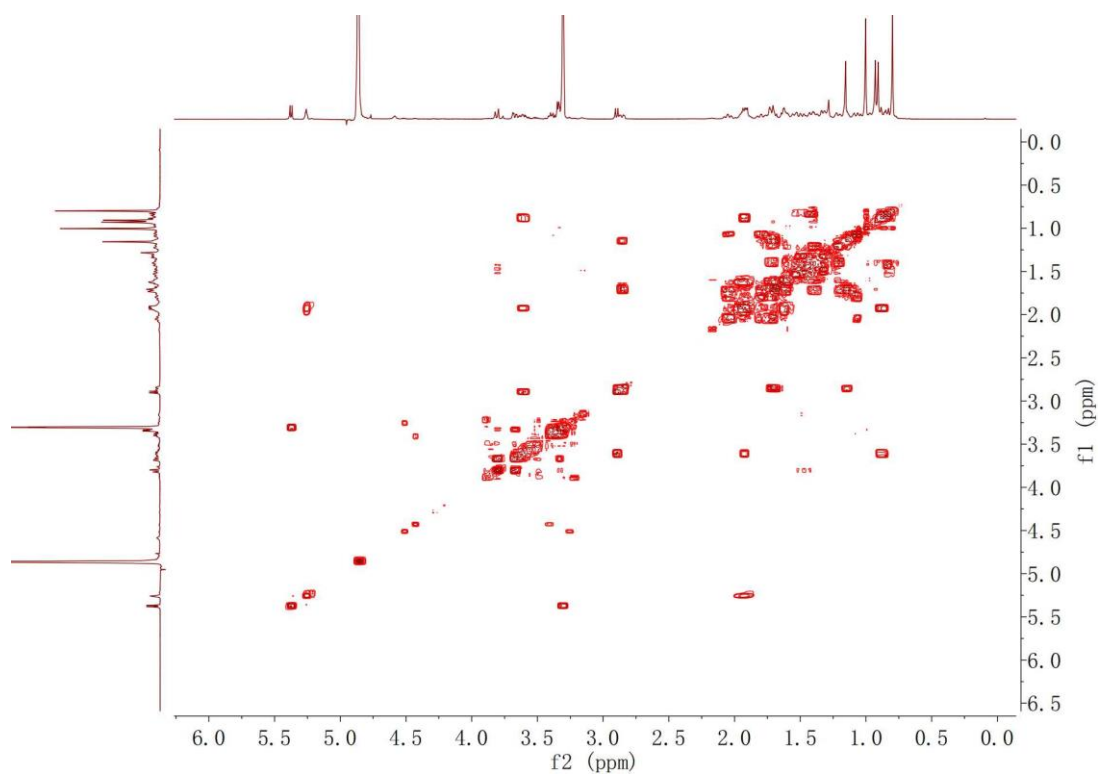
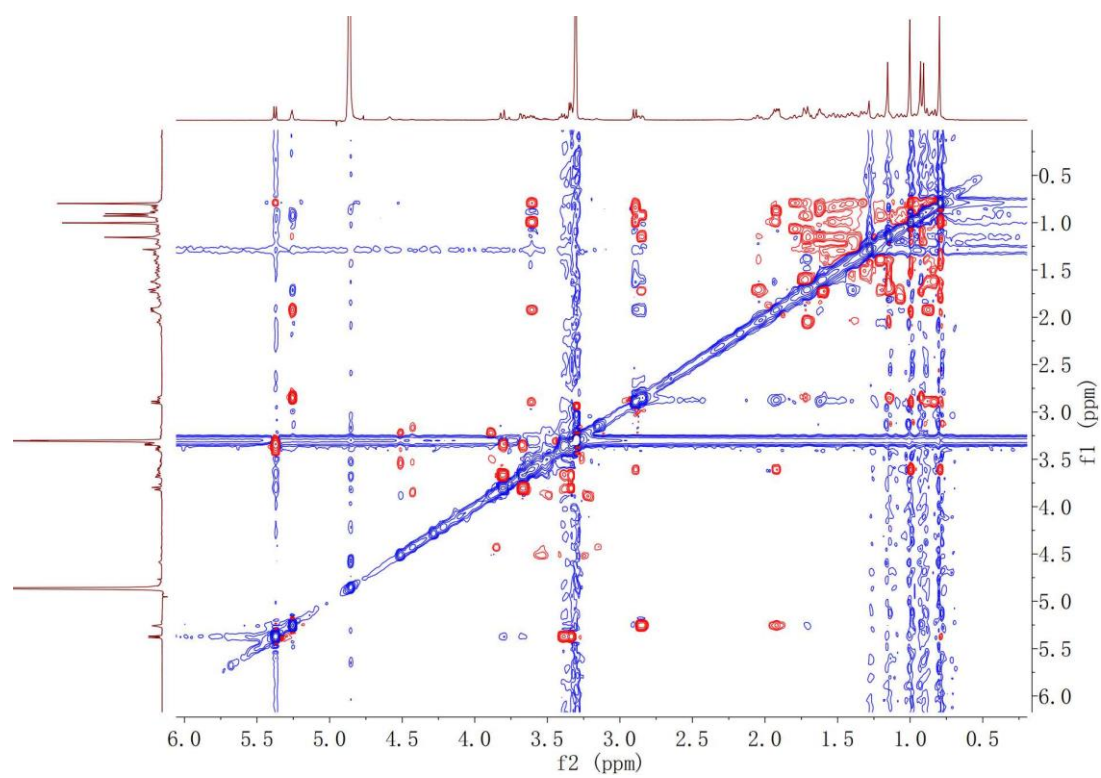


Figure S27.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 3.



**Figure S28.** ROESY spectrum of compound 3.

Formula Predictor Report - ZKF17.lcd

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Data File: E:\DATA\2022\1021\1\ZKF17.lcd

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2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	10	60	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: OR

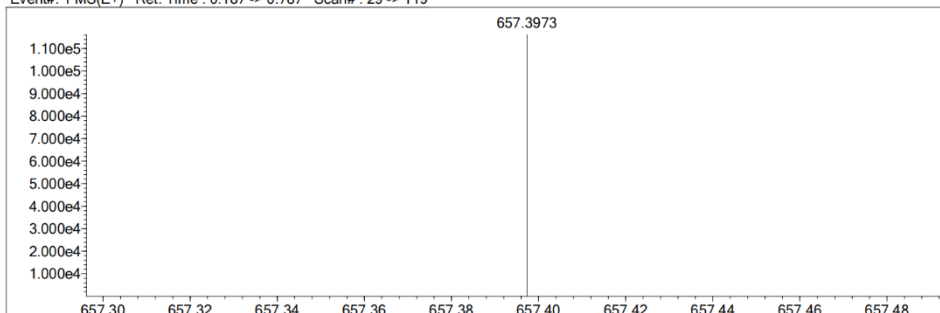
Electron Ions: both

Use MSn Info: yes

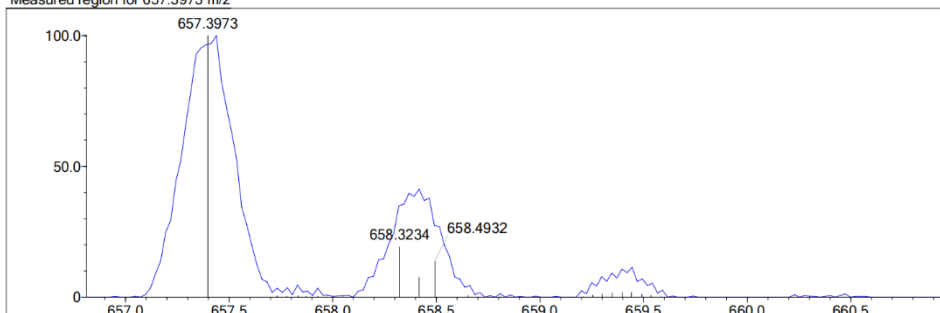
Isotope Res: 10000

Max Results: 30

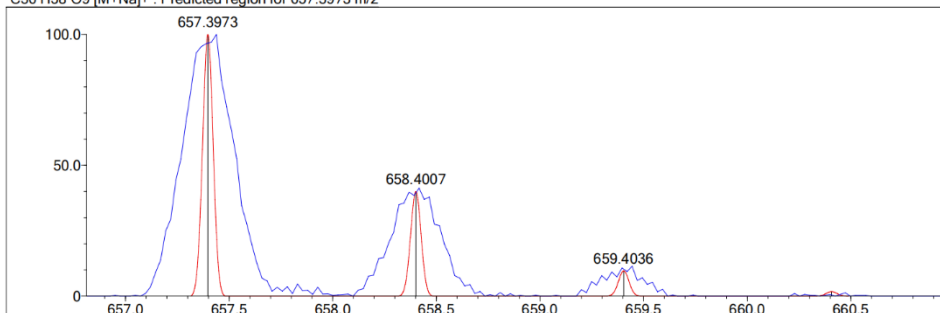
Event#: 1 MS(E+) Ret. Time : 0.187 -&gt; 0.787 Scan#: 29 -&gt; 119



