Electronic Supplementary Material (ESI) for Food & Function.

Supplementary information

Dual effects of cardamonin/alpinetin and their acrolein adducts on scavenging acrolein and anti-bacteria from *Alpinia katsumadai Hayata* as a spice in roasted meat

Yang Lu,[a] Juan Liu, [a] Jiaqi Tong, [a] Chenxiao Zhang,[a] Yi Duan,[a] Xiaoli Song, [a] Yongling Lu, [a] Lishuang Lv[a]*

[a]Department of Food Science and Technology, School of Food Science and Pharmaceutical Engineering, Nanjing Normal University, 2 Xuelin Road, Nanjing, Jiangsu 210023, People's Republic of China

Corresponding author: Dr. Lishuang Lv, Telephone/Fax: +86 25-85898183; E-mail address: lishuanglv@126.com; lulishuang@njnu.edu.cn

Supplementary Information

Table S1 Quantification of CAR and ALP by reacting at different temperatures for 60 min. [a]

Transformation	Compound	Concentration and proportion	Temperature (℃)				
			37	60	80	100	120
CAR ⇓ ALP	CAR	Concentration (mmol/L)	4.937 ± 0.077	4.487 ± 0.1841	4.004 ± 0.205	2.817 ± 0.188	2.139 ± 0.106
		Conversion rate (%)	1.26 ± 1.54	10.26 ± 3.68	19.92 ± 4.1	43.65 ± 3.76	57.22 ± 2.12
	ALP	Concentration (mmol/L)	0.066 ± 0.015	0.489 ± 0.012	0.945 ± 0.036	2.151 ± 0.145	2.967 ± 0.1376
		Yield (%)	1.32 ± 0.3	9.78 ± 0.24	18.9 ± 0.72	43.02 ± 2.90	59.34 ± 2.75
		Deviation rate (%)	4.76	-4.68	-5.12	-1.44	3.70
ALP ⇓ CAR	ALP	Concentration (mmol/L)	4.959 ± 0.036	4.803 ± 0.158	4.204 ± 0.151	3.631 ± 0.22	2.850 ± 0.158
		Conversion rate (%)	0.82 ± 0.72	3.94 ± 3.16	15.92 ± 3.08	27.38 ± 4.40	43.00 ± 3.16
	CAR	Concentration (mmol/L)	0.042 ± 0.009	0.205 ± 0.036	0.753 ± 0.310	1.340 ± 0.141	2.057 ± 0.156
		Yield (%)	0.84 ±0.18	4.10 ± 0.72	15.06 ± 6.20	26.80 ± 2.82	41.14 ± 3.12
		Deviation rate (%)	-2.44	4.06	-5.40	-2.12	-4.33

[a]The results are expressed as mean ± standard deviation.

Table S2 Quantification of CAR and ALP by reacting at different pH for 30 min. [a]

Transformation	Compound	Concentration and proportion	pH			
			5	6	7	8
CAR ⇓ ALP	CAR	Concentration (mmol/L)	4.479 ± 0.195	4.233 ± 0.397	3.791 ± 0.023	3.333 ± 0.415
		Conversion rate (%)	10.42 ± 3.9	15.34 ± 7.94	24.18 ± 0.46	33.33 ± 8.3
	ALP	Concentration (mmol/L)	0.494 ± 0.026	0.728 ± 0.323	1.263 ± 0.179	1.750 ± 0.31
		Yield (%)	9.88 ± 0.52	14.56 ± 6.46	25.26 ± 3.58	35.00 ± 6.2
		Deviation rate (%)	-5.18	-5.08	1.08	5.01
ALP ⇓ CAR	ALP	Concentration (mmol/L)	4.593 ± 0.089	4.389 ± 0.238	4.297 ± 0.215	3.785 ± 0.316
		Conversion rate (%)	8.14 ± 1.78	12.22 ± 4.76	14.06 ± 4.30	24.29 ± 6.32
	CAR	Concentration (mmol/L)	0.391 ± 0.027	0.584 ± 0.083	0.659 ± 0.208	1.246 ± 0.306
		Yield (%)	7.82 ± 0.54	11.68 ± 1.66	13.58 ± 4.16	24.92 ± 6.12
		Deviation rate (%)	-3.93	-4.419	-3.41	2.59

[a]The results are expressed as mean ± standard deviation.

Table S3 ^{1}H (400 MHz) and ^{13}C (100 MHz) data of ALP and ALP-ACR

	ALP		ALP-ACR	
	δ_H δ (ppm), J (Hz)	δ_C δ (ppm)	δ_H δ (ppm), J (Hz)	δ_C δ (ppm)
1	-	-	-	-
2	5.49 (dd, J = 12.4)	78.51	5.56 (d, J = 3.3)	78.14/78.32
3	2.62 (dd, J = 16.4,3.1) 2.99 (dd, J = 16.4,12.4)	45.31	2.81 (m)	45.07
4	-	187.84	-	188.39/188.34
5	-	164.51	-	160.15
6	6.08 (d, J = 2.2)	96.09	6.07 (s)	94.17/94.13
7	-	164.83	-	161.02
8	6.01 (d, J = 2.1 Hz)	93.80	-	102.95/102.91
9	-	162.68	-	159.49/159.41
10	-	104.94	-	105.5
11	3.74 (s)	56.09	3.73 (s)	56.12
12	-	-	2.54 (d, J = 7.2)	15.45/15.09
13	-	-	1.84 (m)	27.24/27.07
14	-	-	5.53 (t, J=5.1)	93.15/92.90
1′	-	139.63	-	139.77/139.74
2′	7.44 (m)	126.92	7.42 (m)	126.62
3′	7.44 (m)	128.98	7.42 (m)	129.02
4′	7.44 (m)	128.80	7.42 (m)	128.69
5′	7.44 (m)	128.98	7.42 (m)	129.02
6′	7.44 (m)	126.92	7.42 (m)	126.60

Table S4 ^{1}H (400 MHz) and ^{13}C (100 MHz) data of CAR, CAR-ACR-1 and CAR-ACR-2

	CAR		CAR-ACR-1		CAR-ACR-2	
	δ_H δ (ppm), J (Hz)	δ_C δ (ppm)	δ_H δ (ppm), J (Hz)	δ_C δ (ppm)	δ_H δ (ppm), J (Hz)	δ_C δ (ppm)
1	-	-	-	-	-	-
2	7.85 (d, J = 15.7)	142.28	7.74 (m)	142.55	6.59 (s)	90.48/90.33
3	7.71 (m)	130.80	7.74 (m)	130.90	6.65 (dd, J = 16.1, 3.8)	118.07
4	-	192.23	-	192.51	-	165.32
5	-	163.18	-	161.07	-	156.04
6	6.05 (d, J = 2.2)	92.15	6.03 (s)	92.45	6.03 (s)	93.30
7	-	166.82	-	160.53	-	152.25/152.33
8	5.96 (d, J = 2.1)	96.32	-	102.98	-	102.93/102.88
9	-	165.56	-	164.49	-	149.28/149.34
10	-	105.59	-	105.51	-	102.39
11	3.90 (s)	56.50	3.90 (s)	56.62	3.72 (s)	55.78
12	-	-	2.55 (d, J = 6.8)	14.90	2.65 (m)/2.44 (t, J = 6.8)	14.06/15.42
13	-	-	1.86 (s)	27.22	1.95 (s)/2.11 (s)	27.55/24.53
14	-	-	5.54 (m)	93.26	5.38 (s)	92.08/91.89
1′	-	135.40	-	135.37	-	134.30
2′	7.71 (m)	128.87	7.74 (m)	128.93	7.74 (m)	129.05
3′	7.46 (m)	129.52	7.46 (dd, J = 5.1, 2.0)	129.56	7.41 (m)	129.36
4′	7.46 (m)	127.96	7.94 (d, J = 15.7)	127.77	7.74 (m)	131.17
5′	7.46 (m)	129.52	7.46 (dd, J = 5.1, 2.0)	129.56	7.41 (m)	129.36
6′	7.71 (m)	128.87	7.74 (m)	128.93	7.74 (m)	129.05

Figure captions:

Fig. S1 ESI-MS^1 and MS^2 (positive ion) spectra of (A) CAR, (B) CAR-ACR-1, (C) CAR-ACR-2, (D) CAR-2ACR, (E) ALP, (F) ALP-ACR and (G) ALP-2ACR.

Fig. S2 High-resolution mass spectrum (MS^1 and MS^2) of ALP-ACR

Fig. S3 ^{1}H-NMR spectrum of ALP-ACR

Fig. S4 ^{13}C-NMR spectrum of ALP-ACR

Fig. S5 HSQC-NMR spectrum of ALP-ACR

Fig. S6 HMBC-NMR spectrum of ALP-ACR

Fig. S7 High-resolution mass spectrum (MS^1 and MS^2) of CAR-ACR-1

Fig. S8 ^{1}H-NMR spectrum of CAR-ACR-1

Fig. S9 ^{13}C-NMR spectrum of CAR-ACR-1

Fig. S10 HSQC-NMR spectrum of CAR-ACR-1

Fig. S11 HMBC-NMR spectrum of CAR-ACR-1

Fig. S12 High-resolution mass spectrum (MS^1 and MS^2) of CAR-ACR-2

Fig. S13 ^{1}H-NMR spectrum of CAR-ACR-2

Fig. S14 ^{13}C-NMR spectrum of CAR-ACR-2

Fig. S15 HSQC-NMR spectrum of CAR-ACR-2

Fig. S16 HMBC-NMR spectrum of CAR-ACR-2

Fig. S17 DEPT-NMR spectrum of CAR-ACR-2

Fig. S18 HPLC-DAD chromatograms of (A) quercetin and (B) myricetin incubated at 100 °C for 0, 5, 15, 60 and 120 min in PBS (0.1M, pH 7.0)

Fig. S19 HPLC-DAD chromatograms of (A) ALP-ACR and (B) CAR-ACR-1 incubated at 100 °C for 0, 5, 15, 60 and 120 min in PBS (pH 7.0).

