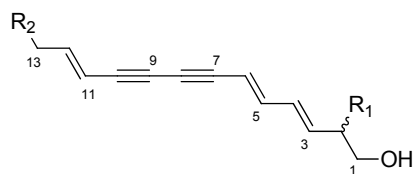
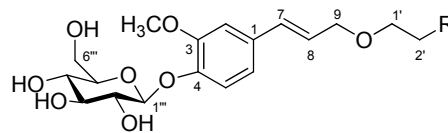


## Supplementary Material

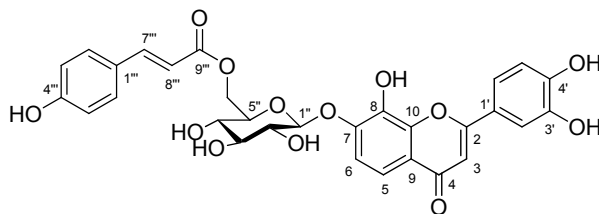


**R<sub>1</sub>**  
**1** O-β-glu  
**1a** OH

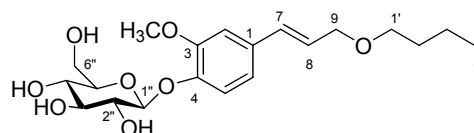
**R<sub>2</sub>**  
**OH**  
**O-β-glu**



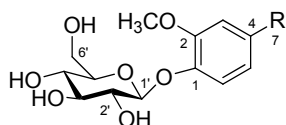
**R**  
**2** OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>  
**2a** H



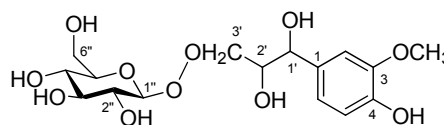
**3**



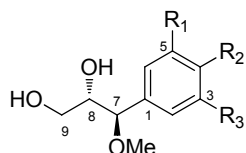
**4**



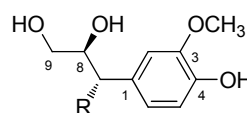
**R**  
**5** CH<sub>2</sub>CHCH<sub>2</sub>  
**6** CH<sub>2</sub>CH<sub>2</sub>OH



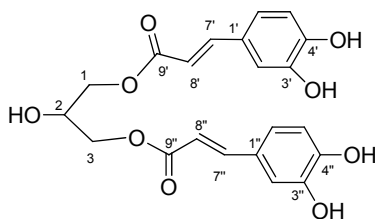
**7**



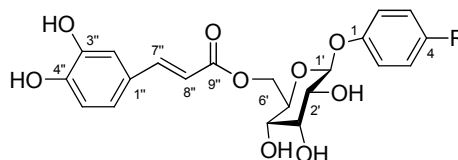
**R<sub>1</sub>** **R<sub>2</sub>** **R<sub>3</sub>**  
**8** OH H OMe  
**9** OMe OH H



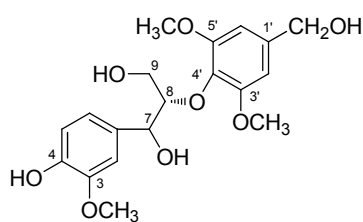
**R**  
**10** H  
**11** OH



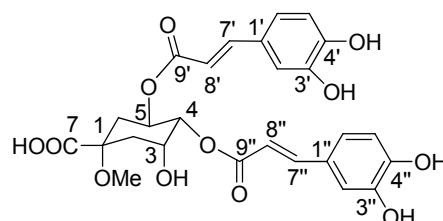
**12**



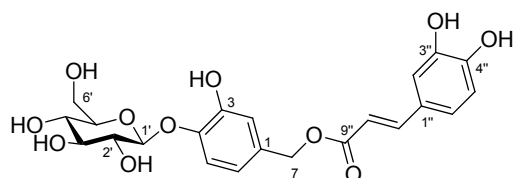
**R**  
**13** OH  
**14** CH<sub>3</sub>CO



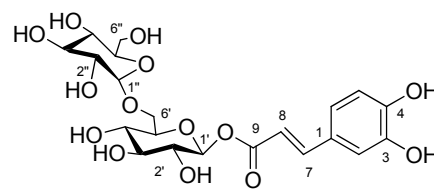
**15**



**16**

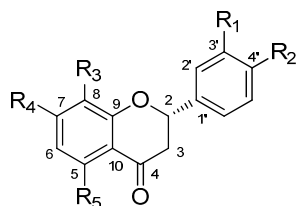
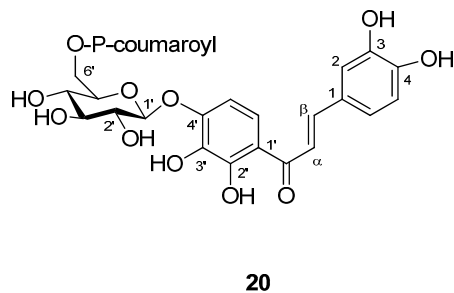
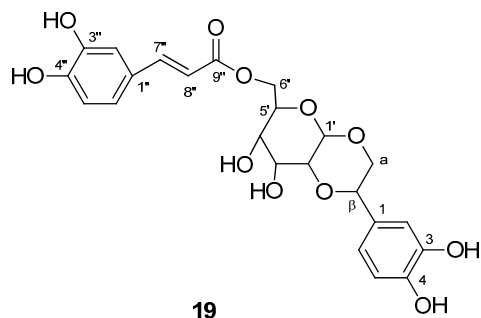


**17**

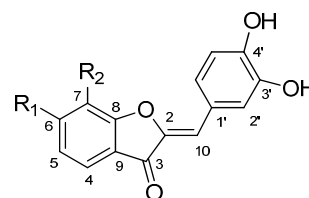


**18**

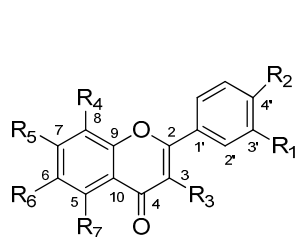
Figure S1. Cont.



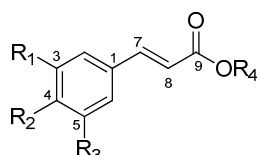
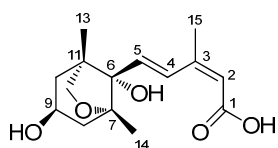
	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>
<b>21</b>	OH	OMe	OH	OGlu-6"-O-Ac	H
<b>22</b>	OH	OMe	OH	OGlu	H
<b>23</b>	OMe	OH	H	OGlu	OH



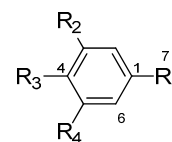
	R <sub>1</sub>	R <sub>2</sub>
<b>32</b>	OH	OGlu-6"-O-Ac
<b>33</b>	OGlu	H
<b>34</b>	OH	OGlu



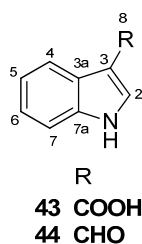
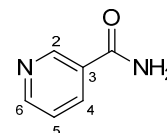
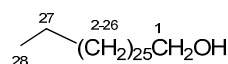
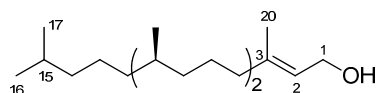
	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
<b>24</b>	H	OH	H	H	OH	H	OH
<b>25</b>	OH	OH	H	H	OGlu-6"-O-protocatechuoyl	OH	OH
<b>26</b>	OH	OH	OGlu	H	OH	H	OH
<b>27</b>	OH	OH	H	OH	OGlu	H	H
<b>28</b>	OH	OH	H	H	OGlu	H	OH
<b>29</b>	OH	OH	H	H	OGlu	OH	OH
<b>30</b>	OH	OH	H	H	OGlu-3"-O-HMG-ester	OH	OH
<b>31</b>	OH	OH	H	H	OGlu-6"-O-Glu	H	OH



	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>
<b>36</b>	OH	OH	H	H
<b>37</b>	OH	OMe	H	CH <sub>2</sub> CH <sub>3</sub>



	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>
<b>38</b>	COOH	OH	OH	H
<b>39</b>	OMe	OMe	H	OMe
<b>40</b>	CHO	H	OMe	OH



<b>43</b>	COOH
<b>44</b>	CHO

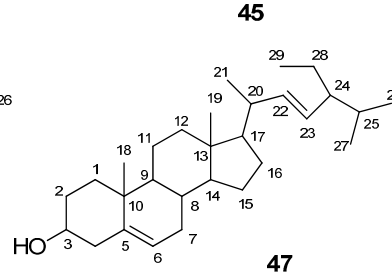
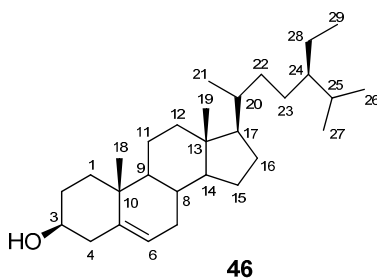


Figure S1. Cont.

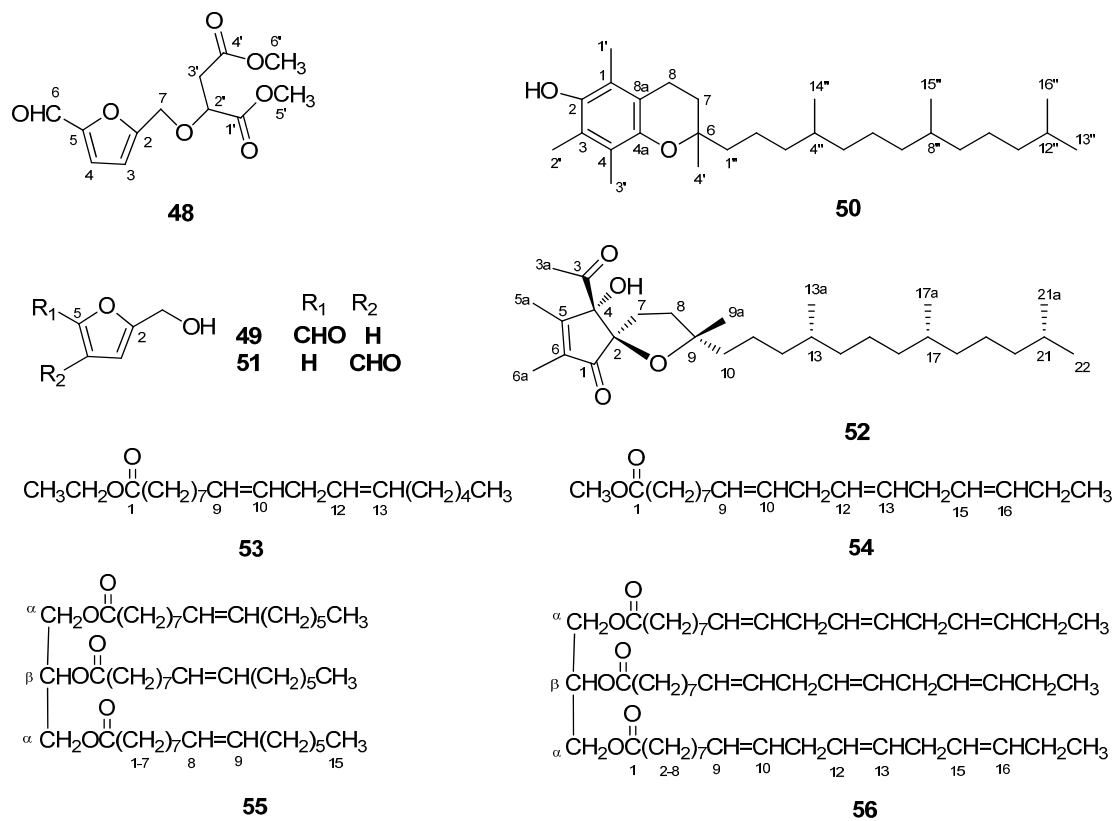


Figure S1. Structures of compounds 1–56.

