Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

A Concise Approach for Determining the Relative Configuration of H-7 and H-8 in 8,4′-oxyneolignans by ^{1}H NMR Spectroscopy

Ya-Nnan Yang, Bing Han, Peng-Fei Yang, Zi-Ming Feng, Jian-Shuang Jiang, and Pei-Cheng Zhang*

State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China

Supporting Information

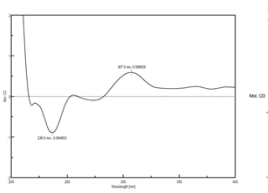
Contents

Experimental section

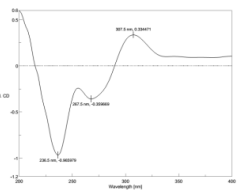
Determination of the absolute configuration of compounds A-1–A-6, B-1–B-4, and C-1–C-3 by measurement of the electronic circular dichroism (ECD) spectrum. The relative configurations of compounds A-1–A-6, B-1–B-4, and C-1–C-3 were determined by the chemical shifts difference of H-9a and H-9b (Table S1). Then, the absolute configurations of these compounds were characterized by electronic circular dichroism (ECD) analysis. The literature survey indicated that (8*S*)-8,4′-oxyneolignans induce positive Cotton effects at 230−250 nm, while (8*R*)-8,4′-oxyneolignans induce negative Cotton effects at 230−250 nm.[1–3] These results, combined with their ECD spectra (Figure S1), allowed the assignment of the absolute configurations of C-7 and C-8 (Table S2).

Table S1. Determination of the relative configurations of compounds A-1–A-6, B-1–B-4, and C-1–C-3.

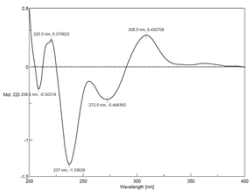
No.	A-1	A-2	A-3	A-4	A-5	A-6	B-1	B-2	B-3	B-4	C-1	C-2	C-3
Relative configuration	*erythro*	*threo*	*erythro*	*threo*	*erythro*	*threo*	*erythro*	*threo*	*erythro*	*threo*	*erythro*	*threo*	*erythro*



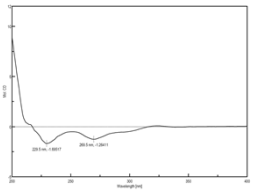
A-1



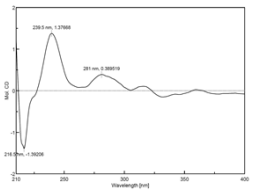
A-2



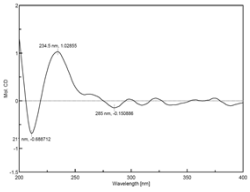
A-3



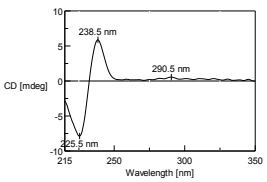
A-4



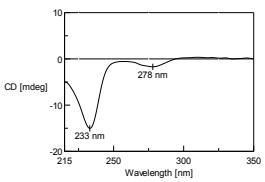
A-5



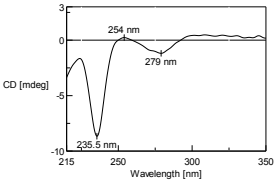
A-6



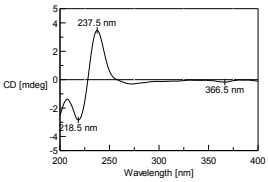
B-1



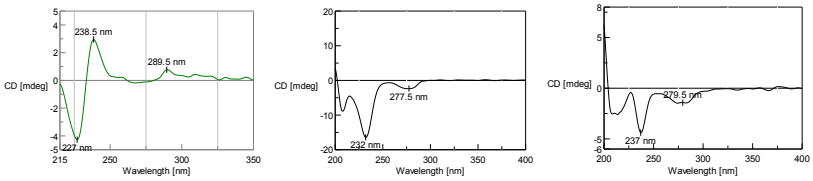
B-2



B-3



B-4



C-1 C-2 C-3

Figure S1. The ECD spectra of compounds A-1–A-6, B-1–B-4, and C-1–C-3.

Table S2. Determination of the absolute configurations of compounds A-1–A-6, B-1–B-4, and C-1–C-3.

No	Name
A-1	(7*S*,8*R*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-7′-en-8-4′-oxyneolignan 9'-*O*-*β*-D-glucopyranoside
A-2	(7*R*,8*R*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-7′-en-8-4'-oxyneolignan 9′-*O*-*β*-D-glucopyranoside
A-3	(7*S*,8*R*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-7′-en-8-4′-oxyneolignan 9′-*O*-*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside
A-4	(7*R*,8*R*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-7′-en-8-4′-oxyneolignan 9'-*O*-*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside
A-5	(7*R*,8*S*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-8,4′-oxyneoligan-9′-*O*-*β*-D-glucopyranoside
A-6	(7*S*,8*S*)-4,7,9,9′-tetrahydroxy-3,3′-dimethoxy-8,4′-oxyneoligan 9′-*O*-*β*-D-glucopyranoside
B-1	(7*R*,8*S*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 3′-*O*-*β*-D-glucopyranoside
B-2	(7*R*,8*R*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 3′-*O*-*β*-D-glucopyranoside
B-3	(7*S*,8*R*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 3′-*O*-*β*-D-glucopyranoside
B-4	(7*S*,8*S*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 3′-*O*-*β*-D-glucopyranoside
C-1	(7*R*,8*S*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 4-*O*-*β*-D-glucopyranoside
C-2	(7*R*,8*R*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 4-*O*-*β*-D-glucopyranoside
C-3	(7*S*,8*R*)-4,7,9,3′,9′-pentahydroxy-3-methoxyl-8-4′-oxyneolignan 4-*O*-*β*-D-glucopyranoside

References:

(1) A. Arnoldi and L. Merlini, *J. Chem. Soc. Perkin Trans. 1*, 1985, 2555−2557.

(2) M. Dellagreca, A. Molinaro, P. Monaco and L. Previtera, *Phytochemistry*, 1994, **35**, 777−779.

(3) L. Fang, D. Du,; G. Z. Ding,; Y. K. Si,; S. S. Yu,; Y. Liu,; W. J. Wang,; S. G. Ma,; S. Xu,; J. Qu,; J. M. Wang and Y. X. Liu, *J. Nat. Prod.*, 2010, **73**, 818−824.

Table S3. ^{1}H NMR Spectroscopic Data for Compounds A-1−A-4 in DMSO-d_6 (500 MHz)

Position	A-1	A-2	A-3	A-4
2	6.98 d (1.5)	6.96 d (2.0)	6.98 d (1.5)	6.96 d (1.5)
5	6.66 d (8.5)	6.67 d (8.0)	6.67 d (8.0)	6.67 d (8.0)
6	6.76 dd (1.5, 8.5)	6.75 dd (2.0, 8.0)	6.76 dd (1.5, 8.0)	6.75 dd (1.5, 8.0)
7	4.69 t (5.0)	4.70 t (4.5)	4.69 t (5.0)	4.70 t (4.0)
8	4.31 q (5.0)	4.26 m	4.30 m	4.27 m
9	3.58 m	3.24 m	3.58 m	3.24 overlap
		3.57 m		3.57 overlap
3-OCH$_3$	3.71 s	3.71 s	3.72 s	3.71 s
2'	7.00 d (1.5)	7.05 d (2.0)	7.01 d (1.5)	7.05 d (1.5)
5'	6.92 d (8.5)	6.97 d (8.0)	6.93 d (8.0)	6.97 d (8.0)
6'	6.85 dd (1.5, 8.5)	6.88 dd (2.0, 8.0)	6.87 dd (1.5, 8.0)	6.88 dd (1.5, 8.0)
7'	6.53 d (15.5)	6.54 d (16.0)	6.56 d (16.0)	6.56 d (15.5)
8'	6.21dt (6.0, 15.5)	6.23dt (6.0, 16.0)	6.22 dt (6.0, 16.0)	6.22 dt (6.0, 15.5)
9'	4.16 dd (6.0, 13.5)	4.17 ddd (1.5, 6.5, 13.0)	4.14 dd (6.0, 13.5)	4.15 dd (6.0, 13.5)
	4.40 dd (6.0, 13.5)	4.40 ddd (1.5, 5.5, 13.0)	4.37 dd (6.0, 13.5)	4.38 dd (6.0, 13.5)
3'-OCH$_3$	3.72 s	3.79 s	3.73 s	3.79 s
1''	4.19 d (7.5)	4.20 d (7.5)	4.19 d (8.0)	4.20 d (8.0)
2''	3.05 overlap	3.05 overlap	3.00 overlap	3.00 overlap
3''	3.08 overlap	3.08 overlap	3.12 m	3.14 t (9.0)
4''	2.98 m	2.99 m	2.97 overlap	2.99 overlap
5''	3.12 overlap	3.14 overlap	3.25 m	3.26 overlap
6''	3.44 m	3.44 m	3.42 dd (7.5, 11.5)	3.43 dd (7.0, 11.5)
	3.67 dd (5.0, 11.0)	3.68 dd (4.5, 12.0)	3.85 overlap	3.86 dd (1.5, 11.5)
1'''			4.88 d (3.0)	4.89 d (3.0)
2'''			3.77 dd (3.0, 6.5)	4.27 m
4'''			3.58 d (9.5)	3.59 d (9.5)
			3.86 d (9.5)	3.87 d (9.5)
5'''			3.32 overlap	3.34 overlap

Table S4. ^{1}H NMR Spectroscopic Data for Compounds A-1−A-4 in DMSO-d_6 (500 MHz)

position	A-5	A-6
2	6.98 d (1.5)	6.97 d (1.5)
5	6.66 d (8.0)	6.68 d (8.0)
6	6.76 dd (1.5, 8.0)	6.76 dd (1.5, 8.0)
7	4.71 d (4.5)	4.71 d (4.5)
8	4.22 m	4.18 m
9	3.55 m	3.22 dd (5.5, 11.0)
		3.55 dd (4.0, 11.0)
3-OCH$_3$	3.70 s	3.72 s
2'	6.77 d (2.0)	6.82 d (2.0)
5'	6.86 d (8.5)	6.92 d (8.5)
6'	6.65 dd (1.5, 8.5)	6.66 dd (2.0, 8.5)
7'	2.57 t (7.5)	2.57 t (7.5)
8'	1.82 m	1.78 m
9'	3.78 m	3.79 dd (6.0, 10.0)
	3.42 m	3.43 dd (6.0, 10.0)
3'-OCH$_3$	3.72 s	3.76 s
1''	4.13 d (8.0)	4.13 d (8.0)
2''	2.95 overlap	2.95 overlap
3''	3.07 overlap	3.07 overlap
4''	3.06 m	3.06 m
5''	3.14 overlap	3.14 overlap
6''	3.43 m	3.43 m
	3.66 dd (6.5, 11.5)	3.66 dd (6.5, 11.5)

Table S5. ^{13}C NMR Spectroscopic Data for Compounds A-1−A-6 in DMSO-d_6 (125 MHz)

position	A-1	A-2	A-3	A-4	A-5	A-6
1	133.2	132.9	133.2	132.9	133.4	132.9
2	111.4	111.0	109.9	110.0	111.2	111.2
3	147.0	147.0	147.0	147.0	147.0	147.0
4	145.4	145.4	145.4	145.4	146.1	145.4
5	114.6	114.6	114.6	114.6	114.7	114.7
6	119.4	119.0	119.4	119.0	119.5	119.1
7	71.6	70.9	71.6	70.9	71.6	71.1
8	83.6	84.3	83.6	84.2	83.9	84.9
9	60.1	60.1	60.1	60.1	60.1	60.1
3-OCH_3	55.4	55.4	55.4	55.4	55.5	55.5
1'	129.5	129.6	129.5	129.6	134.7	134.9
2'	109.8	109.9	109.3	109.9	113.0	113.0
3'	149.7	149.6	149.7	149.6	149.6	149.6
4'	147.9	148.2	147.9	148.2	145.4	146.4
5'	115.3	115.3	115.3	115.3	115.9	116.3
6'	119.5	119.4	119.5	119.4	120.2	120.2
7'	131.5	131.4	131.8	131.7	31.1	31.1
8'	124.0	124.1	123.7	123.8	31.0	31.0
9'	68.7	68.7	68.7	68.6	67.8	67.8
3'-OCH_3	55.6	55.6	55.6	55.6	55.5	55.5
1''	102.1	102.1	101.8	101.8	102.9	102.9
2''	73.5	73.5	73.4	73.4	73.4	73.4
3''	77.0	76.9	76.6	76.6	76.8	76.8
4''	70.1	70.1	70.3	70.3	70.1	70.1
5''	76.8	76.8	75.6	75.6	76.7	76.7
6''	61.1	61.1	67.7	67.7	61.1	61.1
1'''			109.3	109.2		
2'''			75.9	75.9		
3'''			78.8	78.8		
4'''			73.2	73.2		
5'''			63.0	63.1		

Table S6. ^{1}H NMR Spectroscopic Data for Compounds B-1−B-4 in DMSO-d_6 (500 MHz)

position	B-1	B-2	B-3	B-4
2	6.98 d (2.0)	6.98 d (2.0)	6.95 d (2.0)	6.94 d (1.5)
5	6.70 d (8.0)	6.70 d (8.0)	6.70 d (8.0)	6.70 d (8.0)
6	6.78 dd (2.0, 8.0)	6.78 dd (2.0, 8.0)	6.79 overlap	6.79 dd (2.0, 8.0)
7	4.70 t (5.0)	4.72 t (5.5)	4.78 overlap	4.74 overlap
8	4.19 m	4.09 m	4.10 m	4.13 m
9	3.49 m	3.29 m	3.47 m	3.24 m
	3.64 dd (6.0, 11.5)	3.51 m	3.65 m	3.51 m
3-OCH$_3$	3.73 s	3.73 s	3.73 s	3.72 s
2'	6.95 d (2.0)	6.95 d (2.0)	6.96 d (2.0)	6.96 d (2.0)
5'	6.83 d (8.0)	6.94 d (8.0)	6.79 overlap	6.97 d (8.0)
6'	6.72 dd (2.0, 8.0)	6.72 dd (2.0, 8.0)	6.68 dd (2.0, 8.0)	6.73 dd (2.0, 8.0)
7'	2.50 overlap	2.50 overlap	2.50 overlap	2.50 overlap
8'	1.66 m	1.66 m	1.66 m	1.66 m
9'	3.39 m	3.39 m	3.39 overlap	3.39 m
3'-OCH$_3$				
1''	4.76 d (7.5)	4.80 d (7.0)	4.78 d (7.5)	4.75 overlap
2''	3.28 overlap	3.29 overlap	3.28 overlap	3.28 m
3''	3.25 overlap	3.29 overlap	3.25 overlap	3.25 m
4''	3.16 m	3.16 m	3.16 m	3.16 m
5''	3.25 overlap	3.25 overlap	3.25 overlap	3.22 m
6''	3.45 m	3.45 m	3.45 m	3.45 m
	3.68 m	3.68 m	3.68 m	3.65 m

Table S7. ^{13}C NMR Spectroscopic Data for Compounds B-1−B-4 in DMSO-d_6 (500 MHz)

position	B-1	B-2	B-3	B-4
1	133.1	133.1	133.2	132.9
2	111.2	110.9	111.0	110.8
3	147.1	147.1	147.1	147.1
4	145.5	145.5	145.4	145.6
5	114.8	114.8	114.9	114.8
6	119.6	119.3	119.2	119.3
7	71.3	71.6	71.5	71.7
8	86.0	86.3	86.7	86.1
9	59.8	60.3	60.0	60.1
3-OCH_3	55.7	55.6	55.6	55.6
1'	136.1	135.7	136.2	135.6
2'	117.9	117.9	117.3	118.1
3'	148.3	147.8	148.4	147.8
4'	146.3	147.1	146.6	147.2
5'	118.9	118.0	119.1	118.2
6'	122.3	122.3	122.1	122.3
7'	34.2	34.2	34.2	34.3
8'	31.2	31.1	31.2	31.1
9'	60.1	60.1	60.1	60.1
3'-OCH_3				
1''	101.8	101.7	101.6	101.8
2''	73.7	73.7	73.6	73.6
3''	77.1	77.1	77.1	77.1
4''	69.8	69.8	69.8	69.8
5''	76.4	76.5	76.5	76.5
6''	60.8	60.8	60.8	60.7

Table S8. ^{1}H NMR Spectroscopic Data for Compounds C-1−C-3 in DMSO-d_6 (500 MHz)

position	C-1	C-2	C-3
2	7.03 overlap	7.02 overlap	7.03 d (1.5)
5	7.01 d (8.0)	7.01 d (8.5)	7.01 d (8.5)
6	6.87 dd (1.5, 8.0)	6.85 dd (2.0, 8.5)	6.85 dd (1.5, 8.5)
7	4.78 d (4.5)	4. 78 d (5.5)	4.78 d (4.5)
8	4.00 m	3.96 m	4.00 m
9	3.52 dd (4.0, 12.0)	3.30 dd (6.0, 11.5)	3.50 dd (3.5, 11.5)
	3.61 dd (6.5, 12.0)	3.53 dd (4.0, 11.5)	3.61 dd (6.5, 11.5)
3-OCH$_3$	3.73 s	3.72 s	3.73 s
2'	6.60 d (2.0)	6.61 d (2.0)	6.60 d (2.0)
5'	6.74 d (8.0)	6.93 d (8.0)	6.74 d (8.0)
6'	6.45 dd (2.0, 8.0)	6.48 dd (2.0, 8.0)	6.45 dd (2.0, 8.0)
7'	2.44 t (7.5)	2.45 t (7.5)	2.44 t (7.5)
8'	1.64 m	1.64 m	1.64 m
9'	3.37 overlap	3.38 overlap	3.37 overlap
3'-OCH$_3$			
1''	4.86 d (7.5)	4.85 d (7.5)	4.86 d (7.0)
2''	3.15 m	3.15 m	3.15 m
3''	3.28 overlap	3.28 overlap	3.28 overlap
4''	3.23 overlap	3.23 overlap	3.23 overlap
5''	3.28 overlap	3.28 overlap	3.28 overlap
6''	3.44 m	3.44 dd (5.5, 11.5)	3.45 dd (5.5, 11.5)
	3.63 m	3.63 d (11.5)	3.63 d (11.5)

Table S9. ^{13}C NMR Spectroscopic Data for Compounds C-1−C-3 in DMSO-d_6 (125 MHz)

position	C-1	C-2	C-3
1	135.5	135.8	135.5
2	111.5	111.0	111.5
3	148.4	148.5	148.4
4	145.6	145.7	144.5
5	114.7	114.6	114.6
6	119.1	118.8	119.0
7	71.6	71.7	71.5
8	86.5	86.2	86.6
9	59.9	60.0	59.8
3-OCH_3	55.6	55.5	55.6
1'	136.8	136.6	136.8
2'	116.1	116.0	116.2
3'	148.4	148.5	148.4
4'	144.5	144.6	145.6
5'	119.0	118.6	119.0
6'	118.7	118.2	118.5
7'	34.4	34.4	34.4
8'	31.1	31.1	31.1
9'	60.1	60.2	60.1
3'-OCH_3			
1''	100.1	100.1	100.1
2''	73.2	73.2	73.2
3''	77.0	77.0	77.1
4''	69.6	69.6	69.6
5''	76.9	76.9	76.9
6''	60.6	60.6	60.6

Table S10. ^{1}H NMR Spectroscopic Data for Compounds A-1−A-4 in CD_3OD (500 MHz)

position	A-1	A-2	A-3	A-4
2	7.04 overlap	7.04 d (2.0)	7.04 overlap	7.05 d (1.5)
5	6.74 d (8.0)	6.76 d (8.0)	6.74 d (8.0)	6.77 d (8.0)
6	6.84 dd (2.0, 8.0)	6.87 dd (2.0, 8.0)	6.84 dd (2.0, 8.0)	6.87 dd (1.5, 8.0)
7	4.84 d (5.5)	4.90 d (6.0)	4.84 d (6.0)	4.90 d (5.5)
8	4.39 m	4.32 m	4.39 m	4.32 m
9	3.80 m	3.49 dd (5.5, 12.0)	3.80 m	3.49 dd (5.5, 12.0)
	3.87 m	3.75 dd (4.0, 12.0)	3.87 m	3.75 dd (4.0, 12.0)
3-OCH$_3$	3.82 s	3.84 s	3.83 s	3.84 s
2'	7.04 overlap	7.10 d (2.0)	7.04 overlap	7.10 d (1.5)
5'	6.90 overlap	7.01 d (8.0)	6.89 d (8.0)	7.01 d (8.5)
6'	6.90 overlap	6.94 dd (2.0, 8.0)	6.90 dd (2.0, 8.0)	6.94 dd (1.5, 8.5)
7'	6.59 d (16.0)	6.62 d (16.0)	6.60 d (15.5)	6.63 d (15.5)
8'	6.26 dt (6.5, 16.0)	6.29 dt (6.0, 16.0)	6.26 dt (6.5, 15.5)	6.29 dt (6.5, 15.5)
9'	4.32 ddd (1.5, 6.0, 13.0)	4.32 m	4.32 dd (6.5, 13.0)	4.32 m
	4.51 ddd (1.5, 6.5, 13.0)	4.52 ddd (1.5, 6.0, 13.5)	4.50 dd (6.0, 13.0)	4.51 dd (6.0, 13.5)
3'-OCH$_3$	3.82 s	3.90 s	3.82 s	3.90 s
1''	4.37 d (8.0)	4.37 d (7.5)	4.36 d (8.0)	4.37 d (7.5)
2''	3.24 dd (8.0, 9.0)	3.24 dd (8.0, 9.0)	3.24 dd (8.0, 9.0)	3.24 dd (8.0, 9.0)
3''	3.29 m	3.29 m	3.32 m	3.29 m
4''	3.31 overlap	3.31 overlap	3.31 overlap	3.31 overlap
5''	3.38 m	3.38 m	3.37 m	3.37 m
6''	3.70 m	3.70 dd (5.5, 11.5)	3.64 dd (6.0, 11.5)	3.64 dd (6.5, 11.5)
	3.89 m	3.89 overlap	4.01 m	4.01 m
1'''			5.05 d (2.0)	5.05 d (2.0)
2'''			3.43 m	3.43 m
4'''			3.78 d (9.5)	3.78 d (9.5)
			4.02 d (9.5)	4.02 d (9.5)
5'''			3.60 overlap	3.59 overlap

Table S11. ^{1}H NMR Spectroscopic Data for Compounds A-5−A-6 in CD_3OD (500 MHz)

position	A-5	A-6
2	7.00 br s	7.02 d (1.5)
5	6.72 d (8.5)	6.74 d (8.0)
6	6.81 dd (1.5, 8.5)	6.85 dd (1.5, 8.0)
7	4.81 d (5.5)	4.87 d (5.5)
8	4.29 m	4.20 m
9	3.74 m	3.44 dd (5.0, 12.0)
	3.84 dd (5.5, 12.0)	3.72 dd (4.0, 12.0)
3-OCH_3	3.80 s	3.82 s
2'	6.82 overlap	6.88 d (1.5)
5'	6.80 overlap	6.96 d (8.5)
6'	6.67 dd (1.5, 8.5)	6.73 dd (1.5, 8.5)
7'	2.65 t (8.0)	2.68 t (8.0)
8'	1.89 m	1.90 m
9'	3.92 m	3.92 m
	3.52 m	3.52 m
3'-OCH_3	3.79 s	3.86 s
1''	4.24 d (8.0)	4.24 d (7.5)
2''	3.29 overlap	3.29 overlap
3''	3.35 t (8.5)	3.35 t (8.5)
4''	3.20 t (8.5)	3.20 t (8.5)
5''	3.27 overlap	3.26 overlap
6''	3.66 dd (5.5, 12.0)	3.66 dd (5.0, 12.0)
	3.86 dd (2.0, 12.0)	3.86 dd (2.0, 12.0)

Table S12. ^{13}C NMR Spectroscopic Data for Compounds A-1−A-6 in CD_3OD (125 MHz)

position	A-1	A-2	A-3	A-4	A-5	A-6
1	132.8	132.5	132.7	132.5	132.9	132.5
2	110.6	110.4	110.5	110.5	110.5	110.4
3	147.5	147.6	147.3	147.6	147.4	147.6
4	145.8	145.9	145.6	146.0	145.8	146.0
5	114.4	114.6	114.3	114.6	114.4	114.6
6	119.8	119.5	119.7	119.5	119.8	119.5
7	72.8	72.8	72.7	72.8	72.9	72.9
8	84.9	85.8	84.8	85.9	85.4	86.5
9	61.0	60.7	60.9	60.7	60.9	60.6
3-OCH_3	55.1	55.1	55.0	55.4	55.3	55.3
1'	131.5	132.4	131.4	131.7	136.8	136.9
2'	110.1	110.4	110.1	110.2	112.9	112.8
3'	150.7	150.5	150.5	150.5	150.6	150.4
4'	147.9	148.2	147.7	148.2	146.0	146.3
5'	117.5	117.4	117.4	117.6	118.3	118.4
6'	119.6	119.8	119.5	119.8	120.7	120.9
7'	132.4	132.4	132.4	132.5	31.5	31.5
8'	123.9	123.9	123.8	124.1	31.5	31.5
9'	69.6	69.6	69.6	69.7	68.6	68.6
3'-OCH_3	55.2	55.3	55.2	55.1	55.1	55.1
1''	102.0	102.0	101.8	102.0	103.3	103.3
2''	73.9	73.9	73.7	73.9	73.9	74.0
3''	76.9	76.9	76.7	76.9	76.9	76.9
4''	70.5	70.5	70.4	70.6	70.4	70.4
5''	76.8	76.8	76.7	76.8	76.7	76.7
6''	61.6	61.6	67.3	67.5	61.5	61.5
1'''			109.6	109.8		
2'''			75.6	75.8		
3'''			79.2	79.3		
4'''			73.6	73.8		
5'''			64.2	64.4		

Table S13. ^{1}H NMR Spectroscopic Data for Compounds B-1−B-4 in CD_3OD (500 MHz)

position	B-1	B-2	B-3	B-4
2	6.98 d (2.0)	6.98 d (2.0)	6.95 d (2.0)	6.94 d (1.5)
5	6.70 d (8.0)	6.70 d (8.0)	6.70 d (8.0)	6.70 d (8.0)
6	6.78 dd (2.0, 8.0)	6.78 dd (2.0, 8.0)	6.79 overlap	6.79 dd (2.0, 8.0)
7	4.70 t (5.0)	4.72 t (5.5)	4.78 overlap	4.74 overlap
8	4.19 m	4.09 m	4.10 m	4.13 m
9	3.49 m	3.29 m	3.47 m	3.24 m
	3.64 dd (6.0, 11.5)	3.51 m	3.65 m	3.51 m
3-OCH_3	3.73 s	3.73 s	3.73 s	3.72 s
2'	6.95 d (2.0)	6.95 d (2.0)	6.96 d (2.0)	6.96 d (2.0)
5'	6.83 d (8.0)	6.94 d (8.0)	6.79 overlap	6.97 d (8.0)
6'	6.72 dd (2.0, 8.0)	6.72 dd (2.0, 8.0)	6.68 dd (2.0, 8.0)	6.73 dd (2.0, 8.0)
7'	2.50 overlap	2.50 overlap	2.50 overlap	2.50 overlap
8'	1.66 m	1.66 m	1.66 m	1.66 m
9'	3.39 m	3.39 m	3.39 overlap	3.39 m
3'-OCH_3				
1''	4.76 d (7.5)	4.80 d (7.0)	4.78 d (7.5)	4.75 overlap
2''	3.28 overlap	3.29 overlap	3.28 overlap	3.28 m
3''	3.25 overlap	3.29 overlap	3.25 overlap	3.25 m
4''	3.16 m	3.16 m	3.16 m	3.16 m
5''	3.25 overlap	3.25 overlap	3.25 overlap	3.22 m
6''	3.45 m	3.45 m	3.45 m	3.45 m
	3.68 m	3.68 m	3.68 m	3.65 m

Table S14. ^{13}C NMR Spectroscopic Data for Compounds B-1−B-4 in CD_3OD (125 MHz)

position	B-1	B-2	B-3	B-4
1	132.9	132.7	132.8	132.7
2	110.4	110.4	110.4	110.5
3	147.6	147.7	147.6	147.7
4	145.8	146.0	145.7	146.1
5	114.6	114.6	114.7	114.8
6	119.6	119.6	119.3	119.7
7	72.1	72.9	72.3	73.1
8	85.9	85.8	86.7	86.4
9	60.4	60.4	60.3	60.3
3-OCH_3	55.2	55.2	55.2	55.2
1'	137.0	136.5	137.2	136.8
2'	118.9	118.3	118.2	118.6
3'	148.6	148.1	148.9	148.3
4'	146.6	147.1	146.7	147.4
5'	119.2	117.9	119.2	119.2
6'	123.2	122.9	123.0	123.3
7'	34.1	34.2	34.1	34.2
8'	31.2	31.2	31.3	31.2
9'	60.9	60.9	60.9	60.9
3'-OCH_3				
1''	102.4	102.3	102.4	102.6
2''	73.9	73.9	73.8	73.9
3''	77.0	77.1	77.1	77.0
4''	70.2	70.3	70.2	70.2

Table S15. ^{1}H NMR Spectroscopic Data for Compounds C-1−C-3 in CD_3OD (500 MHz)

position	C-1	C-2	C-3
2	7.09 d (2.0)	7.10 d (2.0)	7.10 d (2.0)
5	7.12 d (8.0)	7.12 d (8.0)	7.12 d (8.0)
6	6.95 dd (2.0, 8.0)	6.95 dd (2.0, 8.0)	6.95 dd (2.0, 8.0)
7	4.88 overlap	4.95 d (5.5)	4.89 overlap
8	4.15 m	4.11 m	4.15 m
9	3.72 dd (3.5, 12.0)	3.48 dd (4.5, 12.0)	3.72 dd (3.5, 12.0)
	3.85 m	3.75 dd (4.5, 12.0)	3.85 m
3-OCH_3	3.83 s	3.83 s	3.83 s
2'	6.60 d (2.0)	6.67 d (2.0)	6.60 d (2.0)
5'	6.70 d (8.0)	6.87 d (8.0)	6.71 d (8.0)
6'	6.52 dd (2.0, 8.0)	6.55 dd (2.0, 8.0)	6.52 dd (2.0, 8.0)
7'	2.54 t (8.0)	2.54 t (7.5)	2.54 t (7.5)
8'	1.77 m	1.77 m	1.77 m
9'	3.54 t (6.5)	3.54 t (6.5)	3.54 t (6.5)
3'-OCH_3			
1''	4.86 d (7.5)	4.86 d (7.5)	4.86 d (7.5)
2''	3.47 m	3.47 m	3.47 m
3''	3.38 overlap	3.38 m	3.34 m
4''	3.39 overlap	3.39 overlap	3.39 overlap
5''	3.45 overlap	3.45 overlap	3.39 overlap
6''	3.68 m	3.68 m	3.68 m
	3.86 m	3.86 m	3.86 m

Table S16. ^{13}C NMR Spectroscopic Data for Compounds C-1−C-3 in CD_3OD (125 MHz)

position	C-1	C-2	C-3
1	136.1	136.3	136.1
2	111.2	111.0	111.2
3	149.3	149.4	149.3
4	146.2	146.3	146.2
5	116.3	116.3	116.3
6	119.5	119.3	119.3
7	72.5	72.6	72.5
8	86.2	86.0	86.2
9	60.6	60.4	60.6
3-OCH_3	55.4	55.3	55.4
1'	137.5	137.2	137.5
2'	116.0	116.0	116.1
3'	146.2	146.3	146.2
4'	148.3	148.0	148.3
5'	118.7	117.7	118.7
6'	119.3	119.3	119.5
7'	34.3	34.3	34.3
8'	31.3	31.3	31.3
9'	61.2	61.0	61.2
3'-OCH_3			
1''	101.7	101.5	101.6
2''	73.7	73.6	73.7
3''	77.0	77.0	77.0
4''	70.1	70.1	70.1
5''	76.6	76.6	76.6
6''	61.0	61.2	61.0

Table S17. ^{1}H NMR Spectroscopic Data for Compounds A-1−A-4 in D_2O (500 MHz)

position	A-1	A-2	A-3	A-4
2	6.83 overlap	6.95 d (1.5)	6.88 d (1.5)	7.00 br s
5	6.72 d (8.0)	6.78 d (8.0)	6.76 d (8.0)	6.84 d (8.0)
6	6.79 dd (1.5, 8.0)	6.85 overlap	6.84 dd (1.5, 8.0)	6.89 overlap
7	4.68 d (8.0)	4.90 d (5.0)	4.72 d (8.0)	4.95 d (4.5)
8	4.58 m	4.57 m	4.62 m	4.63 m
9	3.88 dd (6.5, 12.5)	3.59 dd (6.0, 12.0)	3.92 dd (6.5, 12.0)	3.64 dd (7.0, 13.0)
	4.00 dd (2.5, 12.5)	3.78 dd (3.5, 12.0)	4.03 dd (2.0, 12.0)	3.83 dd (3.5, 13.0)
3-OCH$_3$	3.62 s	3.71 s	3.67 s	3.76 s
2'	6.85 overlap	7.04 d (1.5)	6.90 overlap	7.10 br s
5'	6.85 overlap	6.85 overlap	6.90 overlap	6.91 overlap
6'	6.85 overlap	6.78 overlap	6.90 overlap	6.85 overlap
7'	6.54 d (16.0)	6.53 d (16.0)	6.56 d (15.5)	6.59 d (16.0)
8'	6.16 dt (7.0, 16.0)	6.19 dt (7.0, 16.0)	6.21 dt (6.5, 15.5)	6.26 dt (6.5, 16.0)
9'	4.29 dd (6.0, 13.0)	4.30 dd (7.0, 12.5)	4.35 dd (6.0, 13.0)	4.36 dd (7.0, 12.5)
	4.43 dd (7.0, 13.0)	4.43 dd (6.0, 12.5)	4.44 dd (7.0, 13.0)	4.45 dd (6.0, 12.5)
3'-OCH$_3$	3.60 s	3.80 s	3.66 s	3.86 s
1''	4.46 d (8.0)	4.47 d (7.5)	4.50 d (8.0)	4.51 d (8.0)
2''	3.26 dd (8.0, 9.0)	3.26 dd (7.5, 9.0)	3.30 dd (8.0, 8.5)	3.30 dd (8.0, 8.5)
3''	3.43 dd (9.0, 9.0)	3.43 dd (8.0, 9.0)	3.48 m	3.48 m
4''	3.34 m	3.35 m	3.42 m	3.42 m
5''	3.37 m	3.38 m	3.54 m	3.54 m
6''	3.66 dd (6.0, 12.5)	3.66 dd (5.5, 12.5)	3.72 dd (6.0, 12.0)	3.72 dd (6.0, 12.5)
	3.85 dd (2.5, 12.5)	3.85 dd (2.0, 12.5)	4.00 d (12.0)	4.00 dd (12.5)
1'''			5.08 d (3.0)	5.08 d (3.0)
2'''			3.96 d (3.0)	3.95 d (3.0)
4'''			4.00 overlap	4.00 overlap
			3.86 d (10.5)	3.86 overlap
5'''			3.62 d (6.0)	3.62 d (6.0)
			3.66 overlap	3.66 overlap

Table S18. ^{1}H NMR Spectroscopic Data for Compounds A-5−A-6 in D_2O (500 MHz)

position	A-5	A-6
2	6.80 overlap	6.93 br s
5	6.71 d (8.0)	6.85 d (8.0)
6	6.79 overlap	6.76 d (8.0)
7	4.65 d (8.0)	4.89 d (5.0)
8	4.56 m	4.56 m
9	3.89 m	3.59 m
	4.03 m	3.77 m
3-OCH$_3$	3.63 s	3.80 s
2'	6.66 overlap	6.87 br s
5'	6.66 overlap	6.69 d (8.0)
6'	6.82 (2.0, 8.0)	6.81 (2.5, 8.5)
7'	2.53 t (7.0)	2.59 t (7.0)
8'	1.80 m	1.84 m
9'	3.50 m	3.55 m
	3.82 overlap	3.84 m
3'-OCH$_3$	3.58 s	3.71 s
1''	4.38 d (8.0)	4.38 d (8.0)
2''	3.23 dd (8.0, 9.0)	3.23 dd (8.0, 9.0)
3''	3.43 dd (9.0, 9.0)	3.44 dd (9.0, 9.0)
4''	3.34 m	3.34 m
5''	3.38 m	3.38 m
6''	3.67 dd (6.0, 12.5)	3.67 dd (5.0, 12.5)
	3.82 overlap	3.83 overlap

Table S19. ^{13}C NMR Spectroscopic Data for Compounds A-1−A-6 in D_2O (125 MHz)

position	A-1	A-2	A-3	A-4	A-5	A-6
1	135.2	135.3	135.2	135.3	135.2	134.8
2	114.1	113.8	114.2	113.8	114.0	113.8
3	149.8	150.1	149.8	150.1	149.7	150.9
4	147.4	147.4	147.5	147.4	147.4	148.9
5	117.6	118.0	117.7	118.0	117.4	117.4
6	123.8	122.6	123.8	122.6	123.9	123.9
7	75.3	75.4	75.3	75.3	75.5	75.6
8	86.4	86.0	86.4	86.1	86.5	86.5
9	64.3	63.6	64.3	63.5	64.5	63.7
3-OCH_3	58.5	58.6	58.6	58.7	58.5	58.7
1'	133.6	133.3	133.7	133.4	139.2	139.2
2'	112.5	112.8	112.6	112.8	115.3	115.7
3'	152.0	151.8	152.1	151.8	151.8	151.8
4'	150.0	150.1	150.0	150.1	148.0	148.2
5'	119.2	118.1	119.3	118.0	123.5	122.8
6'	122.6	122.9	122.6	122.8	119.6	118.7
7'	136.4	136.4	136.3	136.2	33.7	33.6
8'	126.0	126.0	126.3	126.3	33.6	33.6
9'	73.2	73.2	73.4	73.4	72.4	72.4
3'-OCH_3	58.2	58.5	58.2	58.5	58.1	58.5
1''	103.8	103.8	104.0	104.1	105.2	105.2
2''	76.0	76.0	76.0	76.0	76.0	76.1
3''	78.8	78.8	78.7	78.6	78.8	78.8
4''	72.5	72.5	72.5	72.4	72.6	72.5
5''	78.7	78.7	77.6	77.6	78.7	78.7
6''	63.6	63.6	70.4	70.3	63.6	63.6

Table S20. ^{1}H NMR Spectroscopic Data for Compounds B-1−B-4 in D_2O (500 MHz)

position	B-1	B-2	B-3	B-4
2	6.91 overlap	6.99 d (1.5)	6.89 br s	6.97 d (1.5)
5	6.77 d (8.0)	6.83 d (8.0)	6.74 d (8.0)	6.82 overlap
6	6.89 overlap	6.89 dd (1.5, 8.0)	6.87 overlap	6.91 dd (1.5, 8.0)
7	4.81 overlap	4.92 d (5.5)	4.80 overlap	4.93 overlap
8	4.63 m	4.54 m	4.52 m	4.61 m
9	3.91 dd (5.5,12.5)	3.55 m	3.90 dd (5.5, 12.0)	3.62 dd (5.5, 12.5)
	3.95 dd (2.5,12.5)	3.75 overlap	3.95 dd (2.0, 12.0)	3.80 dd (3.5, 12.5)
3-OCH$_3$	3.66 s	3.75 s	3.68 s	3.71 s
2'	6.89 overlap	6.97 d (1.5)	6.86 overlap	6.95 d (1.5)
5'	6.81 d (8.0)	6.85 d (8.0)	6.78 overlap	6.84 overlap
6'	6.79 dd (1.5, 8.0)	6.80 dd (1.5, 8.0)	6.77 overlap	6.79 dd (1.5, 8.0)
7'	2.51 t (7.0)	2.54 t (7.5)	2.52 t (7.5)	2.54 t (8.0)
8'	1.72 m	1.75 m	1.73 m	1.75 m
9'	3.50 m	3.52 m	3.51 m	3.52 overlap
3'-OCH$_3$				
1''	4.65 d (7.0)	5.06 d (7.5)	4.97 d (7.5)	4.96 d (7.5)
2''	3.48 overlap	3.58 overlap	3.53 overlap	3.56 m
3''	3.29 m	3.51 m	3.48 overlap	3.45 m
4''	3.40 m	3.46 m	3.44 m	3.47 m
5''	3.46 m	3.54 m	3.51 overlap	3.52 m
6''	3.64 dd (5.5,12.5)	3.70 dd (5.5, 12.5)	3.52 overlap	3.69 dd (5.0, 12.5)
	3.67 dd (2.0,12.5)	3.88 dd (2.0, 12.5)	3.70 overlap	3.86 dd (1.5, 12.5)

Table S21. ^{13}C NMR Spectroscopic Data for Compounds B-1−B-4 in D_2O (125 MHz)

position	B-1	B-2	B-3	B-4
1	135.5	135.3	135.5	135.4
2	114.0	113.8	114.0	113.9
3	150.1	150.2	150.0	150.2
4	147.6	147.5	147.5	147.5
5	118.0	118.1	118.0	118.2
6	123.9	122.8	123.4	122.8
7	74.7	75.6	75.0	75.5
8	85.2	87.2	87.2	86.4
9	63.5	63.4	63.7	63.6
3-OCH_3	58.7	58.8	58.7	58.7
1'	139.5	139.6	140.0	139.4
2'	121.3	120.3	121.3	120.4
3'	148.7	149.3	149.6	149.0
4'	148.4	148.7	148.1	149.0
5'	120.2	119.9	119.2	120.0
6'	126.6	126.3	125.8	126.4
7'	36.0	36.0	36.0	36.0
8'	33.5	33.6	33.6	33.5
9'	63.8	63.8	63.8	63.8
3'-OCH_3				
1''	103.4	103.5	103.0	103.6
2''	75.9	75.9	75.9	75.9
3''	78.9	79.0	78.9	79.0
4''	72.3	72.4	72.4	72.3
5''	78.4	78.5	78.5	78.4
6''	63.3	63.4	63.5	63.4

Table S22. ^{1}H NMR Spectroscopic Data for Compounds C-1−C-3 in D_2O (500 MHz)

position	C-1	C-2	C-3
2	6.95 overlap	7.03 d (1.5)	6.96 d (2.0)
5	7.00 d (8.0)	7.04 d (8.5)	7.00 d (8.5)
6	6.94 dd (1.5, 8.0)	6.93 dd (1.5, 8.5)	6.94 dd (2.0, 8.5)
7	4.78 overlap	4.98 overlap	4.79 overlap
8	4.51 m	4.51 m	4.51 m
9	3.91 dd (6.0, 12.0)	3.66 dd (6.0, 12.5)	3.92 dd (6.5, 12.0)
	3.98 dd (2.5, 12.0)	3.83 dd (4.0, 12.5)	3.98 dd (3.0, 12.5)
3-OCH$_3$	3.70 s	3.74 s	3.71 s
2'	6.56 overlap	6.69 overlap	6.58 overlap
5'	6.72 d (8.5)	6.71 d (8.5)	6.73 d (8.5)
6'	6.57 overlap	6.56 dd (1.5, 8.5)	6.57 overlap
7'	2.44 t (7.5)	2.46 t (7.5)	2.45 t (7.0)
8'	1.70 m	1.71 m	1.71 m
9'	3.51 m	3.50 m	3.51 m
3'-OCH$_3$			
1''	4.96 d (7.0)	4.98 overlap	4.97 d (7.5)
2''	3.53 overlap	3.52 overlap	3.53 overlap
3''	3.53 overlap	3.52 overlap	3.53 overlap
4''	3.45 m	3.46 m	3.45 m
5''	3.53 overlap	3.52 overlap	3.53 overlap
6''	3.71 m	3.71 dd (5.5, 12.5)	3.70 dd (5.0, 12.5)
	3.84 m	3.86 dd (2.0, 12.5)	3.85 dd (2.0, 12.5)

Table S23. ^{13}C NMR Spectroscopic Data for Compounds C-1−C-3 in D_2O (125 MHz)

position	C-1	C-2	C-3
1	138.1	138.4	138.2
2	114.1	113.7	114.4
3	151.1	151.4	151.0
4	148.1	147.8	148.0
5	118.4	118.7	118.5
6	123.5	122.3	123.1
7	75.1	75.2	75.0
8	86.4	86.5	86.3
9	64.1	63.7	64.1
3-OCH_3	58.5	58.5	58.5
1'	139.8	139.6	139.7
2'	118.5	118.7	118.6
3'	148.6	148.4	148.5
4'	146.5	146.9	146.4
5'	119.8	118.8	119.6
6'	123.0	123.1	123.1
7'	36.0	36.0	36.0
8'	33.5	33.4	33.5
9'	63.9	63.9	63.9
3'-OCH_3			
1''	103.4	103.4	103.4
2''	75.7	75.7	75.7
3''	78.9	78.9	78.9
4''	72.2	72.1	72.2
5''	78.4	78.4	78.4
6''	63.3	63.3	63.3

Table S24. ^{1}H NMR Spectroscopic Data for Compounds A-1−A-4 in CD_3COOD (500 MHz)

position	A-1	A-2	A-3	A-4
2	7.09 d (2.0)	7.08 d (2.0)	7.07 d (1.5)	7.05 d (1.5)
5	6.84 d (8.5)	6.85 d (8.5)	6.82 d (8.0)	6.83 d (8.0)
6	6.92 overlap	6.92 dd (2.0, 8.5)	6.88 overlap	6.90 dd (1.5, 8.0)
7	4.99 d (6.0)	5.03 d (6.5)	4.96 d (6.0)	5.00 d (7.0)
8	4.45 m	4.36 m	4.42 m	4.35 m
9	3.87 m	3.62 dd (5.0, 11.0)	3.86 m	3.61 m
	3.98 m	3.82 dd (3.5, 11.0)	3.97 m	3.80 m
3-OCH_3	3.86 s	3.86 s	3.84 s	3.84 s
2'	7.04 d (2.0)	7.07 d (2.0)	7.02 s	7.07 s
5'	6.92 overlap	7.10 d (8.5)	6.87 d (8.0)	7.06 d (8.0)
6'	6.92 overlap	6.96 dd (2.0, 8.5)	6.91 d (8.0)	6.95 dd (1.5, 8.0)
7'	6.58 d (16.0)	6.61 d (16.0)	6.57 d (16.0)	6.59 d (16.5)
8'	6.25 dt (6.0, 16.0)	6.28 dt (6.0, 16.0)	6.23 dt (6.0, 16.0)	6.26 dt (6.0, 16.5)
9'	4.31 dd (6.5, 13.5)	4.33 m	4.33 dd (7.0, 13.0)	4.32 dd (6.5, 13.5)
	4.52 dd (6.5, 13.5)	4.52 dd (5.5, 13.5)	4.50 overlap	4.50 overlap
3'-OCH_3	3.88 s	3.94 s	3.86 s	3.92 s
1''	4.55 d (8.0)	4.56 d (7.5)	4.50 d (8.0)	4.50 d (7.5)
2''	3.62 overlap	3.61 overlap	3.49 dd (8.0, 9.0)	3.49 dd (8.0, 9.0)
3''	3.73 t (9.0)	3.73 t (9.0)	3.68 m	3.69 m
4''	3.62 overlap	3.61 overlap	3.55 overlap	3.57 overlap
5''	3.50 m	3.50 m	3.59 m	3.59 m
6''	3.88 overlap	3.89 m	4.03 m	4.01 m
	4.00 m	4.01 dd (2.5, 12.5)		
1'''			5.15 d (2.0)	5.15 d (2.0)
2'''			4.06 d (2.0)	4.07 d (2.0)
4'''			3.91 overlap	3.89 d (10.0)
			3.96 overlap	3.98 d (10.0)
5'''			3.77 d (3.5)	3.77 d (4.0)

Table S25. ^{1}H NMR Spectroscopic Data for Compounds A-5−A-6 in CD_3COOD (500 MHz)

position	A-5	A-6
2	7.06 d (1.5)	7.04 s
5	6.81 overlap	6.83 d (8.0)
6	6.69 d (8.0)	6.89 dd (1.5, 8.0)
7	4.95 d (5.5)	4.99 d (7.0)
8	4.34 m	4.24 m
9	3.82 overlap	3.56 m
	3.95 m	3.77 dd (3.0, 12.5)
3-OCH_3	3.83 s	3.84 s
2'	6.81 overlap	6.86 d (1.5)
5'	6.81 overlap	7.03 d (8.0)
6'	6.87 dd (2.0, 8.0)	6.74 dd (1.5, 8.0)
7'	2.64 t (7.0)	2.66 t (7.5)
8'	1.90 m	1.91 m
9'	3.92 m	3.92 m
3'-OCH_3	3.83 s	3.89 s
1''	4.43 d (8.0)	4.43 d (8.0)
2''	3.45 dd (8.0, 9.0)	3.46 dd (8.0, 9.0)
3''	3.70 t (9.0)	3.70 t (9.0)
4''	3.60 t (9.0)	3.60 t (9.0)
5''	3.49 m	3.49 m
6''	3.85 overlap	3.85 overlap
	3.98 m	3.98 m

Table S26. ^{13}C NMR Spectroscopic Data for Compounds A-1−A-6 in CD_3COOD (125 MHz)

position	A-1	A-2	A-3	A-4	A-5	A-6
1	133.1	132.4	133.2	132.6	133.2	132.4
2	111.2	111.2	111.3	111.3	111.1	111.2
3	147.9	148.1	148.0	148.1	147.9	148.1
4	146.4	146.7	146.4	146.7	146.3	146.7
5	115.4	115.6	115.5	115.6	115.4	115.6
6	120.9	121.0	121.0	121.1	120.9	120.9
7	73.8	74.6	73.9	74.7	73.8	74.6
8	85.9	87.5	86.0	87.5	86.5	88.2
9	61.7	61.6	61.8	61.7	61.7	61.6
3-OCH_3	56.3	56.3	56.4	56.5	56.4	56.4
1'	133.0	133.2	133.2	133.4	138.4	138.7
2'	111.1	111.0	111.3	111.3	113.7	113.6
3'	151.8	151.7	151.9	151.8	151.7	151.7
4'	148.3	148.7	148.3	148.7	146.3	146.7
5'	119.6	120.1	119.8	120.2	120.4	121.1
6'	120.9	121.1	121.0	121.1	121.9	122.1
7'	133.6	133.5	133.7	133.6	32.5	32.5
8'	125.0	125.1	125.1	125.3	32.1	32.2
9'	70.8	70.8	70.8	70.8	69.9	69.9
3'-OCH_3	56.4	56.4	56.5	56.5	56.3	56.4
1''	102.4	102.4	102.4	102.4	103.5	103.5
2''	74.6	74.6	74.6	74.6	74.6	74.6
3''	77.2	77.2	77.4	77.3	77.2	77.2
4''	70.9	70.9	71.1	71.1	70.9	70.9
5''	76.6	76.6	76.0	76.0	76.5	76.5
6''	62.3	62.3	68.0	68.0	62.2	62.2
1'''			110.1	109.8		
2'''			78.3	78.2		
3'''			81.0	81.0		
4'''			74.7	74.7		
5'''			65.9	65.9		

Table S27. ^{1}H NMR Spectroscopic Data for Compounds B-1−B-4 in CD_3COOD (500 MHz)

position	B-1	B-2	B-3	B-4
2	7.07 overlap	7.08 overlap	7.03 s	7.05 s
5	6.84 d (8.0)	6.83 d (8.0)	6.83 overlap	6.84 d (8.0)
6	6.91 dd (1.5, 8.0)	6.90 d (8.0)	6.88 overlap	6.93 d (8.0)
7	5.00 d (6.0)	5.02 d (6.5)	5.03 d (6.0)	5.06 d (7.0)
8	4.20 m	4.41 m	4.39 m	4.38 m
9	3.86 m	3.62 m	3.81 m	3.53 overlap
	3.99 m	3.84 overlap	3.99 m	3.81 overlap
3-OCH_3	3.83 s	3.84 s	3.84 s	3.83 s
2'	7.07 overlap	7.08 overlap	7.08 s	7.10 s
5'	6.81 overlap	7.00 d (8.0)	6.83 overlap	7.05 overlap
6'	6.81 overlap	6.83 overlap	6.88 overlap	6.87 d (8.0)
7'	2.60 t (7.5)	2.61 t (7.5)	2.61 t (7.5)	2.62 t (7.5)
8'	1.84 m	1.85 m	1.85 m	1.86 m
9'	3.66 m	3.67 m	3.67 m	3.67 m
3'-OCH_3				
1''	4.93 d (7.5)	5.04 d (7.0)	5.01 d (8.0)	4.96 d (7.0)
2''	3.72 overlap	3.75 overlap	3.74 m	3.72 m
3''	3.74 m	3.77 overlap	3.77 m	3.76 m
4''	3.69 overlap	3.69 m	3.70 m	3.67 overlap
5''	3.56 m	3.61 overlap	3.61 m	3.53 overlap
6''	3.87 m	3.87 m	3.87 m	3.87 m
	4.00 m	4.00 d (10.5)	4.01 m	3.98 d (11.0)

Table S28. ^{13}C NMR Spectroscopic Data for Compounds B-1−B-4 in CD_3COOD (125 MHz)

position	B-1	B-2	B-3	B-4
1	133.2	133.7	132.8	132.5
2	111.1	111.2	110.8	111.3
3	148.1	148.1	148.0	148.2
4	146.4	146.6	146.3	146.7
5	115.6	115.6	115.6	115.7
6	120.9	121.0	120.5	121.1
7	73.5	74.5	73.6	74.6
8	86.4	86.8	86.9	87.0
9	61.3	61.6	61.3	61.2
3-OCH_3	56.5	56.4	56.4	56.4
1'	138.3	138.0	138.4	138.2
2'	120.9	120.6	120.7	121.3
3'	149.2	148.9	149.5	149.0
4'	147.7	148.1	147.6	148.1
5'	120.5	119.8	120.3	120.3
6'	125.0	124.9	124.8	125.1
7'	34.3	34.4	34.3	34.4
8'	32.0	32.0	32.1	32.0
9'	62.2	62.2	62.2	62.2
3'-OCH_3				
1''	103.2	103.3	103.2	103.4
2''	74.7	74.7	74.6	74.7
3''	77.1	77.2	77.1	77.1
4''	70.6	70.6	70.6	70.6
5''	76.8	76.9	76.8	76.8
6''	62.1	62.1	62.1	62.0

Table S29. ^{1}H NMR Spectroscopic Data for Compounds C-1−C-3 in CD_3COOD (500 MHz)

position	C-1	C-2	C-3
2	7.11 overlap	7.11 d (2.0)	7.11 s
5	7.12 overlap	7.10 d (8.0)	7.12 d (8.0)
6	6.97 d (8.0)	6.97 dd (2.0, 8.0)	6.97 d (8.0)
7	5.06 d (5.5)	5.11 d (6.0)	5.07 d (5.5)
8	4.35 m	4.29 m	4.35 m
9	3.86 m	3.61 m	3.85 m
	3.99 m	3.88 dd (3.5, 12.0)	3.99 m
3-OCH_3	3.82 s	3.83 s	3.82 s
2'	6.73 s	6.75 d (2.0)	6.73 s
5'	6.77 d (8.0)	6.89 d (8.0)	6.78 d (8.0)
6'	6.56 d (8.0)	6.58 dd (2.0, 8.0)	6.56 d (8.0)
7'	2.55 t (7.5)	2.56 t (7.5)	2.55 t (7.5)
8'	1.83 m	1.83 m	1.83 m
9'	3.65 overlap	3.66 m	3.66 m
3'-OCH_3			
1''	4.98 d (7.5)	4.86 d (7.5)	4.98 d (7.5)
2''	3.67 m	3.70 m	3.67 m
3''	3.77 m	3.79 m	3.79 m
4''	3.65 overlap	3.64 overlap	3.65 overlap
5''	3.61 m	3.61 overlap	3.61 m
6''	3.87 overlap	3.87 m	3.86 overlap
	4.00 overlap	3.97 dd (2.0, 12.5)	4.00 overlap

Table S30. ^{13}C NMR Spectroscopic Data for Compounds C-1−C-3 in CD_3COOD (125 MHz)

position	C-1	C-2	C-3
1	136.6	136.6	136.6
2	112.0	112.0	112.1
3	150.6	150.6	150.6
4	146.8	146.9	146.8
5	118.2	118.1	118.3
6	120.5	120.4	120.4
7	73.7	74.1	73.6
8	85.7	86.2	85.7
9	61.5	61.4	61.5
3-OCH_3	56.4	56.3	56.4
1'	138.4	138.4	138.3
2'	117.0	117.0	117.0
3'	148.5	148.4	148.5
4'	144.5	144.9	146.8
5'	118.9	118.7	118.8
6'	120.8	120.7	120.8
7'	34.5	34.5	34.5
8'	32.1	32.1	32.1
9'	62.4	62.4	62.4
3'-OCH_3			
1''	102.2	102.1	102.2
2''	74.5	74.5	74.5
3''	76.9	76.9	76.9
4''	70.5	70.5	70.5
5''	76.7	76.7	76.8
6''	62.1	62.1	62.1