Fig. S1 ESI-MS^1 and MS^2 (positive ion) spectra of (A) CAR, (B) CAR-ACR-1, (C) CAR-ACR-2, (D) CAR-2ACR, (E) ALP, (F) ALP-ACR and (G) ALP-2ACR.

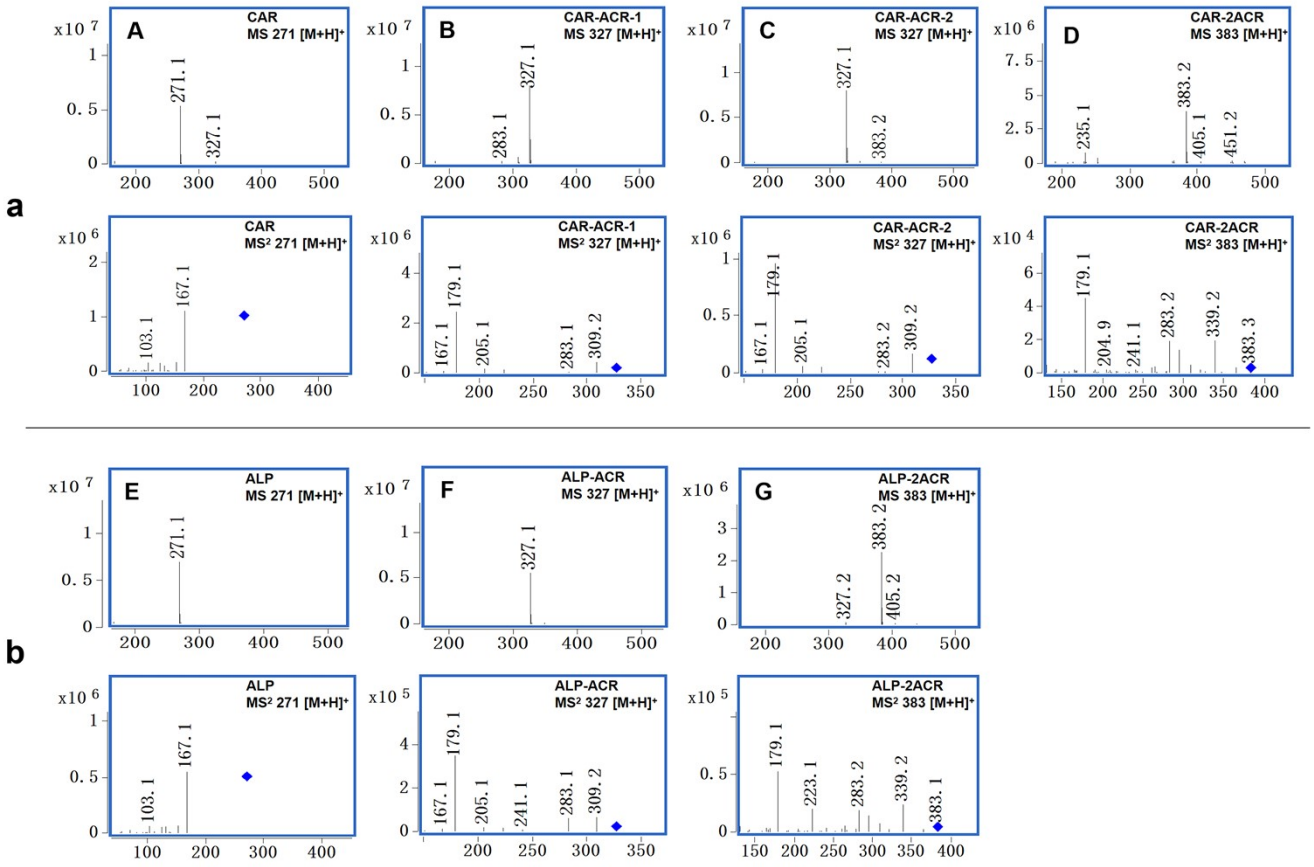

Fig. S2 High-resolution mass spectrum (MS^1 and MS^2) of ALP-ACR