Measured region for 657.3973 m/z



C36 H58 O9 [M+Na]+ : Predicted region for 657.3973 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C36 H58 O9	[M+Na]+	657.3973	657.3973	-0.0	0.00	8.0

Figure S29. HRESI-MS spectra of compound 3.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058  
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 17-OCT-2022

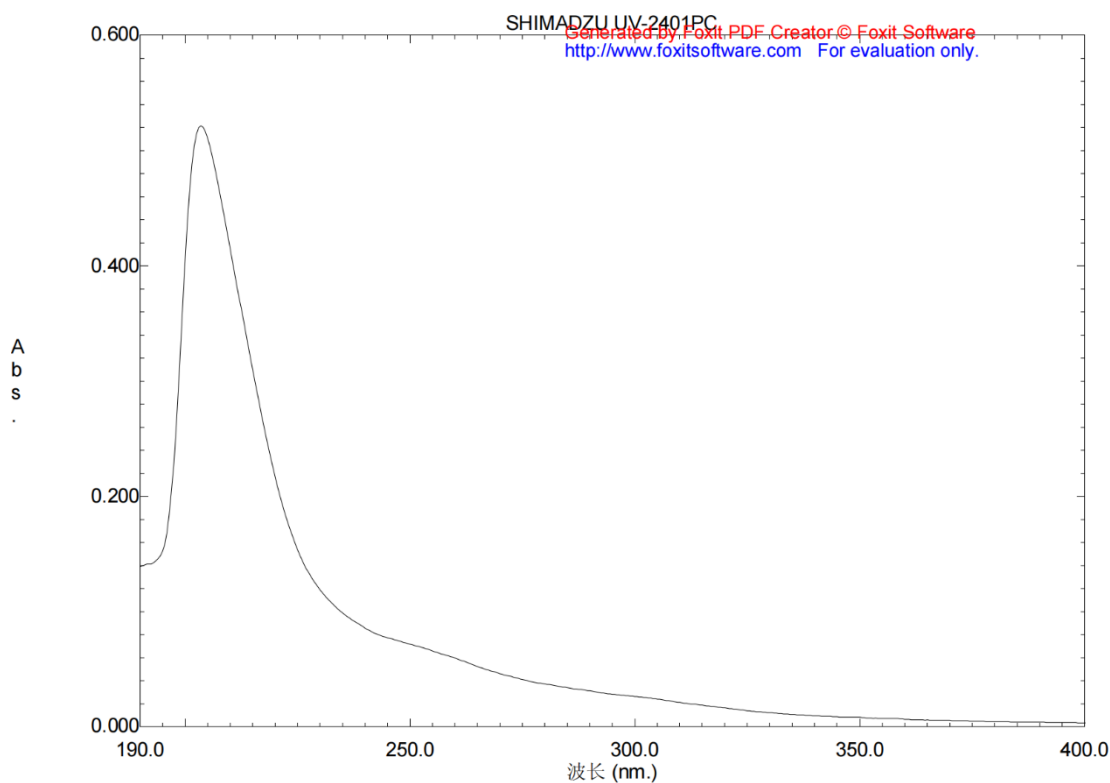
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Time Delay : Disabled

Delay between Measurement : Disabled

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5	23.14	0.64	2.76	23.84	22.67					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	ZKF17	07:15:53 PM	23.84	SR	0.041	589	100.00	0.172	18.6	
2	ZKF17	07:15:59 PM	22.67	SR	0.039	589	100.00	0.172	18.6	
3	ZKF17	07:16:06 PM	22.67	SR	0.039	589	100.00	0.172	18.6	
4	ZKF17	07:16:12 PM	23.84	SR	0.041	589	100.00	0.172	18.6	
5	ZKF17	07:16:18 PM	22.67	SR	0.039	589	100.00	0.172	18.5	

**Figure S30.** Optical rotations spectrum of compound 3.



文件名: ZKF17

ZKF17 ———

创建于: 14:44 22-10-20

数据: 原始

样品浓度: 0.0573毫克/毫升

溶剂: 甲醇

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.5

否. 波长 (nm.) Abs.  
1 203.50 0.5213

**Figure S31.** UV spectrum of compound 3.

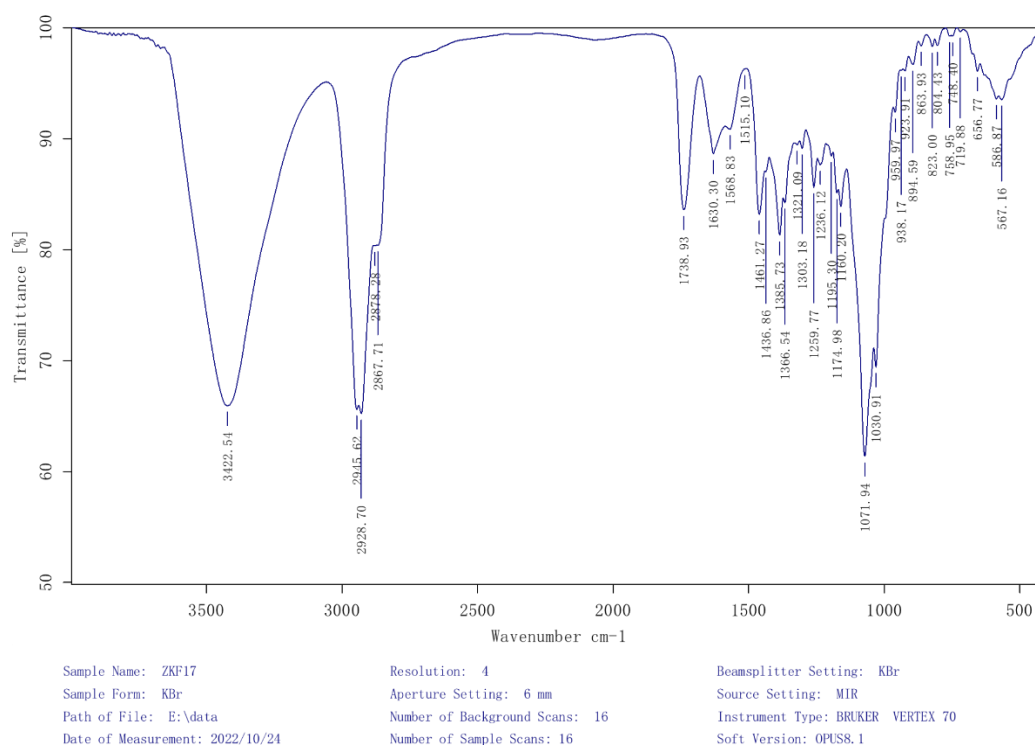


Figure S32. IR spectrum of compound 3.

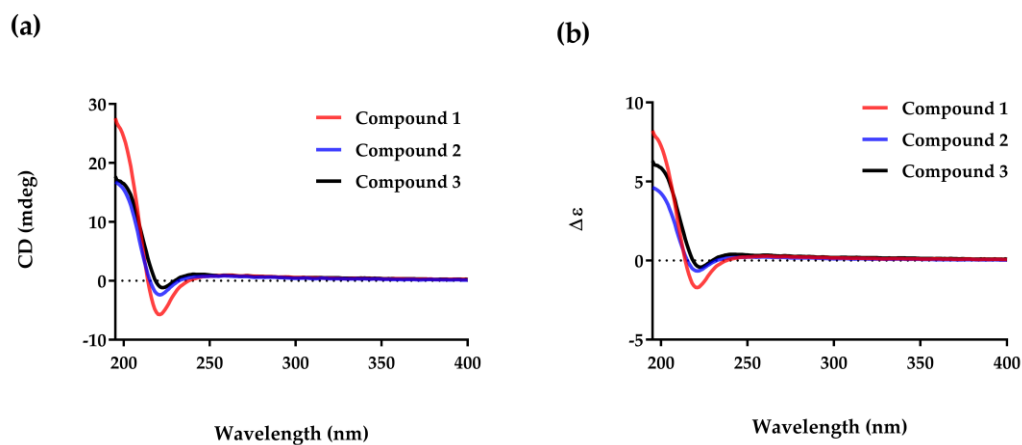


Figure S33. The CD spectra of compounds 1, 2, and 3 in MeOH.