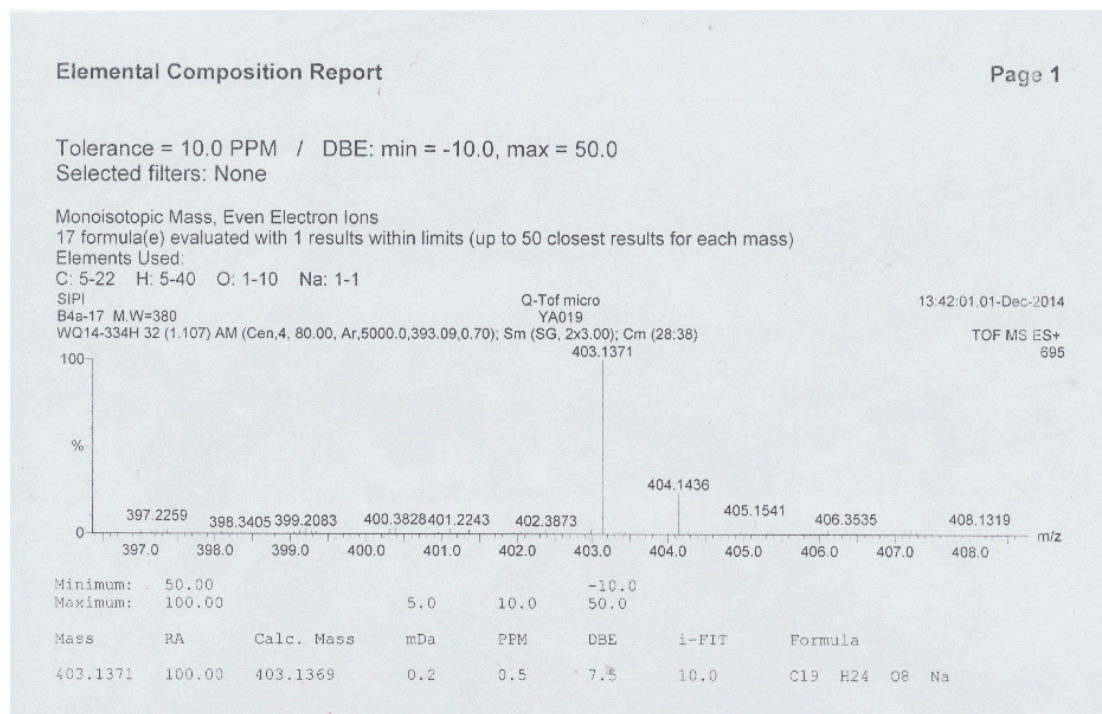
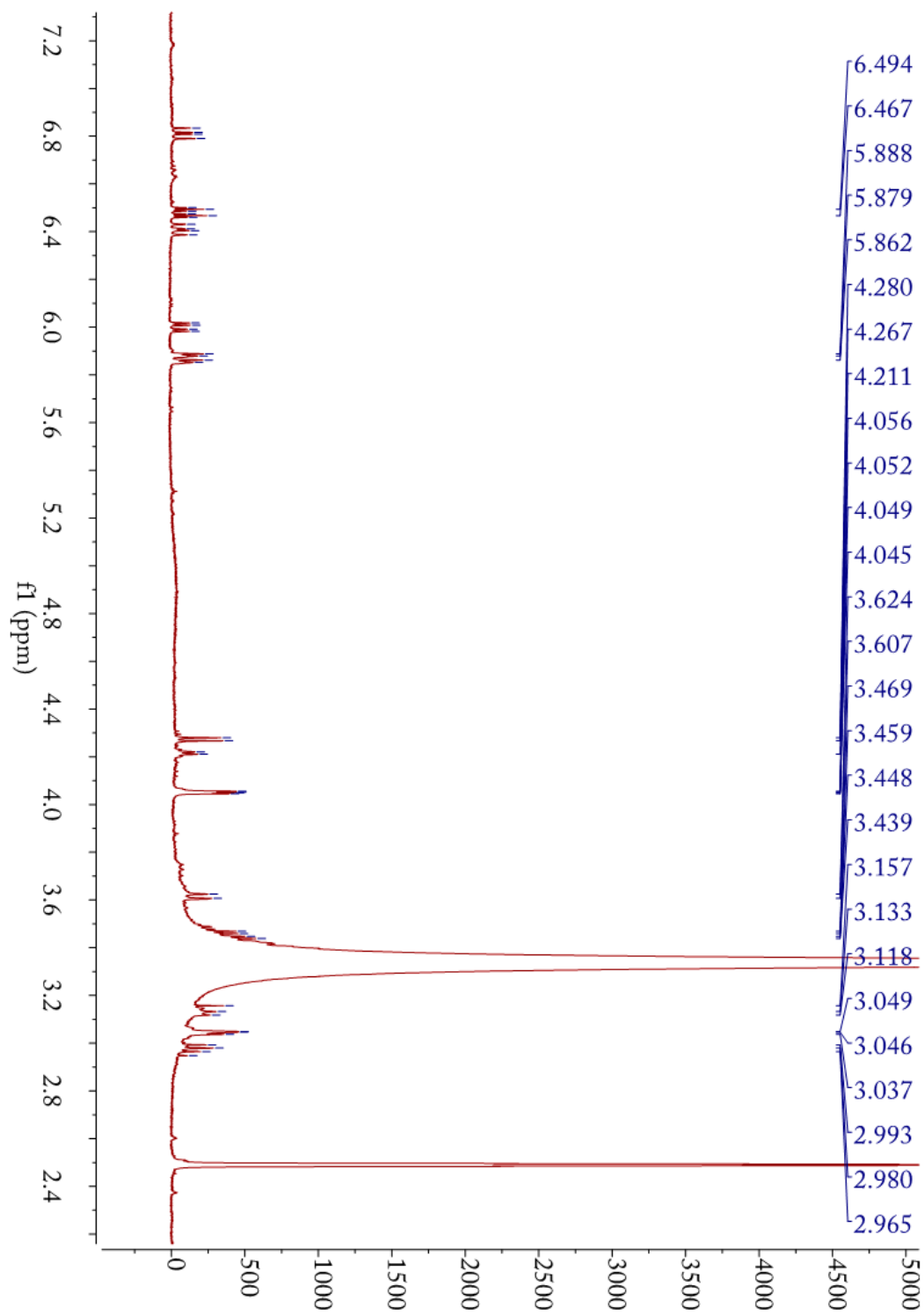
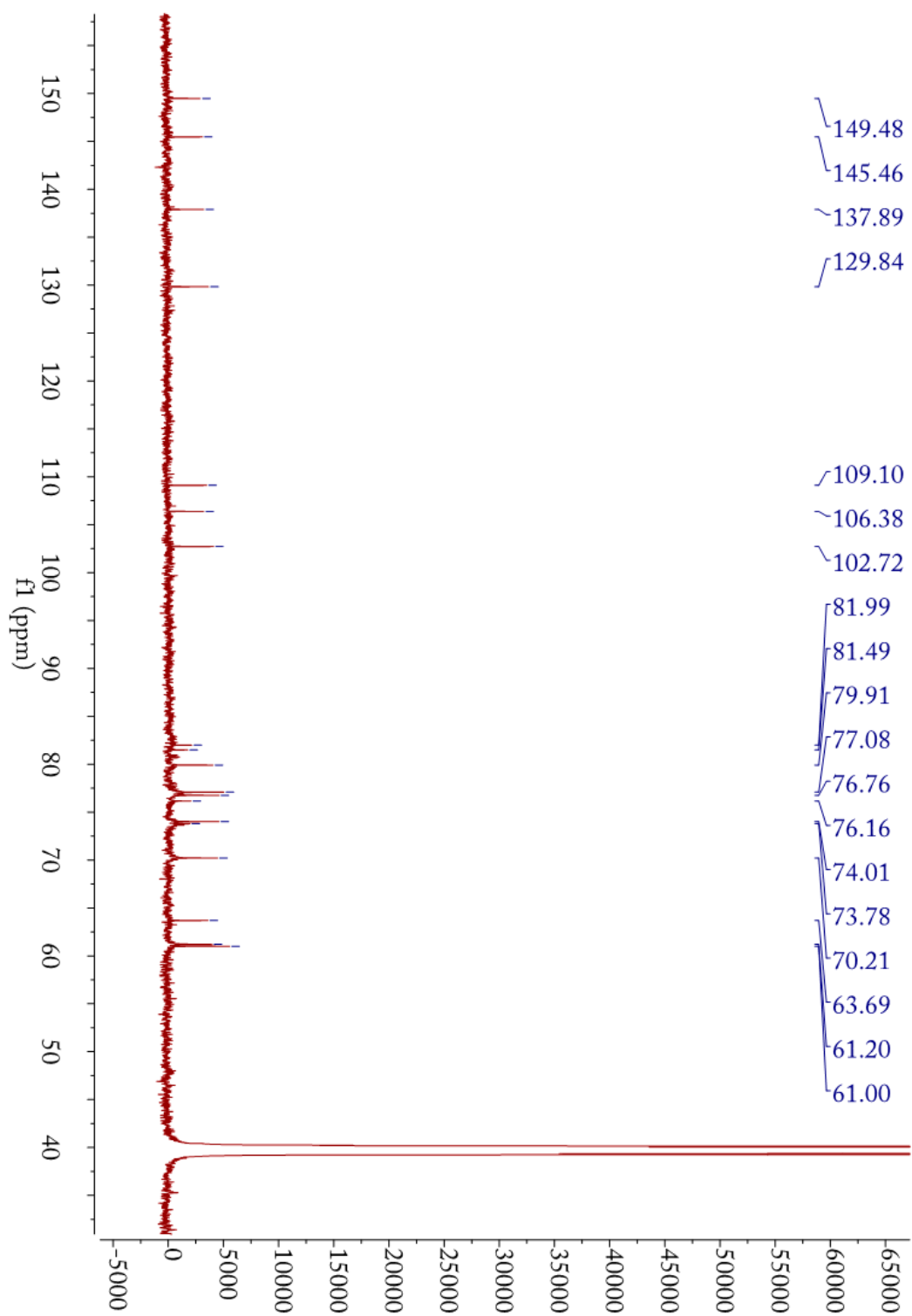


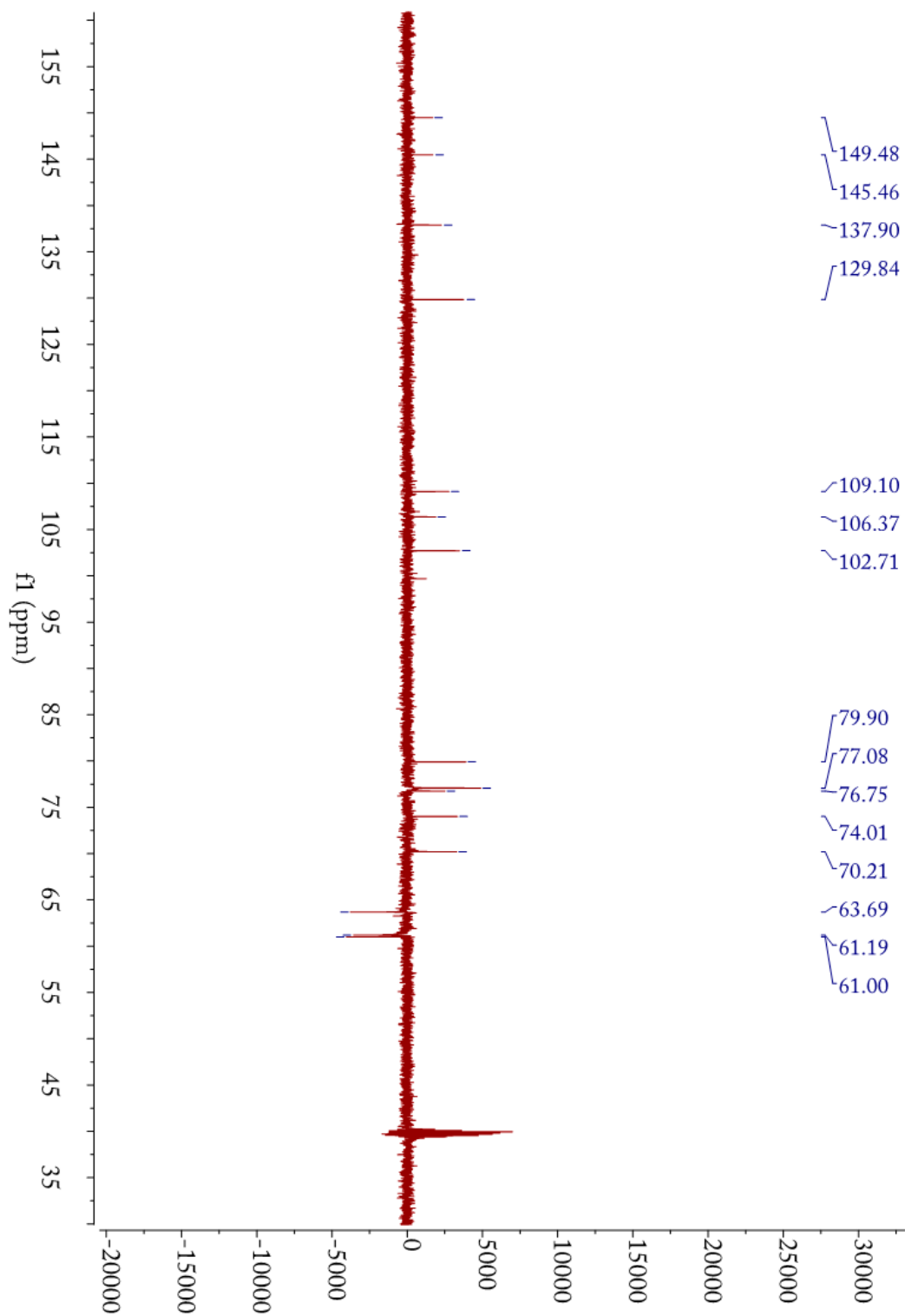
Figure S2. HRESI mass spectrum of compound 1.



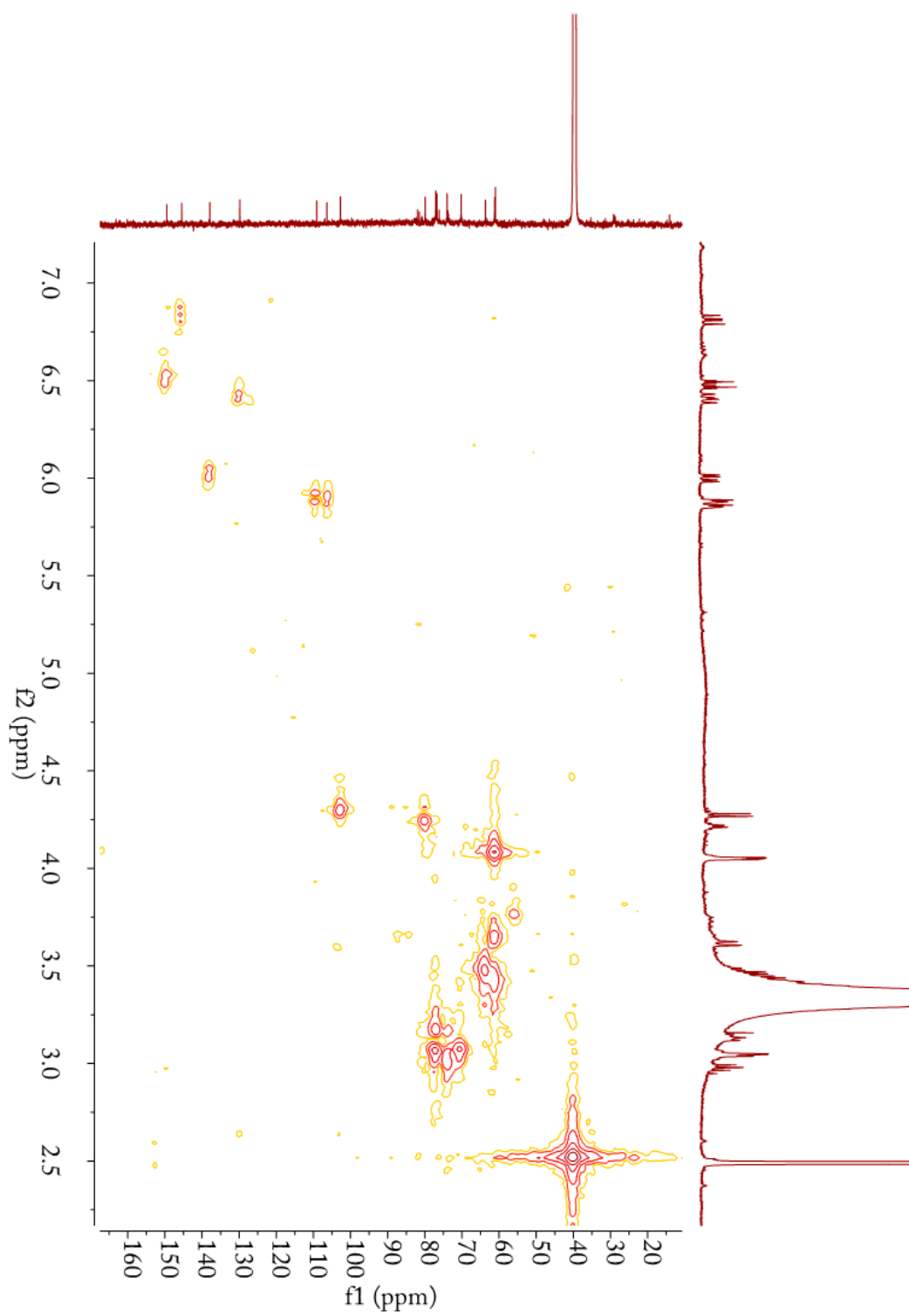
**Figure S3.**  $^1\text{H-NMR}$  spectrum of compound **1** (600 MHz, in  $\text{DMSO-}d_6$ ).