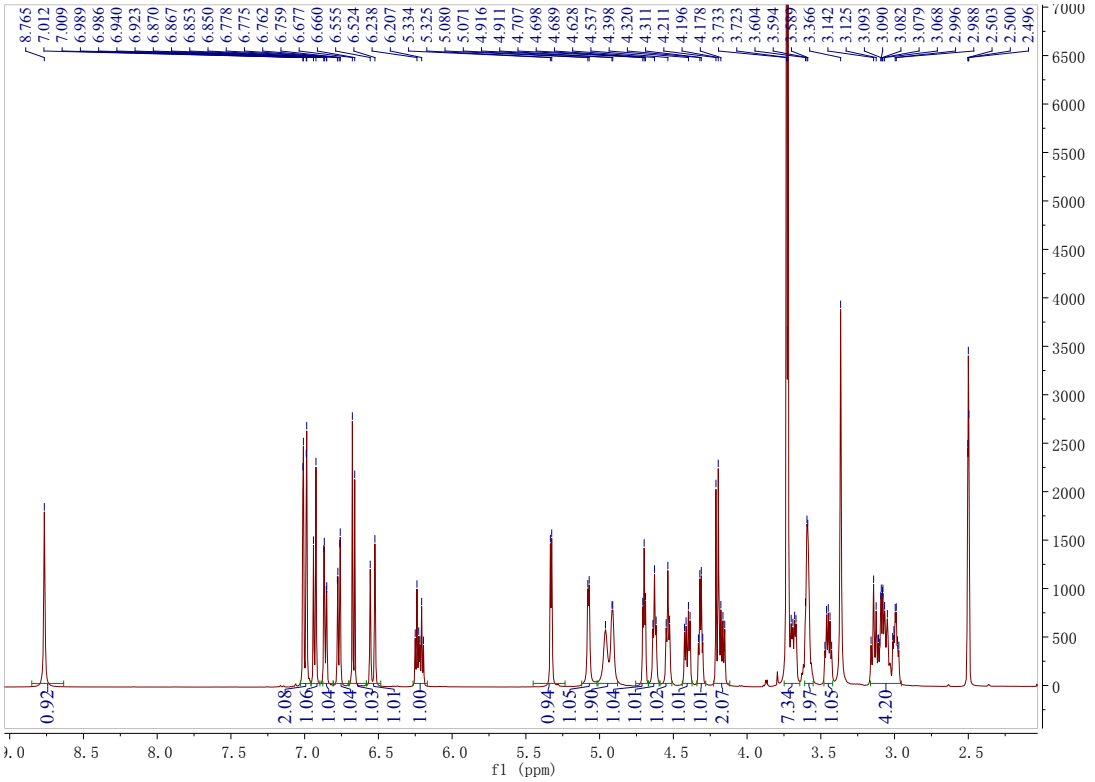


Figure S2. The ^{1}H-NMR spectrum of A-1 in DMSO-d_6

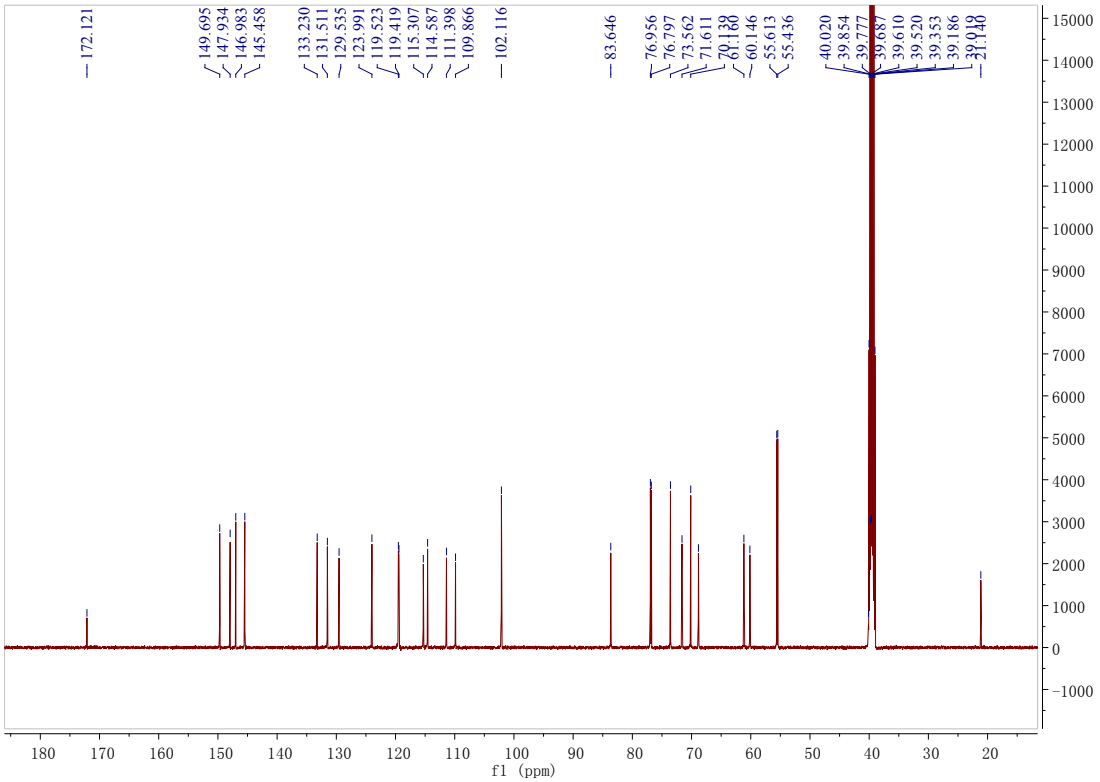


Figure S3. The ^{13}C-NMR spectrum of A-1 in DMSO-d_6

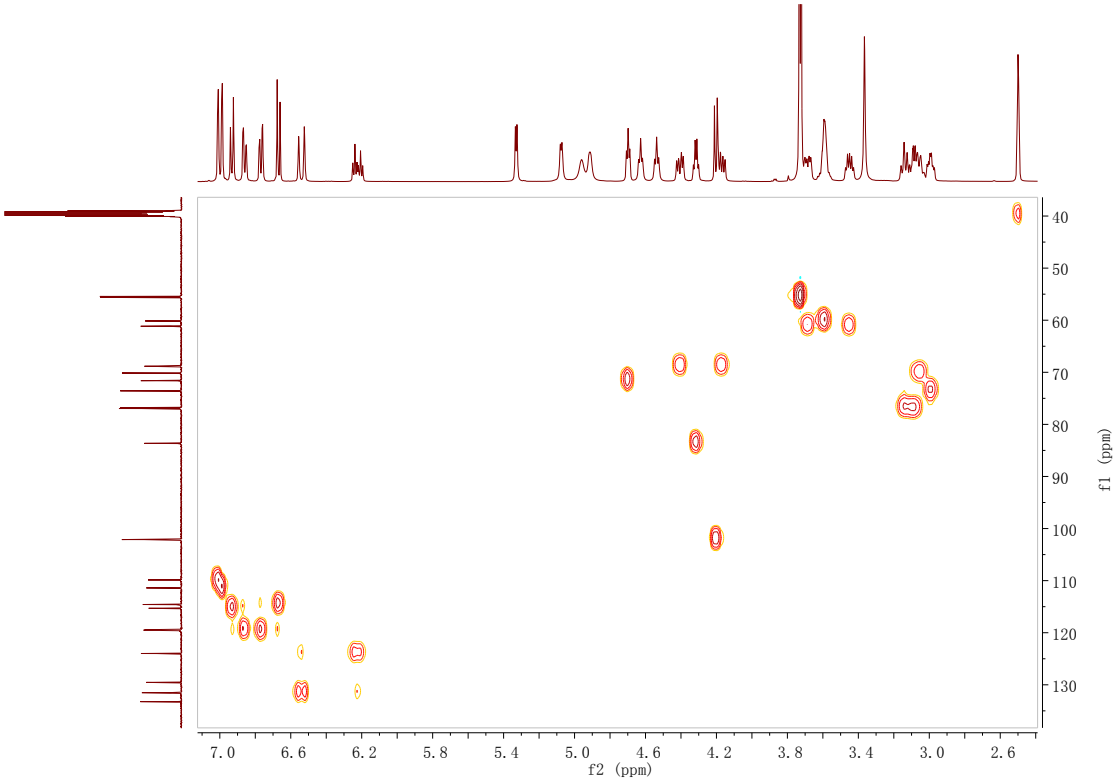


Figure S4. The HSQC spectrum of A-1 in DMSO-d_6

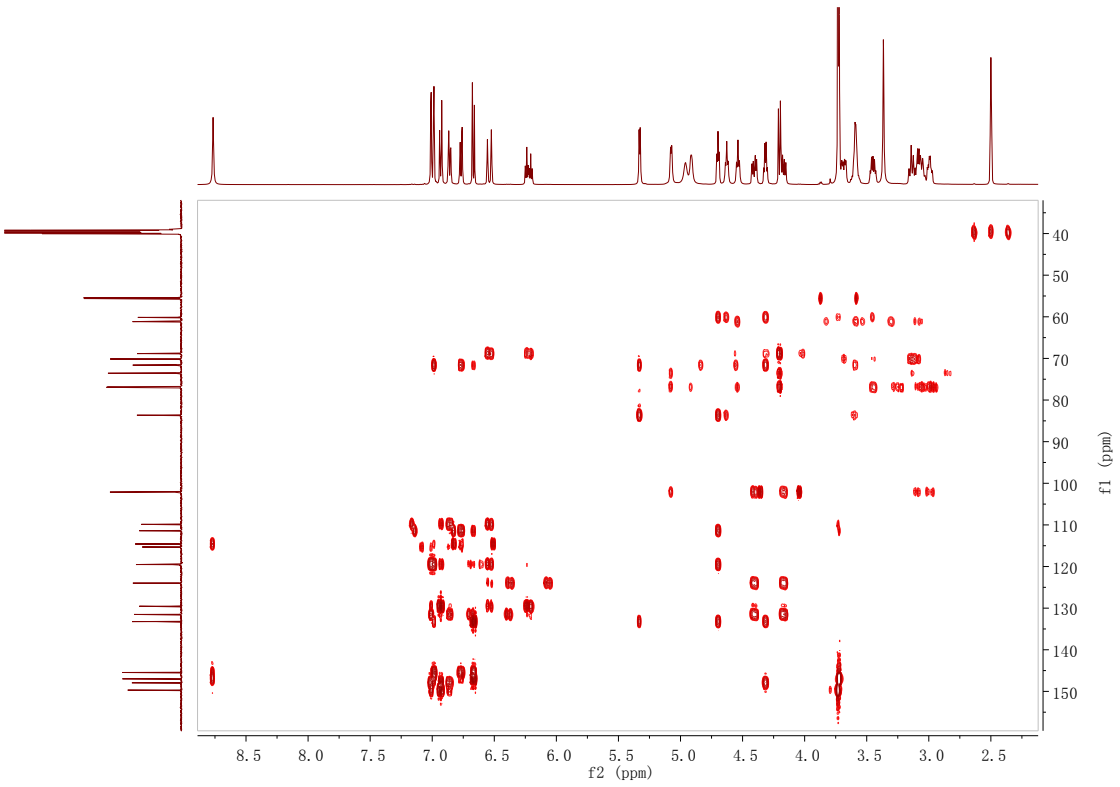


Figure S5. The HMBC spectrum of A-1 in DMSO-d_6

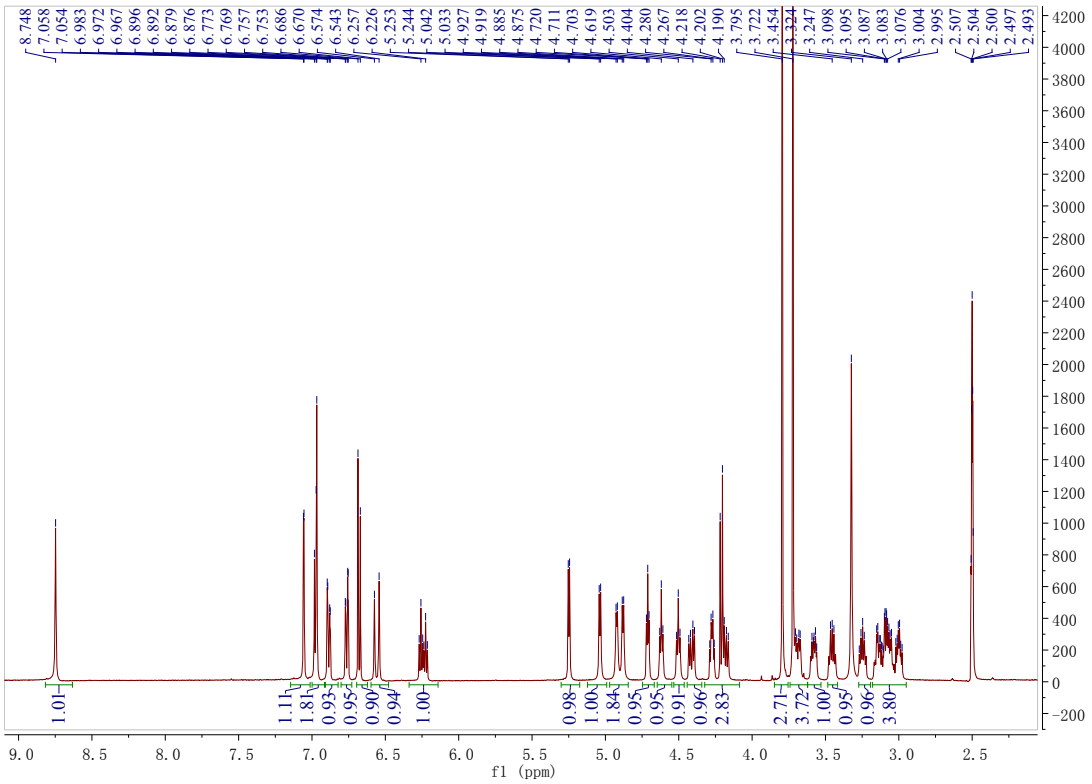


Figure S6. The ^{1}H-NMR spectrum of A-2 in DMSO-d_6

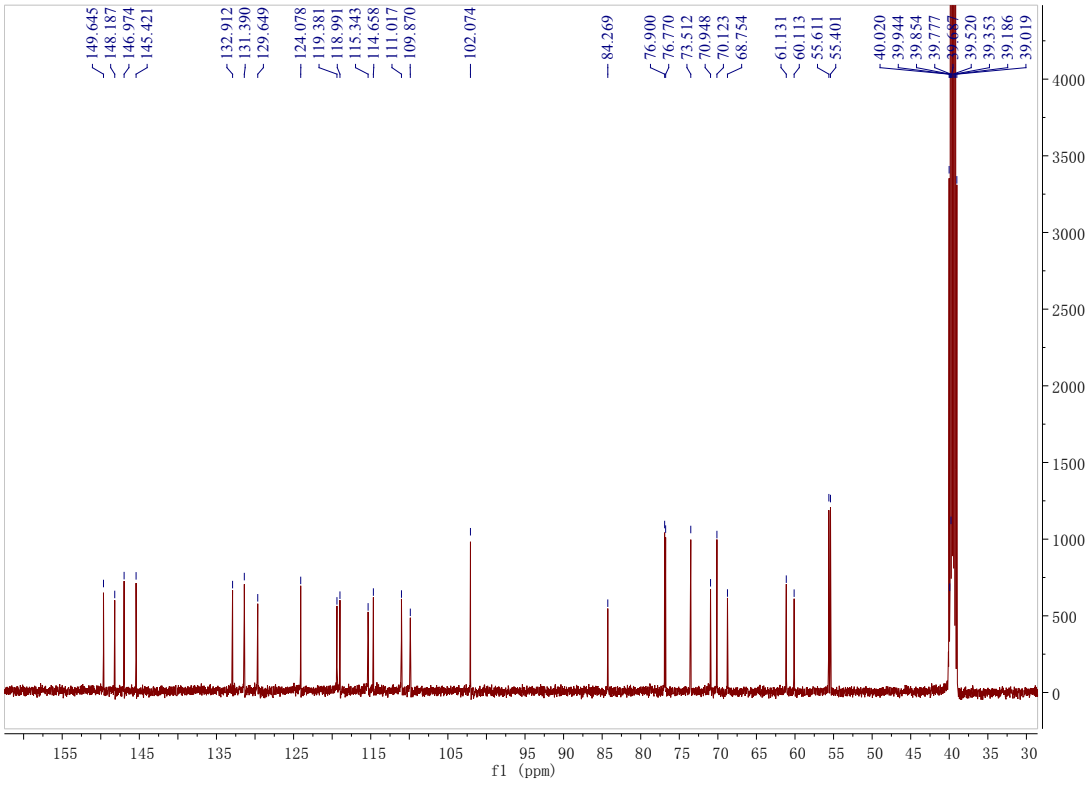


Figure S7. The ^{13}C-NMR spectrum of A-2 in DMSO-d_6

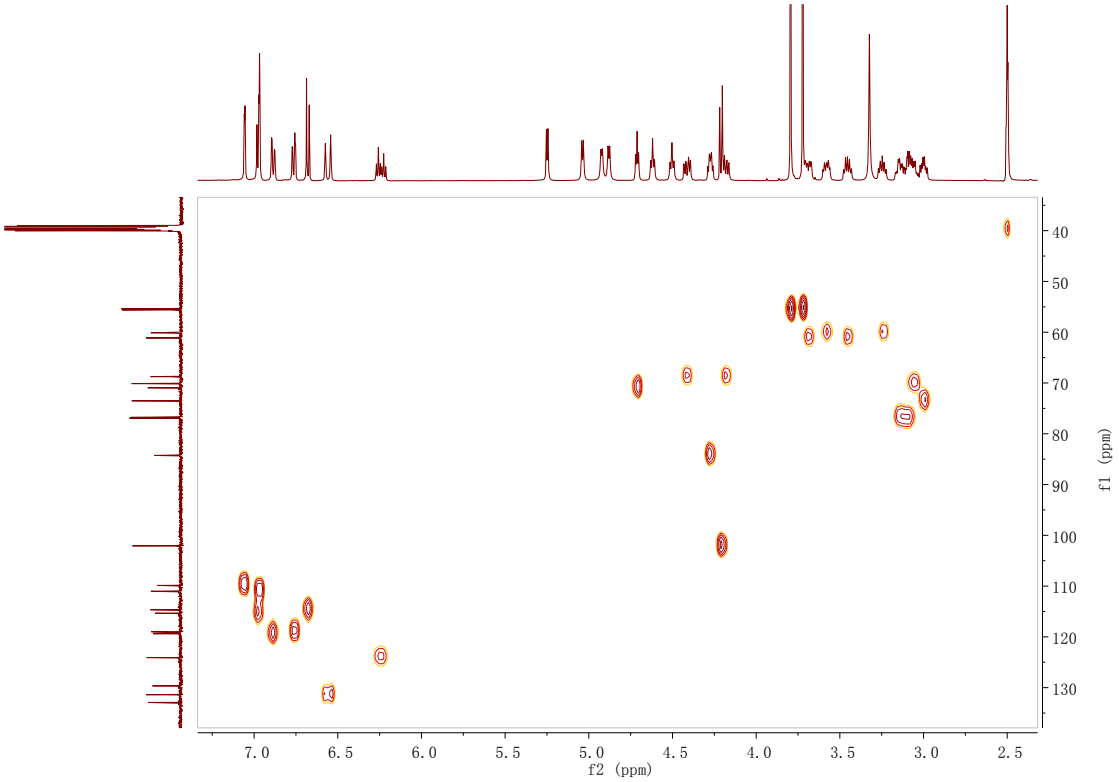


Figure S8. The HSQC spectrum of A-2 in DMSO-d_6

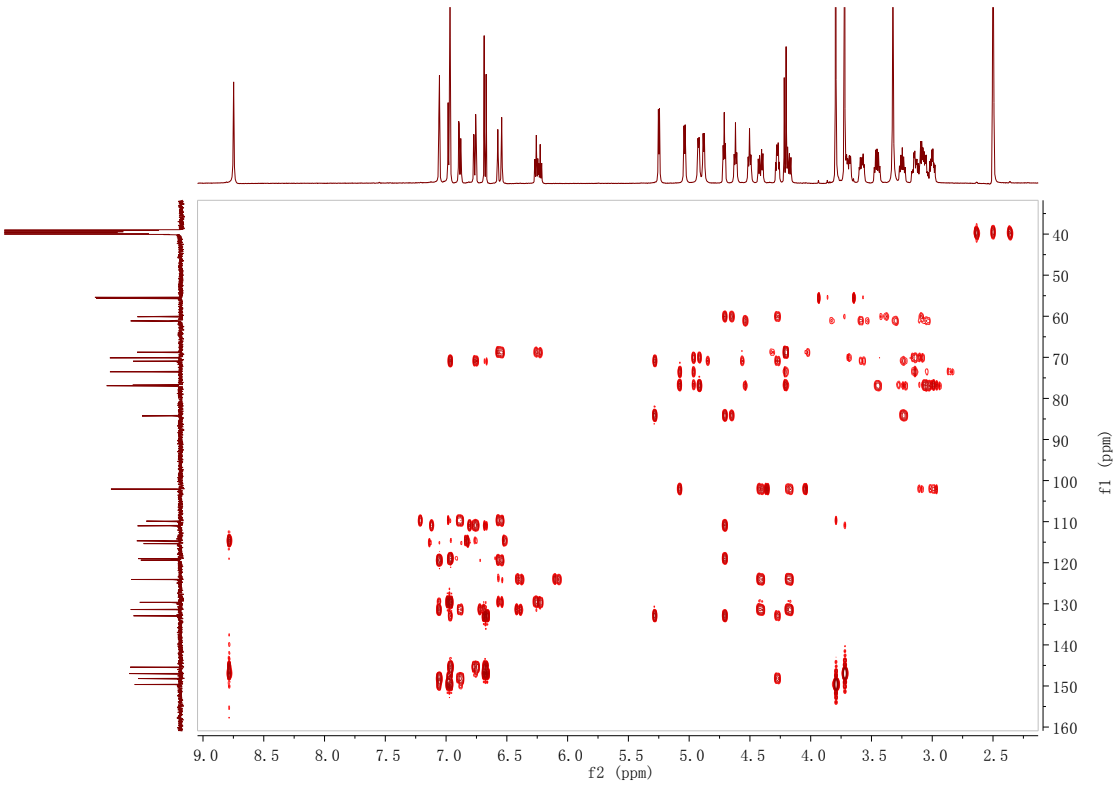


Figure S9. The HMBC spectrum of A-2 in DMSO-d_6

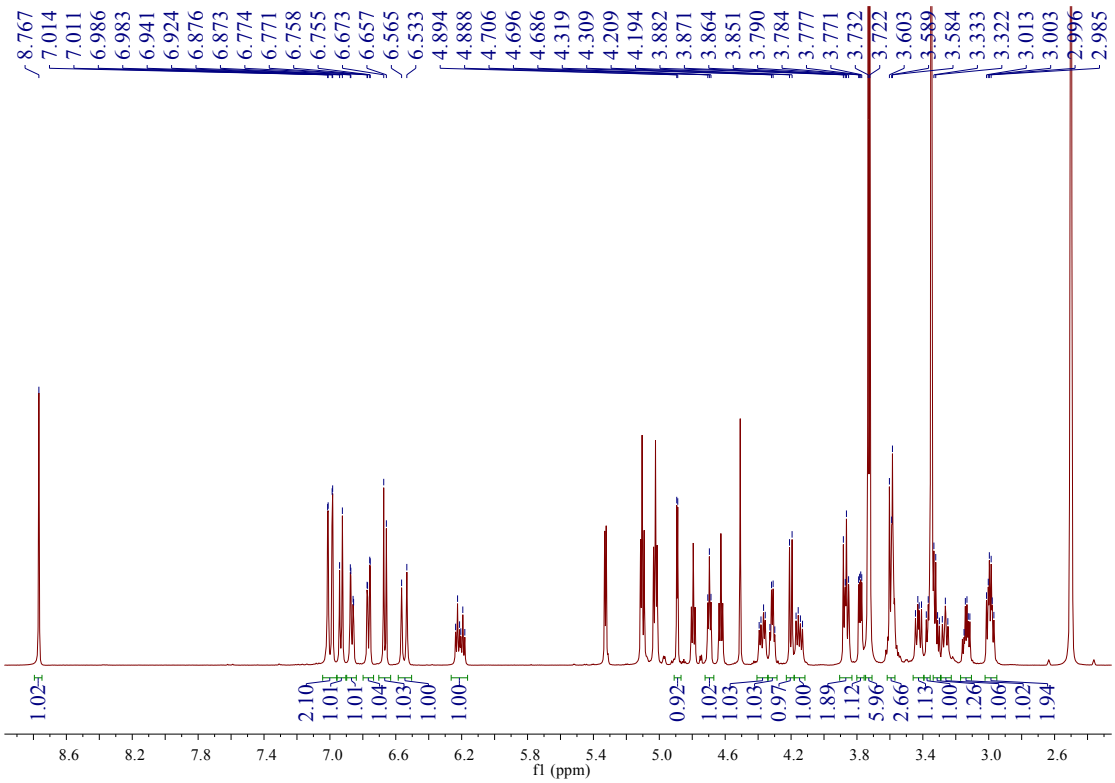


Figure S10. The ^{1}H-NMR spectrum of A-3 in DMSO-d_6

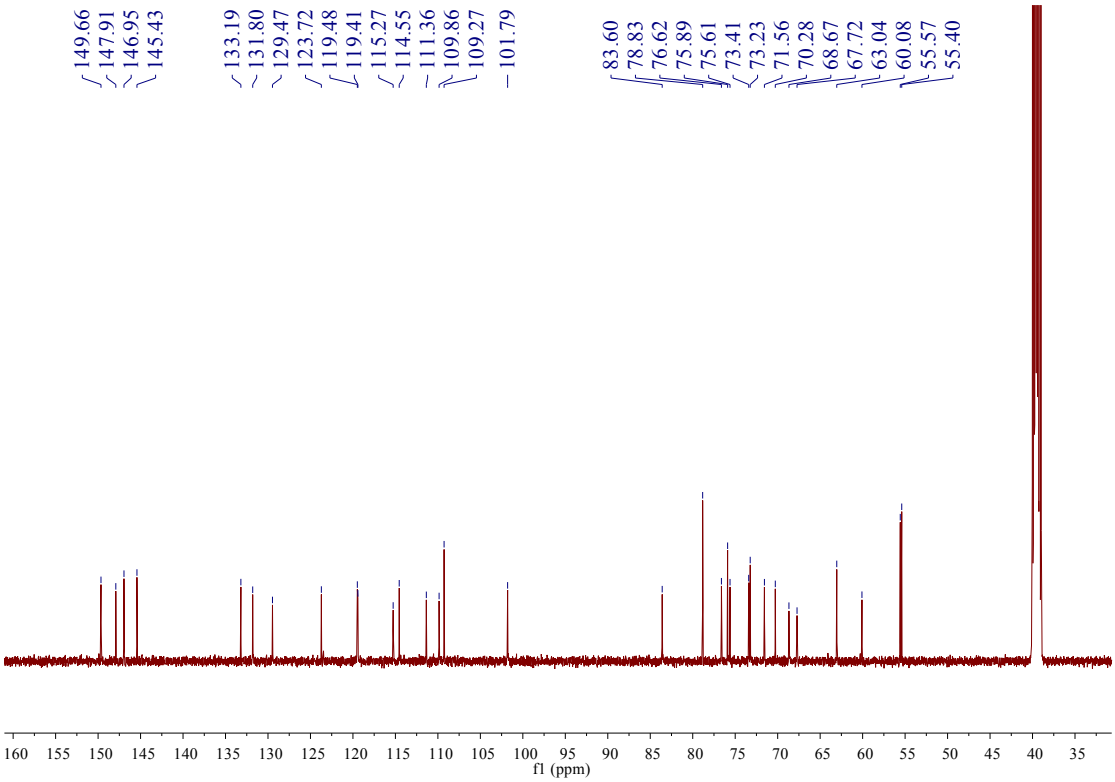


Figure S11. The ^{13}C-NMR spectrum of A-3 in DMSO-d_6

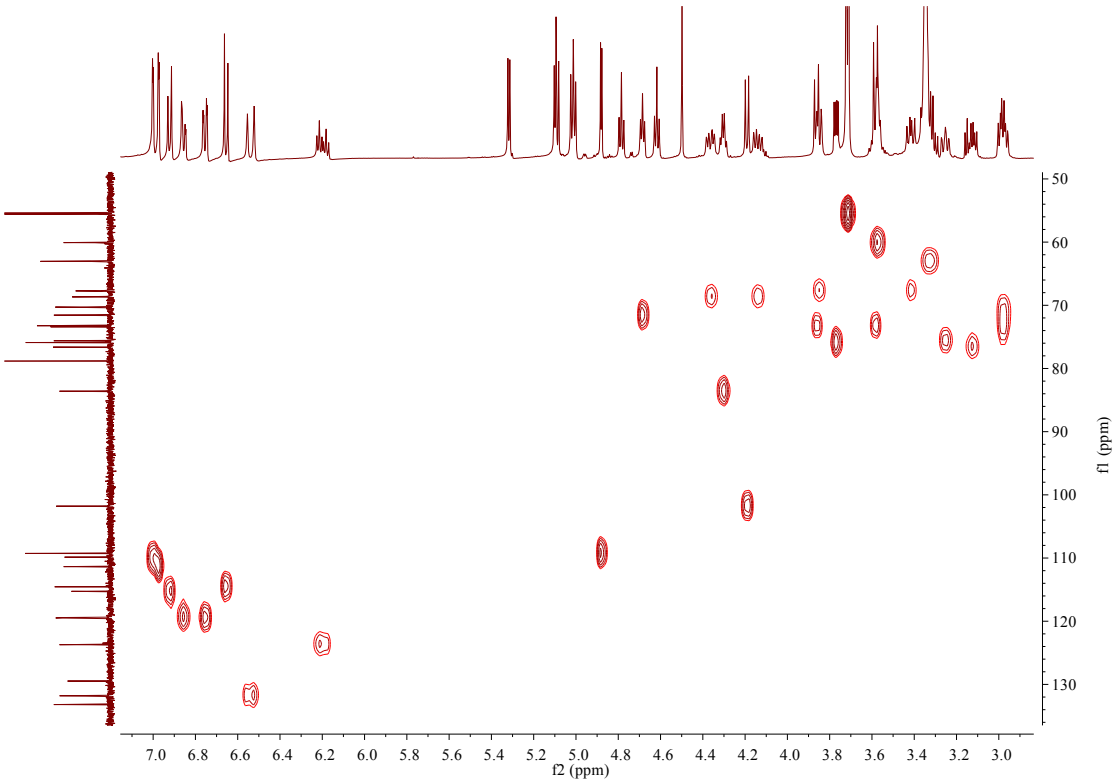


Figure S12. The HSQC spectrum of A-3 in DMSO-d_6

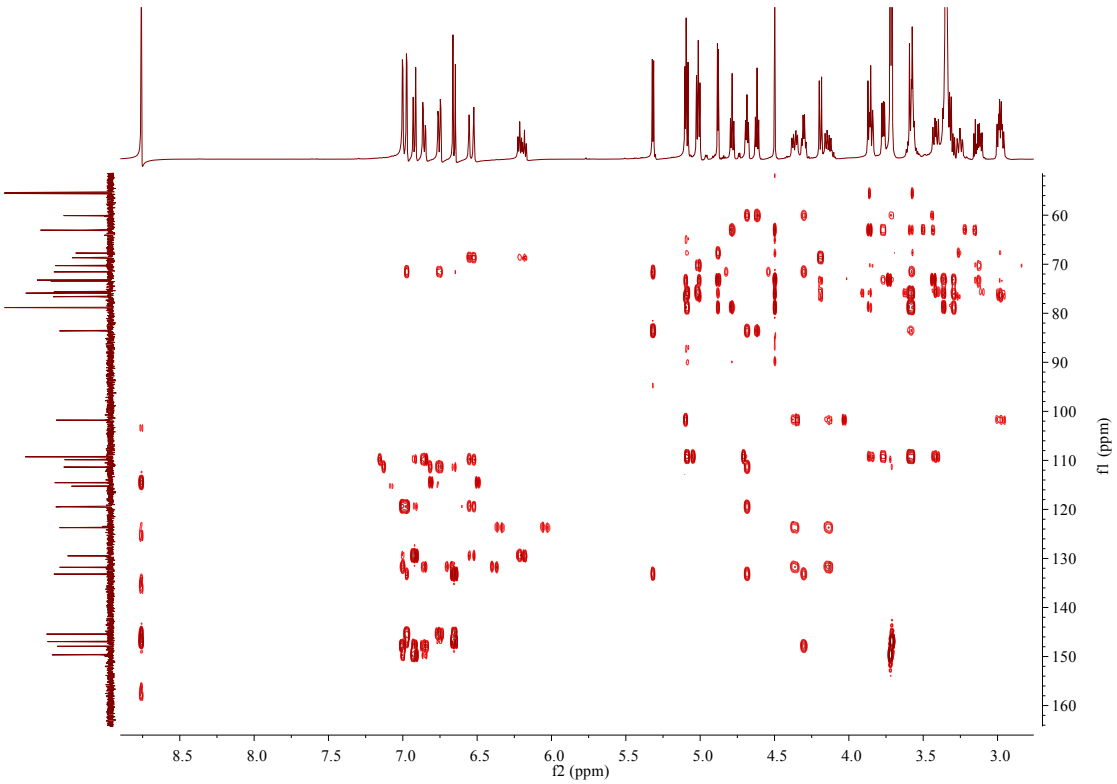


Figure S13. The HMBC spectrum of A-3 in DMSO-d_6

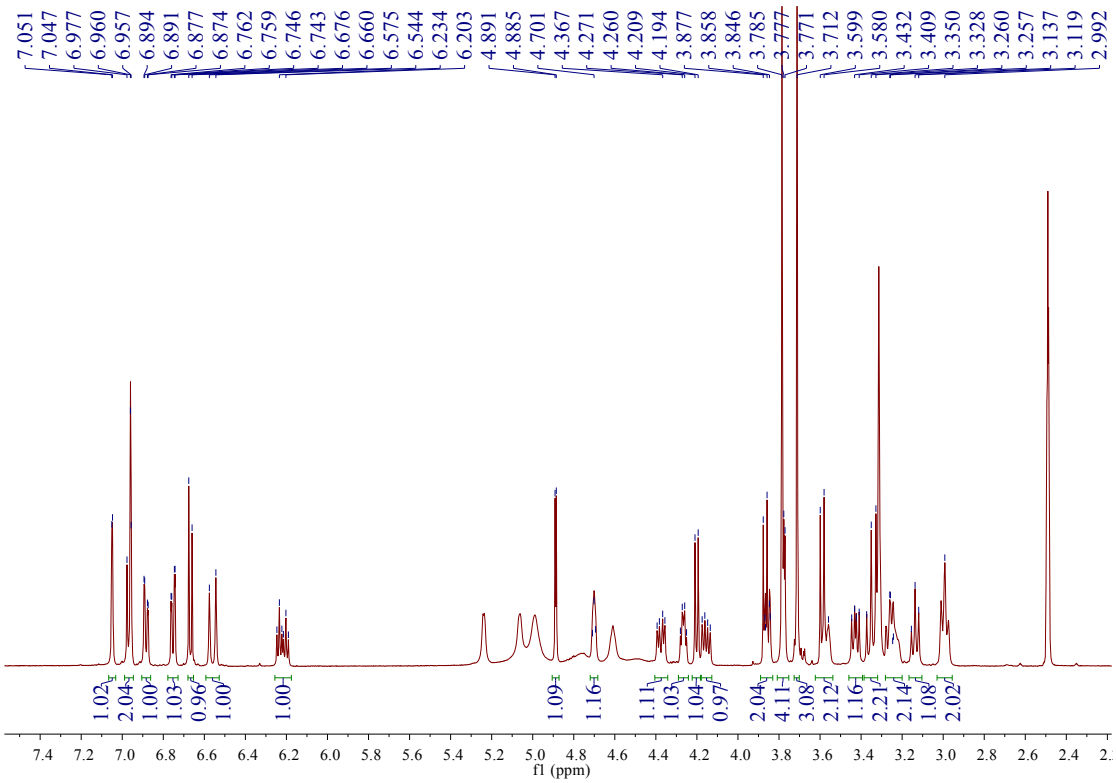


Figure S14. The ^{1}H-NMR spectrum of A-4 in DMSO-d_6

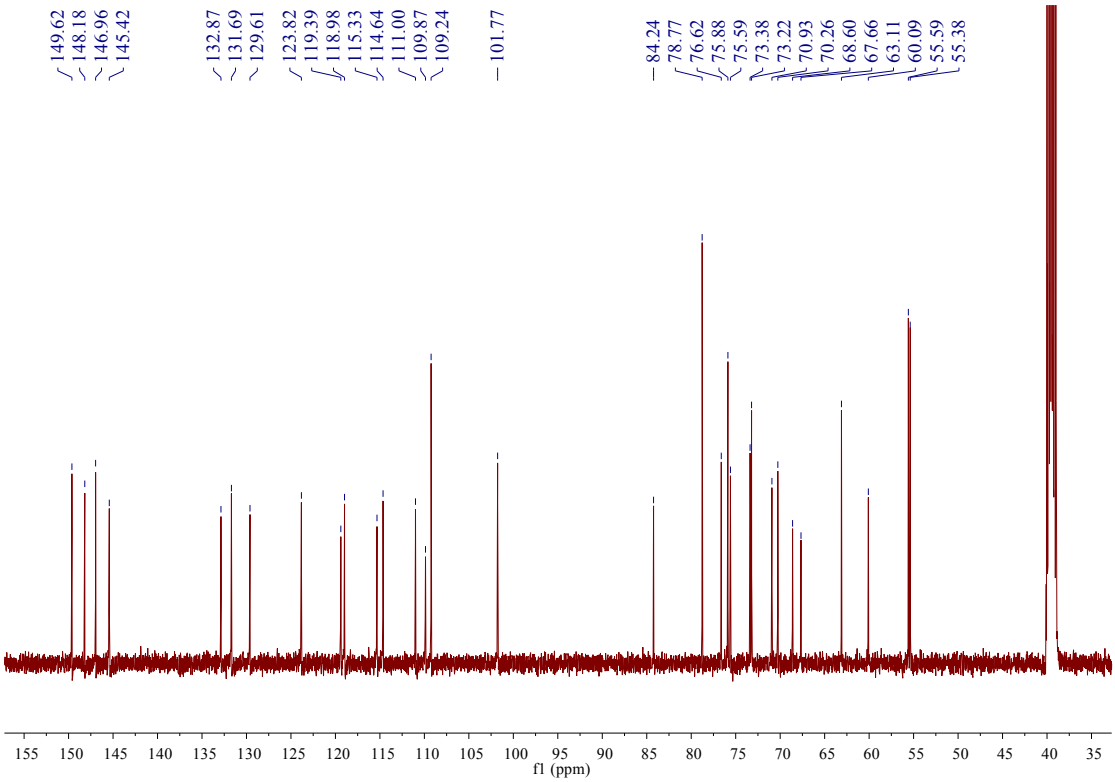


Figure S15. The ^{13}C-NMR spectrum of A-4 in DMSO-d_6

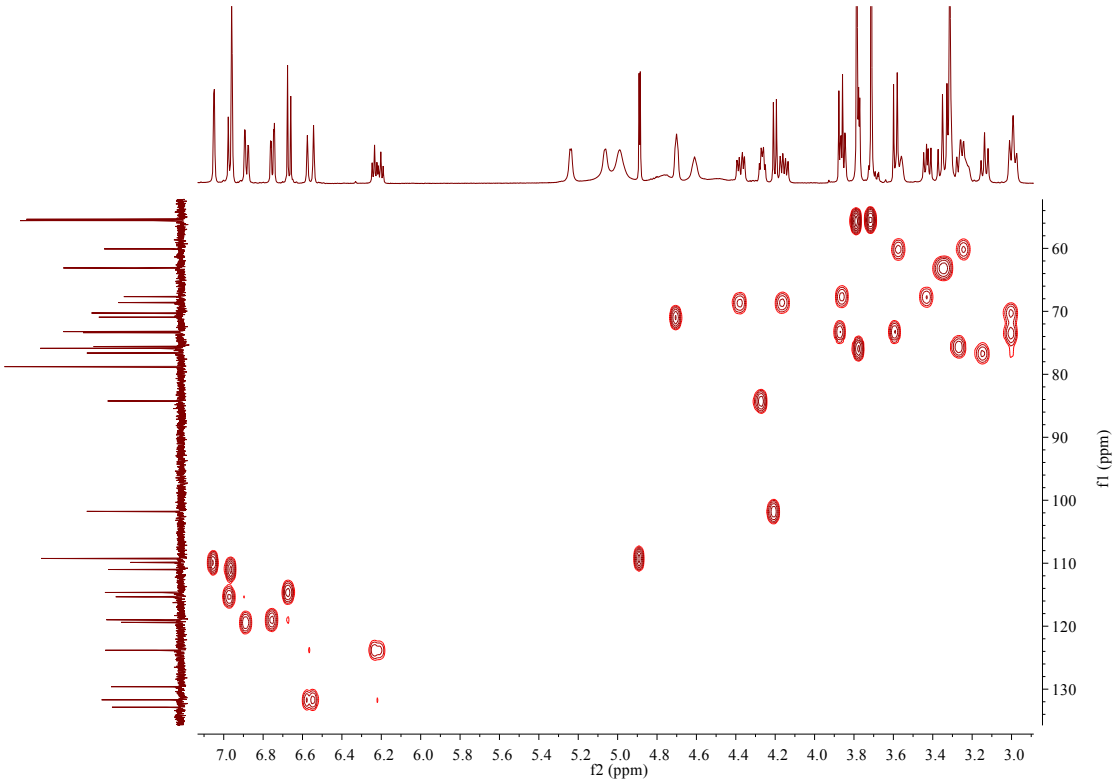


Figure S16. The HSQC spectrum of A-4 in DMSO-d_6

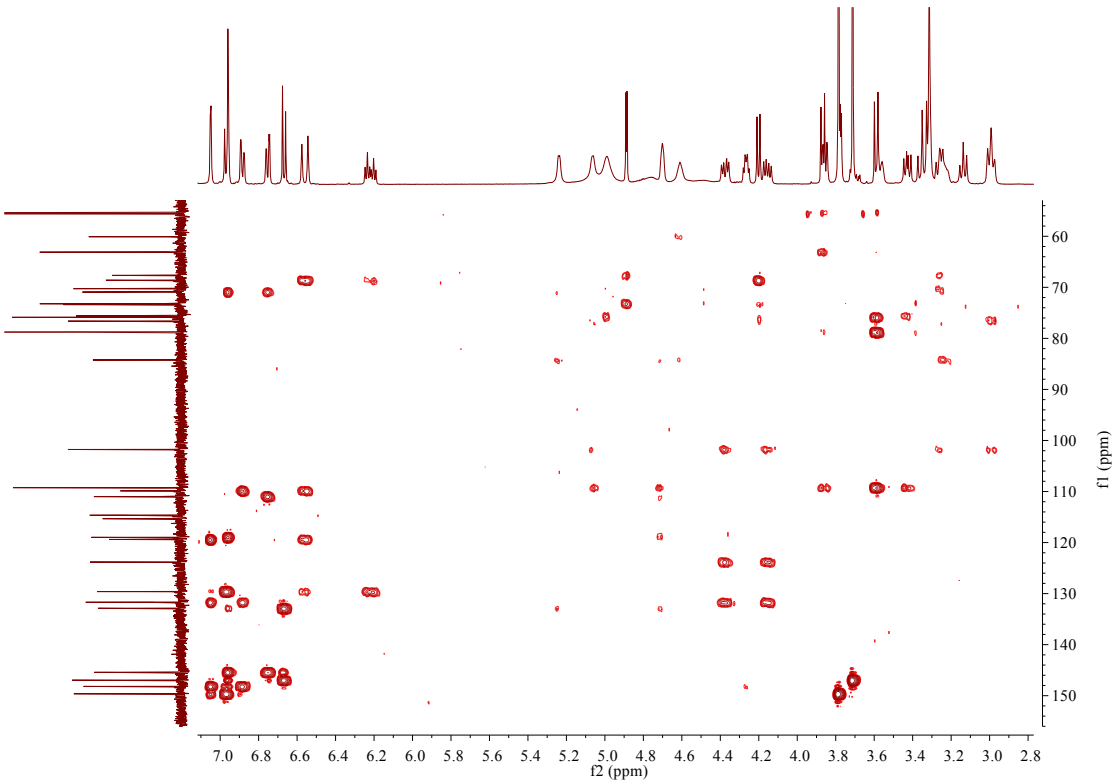


Figure S17. The HMBC spectrum of A-4 in DMSO-d_6

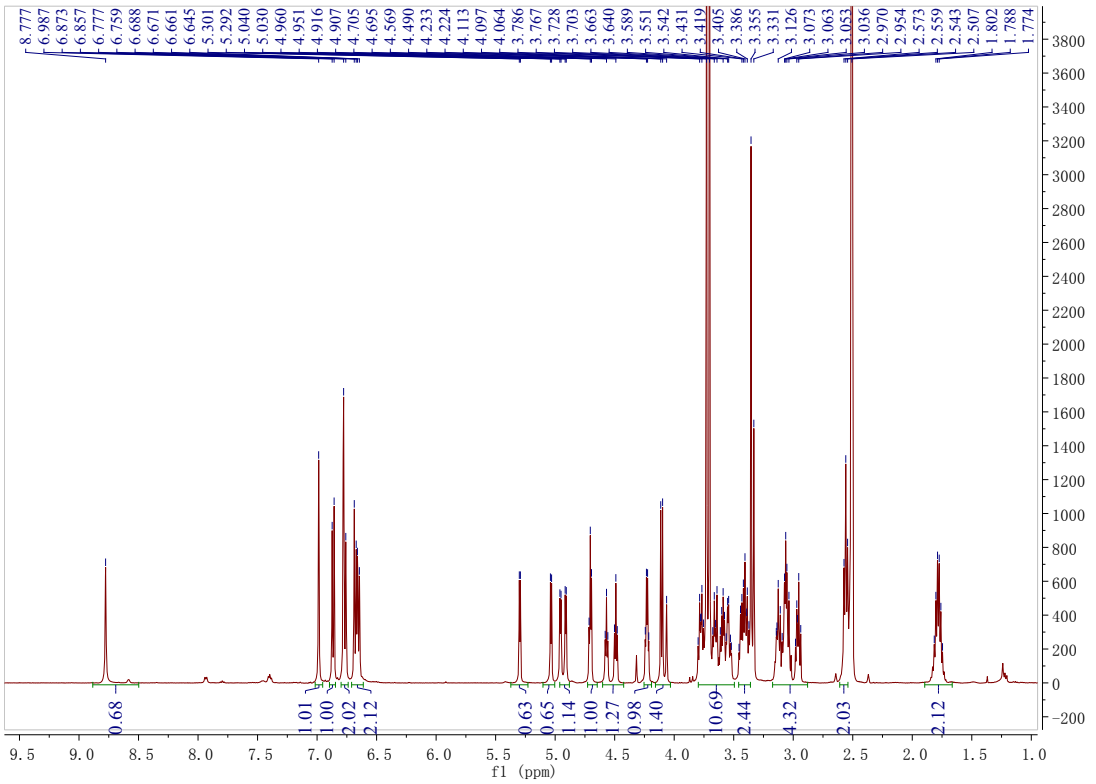


Figure S18. The ^{1}H-NMR spectrum of A-5 in DMSO-d_6

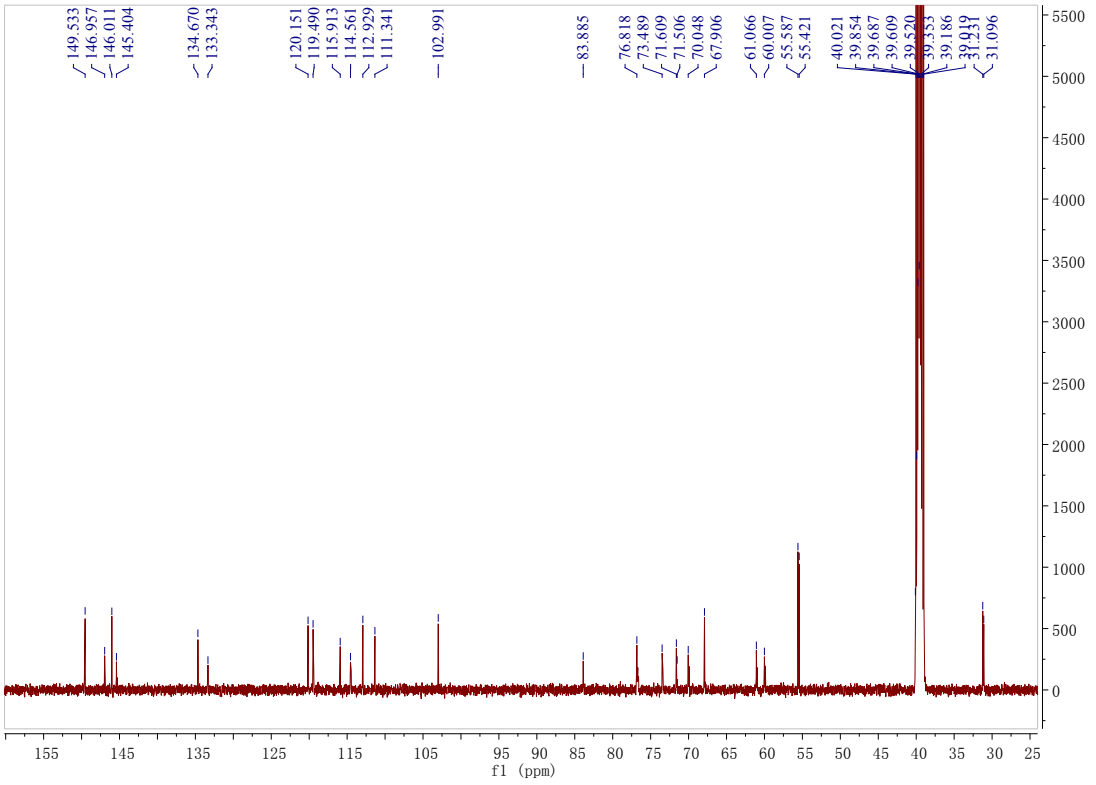


Figure S19. The ^{13}C-NMR spectrum of A-5 in DMSO-d_6

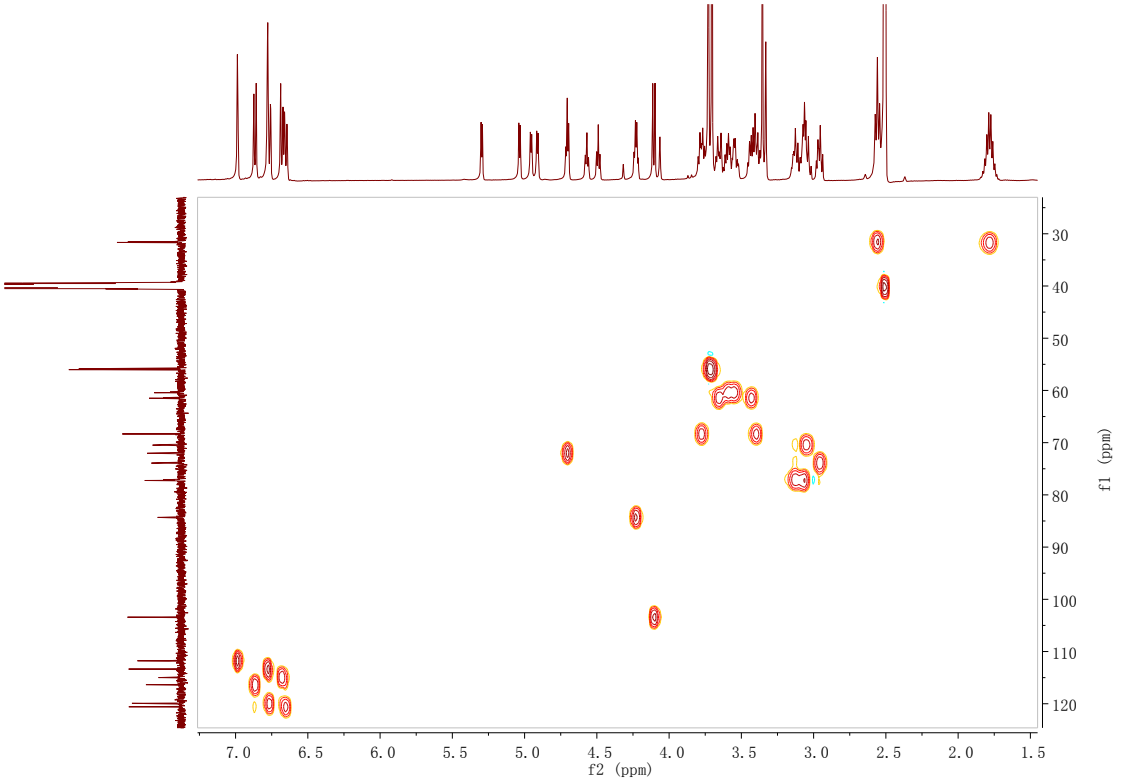


Figure S20. The HSQC spectrum of A-5 in DMSO-d_6

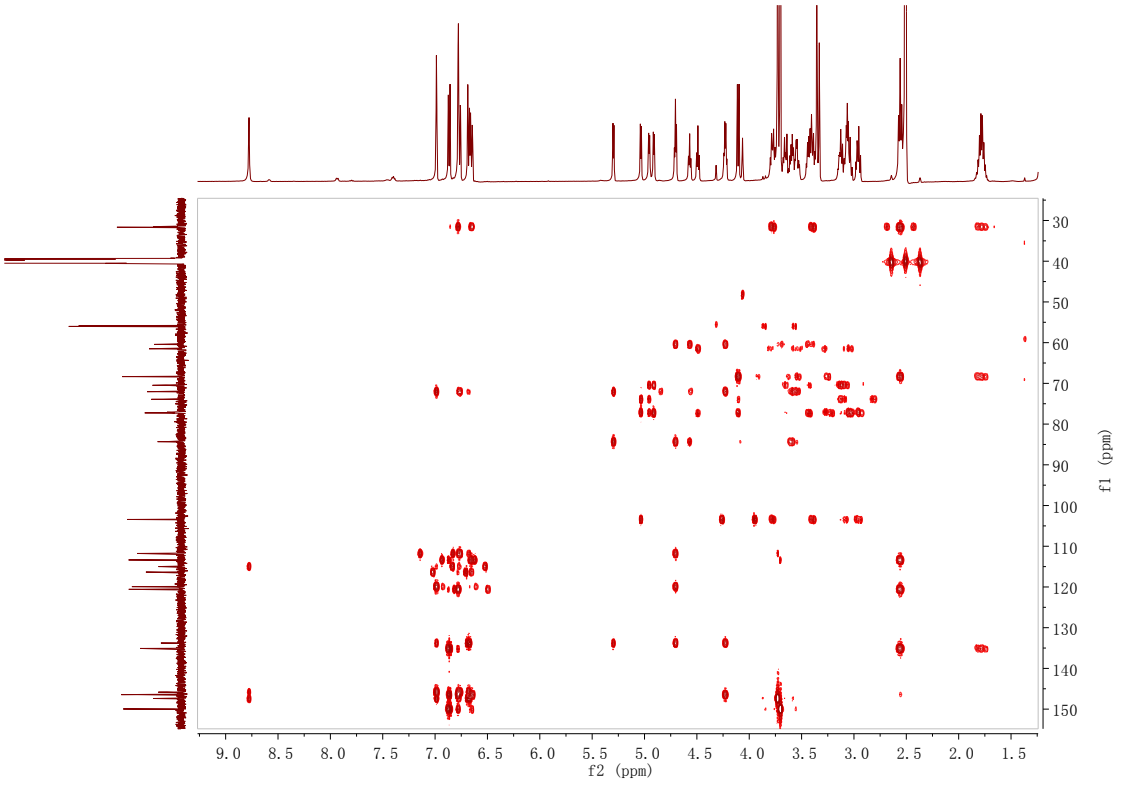


Figure S21. The HMBC spectrum of A-5 in DMSO-d_6

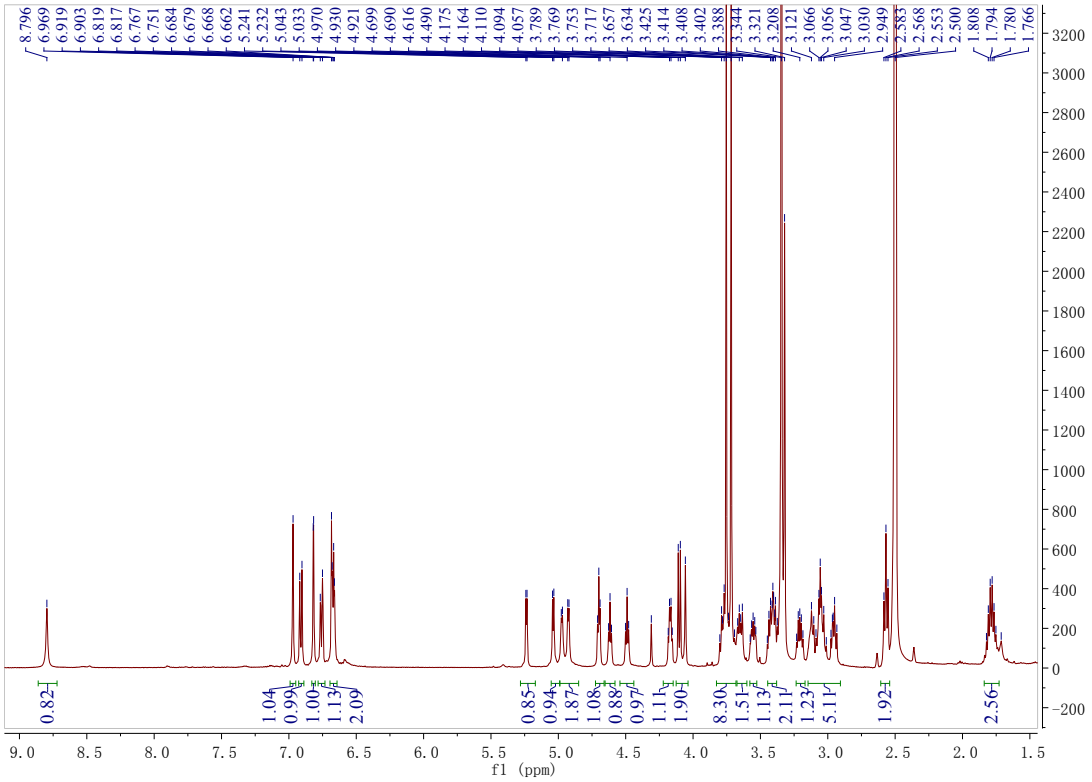


Figure S22. The ^{1}H-NMR spectrum of A-6 in DMSO-d_6

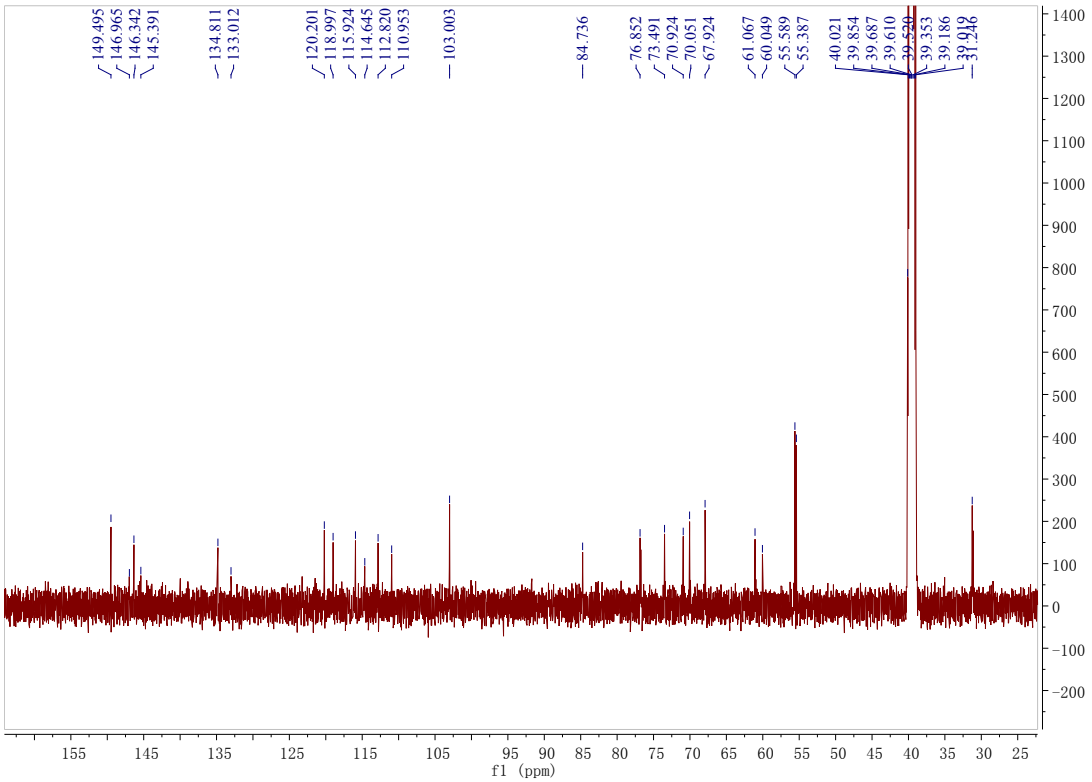


Figure S23. The ^{13}C-NMR spectrum of A-6 in DMSO-d_6

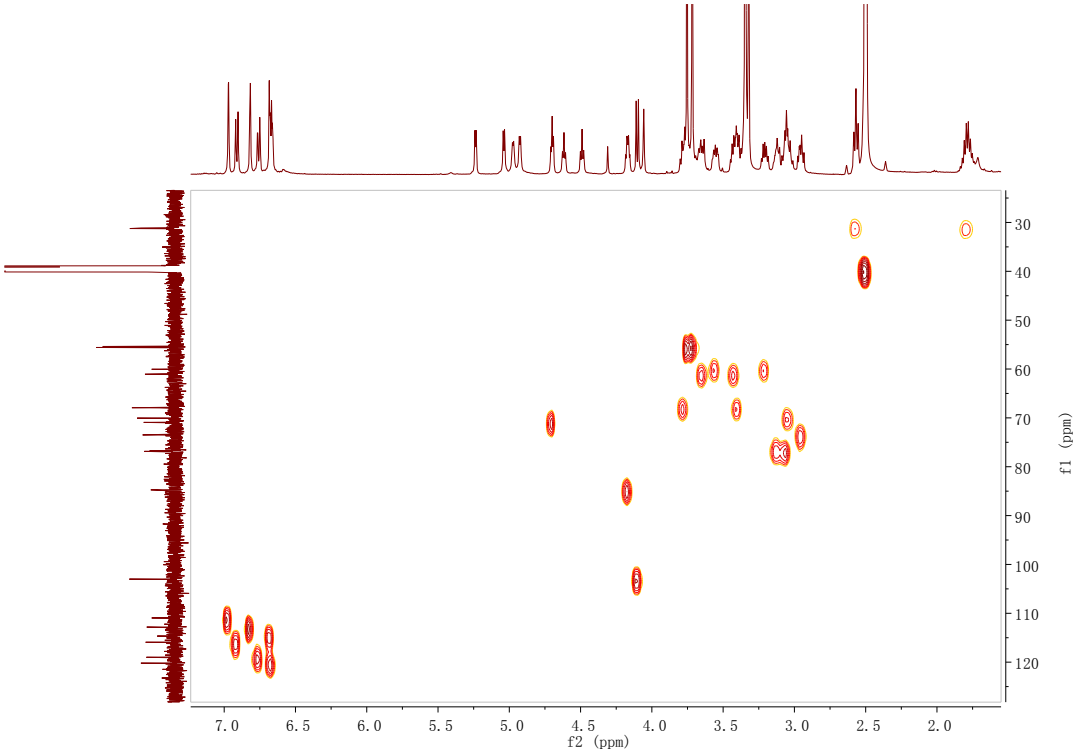


Figure S24. The HSQC spectrum of A-6 in DMSO-d_6

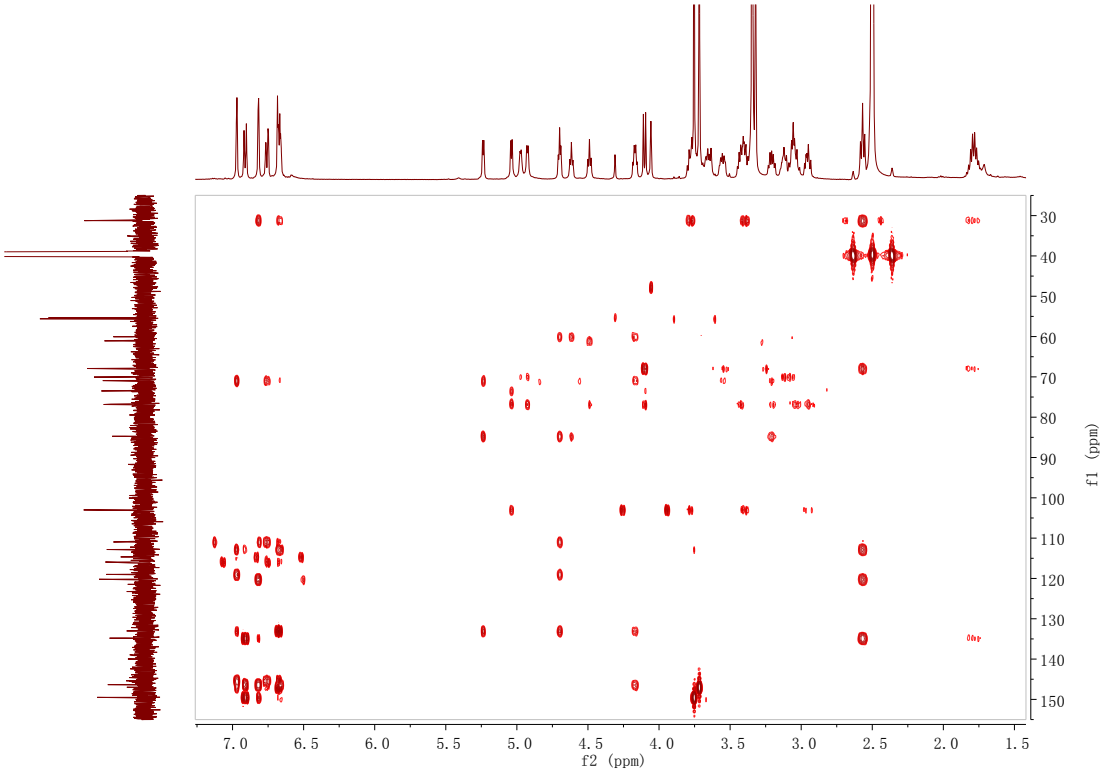


Figure S25. The HMBC spectrum of A-6 in DMSO-d_6

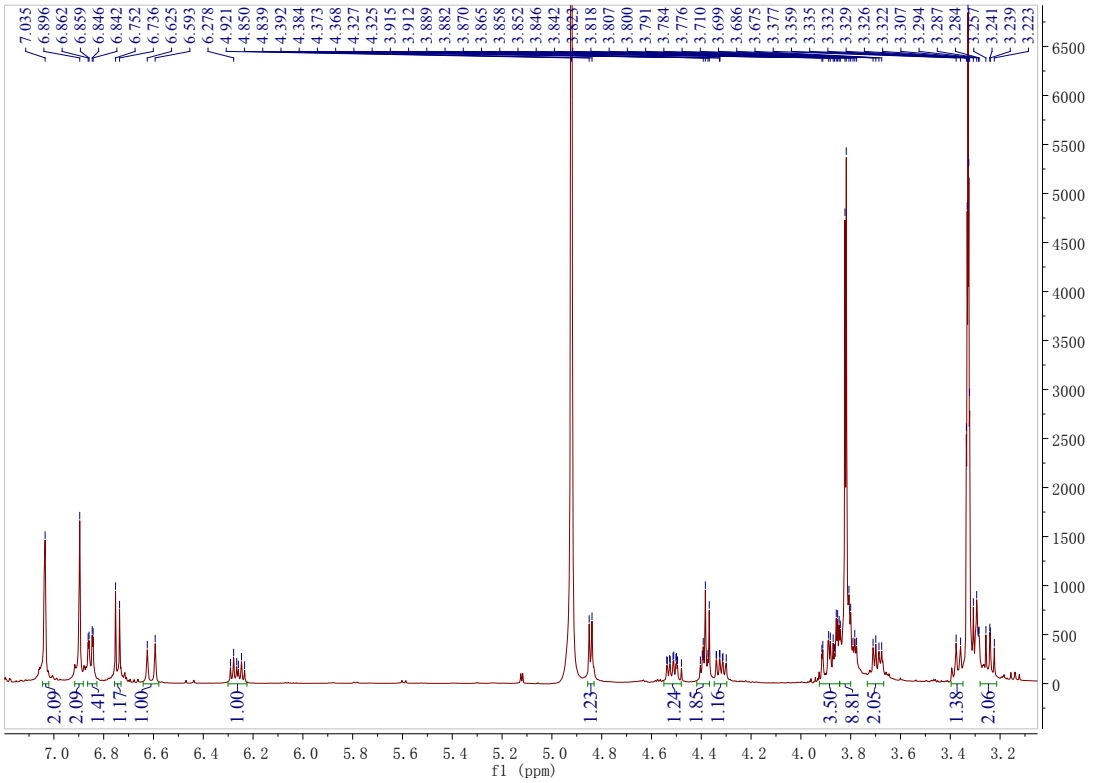


Figure S26. The ^{1}H-NMR spectrum of A-1 in CD_3OD

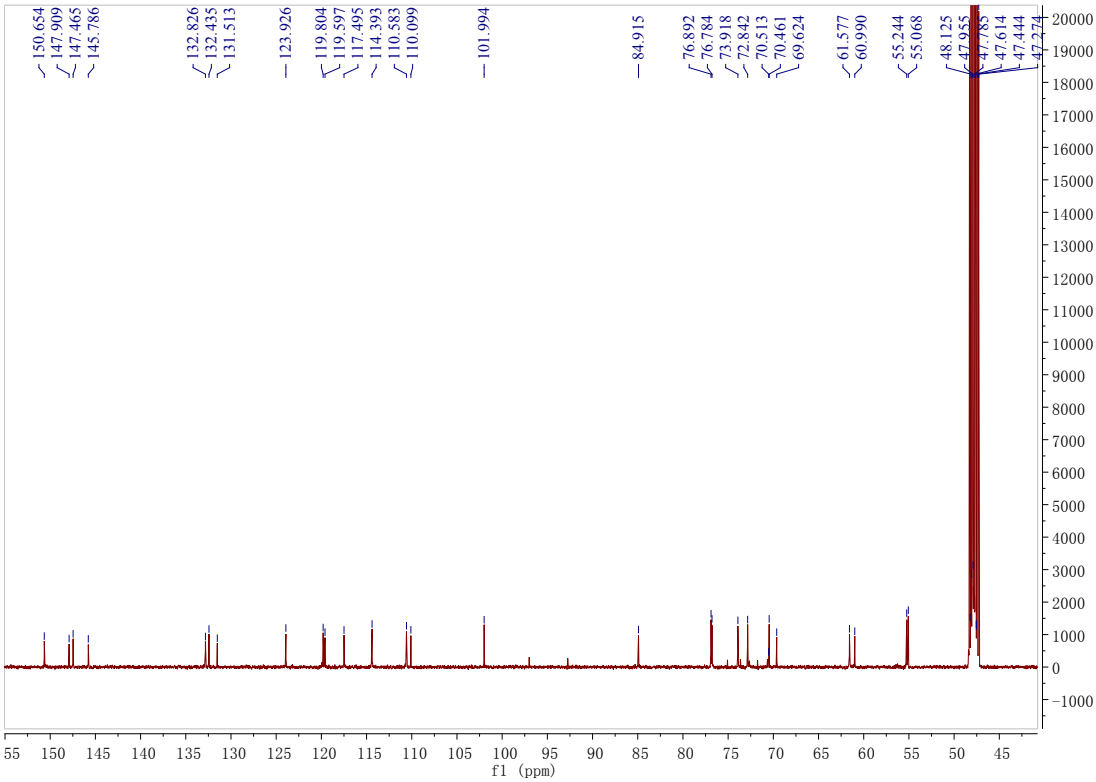


Figure S27. The ^{13}C-NMR spectrum of A-1 in CD_3OD

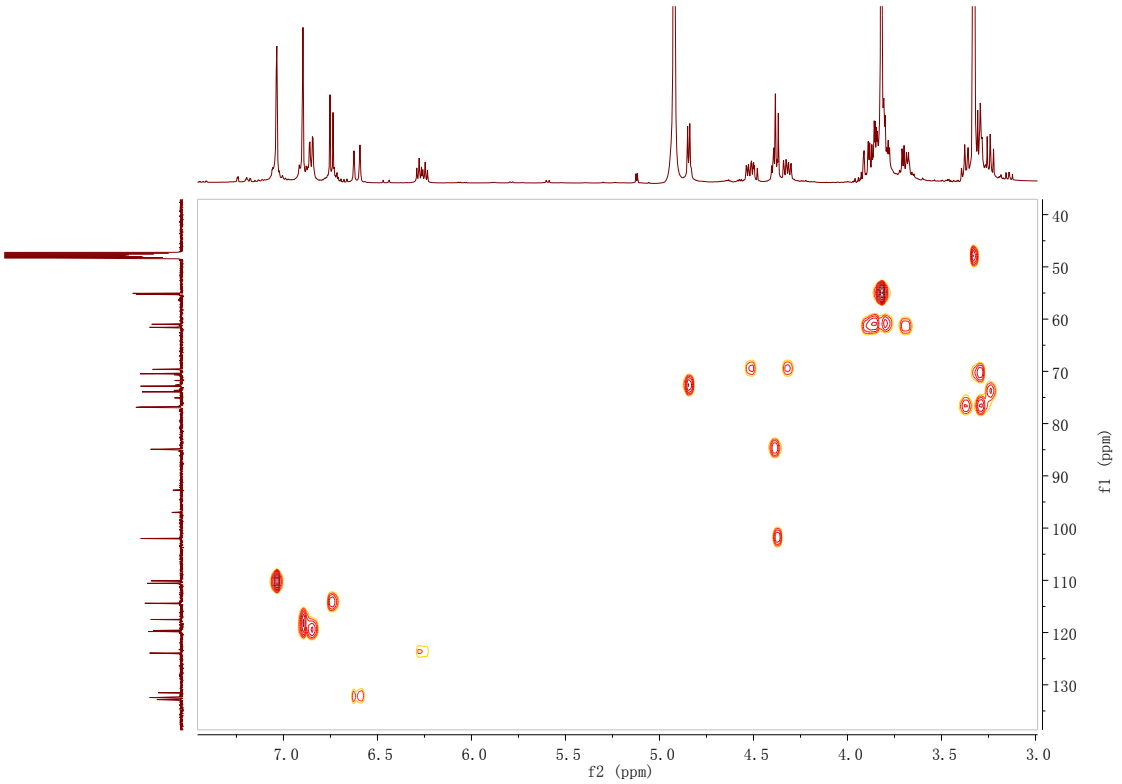