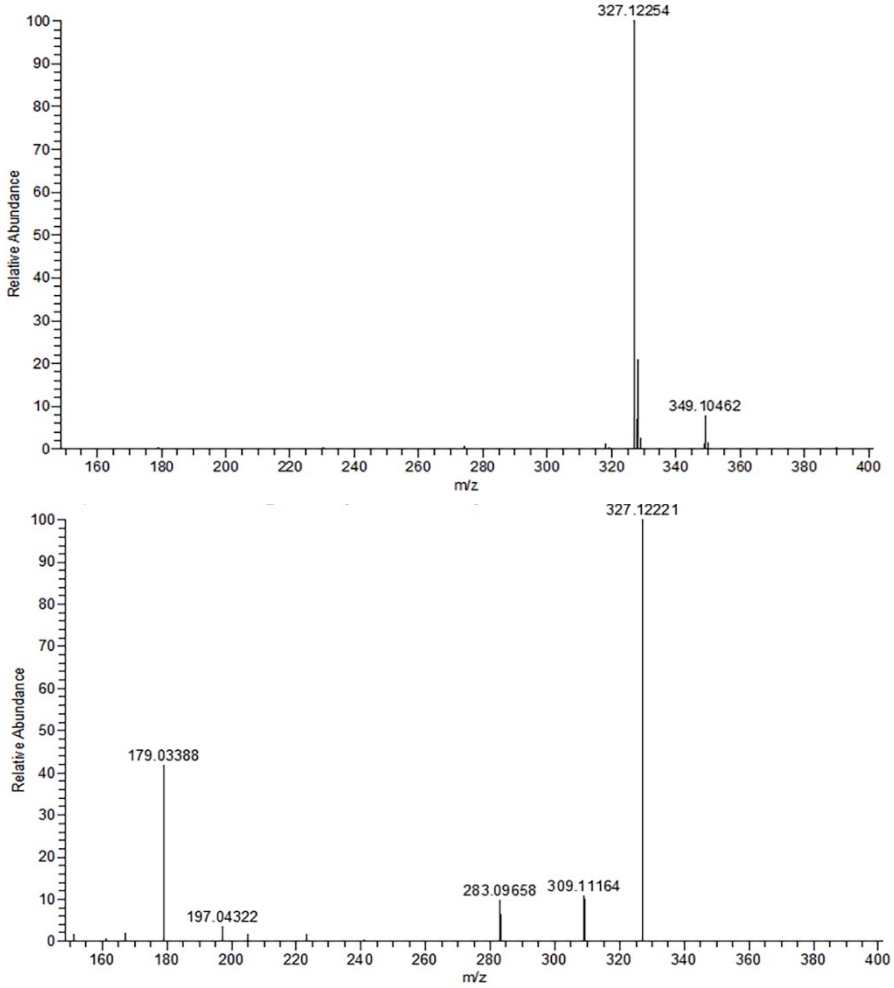

Fig. S3 ^{1}H-NMR spectrum of ALP-ACR

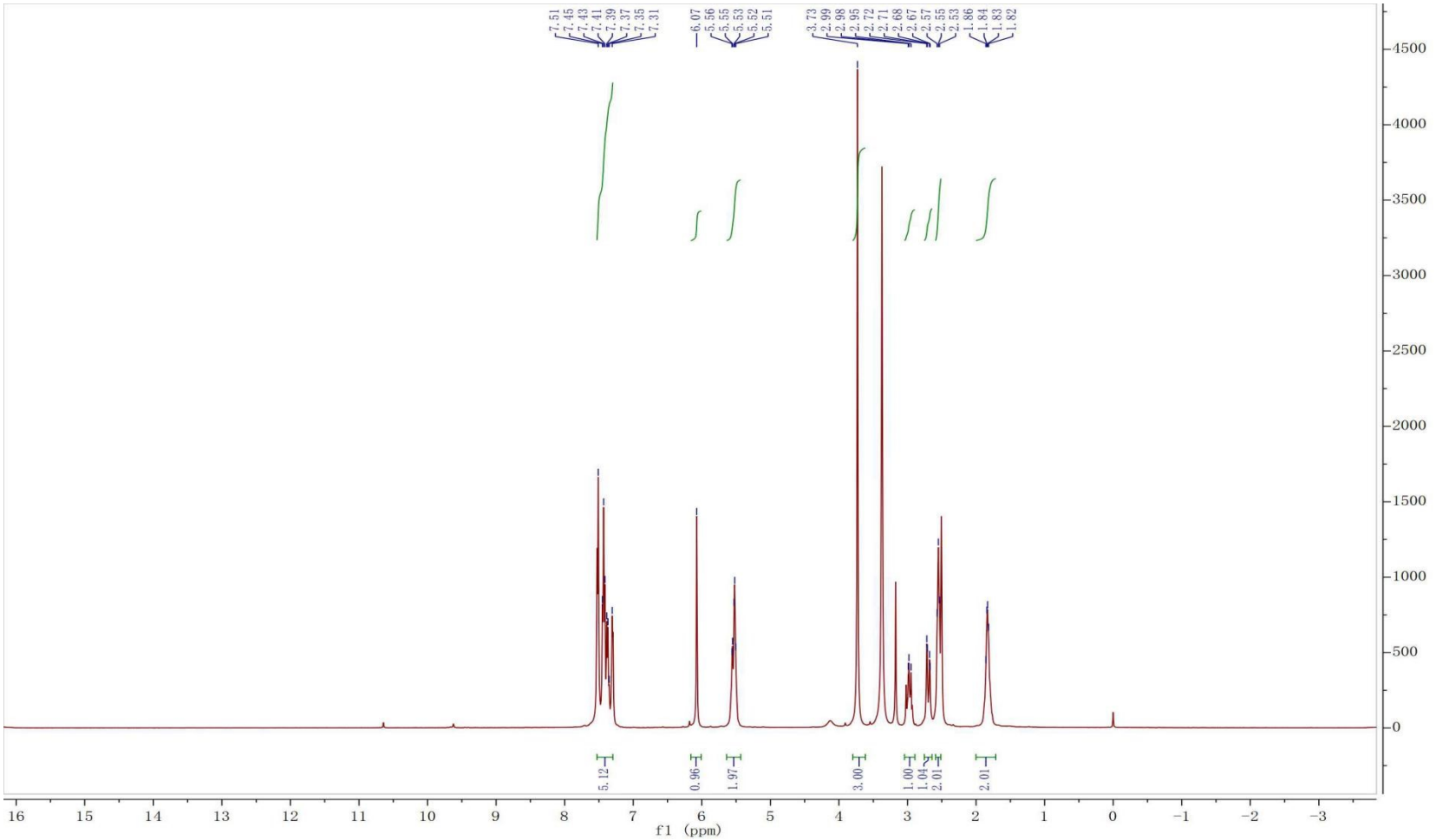

Fig. S4 ^{13}C-NMR spectrum of ALP-ACR

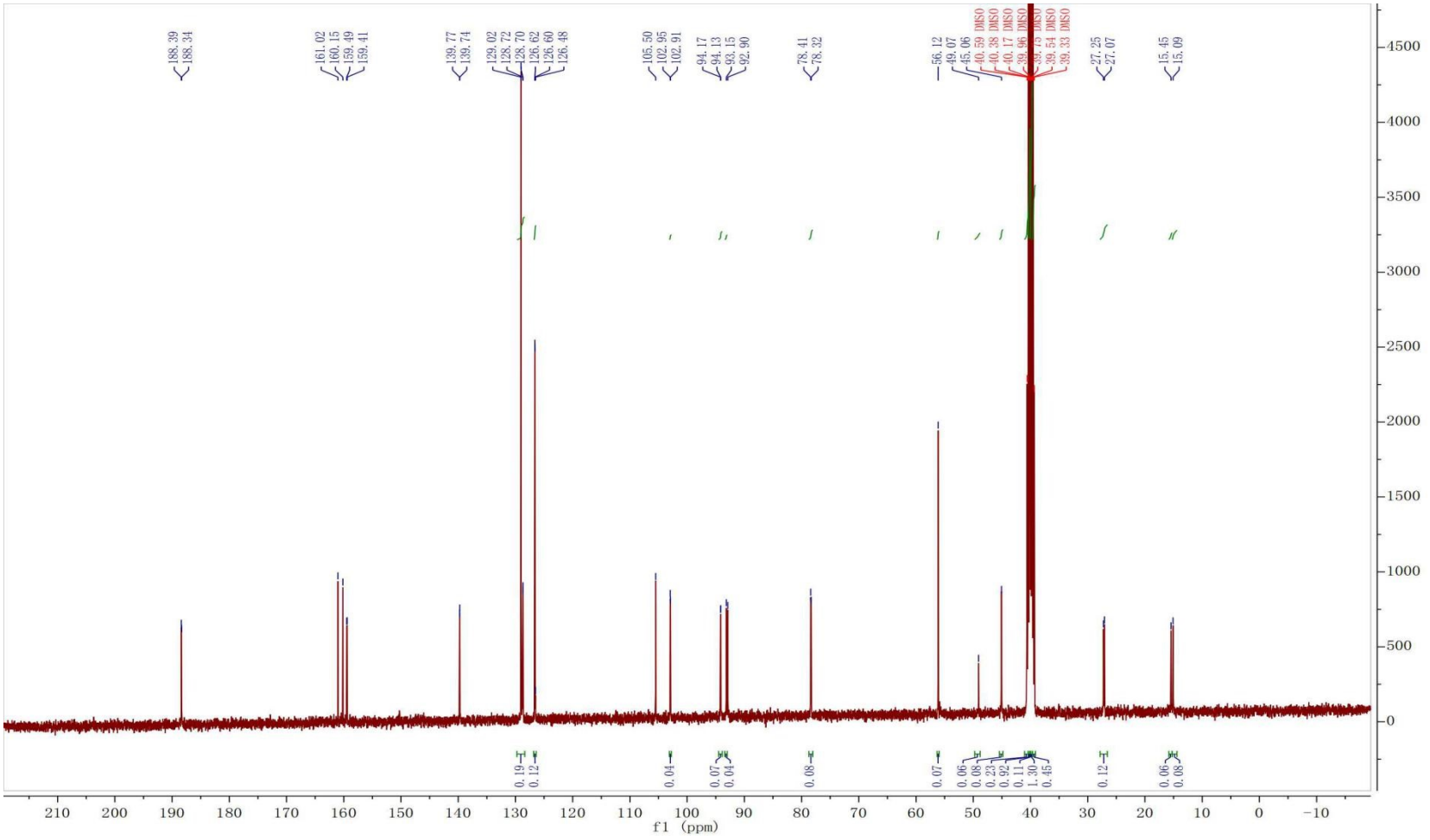

Fig. S5 HSQC-NMR spectrum of ALP-ACR

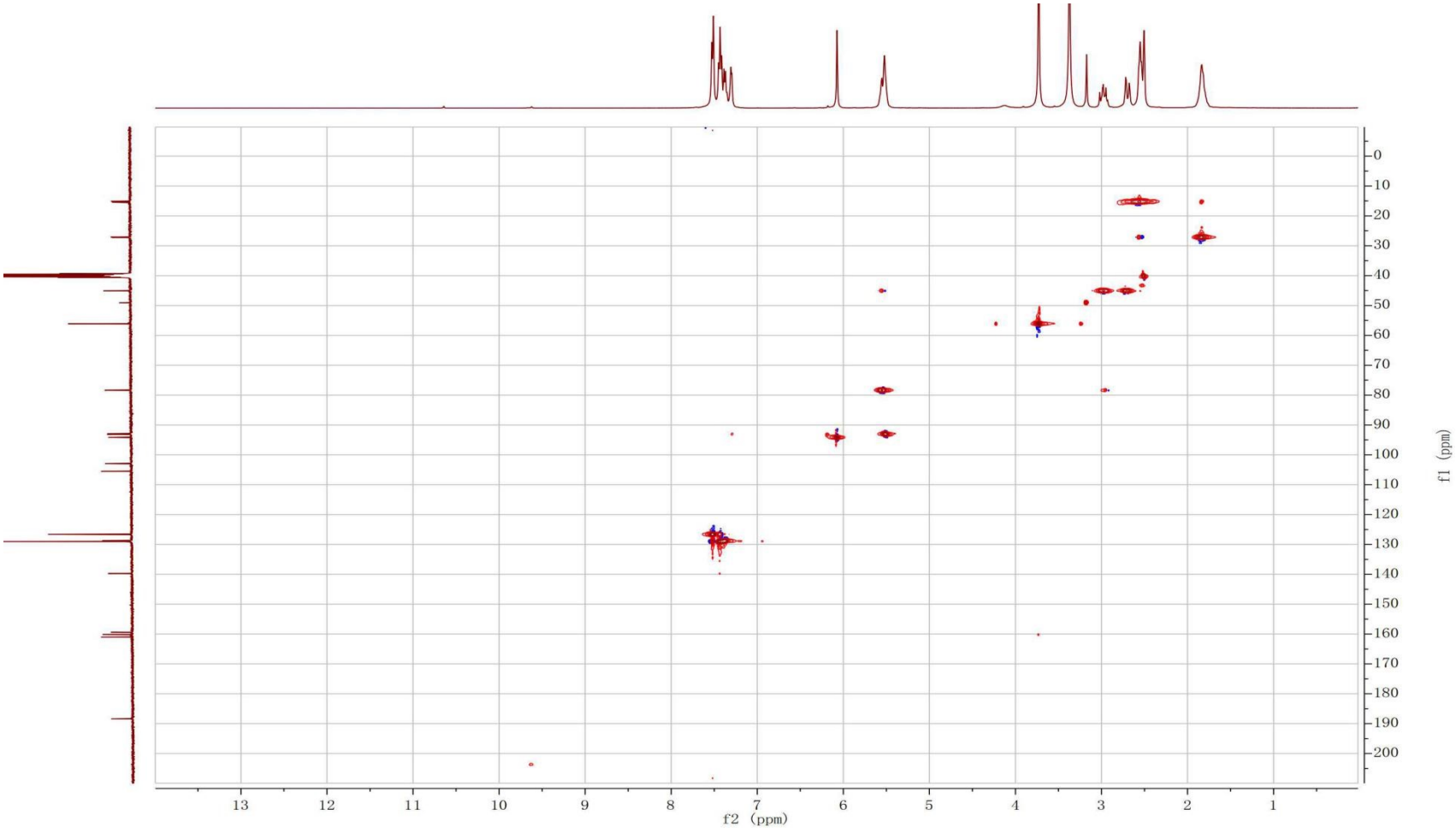