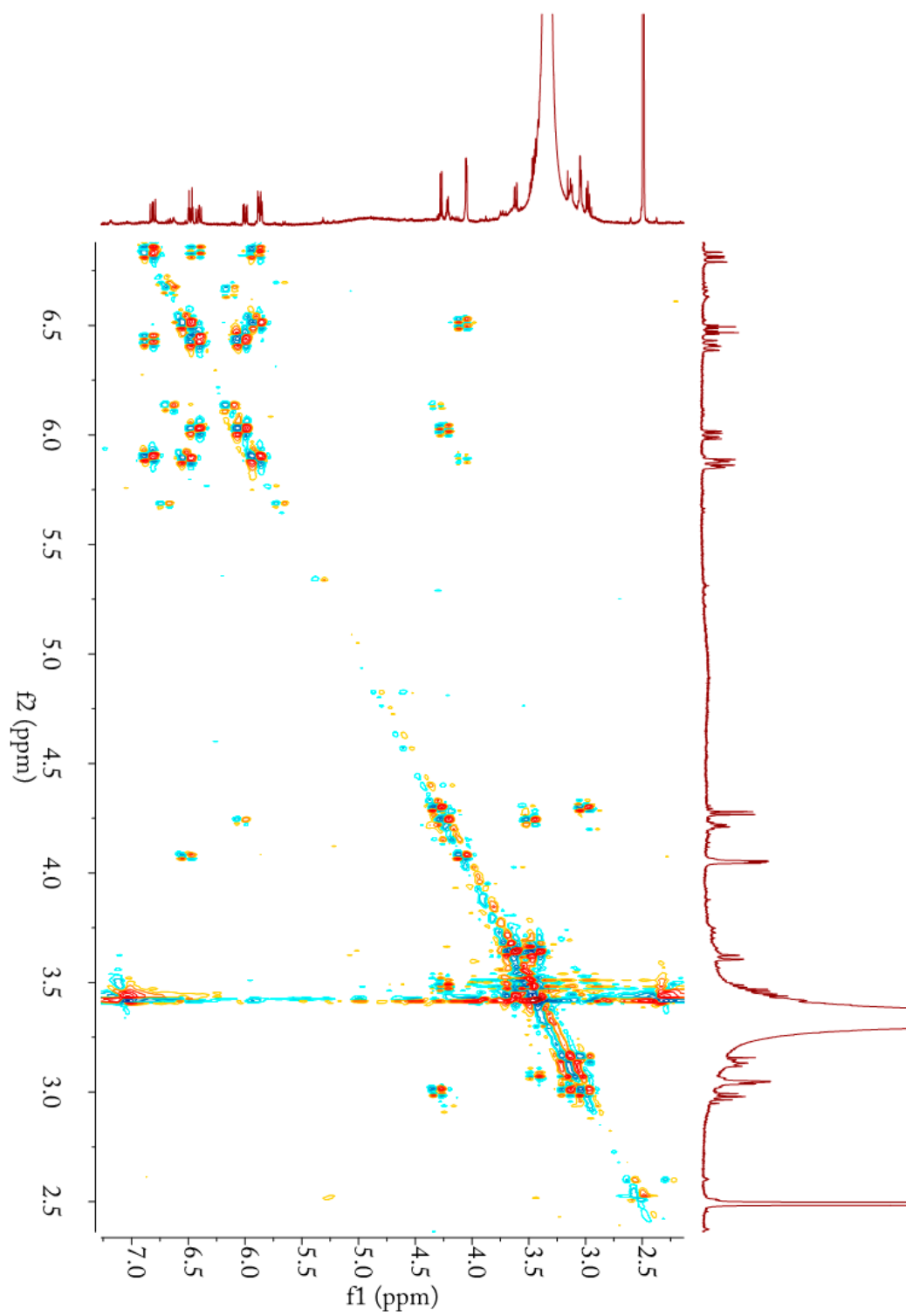
**Figure S4.**  $^{13}\text{C}$ -NMR spectrum of compound **1** (150 MHz, in  $\text{DMSO-}d_6$ ).



**Figure S5.** DEPT spectrum of compound **1** (150 MHz, in DMSO-*d*<sub>6</sub>).

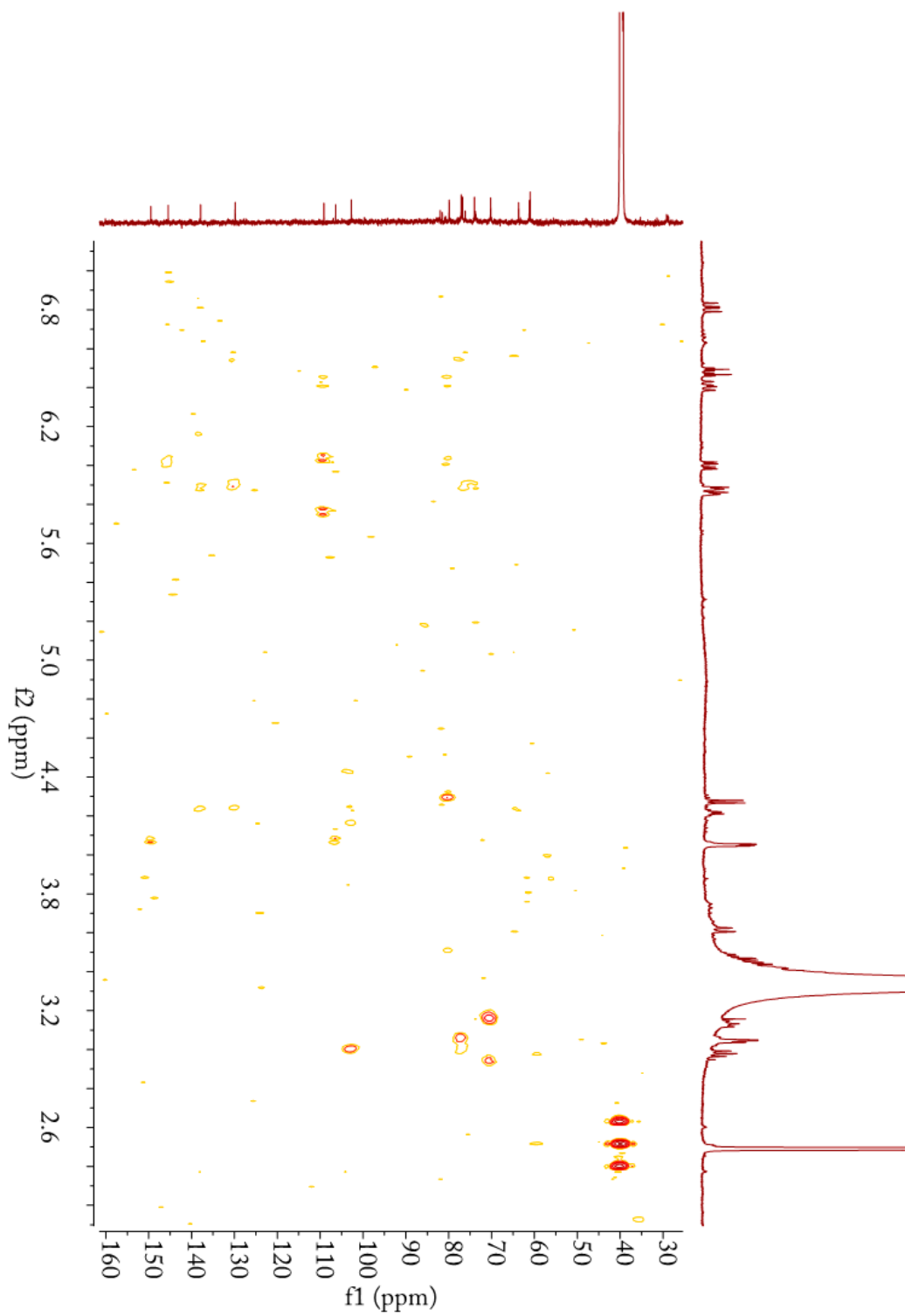


**Figure S6.** HSQC spectrum of compound **1** (600 MHz, in DMSO-*d*<sub>6</sub>).



**Figure S7.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** (600 MHz, in  $\text{DMSO-}d_6$ ).



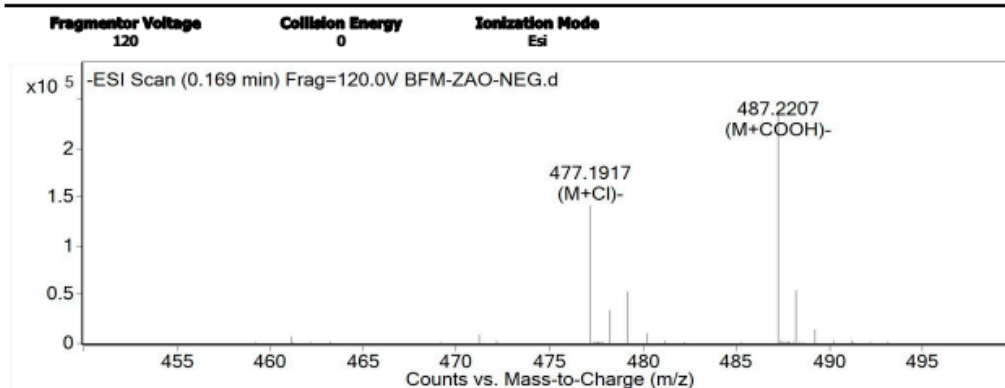


**Figure S8.** HMBC spectrum of compound **1** (600 MHz, in  $\text{DMSO-}d_6$ ).

## Qualitative Analysis Report

<b>Data Filename</b>	BFM-ZAO.d	<b>Sample Name</b>	BFM-ZAO
<b>Sample Type</b>	Sample	<b>Position</b>	P1-D7
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	TEST-POS-01-WL.m	<b>Acquired Time</b>	11/11/2014 4:26:53 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			
<b>Data Filename</b>	BFM-ZAO-NEG.d	<b>Sample Name</b>	BFM-ZAO
<b>Sample Type</b>	Sample	<b>Position</b>	P1-D7
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	TEST-NEG-01-WL.m	<b>Acquired Time</b>	11/11/2014 4:58:04 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
68.9962		96757		
112.9858		179609		
477.1917	1	142017	C22 H34 Cl O9	(M+Cl)-
479.1905	1	53192	C22 H34 Cl O9	(M+Cl)-
487.2207	1	239659	C23 H35 O11	(M+COOH)-
488.2235	1	53870	C23 H35 O11	(M+COOH)-
955.9719	1	100294		
966.0007		50450		
982.9899		50093		
1033.9868		33735		