Figure S28. The HSQC spectrum of A-1 in CD_3OD

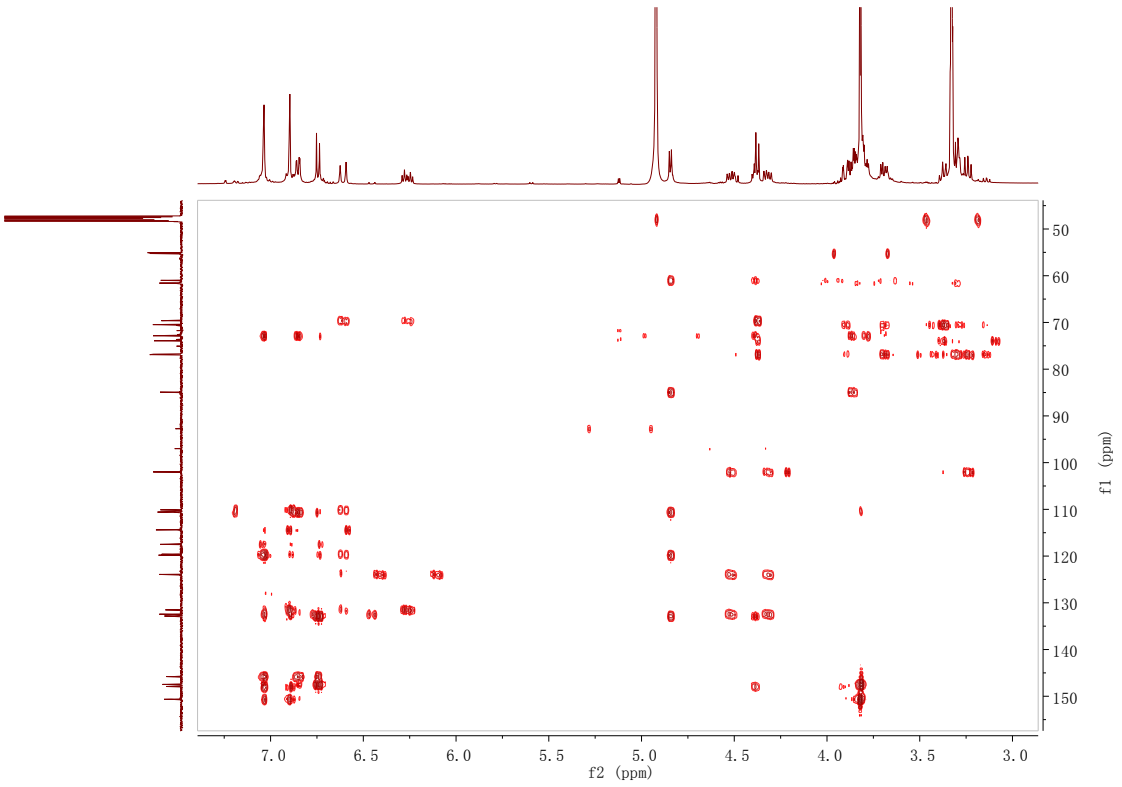


Figure S29. The HMBC spectrum of A-1 in CD_3OD

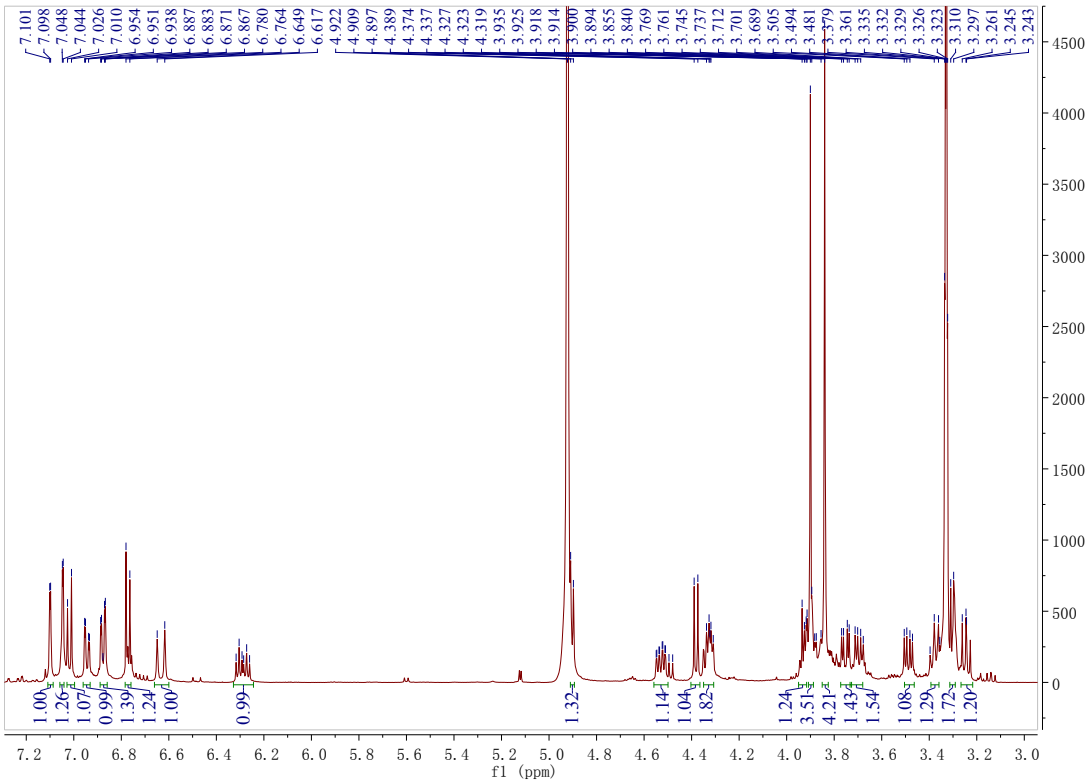


Figure S30. The ^{1}H-NMR spectrum of A-2 in CD_3OD

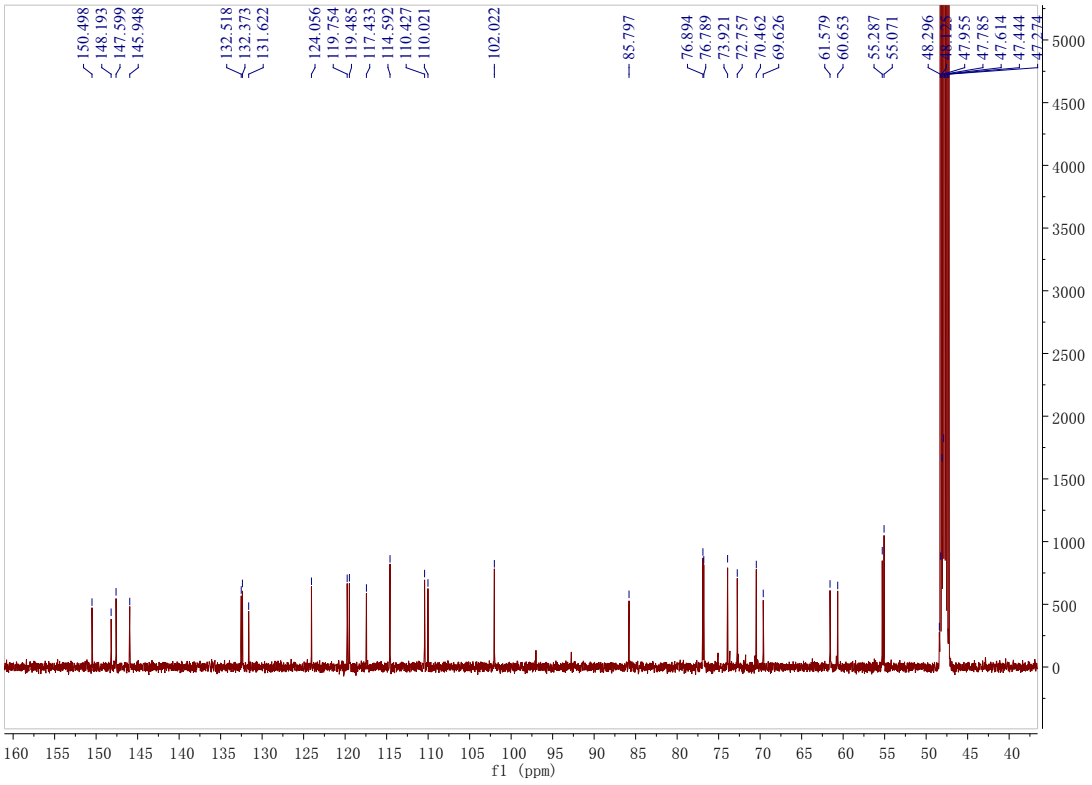


Figure S31. The ^{13}C-NMR spectrum of A-2 in CD_3OD

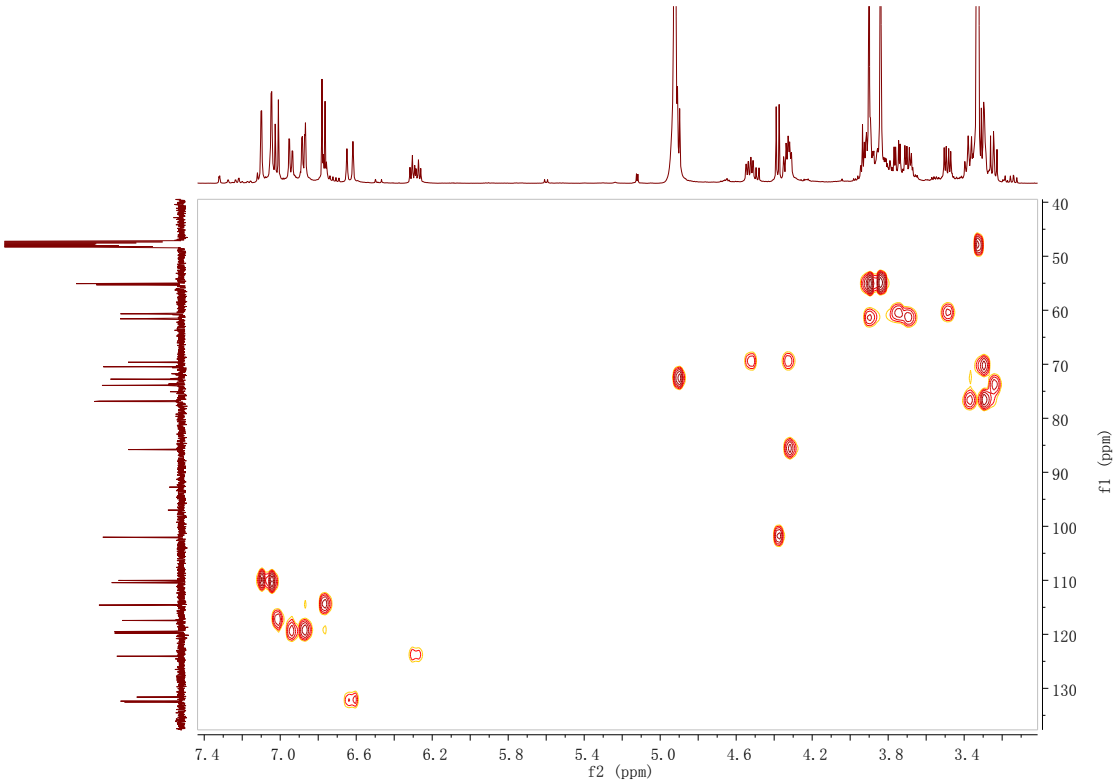


Figure S32. The HSQC spectrum of A-2 in CD_3OD

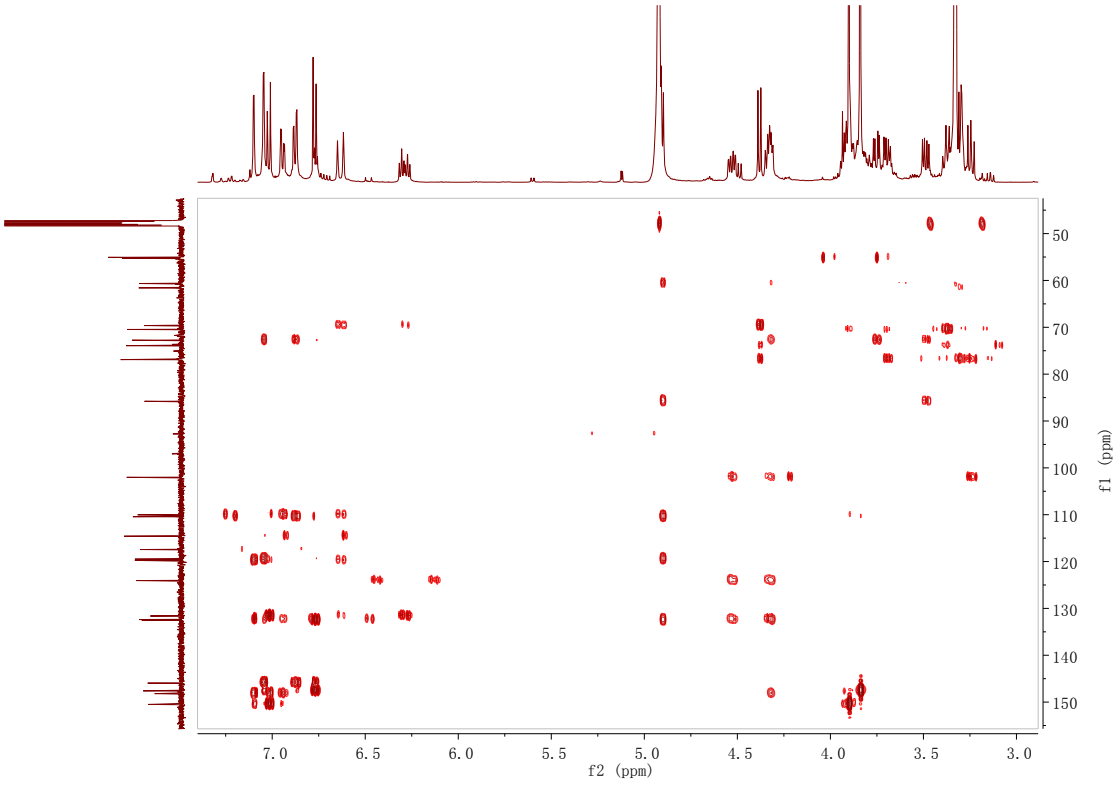


Figure S33. The HMBC spectrum of A-2 in CD_3OD

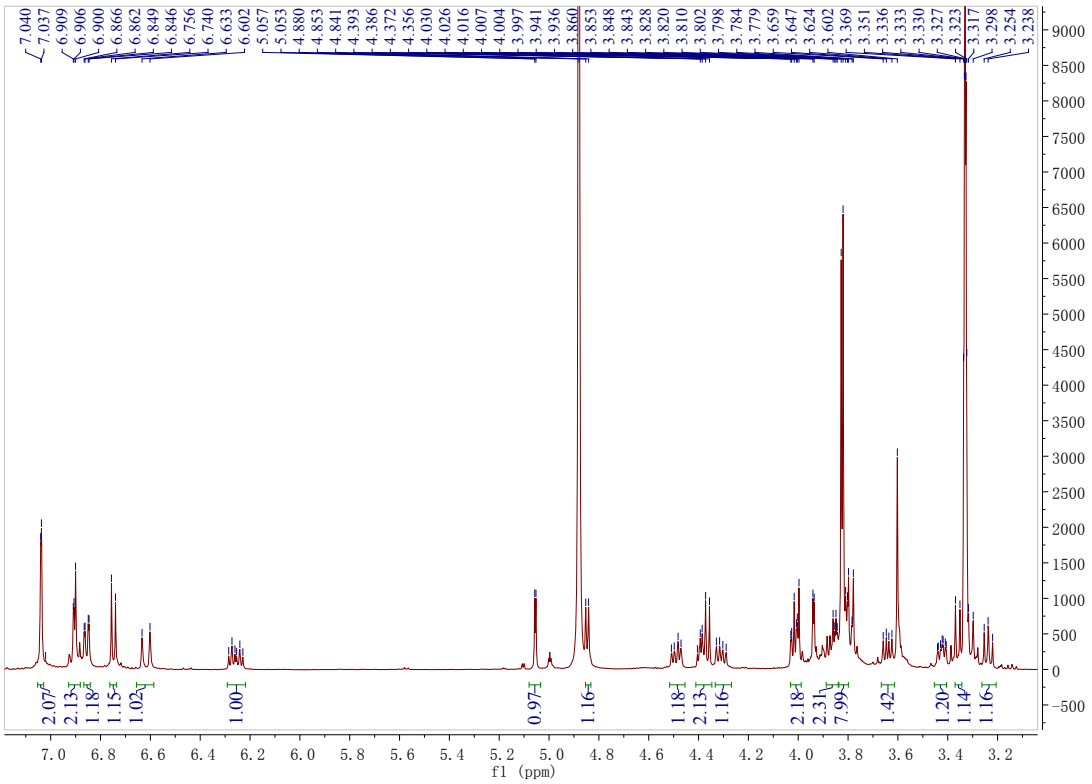


Figure S34. The ^{1}H-NMR spectrum of A-3 in CD_3OD

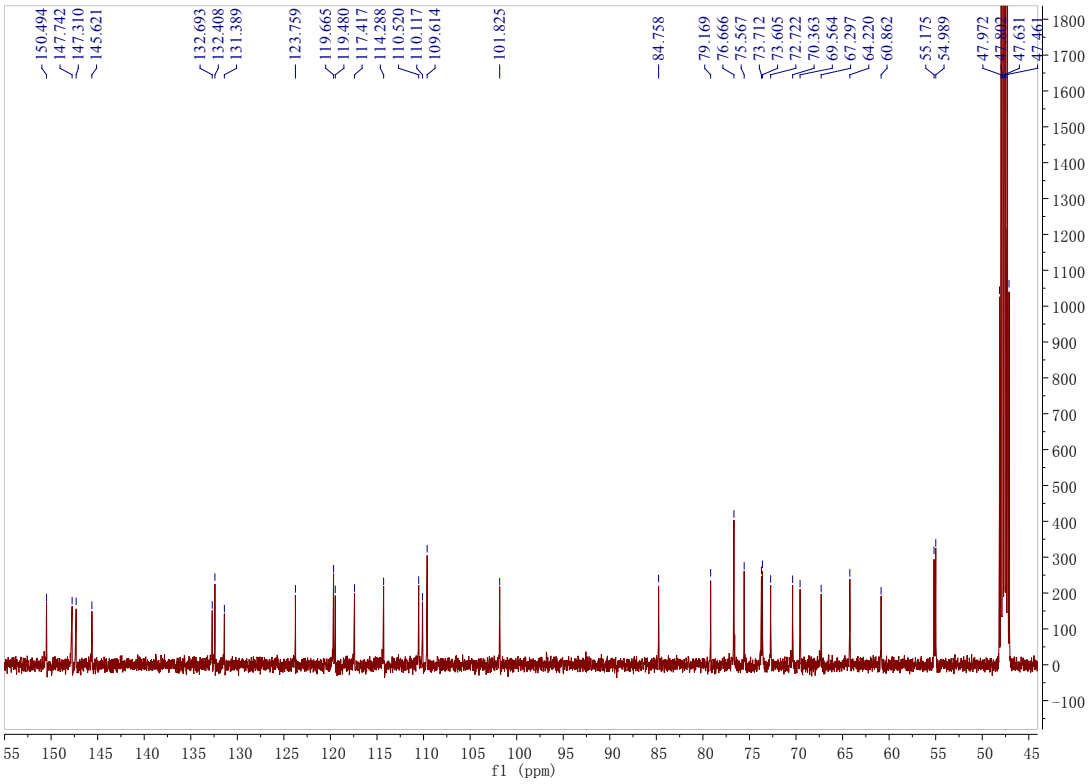


Figure S35. The ^{13}C-NMR spectrum of A-3 in CD_3OD

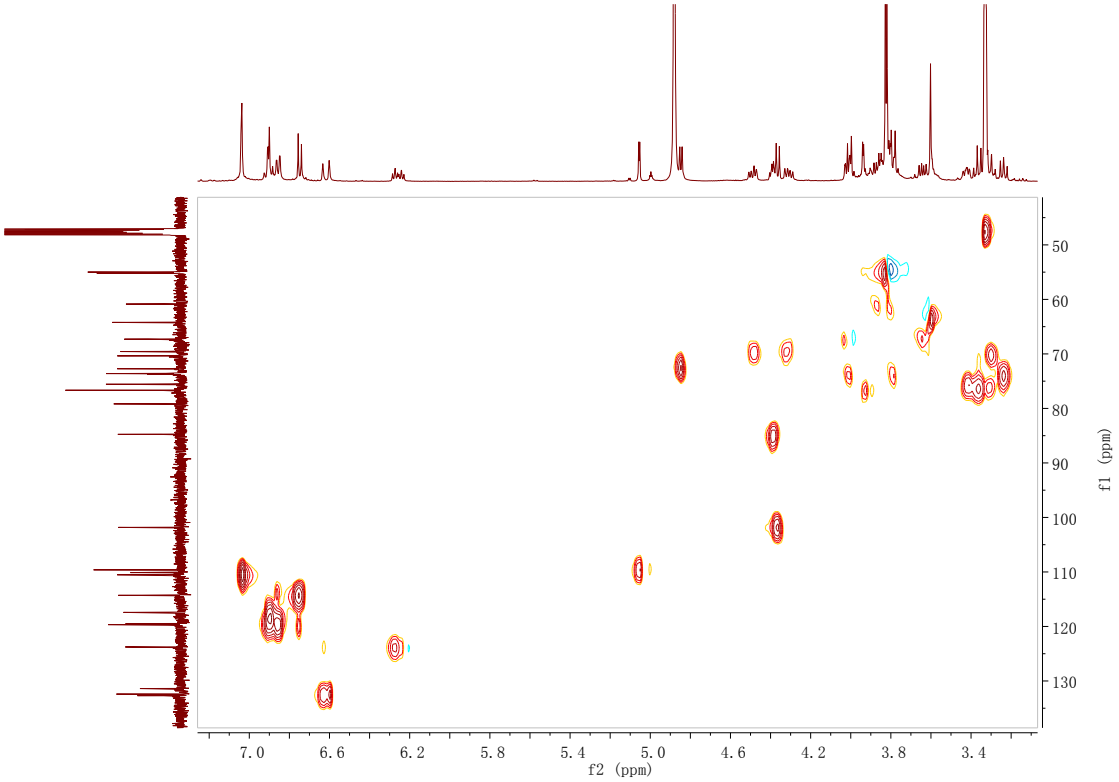


Figure S36. The HSQC spectrum of A-3 in CD_3OD

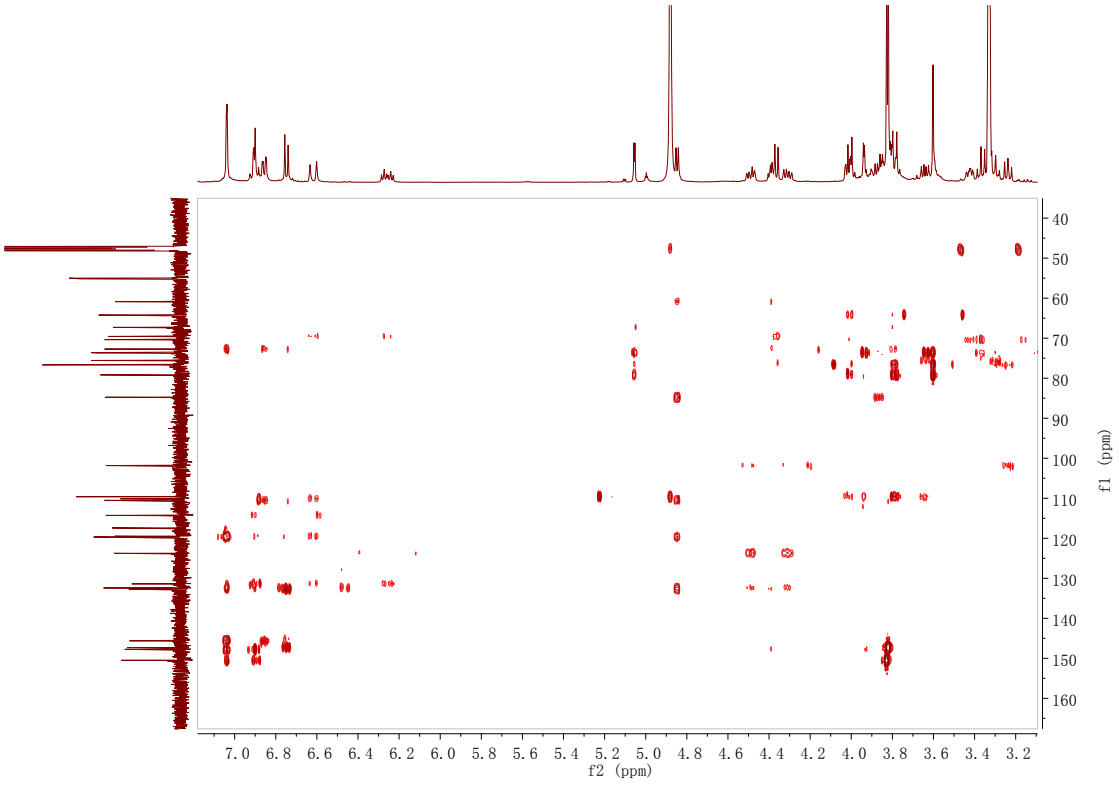


Figure S37. The HMBC spectrum of A-3 in CD_3OD

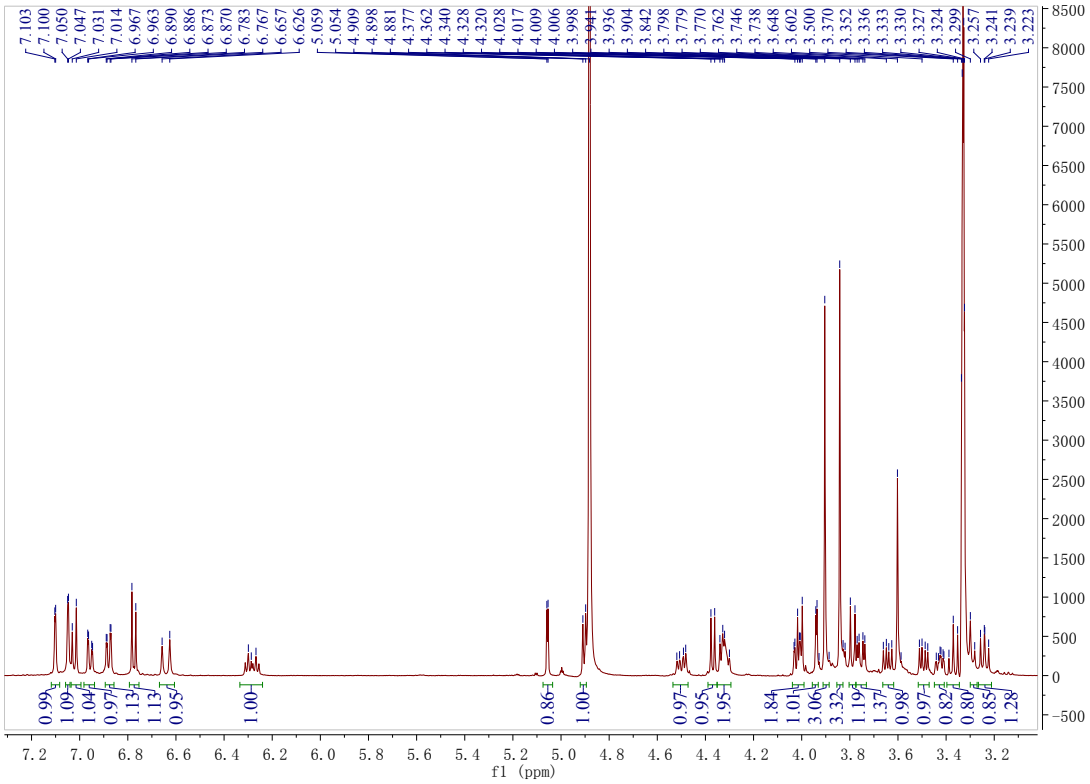


Figure S38. The ^{1}H-NMR spectrum of A-4 in CD_3OD

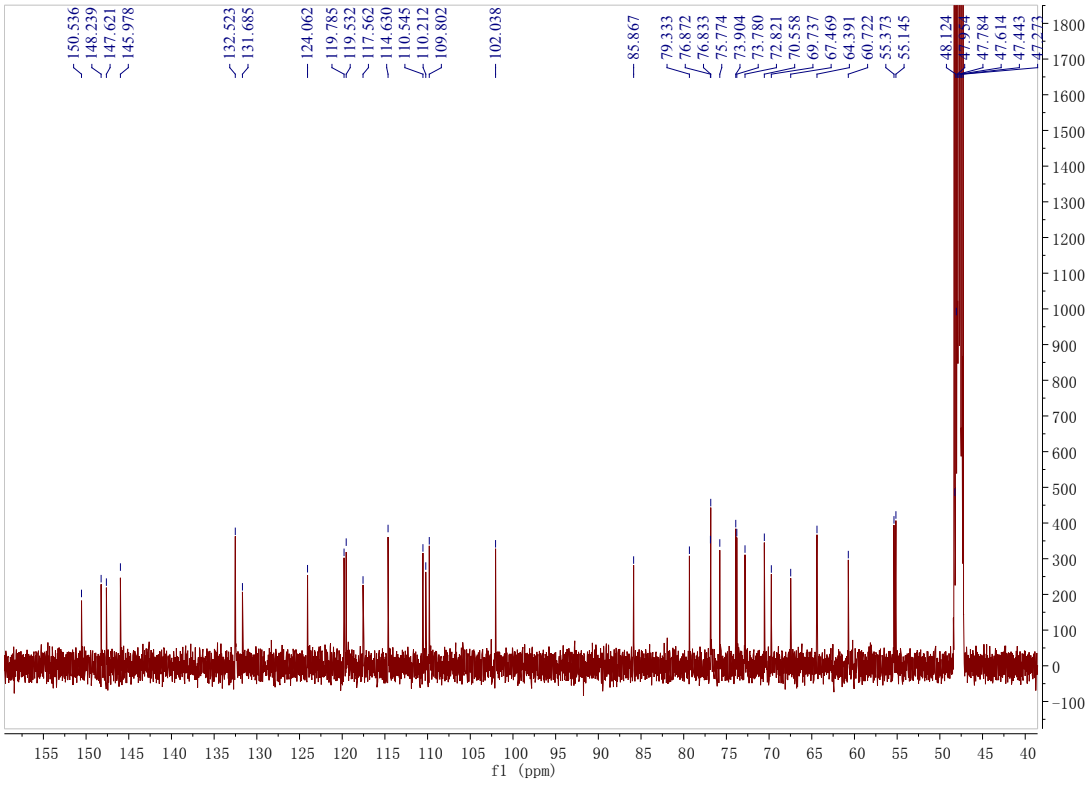


Figure S39. The ^{13}C-NMR spectrum of A-4 in CD_3OD

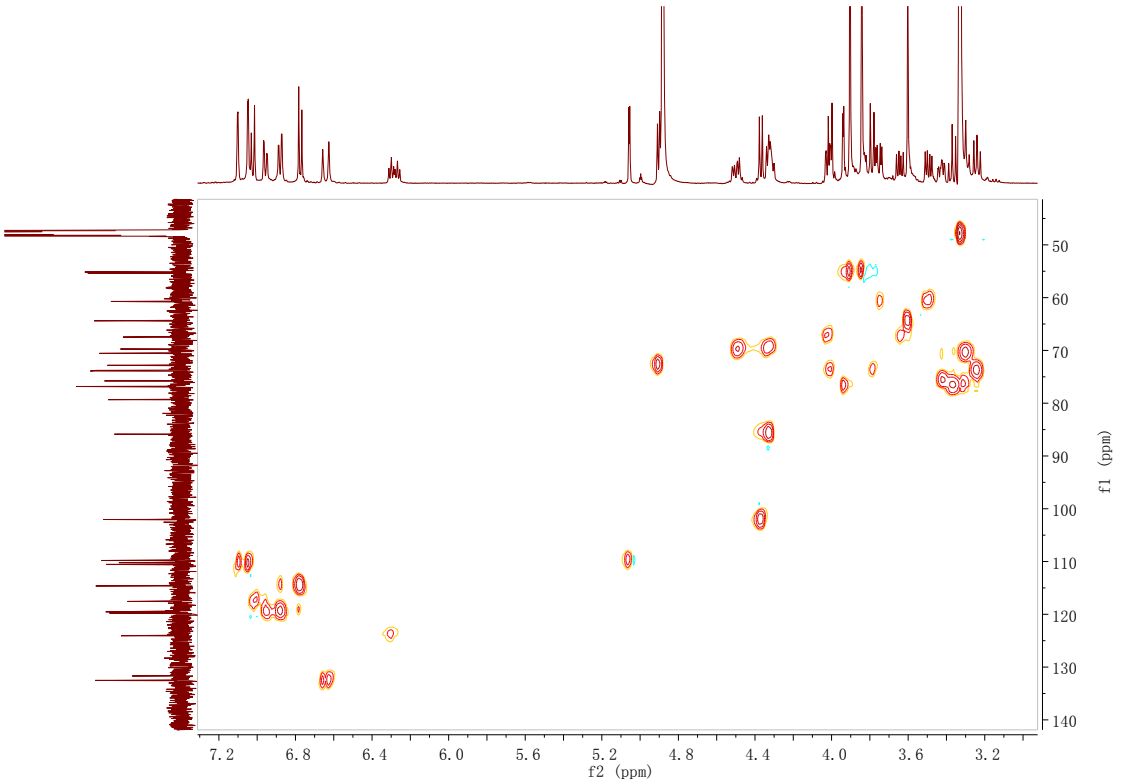


Figure S40. The HSQC spectrum of A-4 in CD_3OD

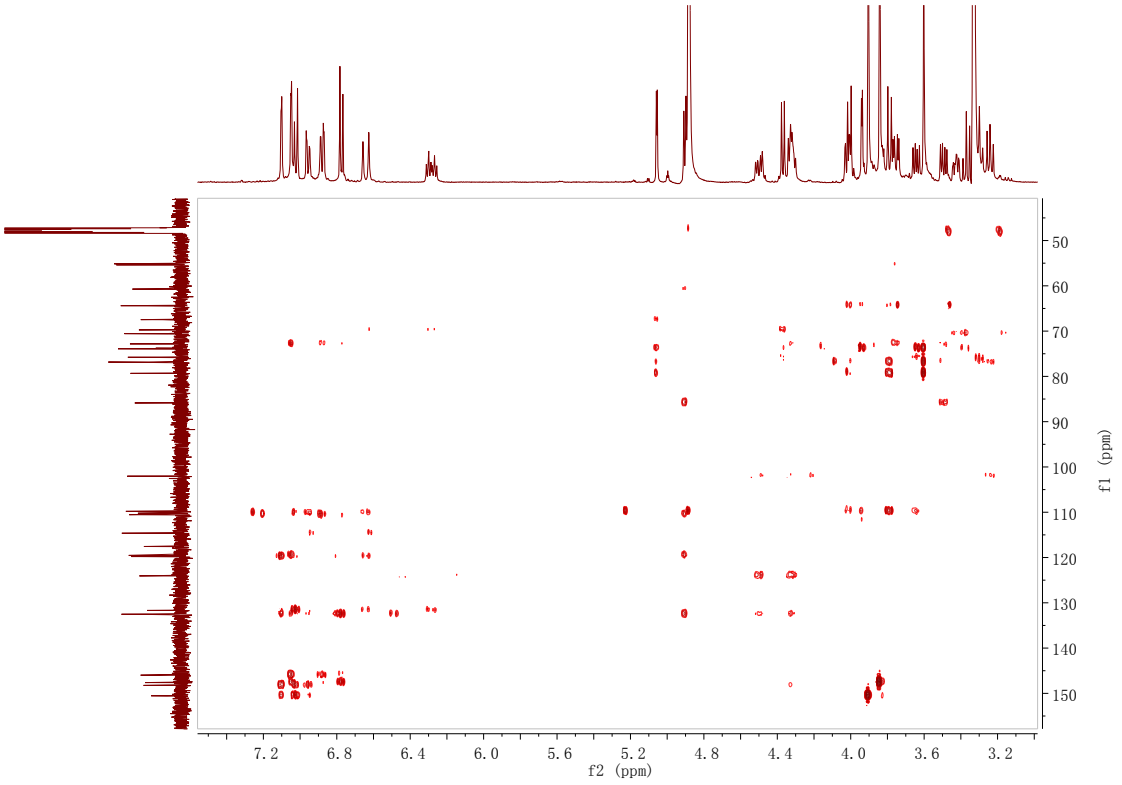


Figure S41. The HMBC spectrum of A-4 in CD_3OD

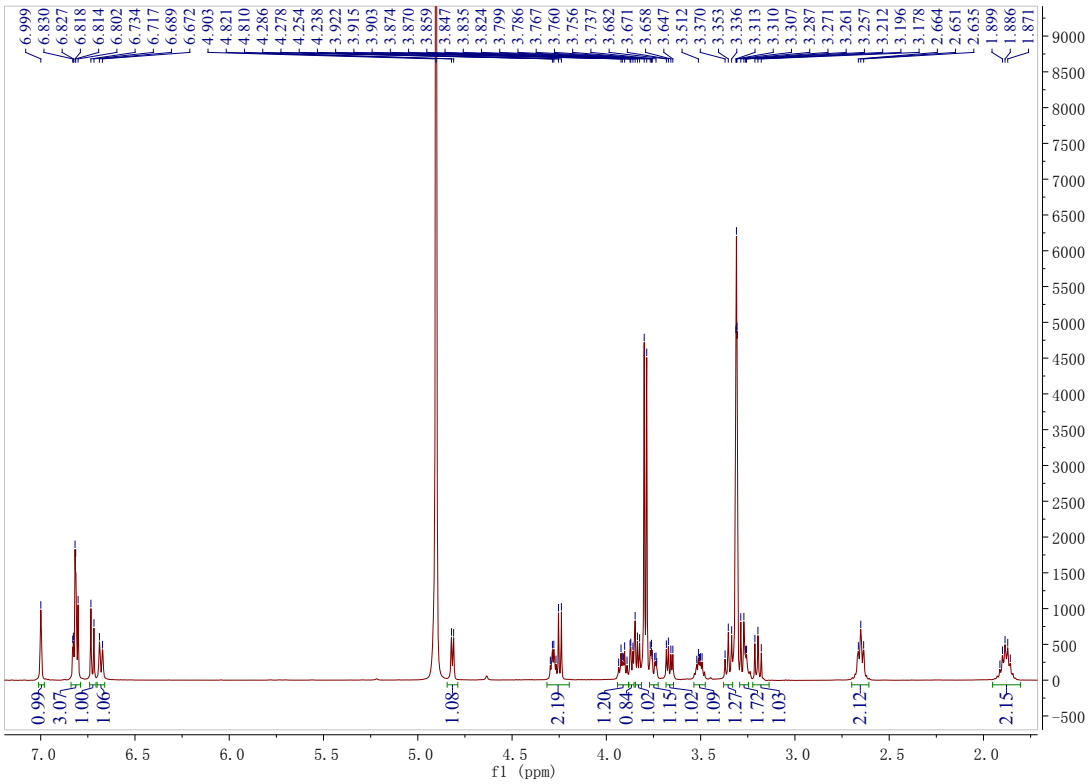


Figure S42. The ^{1}H-NMR spectrum of A-5 in CD_3OD

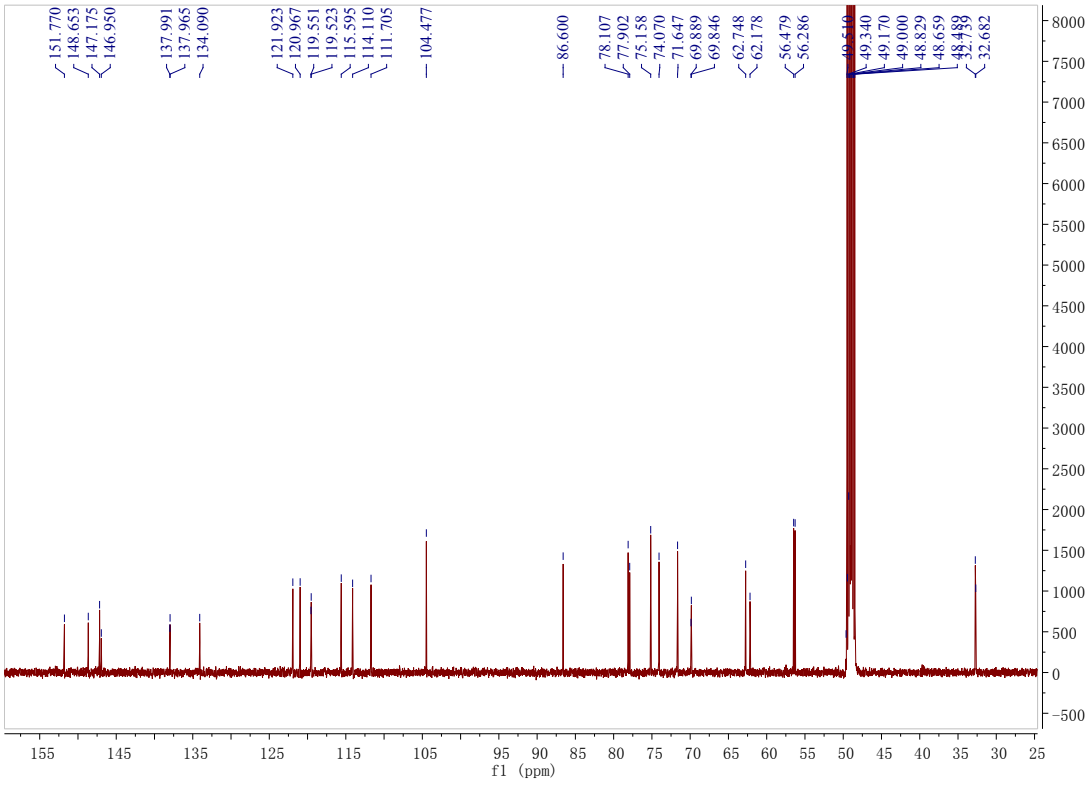


Figure S43. The ^{13}C-NMR spectrum of A-5 in CD_3OD

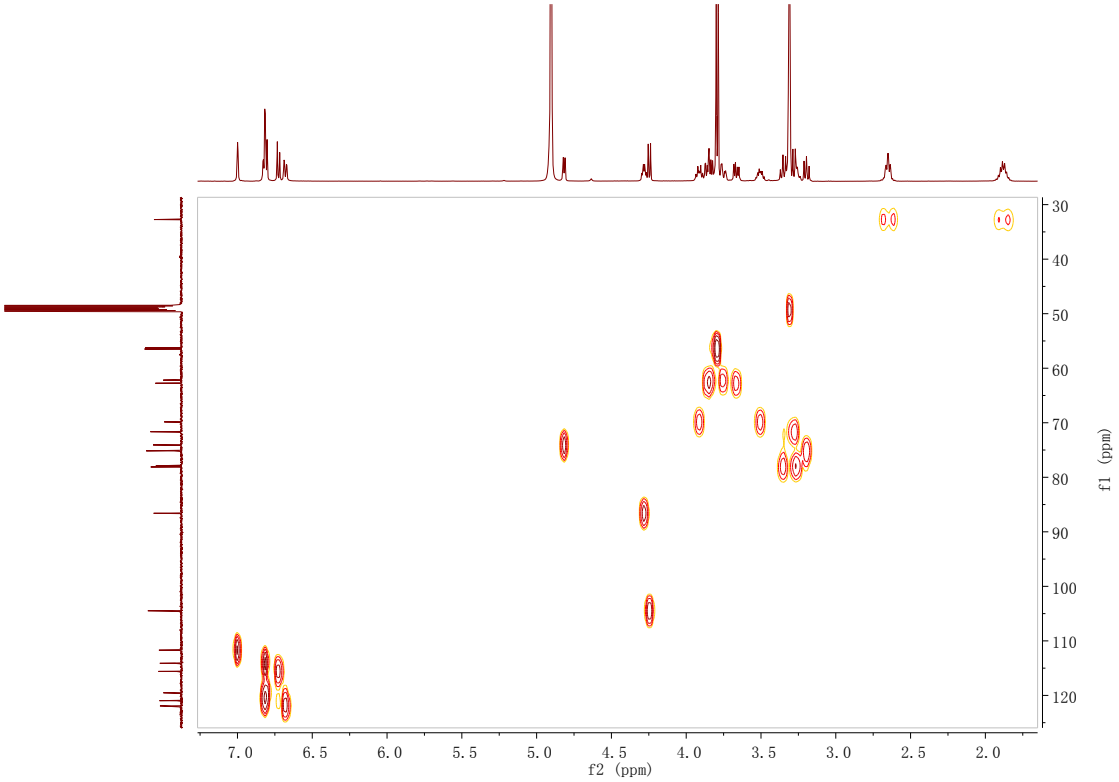


Figure S44. The HSQC spectrum of A-5 in CD_3OD

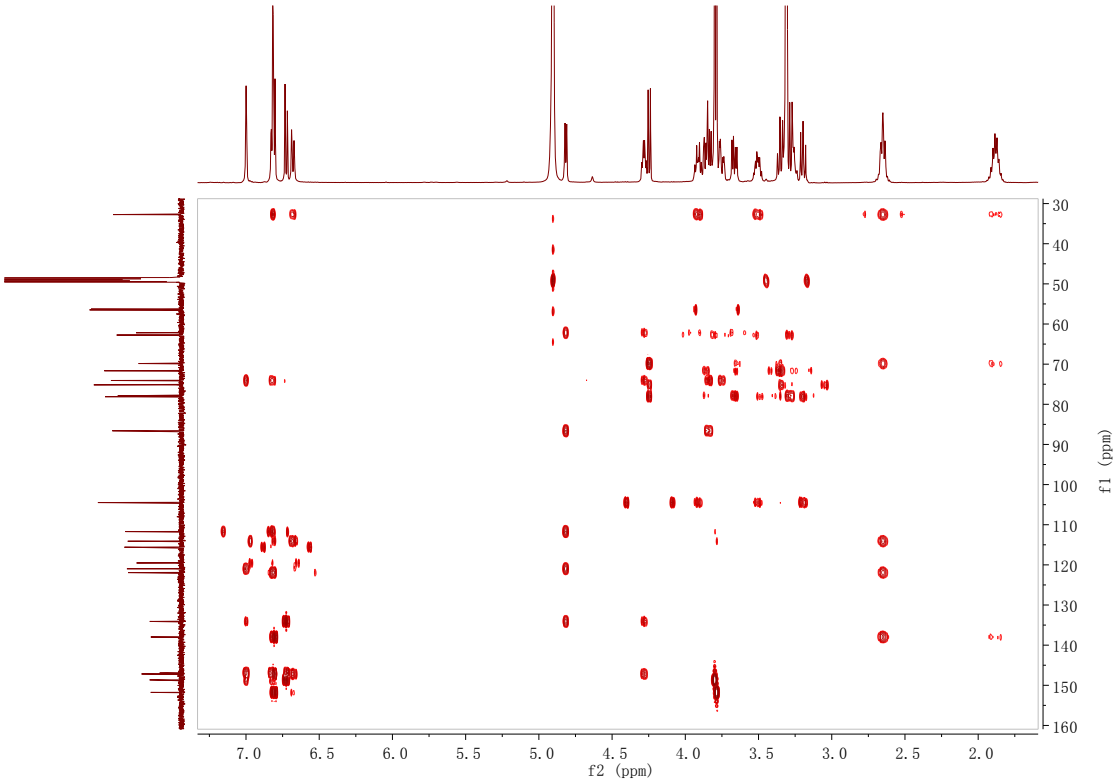


Figure S45. The HMBC spectrum of A-5 in CD_3OD

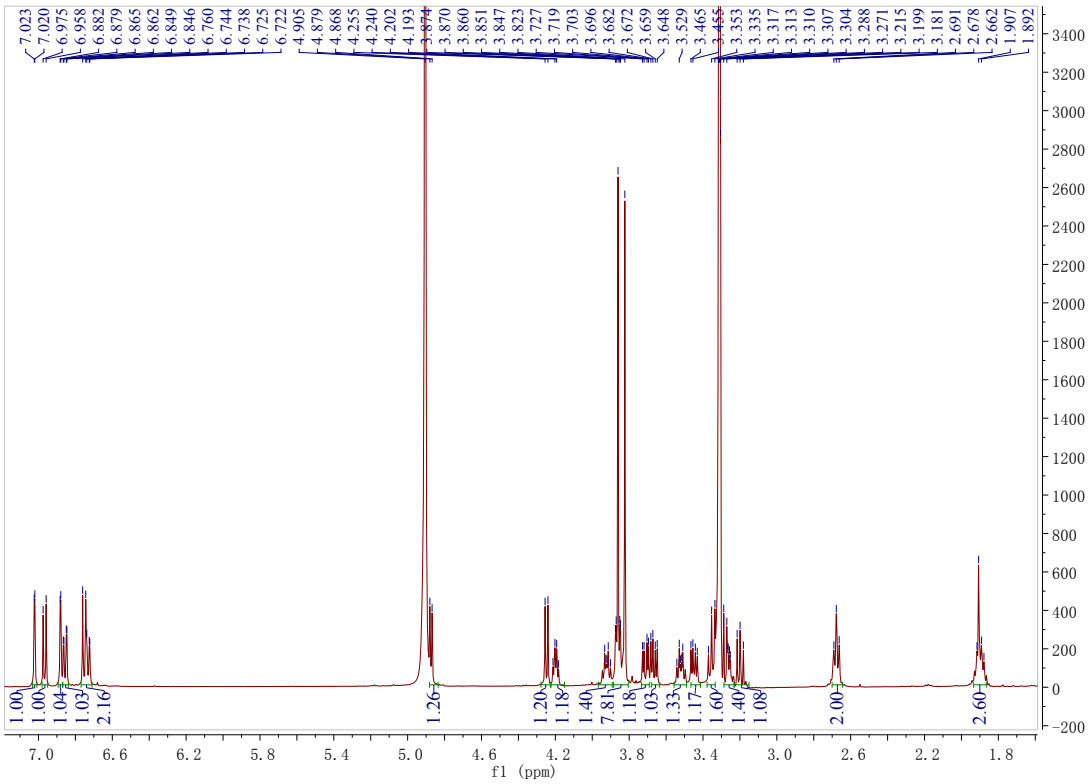


Figure S46. The ^{1}H-NMR spectrum of A-6 in CD_3OD

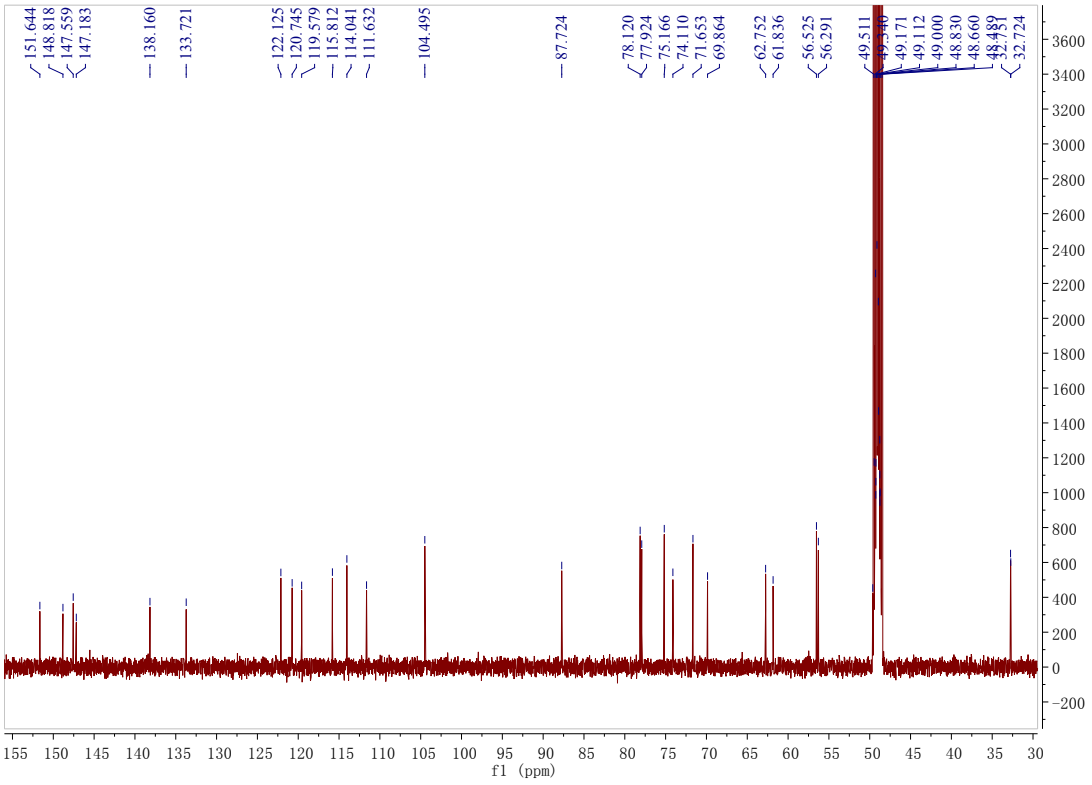


Figure S47. The ^{13}C-NMR spectrum of A-6 in CD_3OD

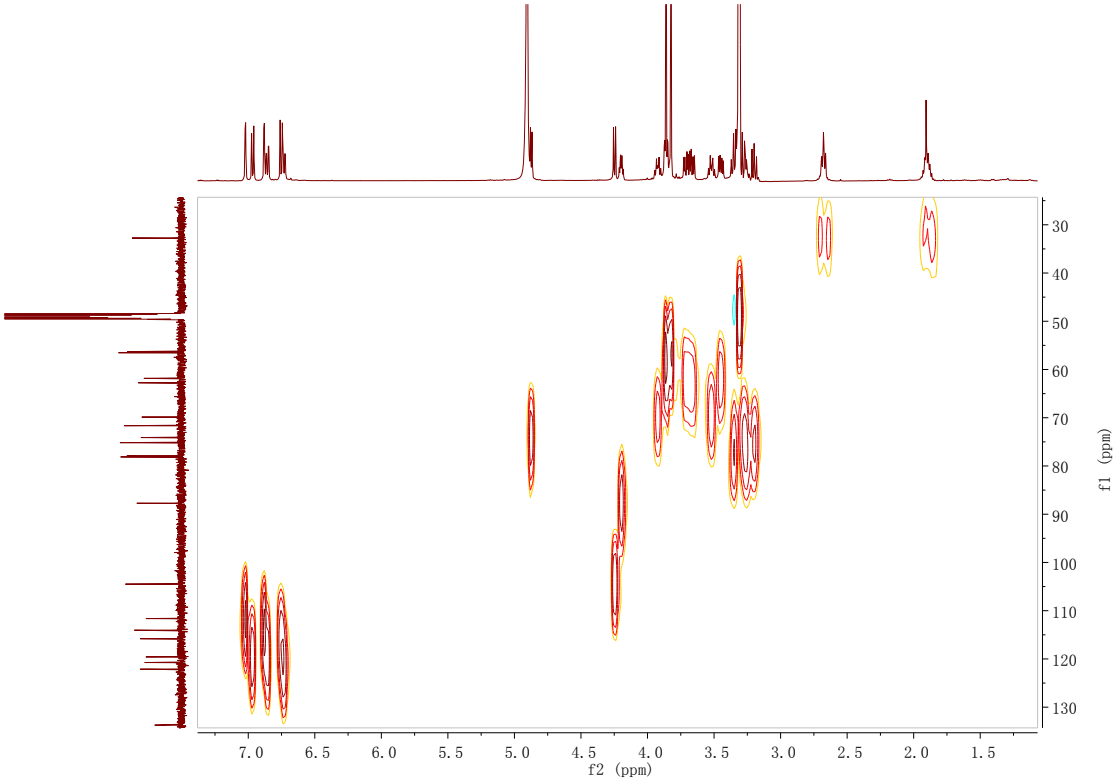


Figure S48. The HSQC spectrum of A-6 in CD_3OD

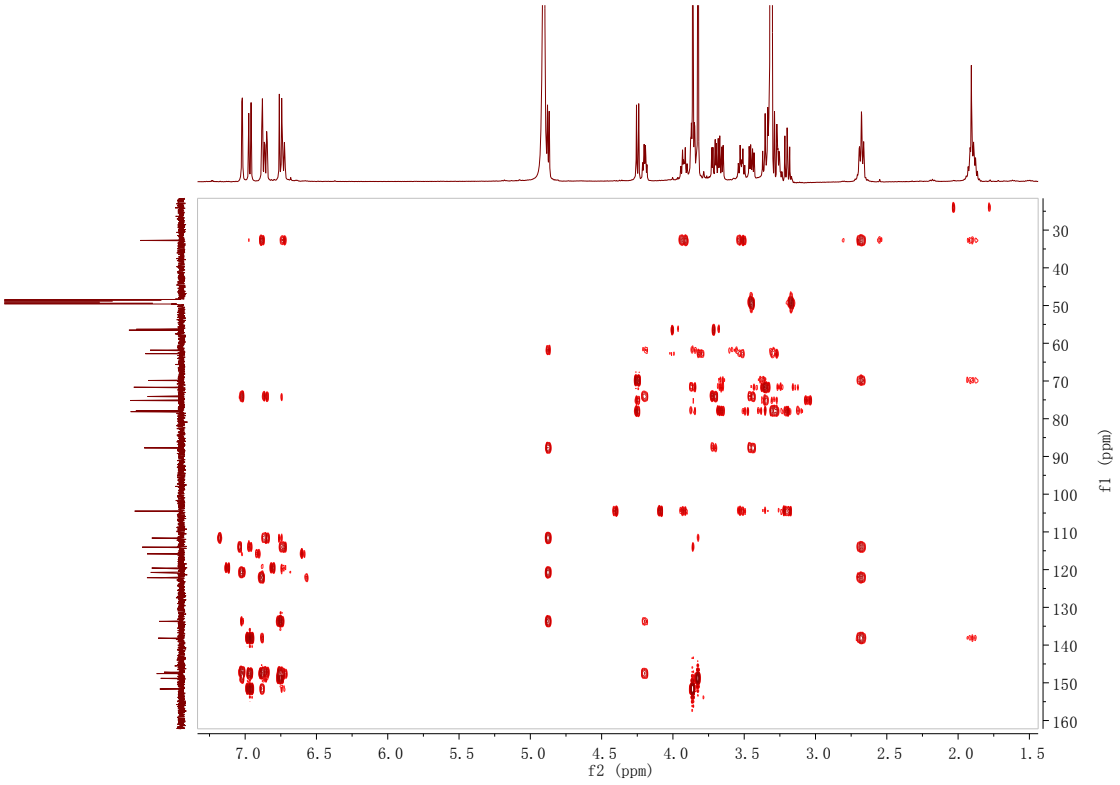


Figure S49. The HMBC spectrum of A-6 in CD_3OD

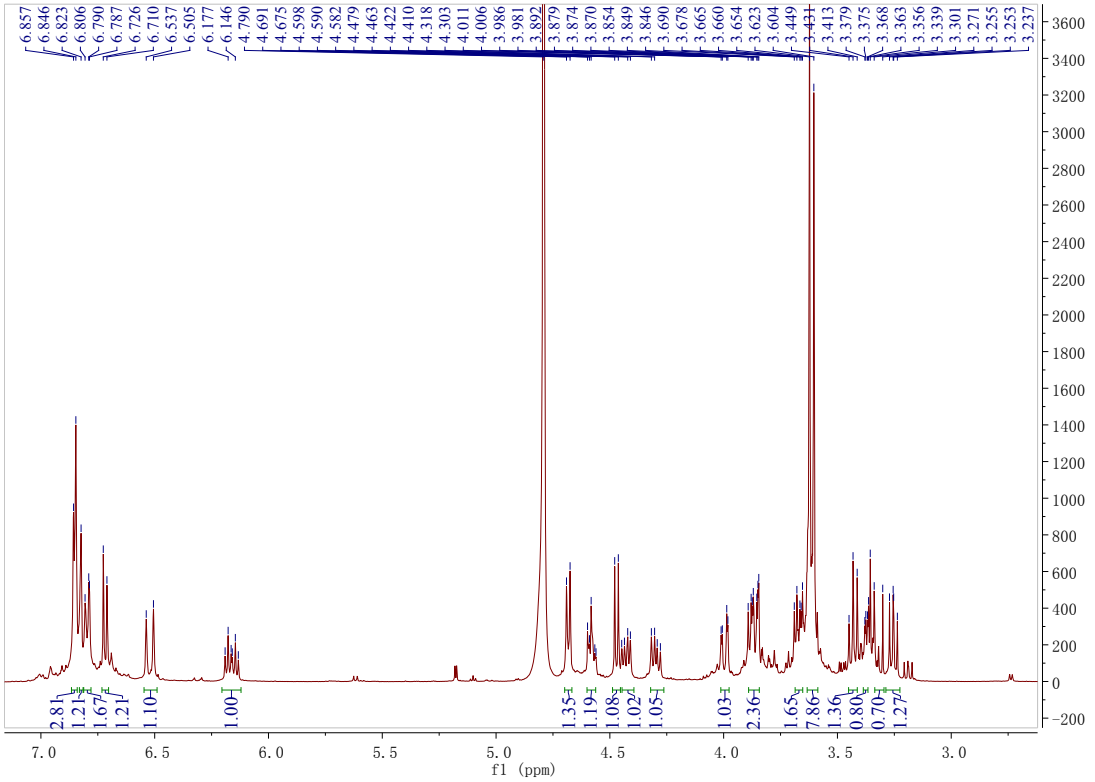


Figure S50. The ^{1}H-NMR spectrum of A-1 in D_2O

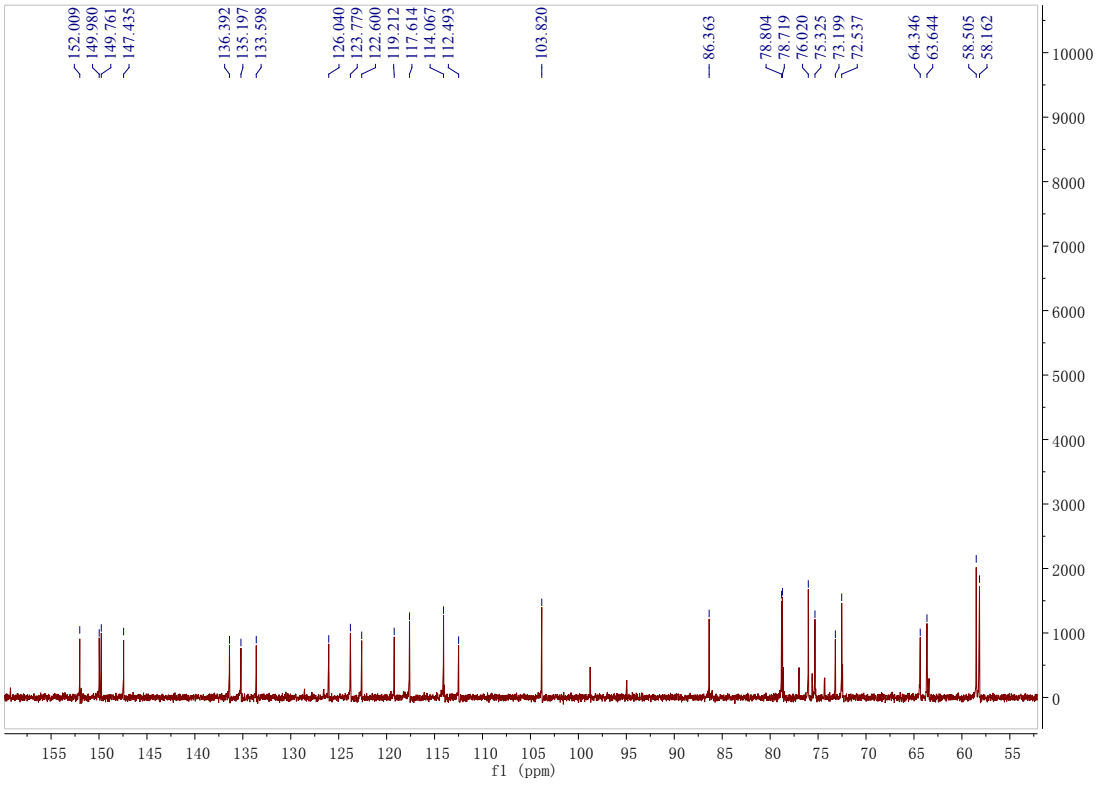


Figure S51. The ^{13}H-NMR spectrum of A-1 in D_2O

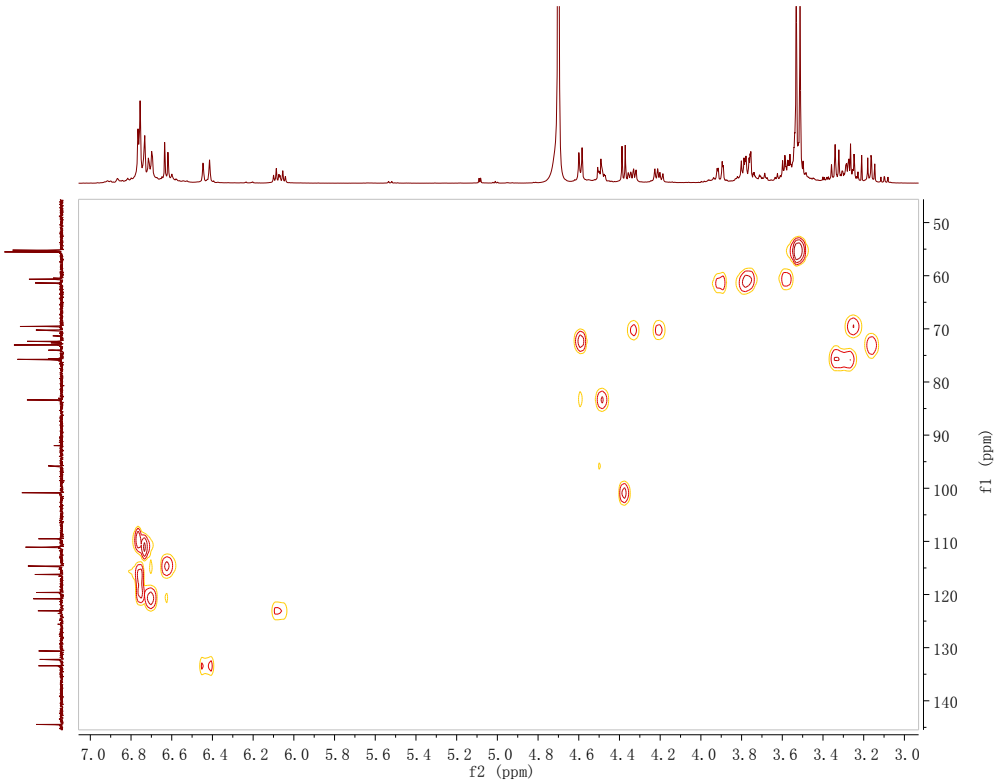


Figure S52. The HSQC spectrum of A-1 in D_2O

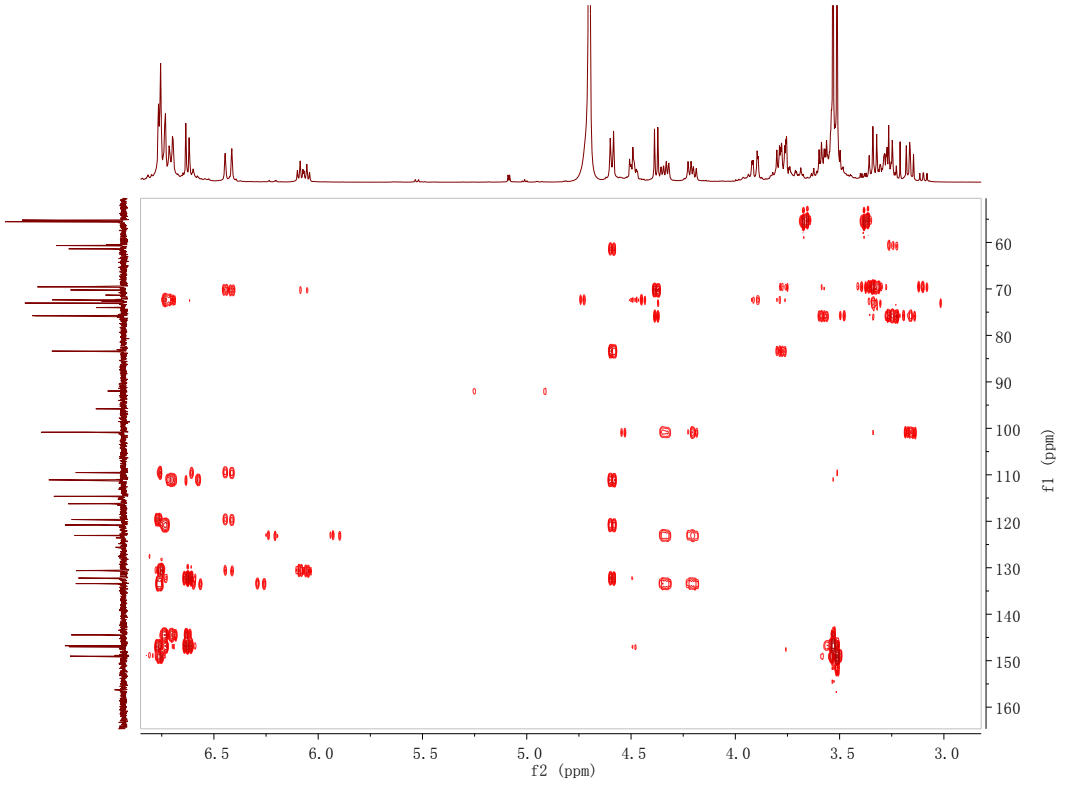


Figure S53. The HMBC spectrum of A-1 in D_2O

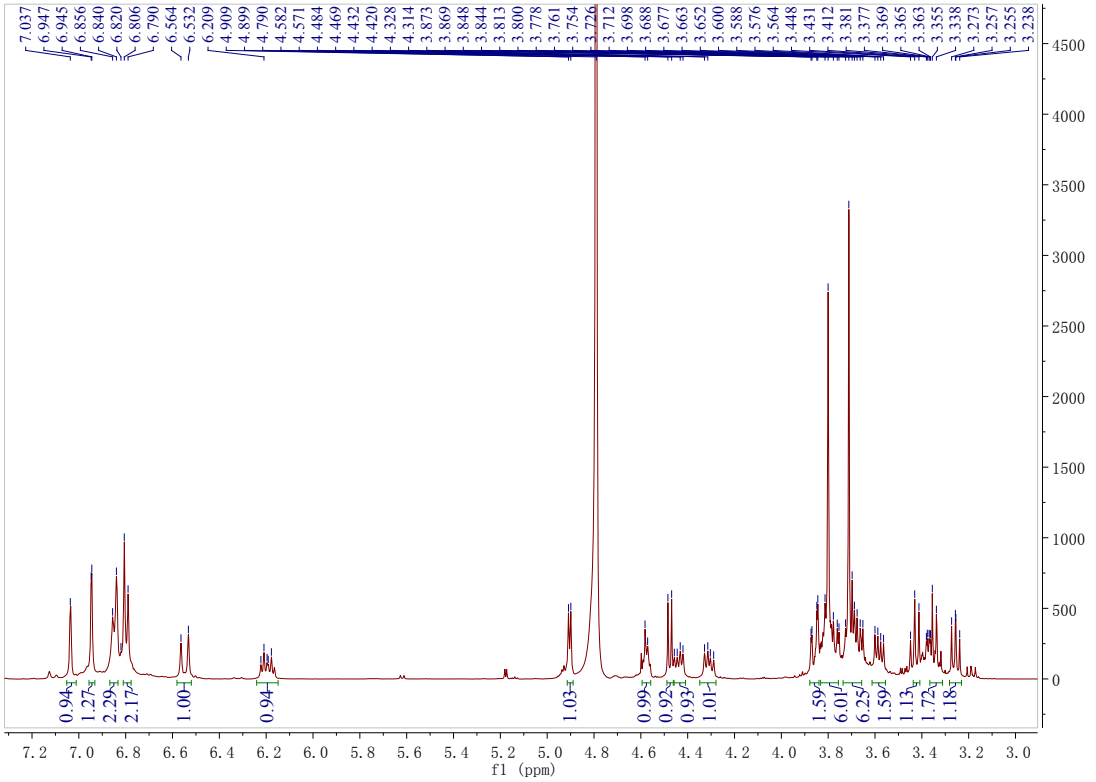


Figure S54. The ^{1}H-NMR spectrum of A-2 in D_2O

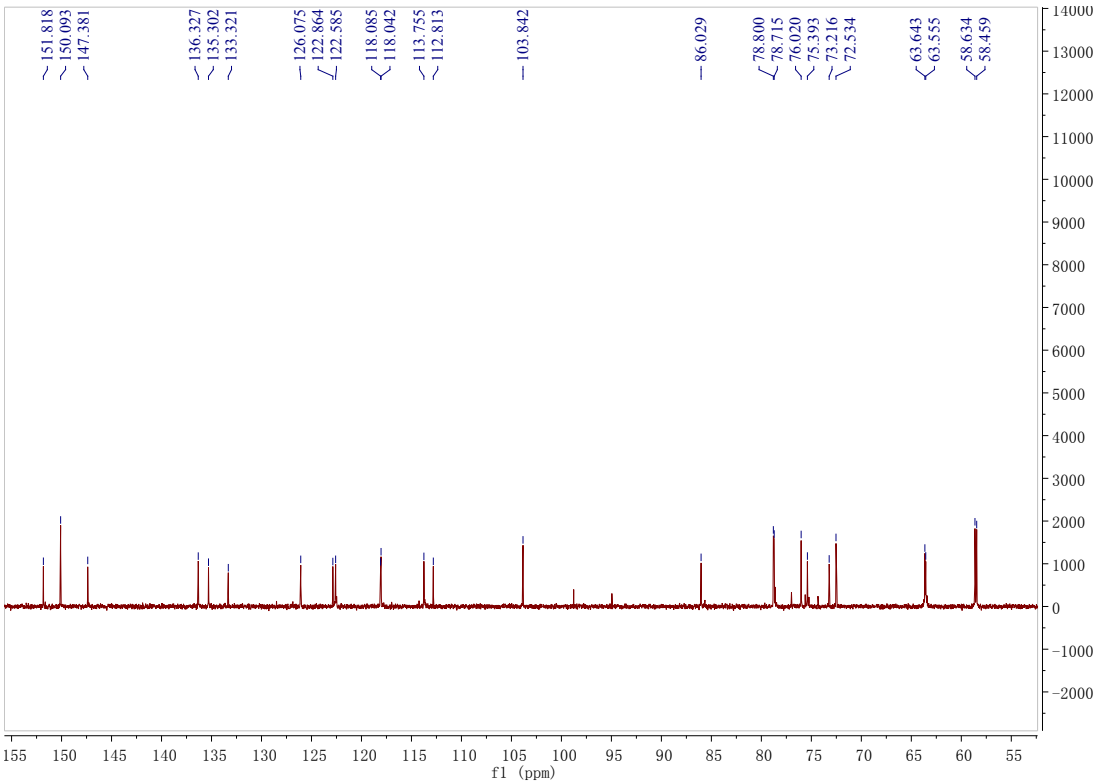