Fig. S6 HMBC-NMR spectrum of ALP-ACR

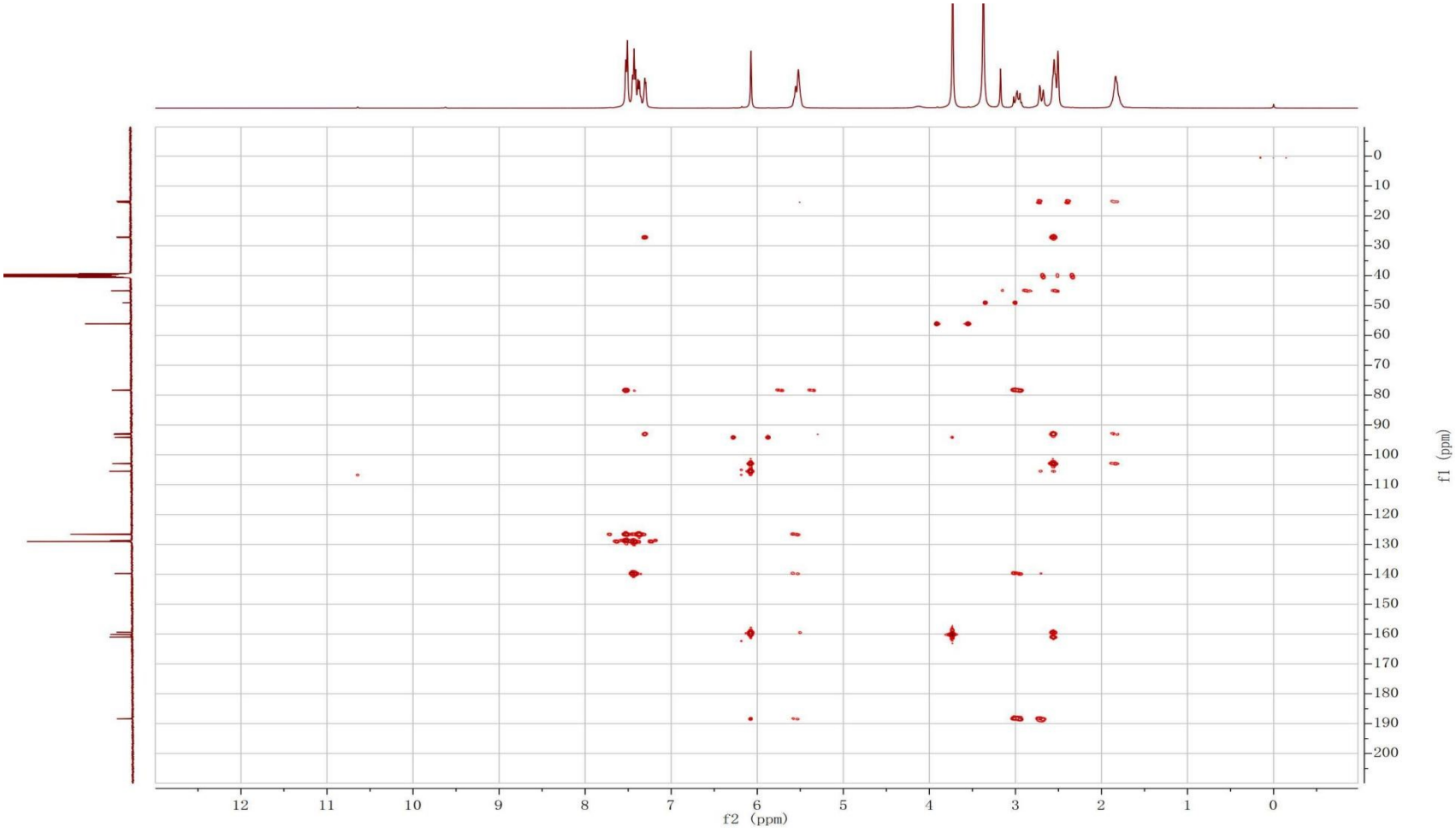

Fig. S7 High-resolution mass spectrum (MS^1 and MS^2) of CAR-ACR-1

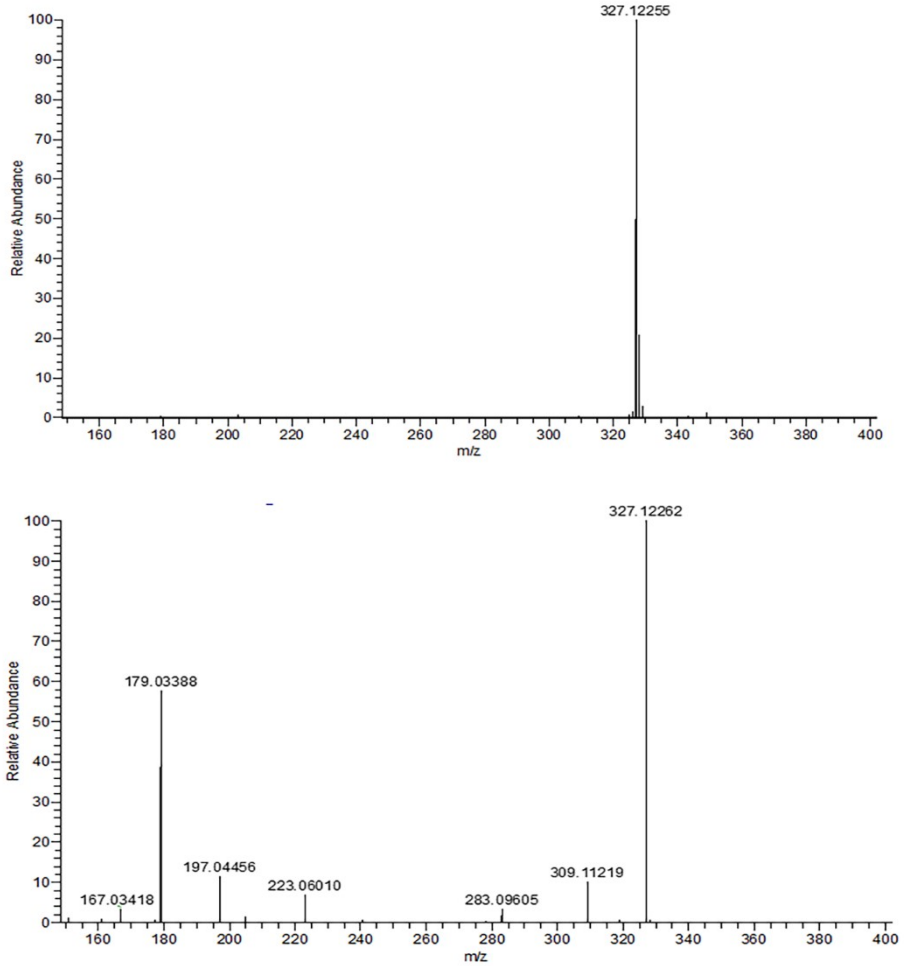

Fig. S8 ^{1}H-NMR spectrum of CAR-ACR-1

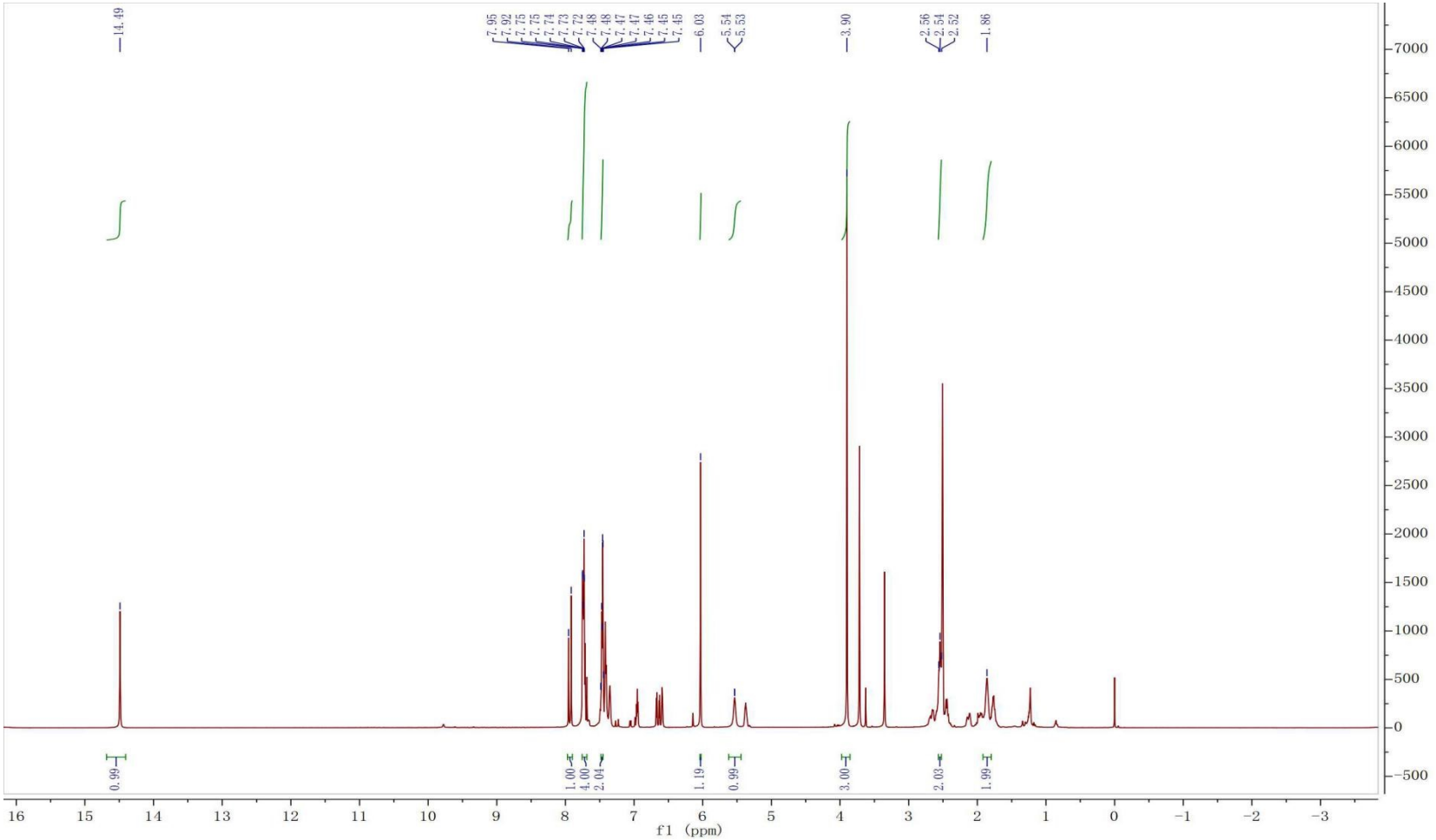