#### Formula Calculator Element Limits

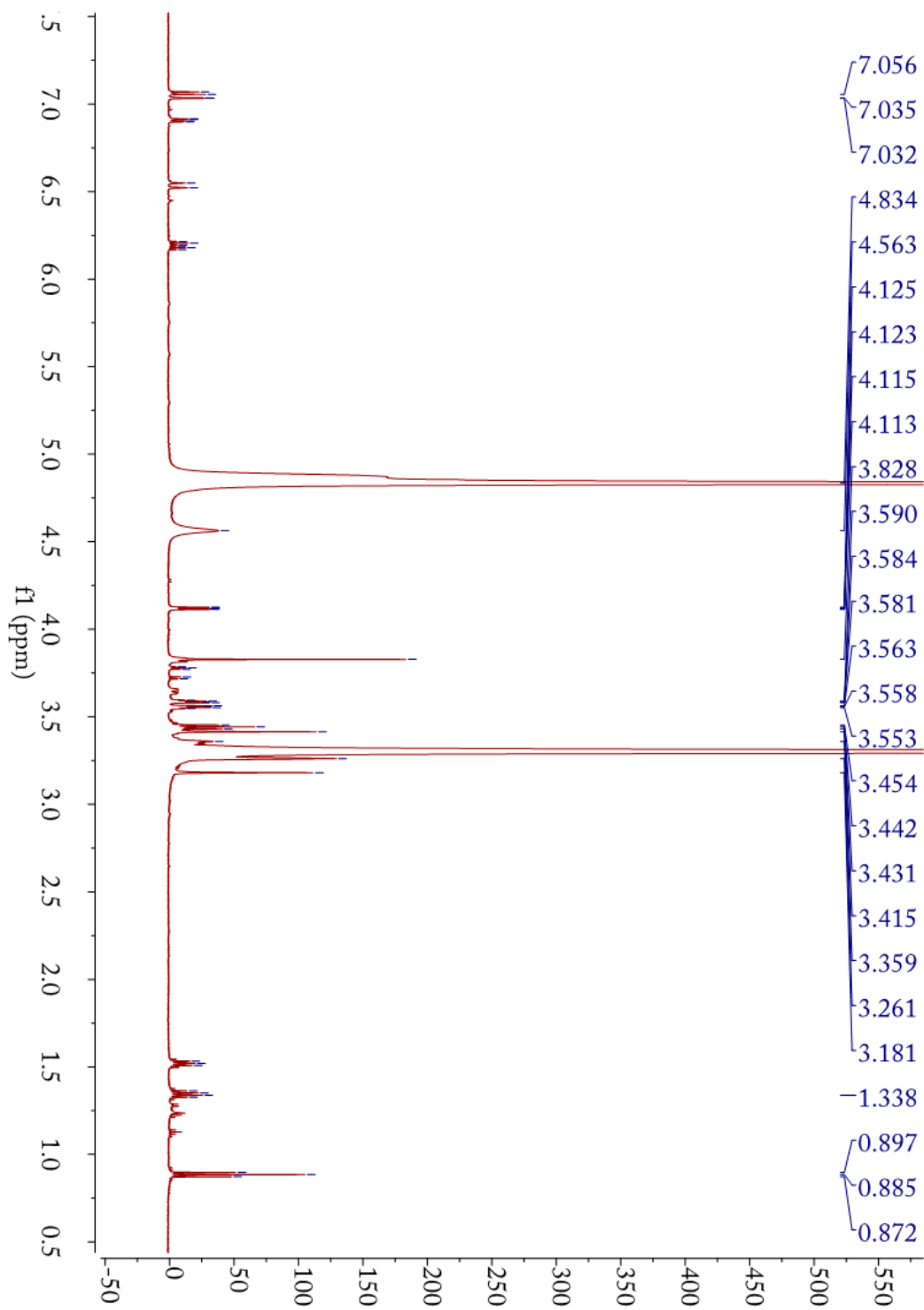
Element	Min	Max
C	3	60
H	0	120
O	0	20

#### Formula Calculator Results

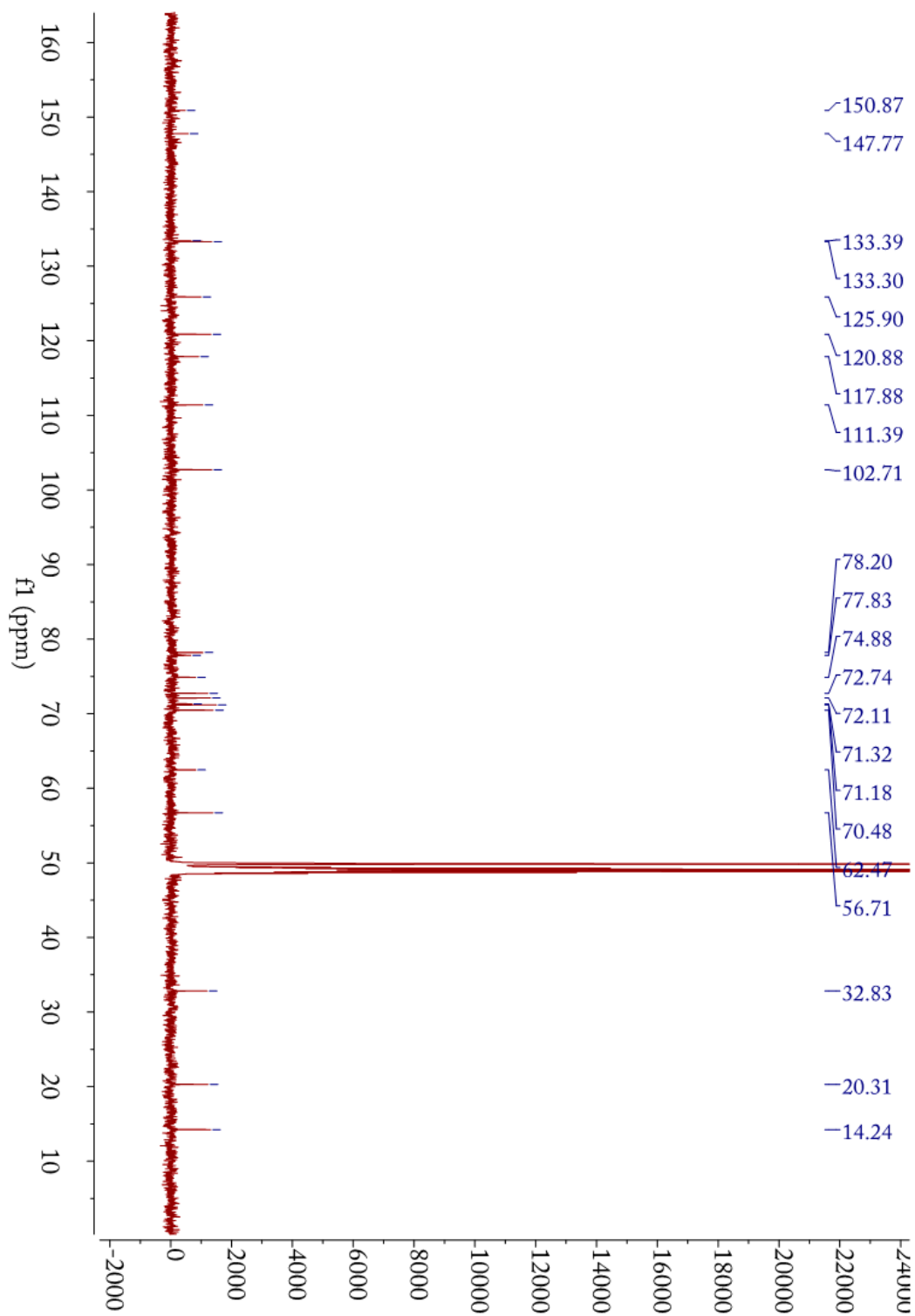
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C22 H34 O9	TRUE	442.2223	442.2203	-4.64	C22 H34 Cl O9	90.72
C22 H34 O9	TRUE	442.2225	442.2203	-5.02	C23 H35 O11	88

--- End Of Report ---

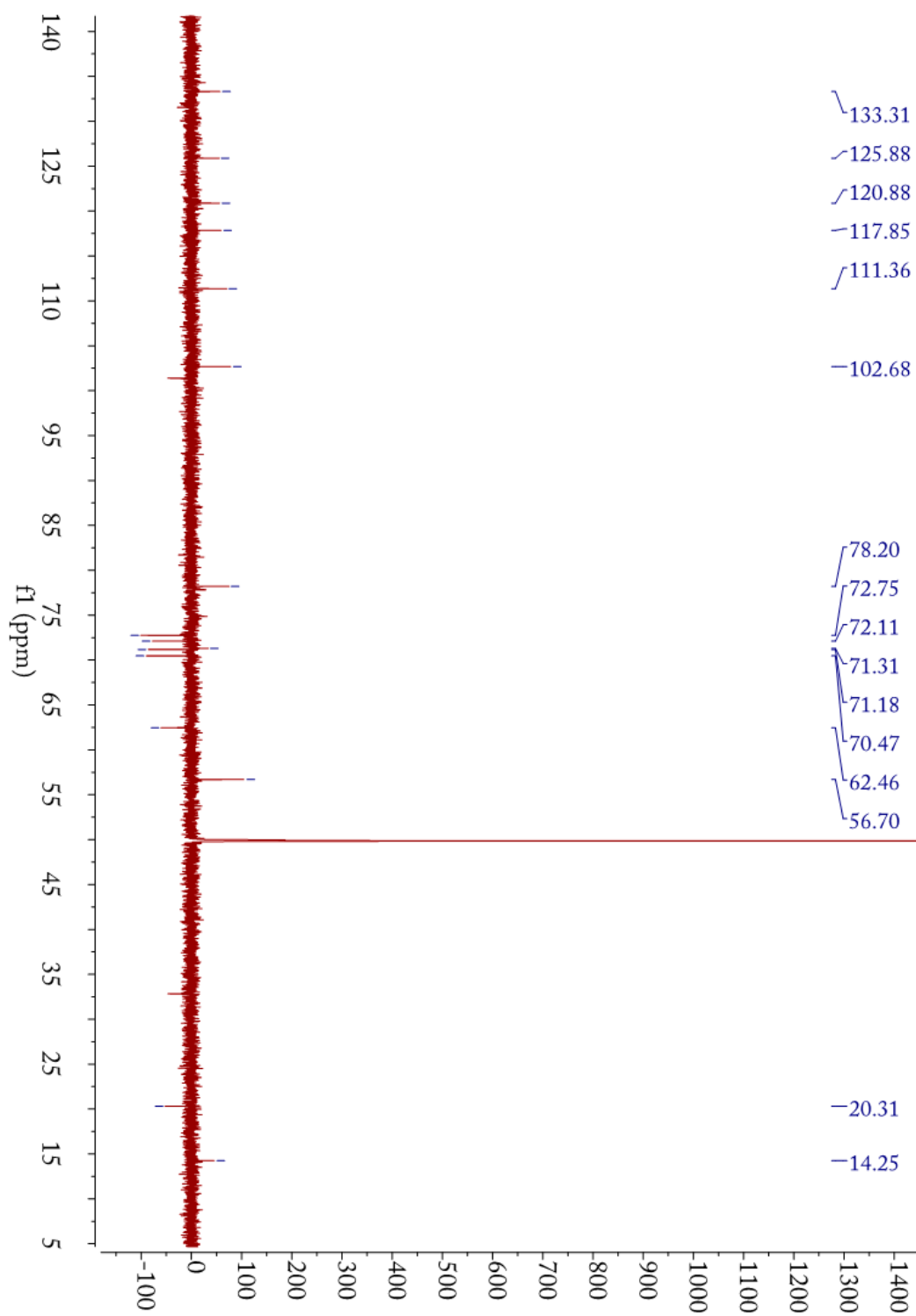
Figure S9. HRESI mass spectrum of compound 2.



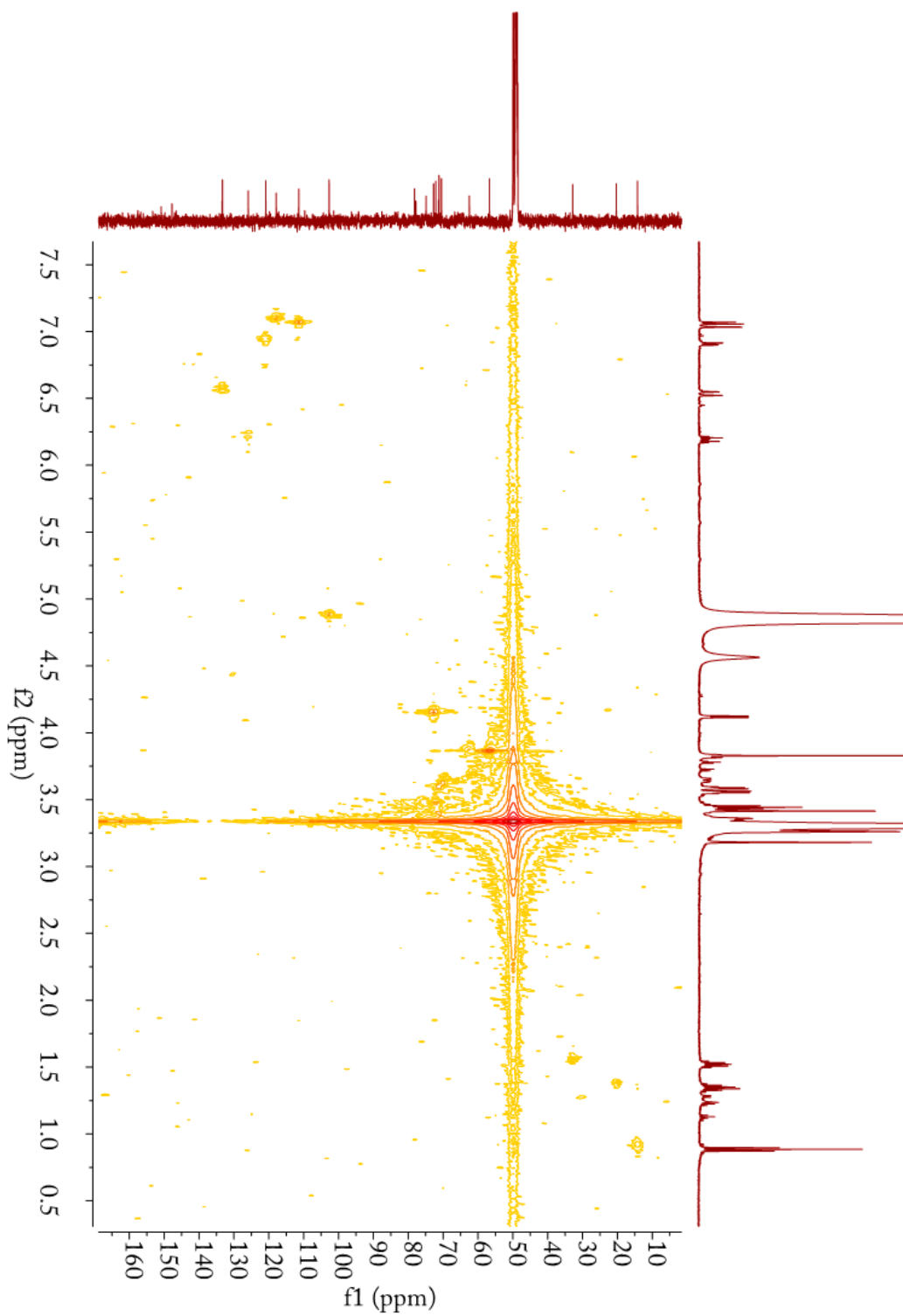
**Figure S10.**  $^1\text{H-NMR}$  spectrum of compound **2** (600 MHz, in  $\text{CD}_3\text{OD}$ ).



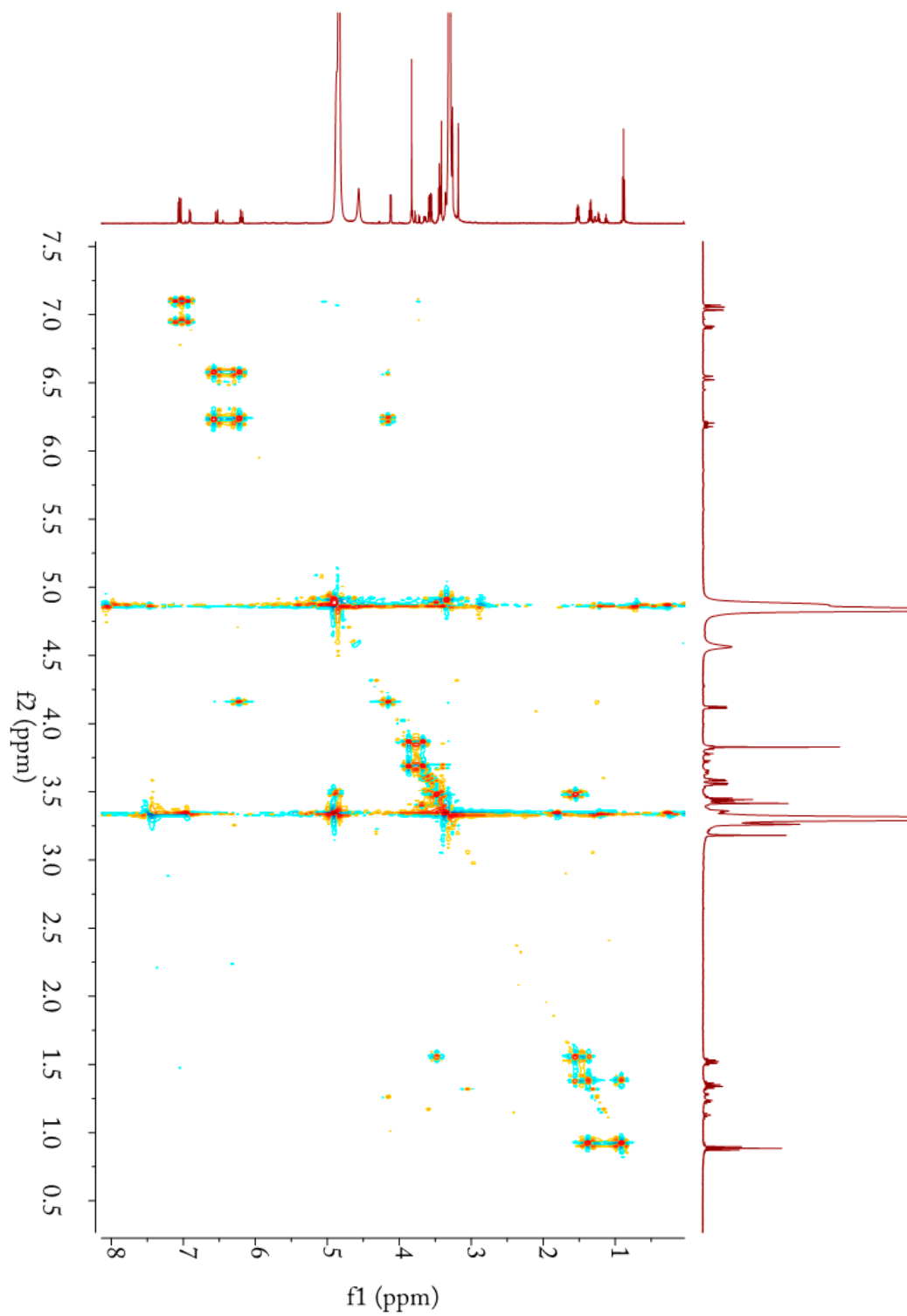
**Figure S11.**  $^{13}\text{C}$ -NMR spectrum of compound 2 (150 MHz, in  $\text{CD}_3\text{OD}$ ).