Figure S55. The ^{13}C-NMR spectrum of A-2 in D_2O

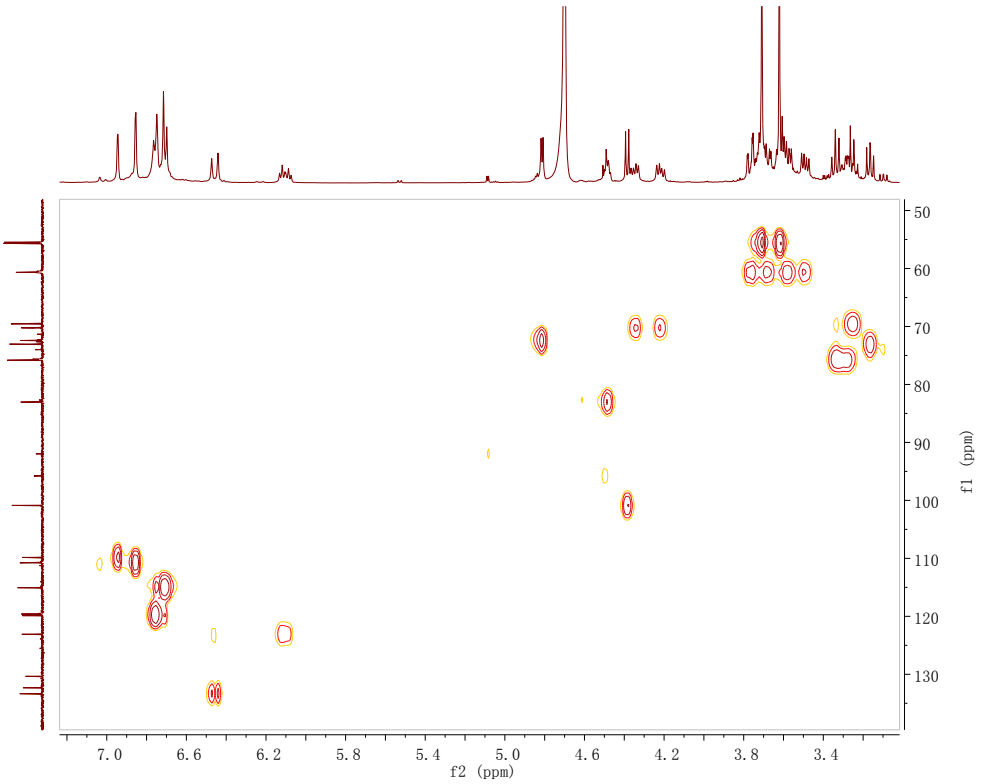


Figure S56. The HSQC spectrum of A-2 in D_2O

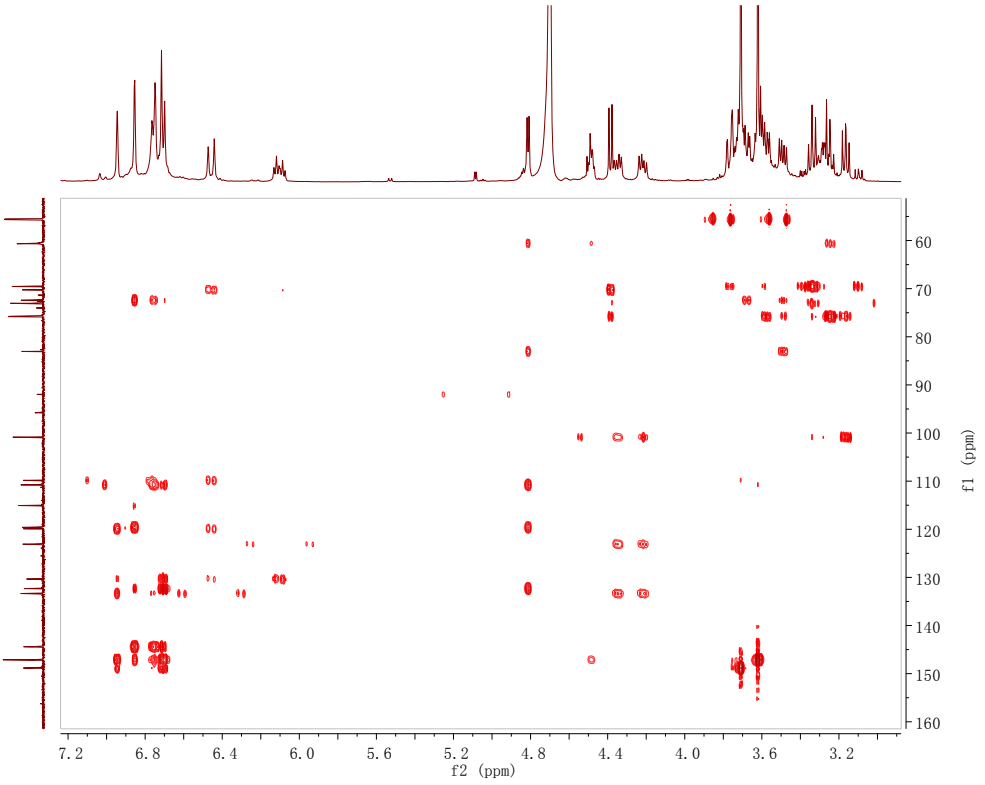


Figure S57. The HMBC spectrum of A-2 in D_2O

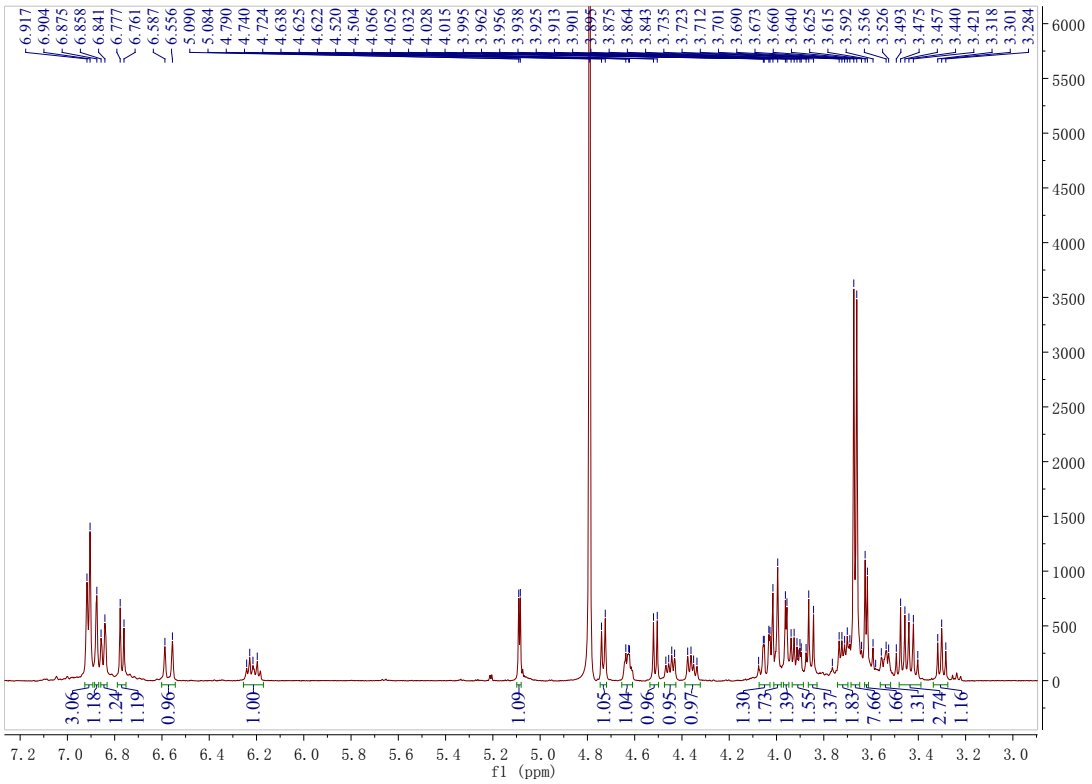


Figure S58. The ^{1}H-NMR spectrum of A-3 in D_2O

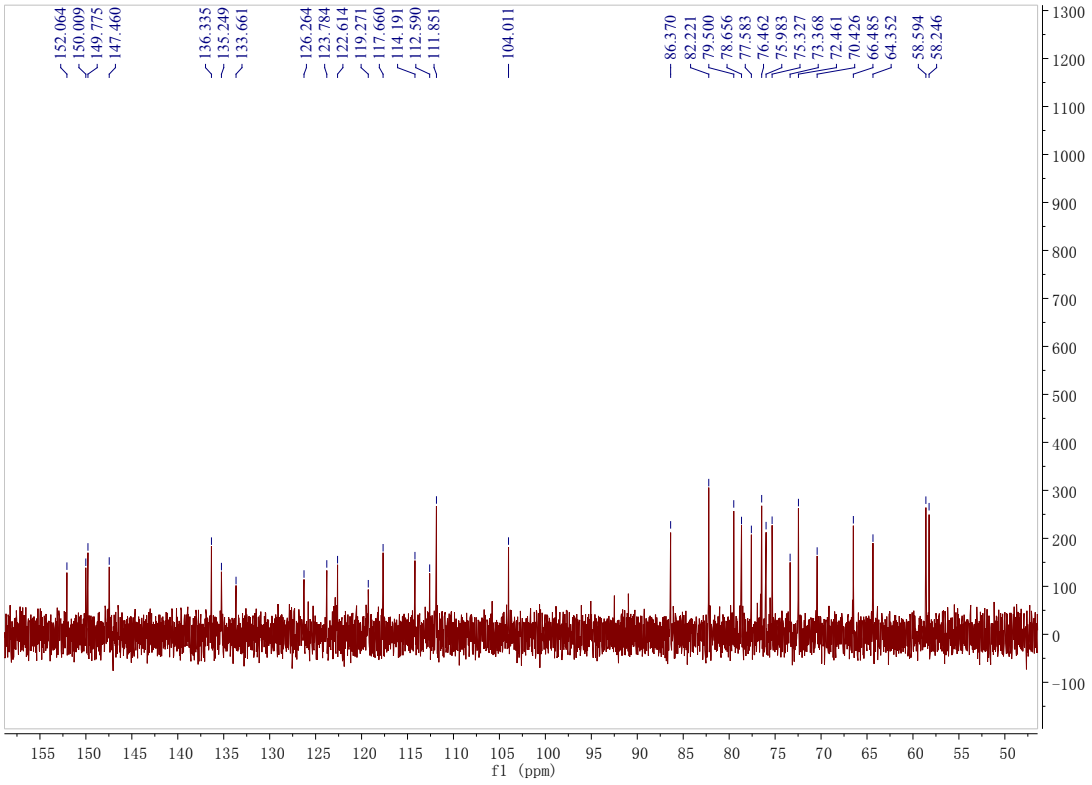


Figure S59. The ^{13}C-NMR spectrum of A-3 in D_2O

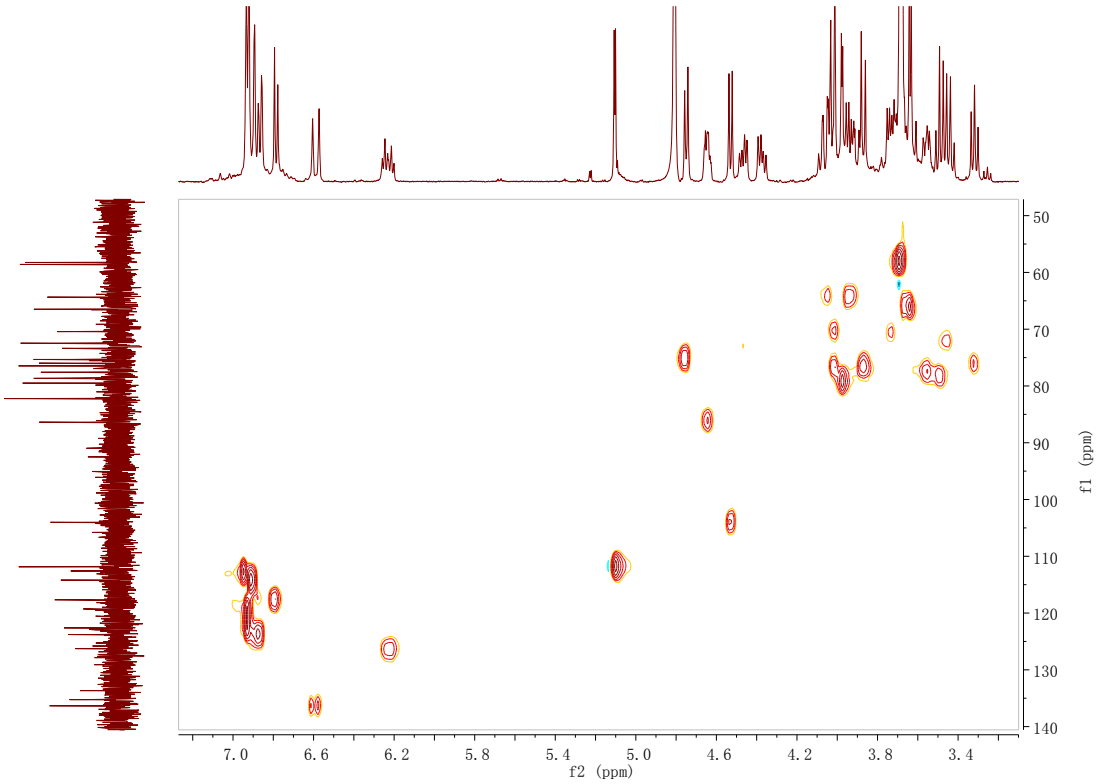


Figure S60. The HSQC spectrum of A-3 in D_2O

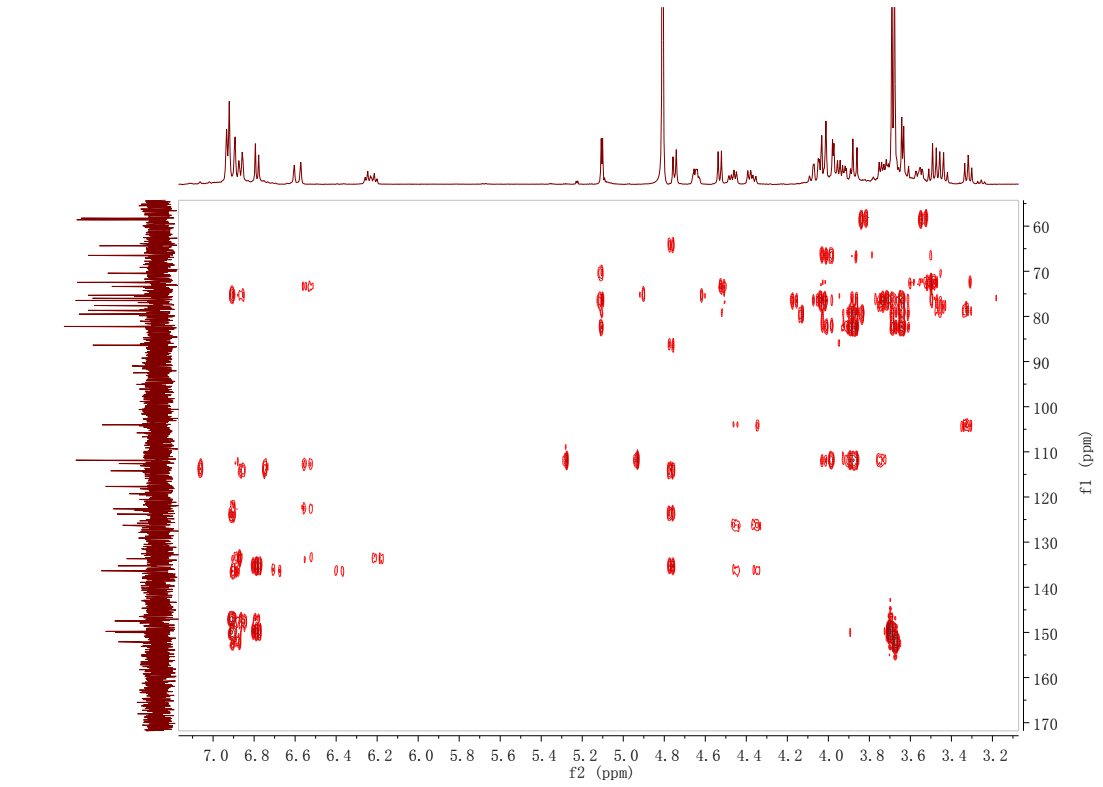


Figure S61. The HMBC spectrum of A-3 in D_2O

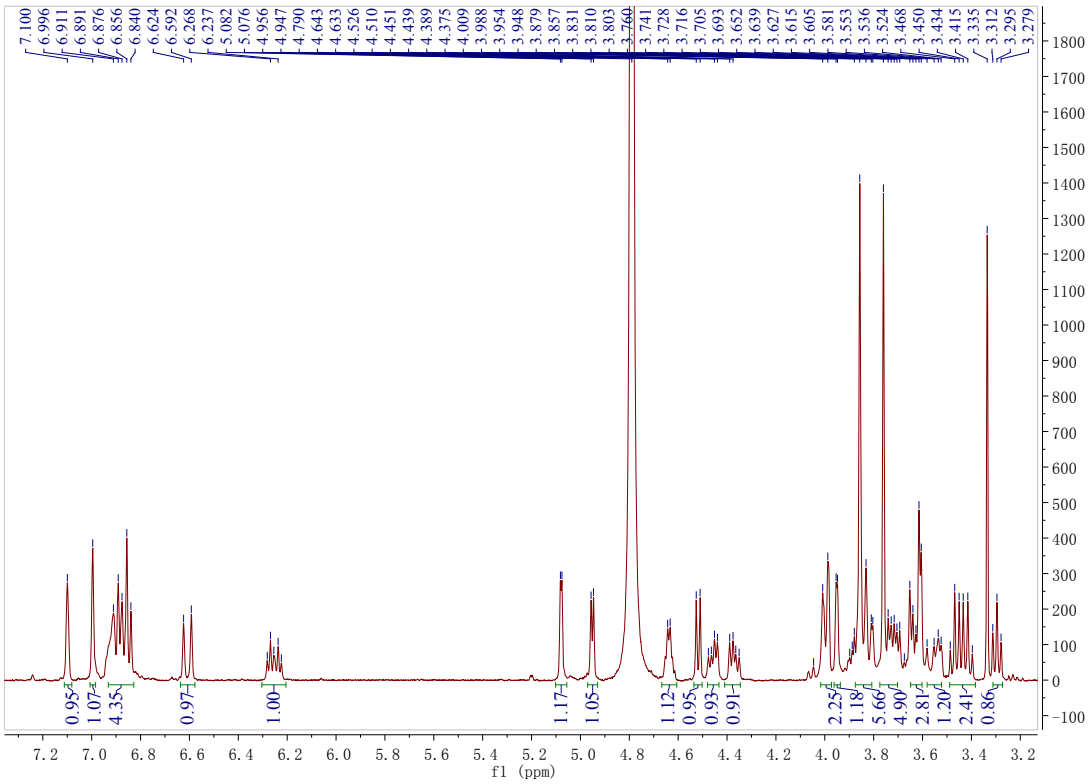


Figure S62. The ^{1}H-NMR spectrum of A-4 in D_2O

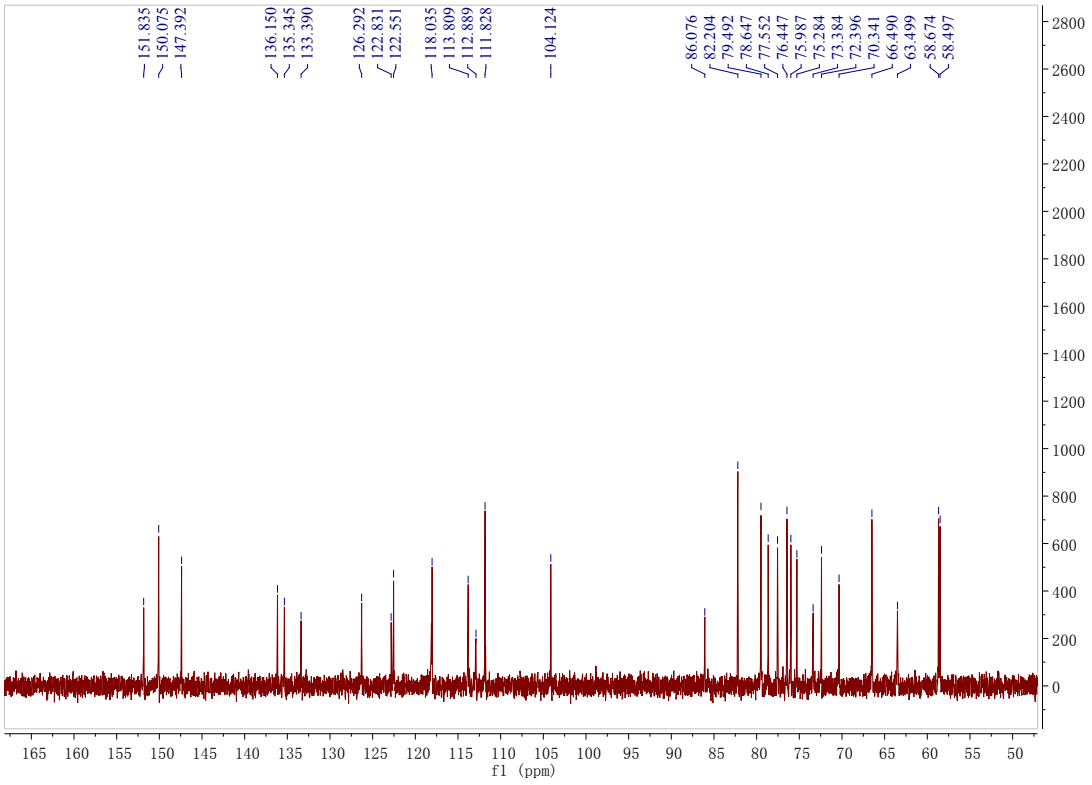


Figure S63. The ^{13}C-NMR spectrum of A-4 in D_2O

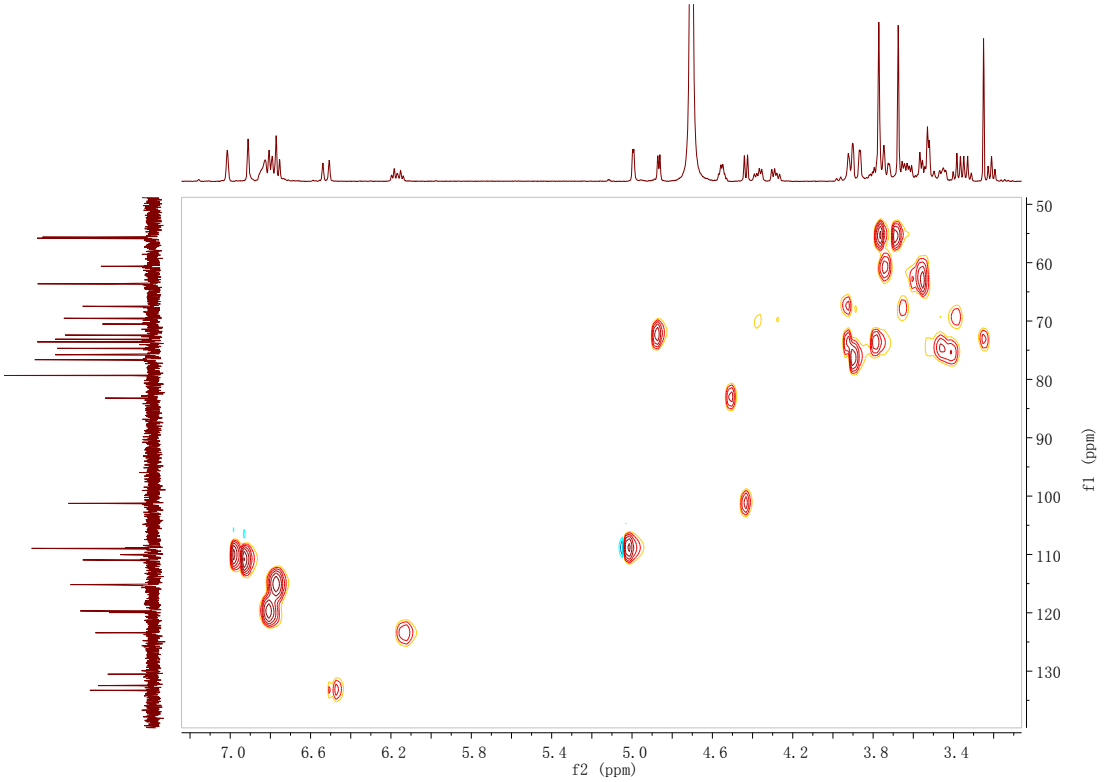


Figure S64. The HSQC spectrum of A-4 in D_2O

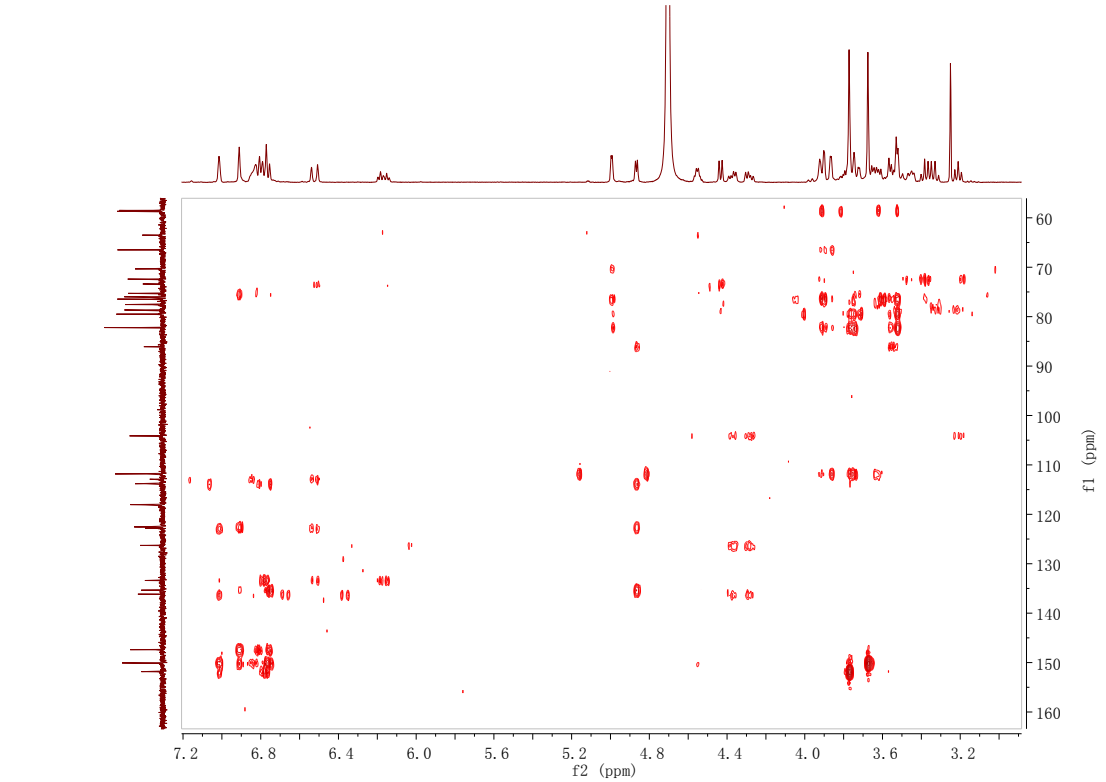


Figure S65. The HMBC spectrum of A-4 in D_2O

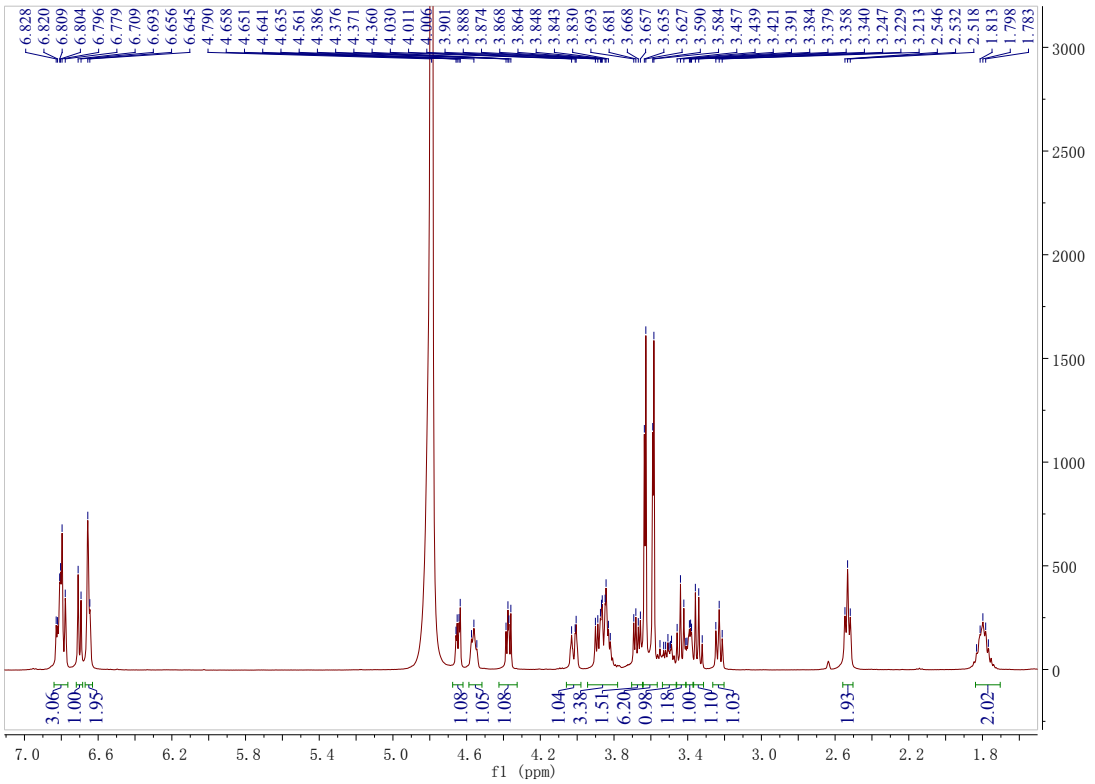


Figure S66. The ^{1}H-NMR spectrum of A-5 in D_2O

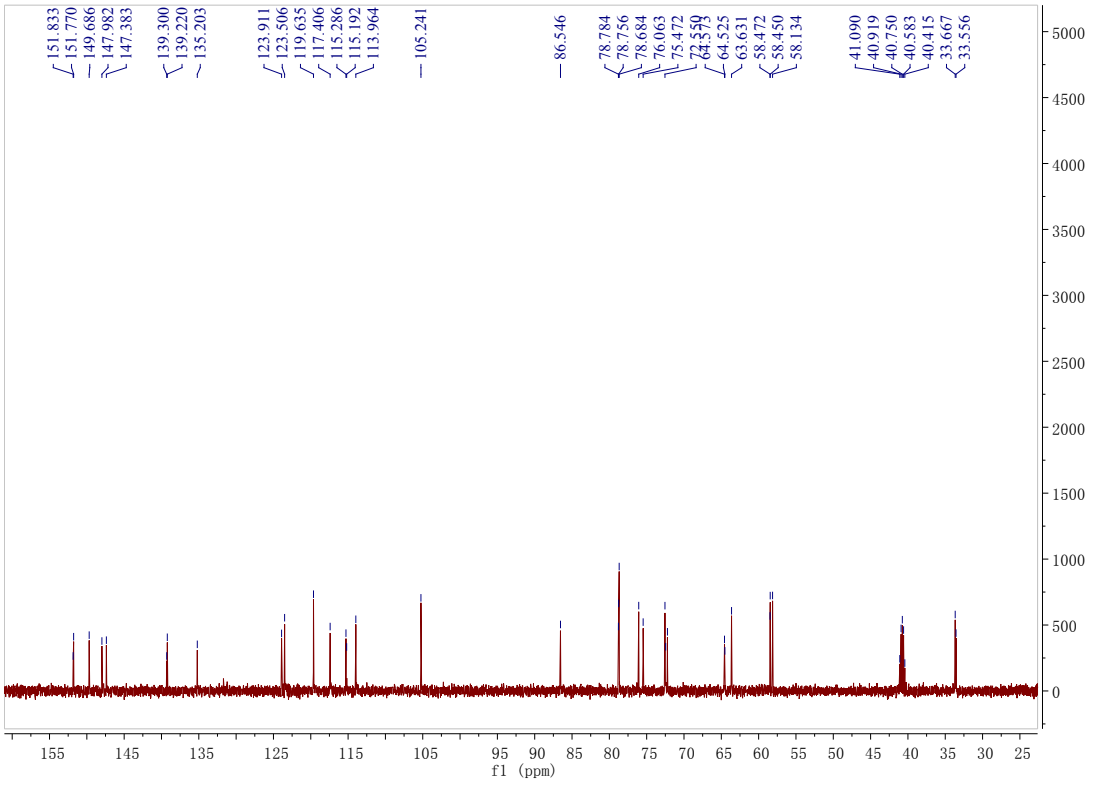


Figure S67. The ^{13}C-NMR spectrum of A-5 in D_2O

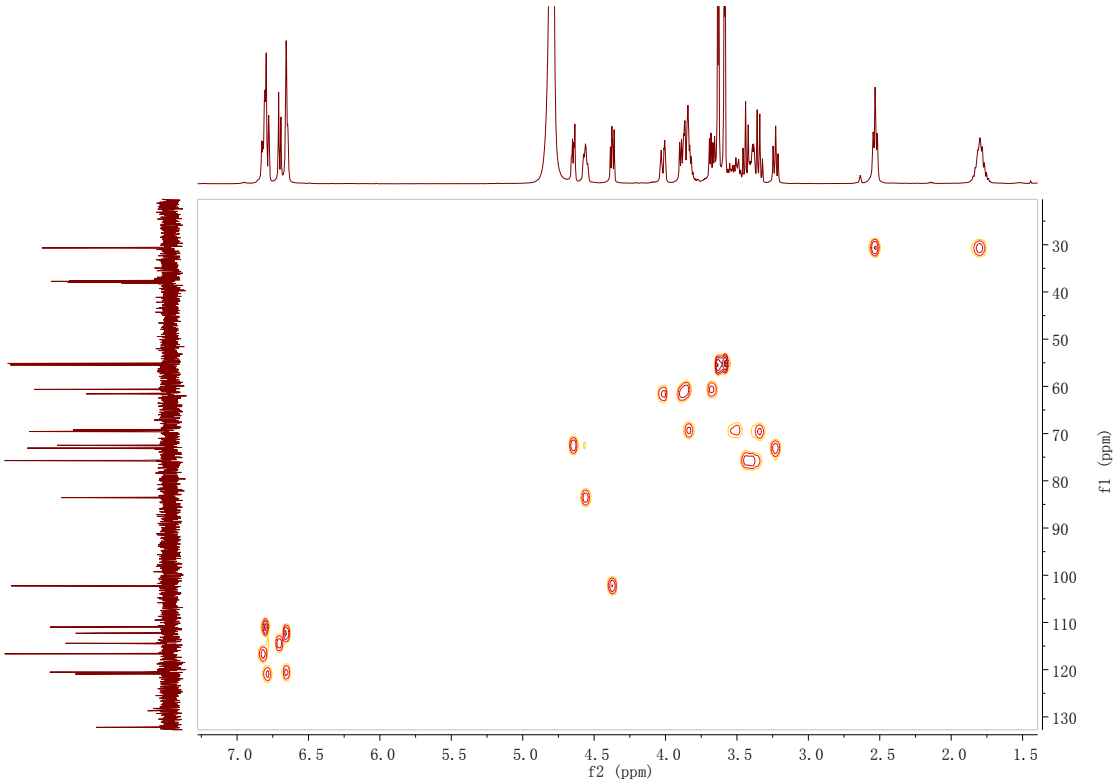


Figure S68. The HSQC spectrum of A-5 in D_2O

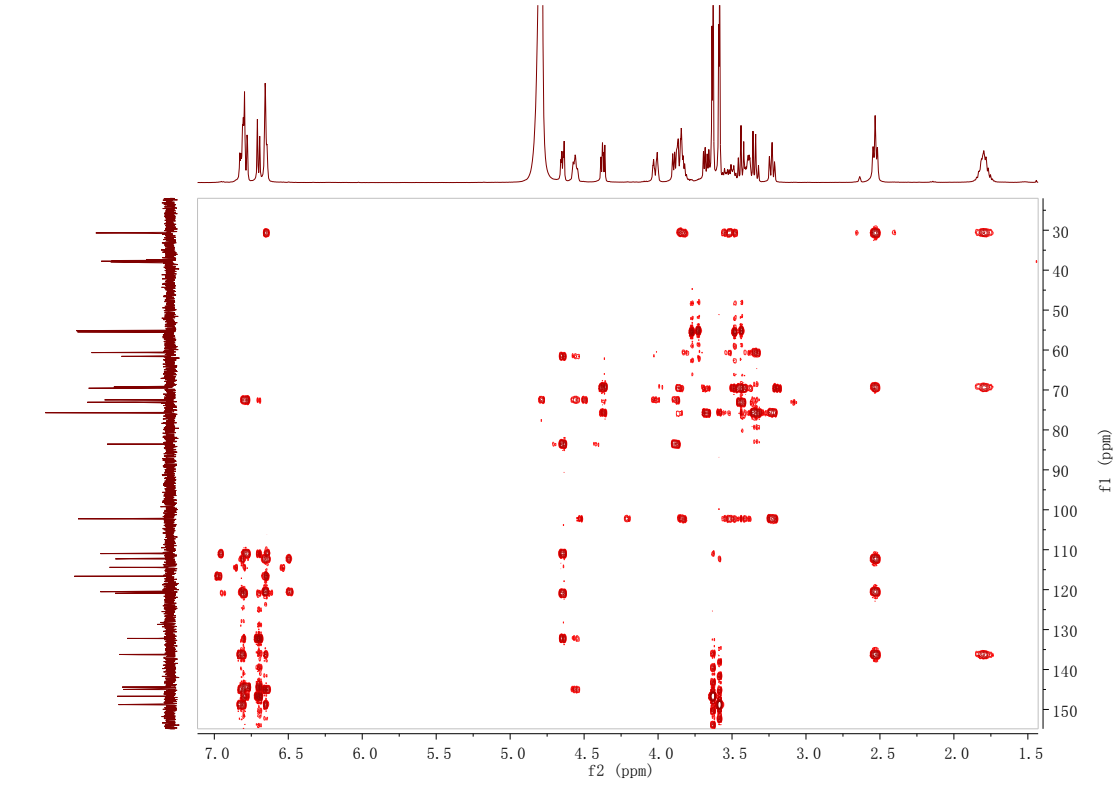


Figure S69. The HMBC spectrum of A-5 in D_2O

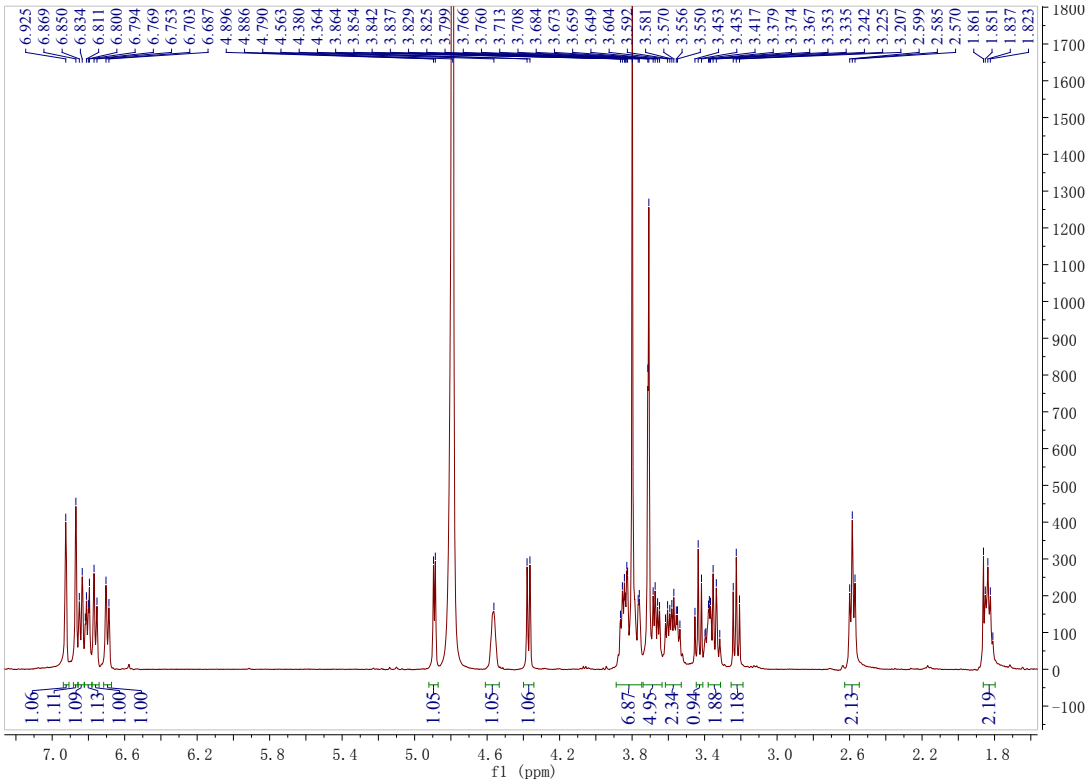


Figure S70. The ^{1}H-NMR spectrum of A-6 in D_2O

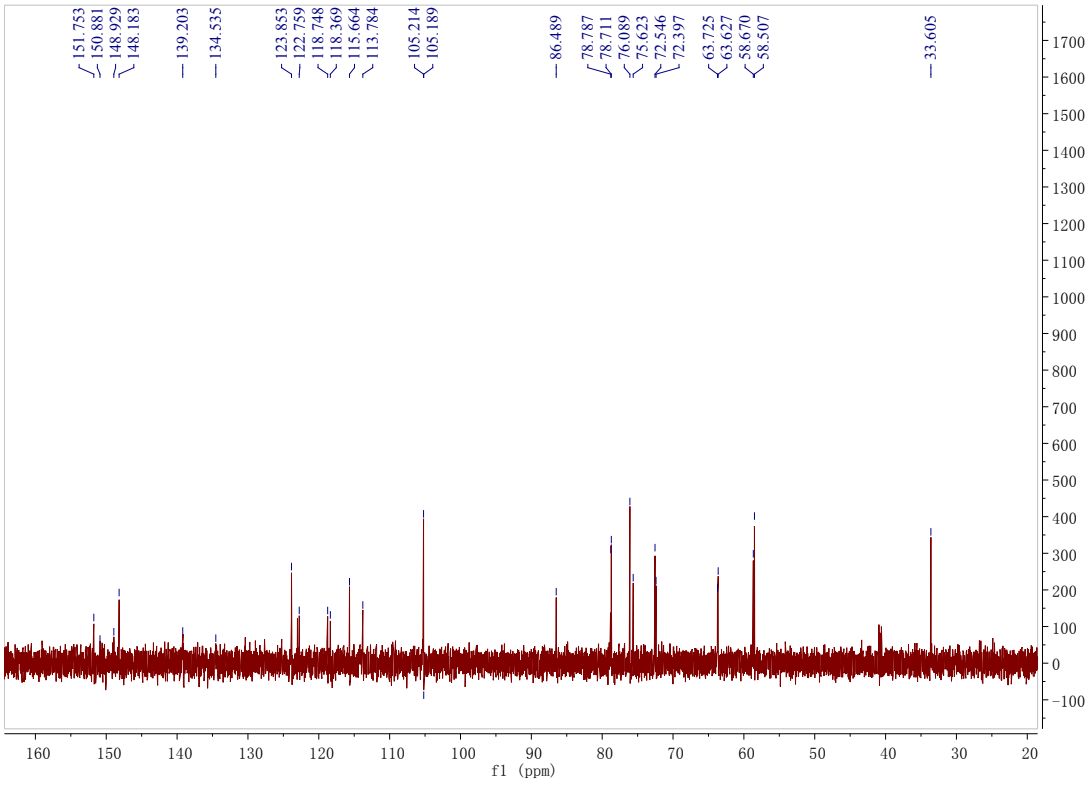


Figure S71. The ^{13}C-NMR spectrum of A-6 in D_2O

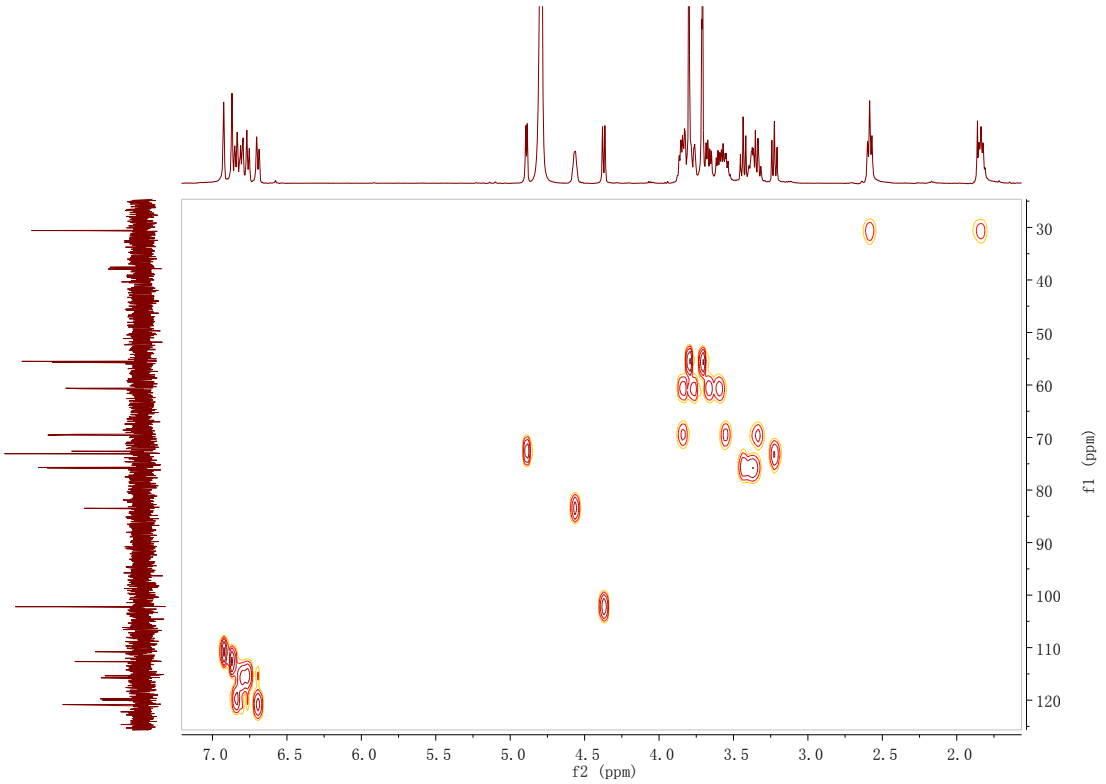


Figure S72. The HSQC spectrum of A-6 in D_2O

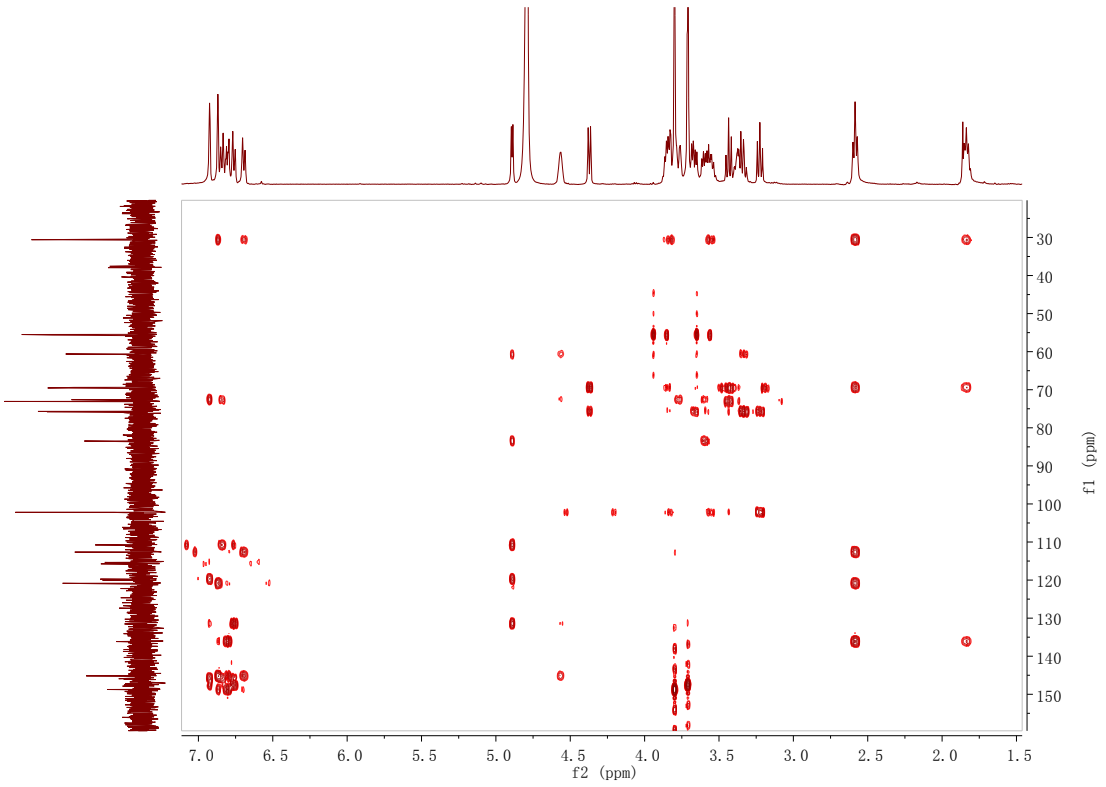


Figure S73. The HMBC spectrum of A-6 in D_2O

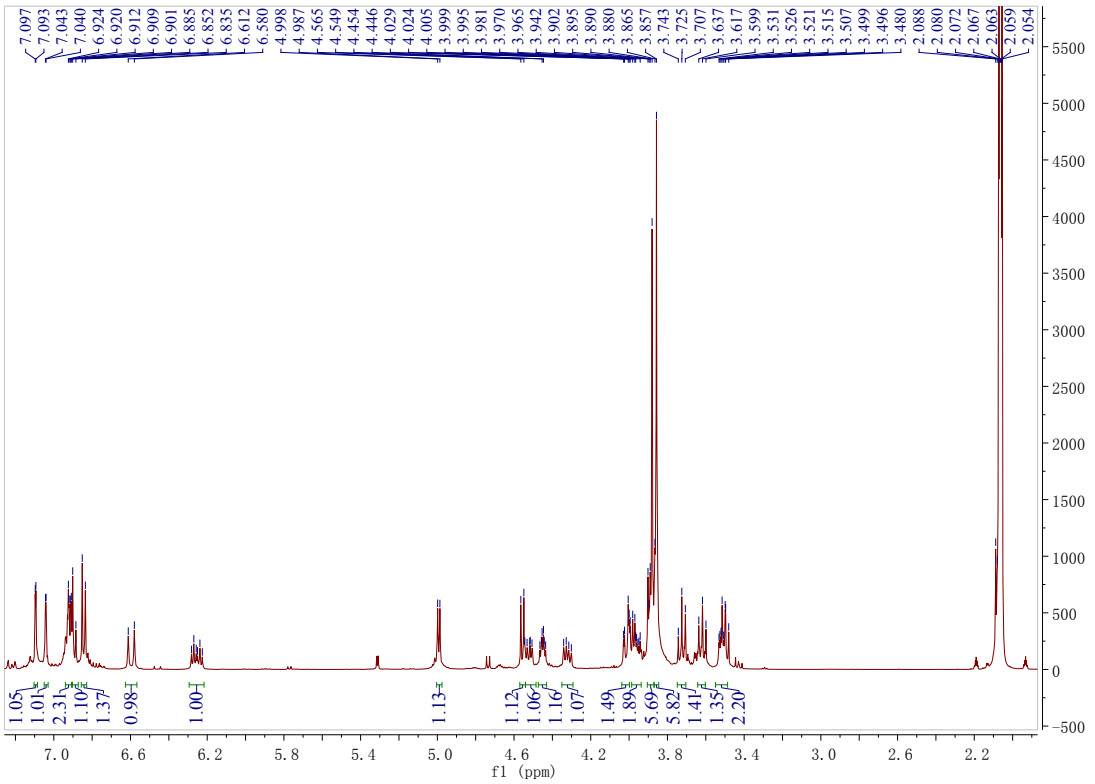


Figure S74. The ^{1}H-NMR spectrum of A-1 in CD_3COOD

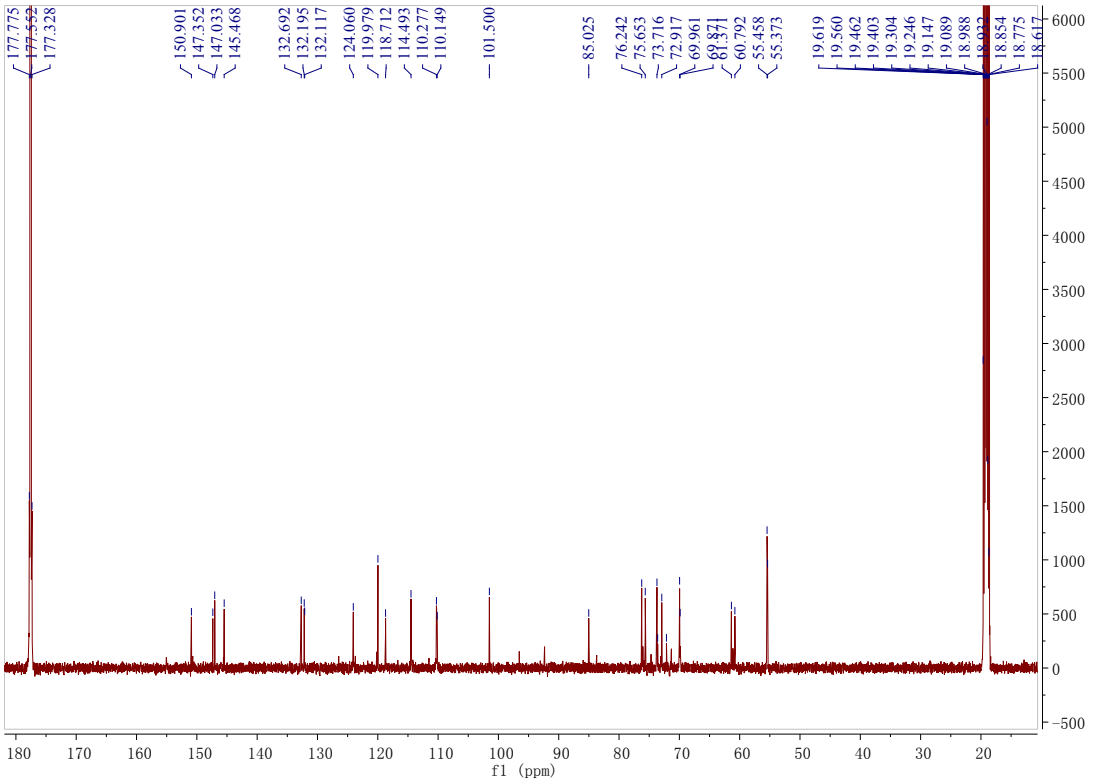


Figure S75. The ^{13}C-NMR spectrum of A-1 in CD_3COOD

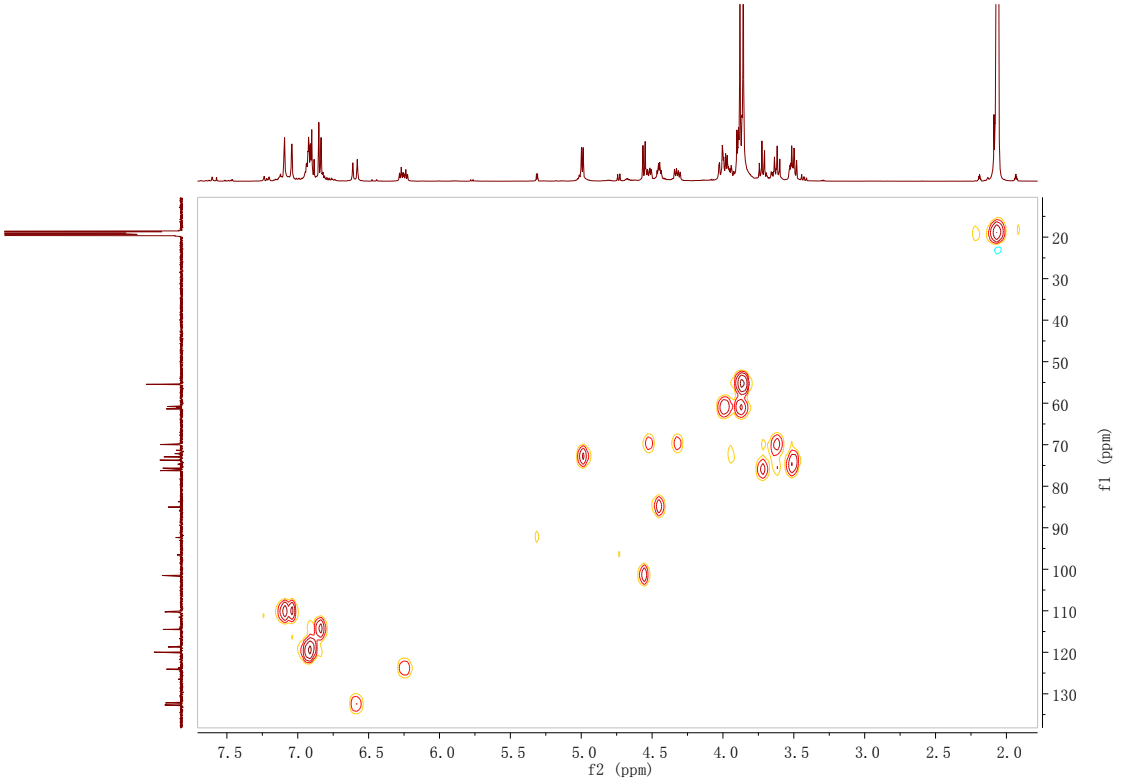


Figure S76. The HSQC spectrum of A-1 in CD_3COOD

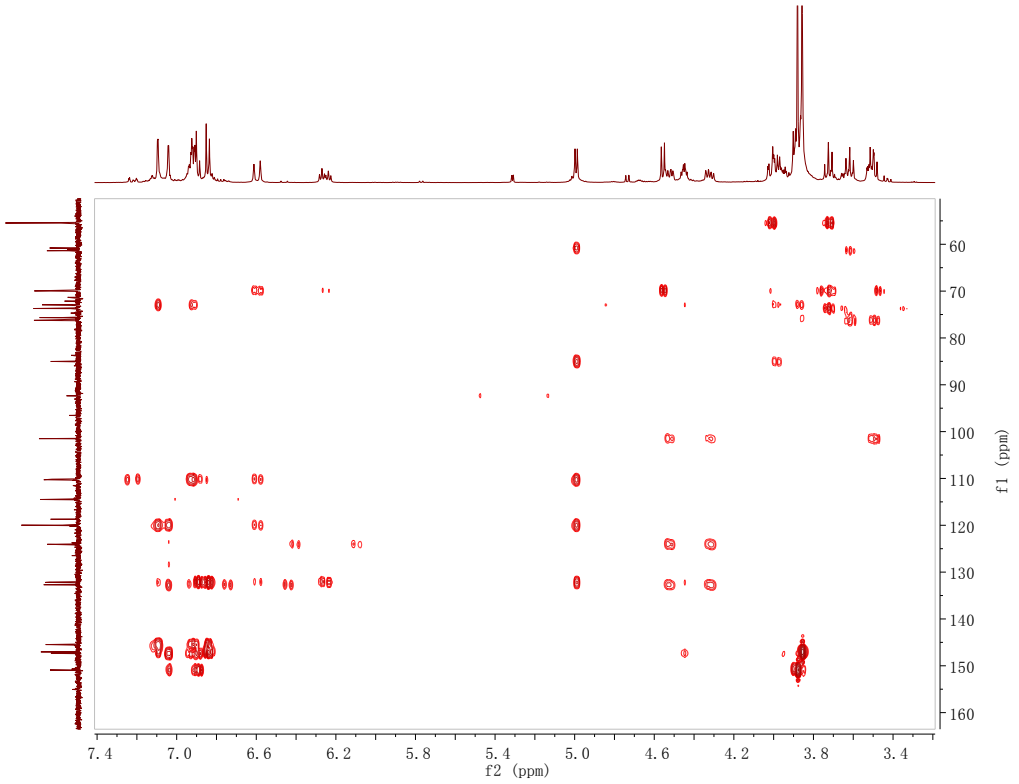


Figure S77. The HMBC spectrum of A-1 in CD_3COOD

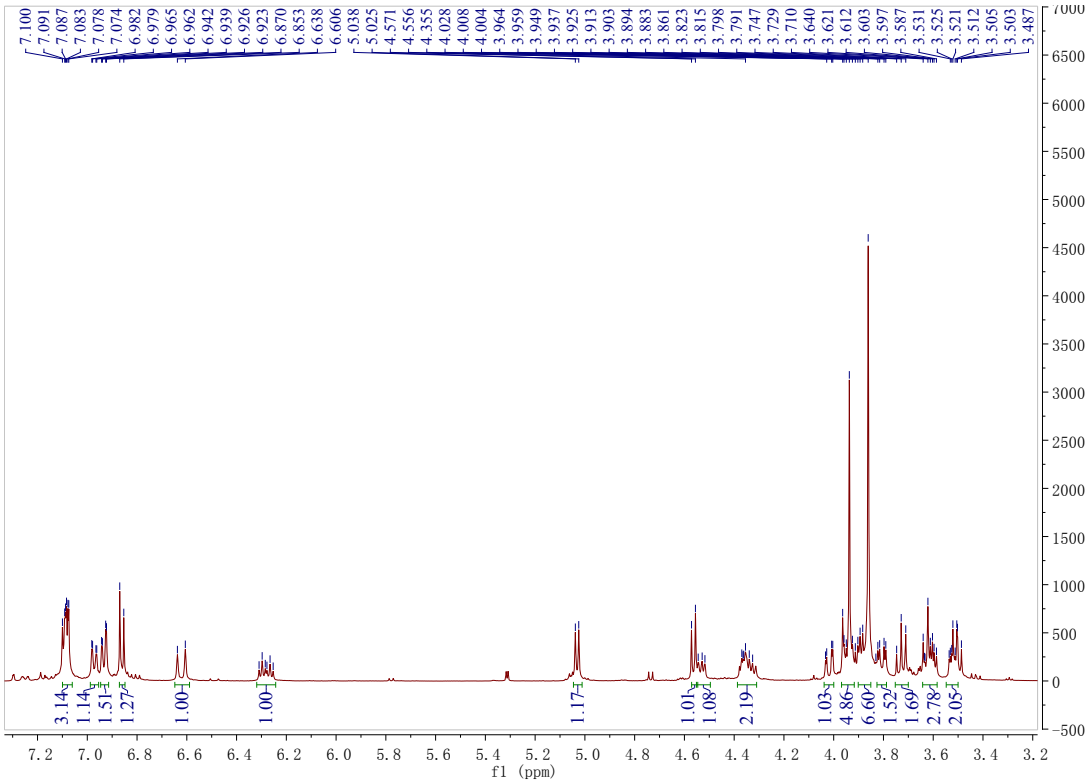


Figure S78. The ^{1}H-NMR spectrum of A-2 in CD_3COOD

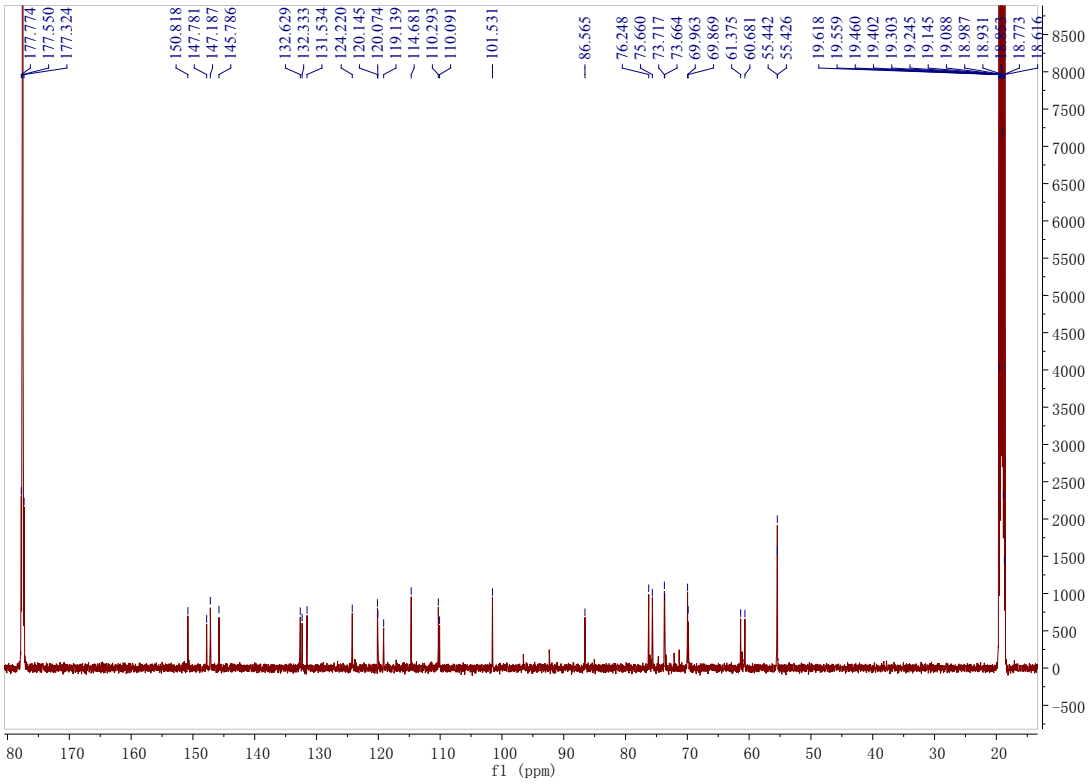


Figure S79. The ^{13}C-NMR spectrum of A-2 in CD_3COOD

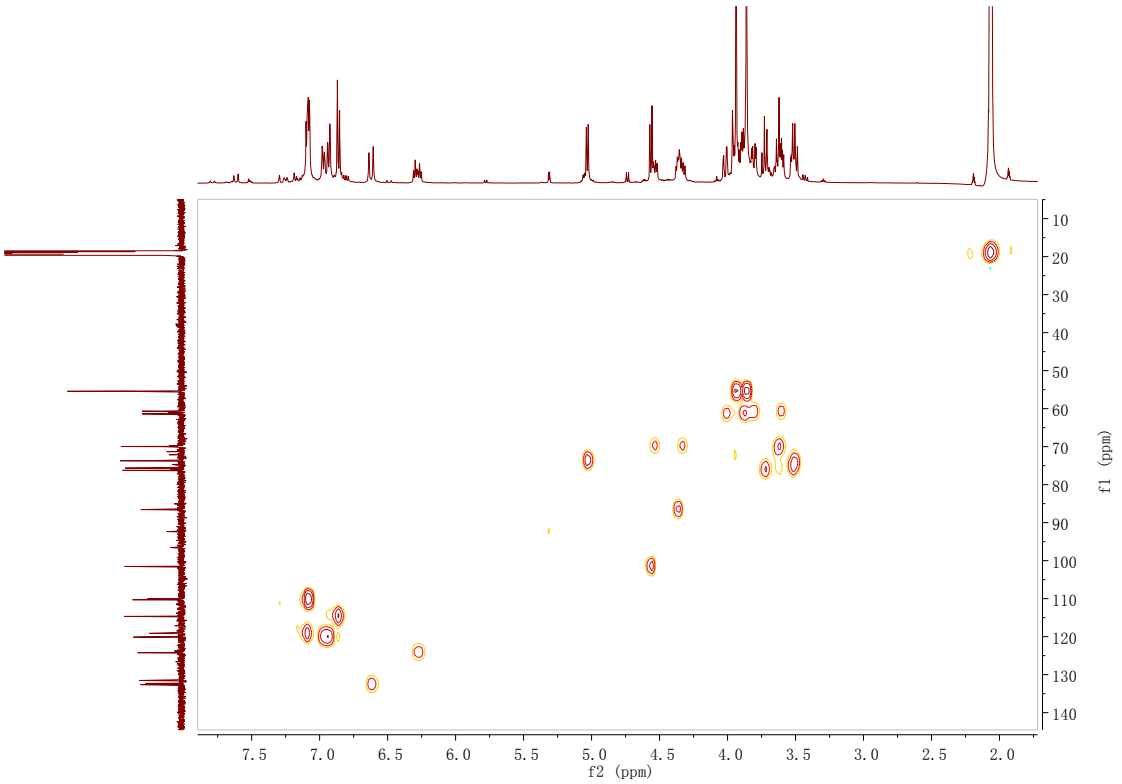


Figure S80. The HSQC spectrum of A-2 in CD_3COOD

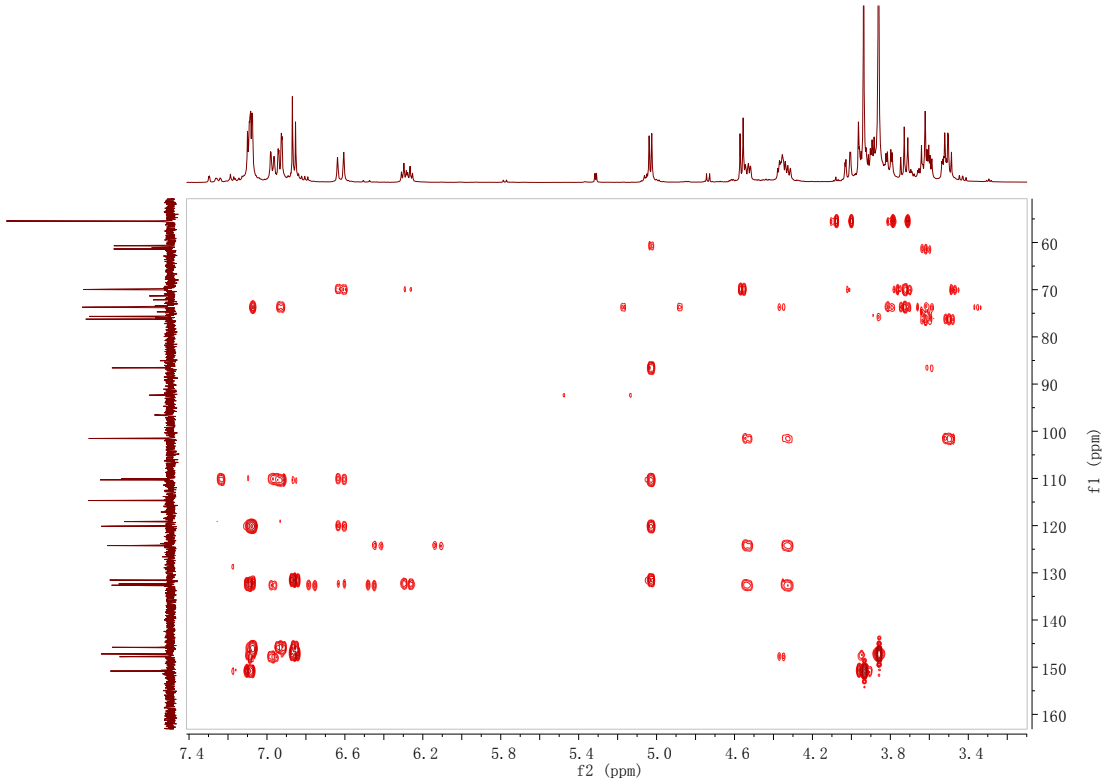


Figure S81. The HMBC spectrum of A-2 in CD_3COOD

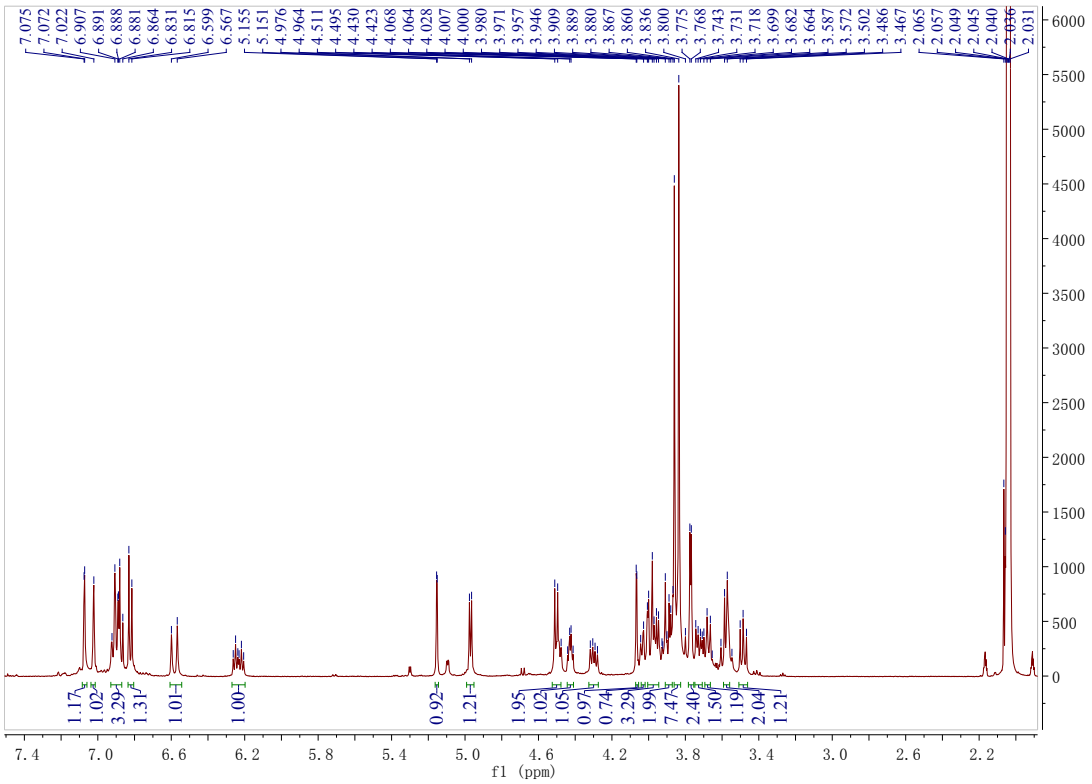


Figure S82. The ^{1}H-NMR spectrum of A-3 in CD_3COOD