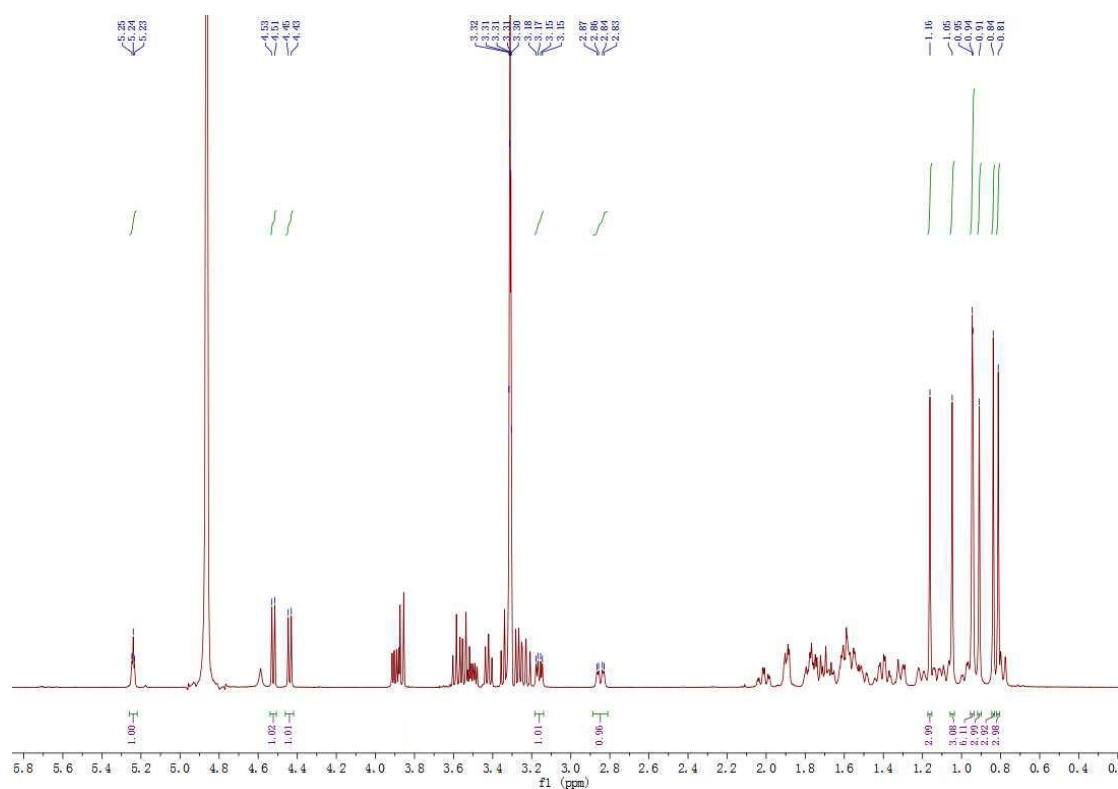


Figure S34. <sup>1</sup>H NMR spectrum of compound 4 (methanol-*d*<sub>4</sub>, 500MHz).

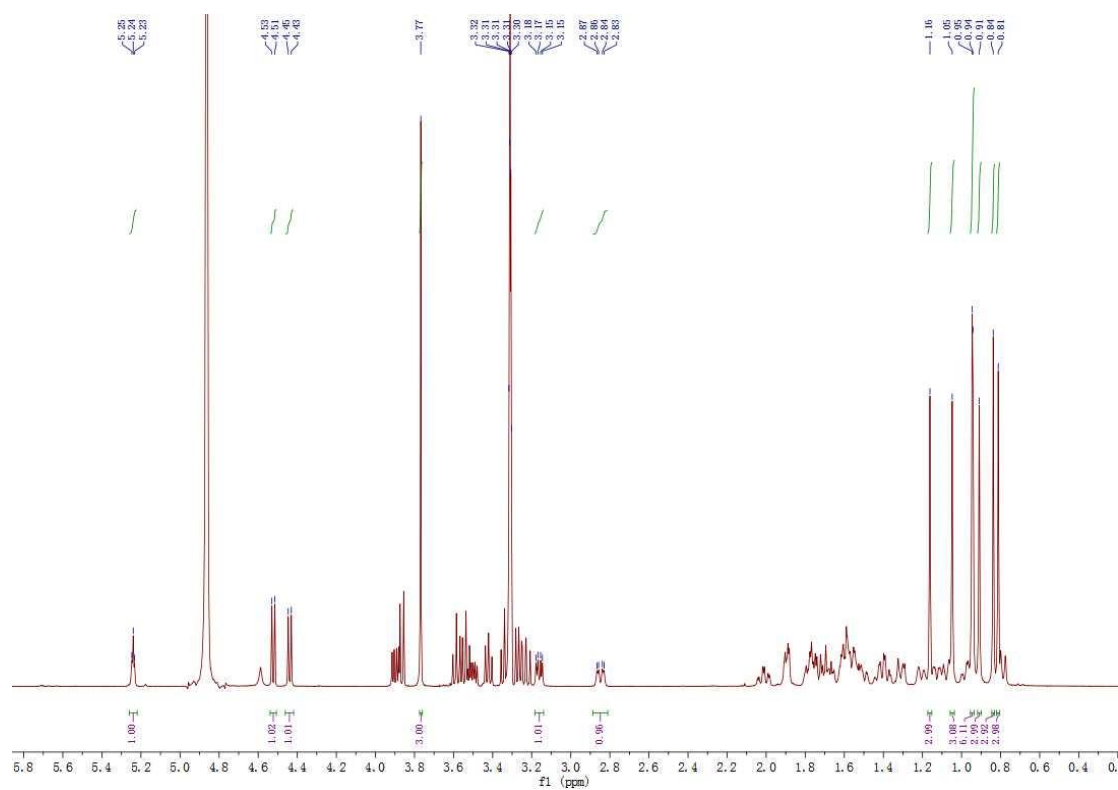


Figure S35. <sup>1</sup>H NMR spectrum of compound 5 (methanol-*d*<sub>4</sub>, 500MHz).

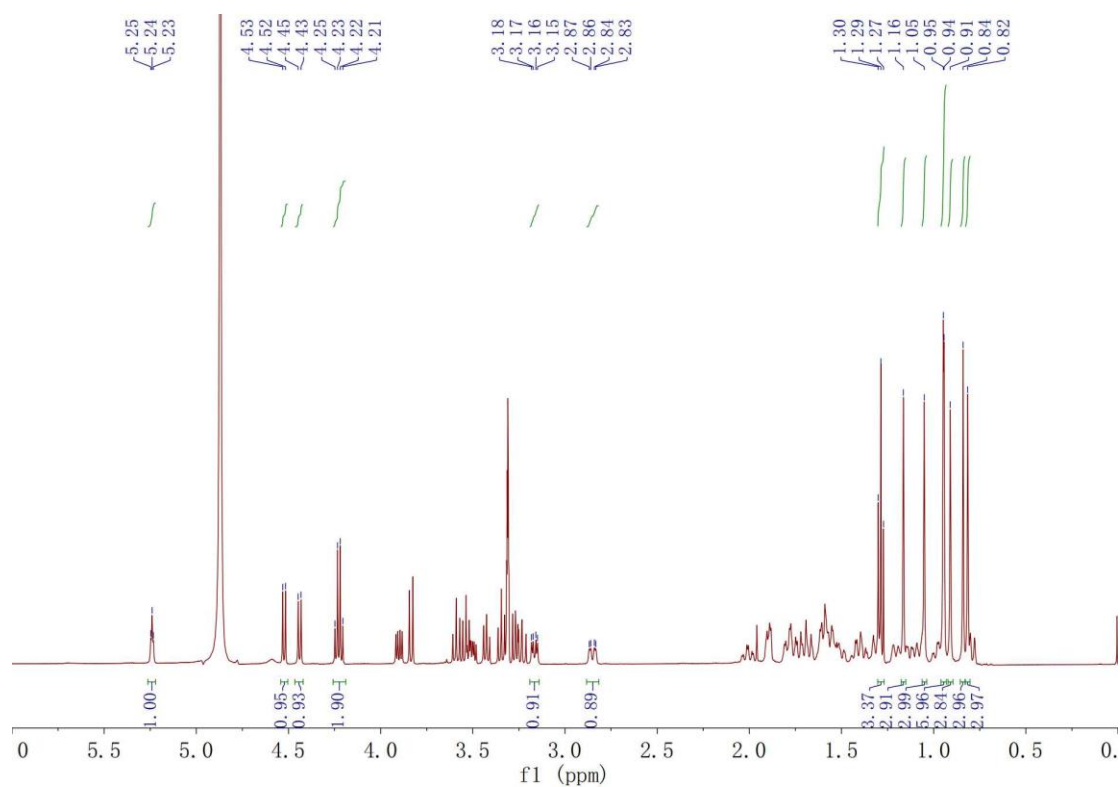


Figure S36. <sup>1</sup>H NMR spectrum of compound 6 (methanol-*d*<sub>4</sub>, 500 MHz).