Fig. S9 ^{13}C-NMR spectrum of CAR-ACR-1

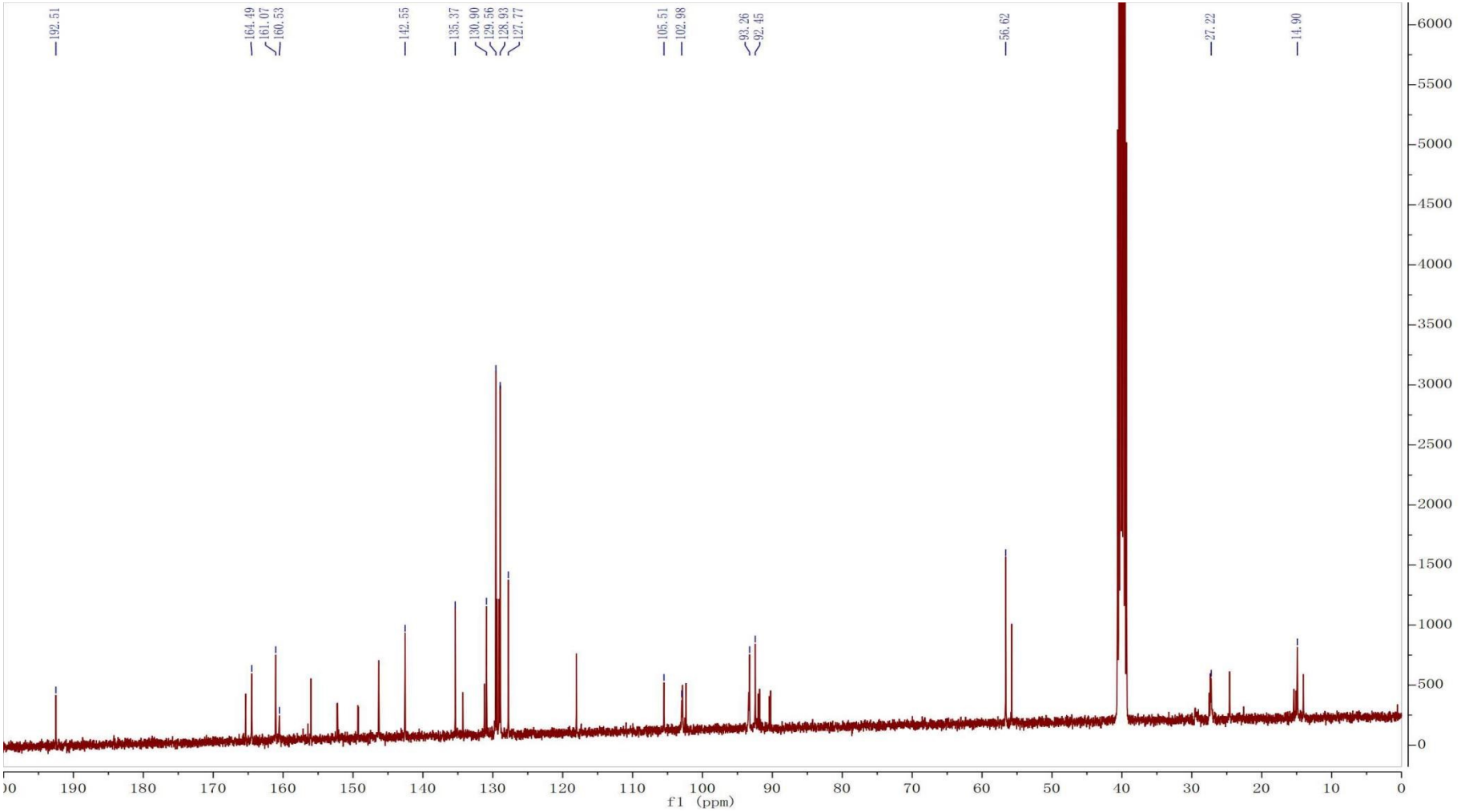

Fig. S10 HSQC-NMR spectrum of CAR-ACR-1

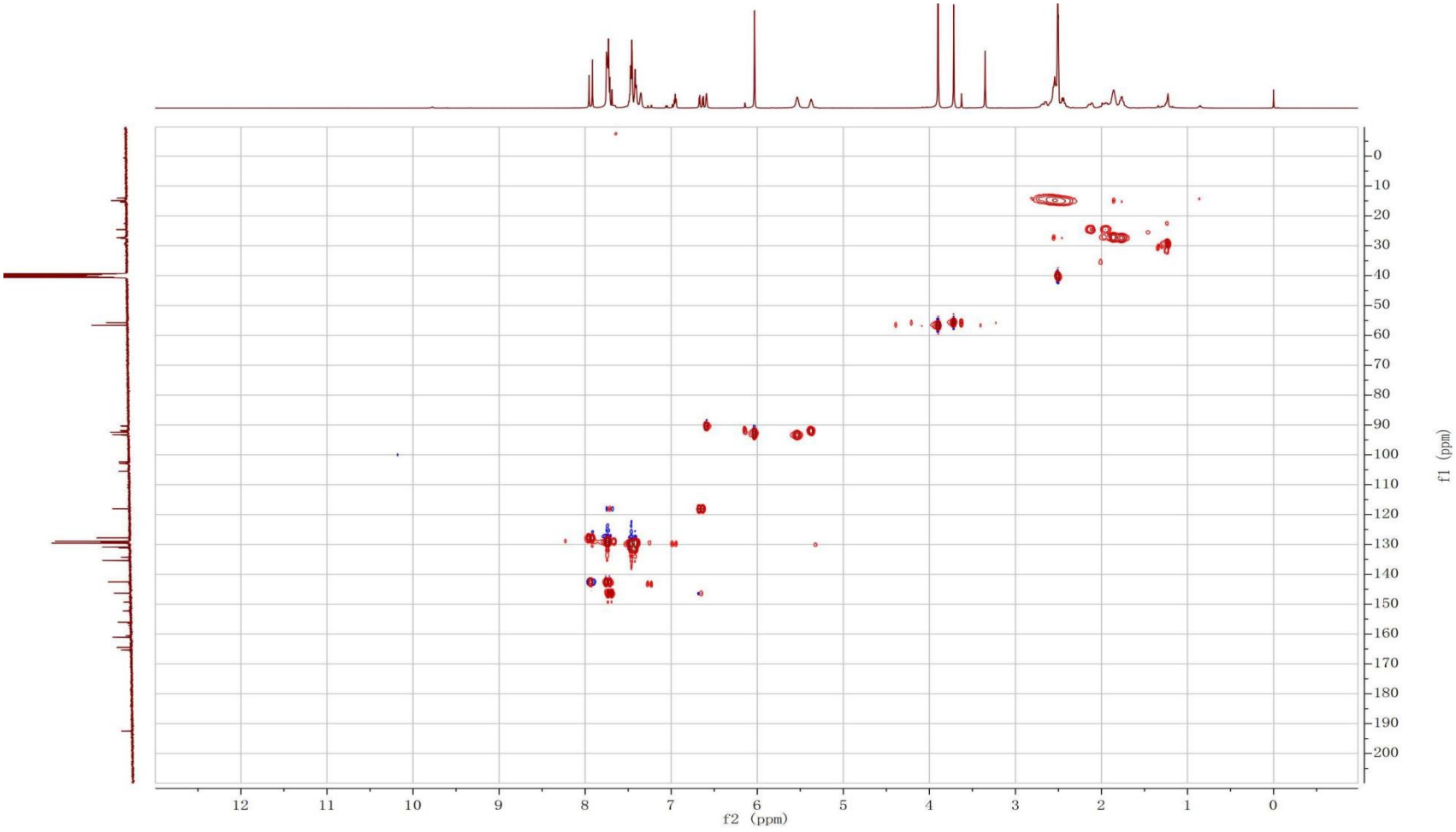

Fig. S11 HMBC-NMR spectrum of CAR-ACR-1

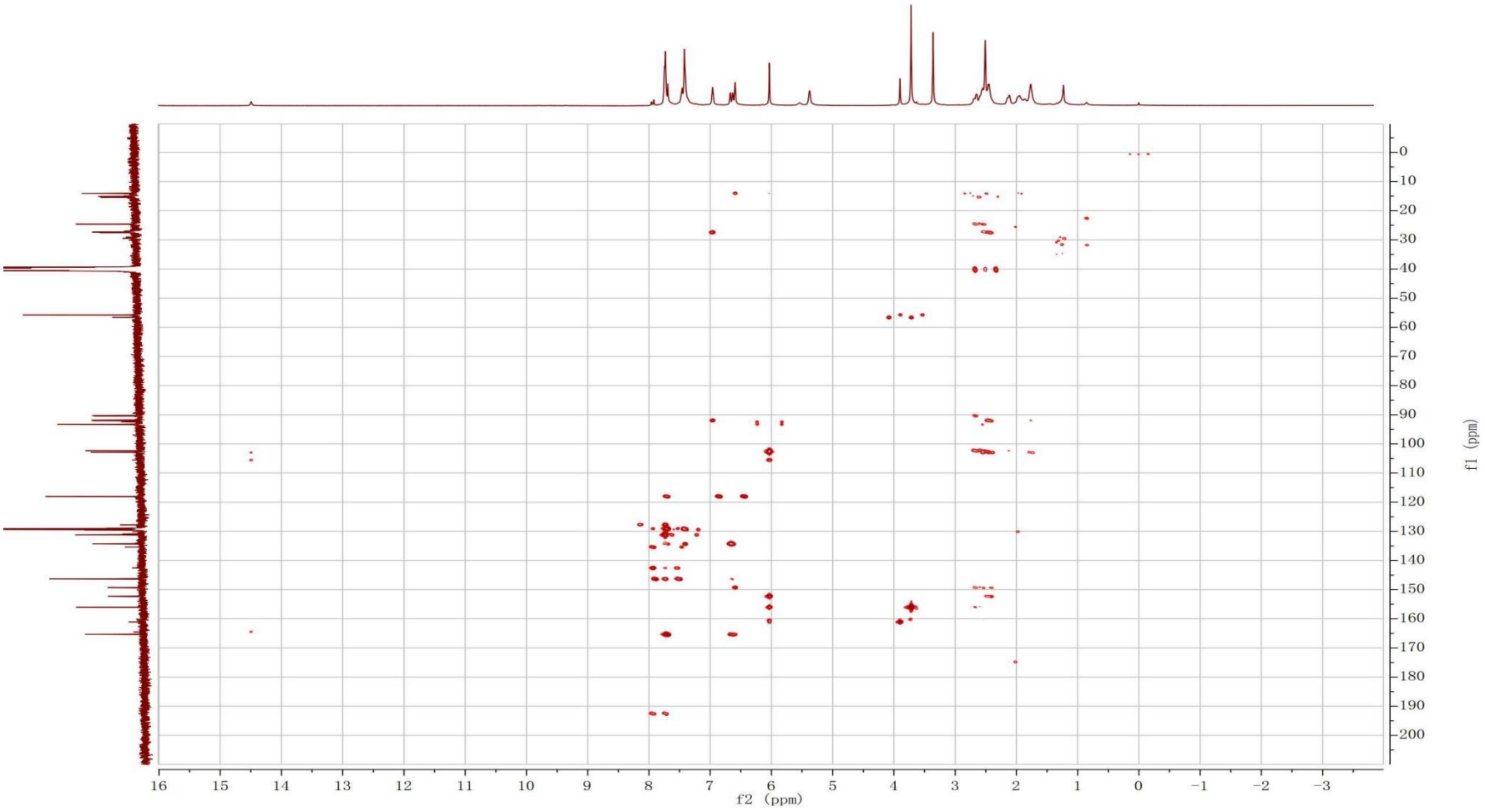