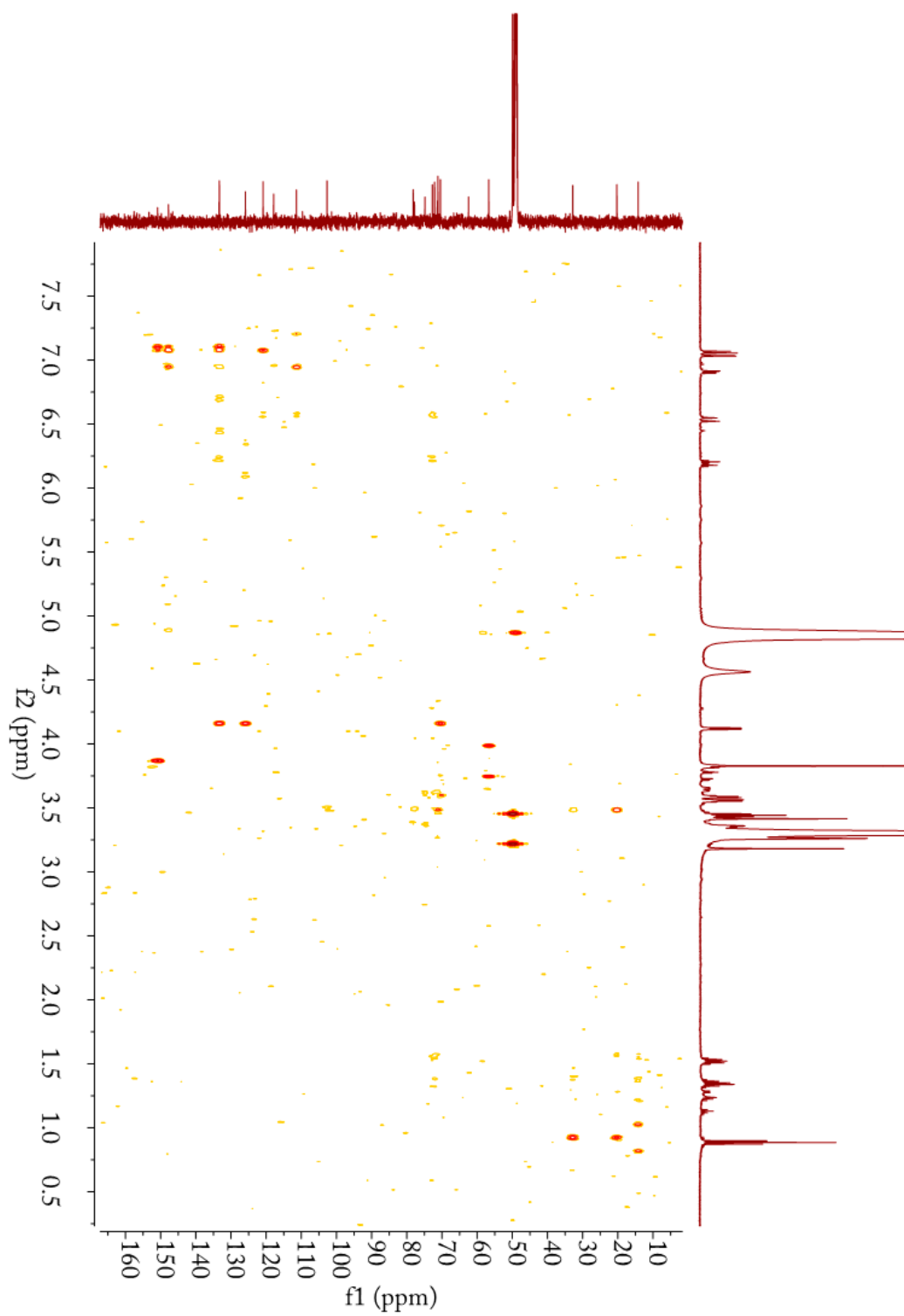
**Figure S12.** DEPT spectrum of compound **2** (150 MHz, in CD<sub>3</sub>OD).



**Figure S13.** HSQC spectrum of compound **2** (600 MHz, in  $\text{CD}_3\text{OD}$ ).



**Figure S14.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** (600 MHz, in  $\text{CD}_3\text{OD}$ ).



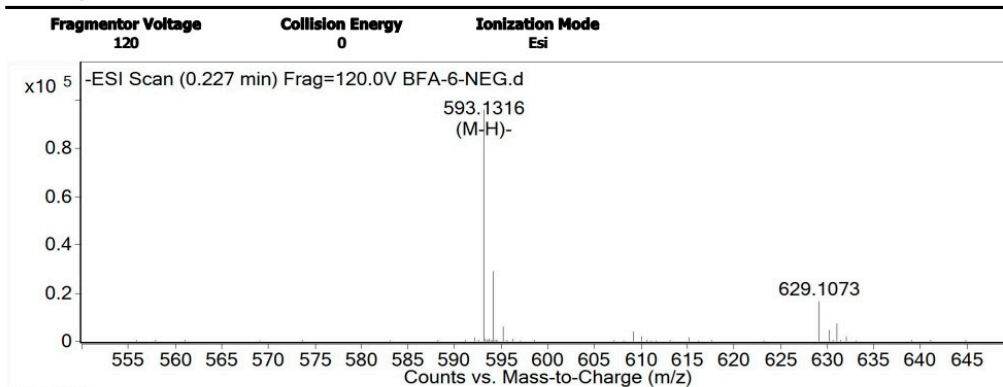
**Figure S15.** HMBC spectrum of compound **2** (600 MHz, in CD<sub>3</sub>OD).



## Qualitative Analysis Report

<b>Data Filename</b>	BFA-6.d	<b>Sample Name</b>	BFA-6
<b>Sample Type</b>	Sample	<b>Position</b>	P1-D8
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	TEST-POS-01-WL.m	<b>Acquired Time</b>	11/11/2014 4:28:31 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			
<b>Data Filename</b>	BFA-6-NEG.d	<b>Sample Name</b>	BFA-6
<b>Sample Type</b>	Sample	<b>Position</b>	P1-D8
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	TEST-NEG-01-WL.m	<b>Acquired Time</b>	11/11/2014 4:59:40 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
68.9963		76658		
112.9857		146937		
160.842		22421		
197.8083		20953		
593.1316	1	96289	C30 H25 O13	(M-H)-
594.1345	1	28955	C30 H25 O13	(M-H)-
955.9712	1	56329		
966.0007	1	60958		
982.9909	1	71446		
1033.9866		25585		

#### Formula Calculator Element Limits

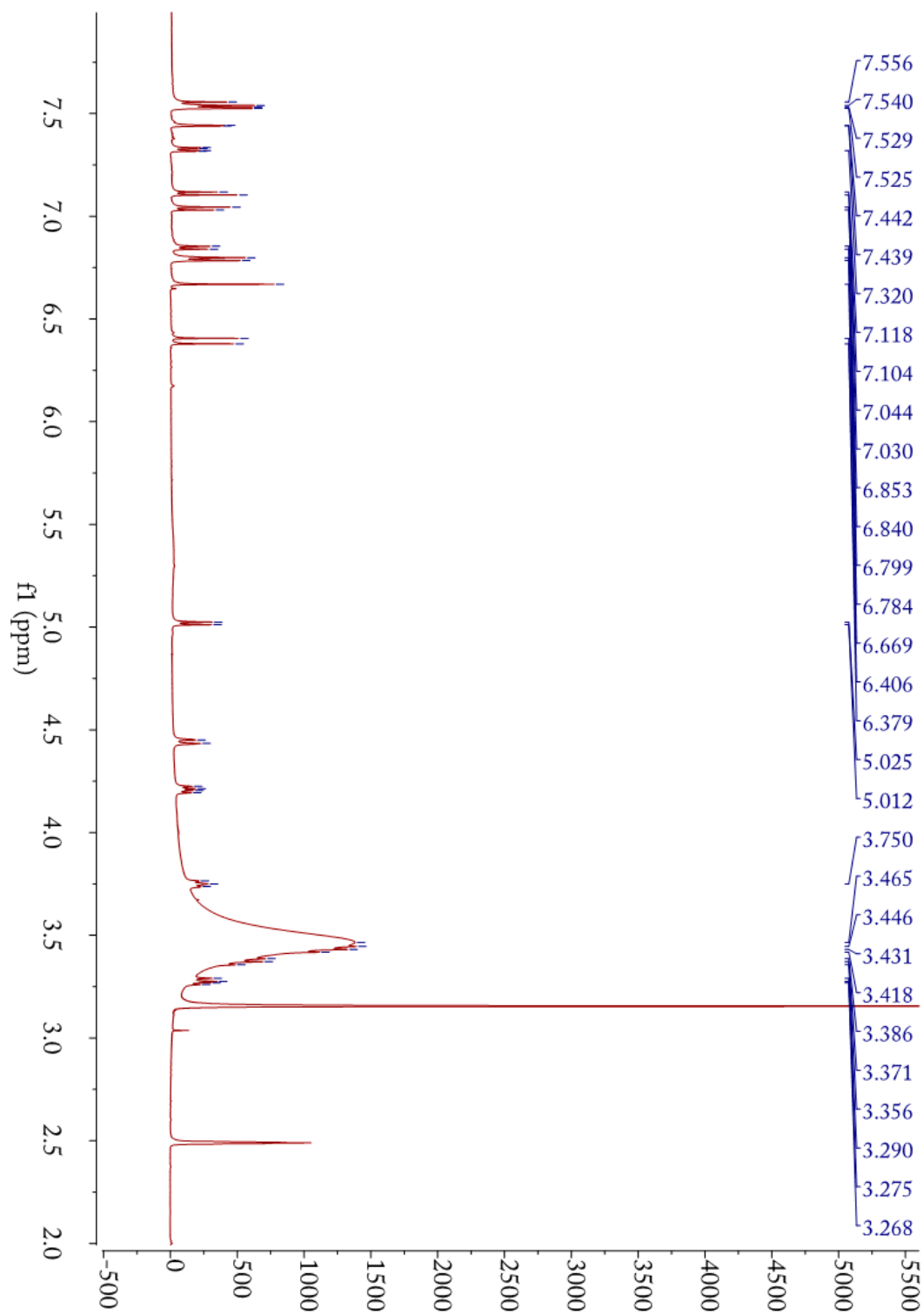
Element	Min	Max
C	3	60
H	0	120
O	0	20

#### Formula Calculator Results

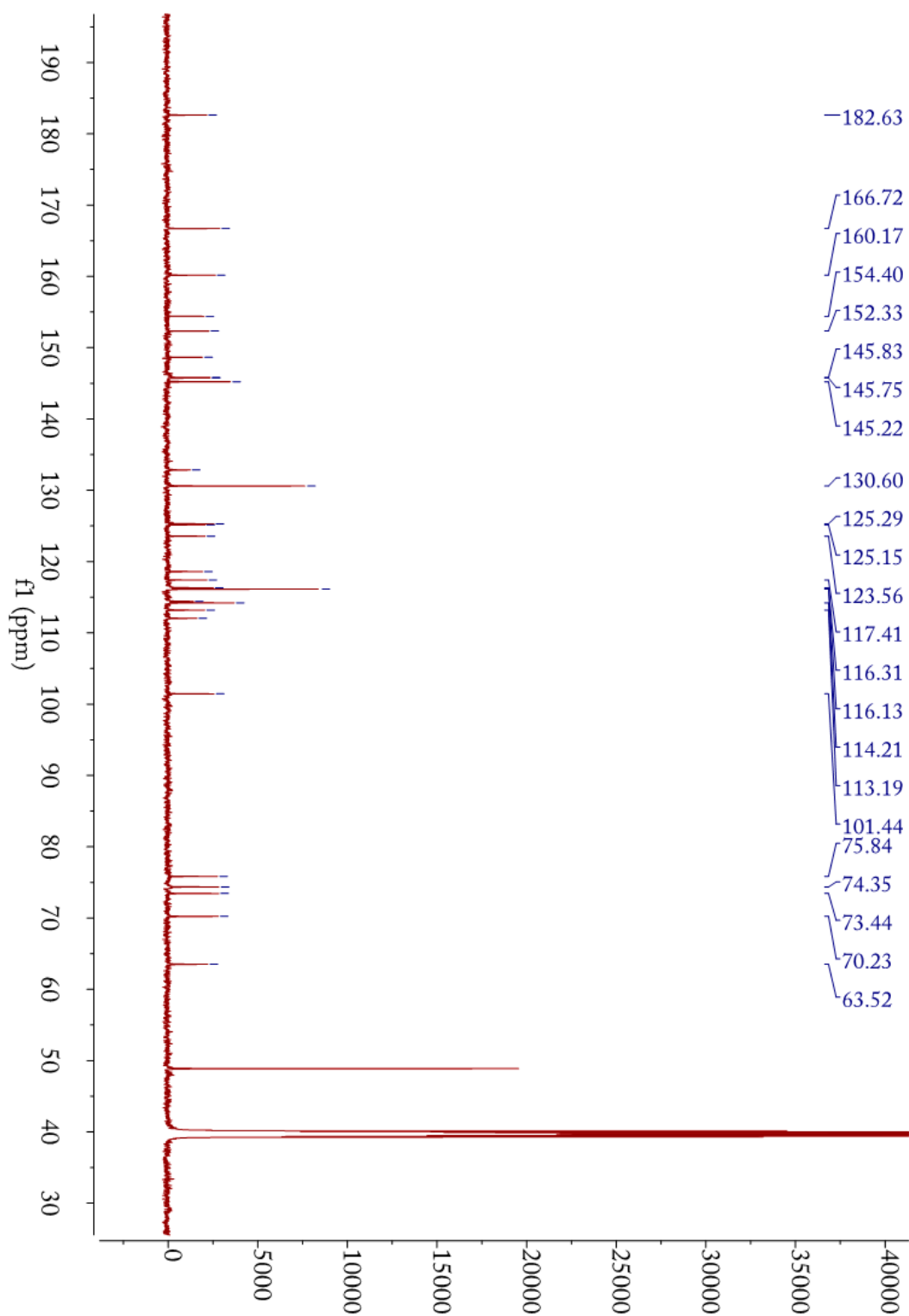
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C30 H26 O13	TRUE	594.1389	594.1373	-2.64	C30 H25 O13	94.26