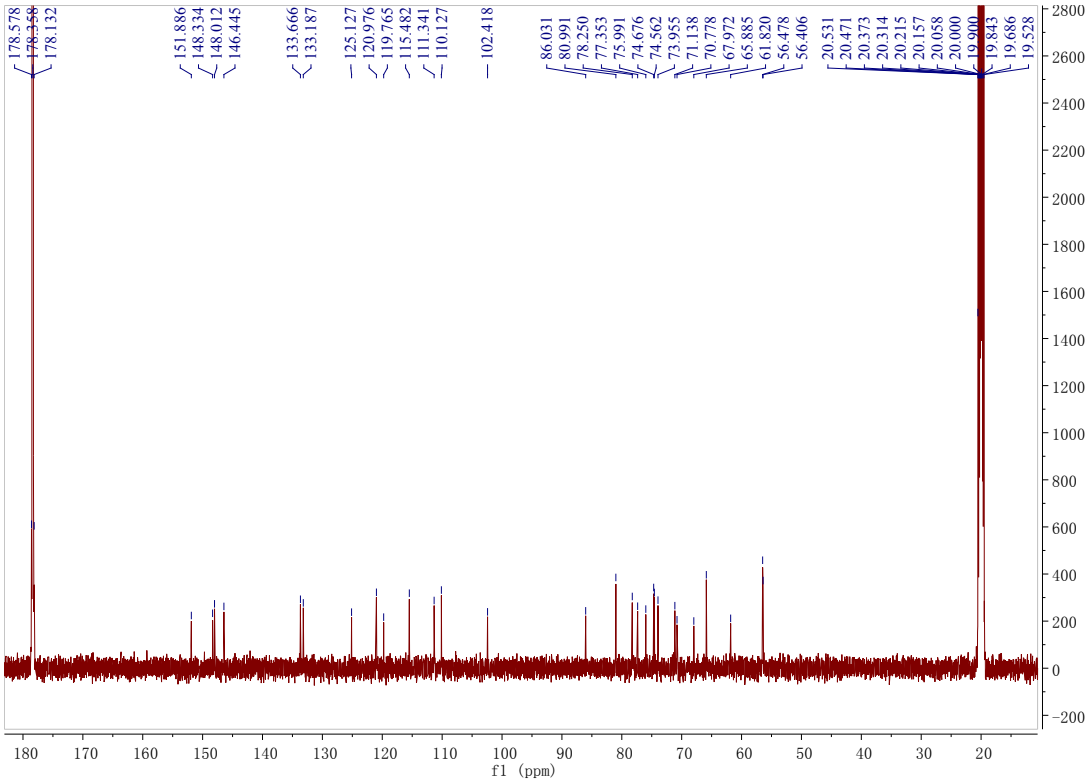


Figure S83. The ^{13}C-NMR spectrum of A-3 in CD_3COOD

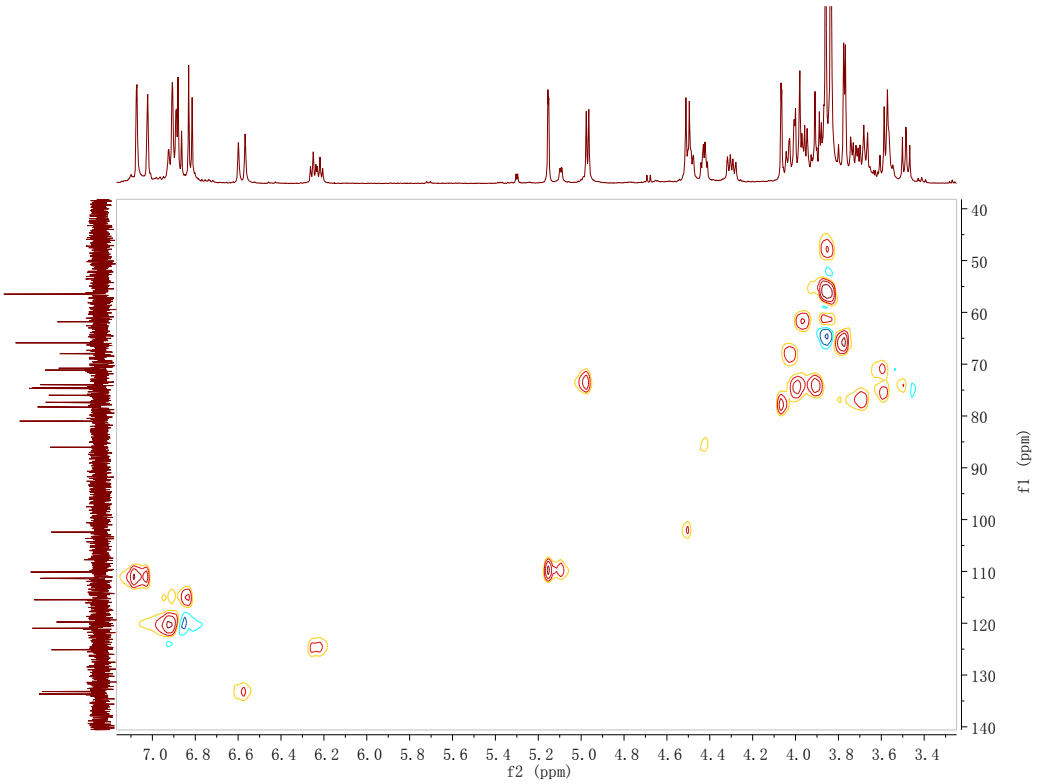


Figure S84. The HSQC spectrum of A-3 in CD_3COOD

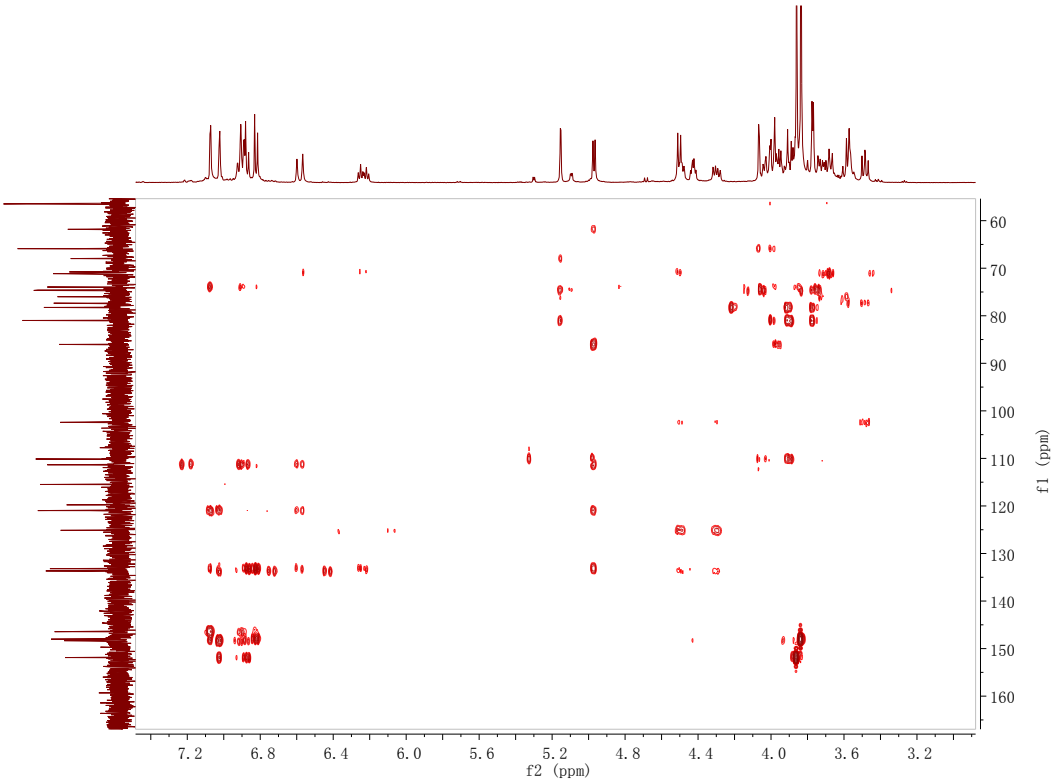


Figure S85. The HMBC spectrum of A-3 in CD_3COOD

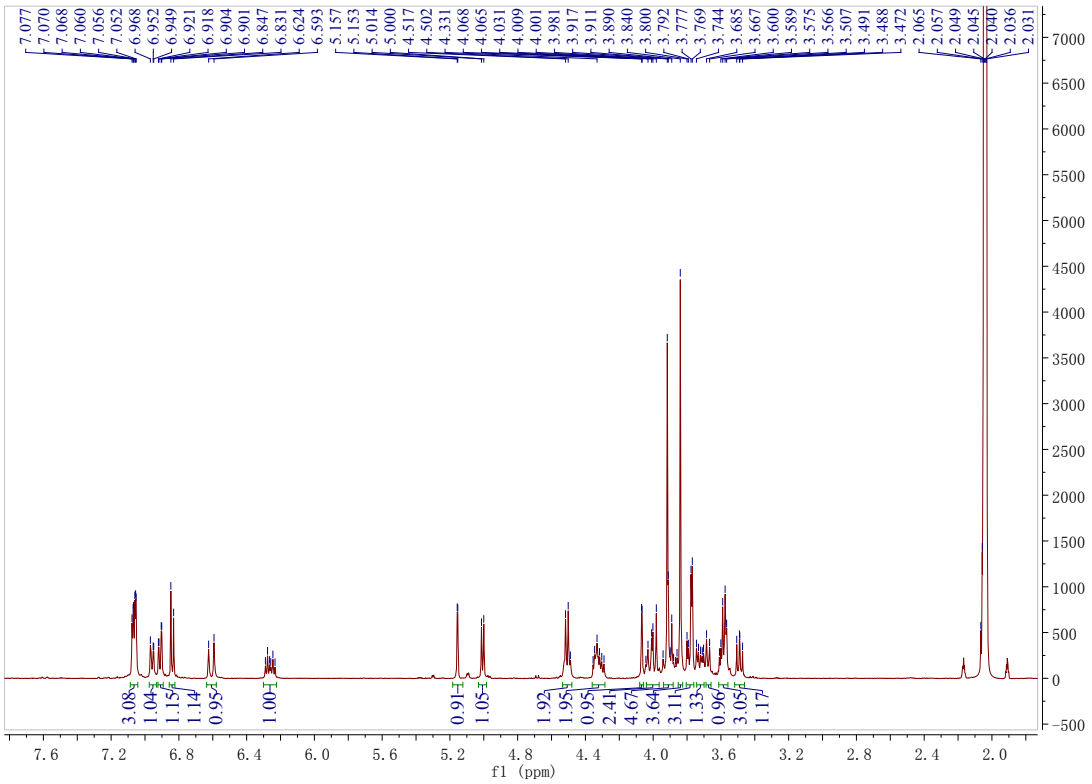


Figure S86. The ^{1}H-NMR spectrum of A-4 in CD_3COOD

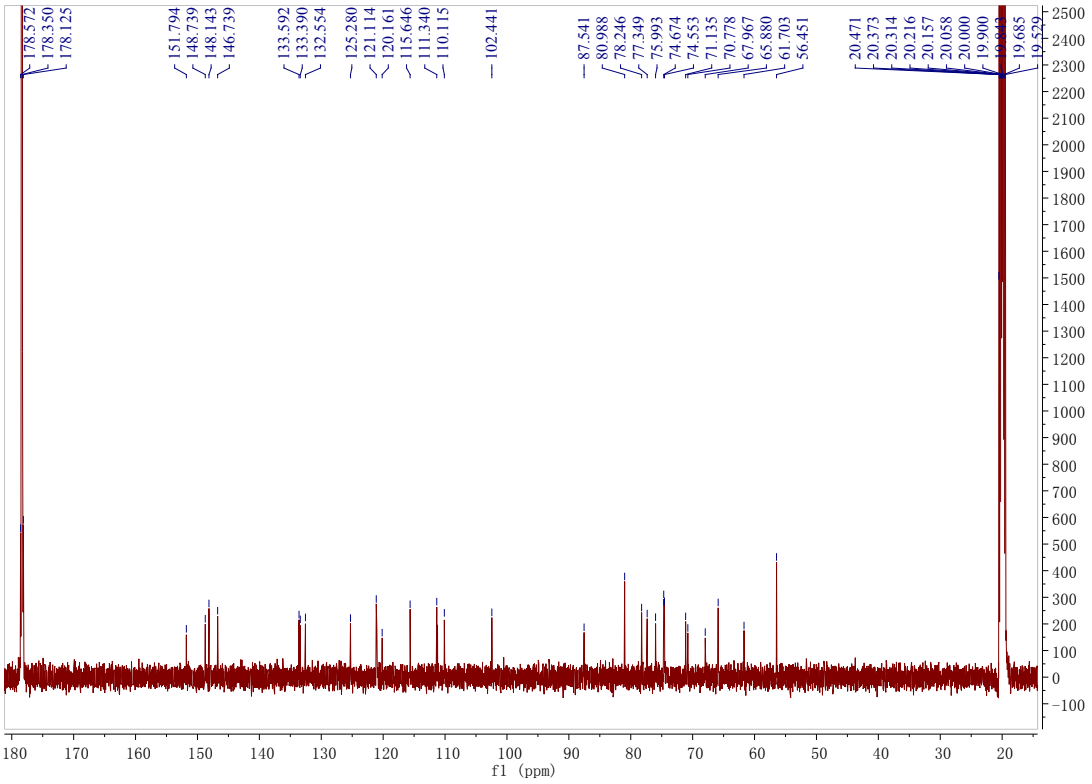


Figure S87. The ^{13}C-NMR spectrum of A-4 in CD_3COOD

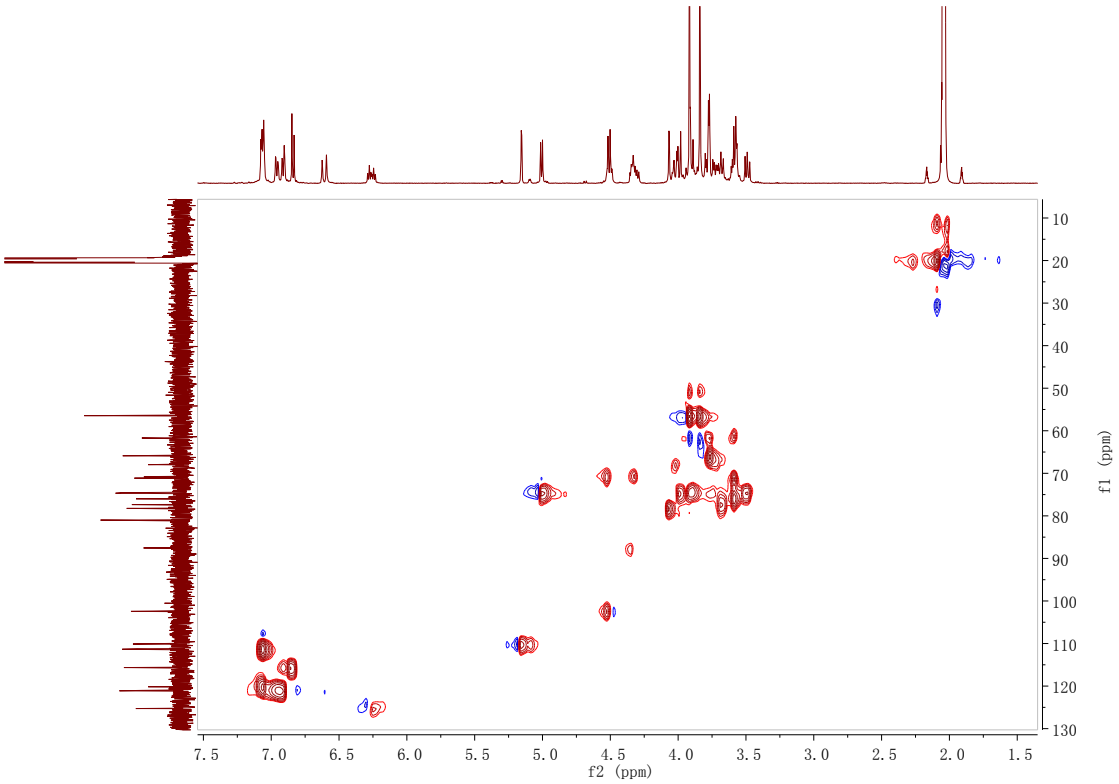


Figure S88. The HSQC spectrum of A-4 in CD_3COOD

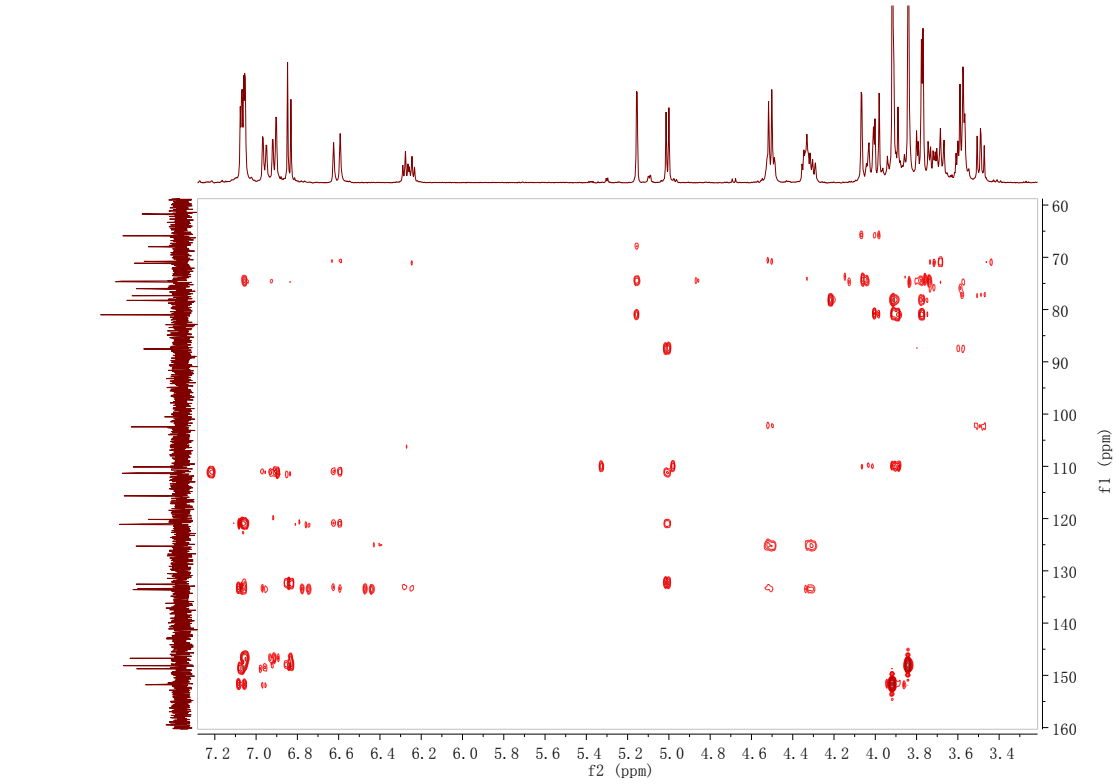


Figure S89. The HMBC spectrum of A-4 in CD_3COOD

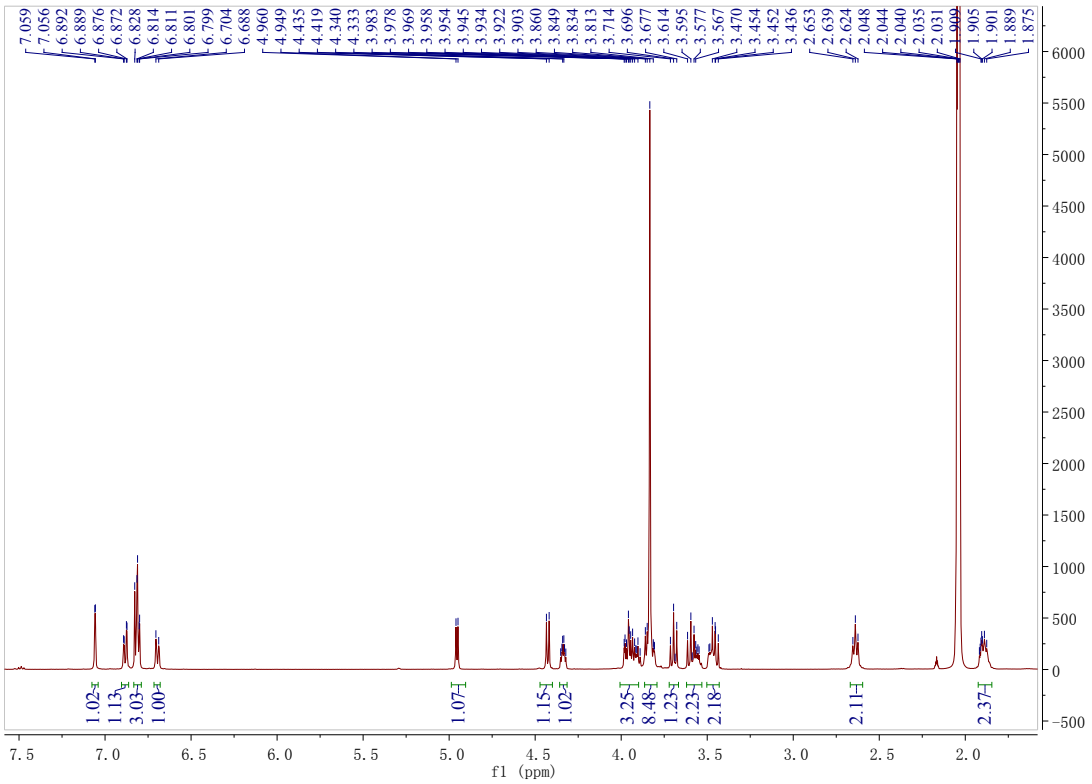


Figure S90. The ^{1}H-NMR spectrum of A-5 in CD_3COOD

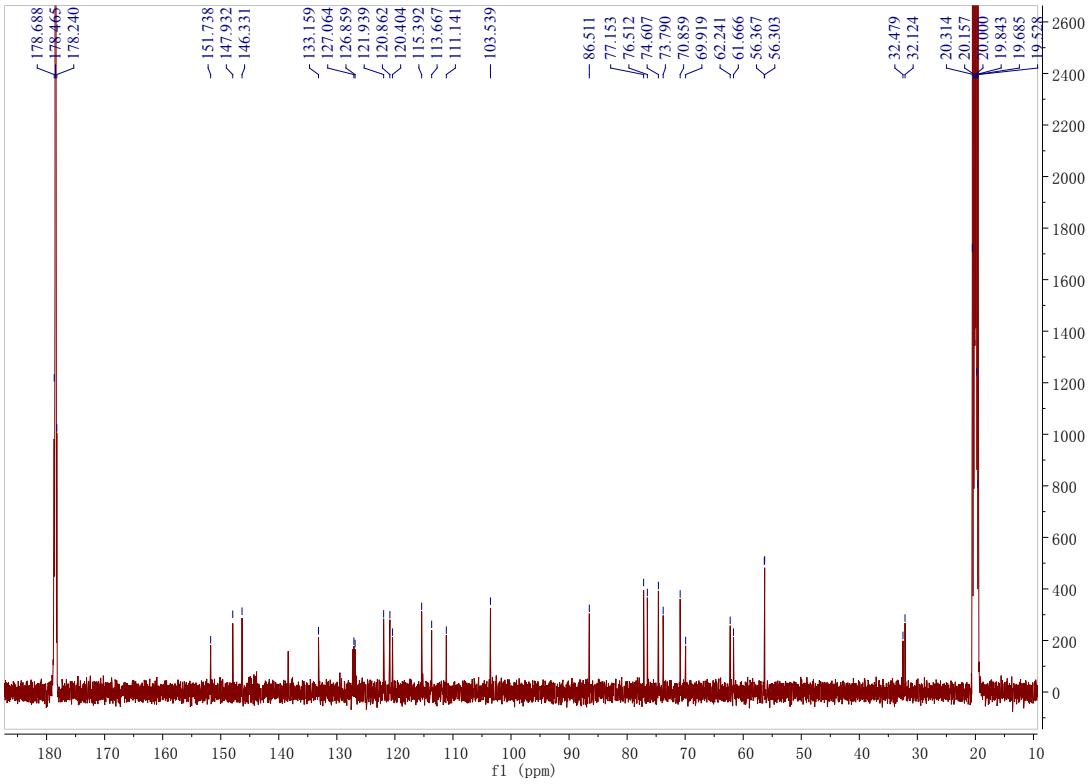


Figure S91. The ^{13}C-NMR spectrum of A-5 in CD_3COOD

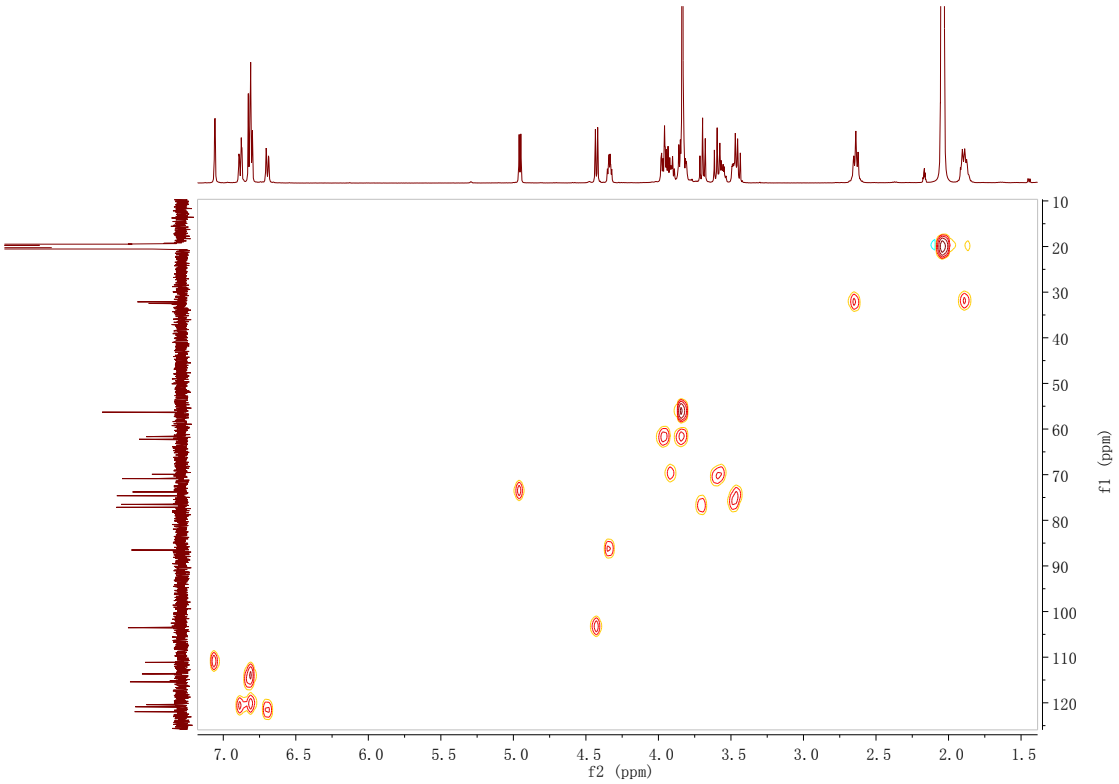


Figure S92. The HSQC spectrum of A-5 in CD_3COOD

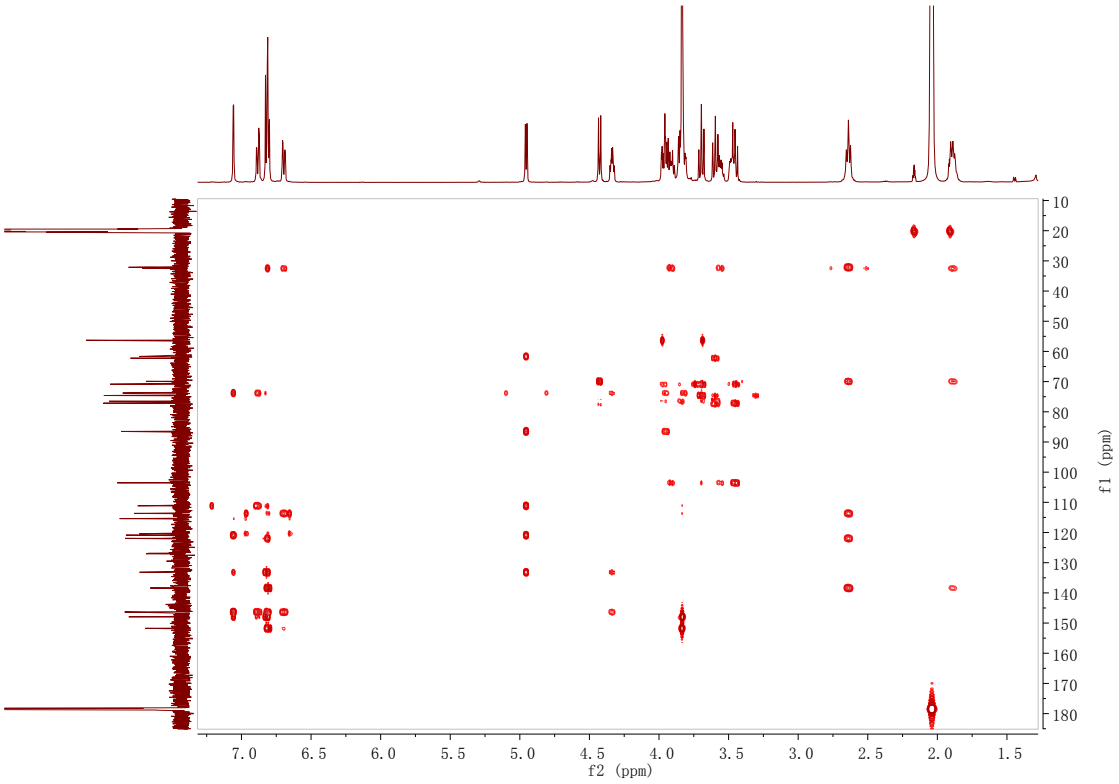


Figure S93. The HMBC spectrum of A-5 in CD_3COOD

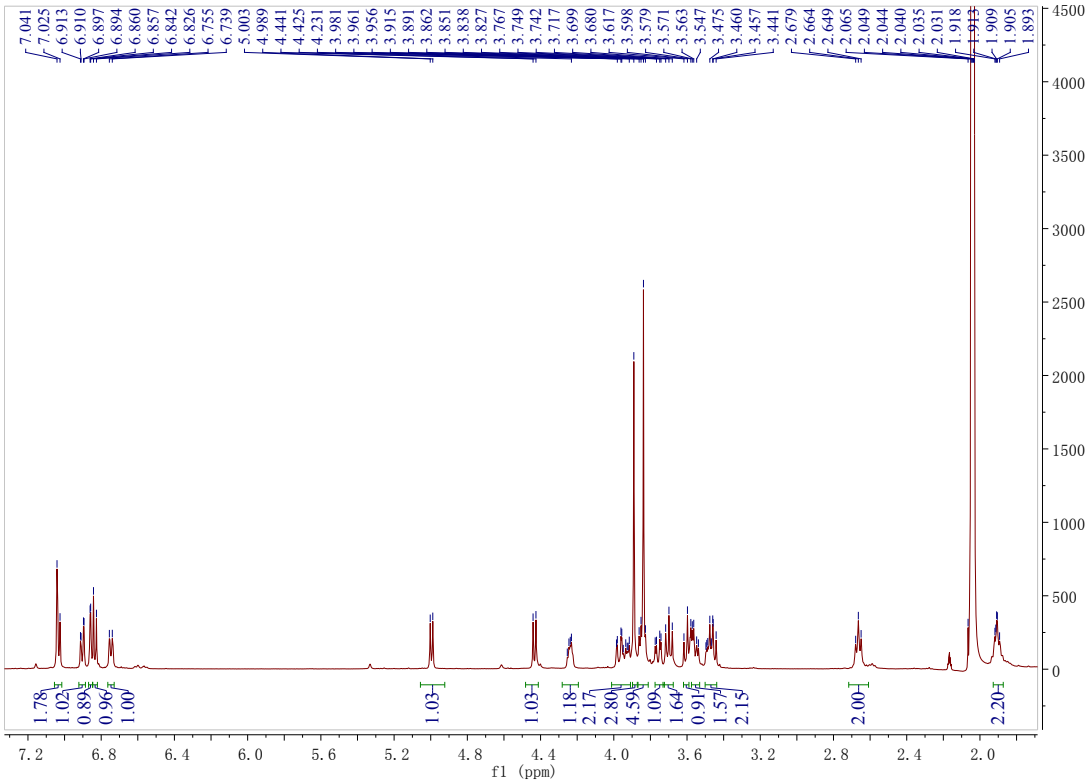


Figure S94. The ^{1}H-NMR spectrum of A-6 in CD_3COOD

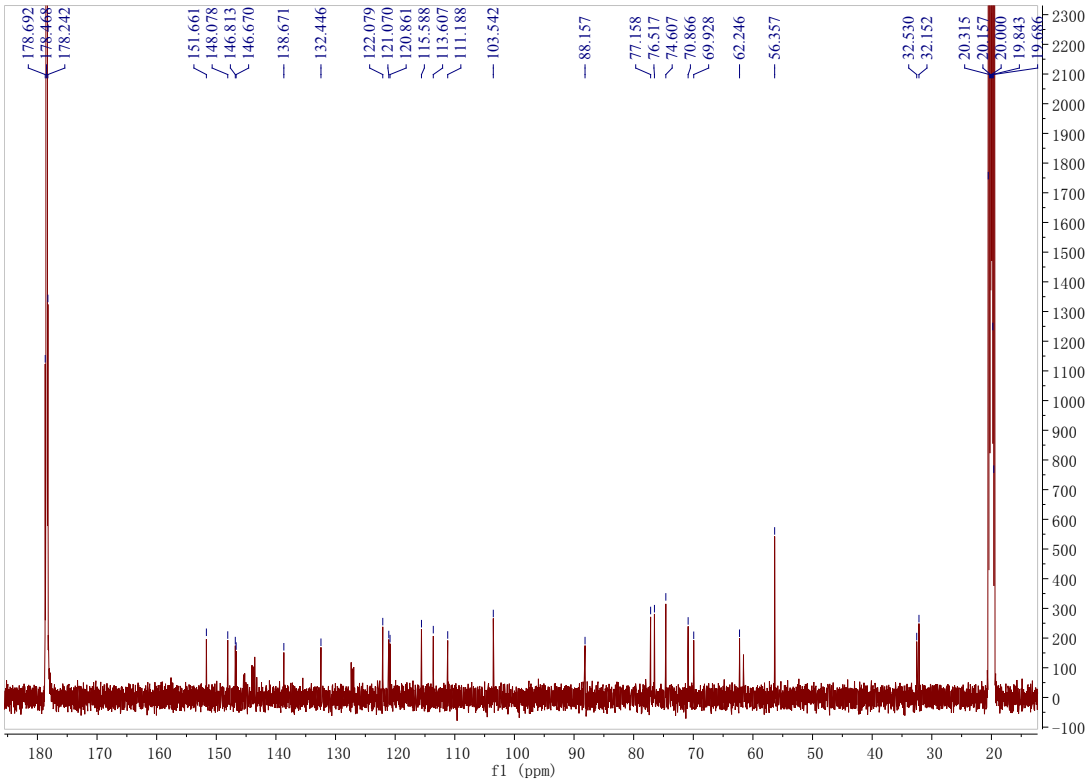


Figure S95. The ^{13}C-NMR spectrum of A-6 in CD_3COOD

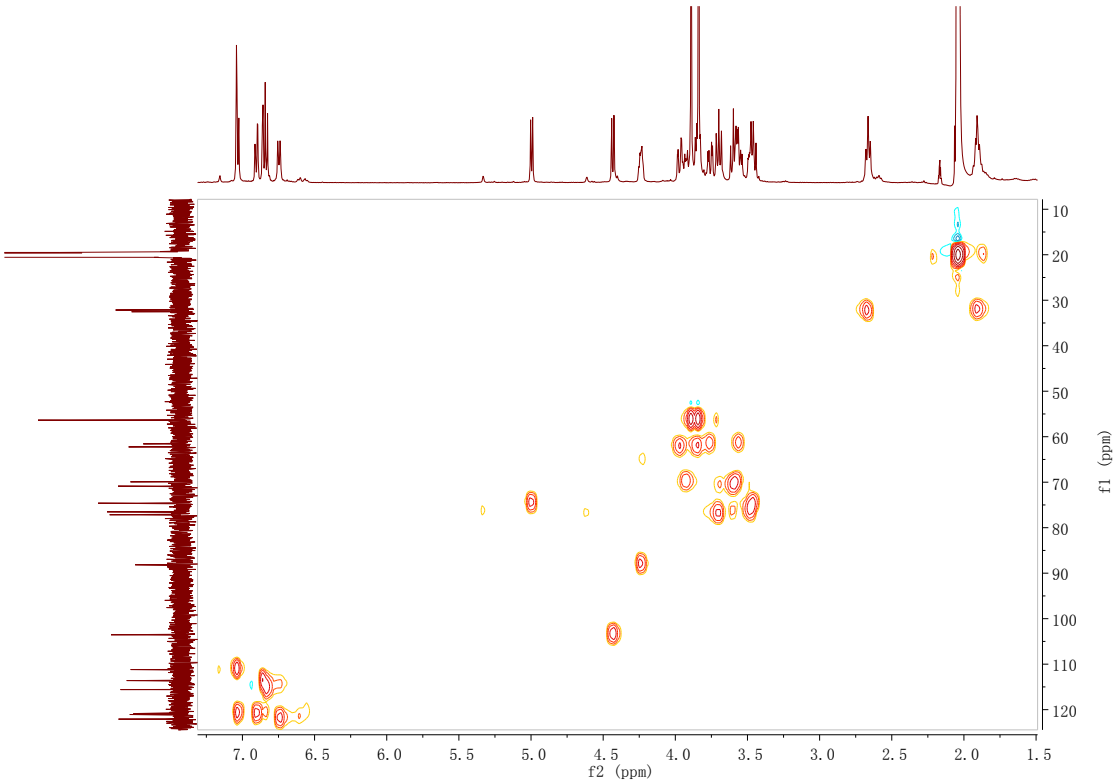


Figure S96. The HSQC spectrum of A-6 in CD_3COOD

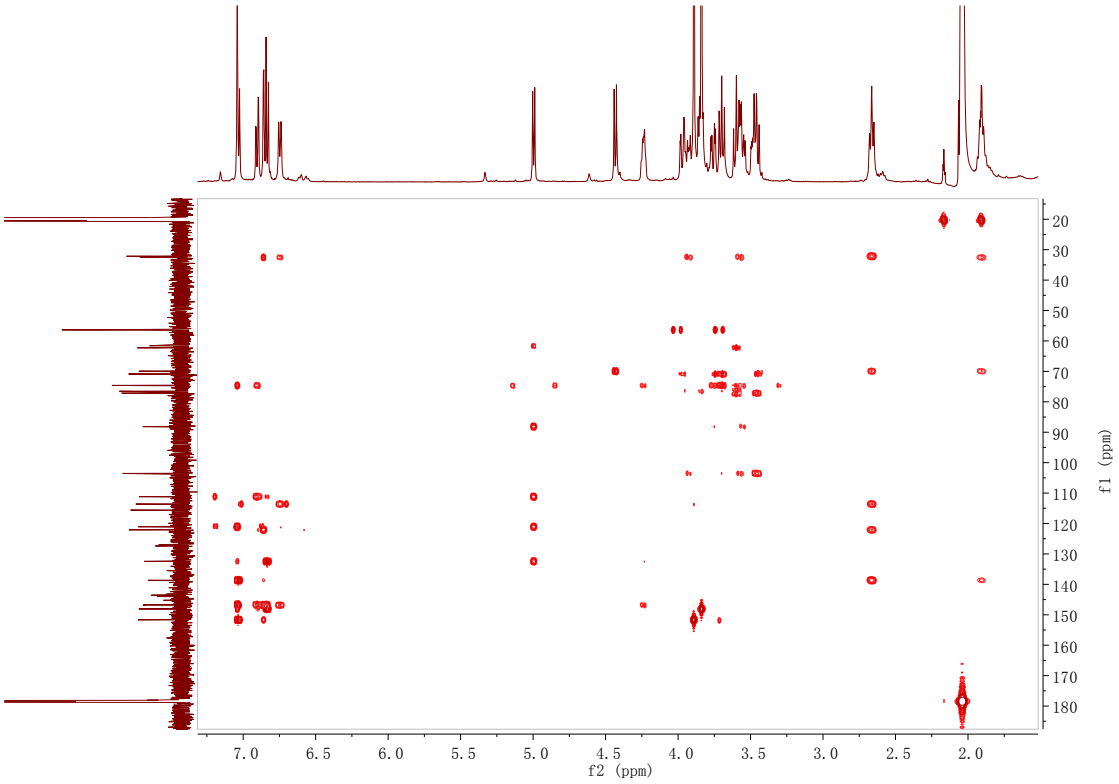


Figure S97. The HMBC spectrum of A-6 in CD_3COOD

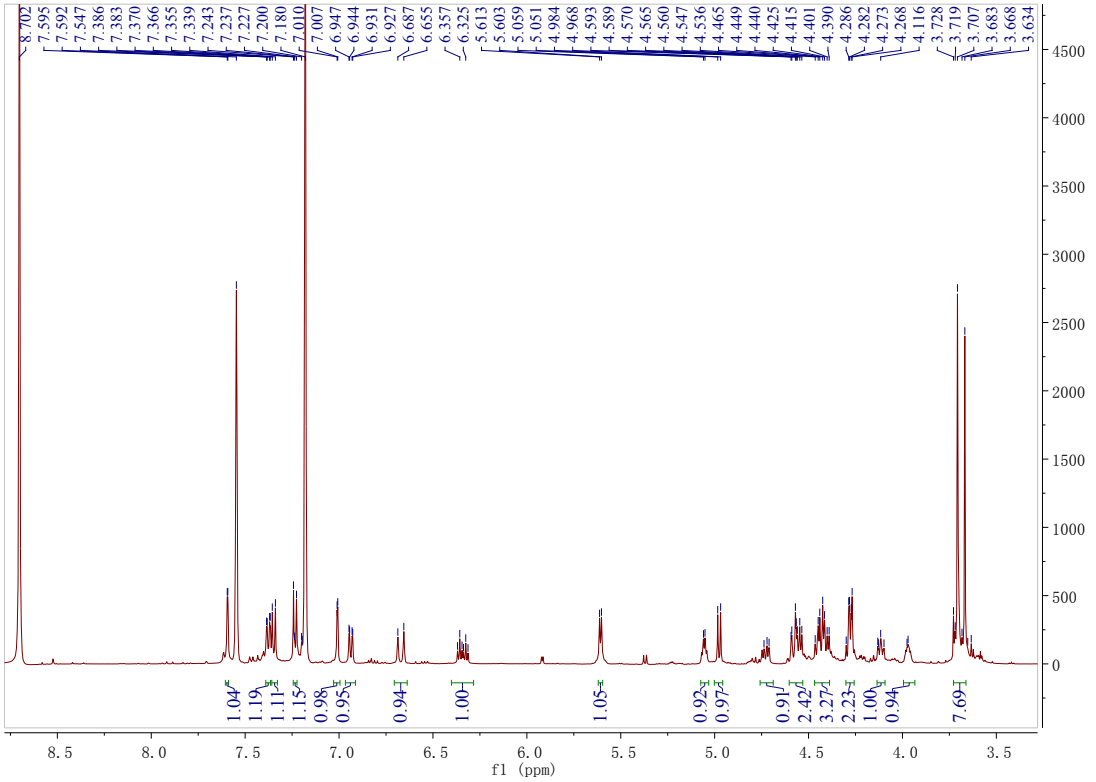


Figure S98. The ^{1}H-NMR spectrum of A-1 in C_5D_5N

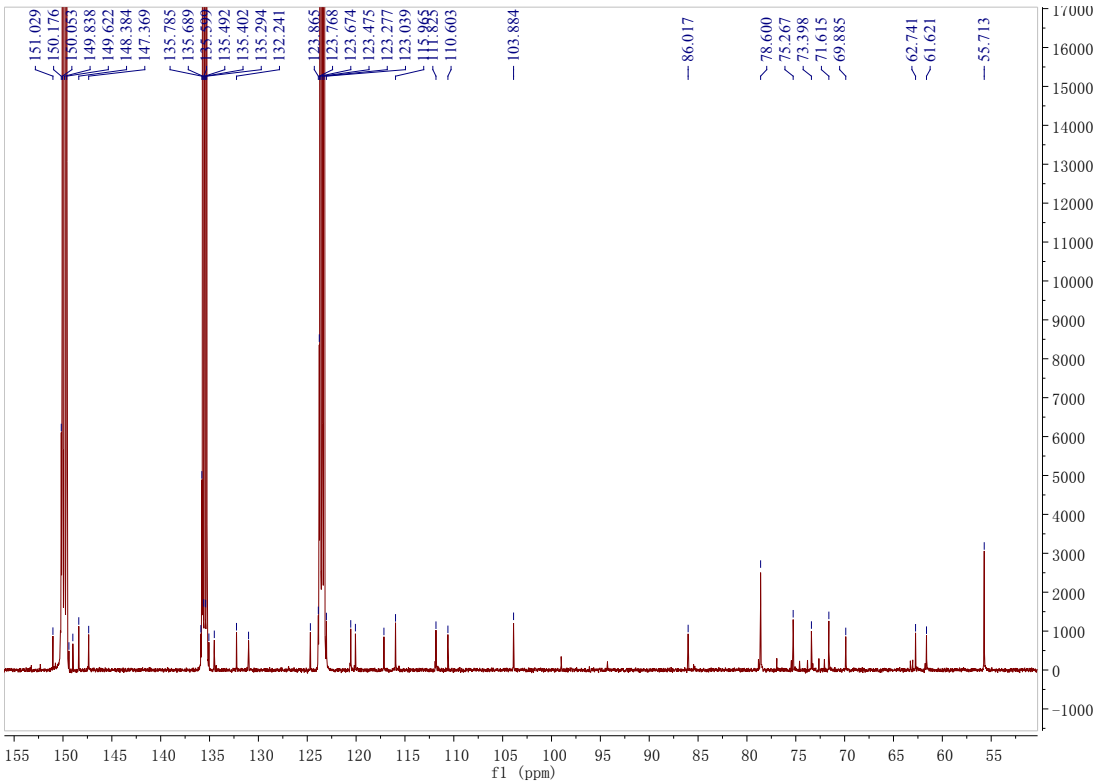


Figure S99. The ^{13}C-NMR spectrum of A-1 in C_5D_5N

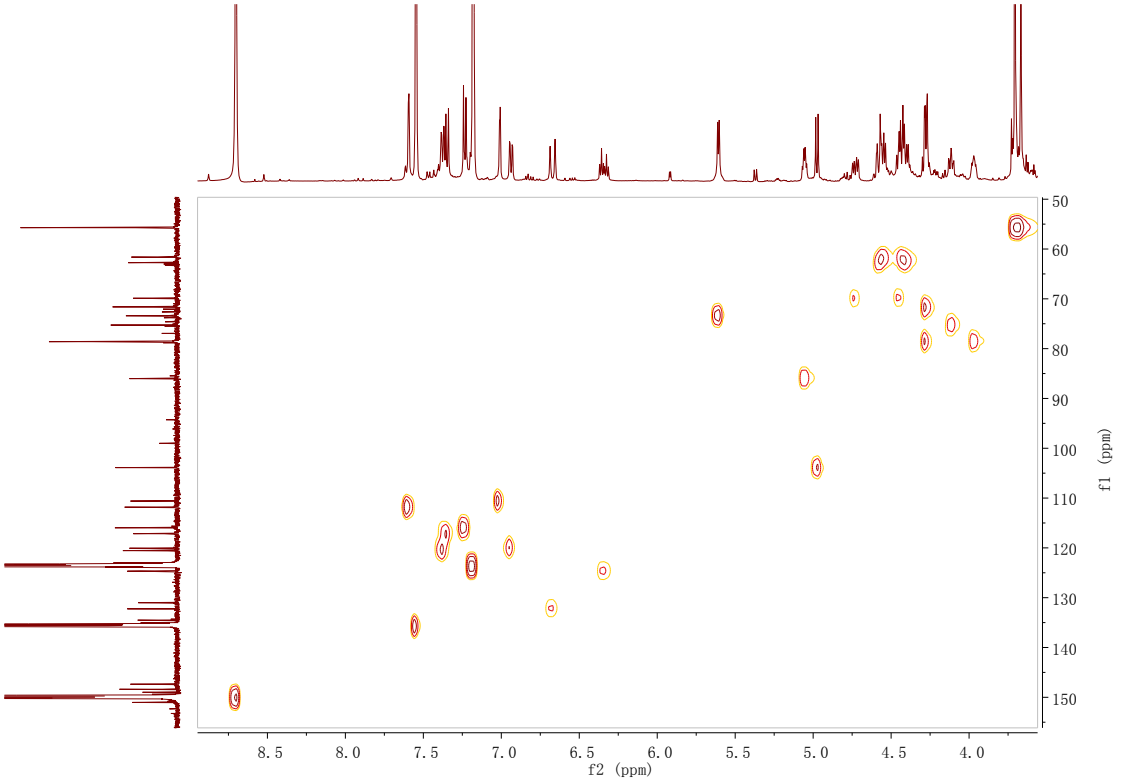


Figure S100. The HSQC spectrum of A-1 in C_5D_5N

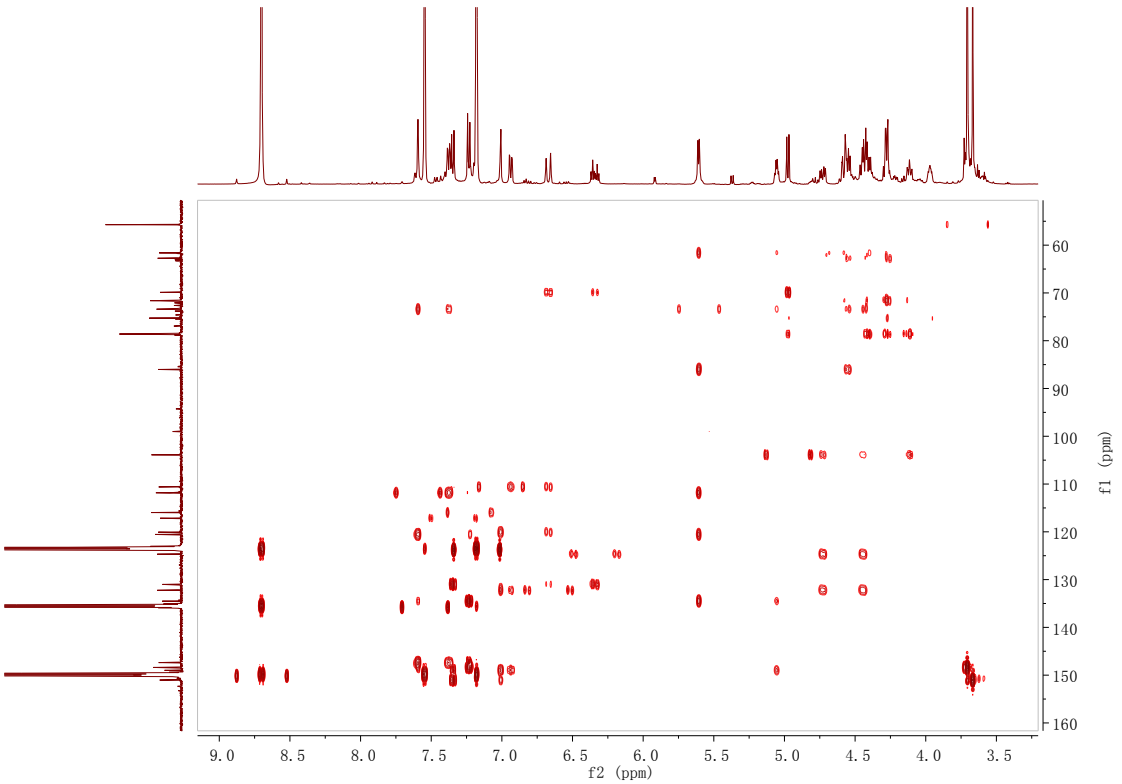


Figure S101. The HMBC spectrum of A-1 in C_5D_5N

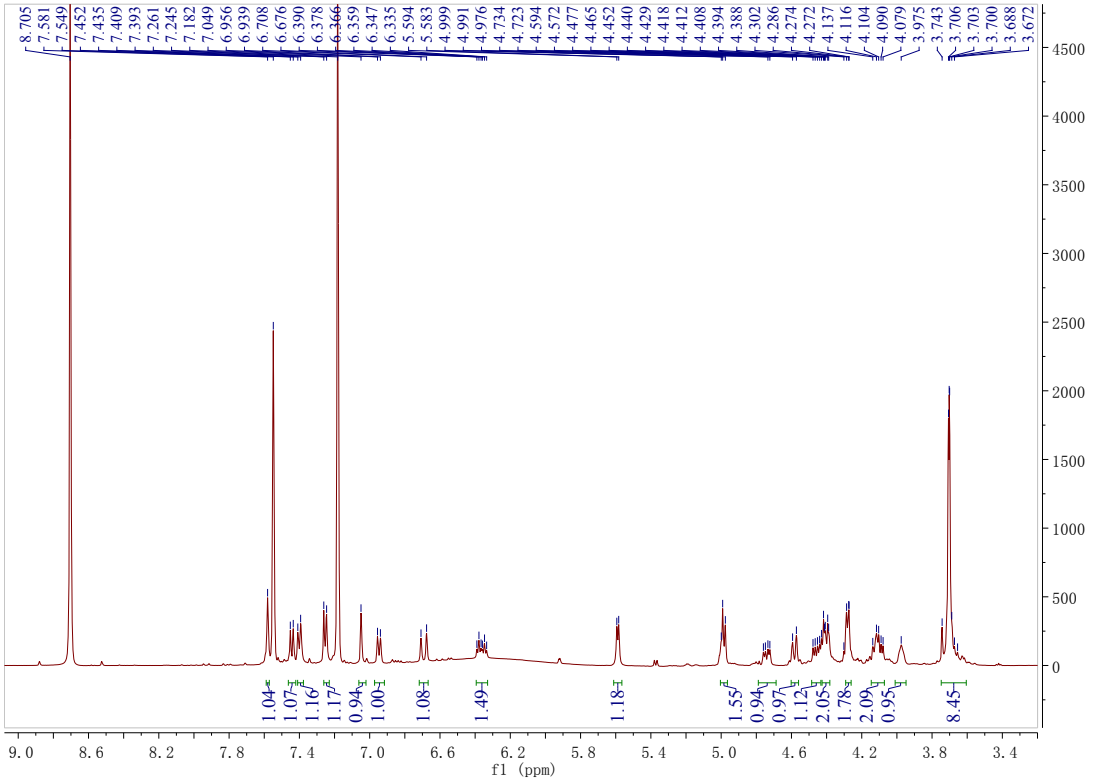


Figure S102. The ^{1}H-NMR spectrum of A-2 in C_5D_5N

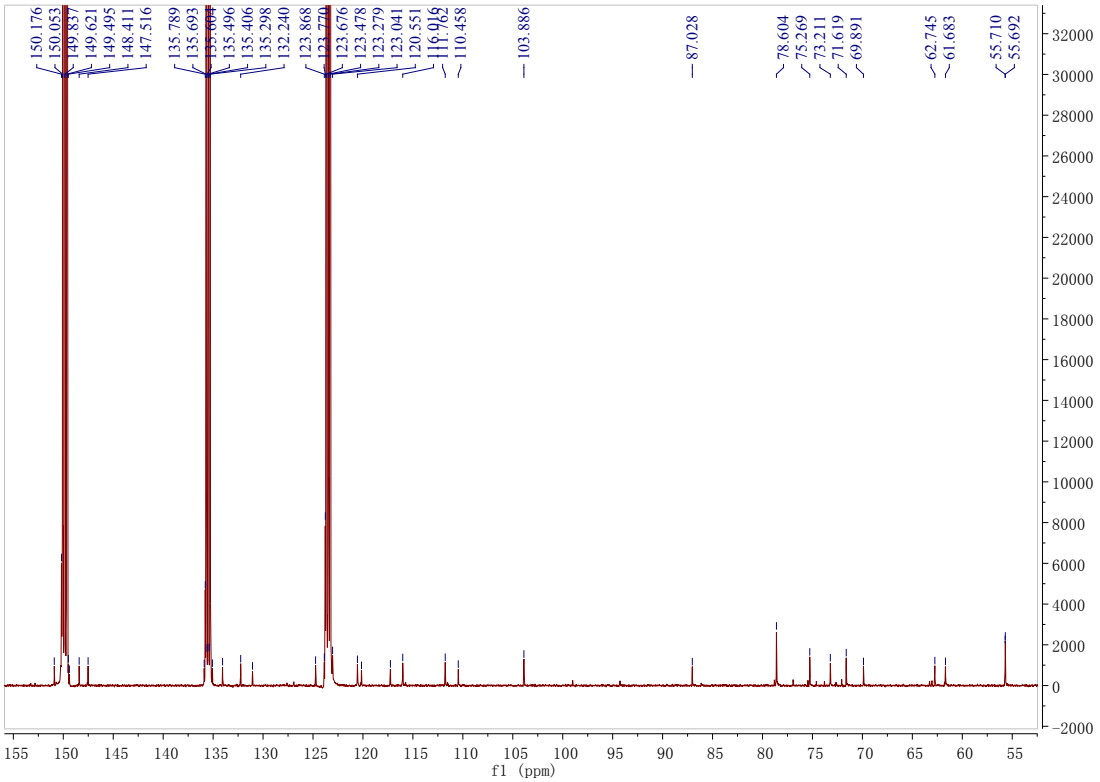


Figure S103. The ^{13}C-NMR spectrum of A-2 in C_5D_5N

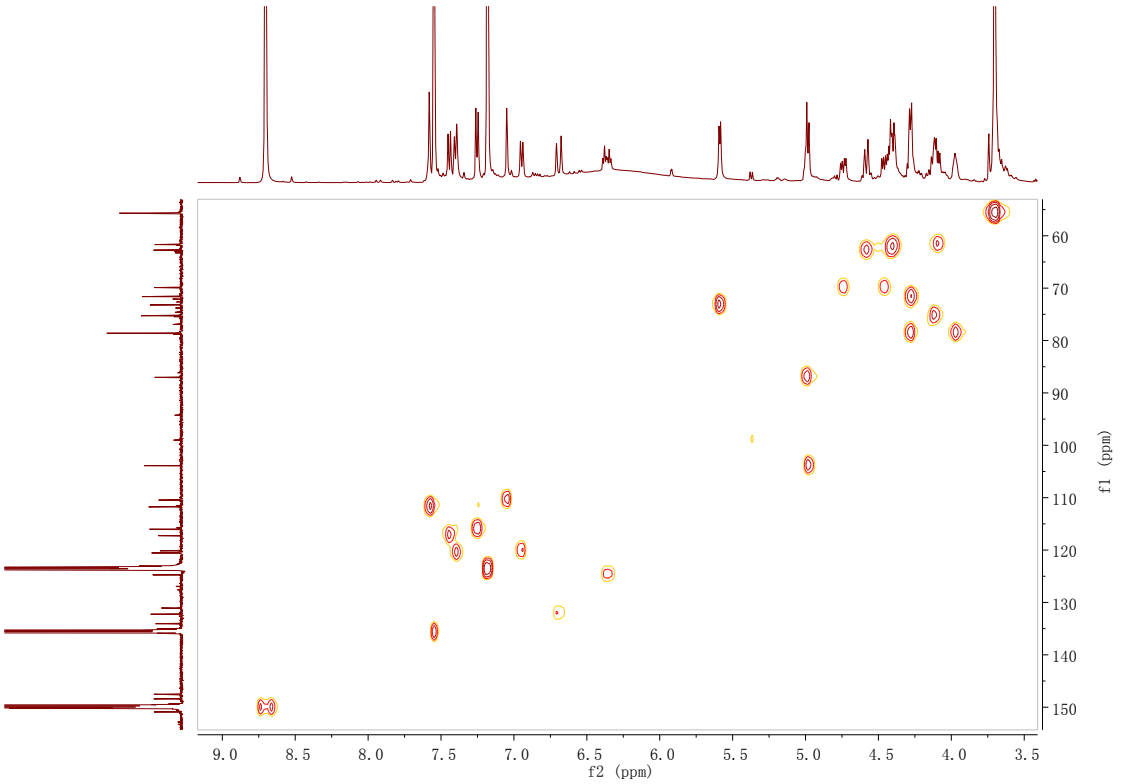


Figure S104. The HSQC spectrum of A-2 in C_5D_5N

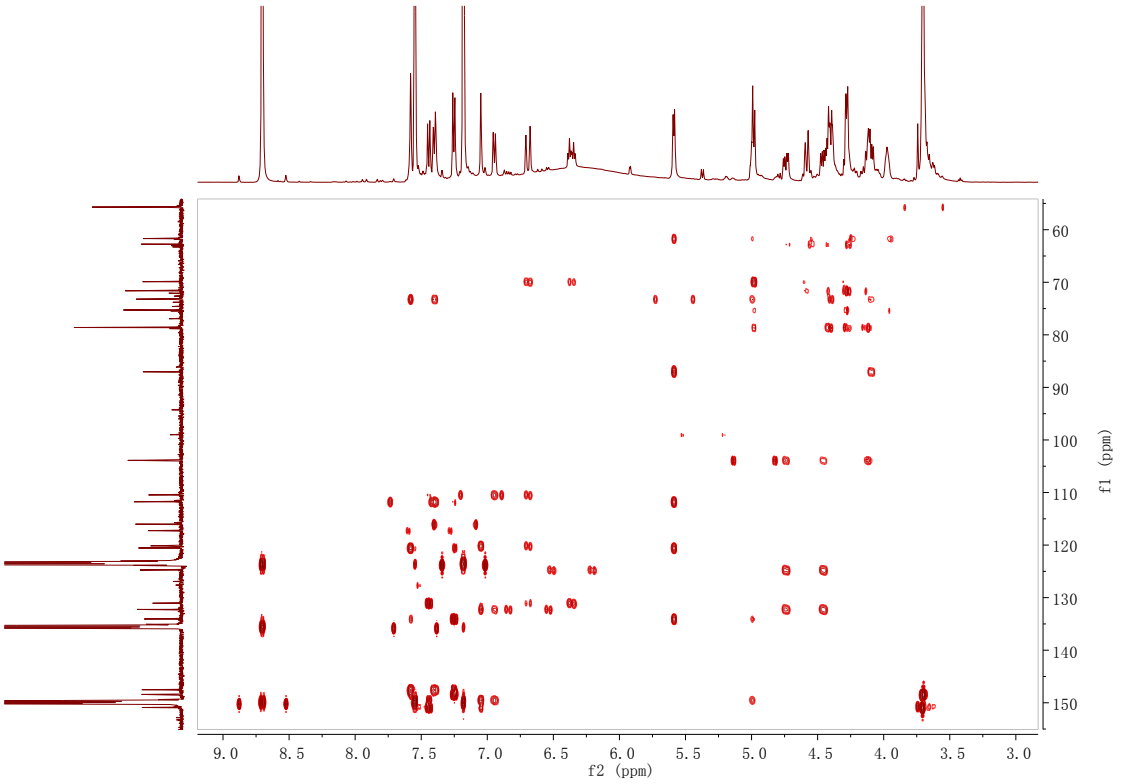


Figure S105. The HMBC spectrum of A-2 in C_5D_5N

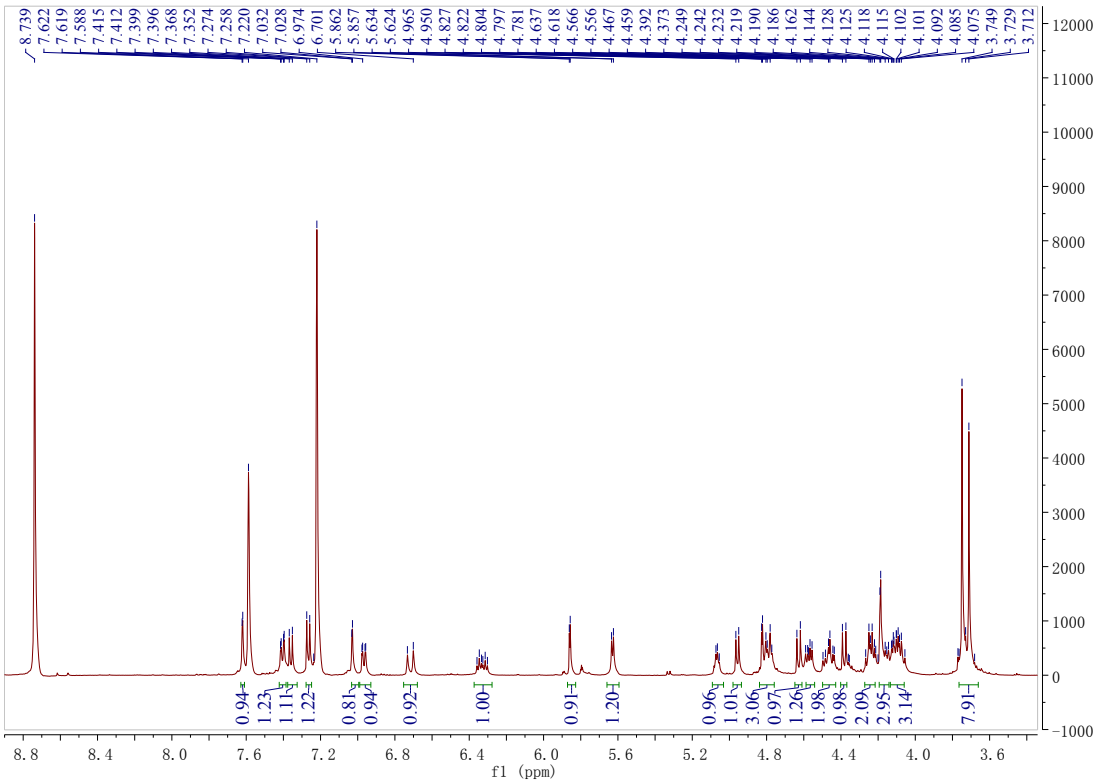


Figure S106. The ^{1}H-NMR spectrum of A-3 in C_5D_5N

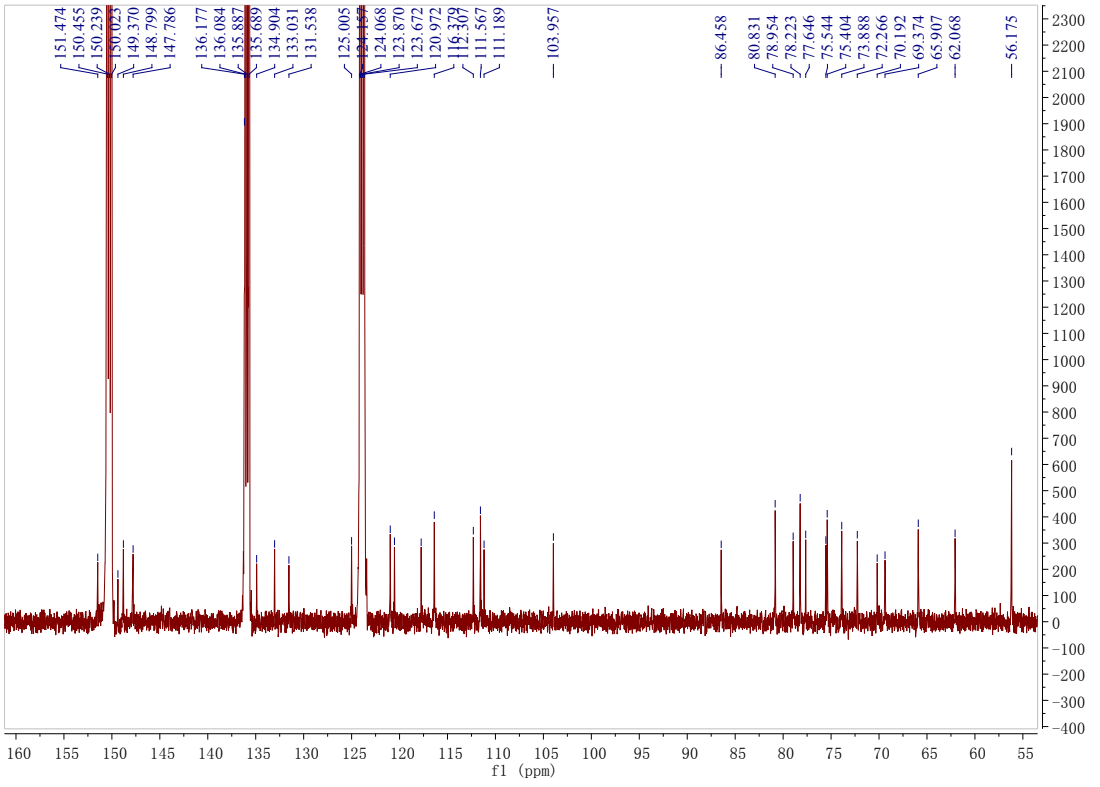


Figure S107. The ^{13}C-NMR spectrum of A-3 in C_5D_5N

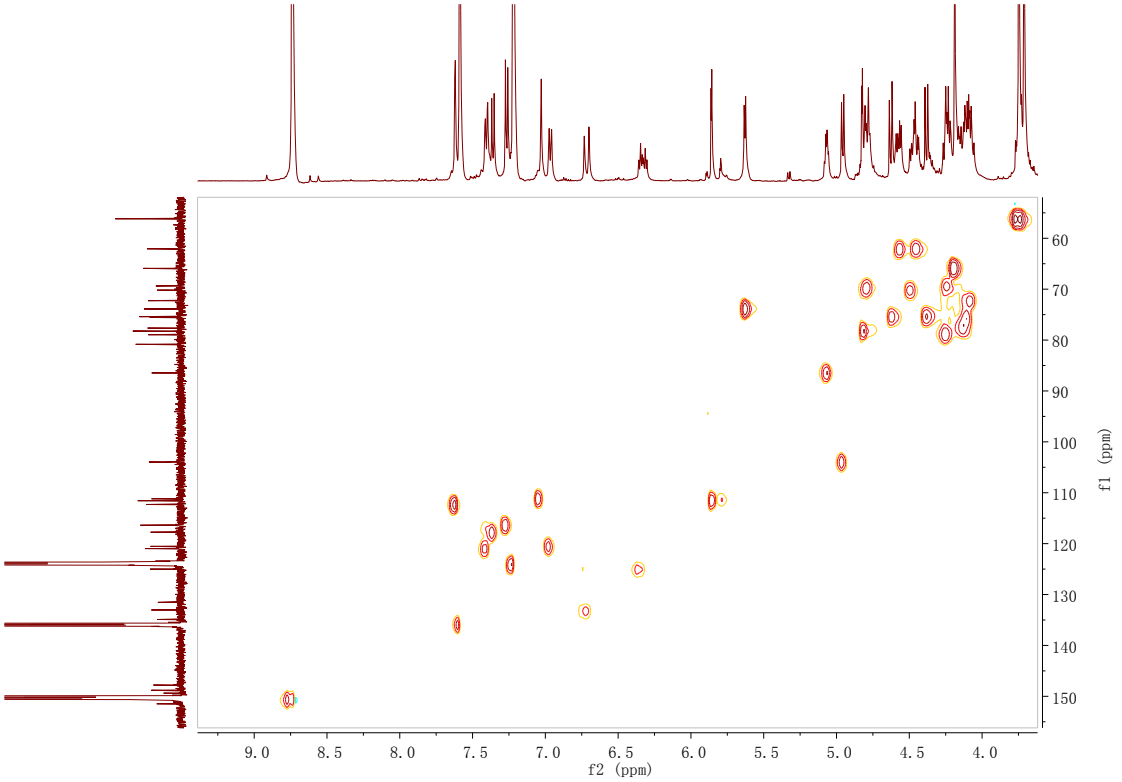


Figure S108. The HSQC spectrum of A-3 in C_5D_5N

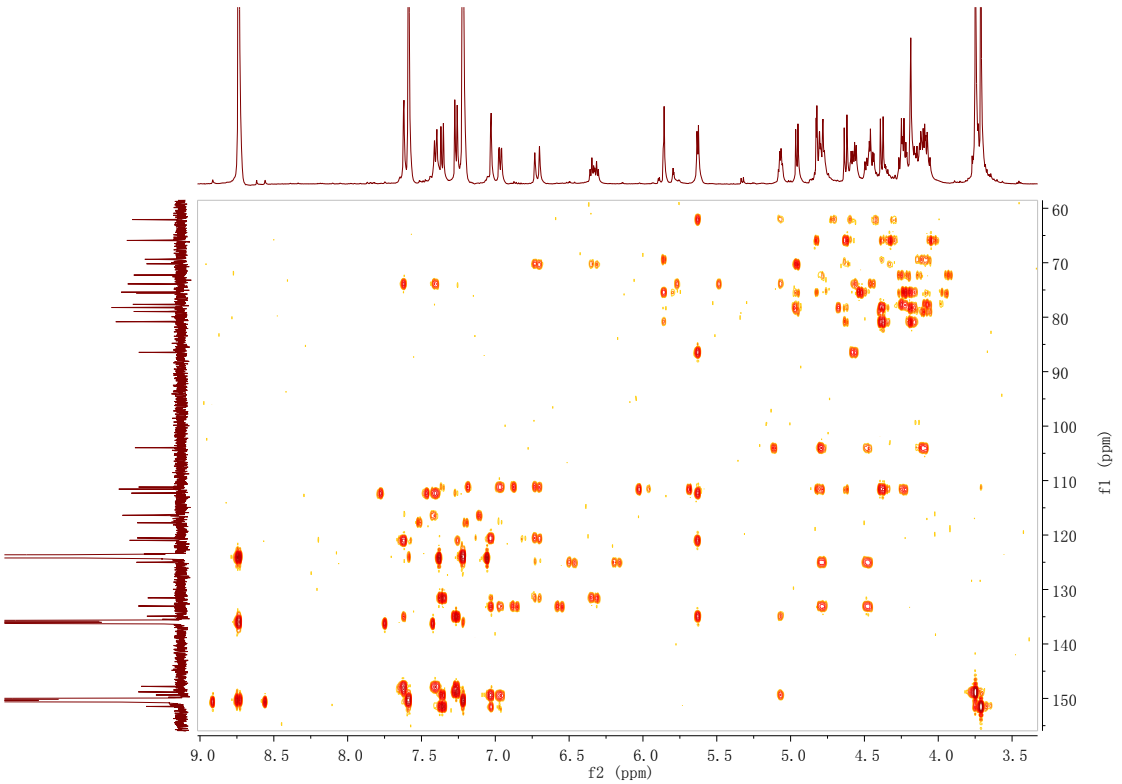