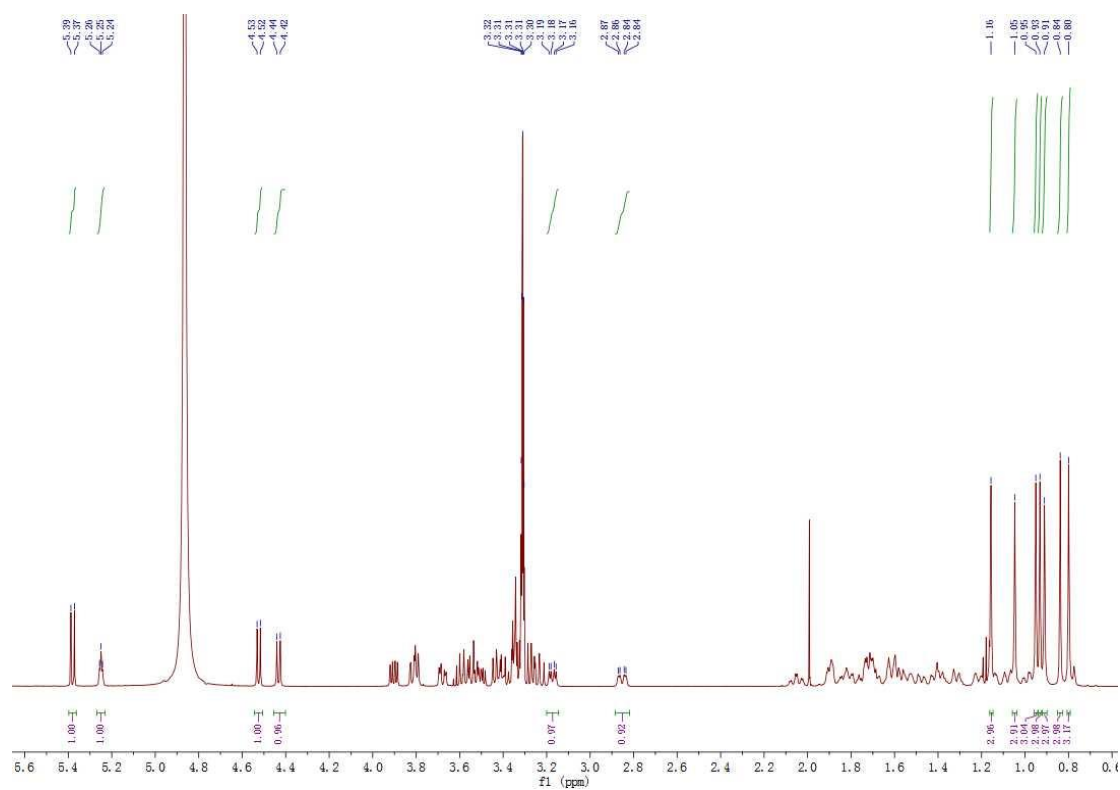


Figure S37. <sup>1</sup>H NMR spectrum of compound 7 (methanol-*d*<sub>4</sub>, 500 MHz).

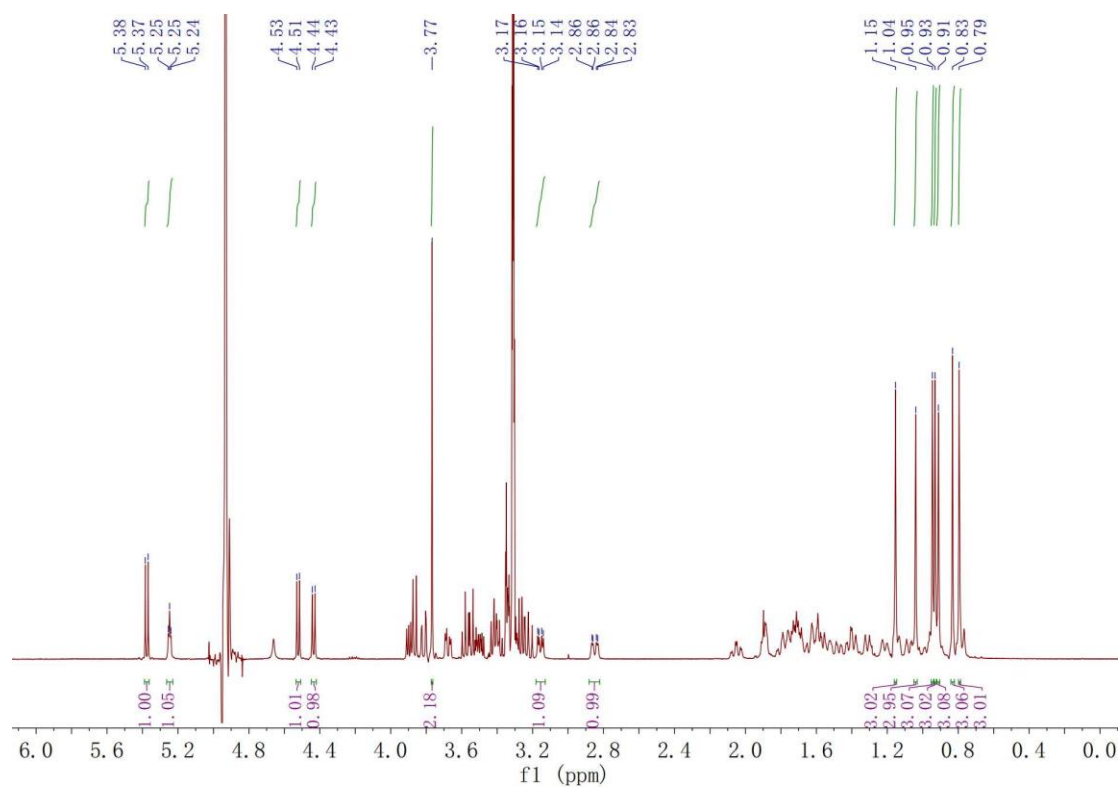


Figure S38. <sup>1</sup>H NMR spectrum of compound 8 (methanol-*d*<sub>4</sub>, 500 MHz).