<b>Fragmentor Voltage</b> 120	<b>Collision Energy</b> 0	<b>Ionization Mode</b> Esi
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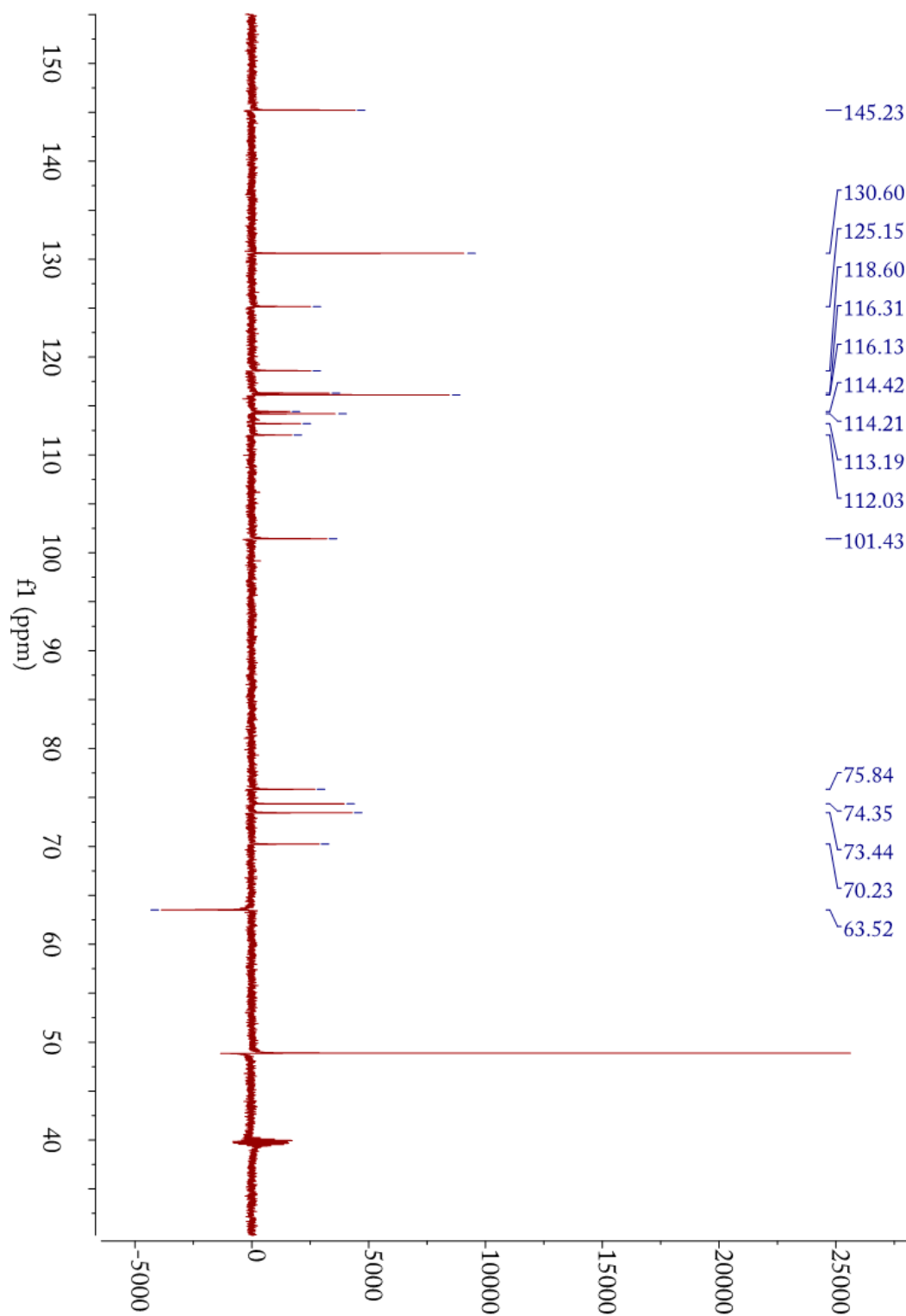
Figure S16. HRESI mass spectrum of compound 3.



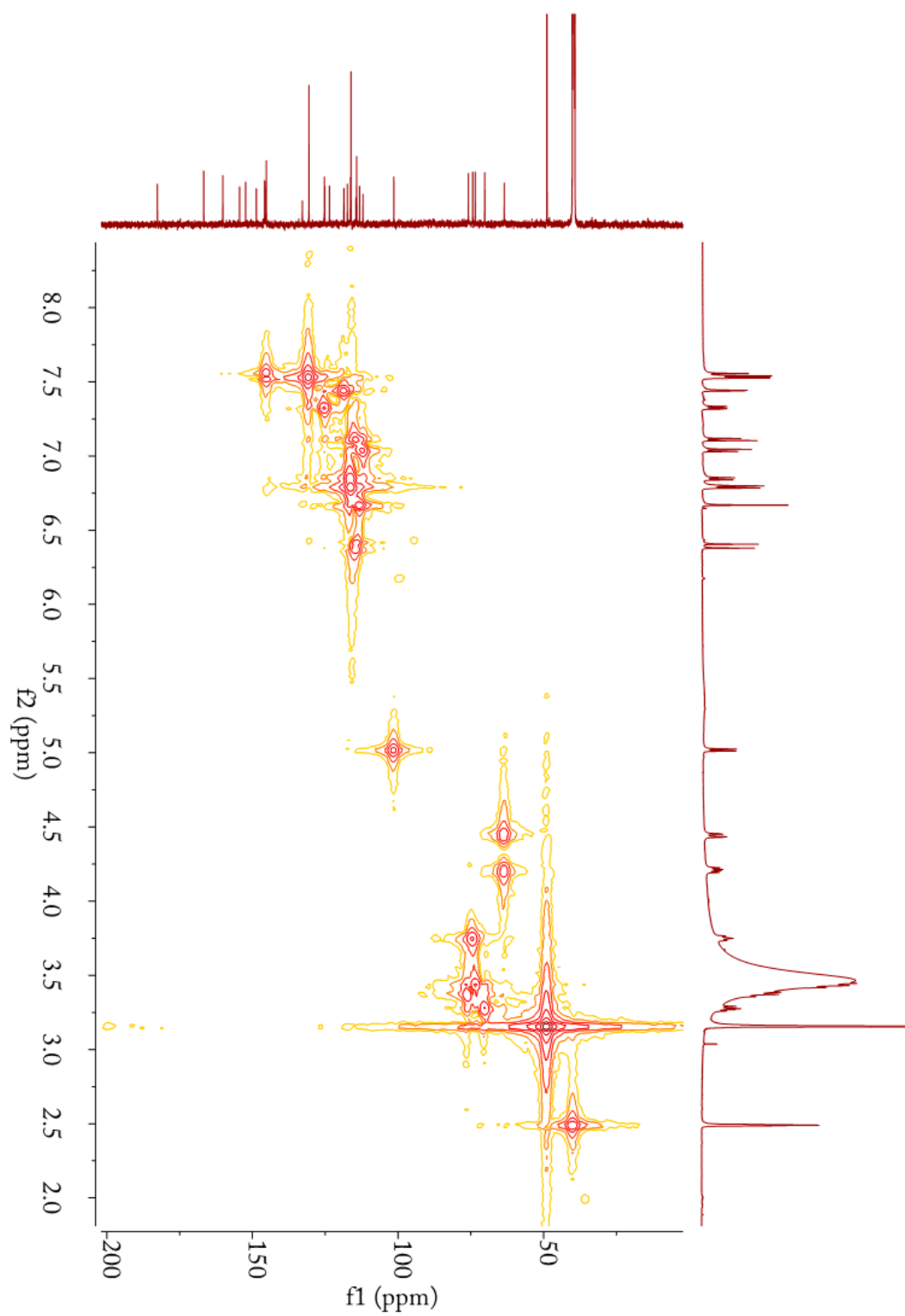
**Figure S17.**  $^1\text{H-NMR}$  spectrum of compound **3** (600 MHz, in  $\text{DMSO-}d_6$ ).



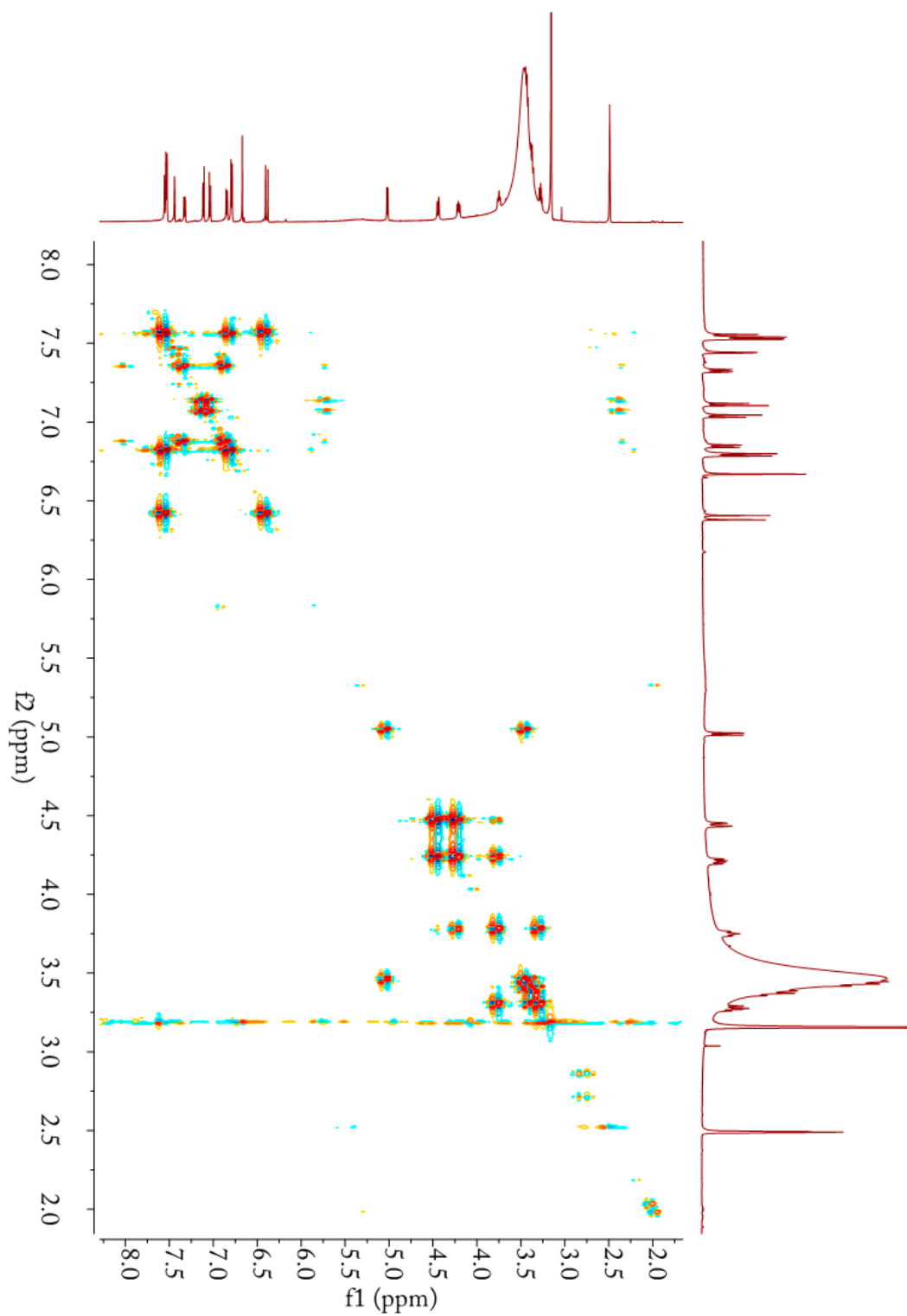
**Figure S18.**  $^{13}\text{C}$ -NMR spectrum of compound **3** (150 MHz, in  $\text{DMSO-}d_6$ ).



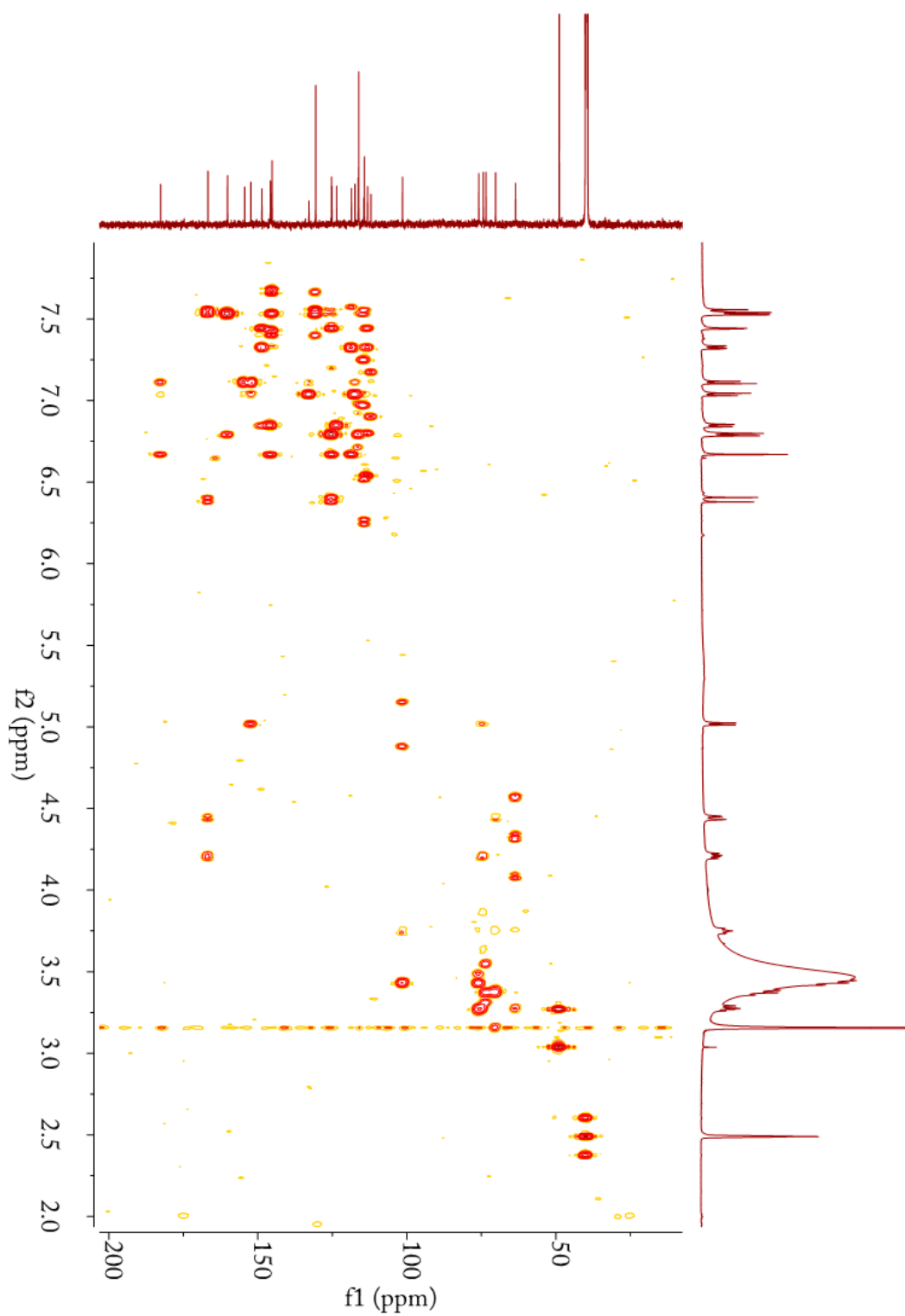
**Figure S19.** DEPT spectrum of compound **3** (150 MHz, in DMSO-*d*<sub>6</sub>).