Figure S109. The HMBC spectrum of A-3 in C_5D_5N

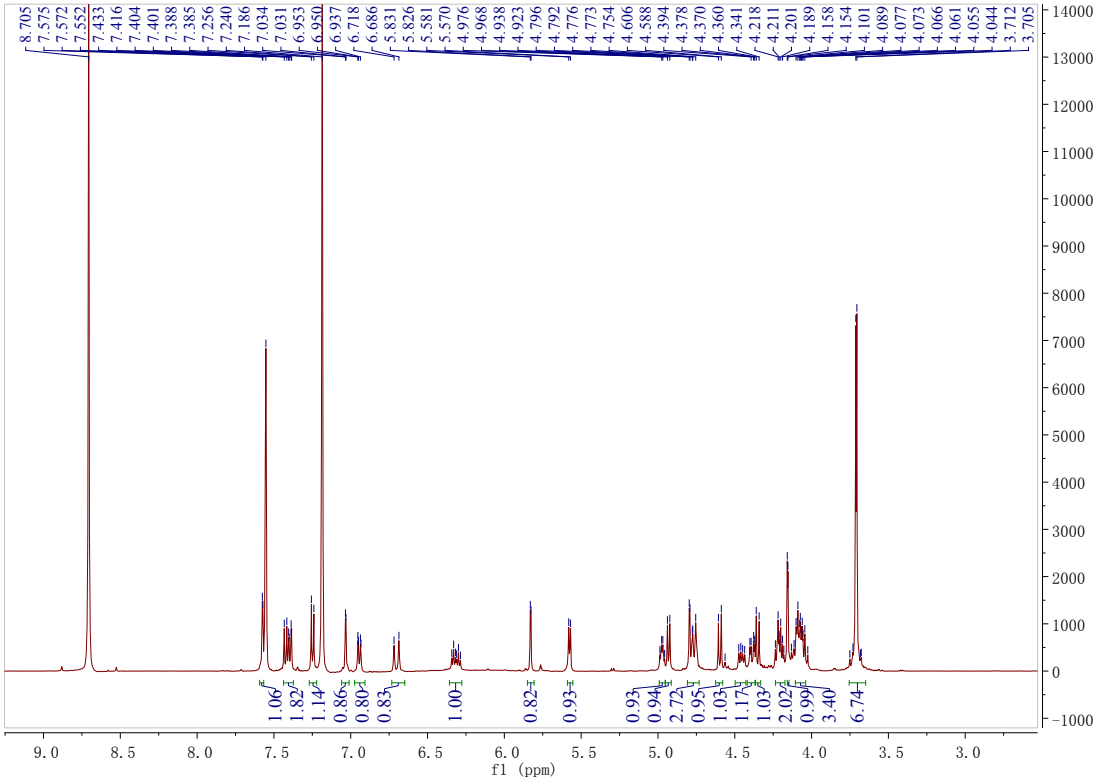


Figure S110. The ^{1}H-NMR spectrum of A-4 in C_5D_5N

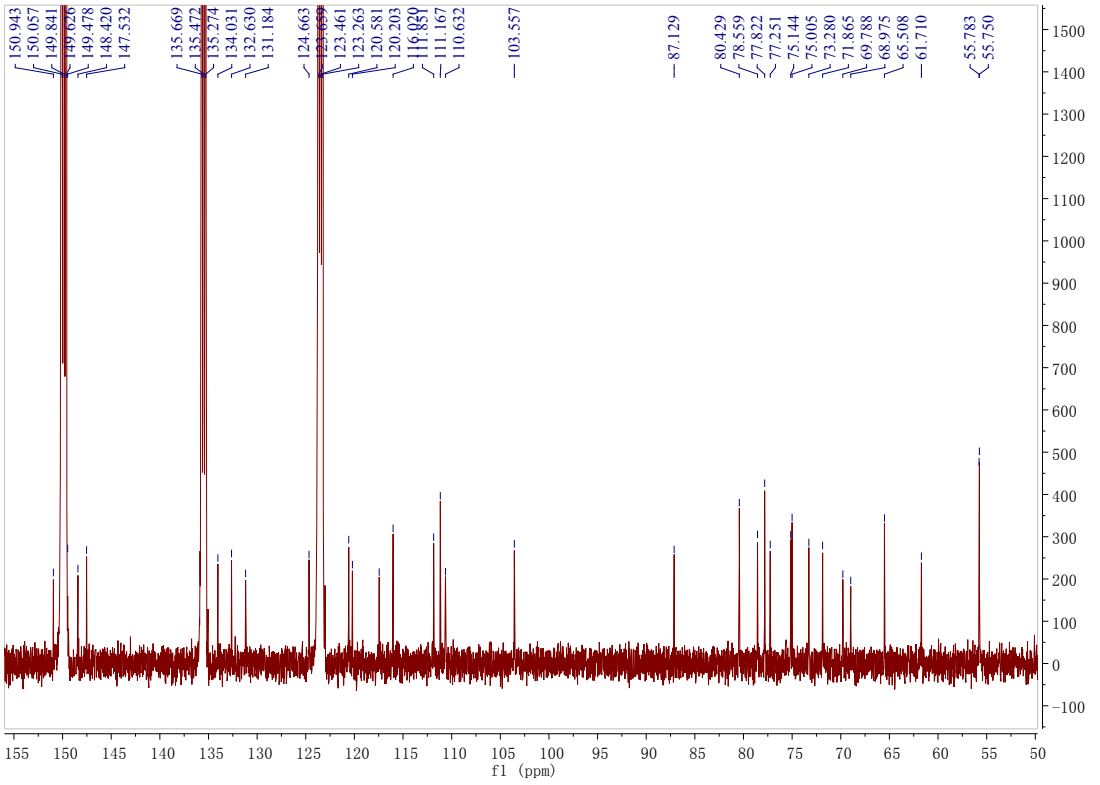


Figure S111. The ^{13}C-NMR spectrum of A-4 in C_5D_5N

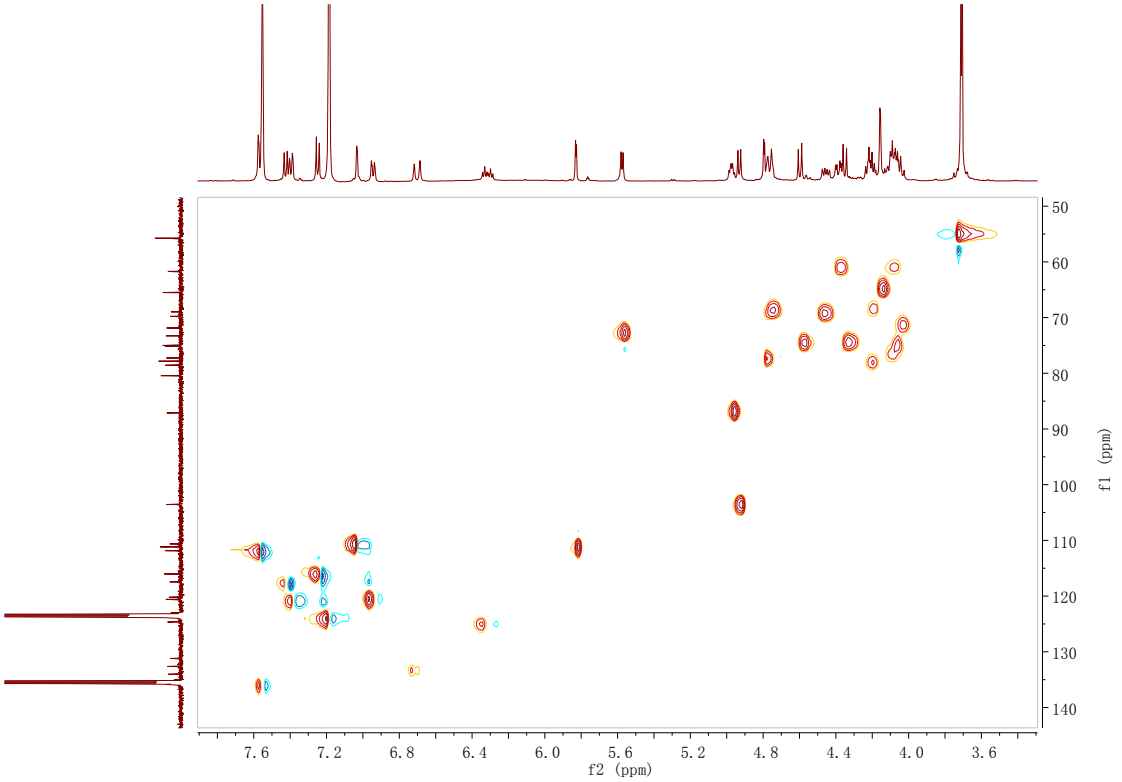


Figure S112. The HSQC spectrum of A-4 in C_5D_5N

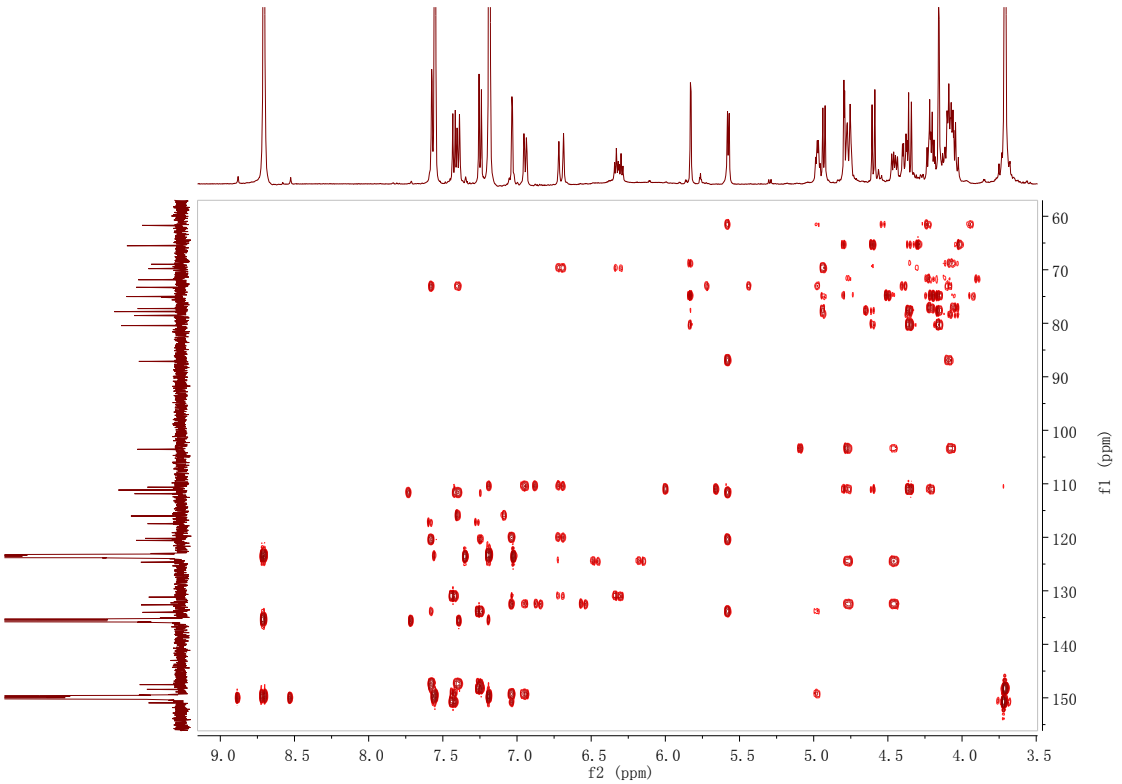


Figure S113. The HMBC spectrum of A-4 in C_5D_5N

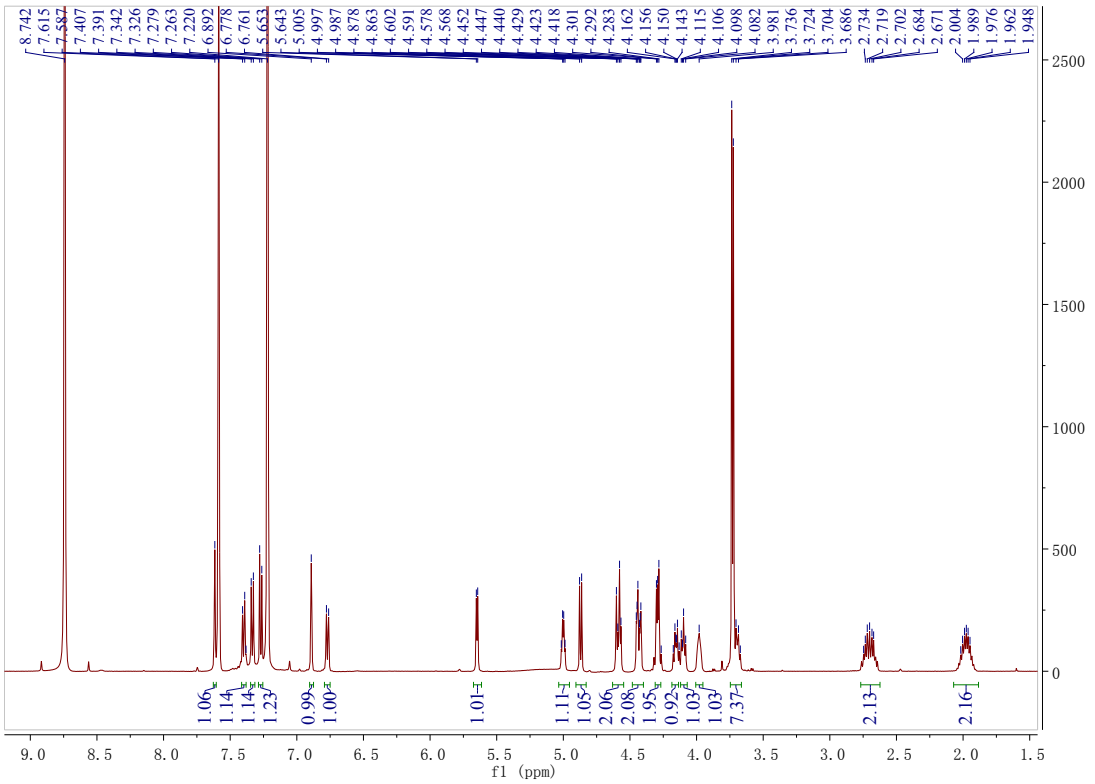


Figure S114. The ^{1}H-NMR spectrum of A-5 in C_5D_5N

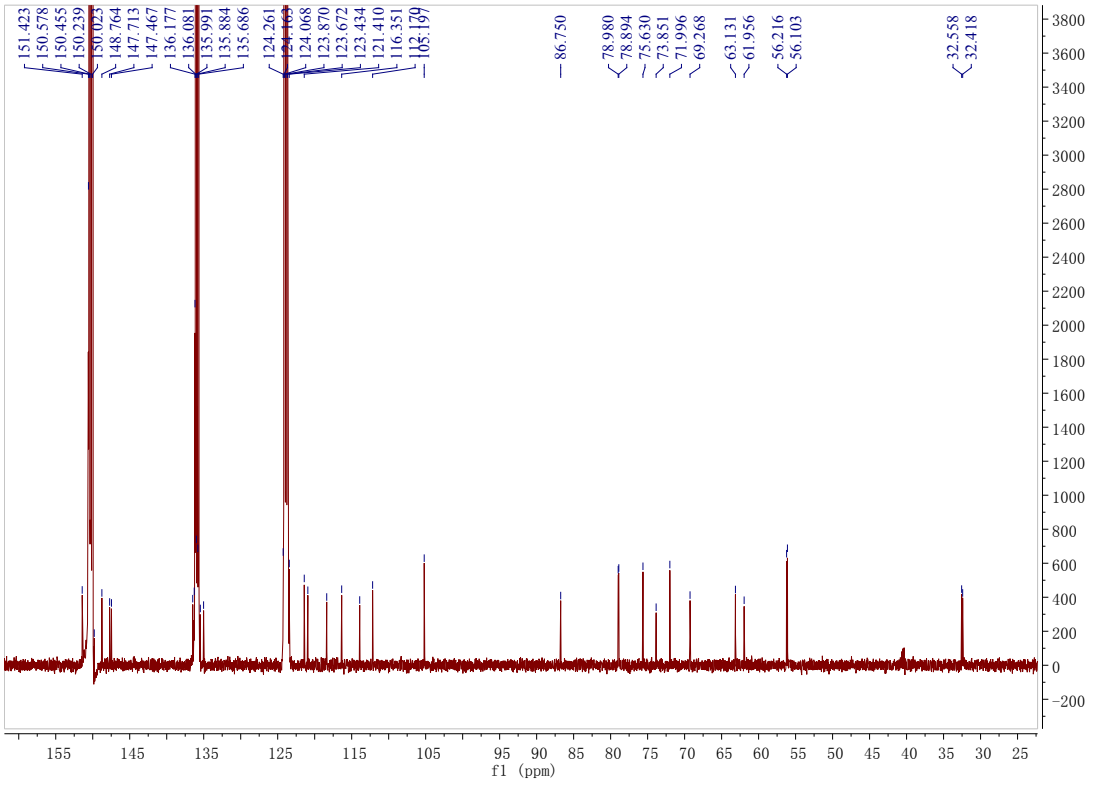


Figure S115. The ^{13}C-NMR spectrum of A-5 in C_5D_5N

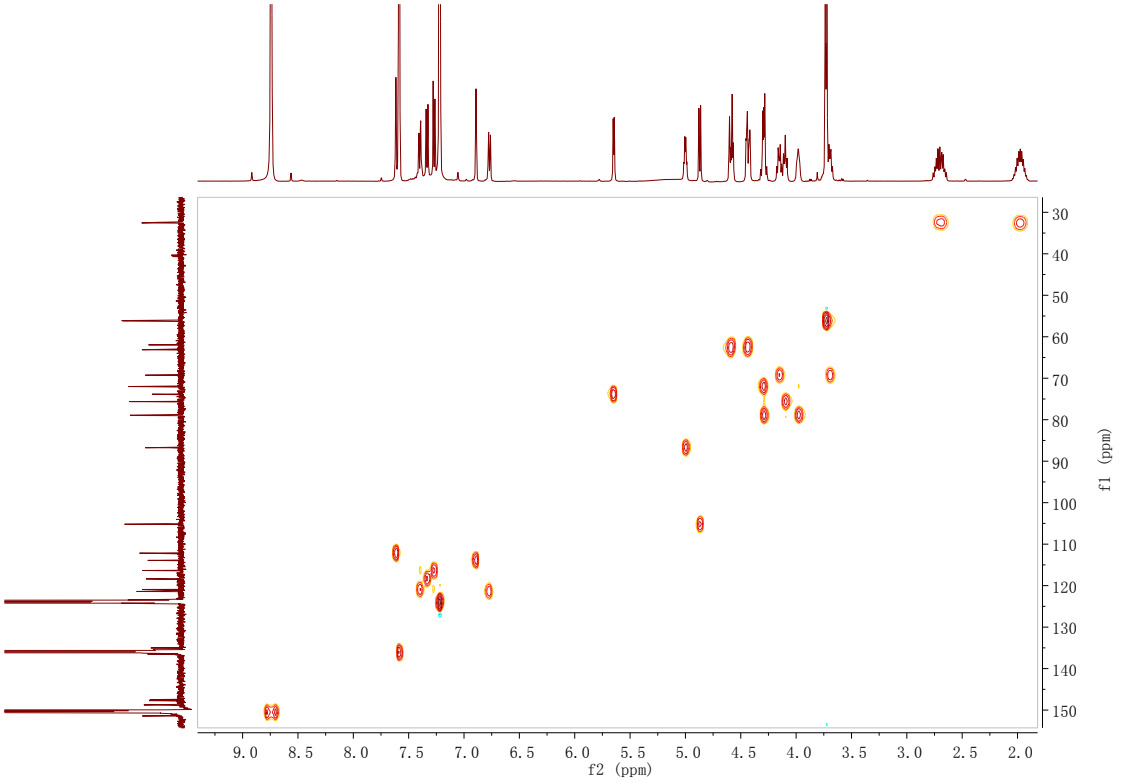


Figure S116. The HSQC spectrum of A-5 in C_5D_5N

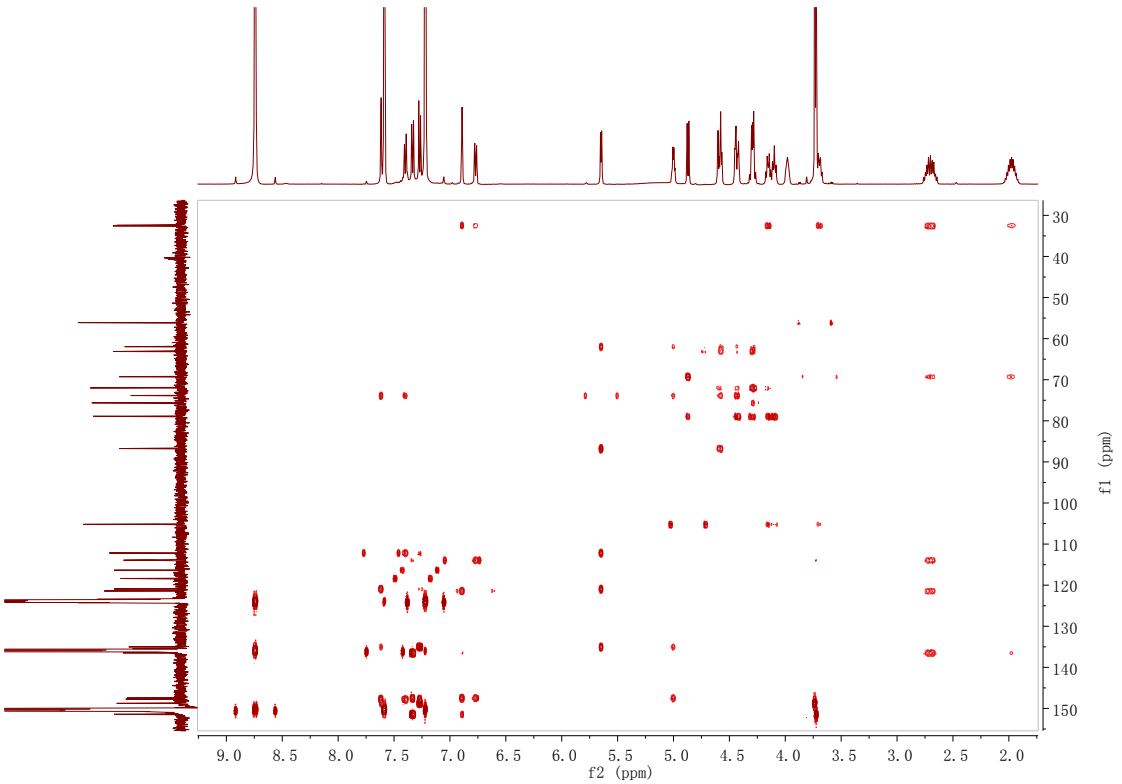


Figure S117. The HMBC spectrum of A-5 in C_5D_5N

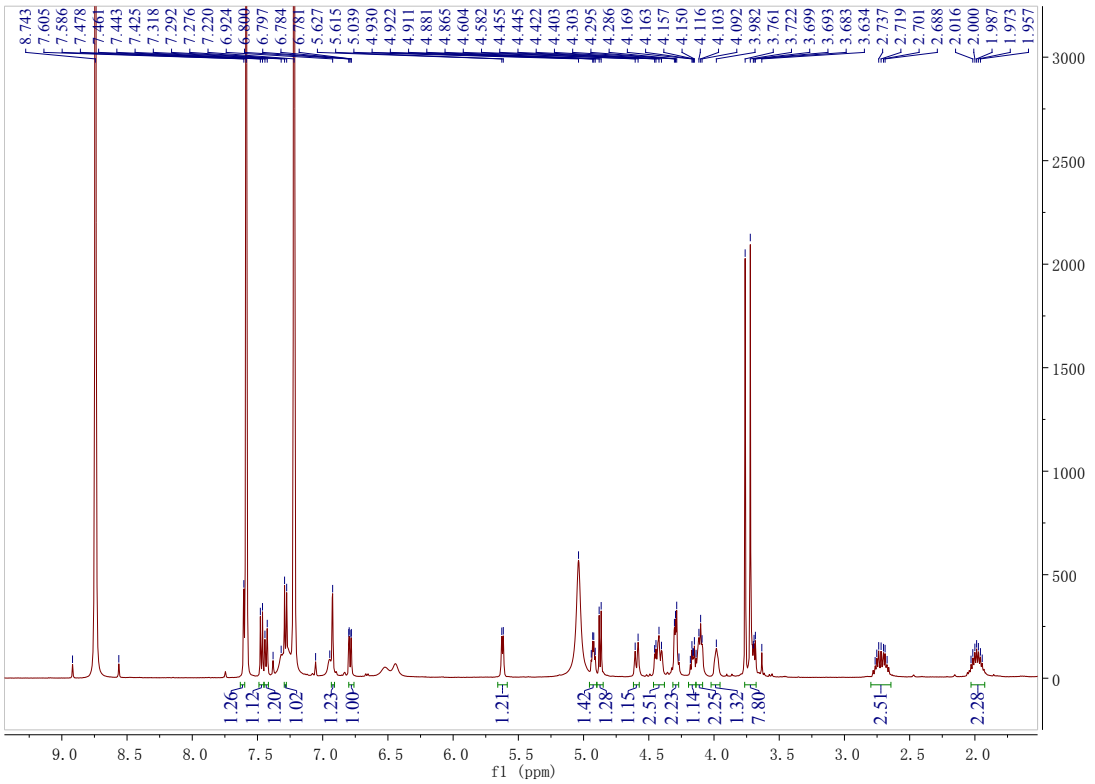


Figure S118. The ^{1}H-NMR spectrum of A-6 in C_5D_5N

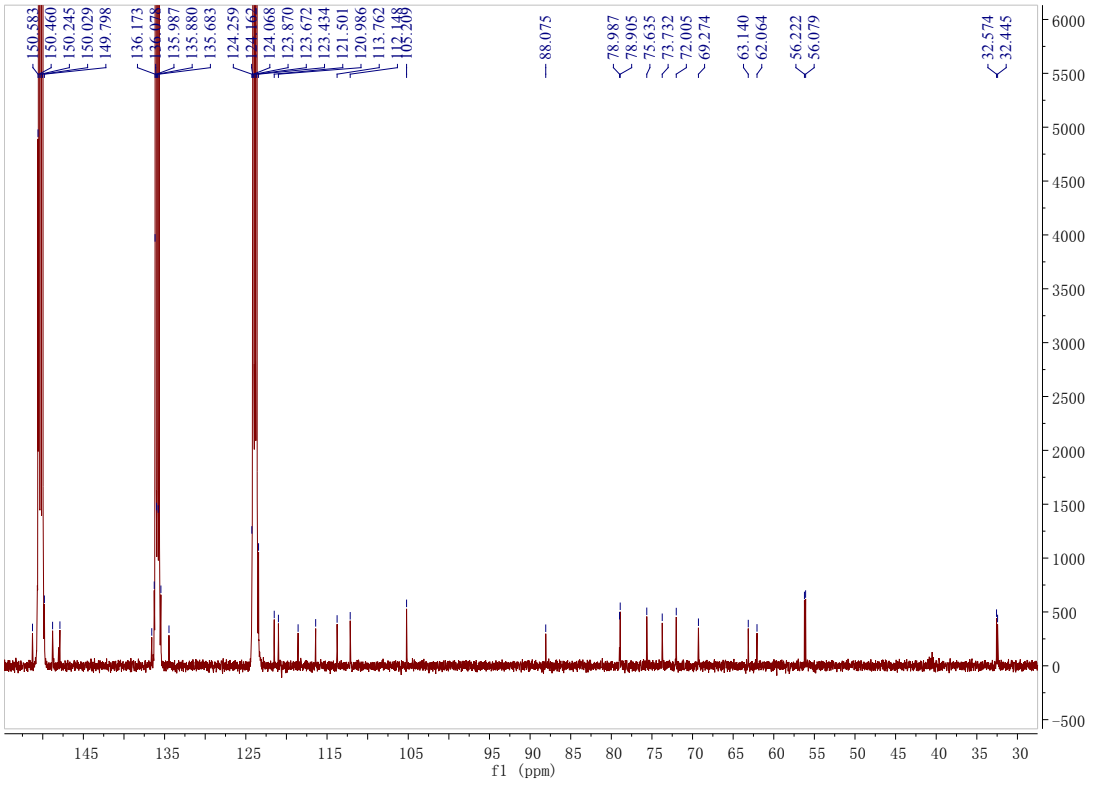


Figure S119. The ^{13}C-NMR spectrum of A-6 in C_5D_5N

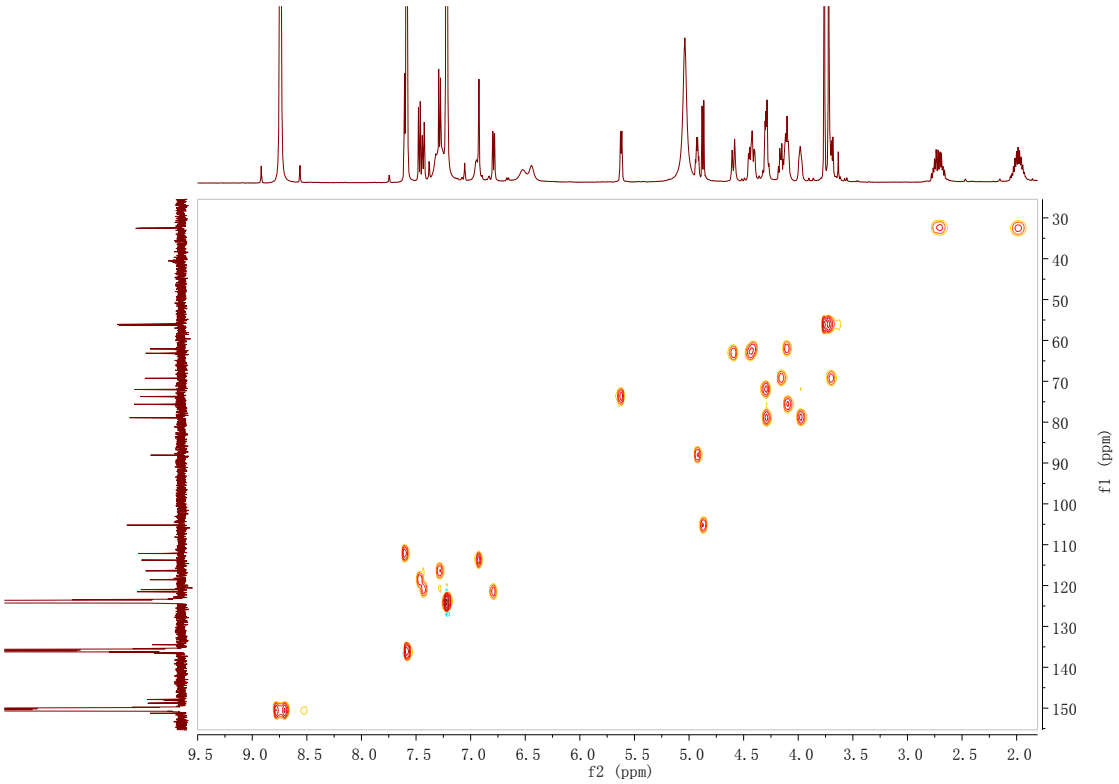


Figure S120. The HSQC spectrum of A-6 in C_5D_5N

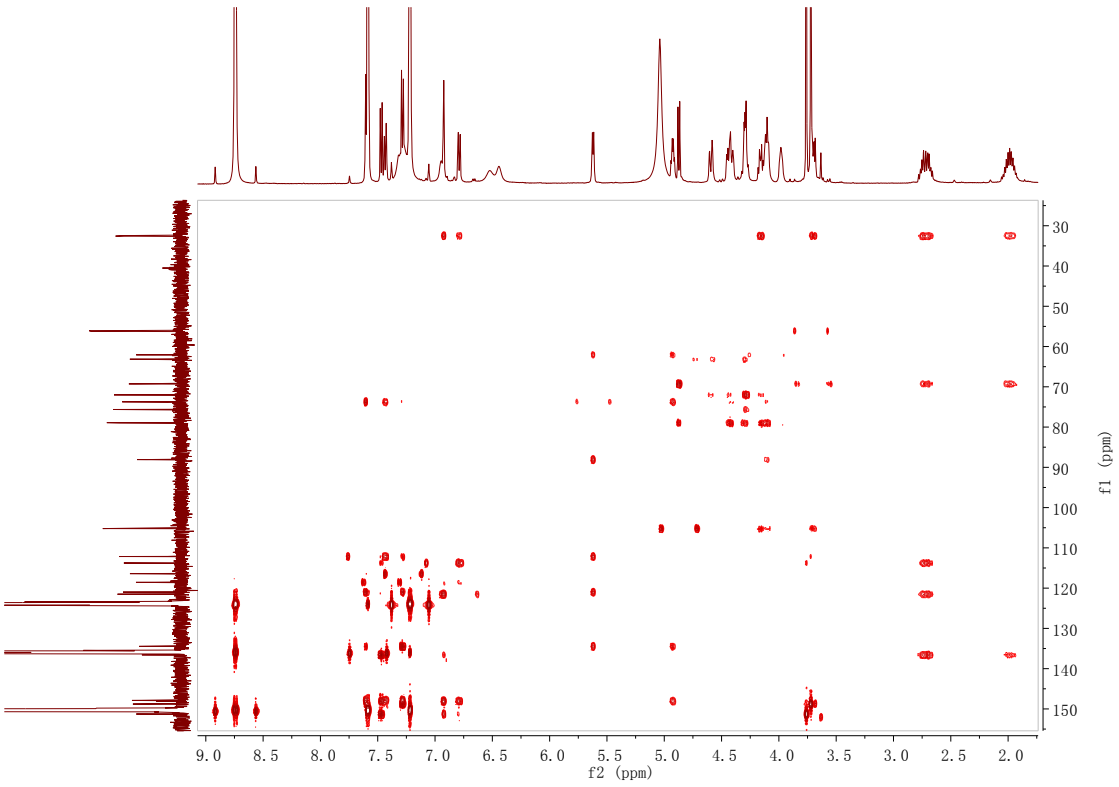


Figure S121. The HMBC spectrum of A-6 in C_5D_5N

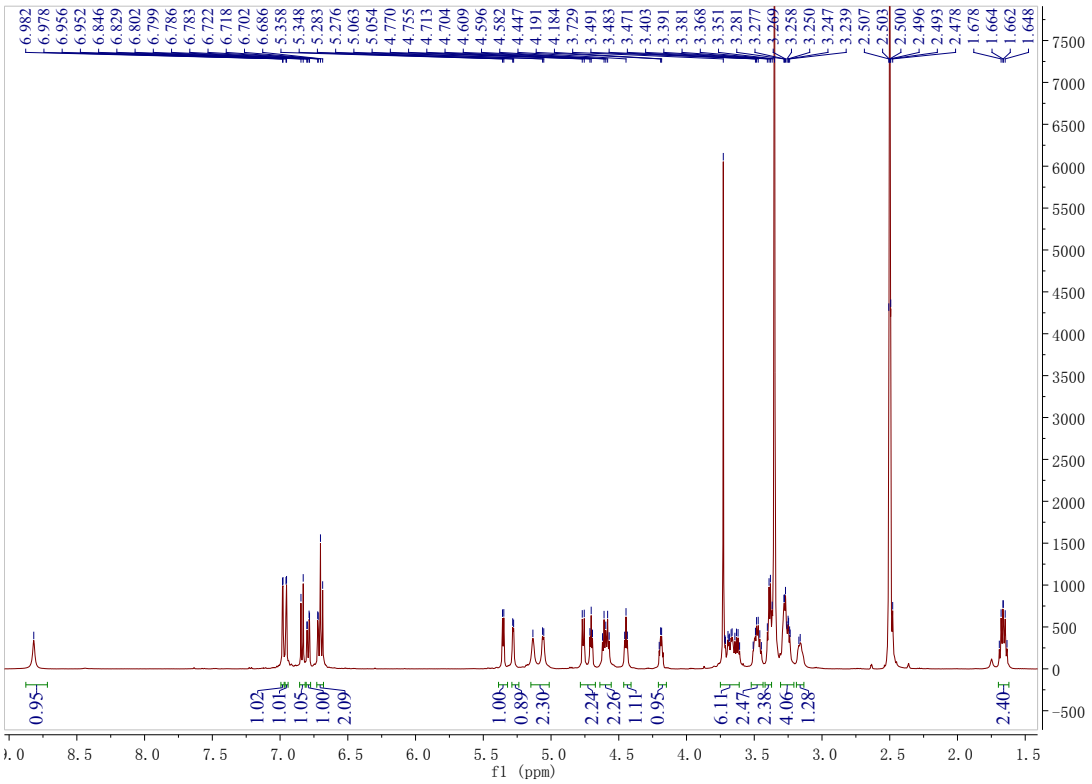


Figure S122. The ^{1}H-NMR spectrum of B-1 in DMSO-d_6

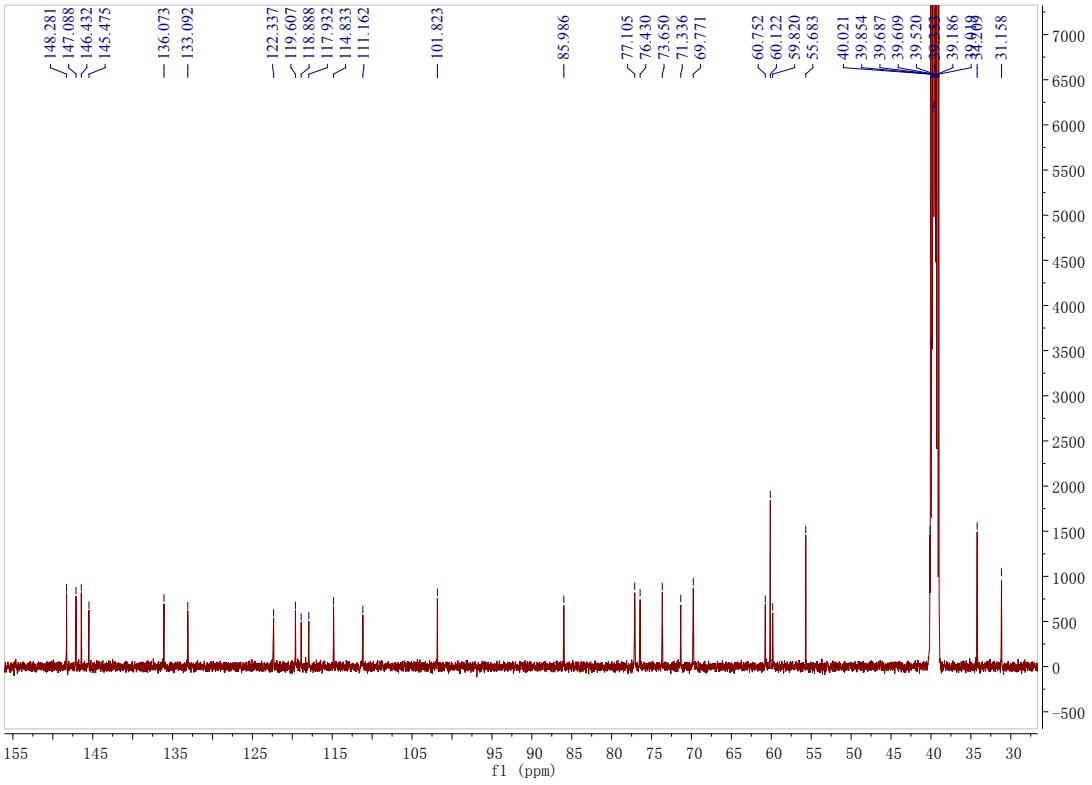


Figure S123. The ^{13}C-NMR spectrum of B-1 in DMSO-d_6

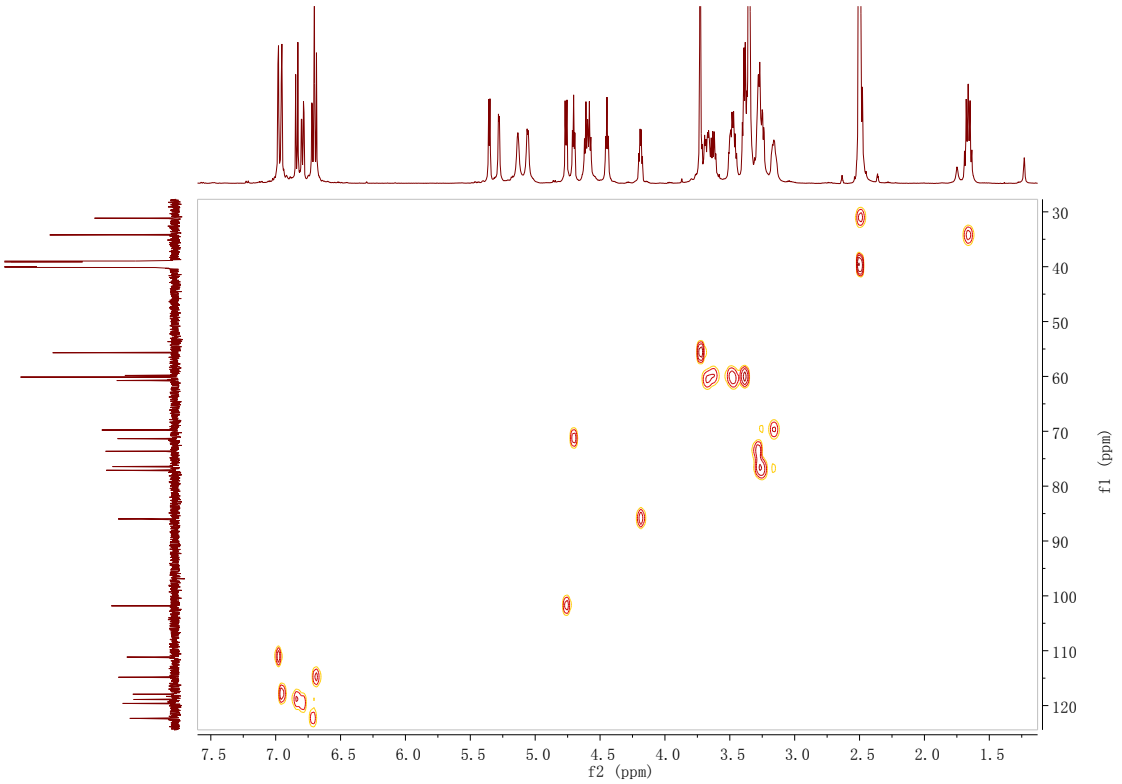


Figure S124. The HSQC spectrum of B-1 in DMSO-d_6

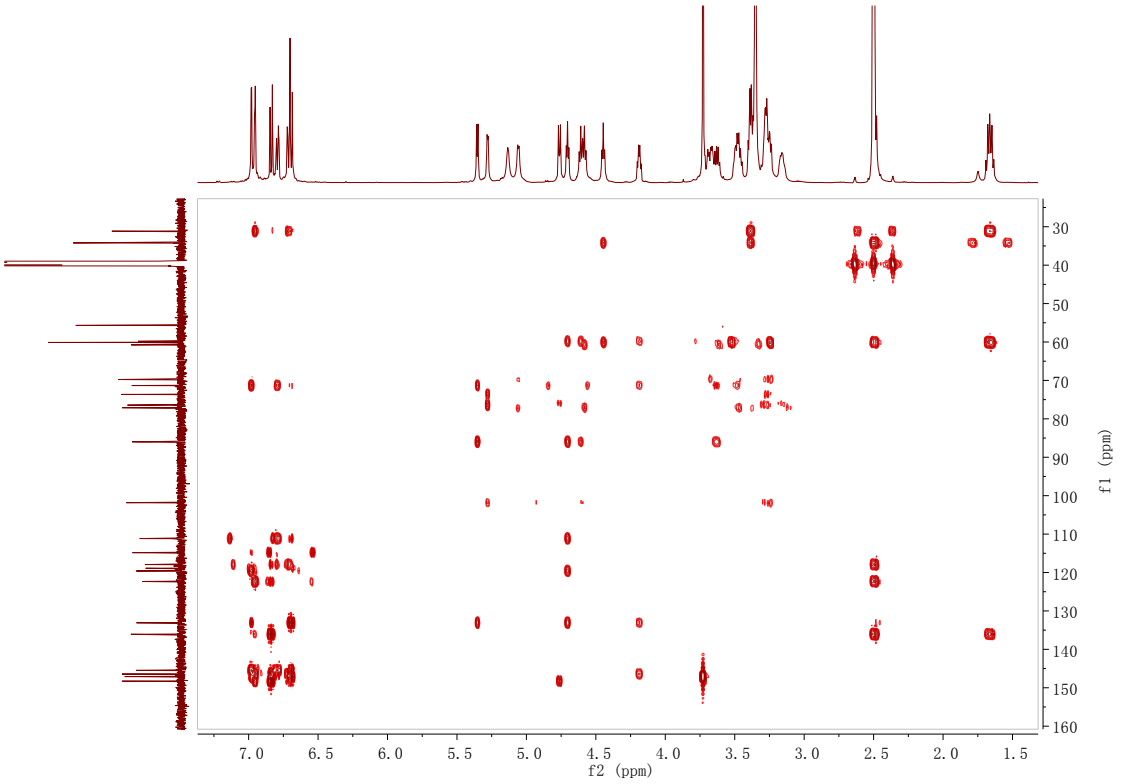


Figure S125. The HMBC spectrum of B-1 in DMSO-d_6

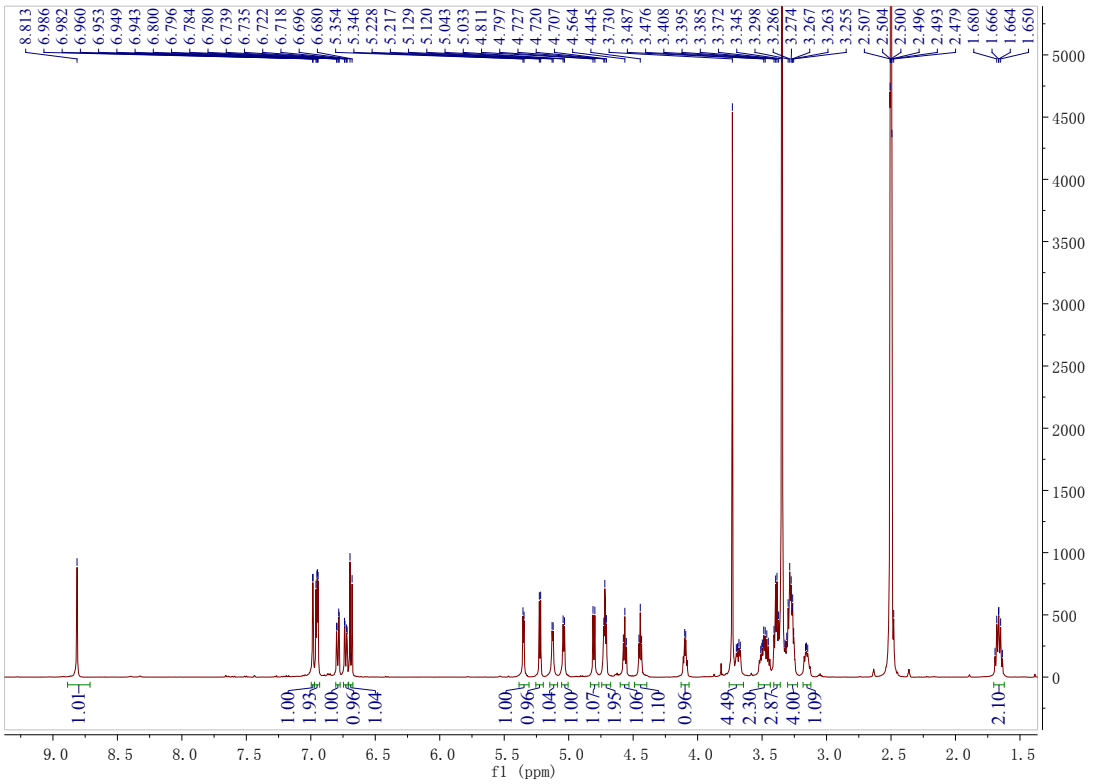


Figure S126. The ^{1}H-NMR spectrum of B-2 in DMSO-d_6

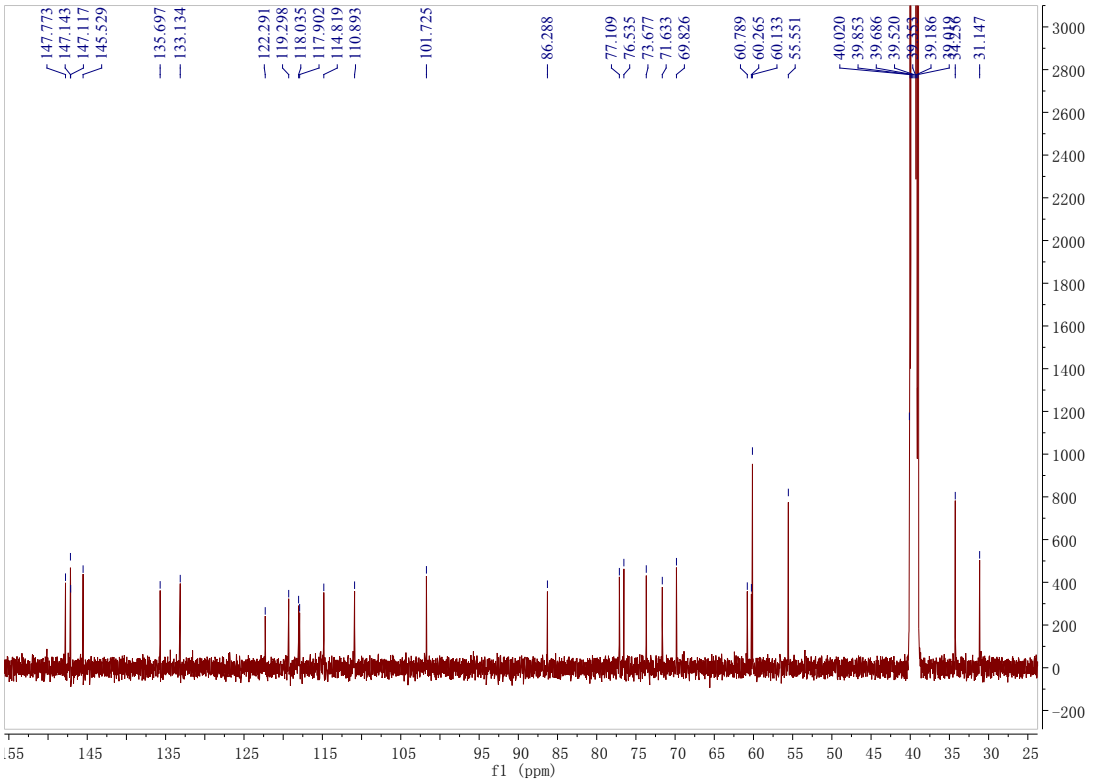


Figure S127. The ^{13}C-NMR spectrum of B-2 in DMSO-d_6

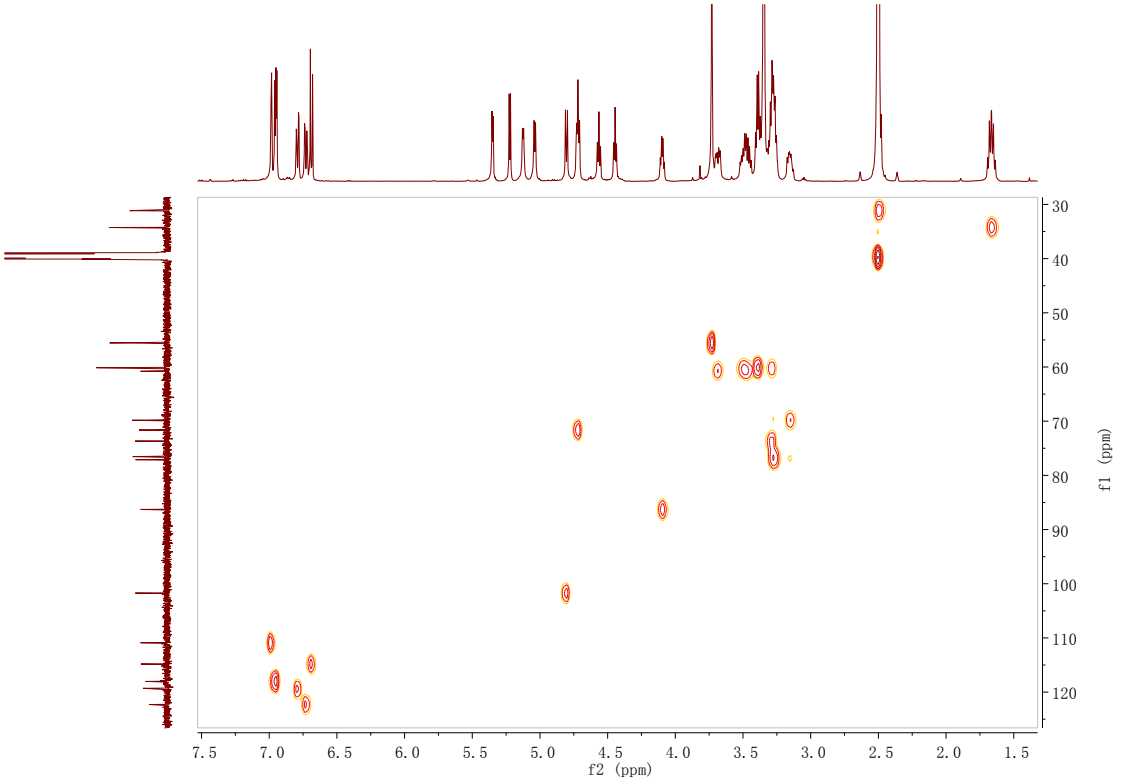


Figure S128. The HSQC spectrum of B-2 in DMSO-d_6

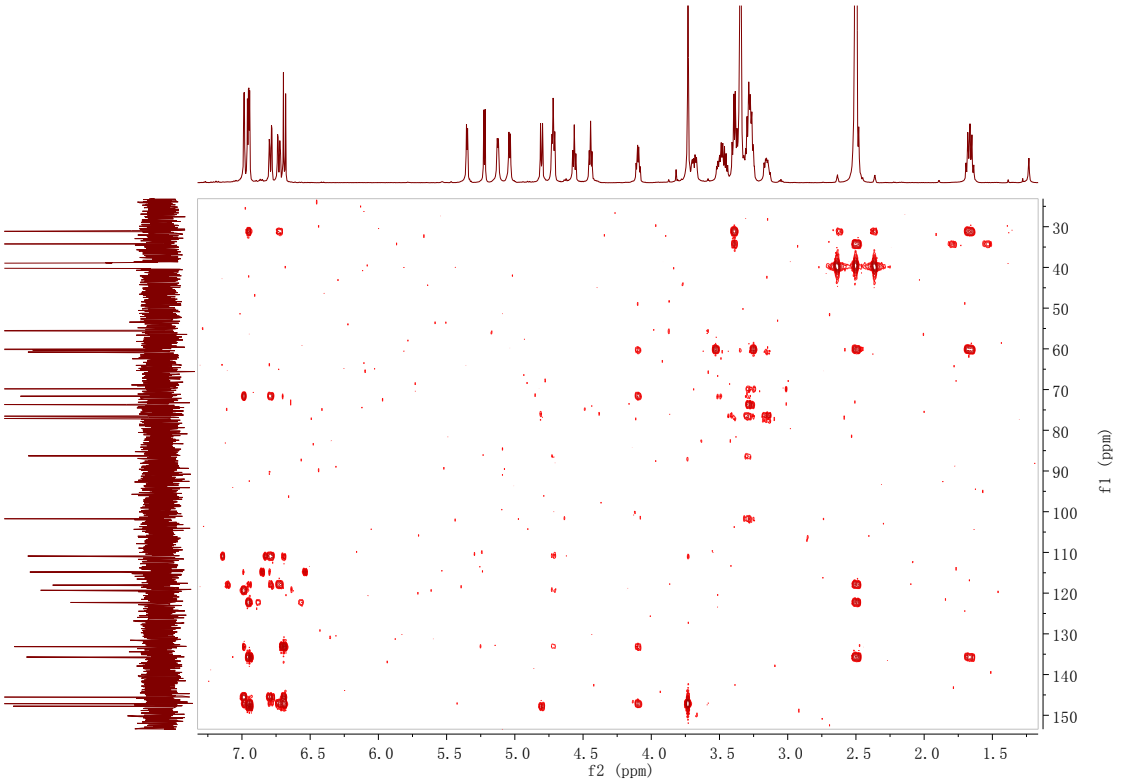


Figure S129. The HMBC spectrum of B-2 in DMSO-d_6

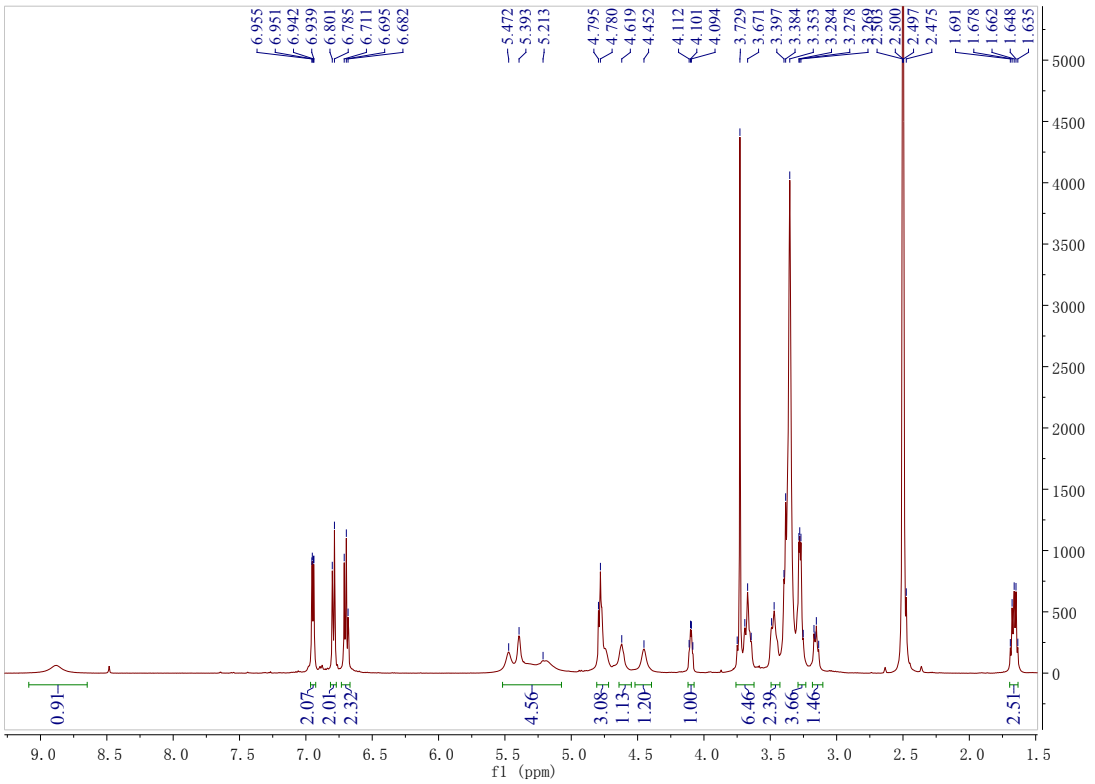


Figure S130. The ^{1}H-NMR spectrum of B-3 in DMSO-d_6

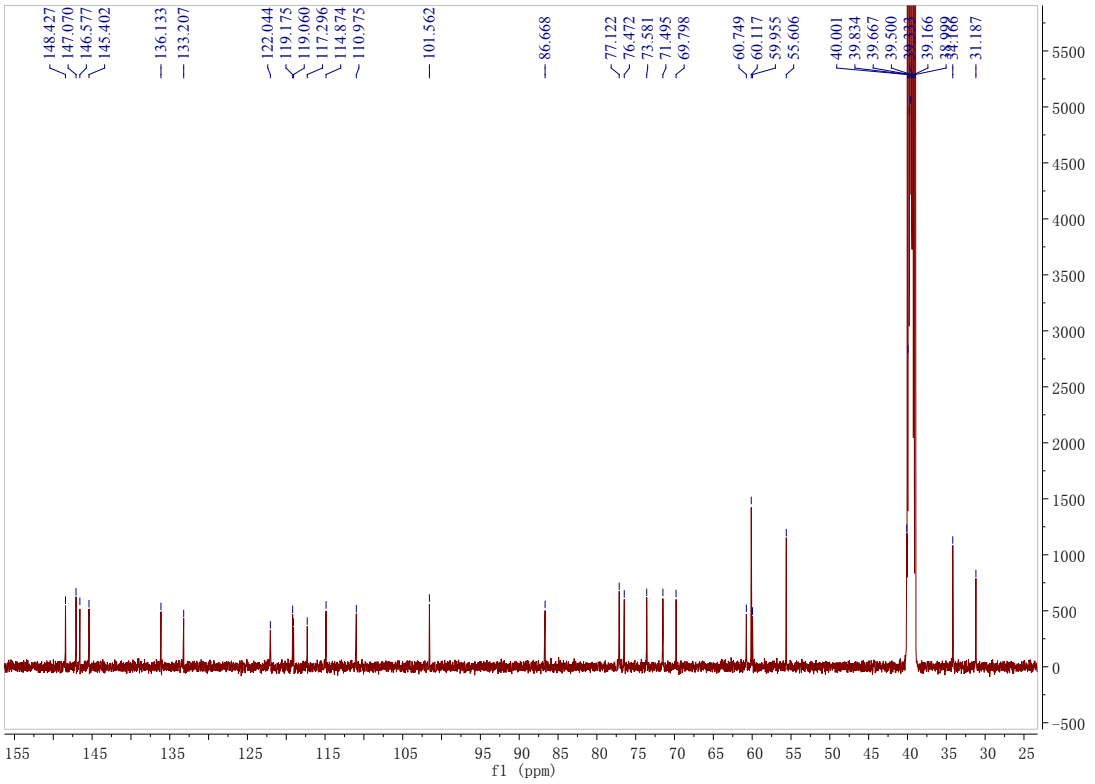


Figure S131. The ^{13}C-NMR spectrum of B-3 in DMSO-d_6

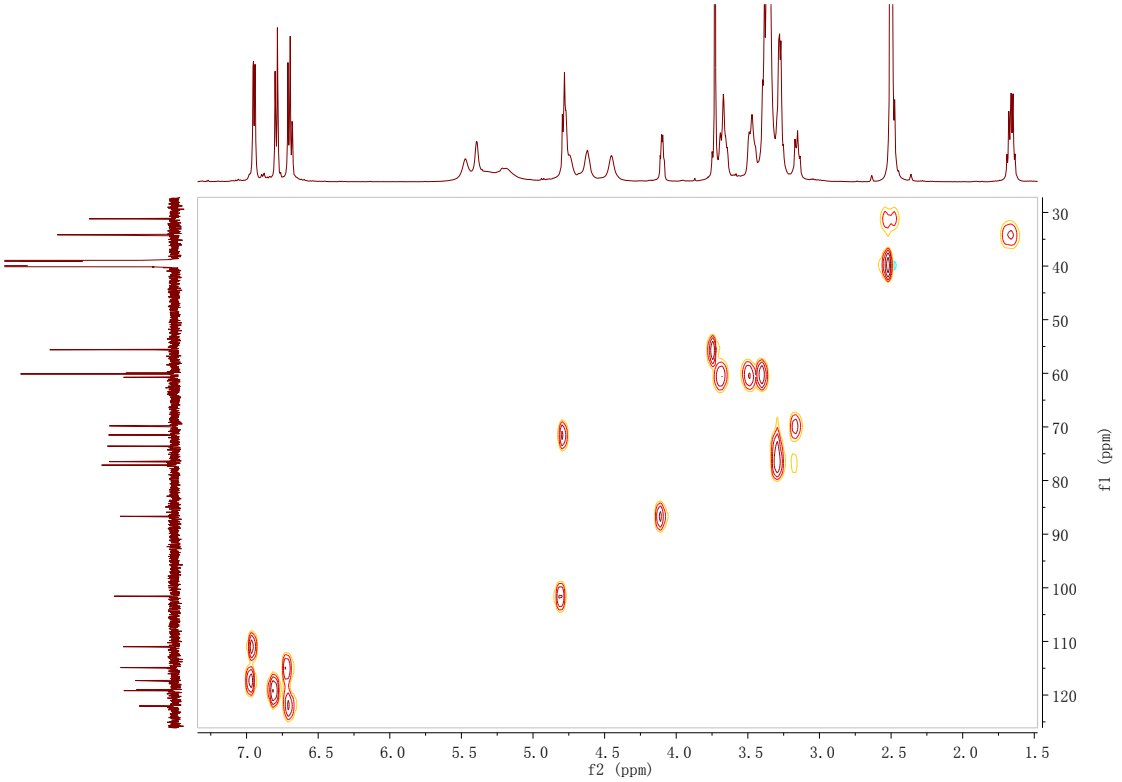


Figure S132. The HSQC spectrum of B-3 in DMSO-d_6

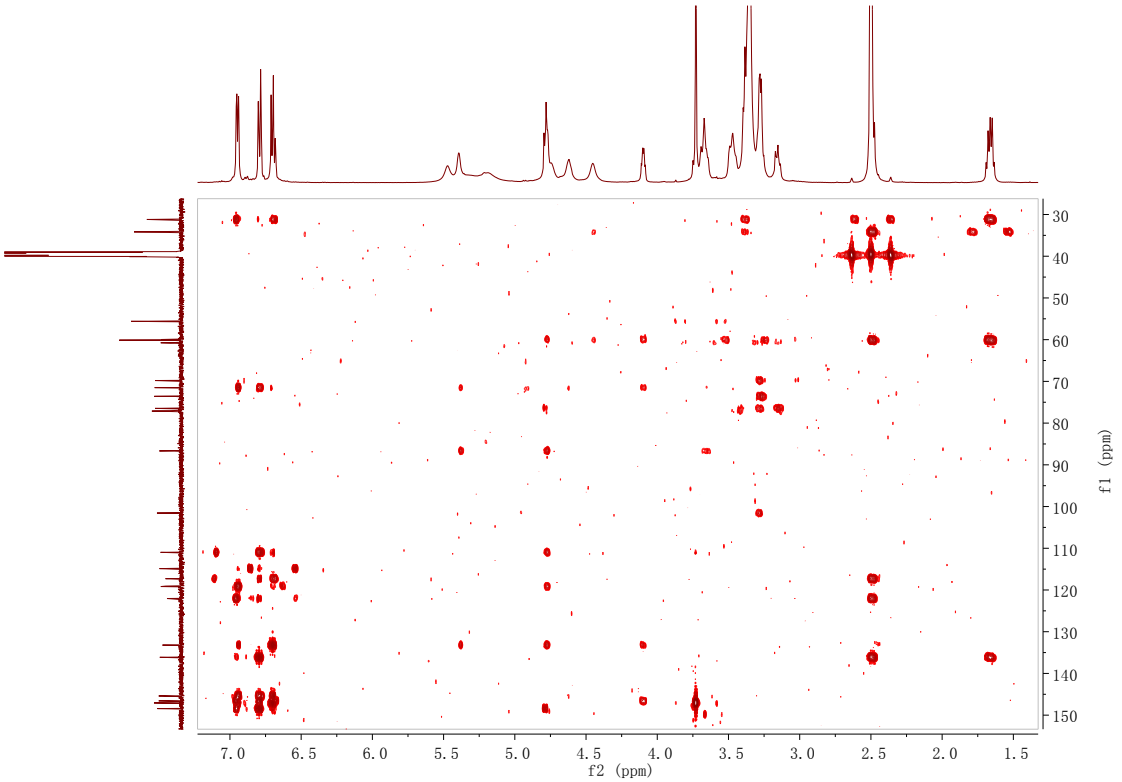


Figure S133. The HMBC spectrum of B-3 in DMSO-d_6

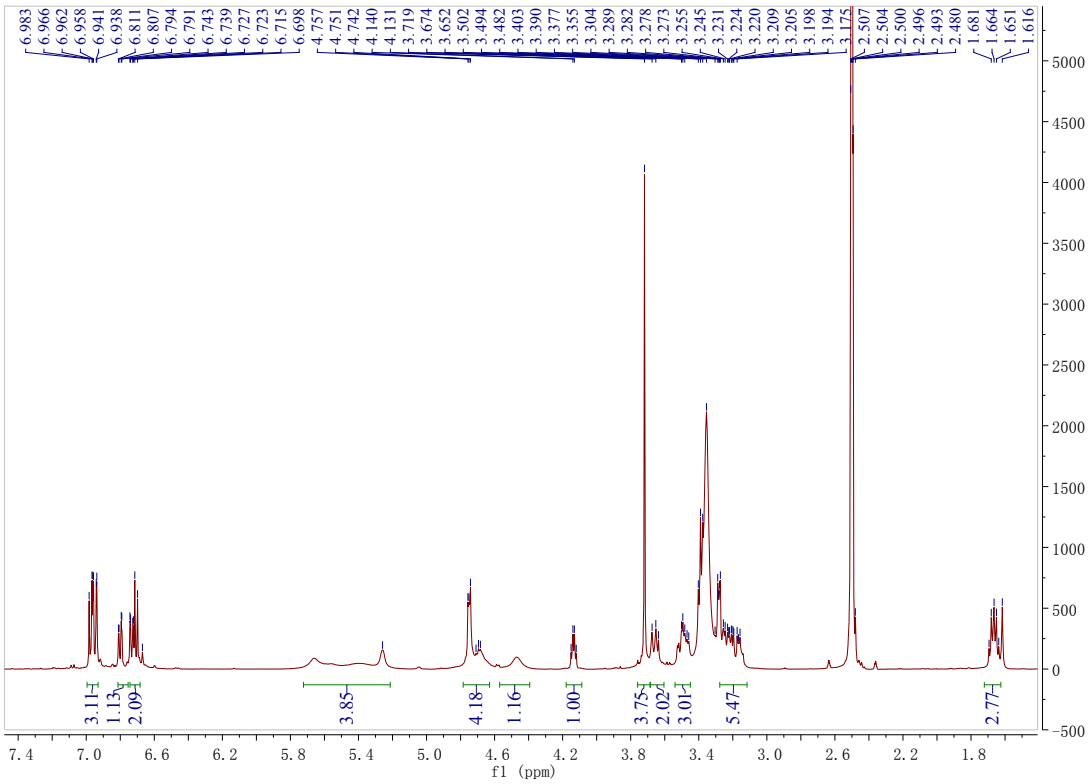


Figure S134. The ^{1}H-NMR spectrum of B-4 in DMSO-d_6

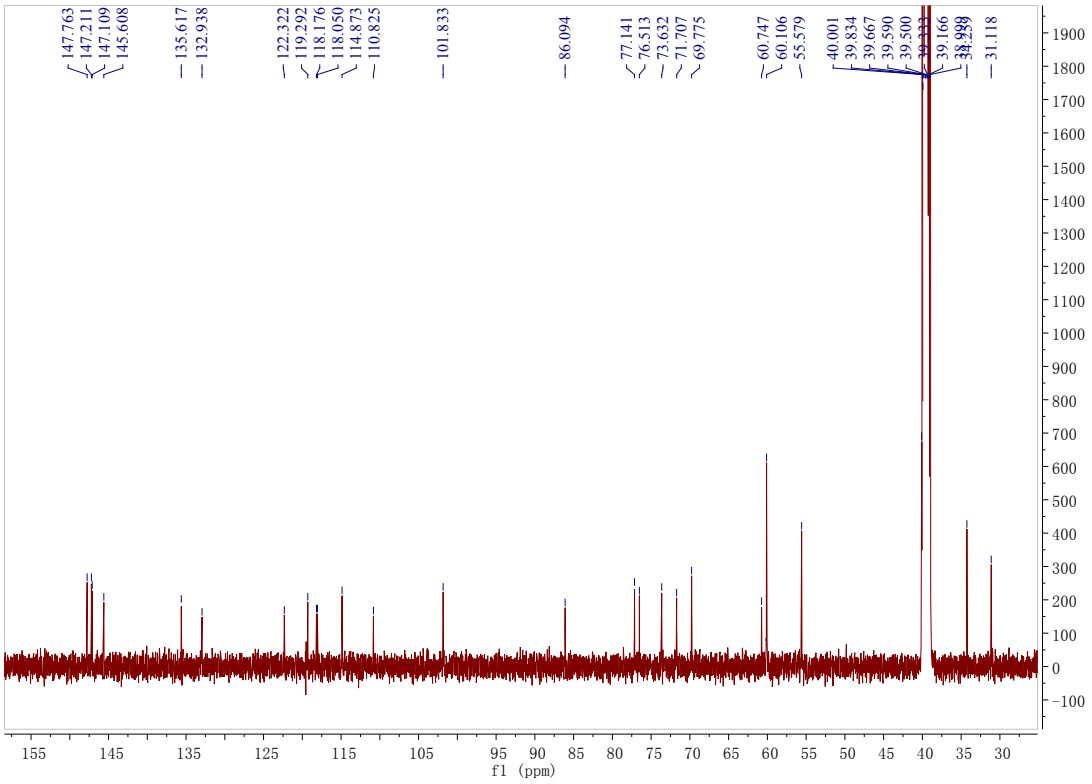