Fig. S12 High-resolution mass spectrum (MS^1 and MS^2) of CAR-ACR-2

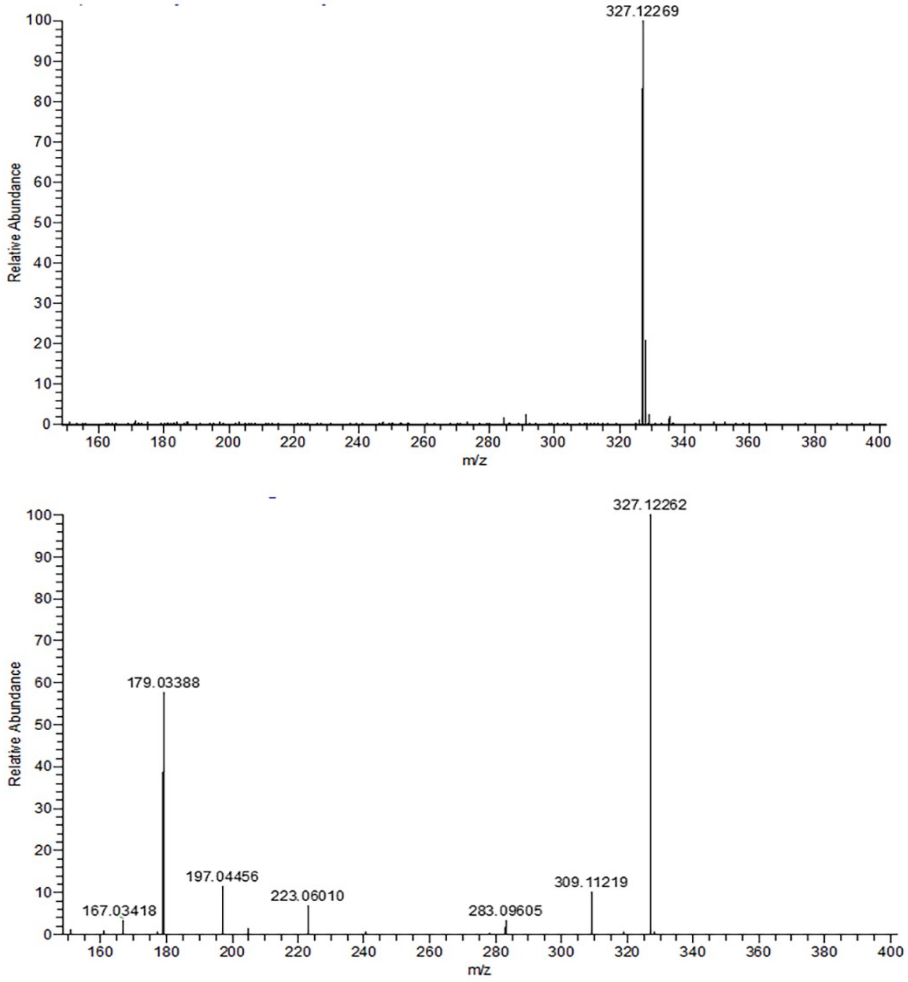

Fig. S13 ^{1}H-NMR spectrum of CAR-ACR-2

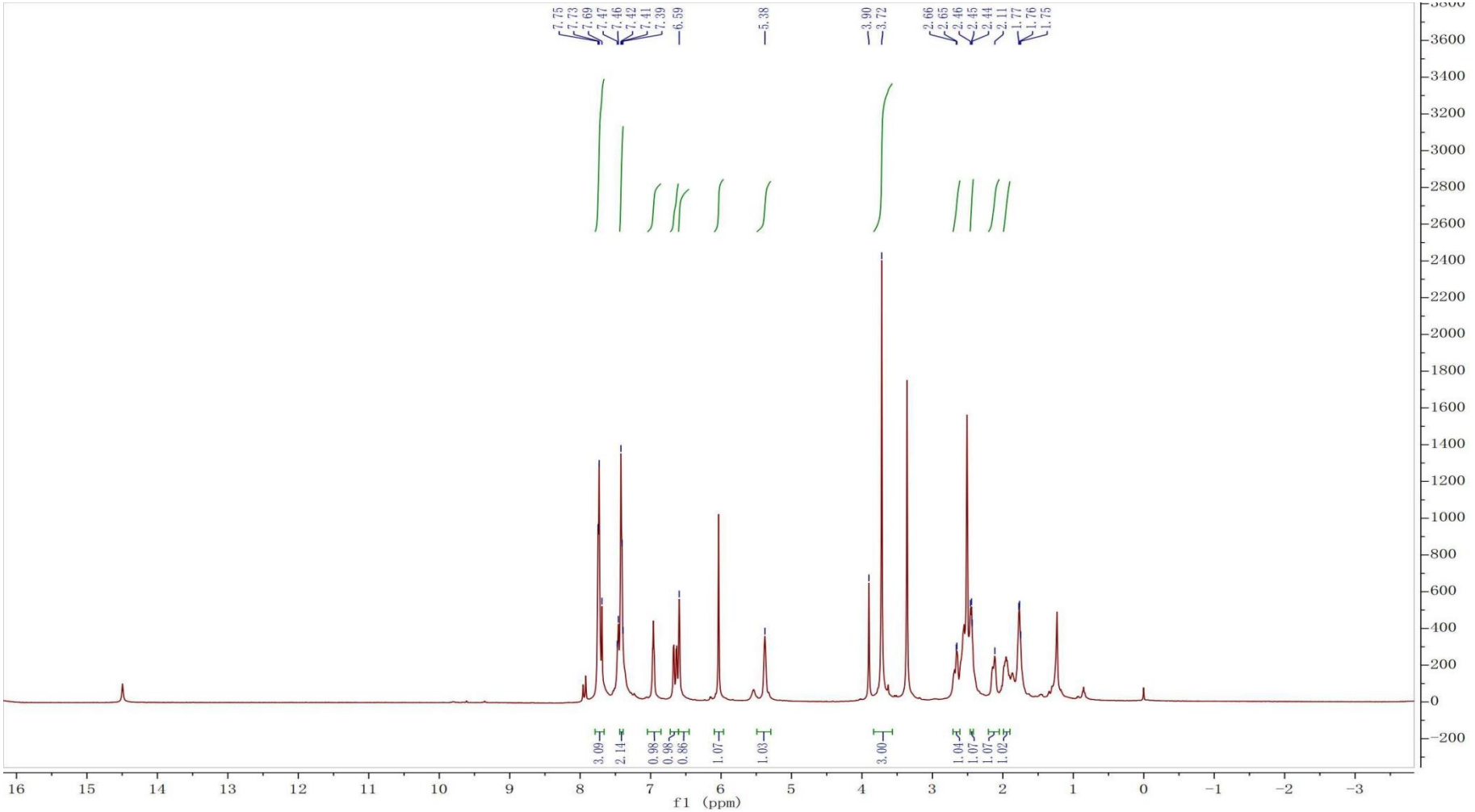

Fig. S14 ^{13}C-NMR spectrum of CAR-ACR-2

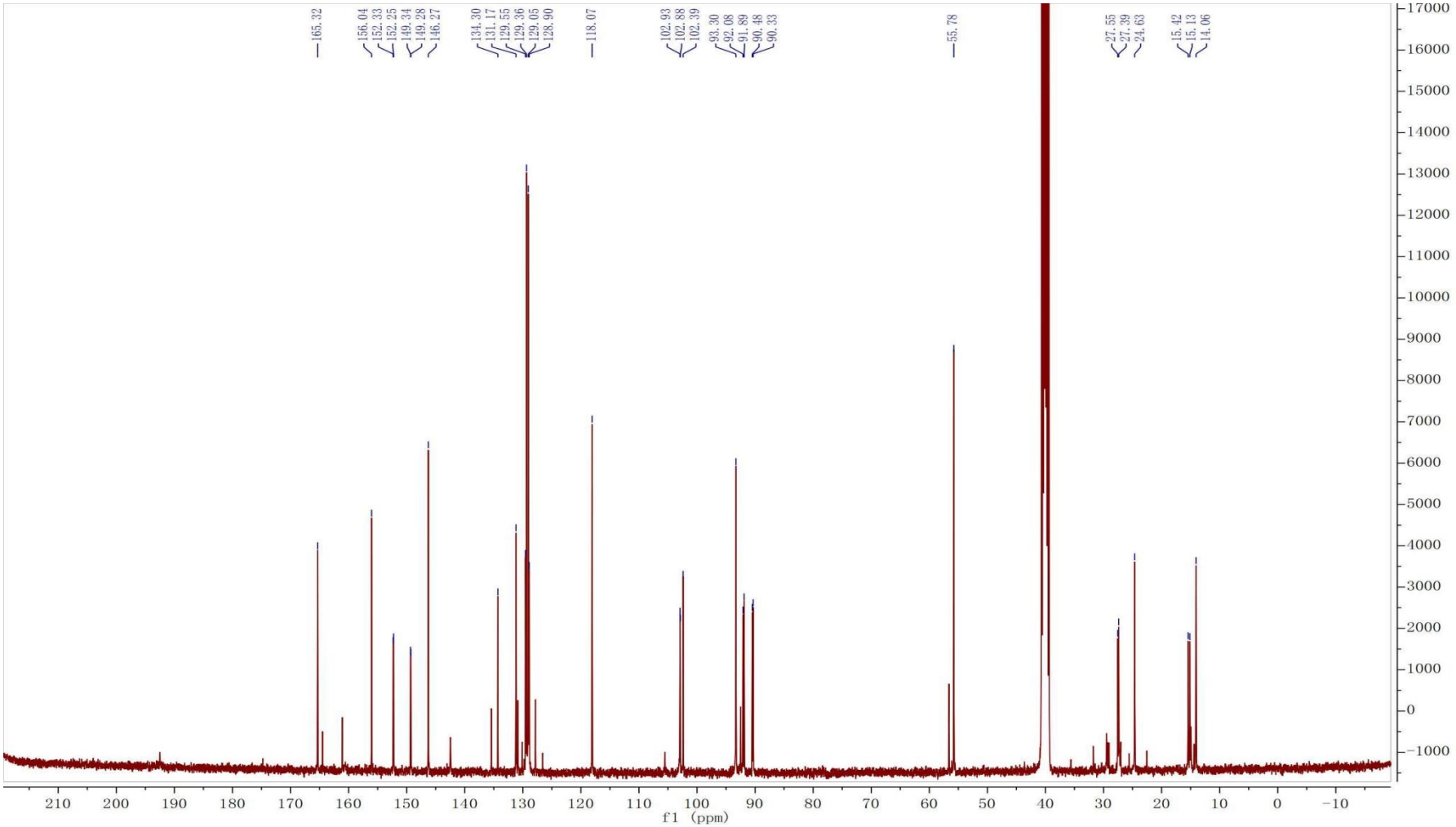