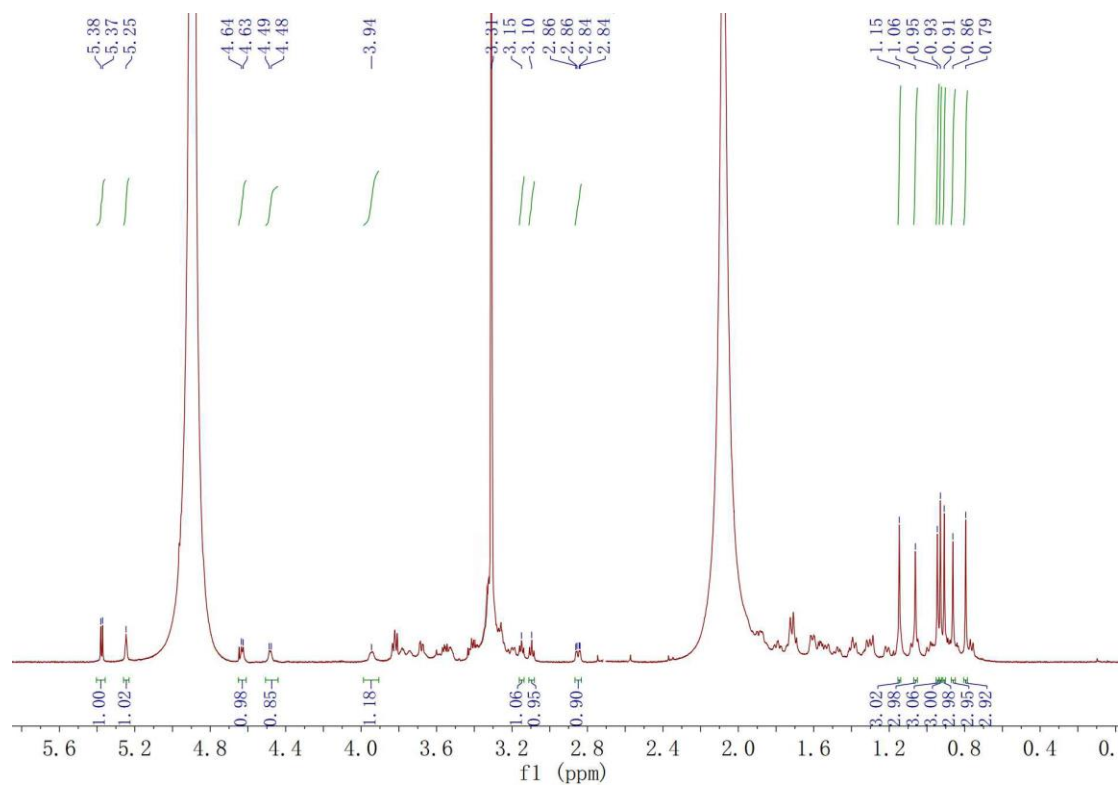


Figure S39. <sup>1</sup>H NMR spectrum of compound 9 (methanol-*d*<sub>4</sub>, 500 MHz).



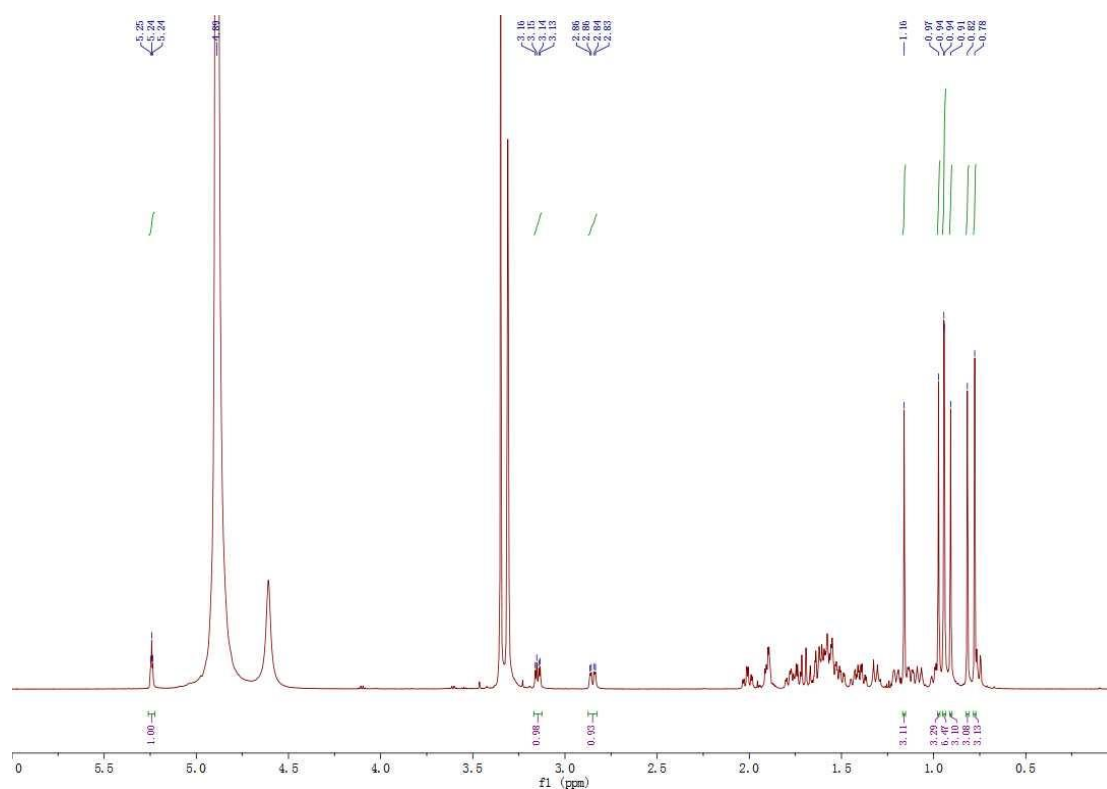


Figure S40. <sup>1</sup>H NMR spectrum of compound **10** (methanol-*d*<sub>4</sub>, 600MHz).

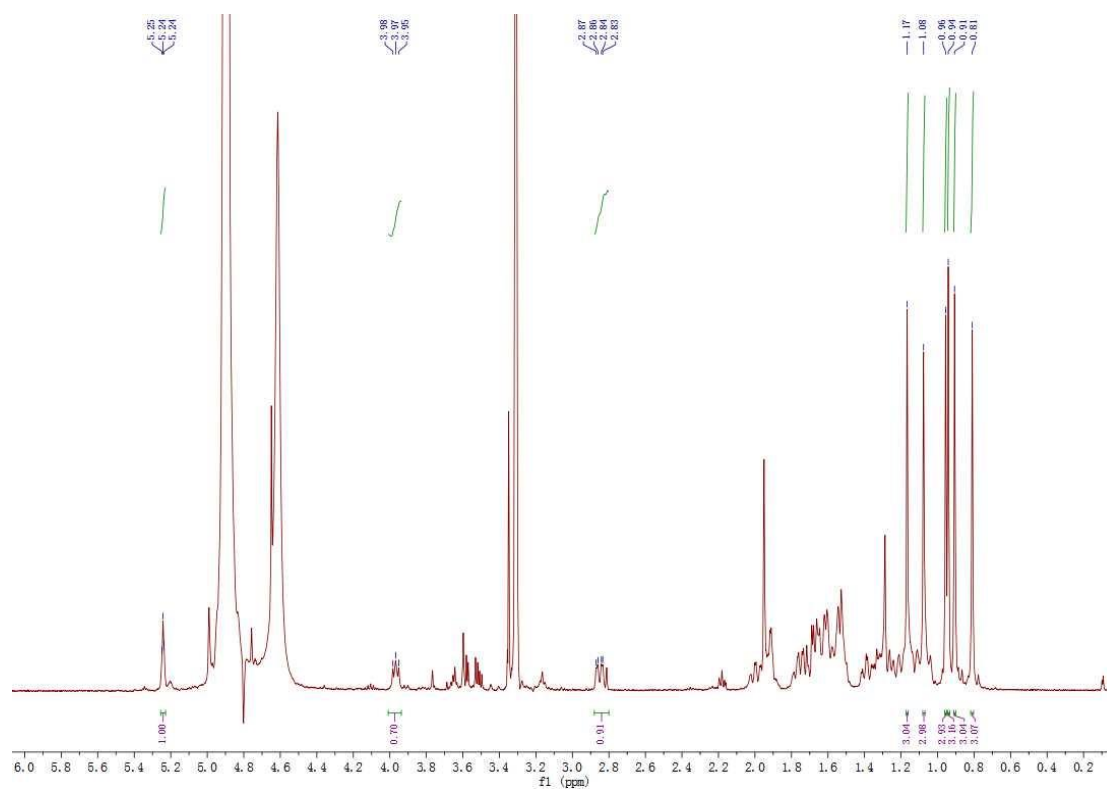


Figure S41. <sup>1</sup>H NMR spectrum of compound **11** (methanol-*d*<sub>4</sub>, 500MHz).