Figure S135. The ^{13}C-NMR spectrum of B-4 in DMSO-d_6

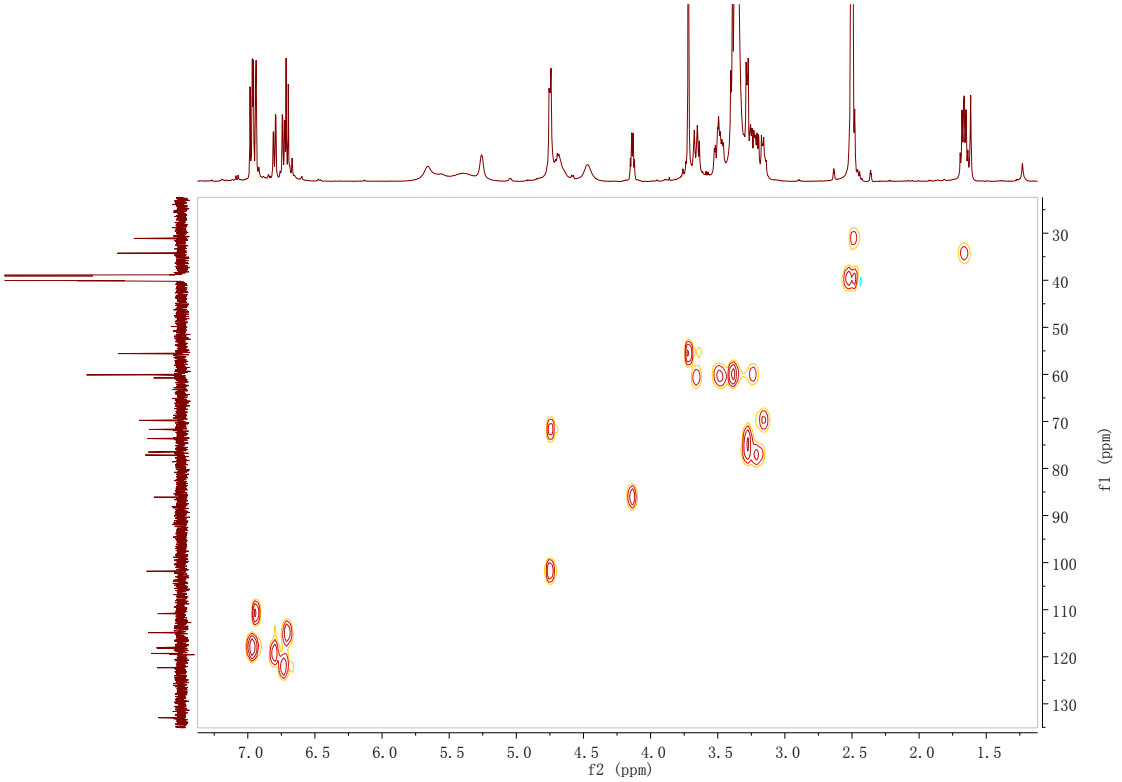


Figure S136. The HSQC spectrum of B-4 in DMSO-d_6

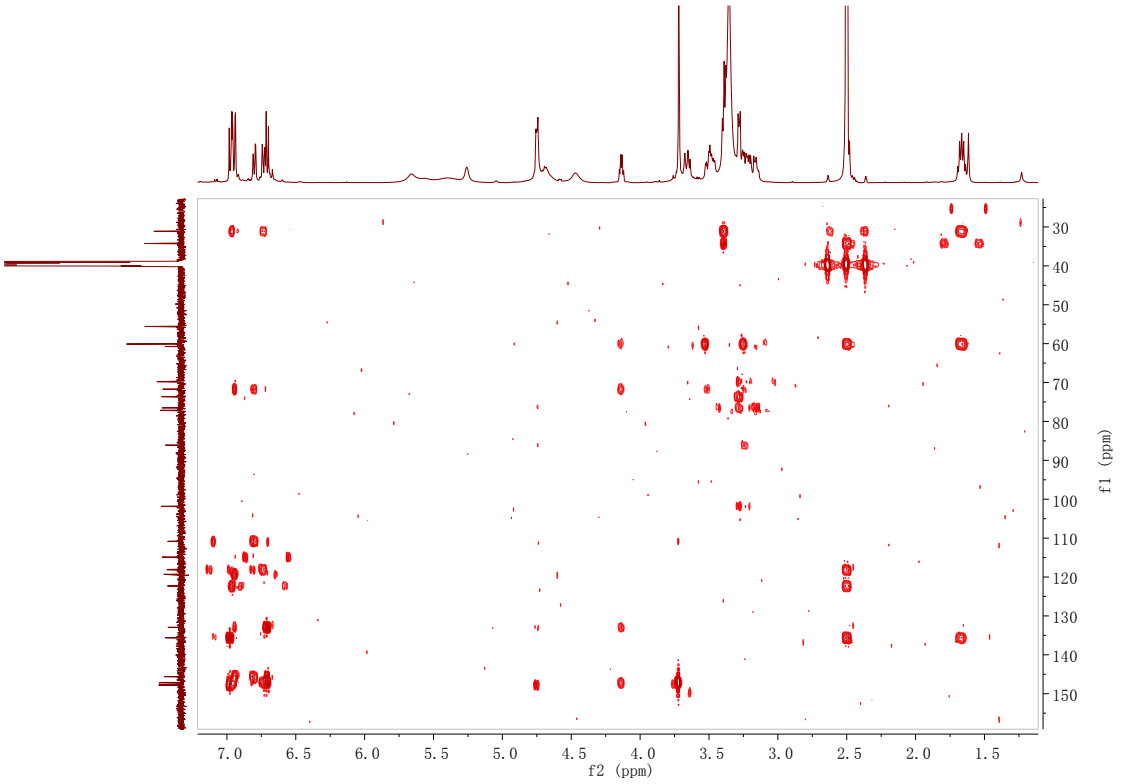


Figure S137. The HMBC spectrum of B-4 in DMSO-d_6

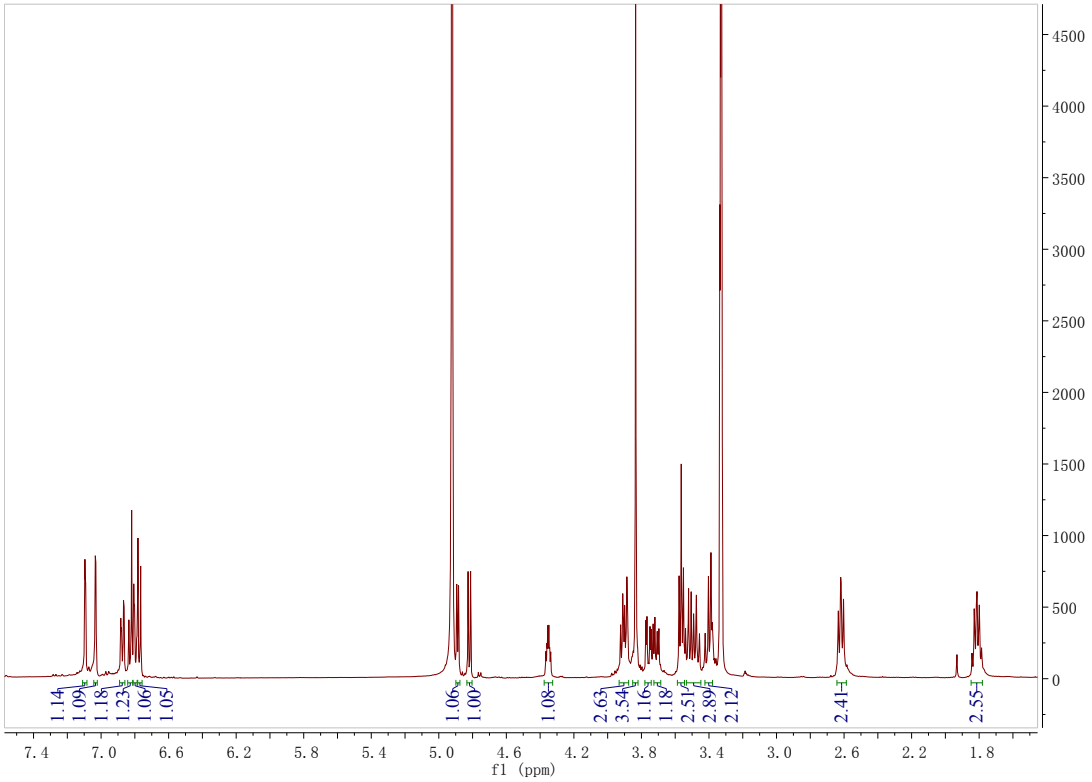


Figure S138. The ^{1}H-NMR spectrum of B-1 in CD_3OD

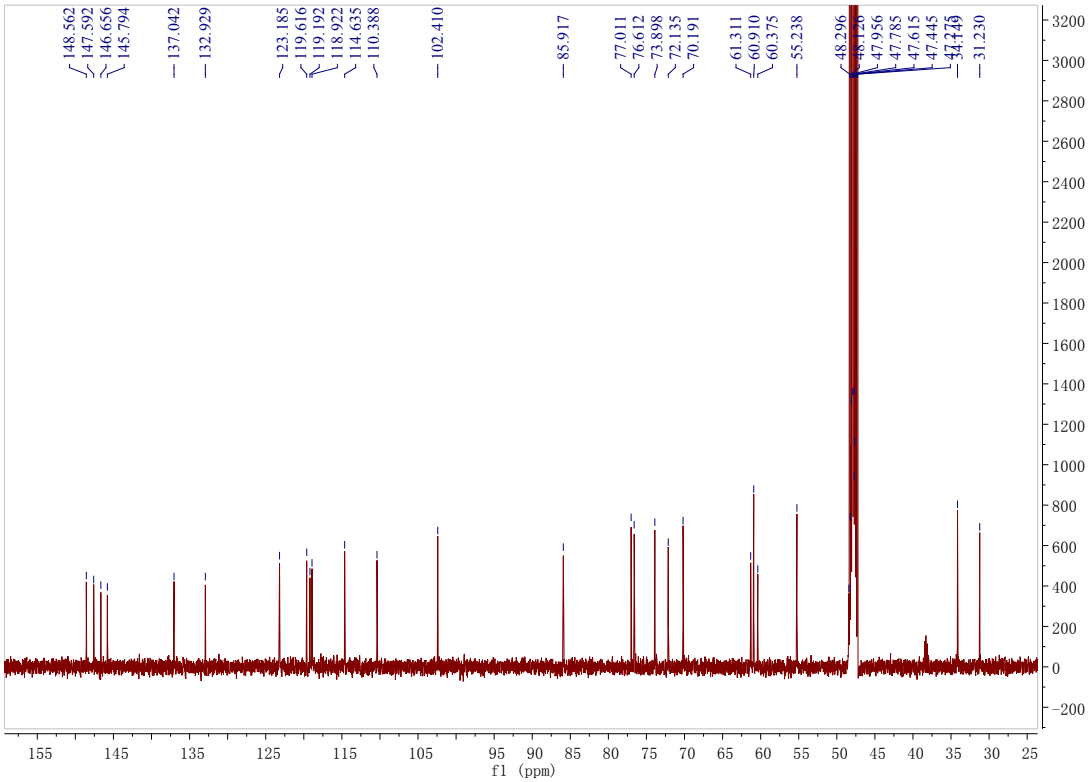


Figure S139. The ^{13}C-NMR spectrum of B-1 in CD_3OD

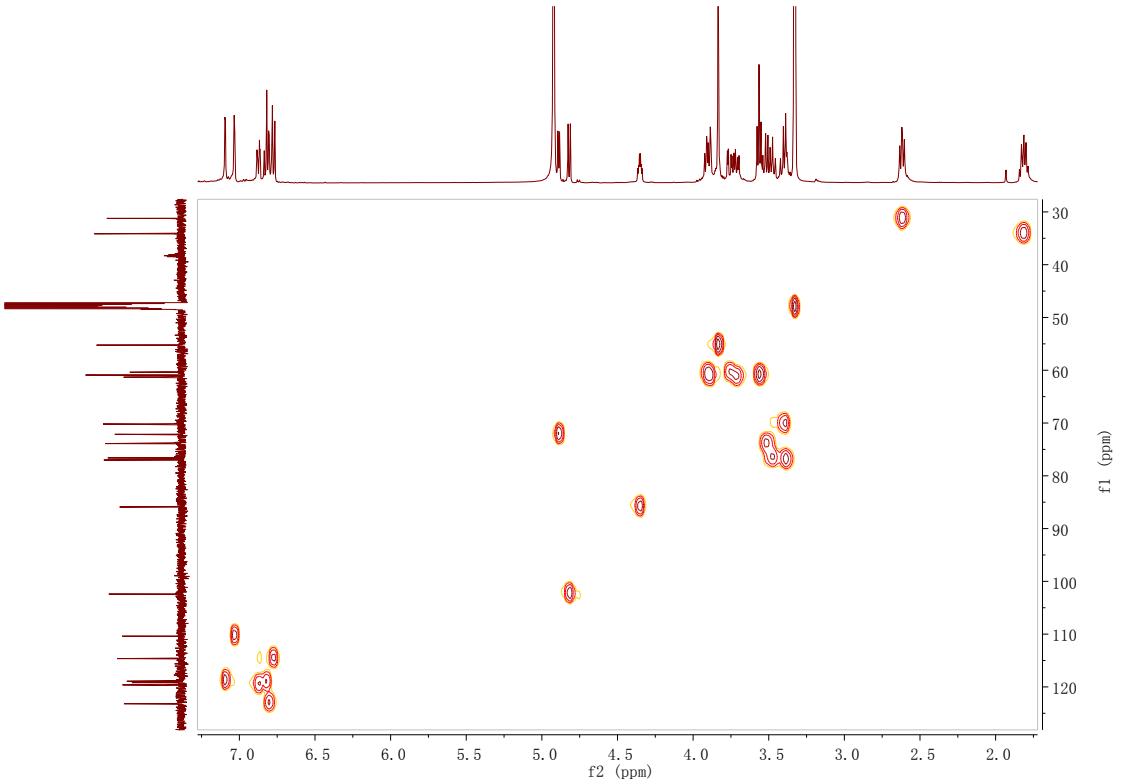


Figure S140. The HSQC spectrum of B-1 in CD_3OD

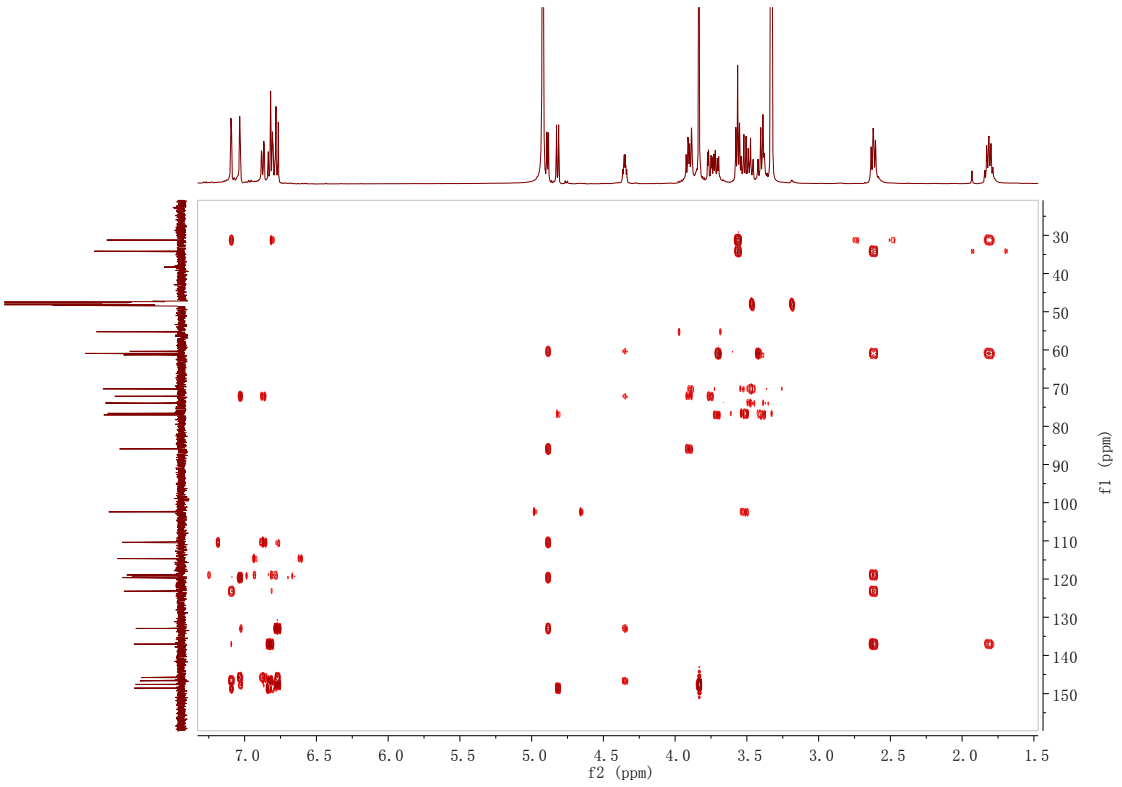


Figure S141. The HMBC spectrum of B-1 in CD_3OD

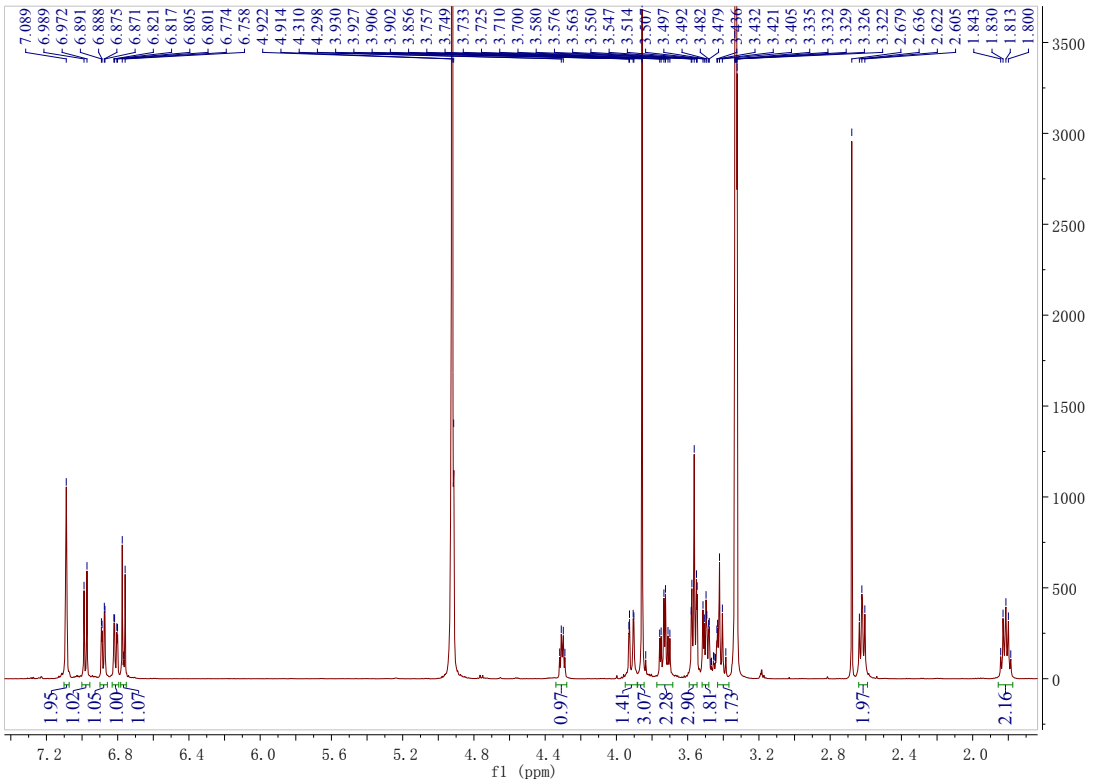


Figure S142. The ^{1}H-NMR spectrum of B-2 in CD_3OD

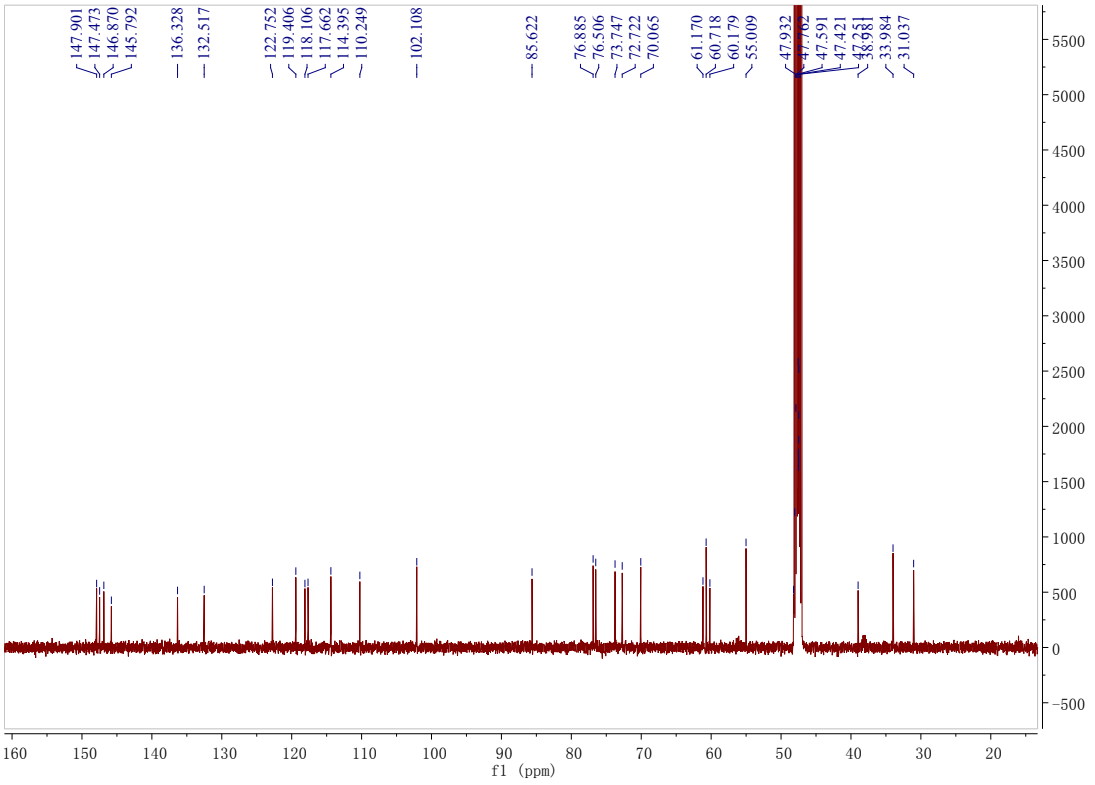


Figure S143. The ^{13}C-NMR spectrum of B-2 in CD_3OD

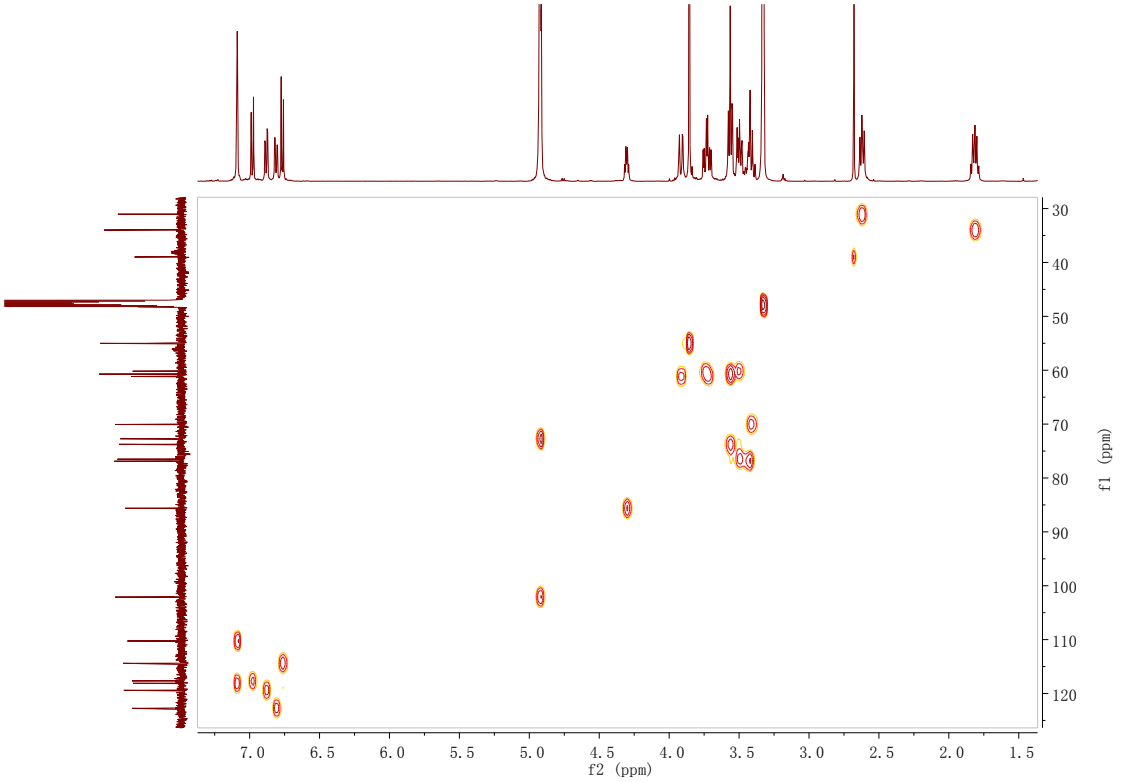


Figure S144. The HSQC spectrum of B-2 in CD_3OD

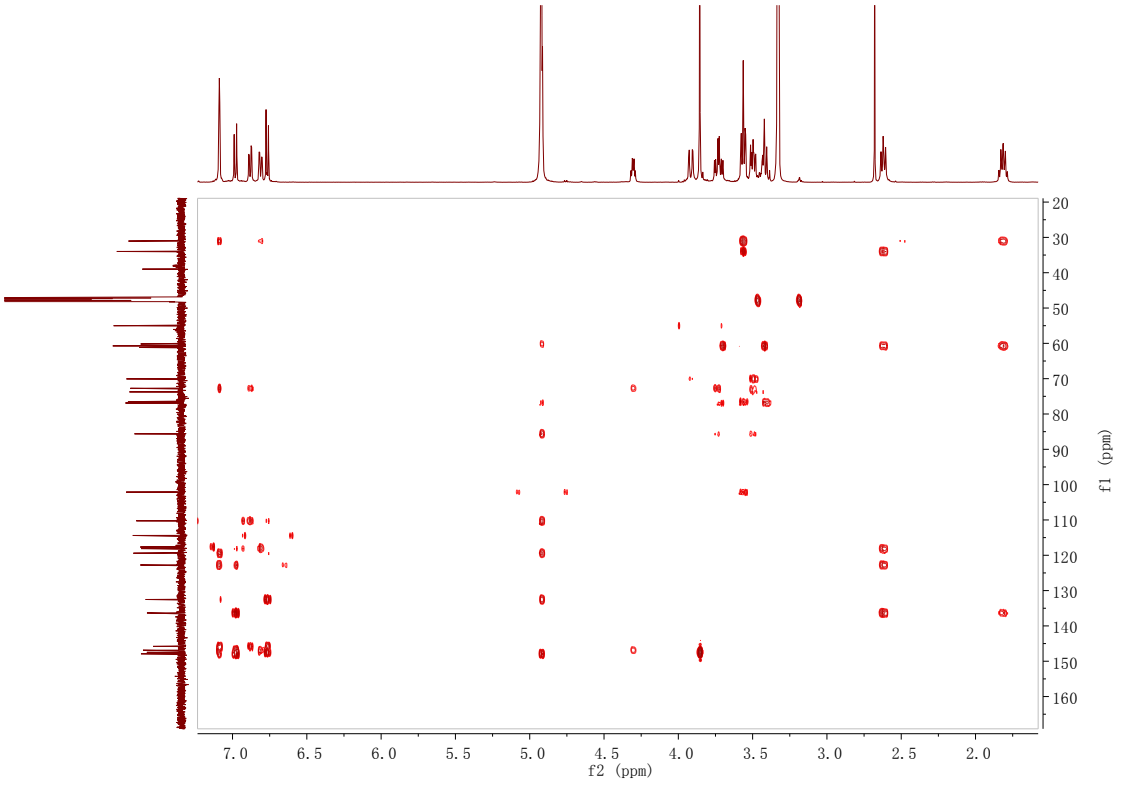


Figure S145. The HMBC spectrum of B-2 in CD_3OD

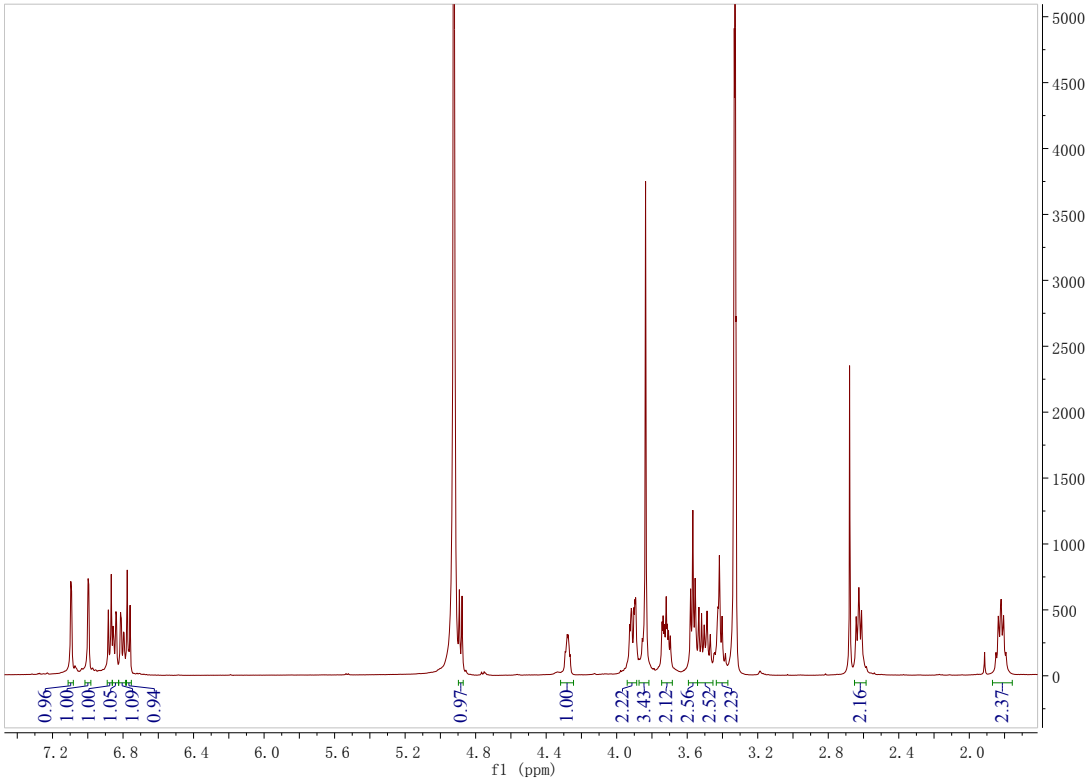


Figure S146. The ^{1}H-NMR spectrum of B-3 in CD_3OD

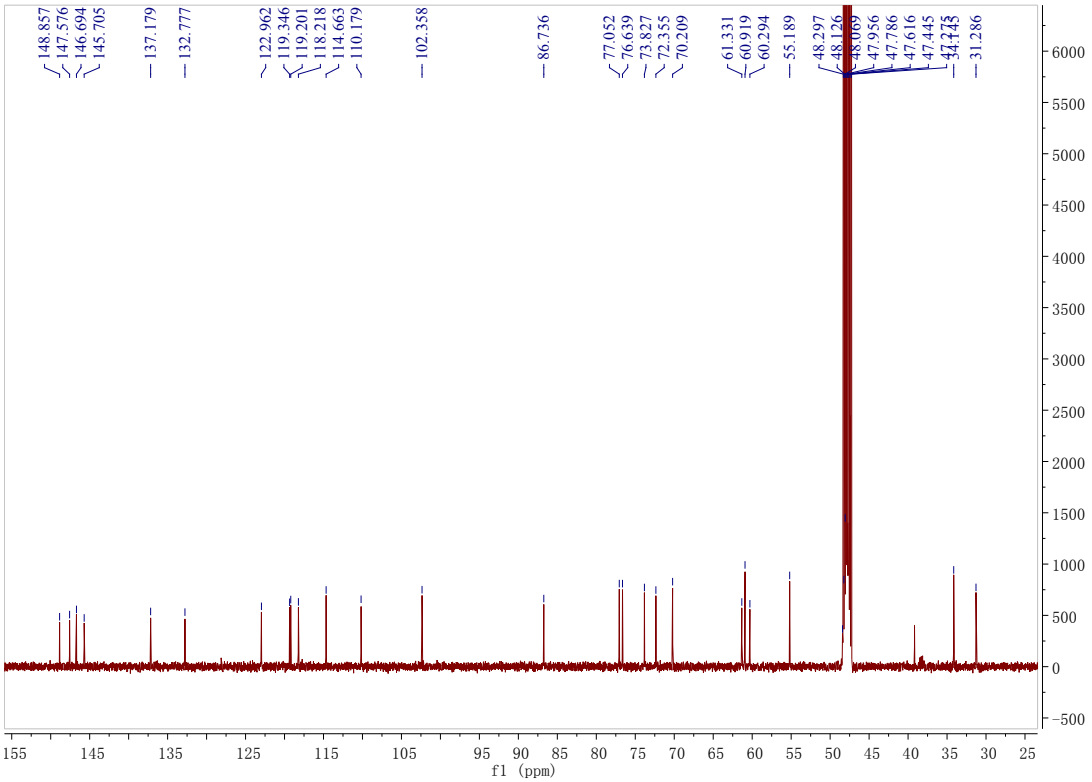


Figure S147. The ^{13}C-NMR spectrum of B-3 in CD_3OD

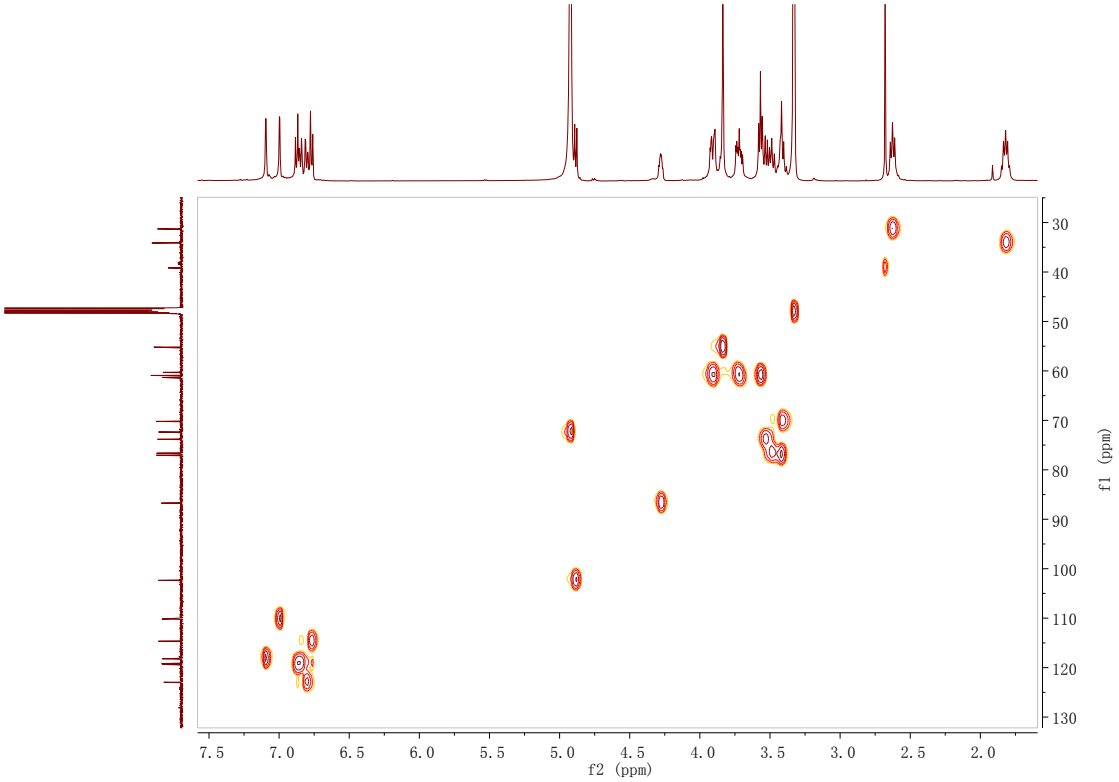


Figure S148. The HSQC spectrum of B-3 in CD_3OD

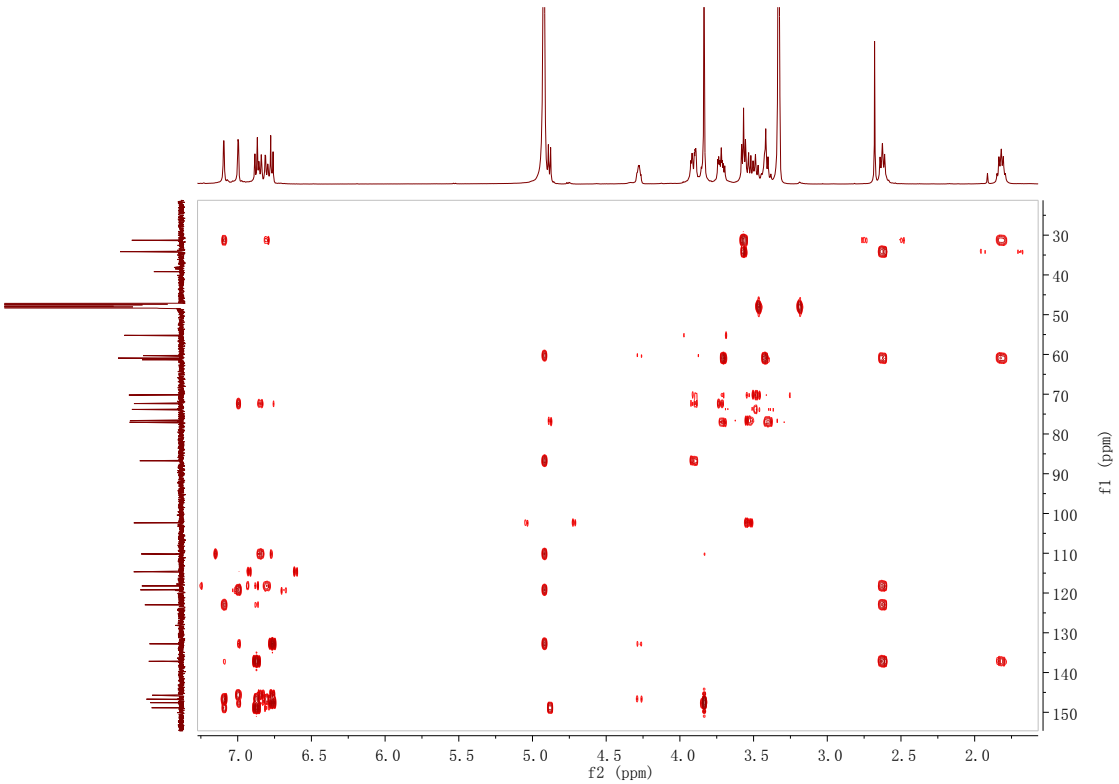


Figure S149. The HMBC spectrum of B-3 in CD_3OD

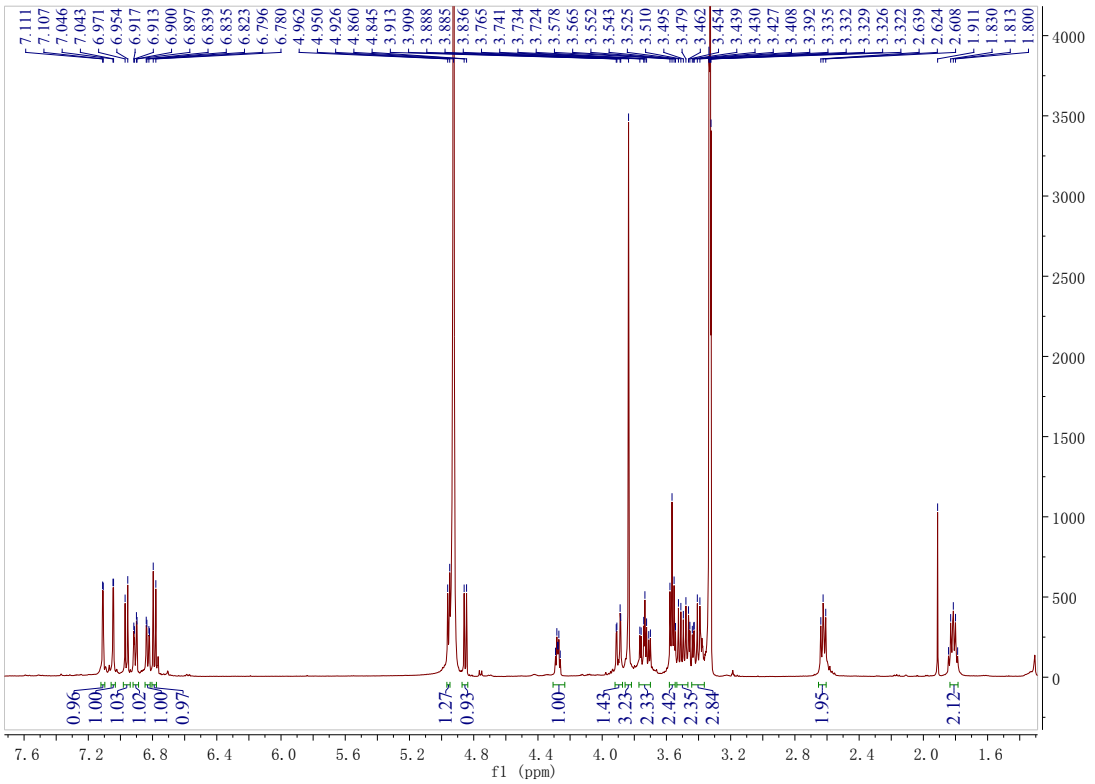


Figure S150. The ^{1}H-NMR spectrum of B-4 in CD_3OD

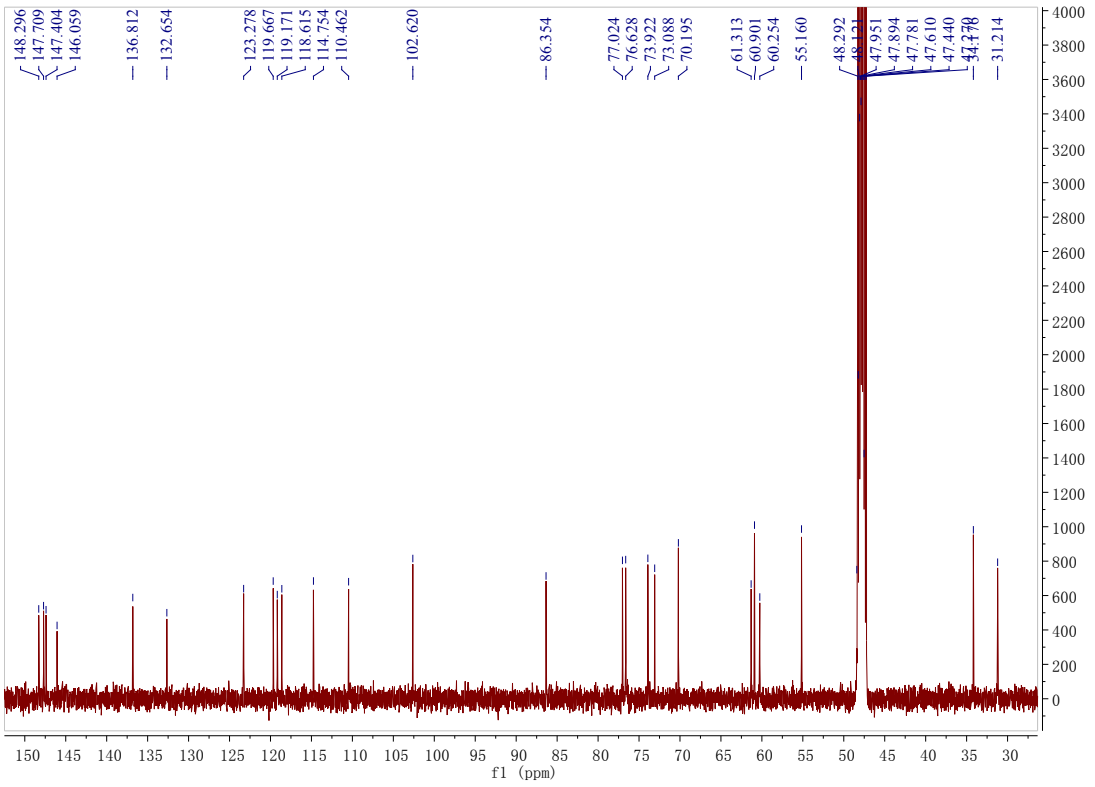


Figure S151. The ^{13}C-NMR spectrum of B-4 in CD_3OD

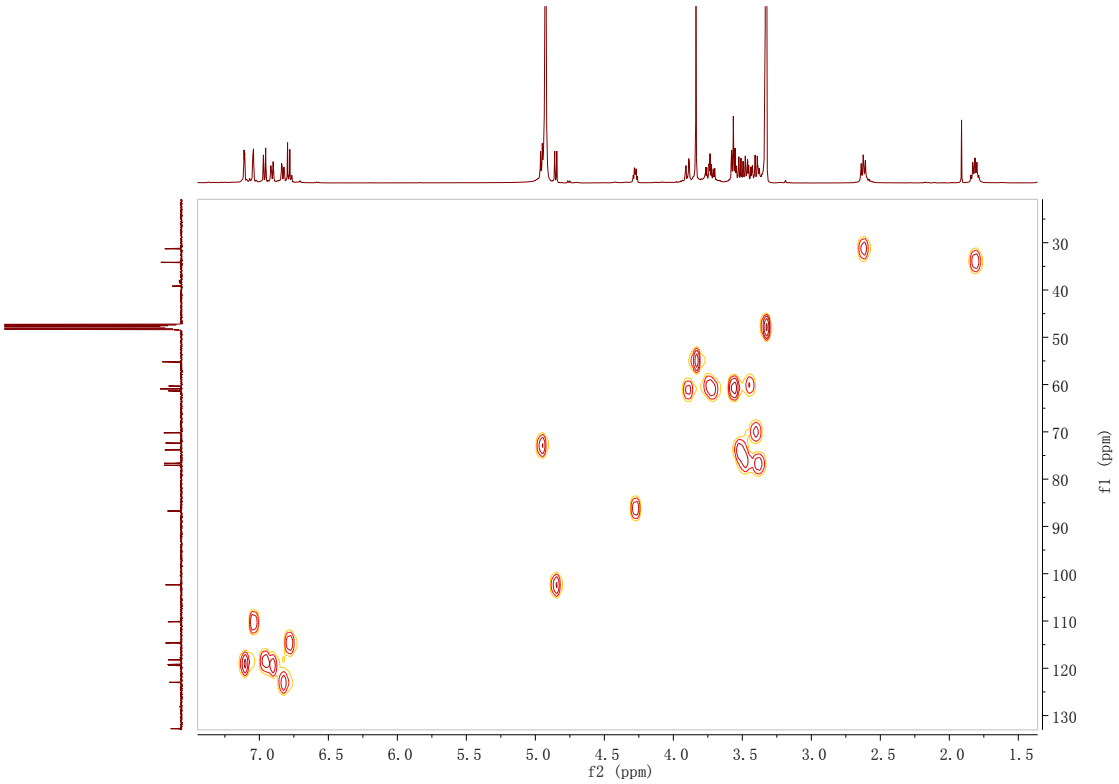


Figure S152. The HSQC spectrum of B-4 in CD_3OD

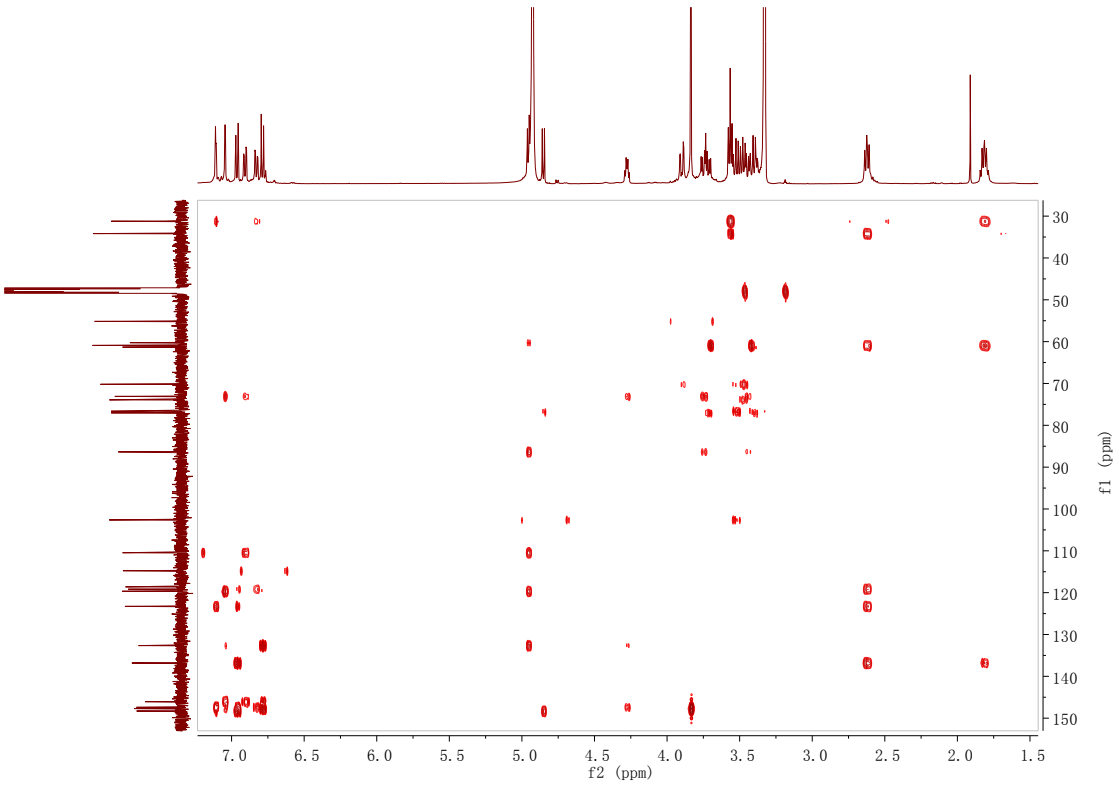


Figure S153. The HMBC spectrum of B-4 in CD_3OD

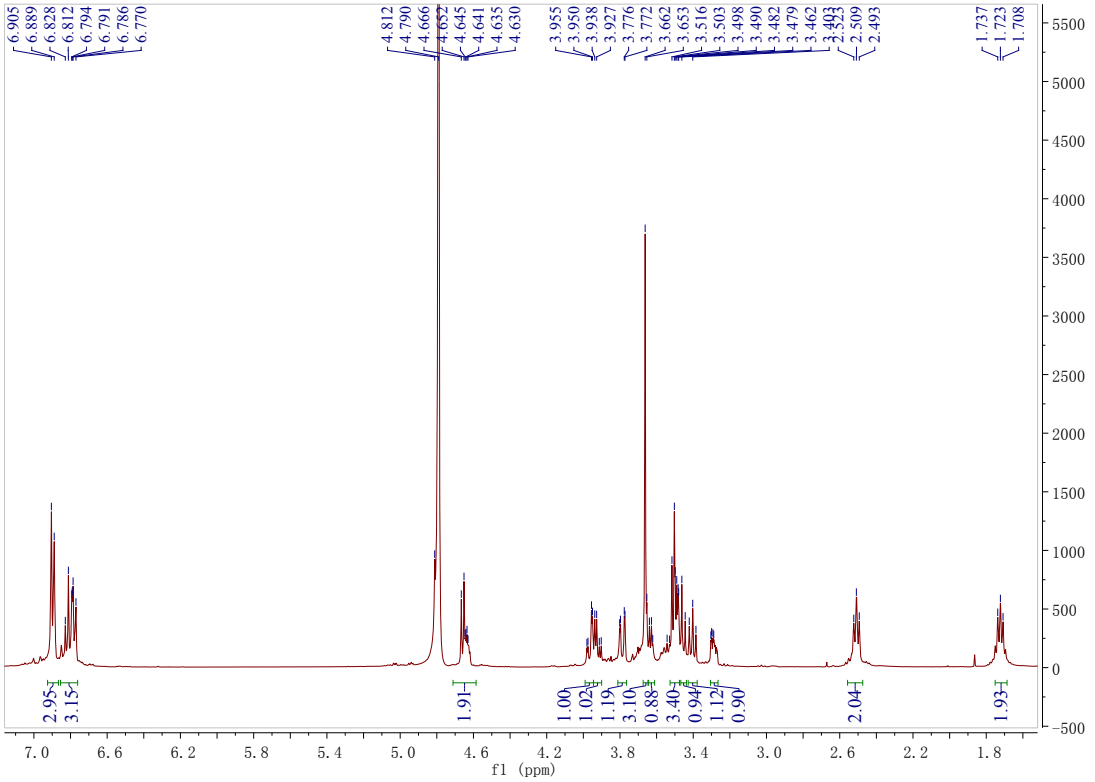


Figure S154. The ^{1}H-NMR spectrum of B-1 in D_2O

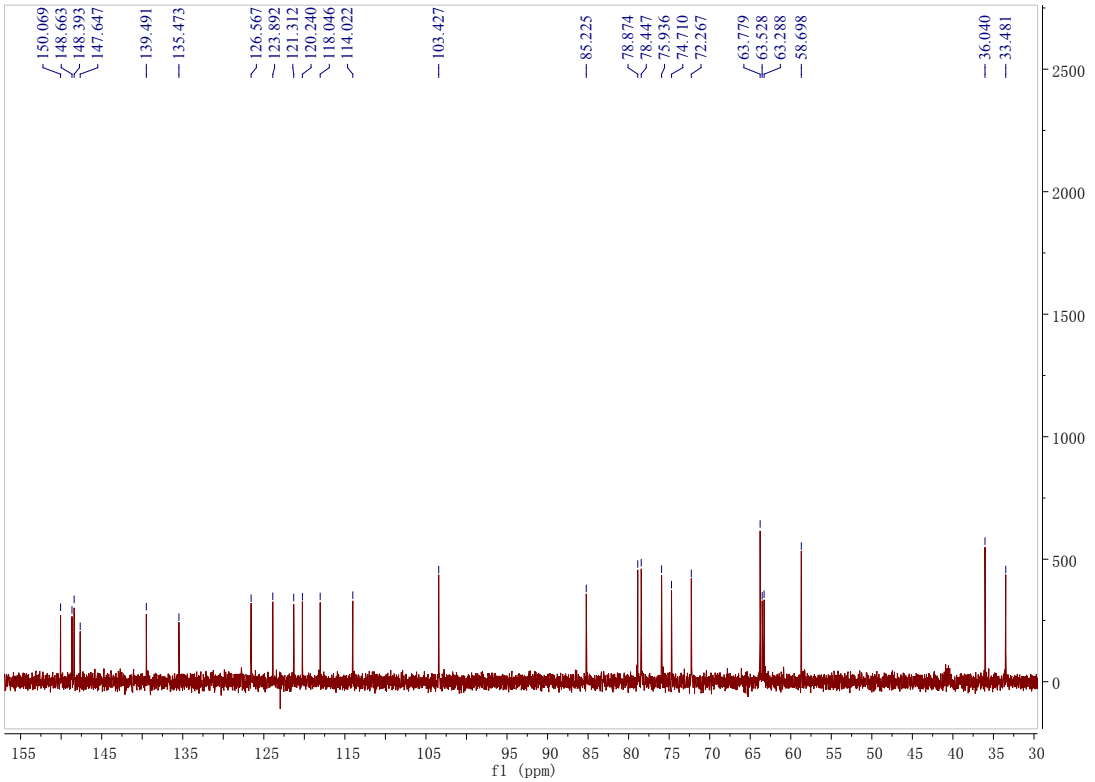


Figure S155. The ^{13}C-NMR spectrum of B-1 in D_2O

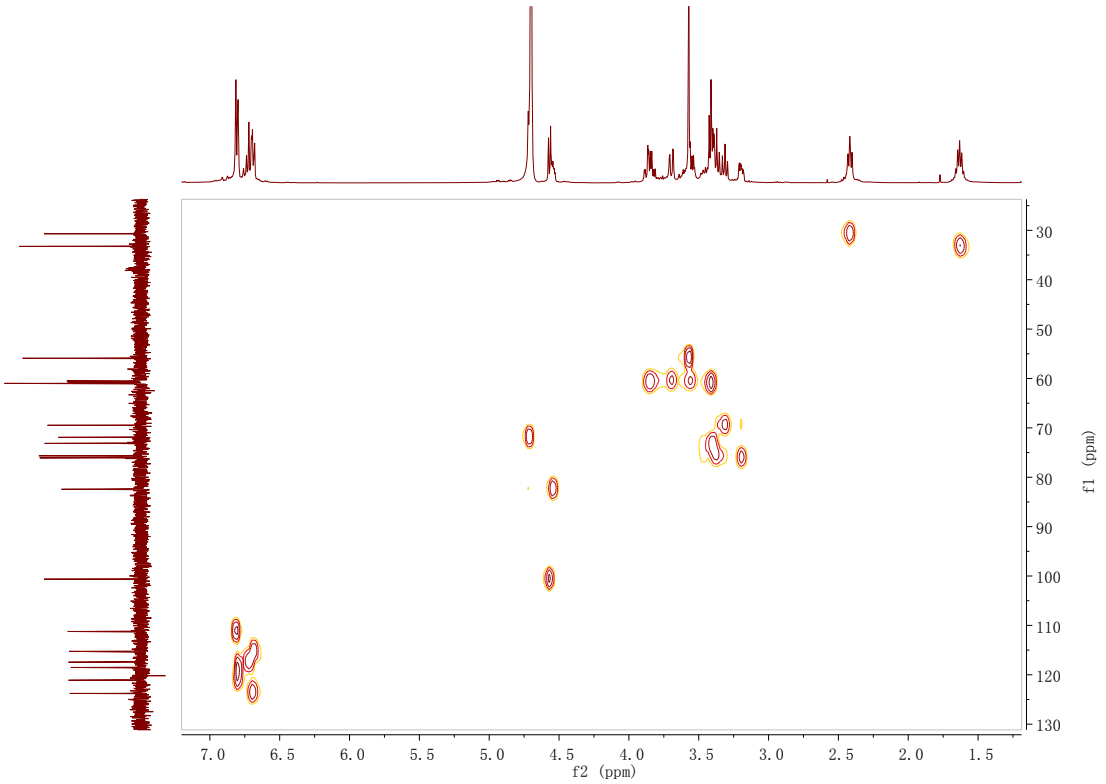


Figure S156. The HSQC spectrum of B-1 in D_2O

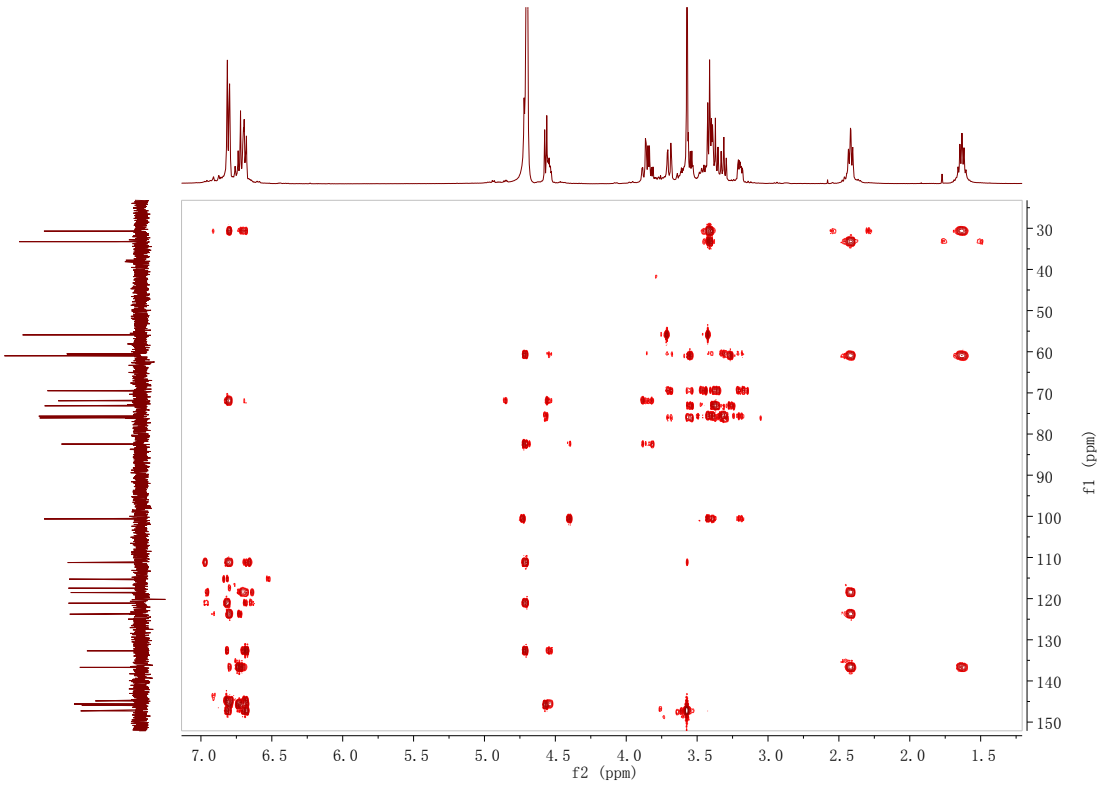


Figure S157. The HMBC spectrum of B-1 in D_2O

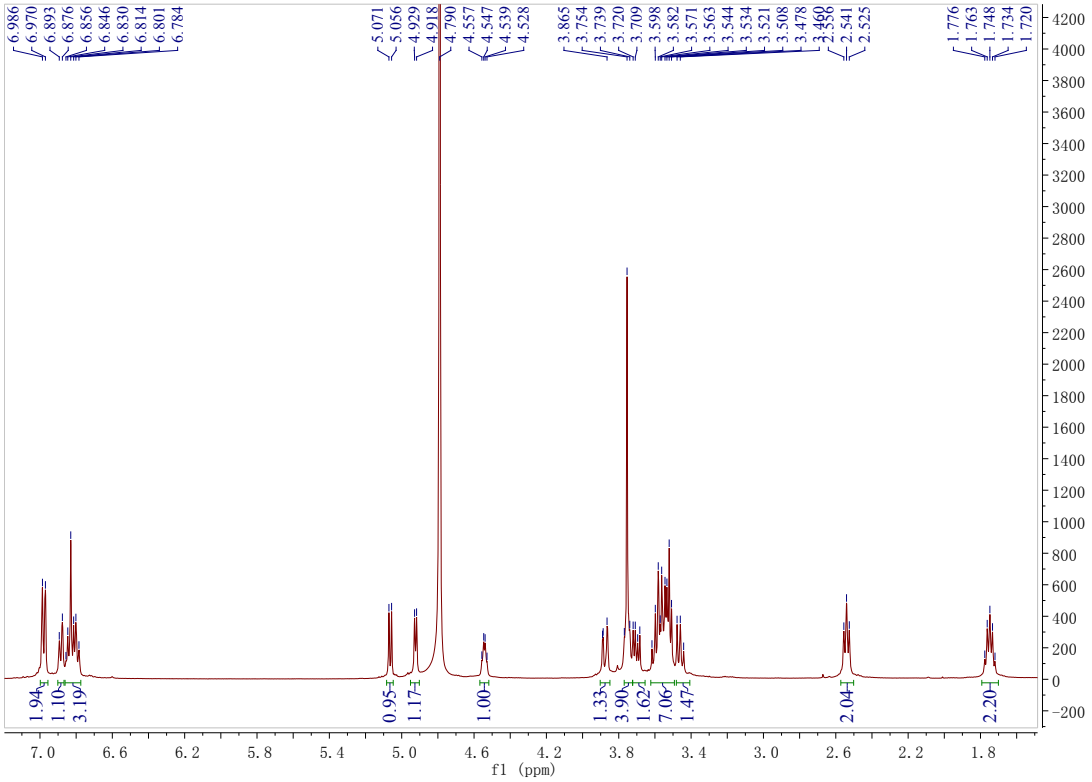


Figure S158. The ^{1}H-NMR spectrum of B-2 in D_2O

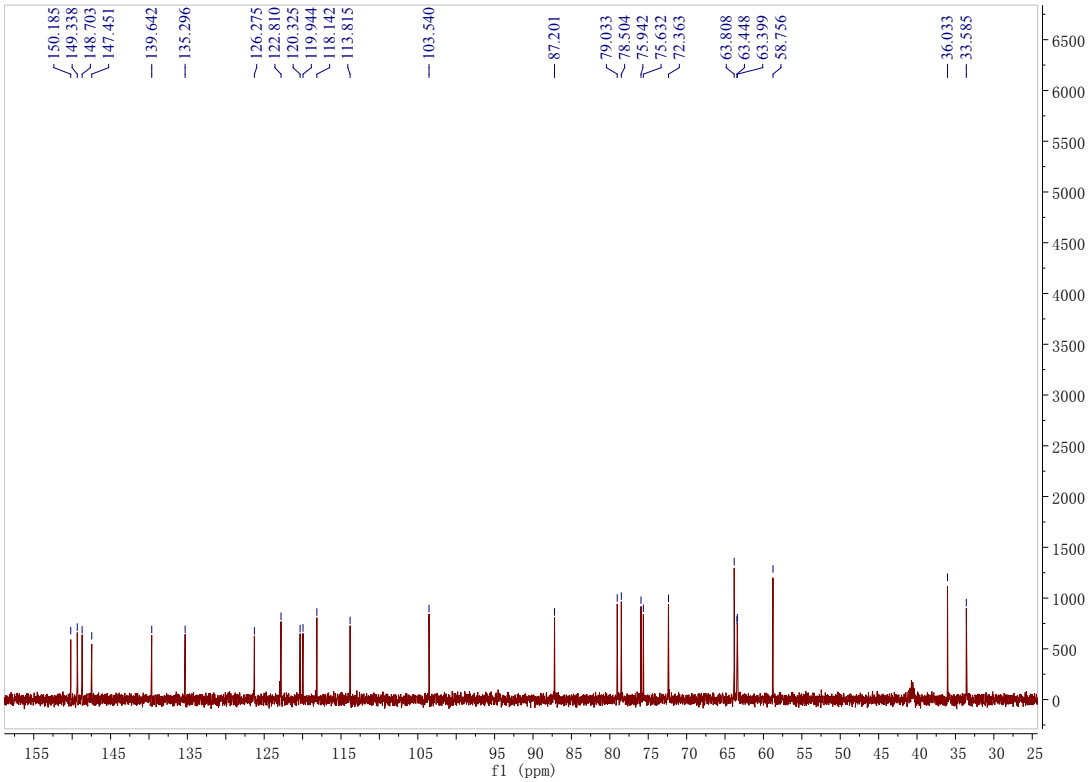


Figure S159. The ^{13}C-NMR spectrum of B-2 in D_2O

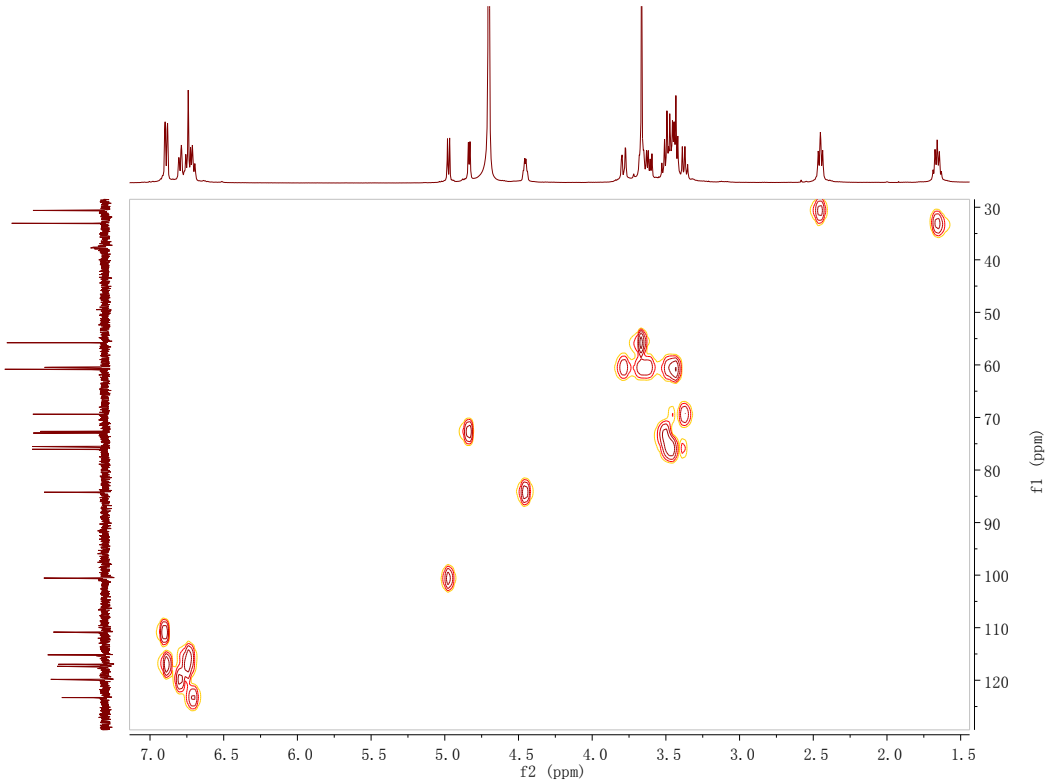


Figure S160. The HSQC spectrum of B-2 in D_2O

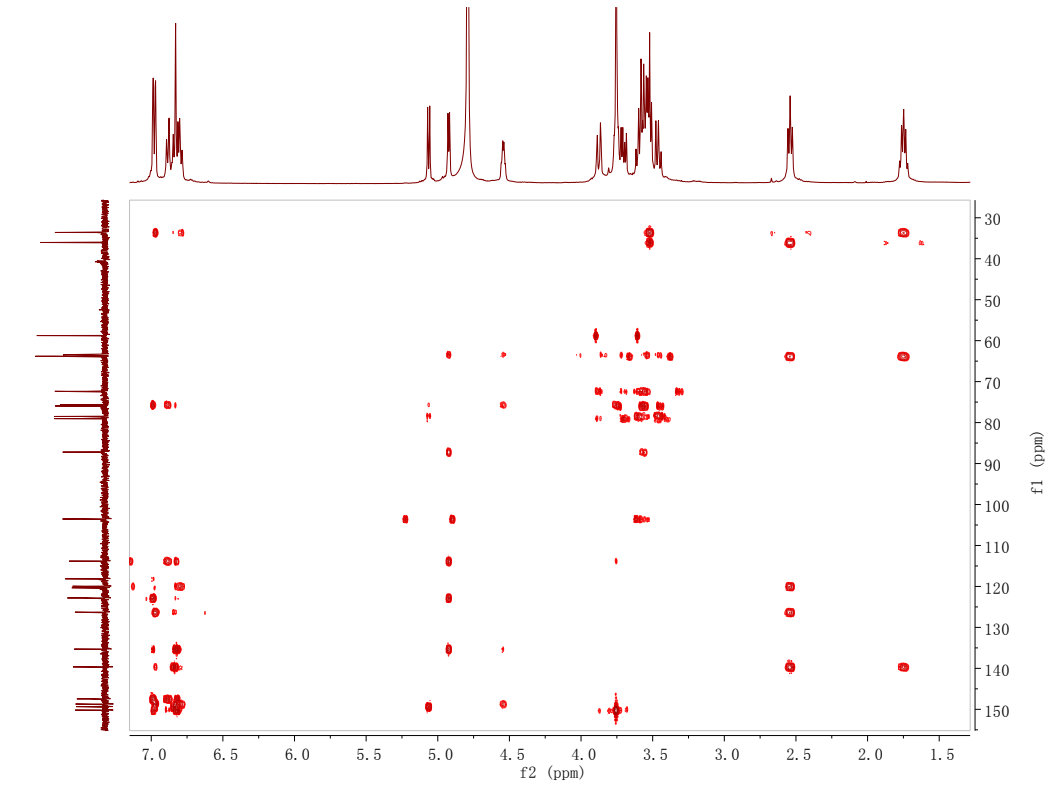


Figure S161. The HMBC spectrum of B-2 in D_2O

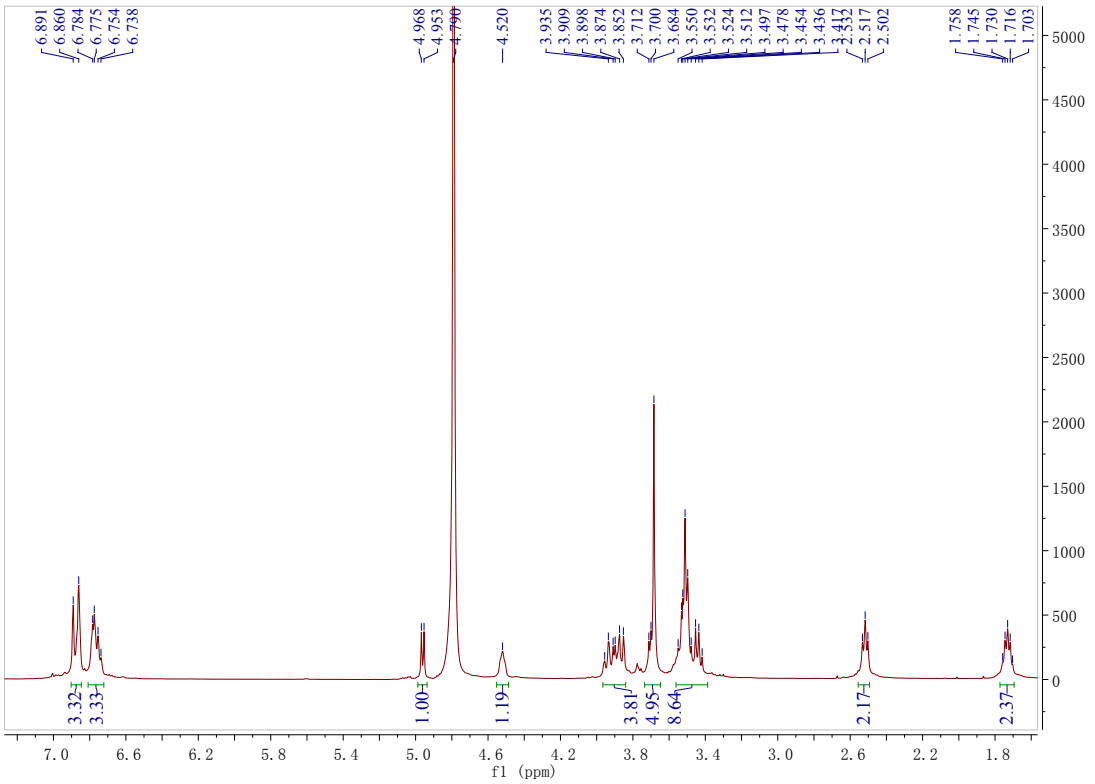