Fig. S15 HSQC-NMR spectrum of CAR-ACR-2

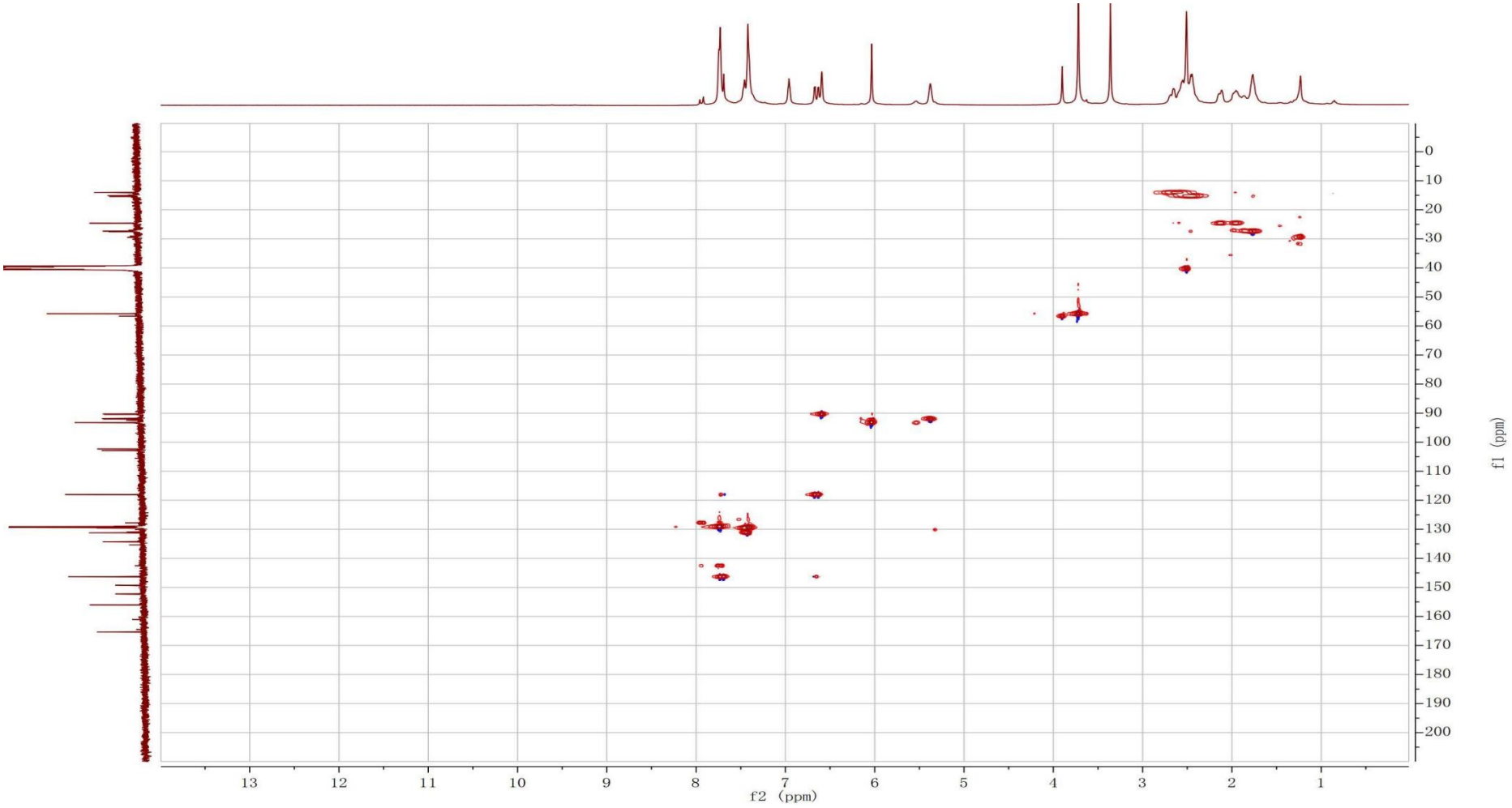

Fig. S16 HMBC-NMR spectrum of CAR-ACR-2

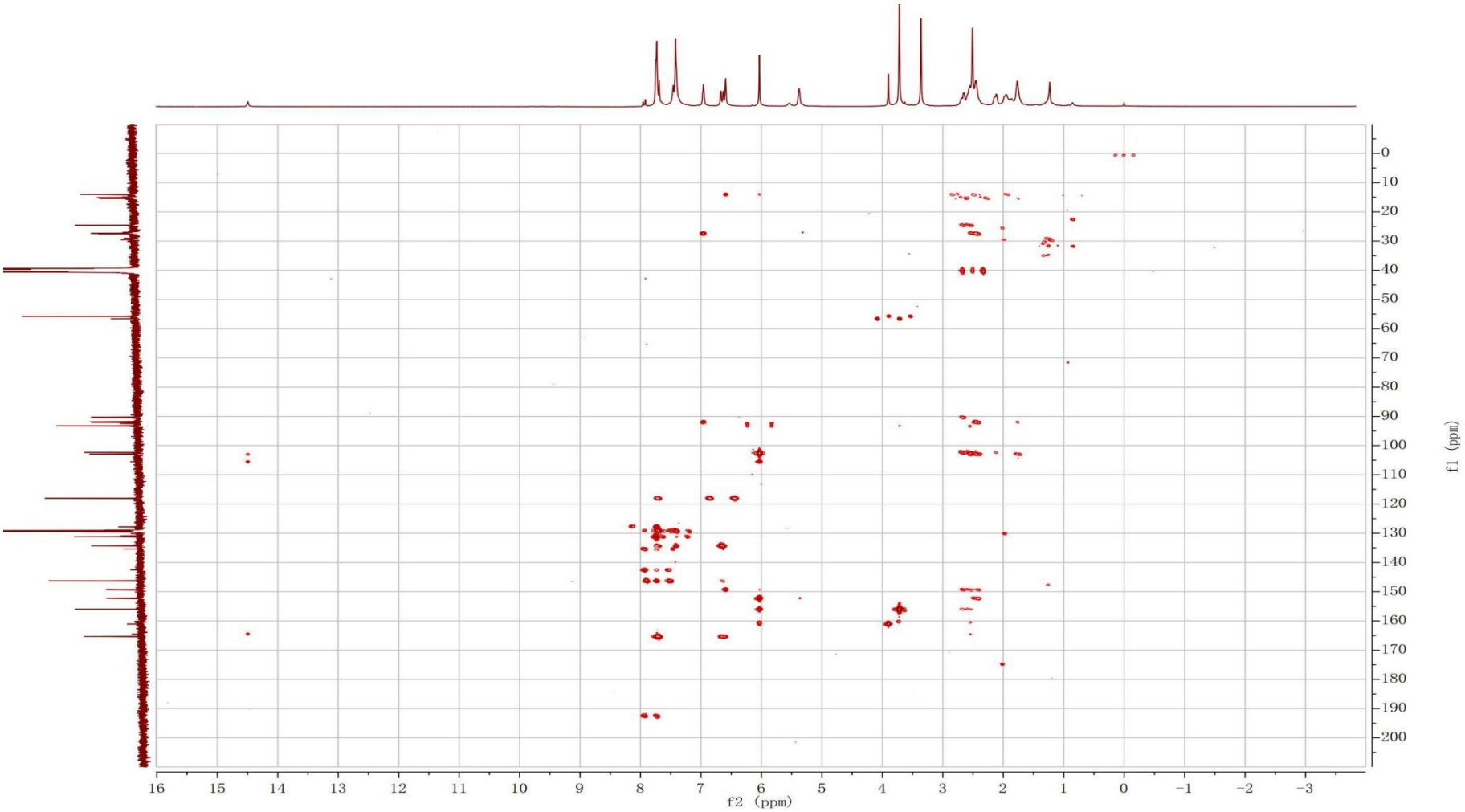

Fig. S17 DEPT-NMR spectrum of CAR-ACR-2

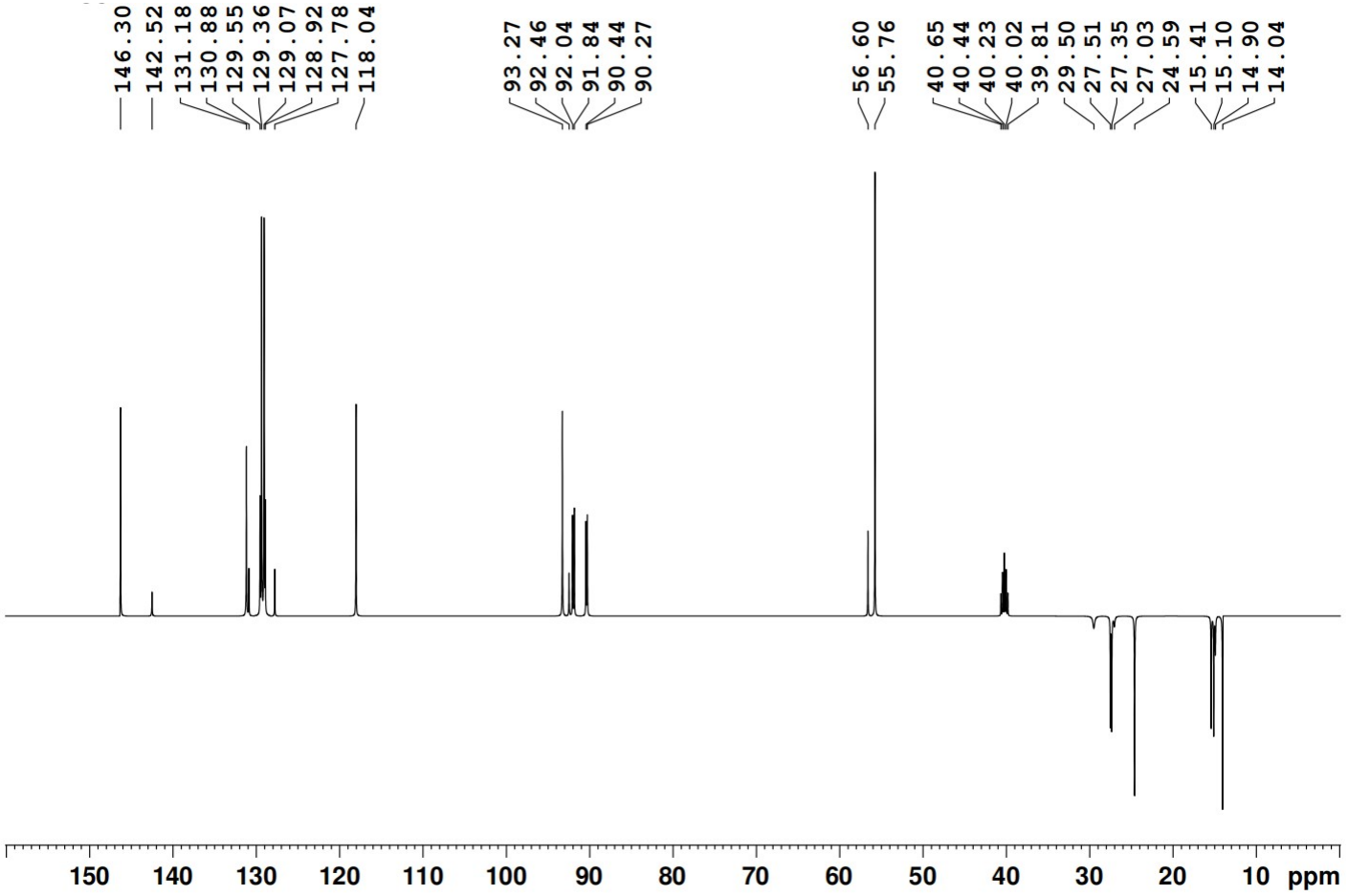