**Figure S20.** HSQC spectrum of compound **3** (600 MHz, in DMSO-*d*<sub>6</sub>).



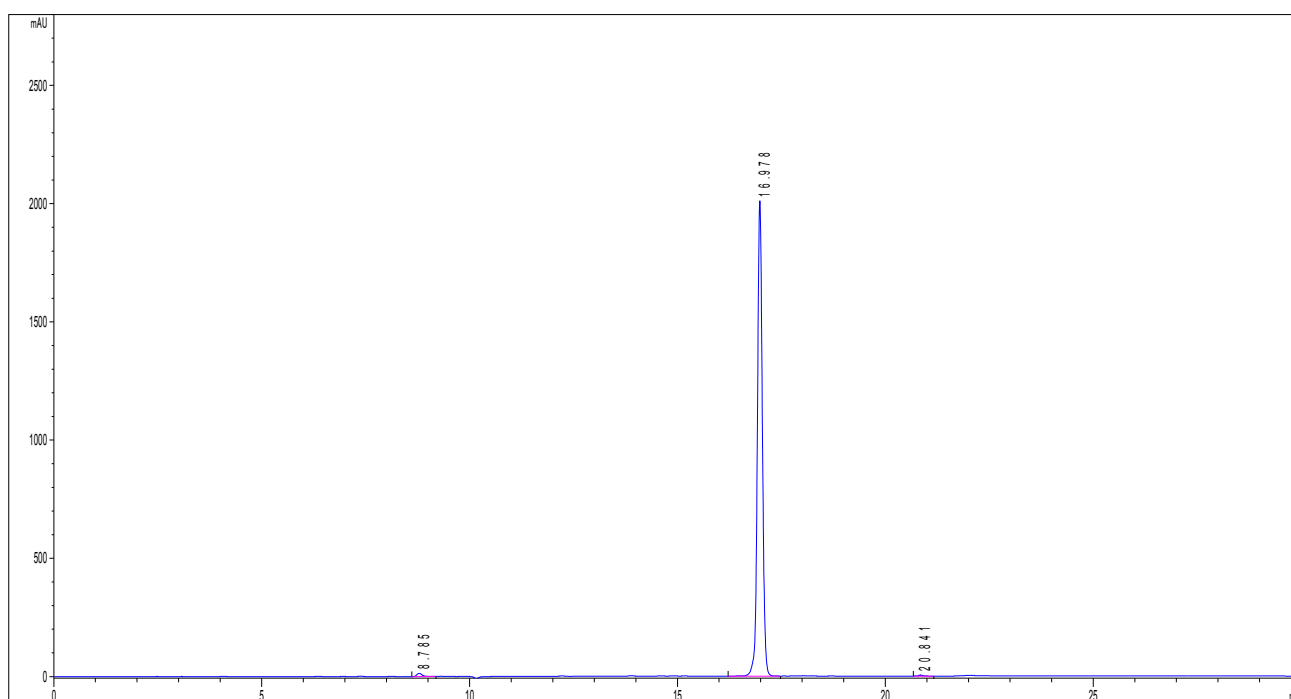
**Figure S21.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3** (600 MHz, in  $\text{DMSO-}d_6$ ).



**Figure S22.** HMBC spectrum of compound **3** (600 MHz, in DMSO-*d*<sub>6</sub>).

Mobile phase of HPLC-DAD analysis for compounds **1**, **2**, **3**, **9**, **15**, **21**, **24**, **51** and EtOH extract of *B. frondosa* with Diamonsil C18 column (250 mm × 4.6 mm, 5.0 μm, Dikma Technologies, Beijing, China)

No.	Time (min)	CH <sub>3</sub> OH (%)	0.1% Aqueous Formic Acid (%)	Flow (mL/min)
1	0.00	10.0	90.0	0.10
	30.00	100.0	0.0	0.10
2	0.00	20.0	80.0	0.10
	80.00	100.0	0.0	0.10

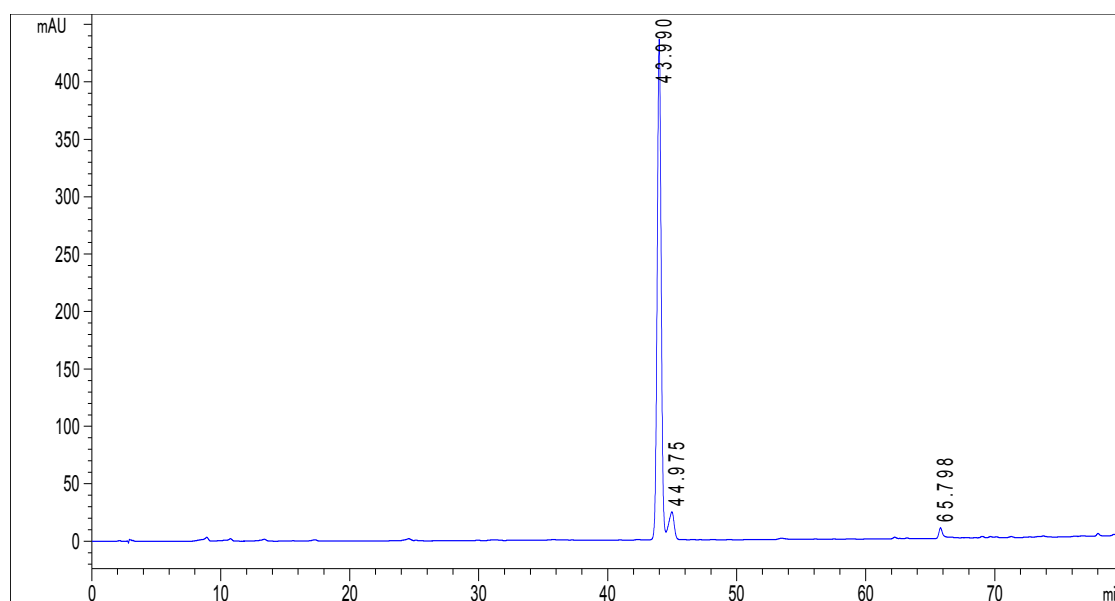


No.	Time	Area	Height	Width	Area%
2	16.978	16638.5	2011	0.1265	99.057

**Figure S23.** HPLC profile of compound 1. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time = 30 min.

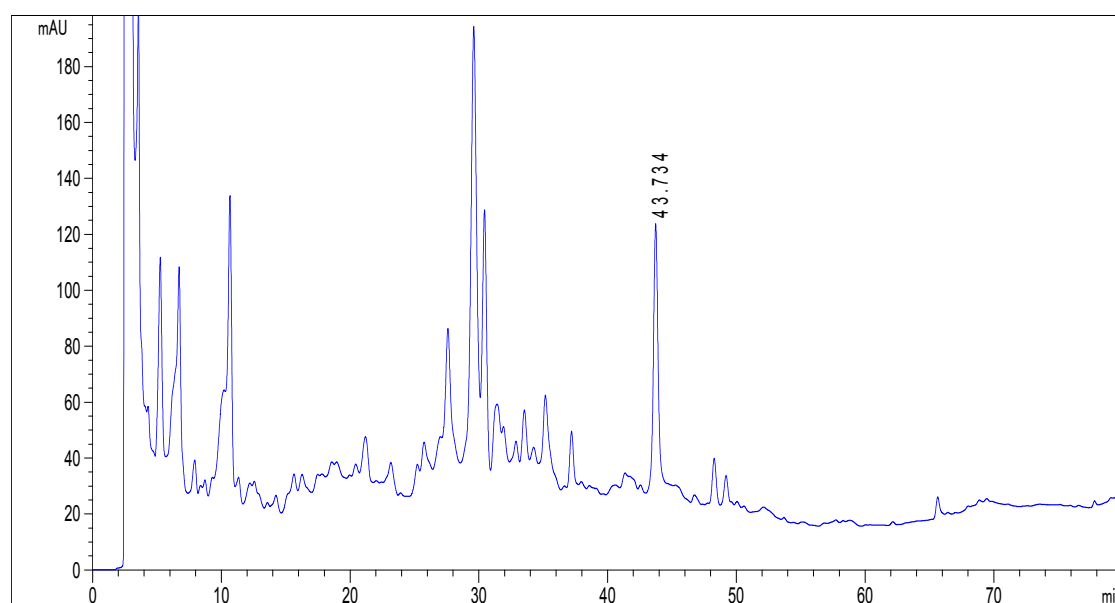


(a)



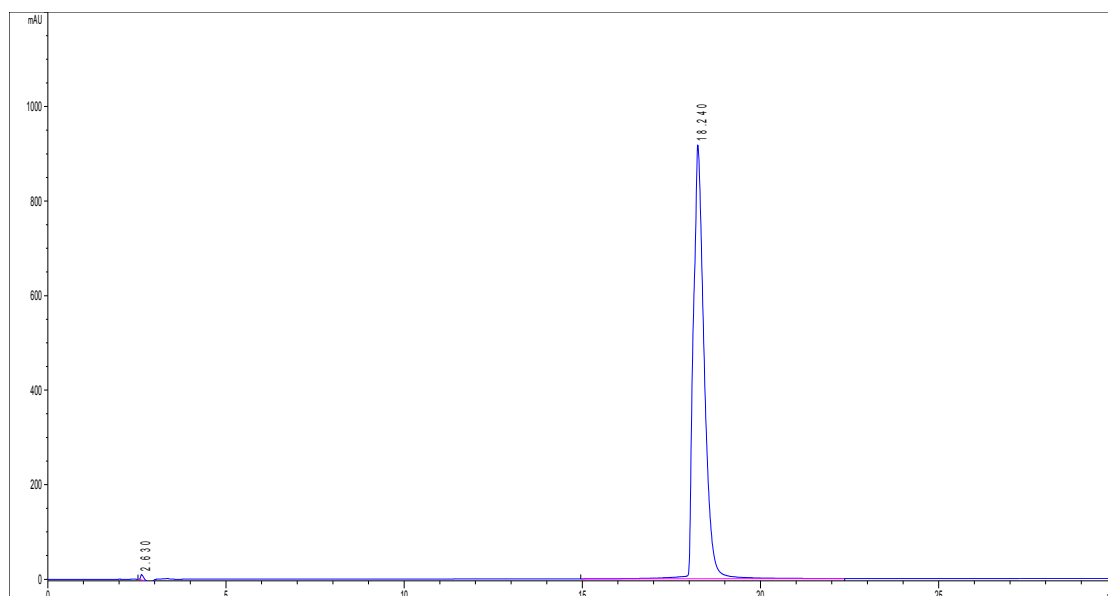
No.	Time	Area	Height	Width	Area%
1	43.99	9331.9	435.9	0.3313	91.239

(b)



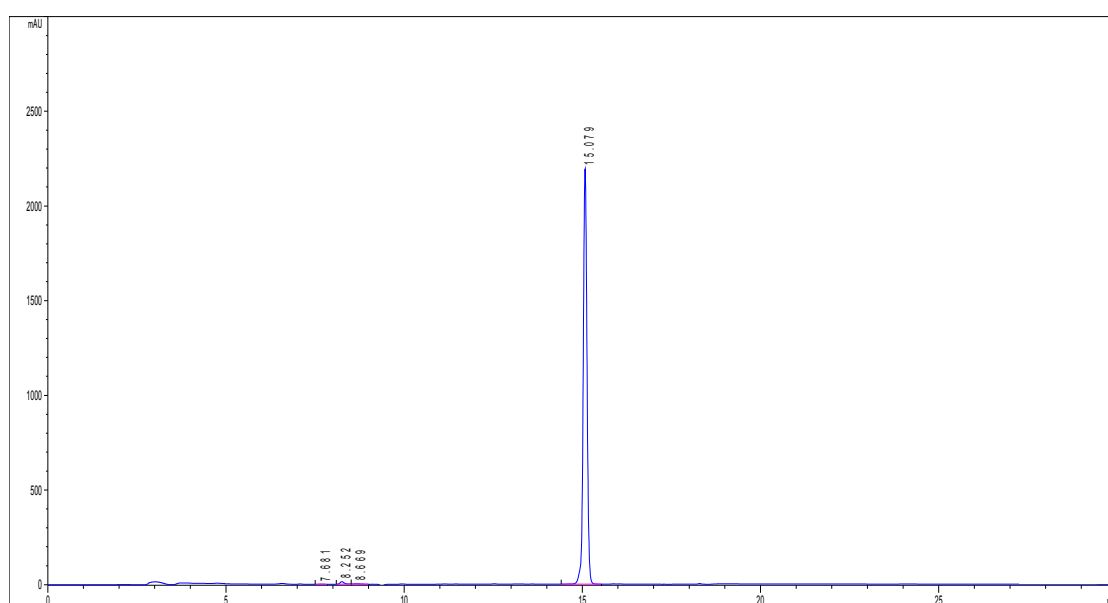
No.	Time	Area	Height	Width	Area%
44	43.734	2421.2	95.3	0.3866	5.307

**Figure S24.** HPLC profiles of compound 2 (a) and EtOH extract of *B. frondosa* (b). Mobile phase of 0 min 20% MeOH–80 min 100% MeOH, Time = 80 min. Compound 2 is a natural chemical constituent, which is identified by HPLC.



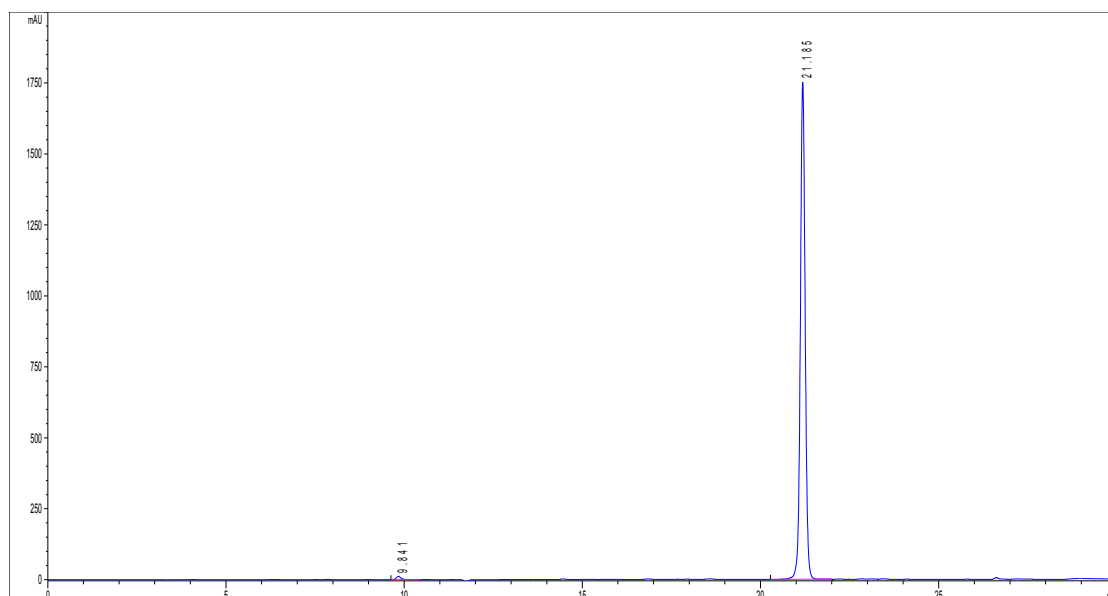
No.	Time	Area	Height	Width	Area%
2	18.24	19459	917.3	0.2955	99.662