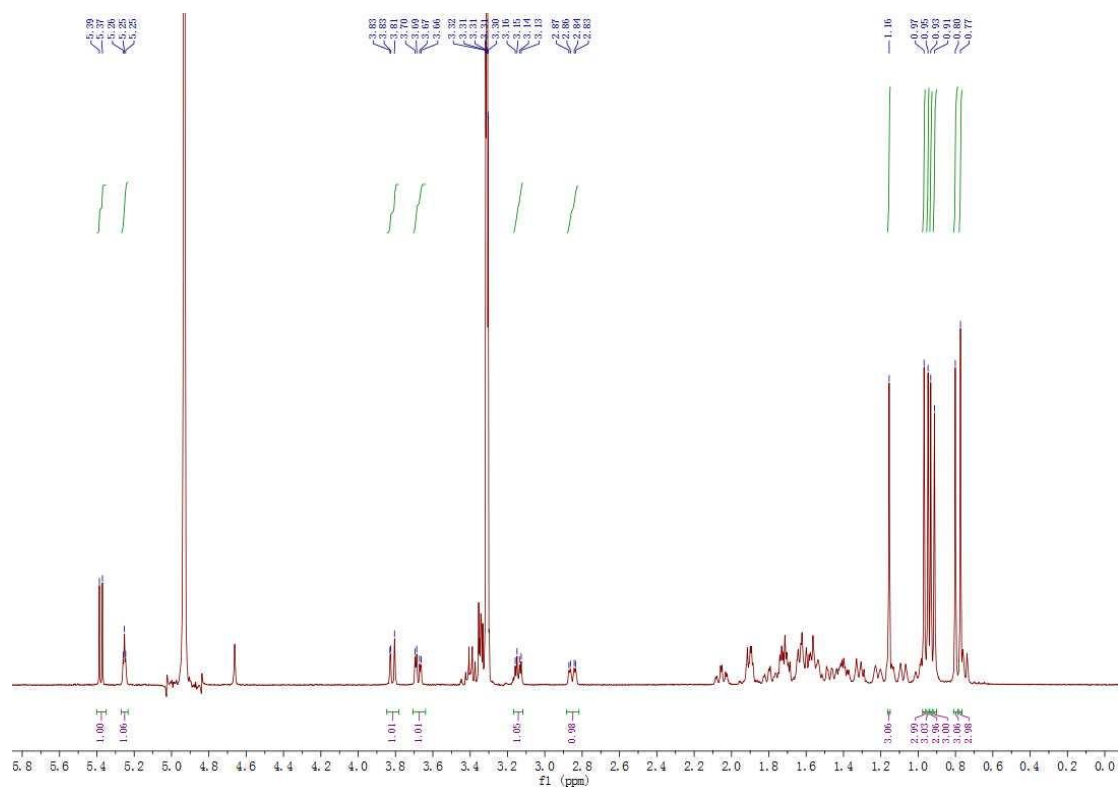


Figure S42. <sup>1</sup>H NMR spectrum of compound 12 (methanol-*d*<sub>4</sub>, 500 MHz).

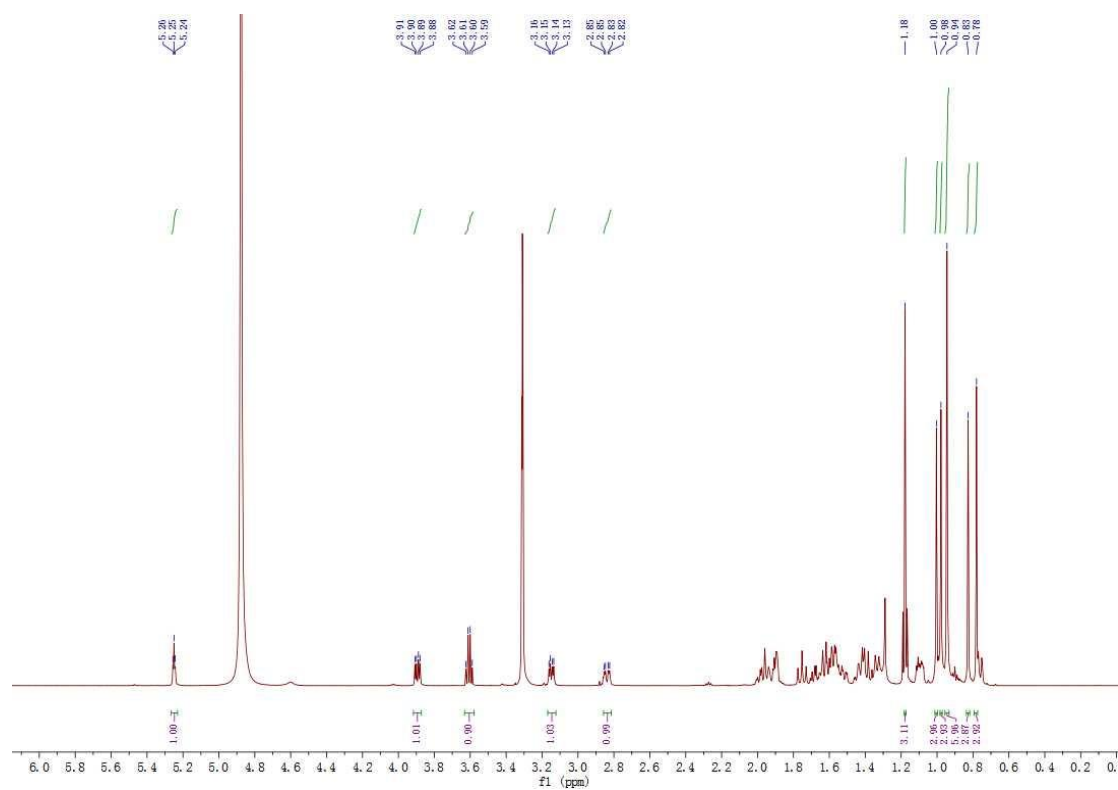
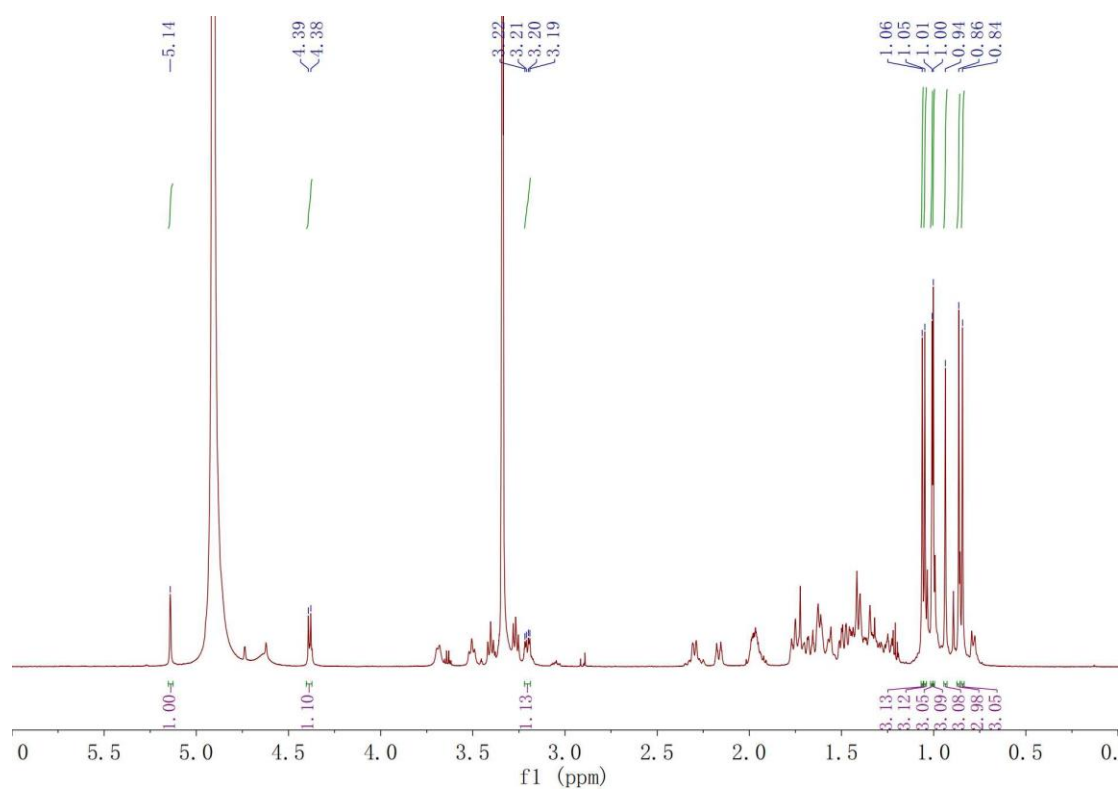
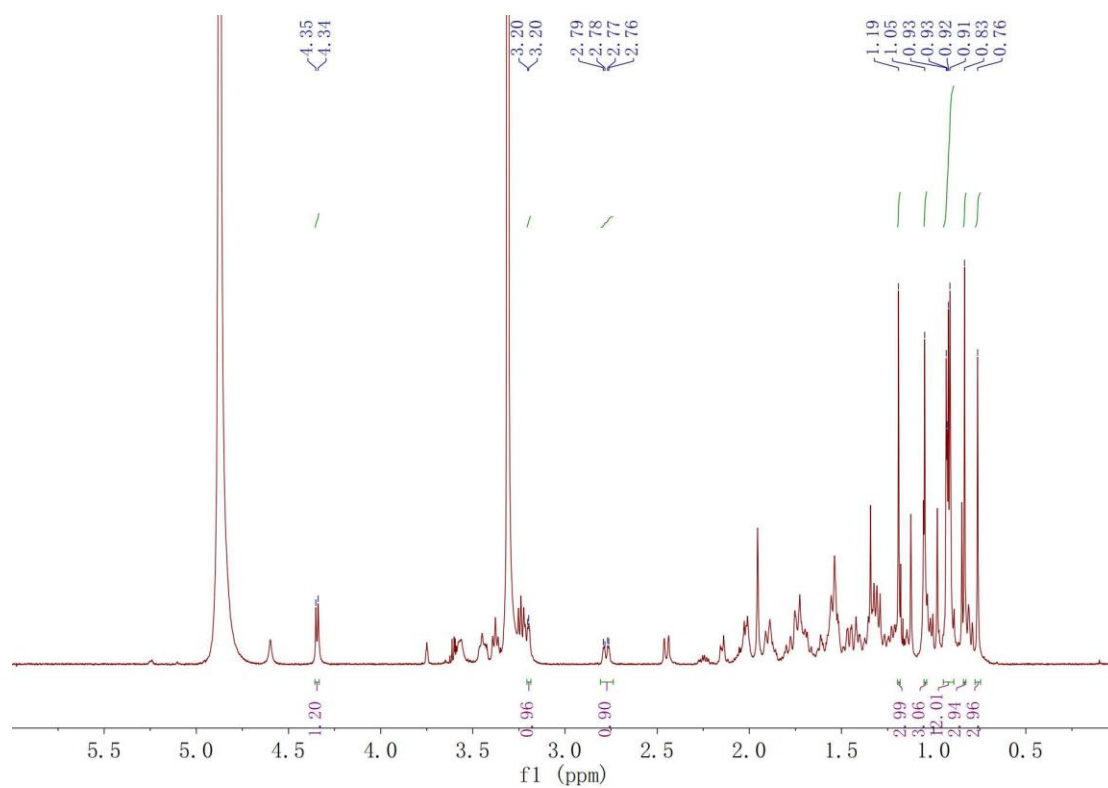