Fig. S18 HPLC-DAD chromatograms of (A) quercetin and (B) myricetin incubated at 100 °C for 0, 5, 15, 60 and 120 min in PBS (pH 7.0)

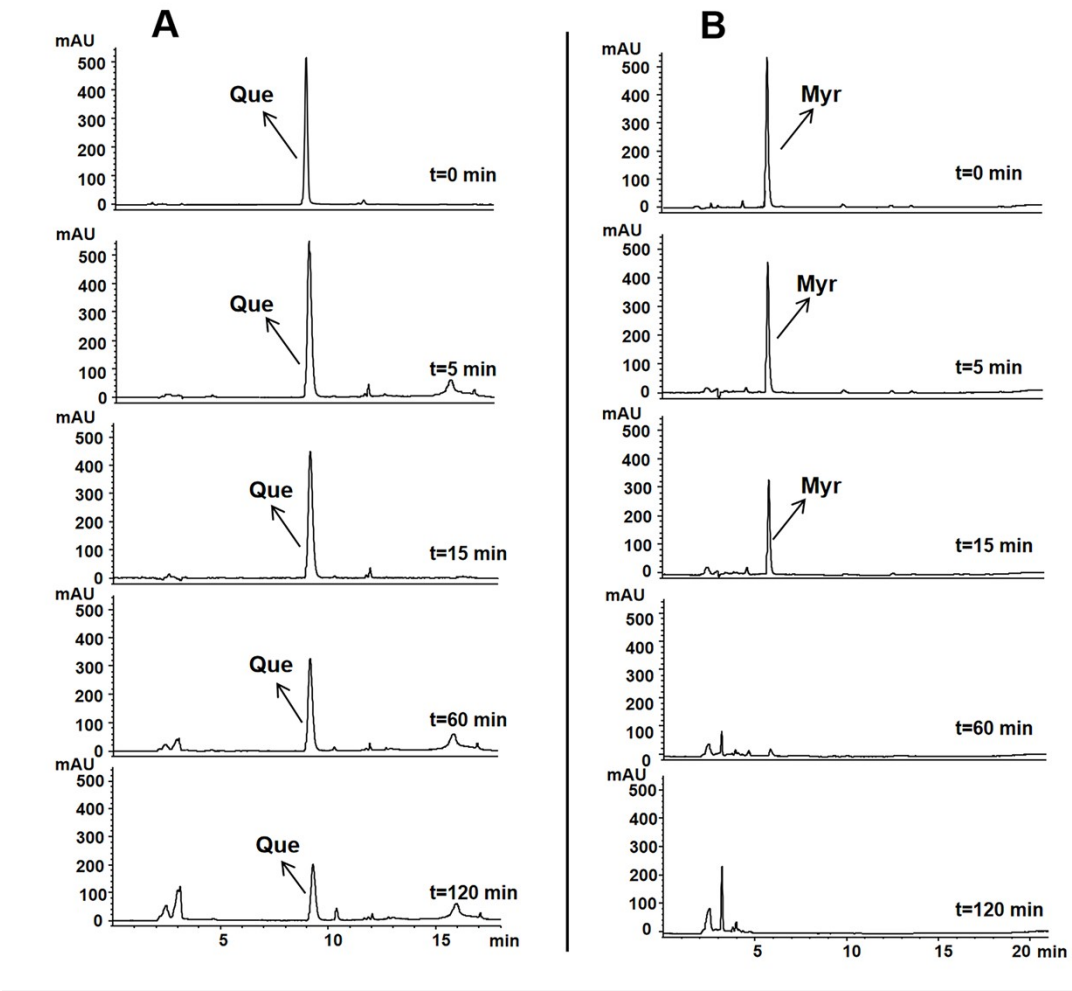

Fig. S19 HPLC-DAD chromatograms of (A) ALP-ACR and (B) CAR-ACR-1 incubated at 100 °C for 0, 5, 15, 60 and 120 min in PBS (pH 7.0).