**Figure S25.** HPLC profile of compound 3. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time = 30 min.



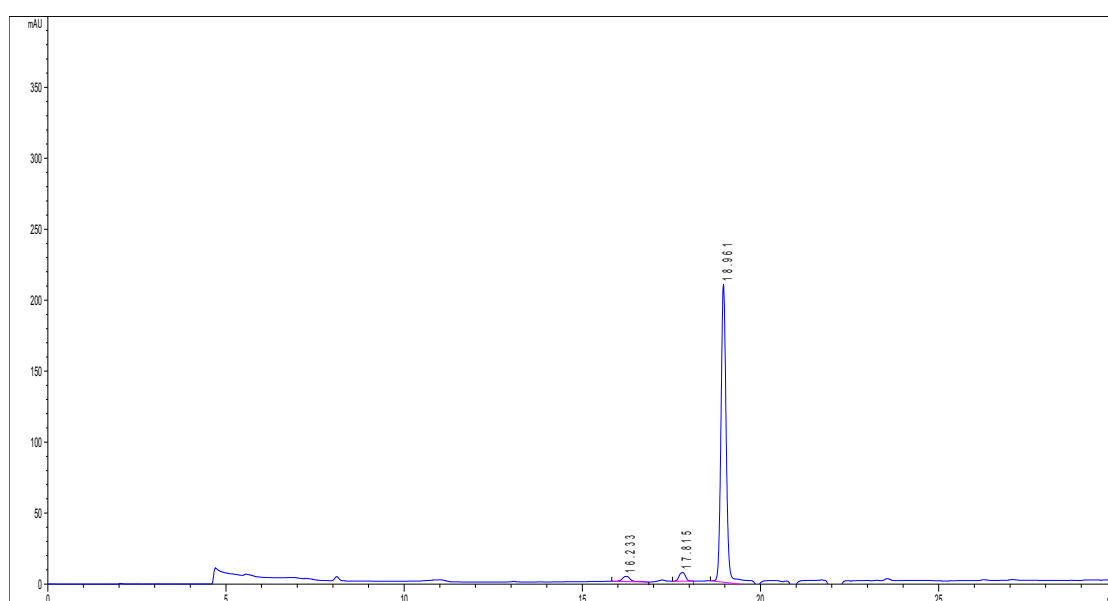
No.	Time	Area	Height	Width	Area%
4	15.079	16115.4	2195.6	0.1136	99.167

**Figure S26.** HPLC profile of compound 9. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time = 30 min.



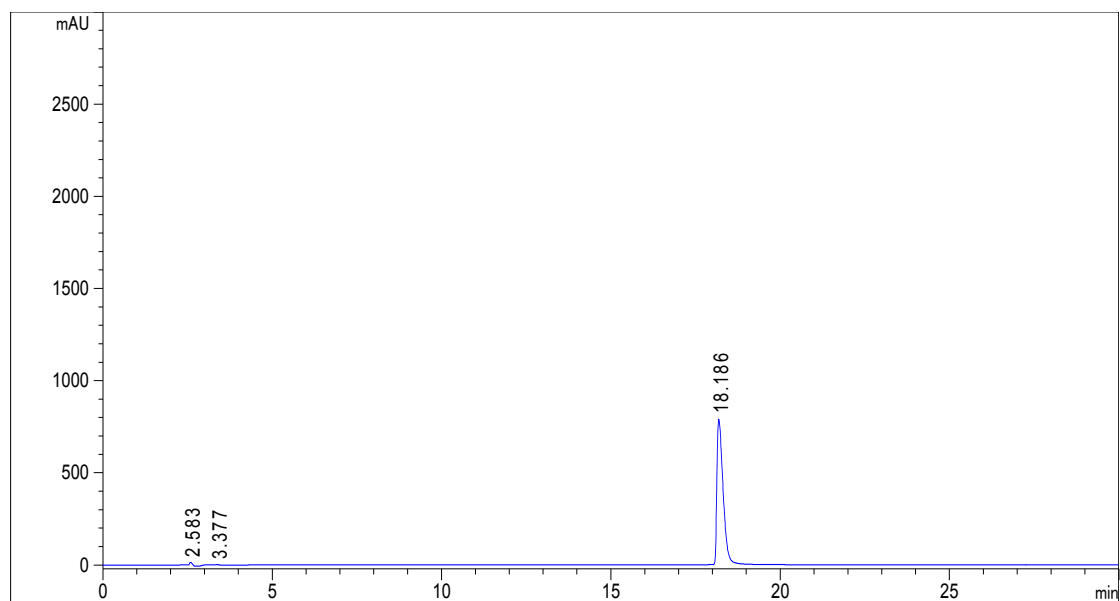
No.	Time	Area	Height	Width	Area%
2	21.185	16489.1	1751	0.1459	99.293

**Figure S27.** HPLC profile of compound **15**. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time =30 min.



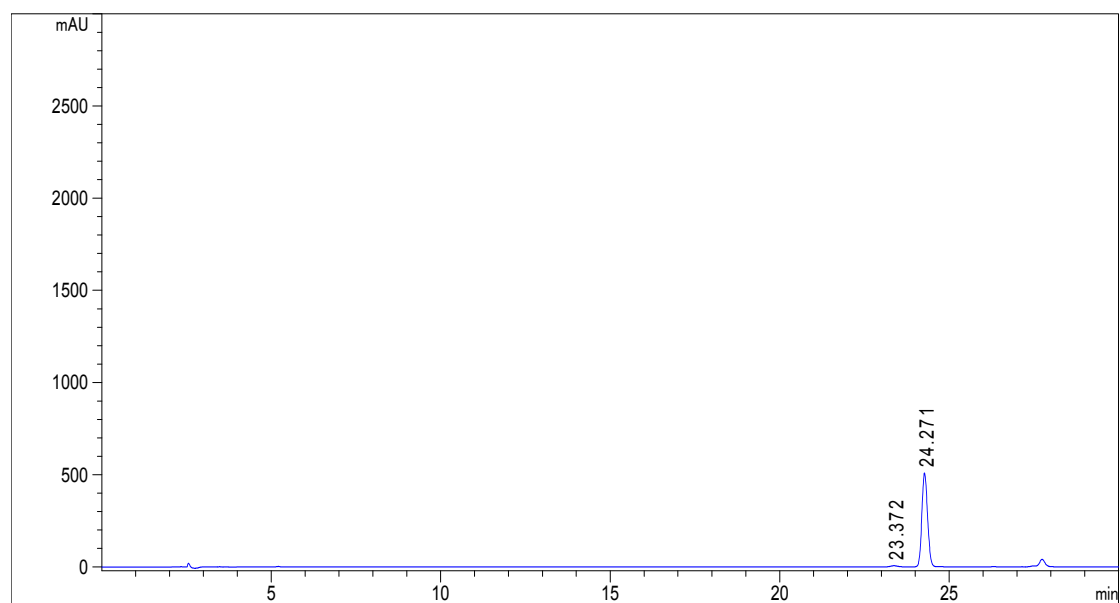
No.	Time	Area	Height	Width	Area%
3	18.961	2189.7	209.8	0.1597	94.127

**Figure S28.** HPLC profile of compound **21**. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time =30 min.



No.	Time	Area	Height	Width	Area%
3	18.186	10208.7	790.4	0.1967	97.939

**Figure S29.** HPLC profile of compound **24**. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time =30 min.



No.	Time	Area	Height	Width	Area%
2	24.271	6150.1	565.5	0.179	97.089

**Figure S30.** HPLC profile of compound **51**. Mobile phase of 0 min 10% MeOH–30 min 100% MeOH, Time =30 min.

**Table S1.** Inhibitory effects of compounds **1–34, 36, 39, 43, 47, 51, 52** (1, 10, 100 µg/mL) on NF-κB in luciferase activity assay.

Compound	Cell	LPS	Compound + LPS		
			C-1 µg/mL	C-10 µg/mL	C-100 µg/mL
1	2132.00 ± 281.13 **	73268.00 ± 4999.01	65479.00 ± 2675.95	62319.67 ± 4230.77 *	59421.67 ± 4993.19 *
2	2132.00 ± 281.13 **	73268.00 ± 4999.01	66488.00 ± 3148.37	62489.67 ± 3724.55 *	56398.67 ± 4119.77
3	2132.00 ± 281.13 **	73268.00 ± 4999.01	68896.00 ± 3696.88	62387.67 ± 3843.46 *	59076.33 ± 6732.61 *
4	2132.00 ± 281.13 **	73268.00 ± 4999.01	68333.00 ± 5552.84	65038.67 ± 5021.67	62632.00 ± 4289.43 *
5	2132.00 ± 281.13 **	73268.00 ± 4999.01	69027.00 ± 4565.20	61769.67 ± 4480.88 *	58630.67 ± 2551.23 **
6	2132.00 ± 281.13 **	73268.00 ± 4999.01	68977.33 ± 4635.98	65313.00 ± 3016.18	60990.67 ± 3209.34 *
7	2132.00 ± 281.13 **	73268.00 ± 4999.01	68038.67 ± 4100.52	67432.00 ± 6221.41	64396.67 ± 5314.31
8	2132.00 ± 281.13 **	73268.00 ± 4999.01	69060.00 ± 4137.77	64708.00 ± 2633.98	60614.67 ± 4016.71 *
9	2132.00 ± 281.13 **	73268.00 ± 4999.01	62253.33 ± 3875.6 *	56677.33 ± 5258.80 *	45549.67 ± 8023.69 **
10	2132.00 ± 281.13 **	73268.00 ± 4999.01	67950.33 ± 4247.37	67385.67 ± 3348.19	58837.00 ± 6131.49 *
11	2132.00 ± 281.13 **	73268.00 ± 4999.01	65528.00 ± 4876.20	64122.33 ± 3531.52	59963.67 ± 3575.50 *
12	2132.00 ± 281.13 **	73268.00 ± 4999.01	67828.33 ± 4365.55	63674.33 ± 4035.83	53432.00 ± 4547.24 **
13	2132.00 ± 281.13 **	73268.00 ± 4999.01	69319.33 ± 4163.59	65280.67 ± 4343.88	56975.67 ± 5995.17 *
14	2132.00 ± 281.13 **	73268.00 ± 4999.01	68371.33 ± 5603.29	63247.67 ± 3694.65 *	58347.33 ± 4447.21 *
15	2132.00 ± 281.13 **	73268.00 ± 4999.01	59902.00 ± 5734.5 *	58715.33 ± 4789.37 *	35417.00 ± 7285.47 **
16	2132.00 ± 281.13 **	73268.00 ± 4999.01	69980.67 ± 4109.9	67088.67 ± 2854.42	63264.67 ± 4006.62
17	2132.00 ± 281.13 **	73268.00 ± 4999.01	68069.33 ± 2254.6	64314.67 ± 3788.37	59662.67 ± 4631.43*
18	2132.00 ± 281.13 **	73268.00 ± 4999.01	65444.67 ± 2904.9	60307.00 ± 3656.06 *	56705.00 ± 5944.80*
19	2132.00 ± 281.13 **	73268.00 ± 4999.01	65878.00 ± 3992.27	64450.67 ± 3680.85	55090.33 ± 4504.16**
20	2132.00 ± 281.13 **	73268.00 ± 4999.01	69457.00 ± 2955.76	65315.33 ± 2724.70	58030.00 ± 5092.78 *
21	2132.00 ± 281.13 **	73268.00 ± 4999.01	61918.33 ± 3548.9 *	50924.00 ± 3502.17 **	45476.00 ± 8498.07 **
22	2132.00 ± 281.13 **	73268.00 ± 4999.01	58070.00 ± 4334.8 *	51643.33 ± 6534.49 *	40122.67 ± 4886.15 **
23	2132.00 ± 281.13 **	73268.00 ± 4999.01	65622.00 ± 3349.58	66220.33 ± 5212.61	59923.33 ± 6084.11 *
24	2132.00 ± 281.13 **	73268.00 ± 4999.01	65046.00 ± 4545.51	64802.33 ± 4082.00	59672.67 ± 3753.96 *
25	2132.00 ± 281.13**	73268.00 ± 4999.01	66629.67 ± 3227.20	63780.33 ± 4066.85	63819.67 ± 4675.25

Table S1. Cont.

Compound	Cell	LPS	Compound + LPS		
			C-1 µg/mL	C-10 µg/mL	C-100 µg/mL
26	2132.00 ± 281.13 **	73268.00 ± 4999.01	65229.67 ± 4410.53	64029.00 ± 4013.51	59010.00 ± 5472.91 *
27	2132.00 ± 281.13 **	73268.00 ± 4999.01	66429.00 ± 3131.58	60575.00 ± 4677.45 *	57566.33 ± 4433.86 *
28	2132.00 ± 281.13 **	73268.00 ± 4999.01	67093.00 ± 3899.88	65215.00 ± 2716.62	59226.00 ± 5025.35 *
29	2132.00 ± 281.13 **	73268.00 ± 4999.01	67276.00 ± 3507.74	63942.33 ± 3294.88	59497.33 ± 4052.66 *
30	2132.00 ± 281.13 **	73268.00 ± 4999.01	67418.00 ± 4181.95	64804.67 ± 3725.58	59233.67 ± 4645.91 *
31	2132.00 ± 281.13 **	73268.00 ± 4999.01	67722.33 ± 2772.07	64602.67 ± 3300.97	58969.00 ± 4565.26 *
32	2132.00 ± 281.13 **	73268.00 ± 4999.01	69157.00 ± 4731.34	63617.00 ± 4047.05	59162.67 ± 4481.74 *
33	2132.00 ± 281.13 **	73268.00 ± 4999.01	67359.00 ± 3514.87	64555.67 ± 4021.52	56640.00 ± 4919.46 *
34	2132.00 ± 281.13 **	73268.00 ± 4999.01	68007.67 ± 4107.68	63242.33 ± 4638.23	52565.67 ± 4279.69 **
36	2132.00 ± 281.13 **	73268.00 ± 4999.01	70055.33 ± 4111.44	64733.33 ± 4174.56	59247.00 ± 4648.29 *
39	2132.00 ± 281.13 **	73268.00 ± 4999.01	67420.00 ± 3259.34	62314.00 ± 4492.91 *	57646.67 ± 3659.60 *
43	2132.00 ± 281.13 **	73268.00 ± 4999.01	66801.00 ± 3696.52	64209.3 ± 3814.68	59015.00 ± 4434.44 *
47	2132.00 ± 281.13 **	73268.00 ± 4999.01	68683.33 ± 4069.28	63742.67 ± 3990.68	62942.00 ± 4080.98
51	2132.00 ± 281.13 **	73268.00 ± 4999.01	61368.33 ± 3827.01 *	51393.67 ± 5605.39 **	38543.67 ± 7726.72 **
52	2132.00 ± 281.13 **	73268.00 ± 4999.01	65899.00 ± 2711.02 *	62089.00 ± 5475.50 **	53650.00 ± 3463.12 **
<b>Ibuprofen</b>	2132.00 ± 281.13 **	73268.00 ± 4999.01	63530.33 ± 4994.17	60789.67 ± 4489.31 *	36894.67 ± 6013.18 **

\*\*  $p < 0.01$ , \*  $p < 0.05$  versus LPS-treated group. Data presented is the mean ± S.D. of samples run in triplicate.