Figure S43. <sup>1</sup>H NMR spectrum of compound 13 (methanol-*d*<sub>4</sub>, 600 MHz).



**Figure S44.** <sup>1</sup>H NMR spectrum of compound **14** (methanol-*d*<sub>4</sub>, 600 MHz).



**Figure S45.** <sup>1</sup>H NMR spectrum of compound **15** (methanol-*d*<sub>4</sub>, 600 MHz).

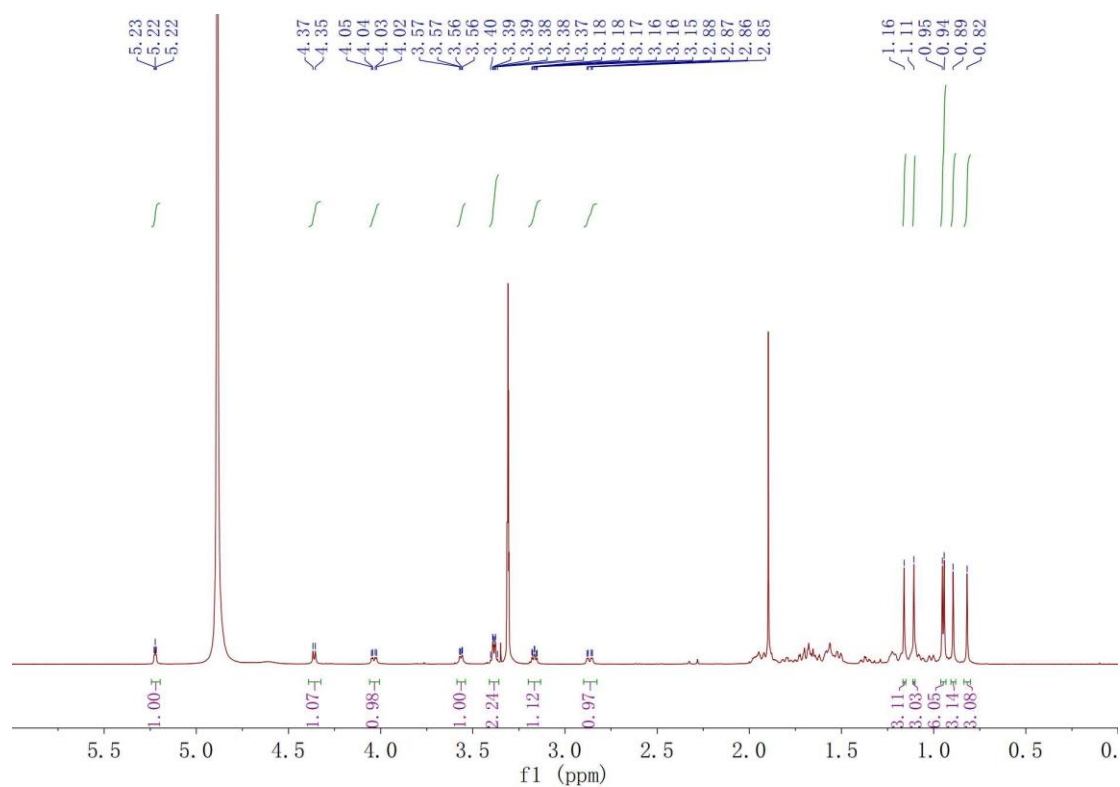


Figure S46. <sup>1</sup>H NMR spectrum of compound 16 (methanol-*d*<sub>4</sub>, 600MHz).

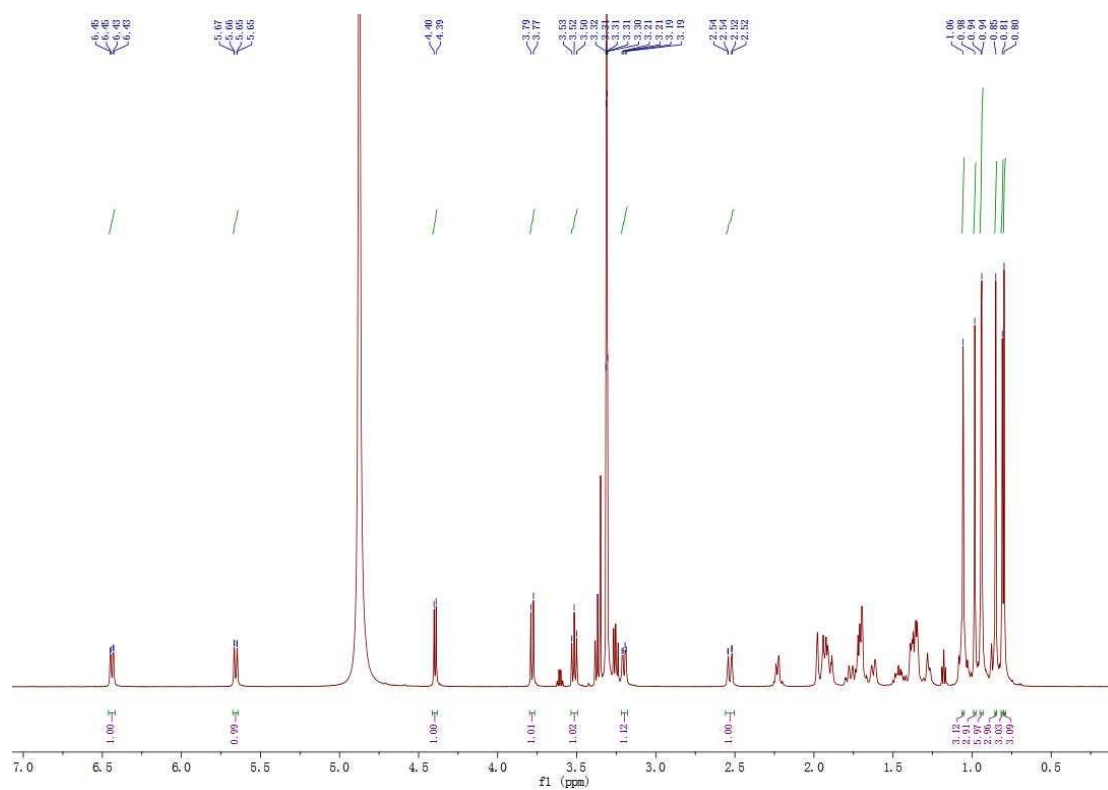


Figure S47. <sup>1</sup>H NMR spectrum of compound 17 (methanol-*d*<sub>4</sub>, 600MHz).

**Table S1.** The data that was used to calculate the IC<sub>50</sub> value for compound 3.

Concentration (μM)	The absorbance was determined at 405 nm		
0	1.8958	1.9019	1.8899
100	0.6803	0.6919	0.7170
50	0.7423	0.7590	0.7817
25	0.8752	0.8998	0.8730
12.5	0.9834	0.9814	1.0439
6.25	1.2902	1.2382	1.2113
3.125	1.4815	1.5014	1.4437
1.5625	1.6101	1.5873	1.5432

**Table S2.** The data that was used to calculate the IC<sub>50</sub> value for compound 9.

Concentration (μM)	The absorbance was determined at 405 nm		
0	1.8958	1.9019	1.8899
100	0.4444	0.4341	0.4423
50	0.4621	0.4971	0.4936
25	0.6253	0.6273	0.6271
12.5	0.7563	0.7374	0.7484
6.25	0.8887	0.9370	0.9375
3.125	1.0034	0.9730	0.9284
1.5625	1.0695	1.1973	1.1694

**Table S3.** The data that was used to calculate the IC<sub>50</sub> value for compound 13.

Concentration (μM)	The absorbance was determined at 405 nm		
0	1.3835	1.3330	1.4915
50	0.4252	0.4282	0.4126
25	0.4835	0.5313	0.4158
12.5	0.6657	0.7189	0.6798
6.25	1.1589	1.1940	1.2485
3.125	1.3230	1.3611	1.4017
1.5625	1.3461	1.3679	1.4208
0.78125	1.3527	1.3974	1.4329

**Table S4.** The data that was used to calculate the IC<sub>50</sub> value for acarbose.

Concentration (μM)	The absorbance was determined at 405 nm		
0	2.1073	2.1278	2.1184
0.012207031	0.2813	0.2694	0.2728

0.006103516	0.4321	0.4114	0.3998
0.003051758	0.6511	0.6945	0.6400
0.001525879	0.9629	0.9268	0.8430
0.000762939	0.8613	0.7828	0.7353
0.00038147	1.3322	1.4116	1.2263
0.000190735	1.3945	1.5378	1.3163

**Table S5.** The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound 3.

Inhibitor concentration ( $\mu\text{M}$ ), Substrate concentration ( $\mu\text{M}$ )	At 40 min, the absorbance at 405 nm			At 60 min, the absorbance at 405 nm		
0, 20	2.389	2.3089	2.3749	3.7430	3.7856	3.7507
0, 10	1.9815	2.0409	2.0955	3.6091	3.6436	3.6622
0, 5	1.4382	1.5183	1.5654	2.8114	2.8911	2.9381
0, 2.5	0.9304	0.9691	0.9855	1.7553	1.8237	1.8345
0, 1.25	0.4709	0.5034	0.5031	1.0150	1.0704	1.0237
10, 20	1.7721	1.7106	1.6819	3.0562	3.0062	2.9897
10, 10	1.3527	1.3746	1.3316	2.6308	2.6593	2.5884
10, 5	0.8755	0.9599	0.8015	1.7481	1.9158	1.4774
10, 2.5	0.6534	0.6553	0.6477	1.3342	1.3436	1.3216
10, 1.25	0.4508	0.4348	0.4538	0.8708	0.8533	0.8824
20, 20	1.3537	1.4013	1.4327	2.5861	2.6594	2.6711
20, 10	1.1342	1.1695	1.1576	2.2100	2.2641	2.2381
20, 5	0.9566	0.9016	0.8443	1.7477	1.7496	1.6806
20, 2.5	0.5977	0.5982	0.6017	1.1970	1.2155	1.1990
20, 1.25	0.4184	0.4411	0.4376	0.8111	0.8186	0.8069
30, 20	1.3338	1.2450	1.3039	2.5147	2.4105	2.4819
30, 10	1.0438	1.0267	1.0430	2.0192	2.0074	2.0523
30, 5	0.8664	0.8472	0.8355	1.6416	1.6235	1.6226
30, 2.5	0.5481	0.5671	0.5655	1.0793	1.0715	1.1152
30, 1.25	0.3996	0.3989	0.3910	0.7365	0.7384	0.7435

**Table S6.** The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound 9.

Inhibitor concentration ( $\mu\text{M}$ ), Substrate concentration ( $\mu\text{M}$ )	At 40 min, the absorbance at 405 nm			At 60 min, the absorbance at 405 nm		
0, 20	1.7770	1.7276	1.6815	3.1858	3.1595	3.1413
0, 10	1.2788	1.2958	1.2796	2.7135	2.7351	2.7318
0, 5	0.9435	0.9631	0.9686	2.0897	2.1274	2.1005
0, 2.5	0.6044	0.6198	0.6389	1.3440	1.397	1.4151

0, 1.25	0.4016	0.4044	0.4167	0.8927	0.8869	0.9061
1, 20	1.1836	1.1608	1.1294	2.5202	2.4940	2.4150
1, 10	0.9300	0.9261	0.8717	2.0569	2.0714	1.9441
1, 5	0.7181	0.6615	0.6738	1.6108	1.4904	1.5321
1, 2.5	0.5198	0.4789	0.4803	1.1546	1.0906	1.0878
1, 1.25	0.3628	0.3418	0.3450	0.7934	0.7671	0.765
15, 20	0.6873	0.6806	0.6860	1.5269	1.5028	1.5141
15, 10	0.5631	0.5584	0.5762	1.2792	1.2649	1.3213
15, 5	0.4552	0.4583	0.4585	1.0338	1.045	1.0553
15, 2.5	0.3533	0.3457	0.3541	0.7855	0.7751	0.8129
15, 1.25	0.2585	0.2579	0.2520	0.5664	0.5730	0.5667
30, 20	0.5788	0.5855	0.5712	1.2477	1.2704	1.2314
30, 10	0.4741	0.4720	0.4750	1.0277	1.0346	1.0411
30, 5	0.3895	0.3841	0.3769	0.8658	0.8555	0.8353
30, 2.5	0.2916	0.2954	0.2993	0.6373	0.6469	0.6562
30, 1.25	0.2282	0.2232	0.2260	0.4892	0.4743	0.4793

Table S7. The data that was used to calculate the  $K_m$ ,  $K_i$ , and  $K_i'$  value for compound 13.

Inhibitor concentration ( $\mu\text{M}$ ), Substrate concentration ( $\mu\text{M}$ )	At 40 min, the absorbance at 405 nm			At 42 min, the absorbance at 405 nm		
0, 20	0.8897	0.8690	0.8560	1.1424	1.1263	1.1087
0, 10	0.6616	0.6628	0.6686	0.8643	0.8834	0.8734
0, 5	0.4742	0.4664	0.4818	0.6329	0.6182	0.6489
0, 2.5	0.3250	0.3233	0.3241	0.4391	0.4361	0.4332
0, 1.25	0.2127	0.2137	0.2167	0.2775	0.2797	0.2780
5, 20	0.6681	0.6589	0.6944	0.8635	0.8479	0.8889
5, 10	0.4885	0.4832	0.5273	0.6347	0.6313	0.6835
5, 5	0.3071	0.3248	0.3327	0.4012	0.4300	0.4372
5, 2.5	0.2150	0.2199	0.2261	0.2822	0.2910	0.2993
5, 1.25	0.1505	0.1474	0.1521	0.1947	0.1927	0.1958
10, 20	0.4291	0.4068	0.4258	0.5371	0.5130	0.5350
10, 10	0.3402	0.3144	0.3391	0.4314	0.3998	0.4320
10, 5	0.2353	0.2200	0.2359	0.2985	0.2826	0.3006
10, 2.5	0.1573	0.1522	0.1615	0.2037	0.1937	0.2067
10, 1.25	0.1138	0.1106	0.1182	0.1411	0.1389	0.1479
20, 20	0.3343	0.3345	0.3517	0.4152	0.4173	0.4392
20, 10	0.2677	0.2821	0.2870	0.3361	0.3527	0.3592
20, 5	0.1987	0.1952	0.2055	0.2515	0.2454	0.2578
20, 2.5	0.1429	0.1453	0.1436	0.1821	0.1830	0.1798
20, 1.25	0.1093	0.1023	0.1057	0.1342	0.1252	0.1290