Figure S162. The ^{1}H-NMR spectrum of B-3 in D_2O

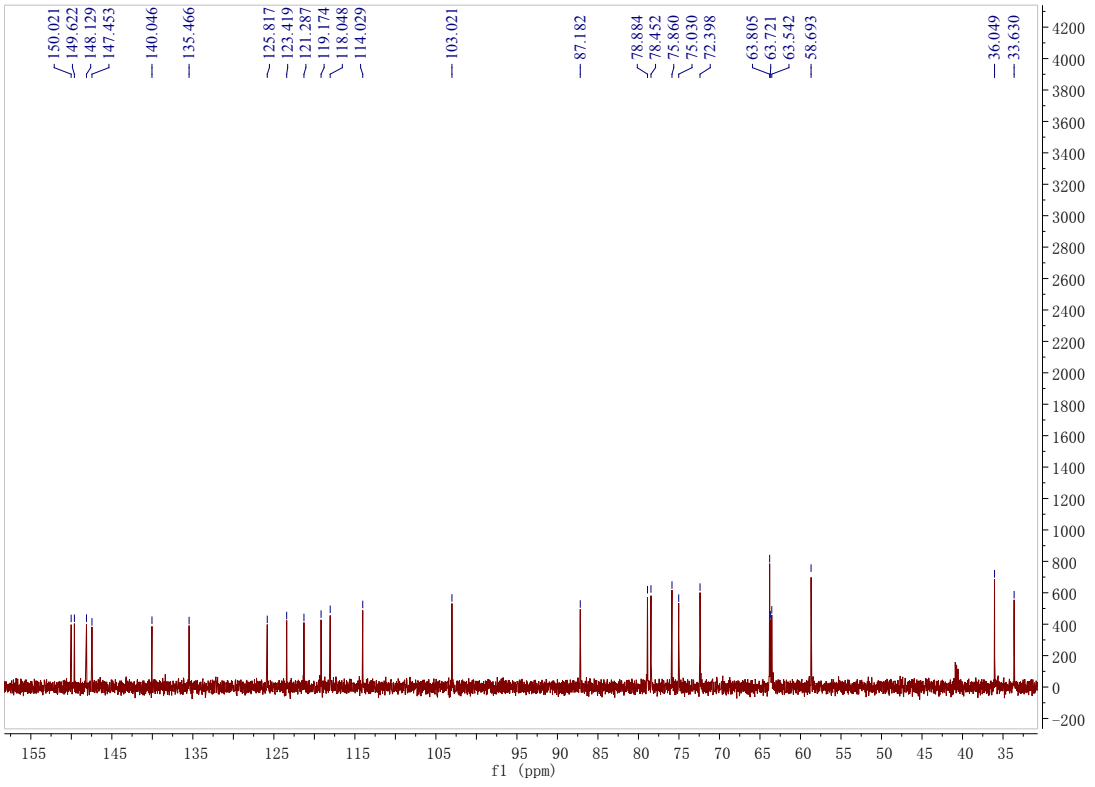


Figure S163. The ^{13}C-NMR spectrum of B-3 in D_2O

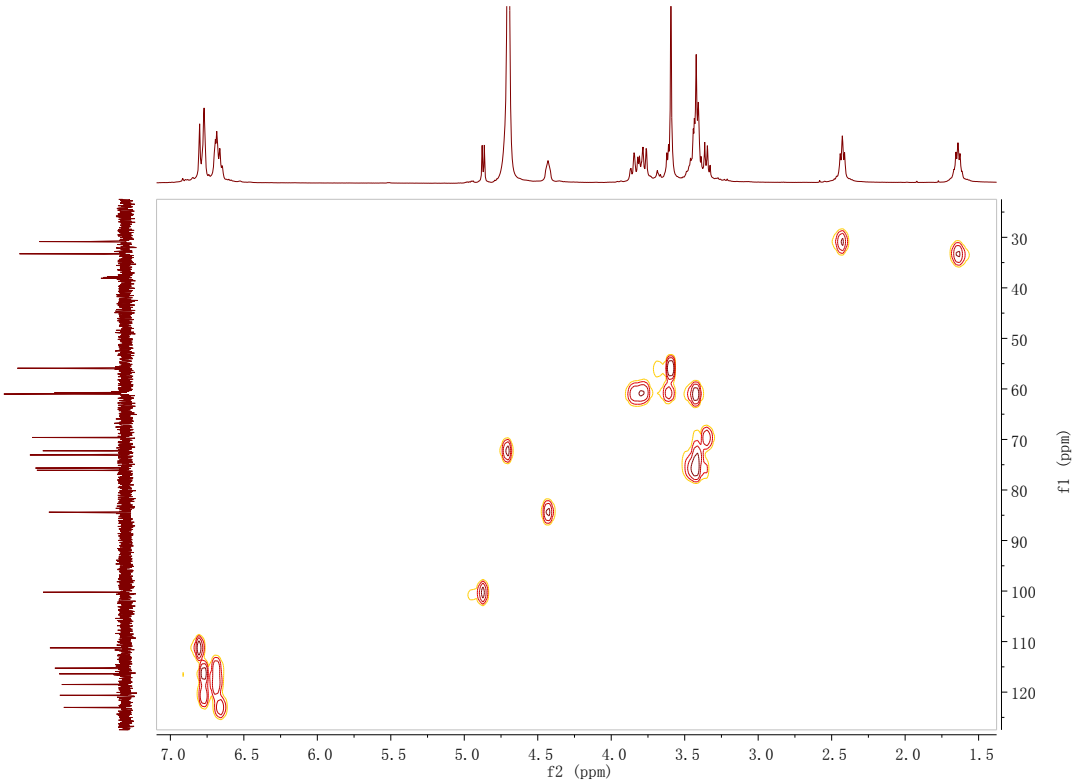


Figure S164. The HSQC spectrum of B-3 in D_2O

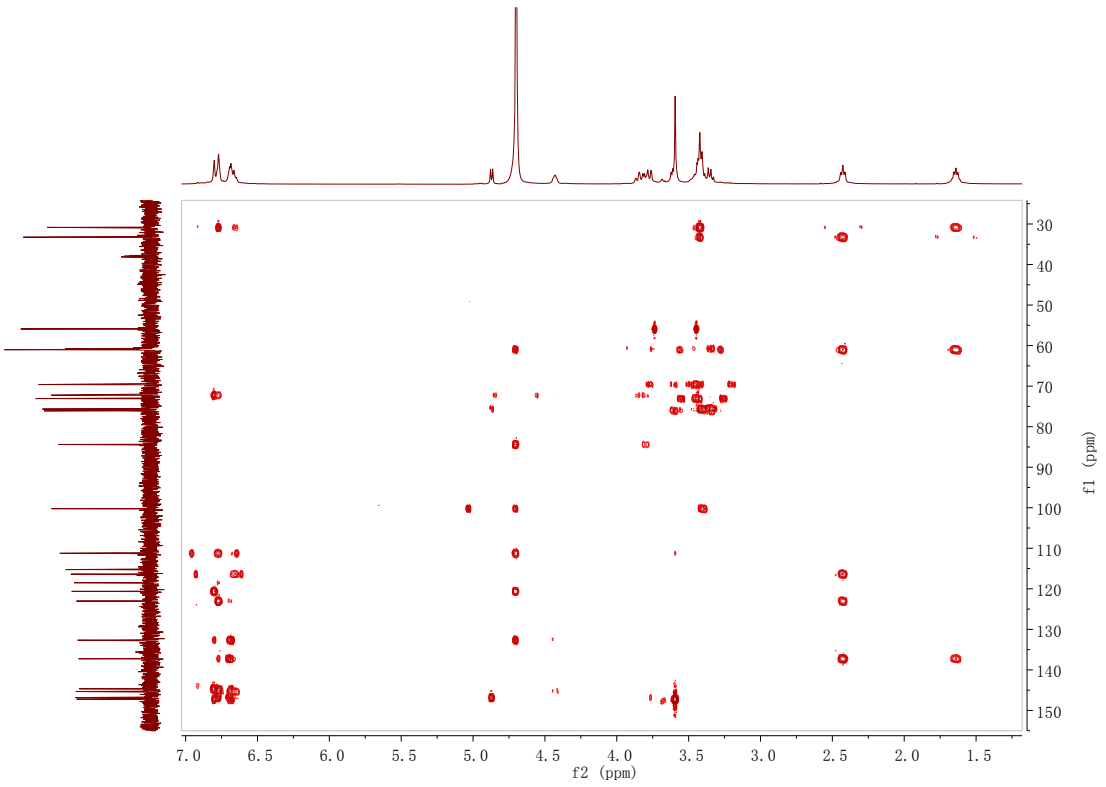


Figure S165. The HMBC spectrum of B-3 in D_2O

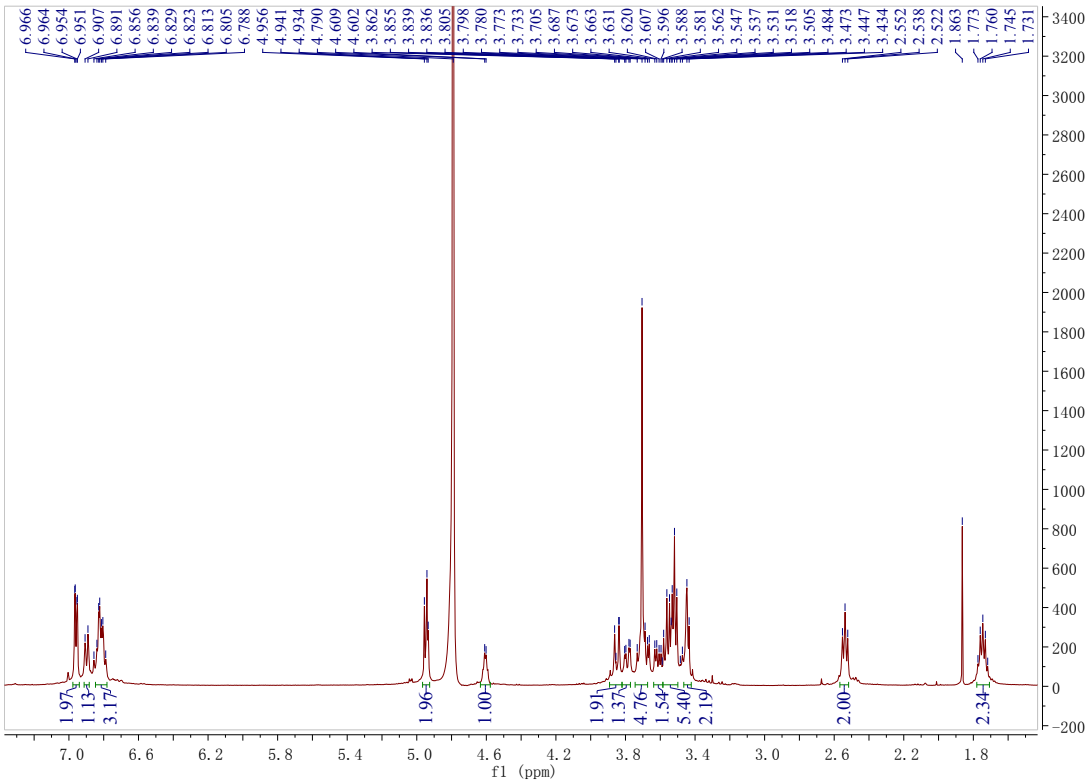


Figure S166. The ^{1}H-NMR spectrum of B-4 in D_2O

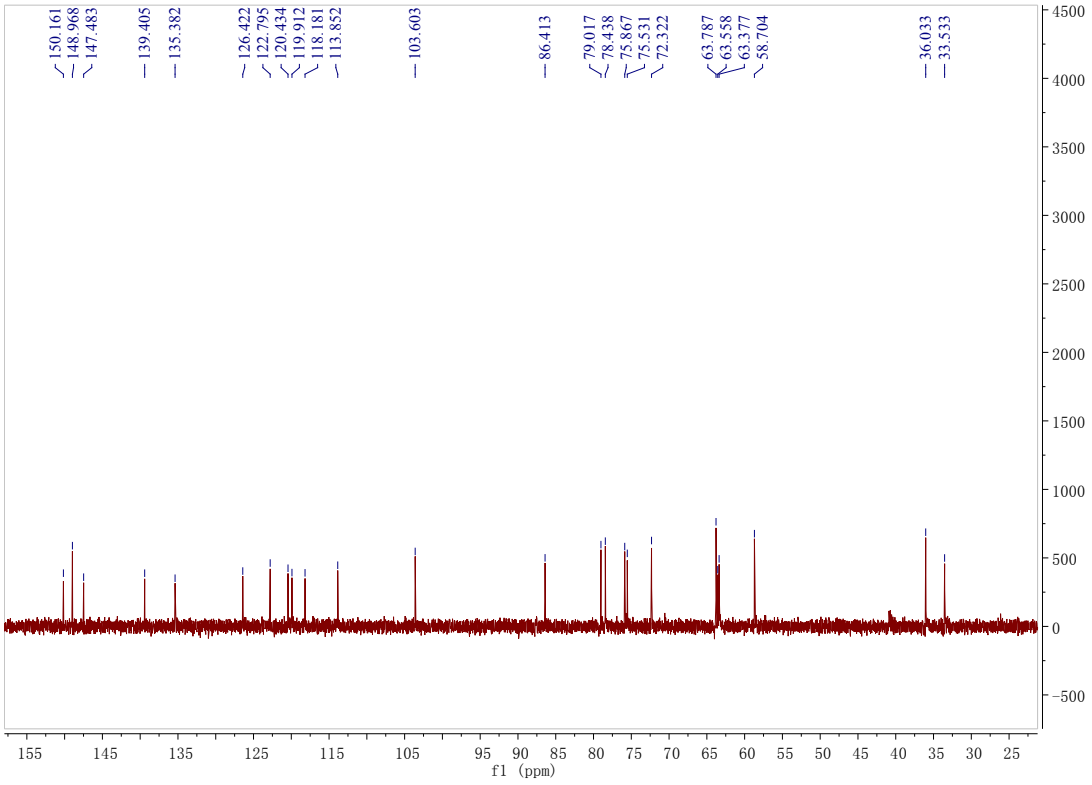


Figure S167. The ^{13}C-NMR spectrum of B-4 in D_2O

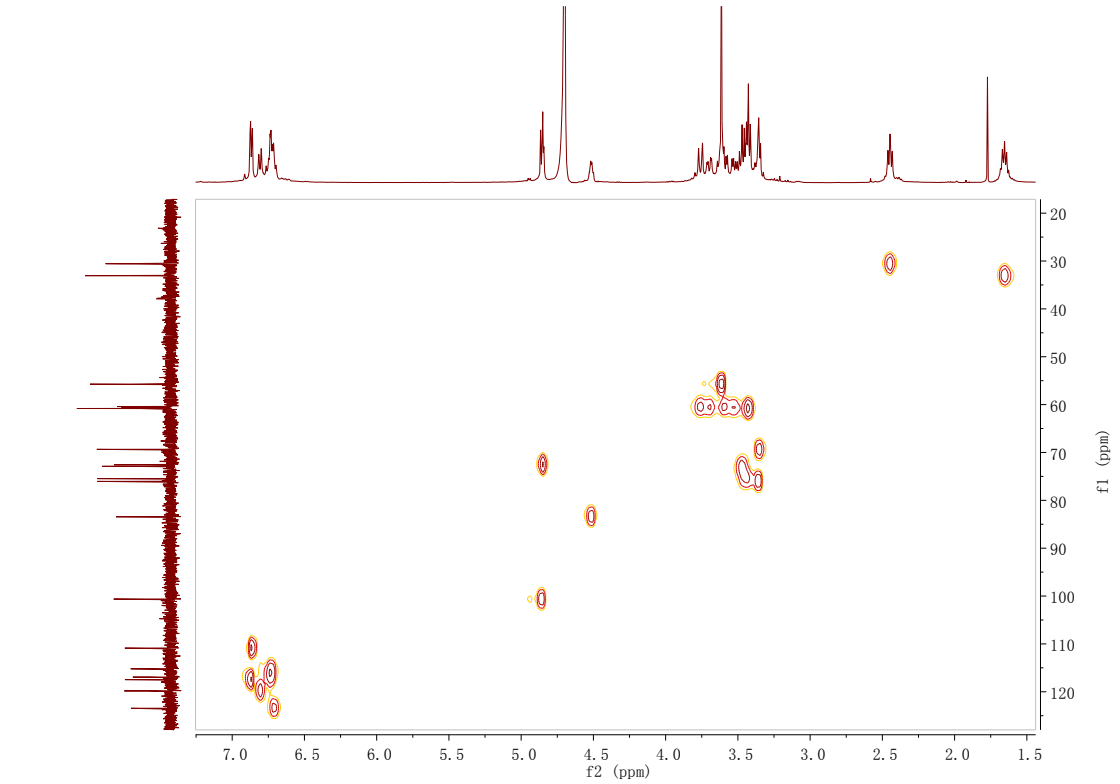


Figure S168. The HSQC spectrum of B-4 in D_2O

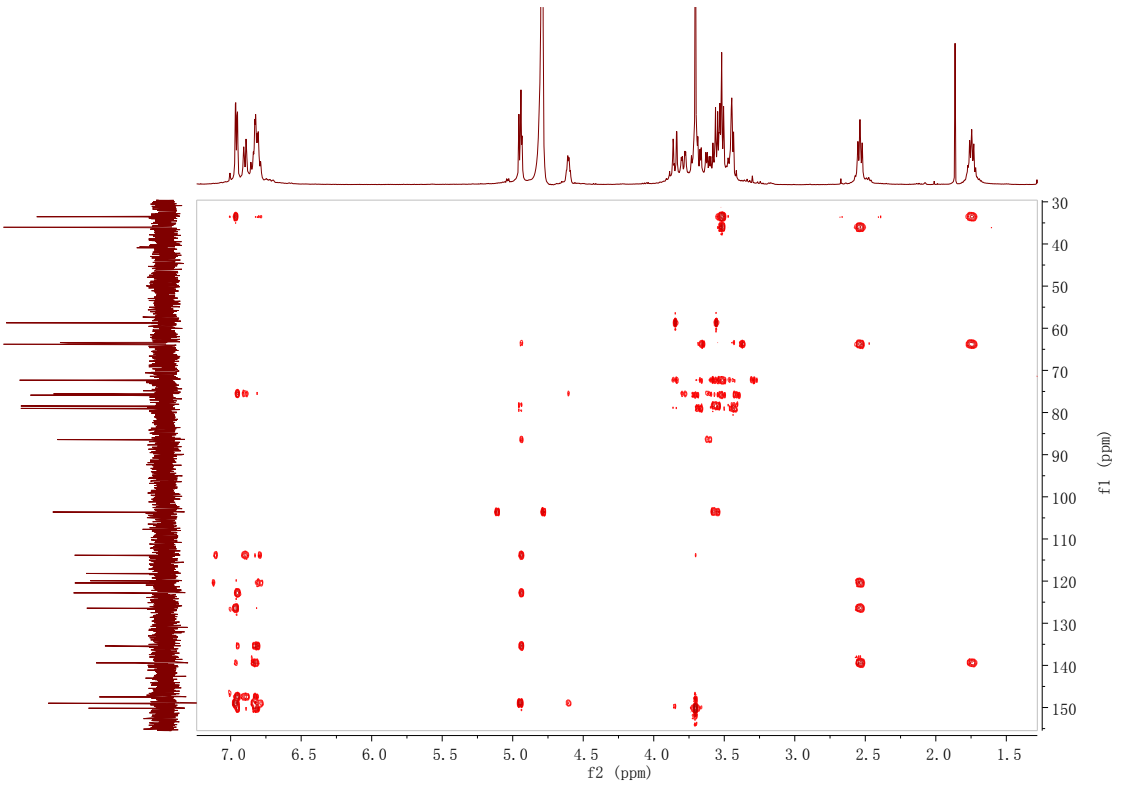


Figure S169. The HMBC spectrum of B-4 in D_2O

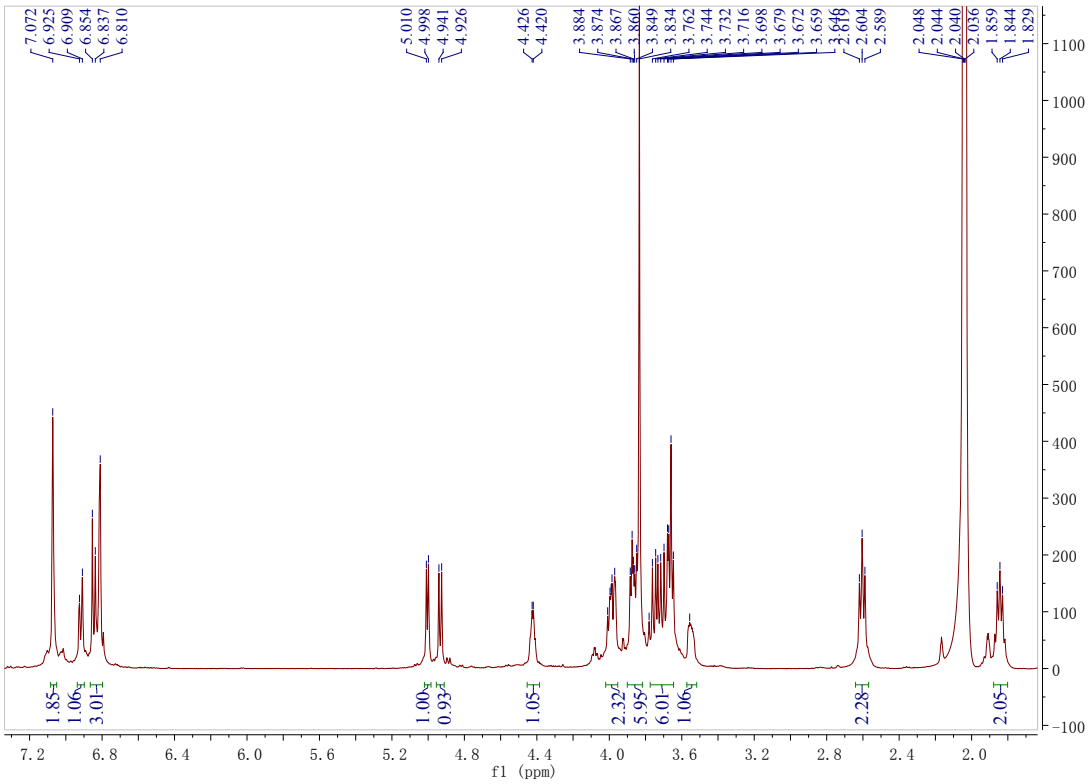


Figure S170. The ^{1}H-NMR spectrum of B-1 in CD_3COOD

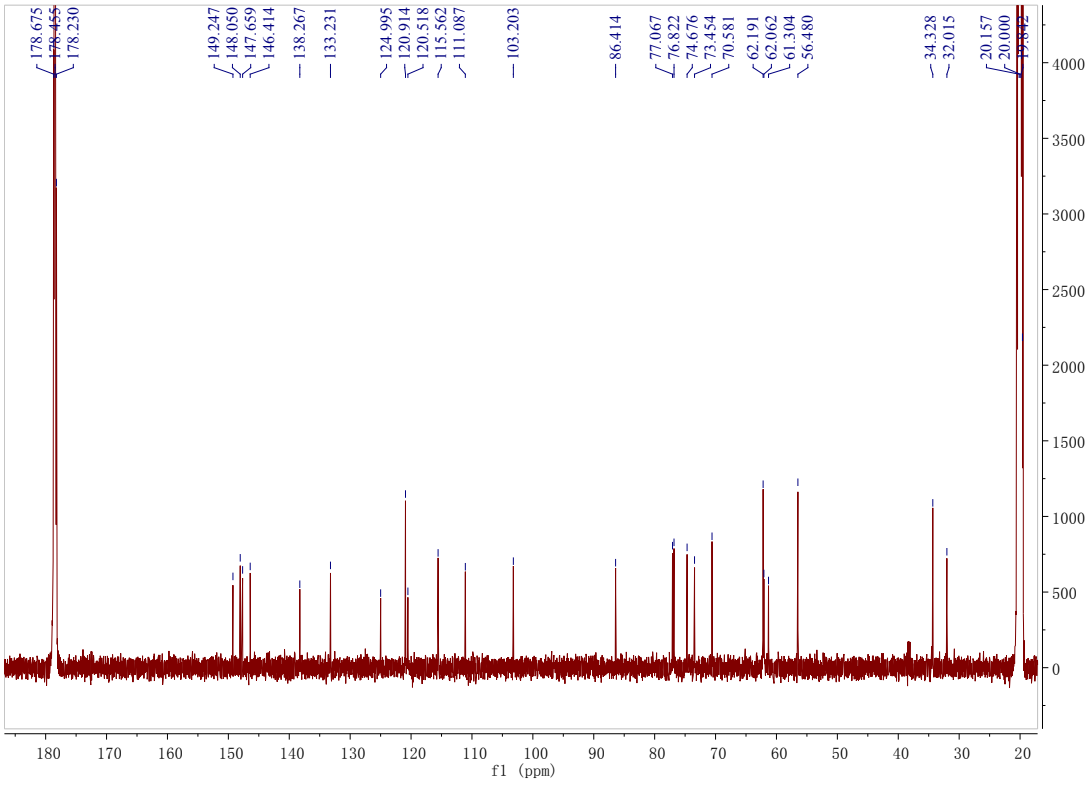


Figure S171. The ^{13}C-NMR spectrum of B-1 in CD_3COOD

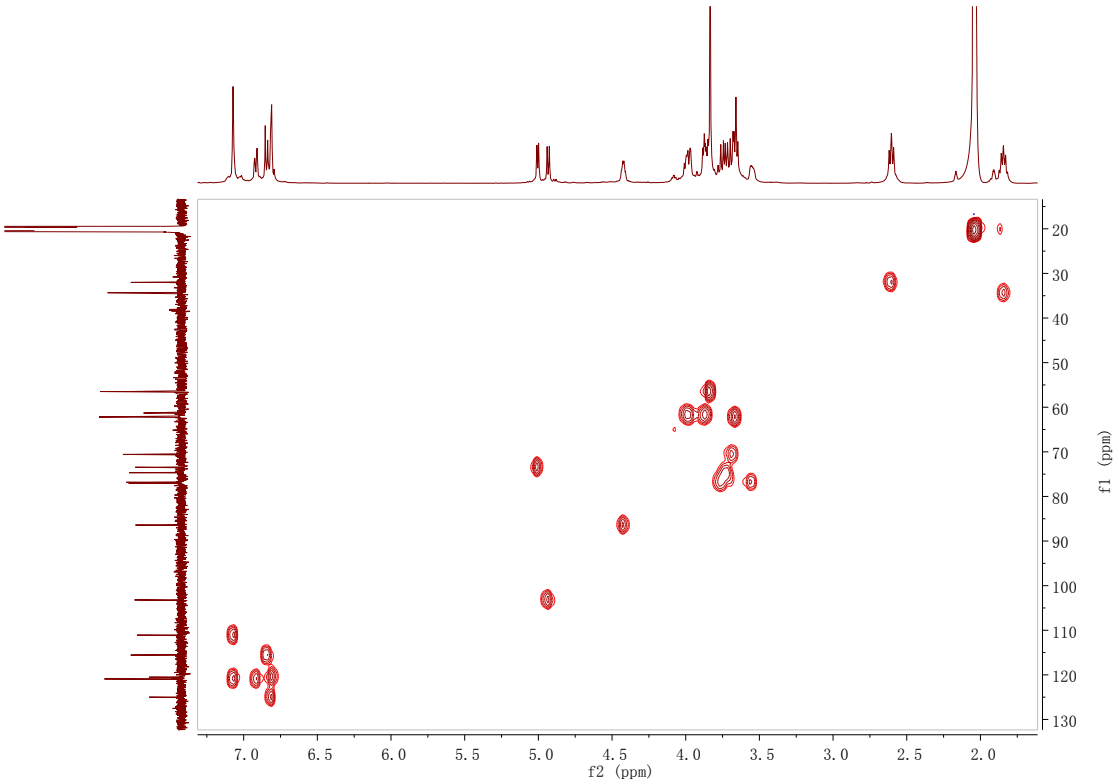


Figure S172. The HSQC spectrum of B-1 in CD_3COOD

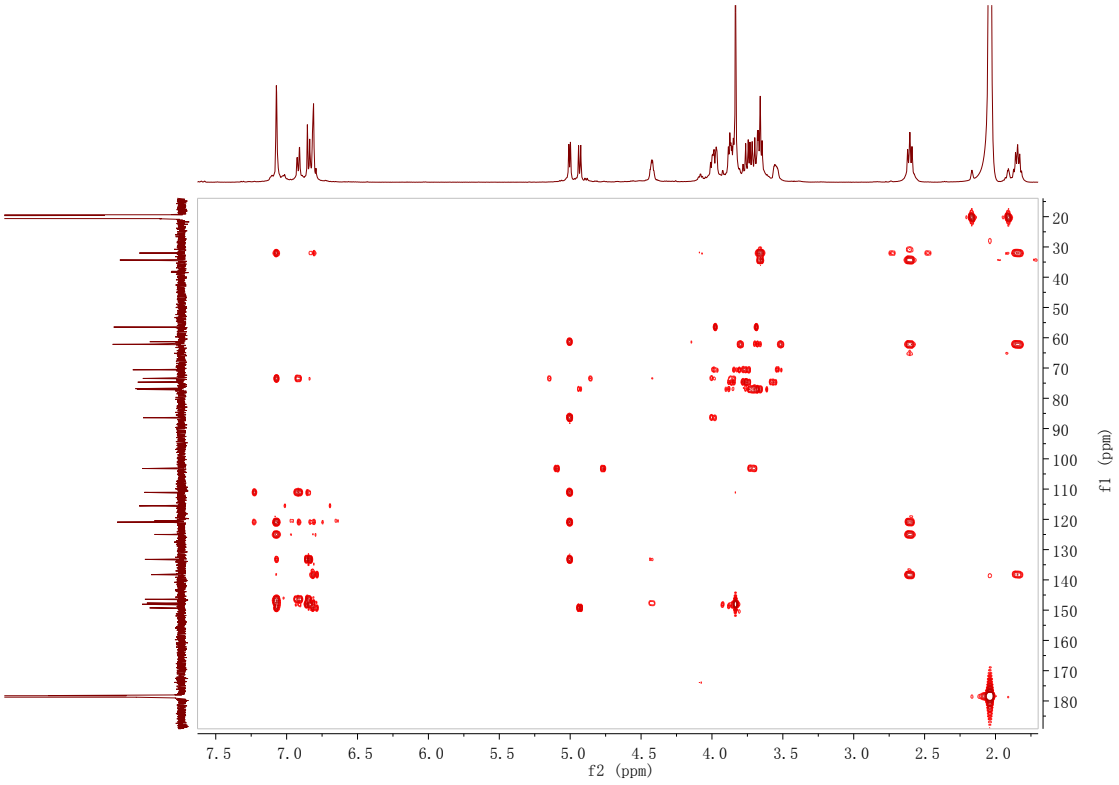


Figure S173. The HMBC spectrum of B-1 in CD_3COOD

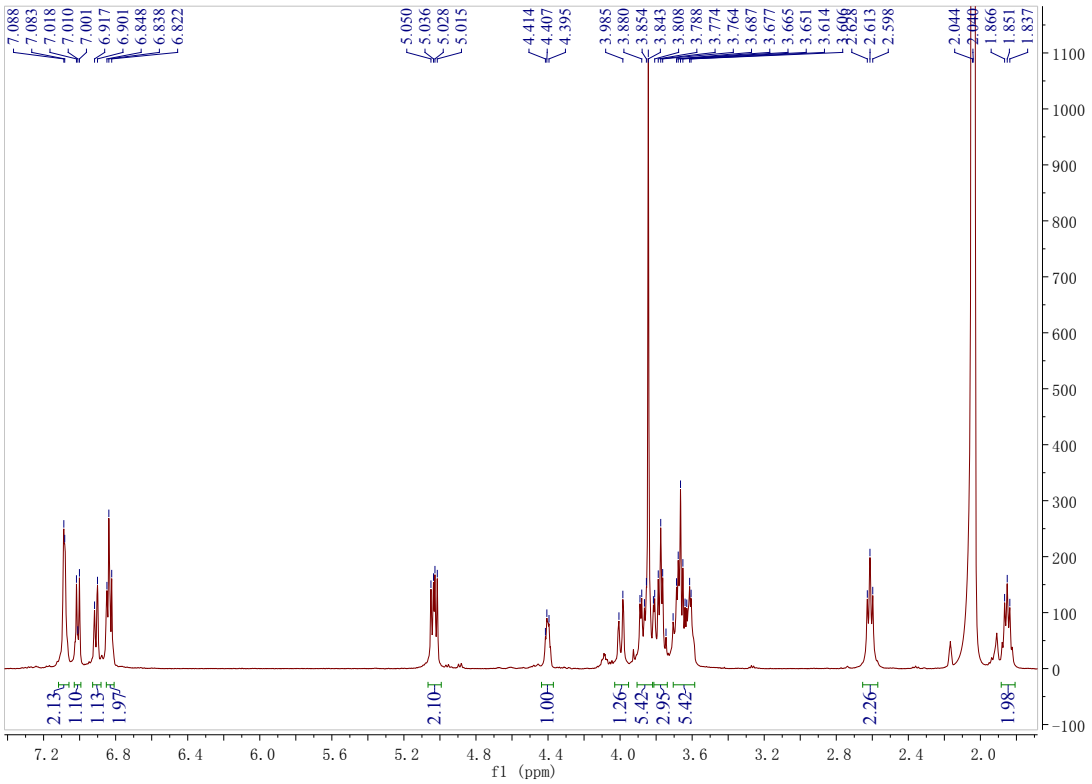


Figure S174. The ^{1}H-NMR spectrum of B-2 in CD_3COOD

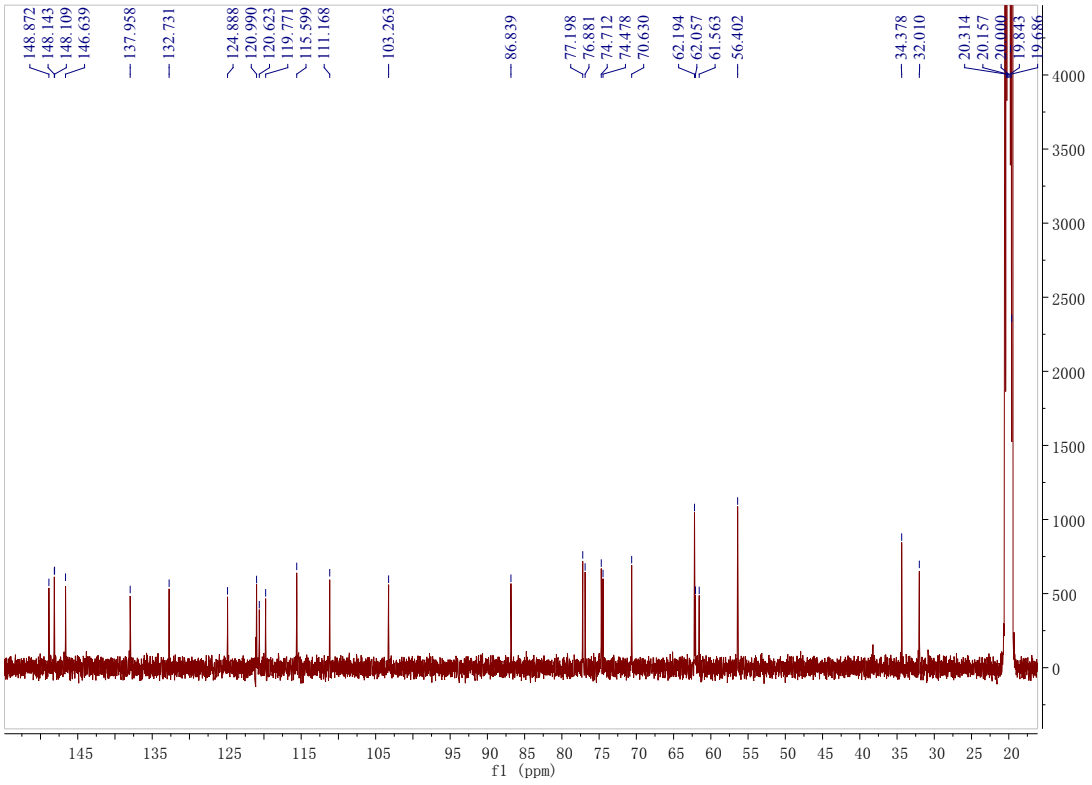


Figure S175. The ^{13}C-NMR spectrum of B-2 in CD_3COOD

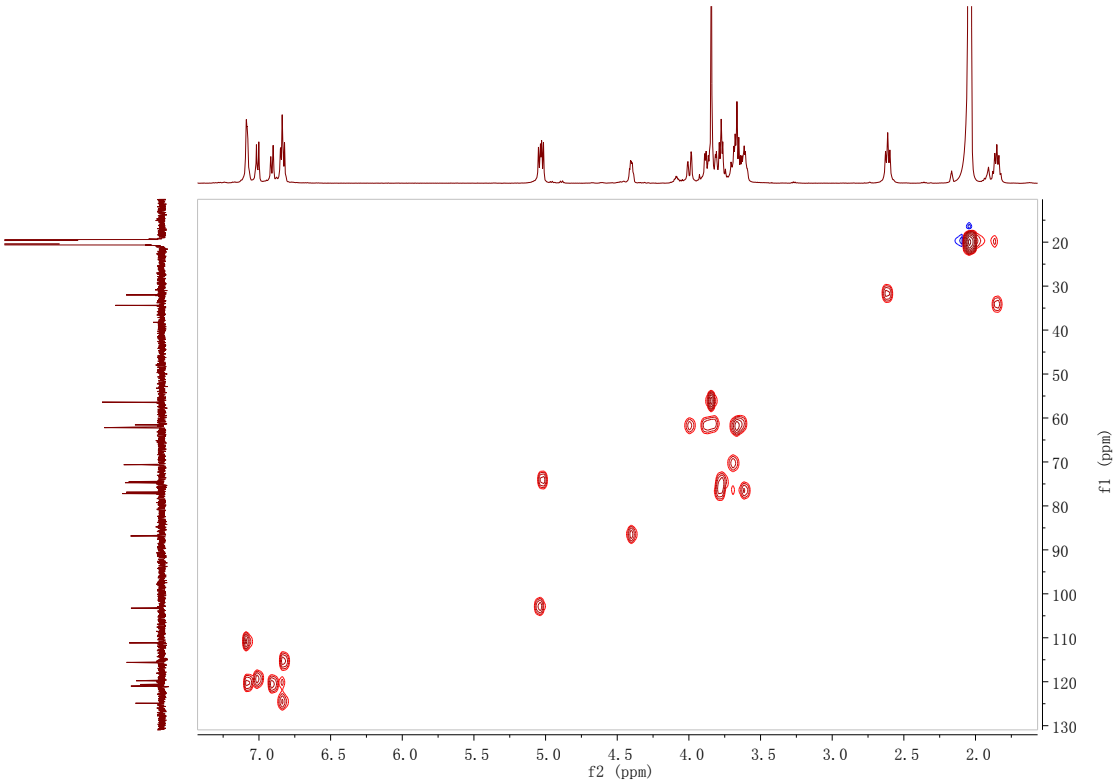


Figure S176. The HSQC spectrum of B-2 in CD_3COOD

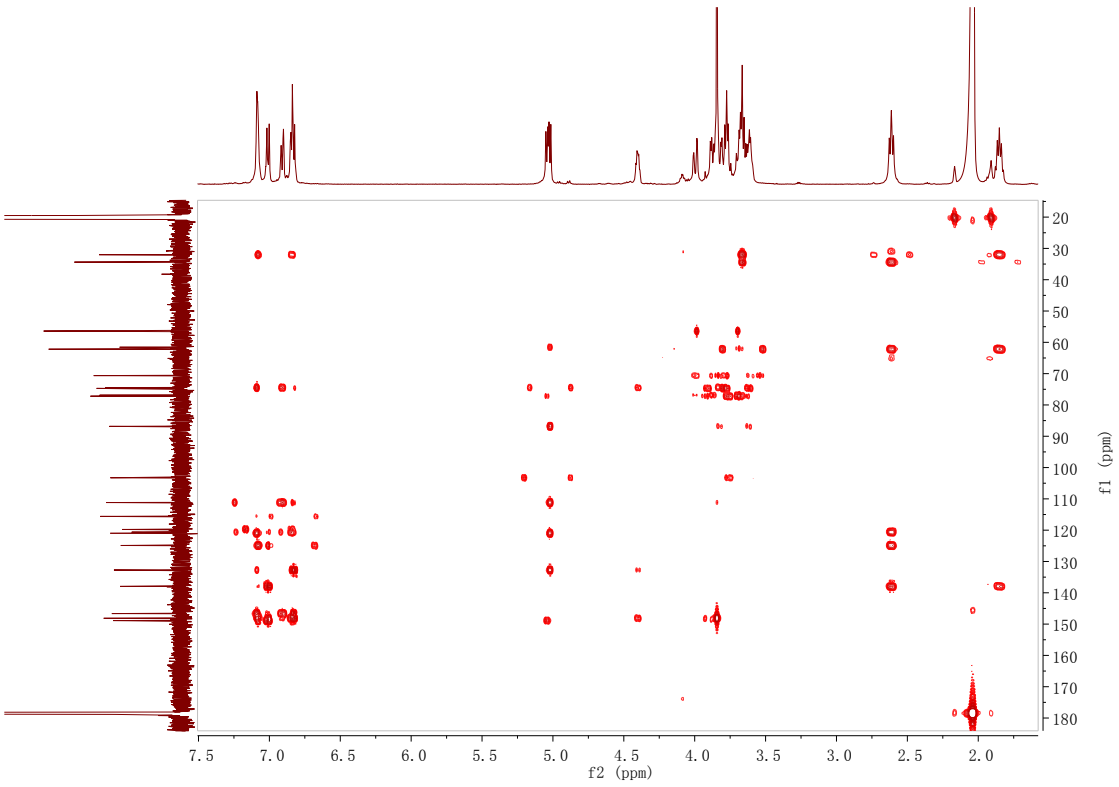


Figure S177. The HMBC spectrum of B-2 in CD_3COOD

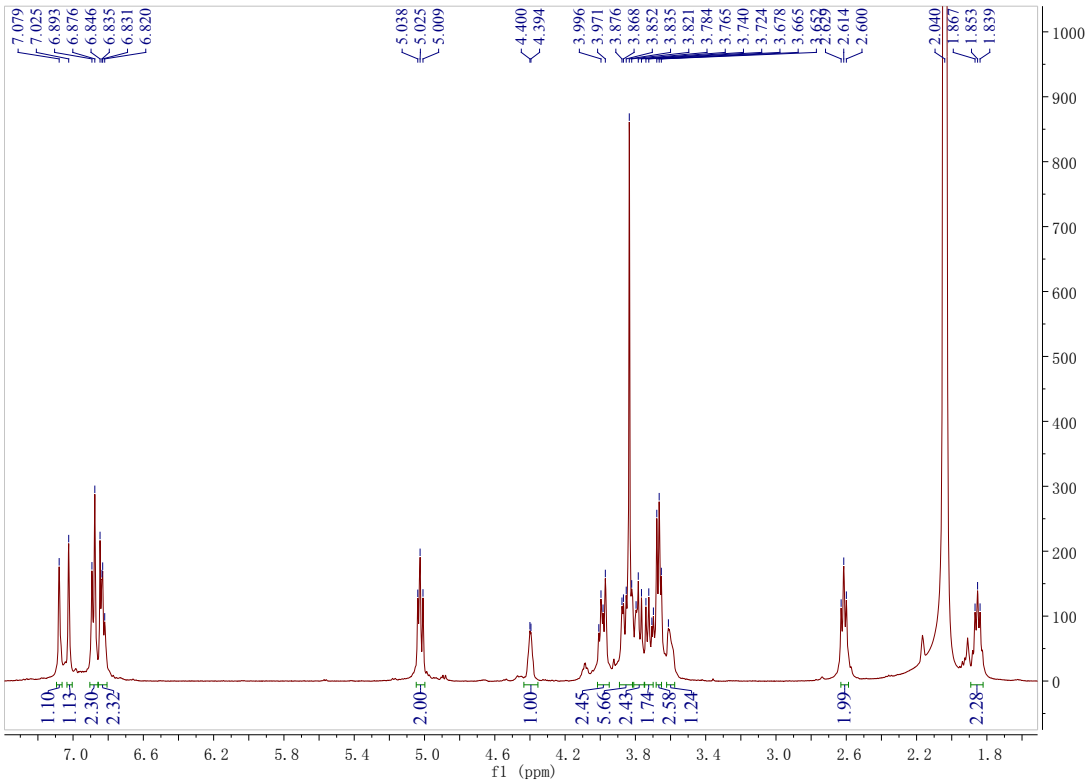


Figure S178. The ^{1}H-NMR spectrum of B-3 in CD_3COOD

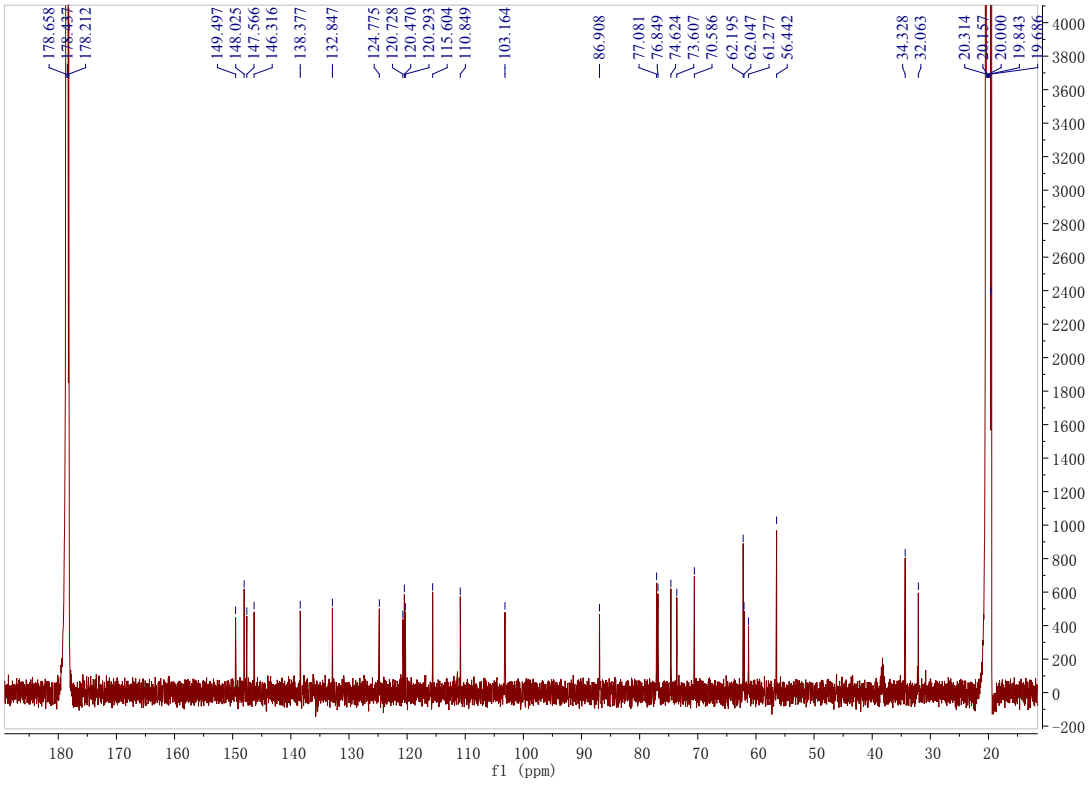


Figure S179. The ^{13}C-NMR spectrum of B-3 in CD_3COOD

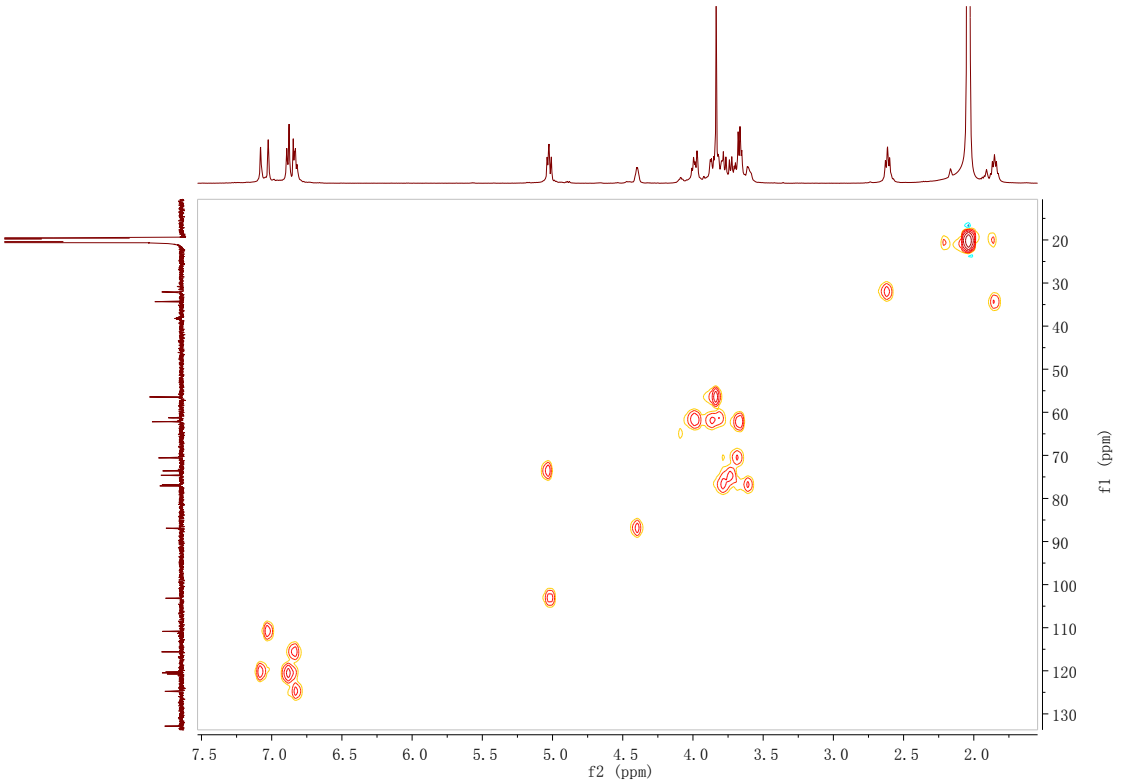


Figure S180. The HSQC spectrum of B-3 in CD_3COOD

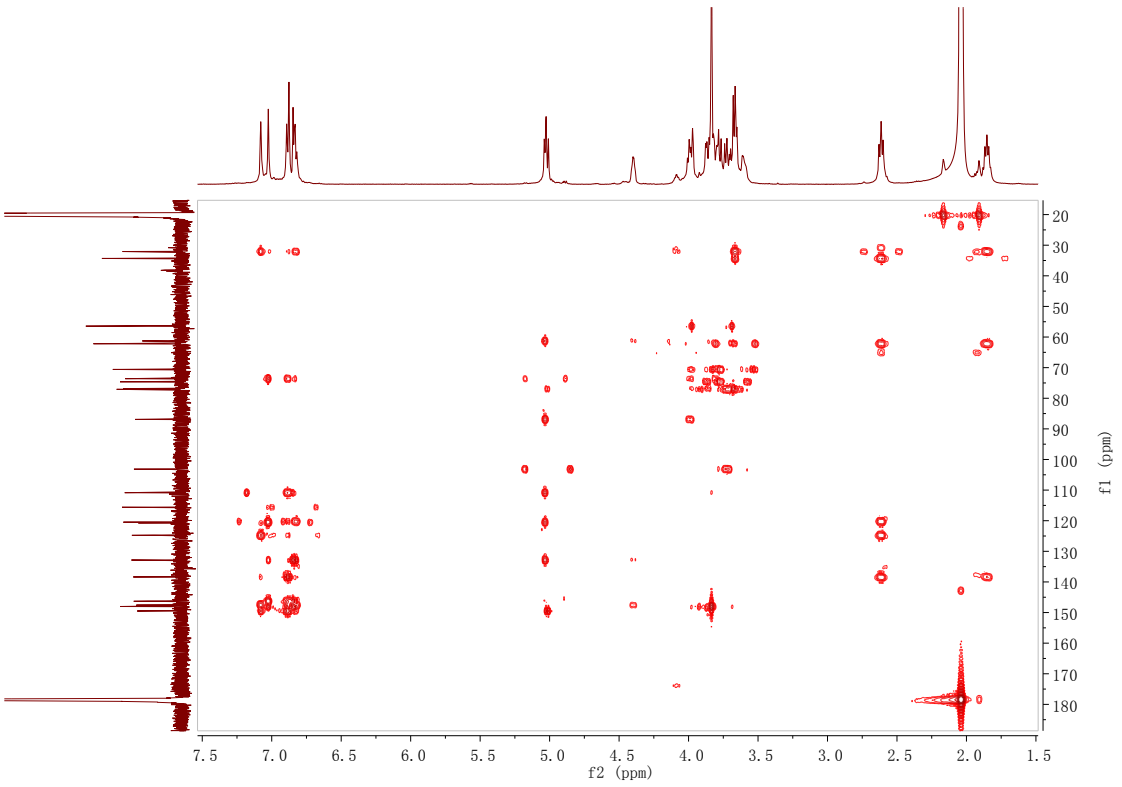


Figure S181. The HMBC spectrum of B-3 in CD_3COOD

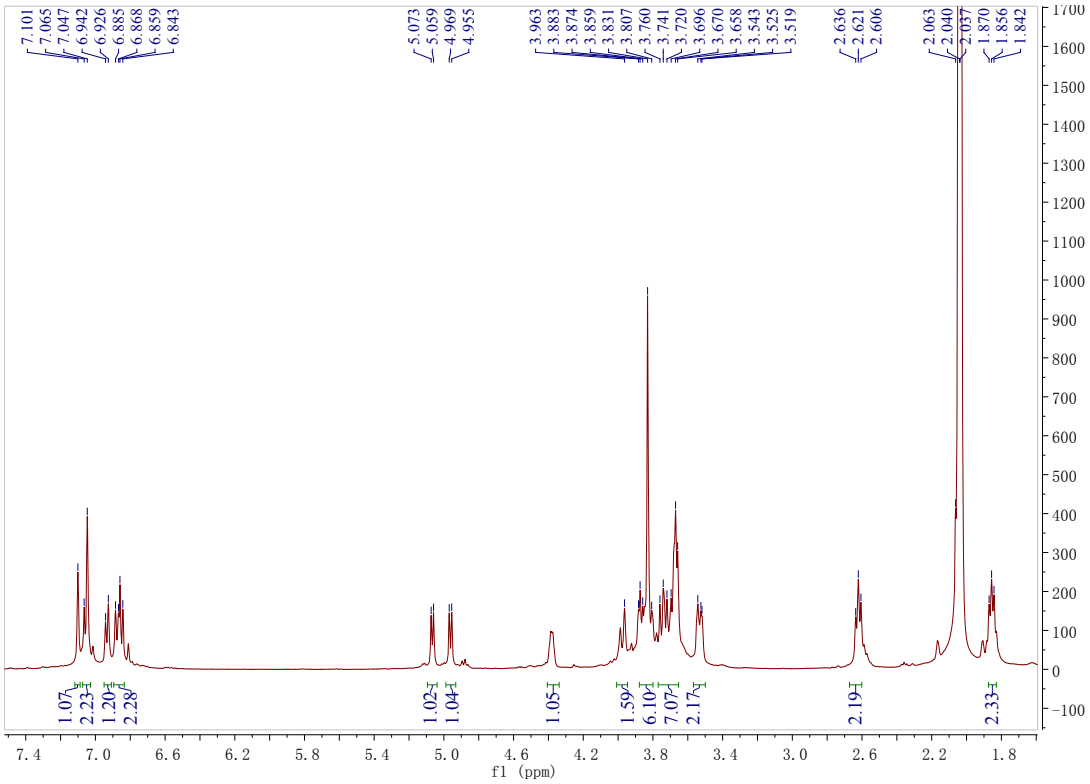


Figure S182. The ^{1}H-NMR spectrum of B-4 in CD_3COOD

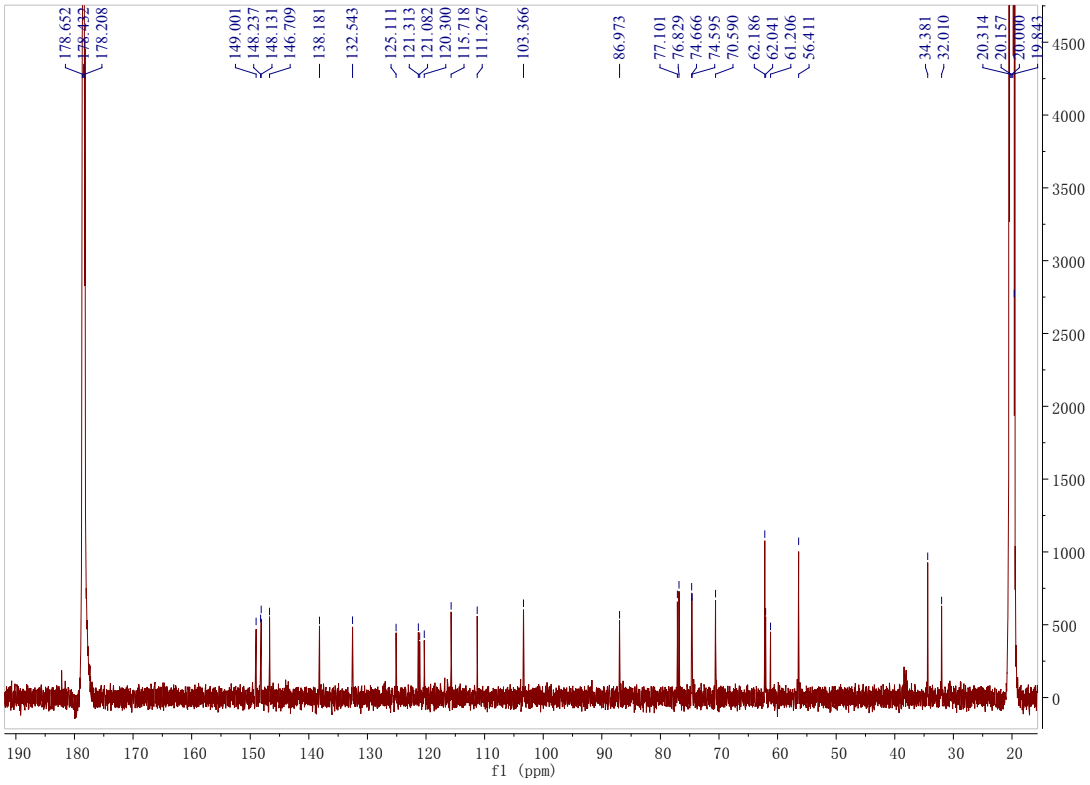


Figure S183. The ^{13}C-NMR spectrum of B-4 in CD_3COOD

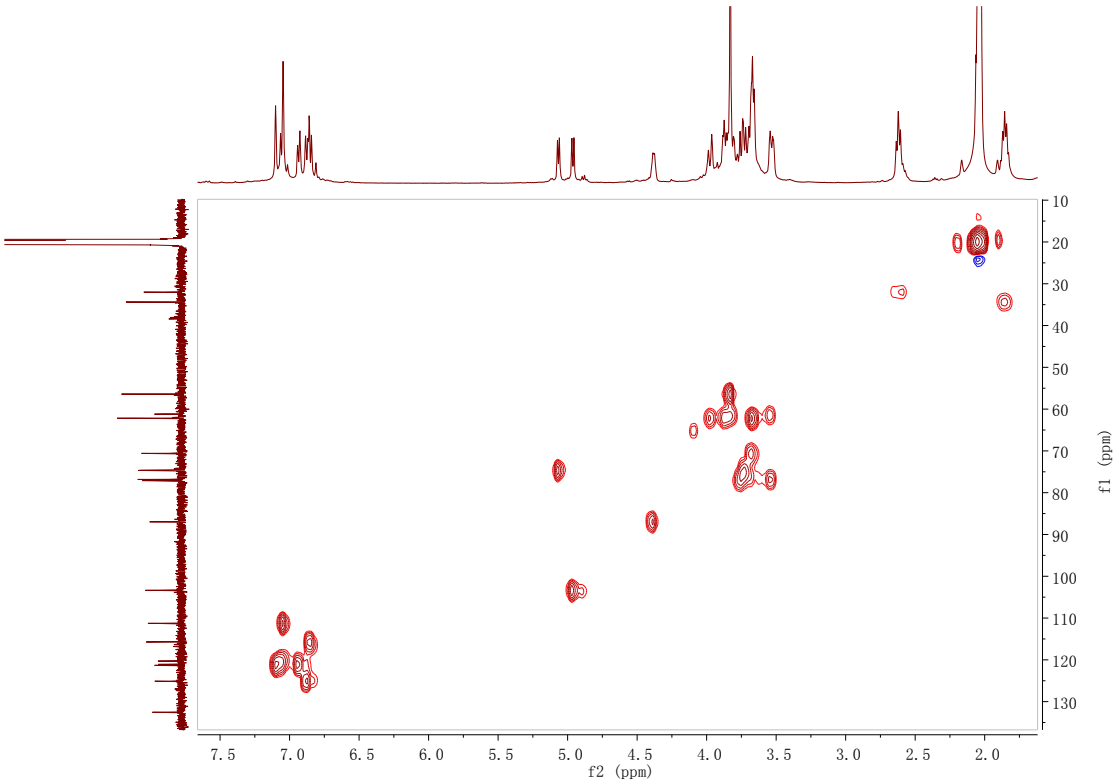


Figure S184. The HSQC spectrum of B-4 in CD_3COOD

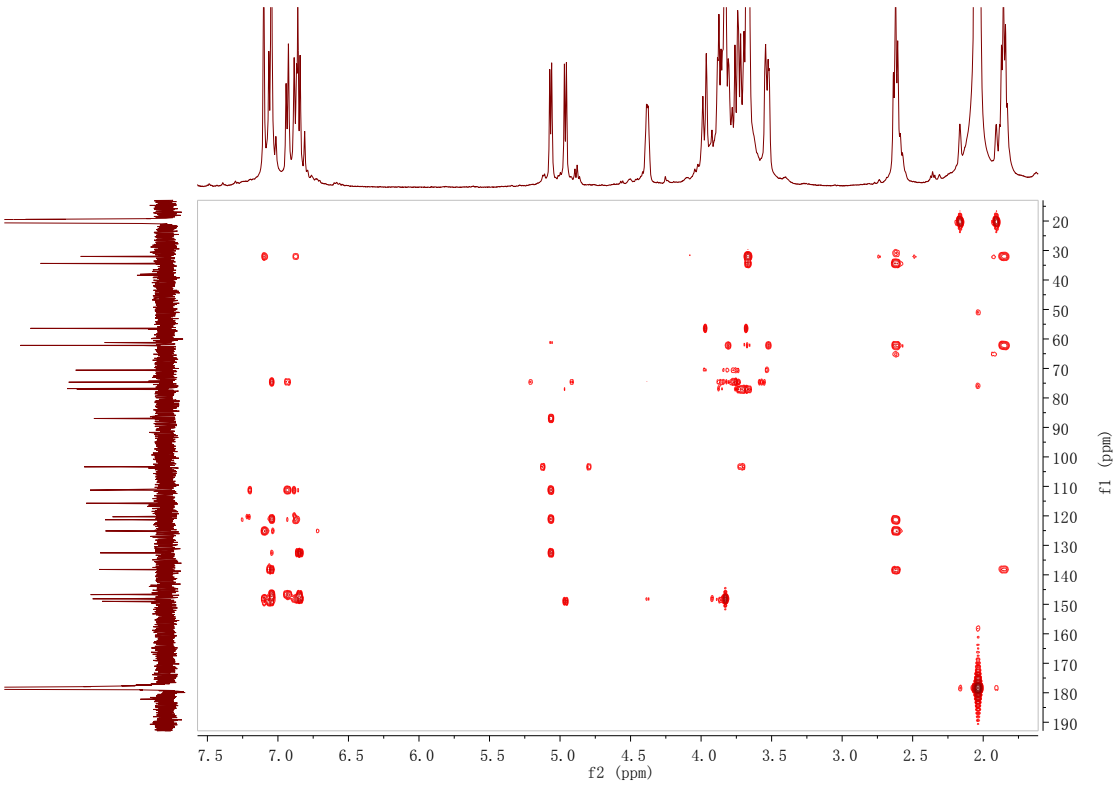


Figure S185. The HMBC spectrum of B-4 in CD_3COOD

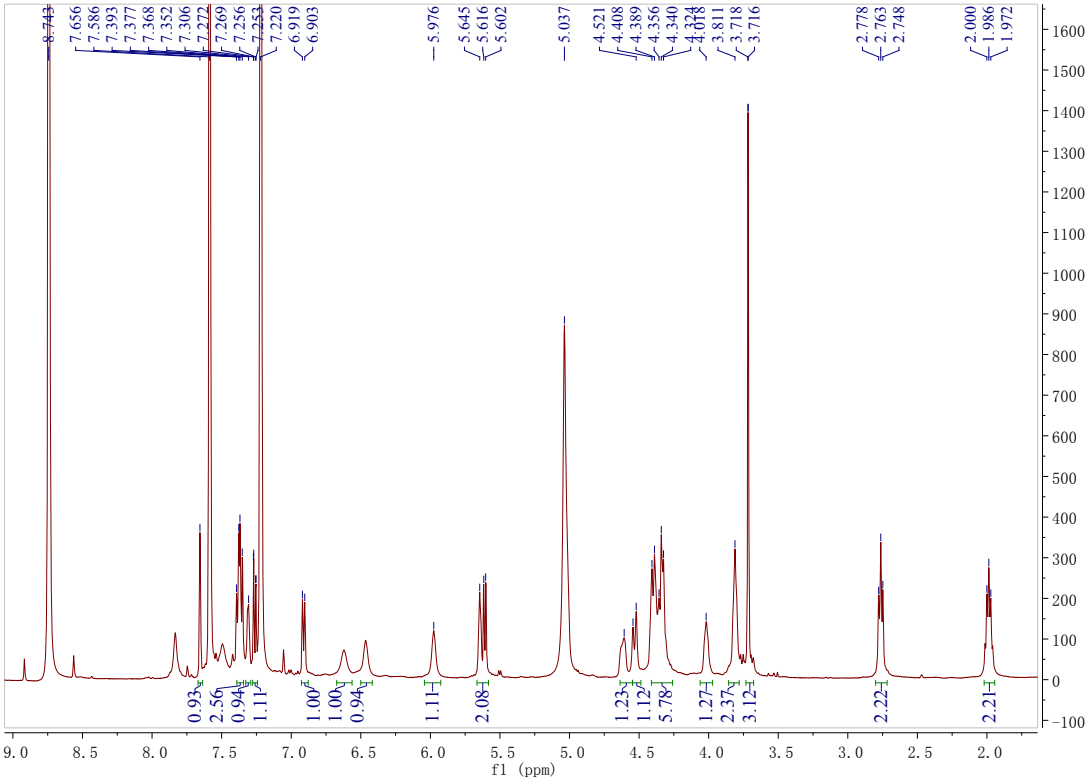


Figure S186. The ^{1}H-NMR spectrum of B-1 in C_5D_5N

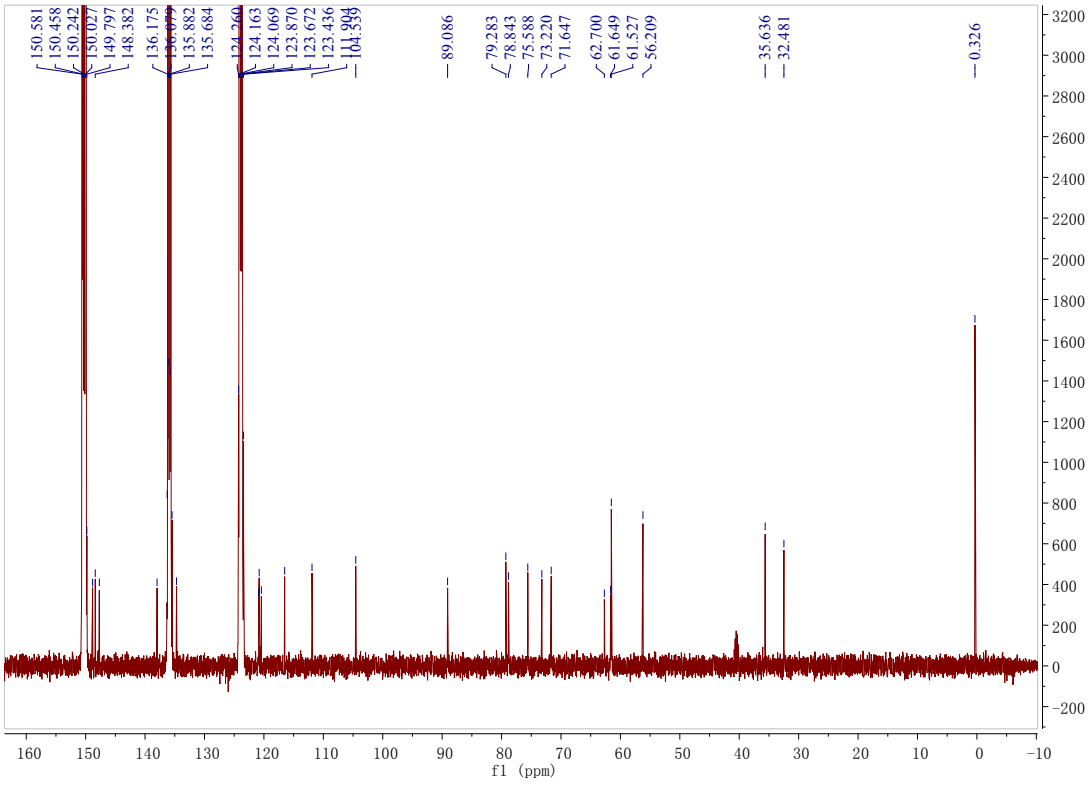


Figure S187. The ^{13}C-NMR spectrum of B-1 in C_5D_5N

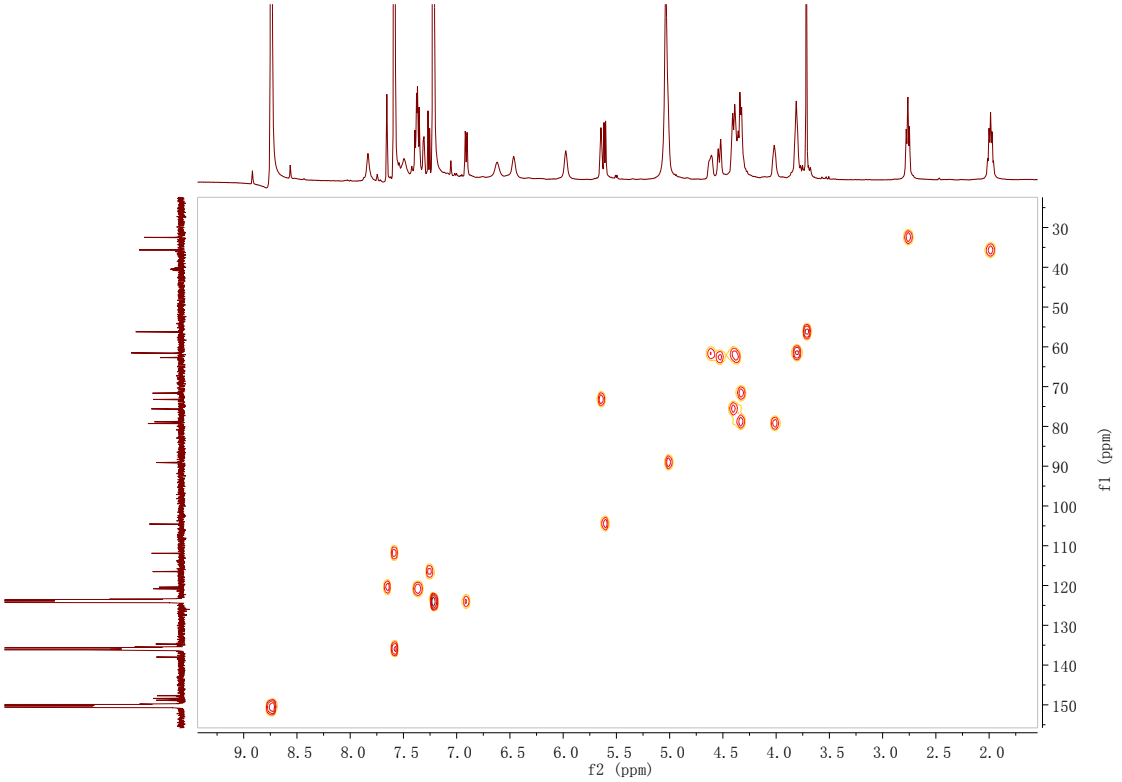


Figure S188. The HSQC spectrum of B-1 in C_5D_5N

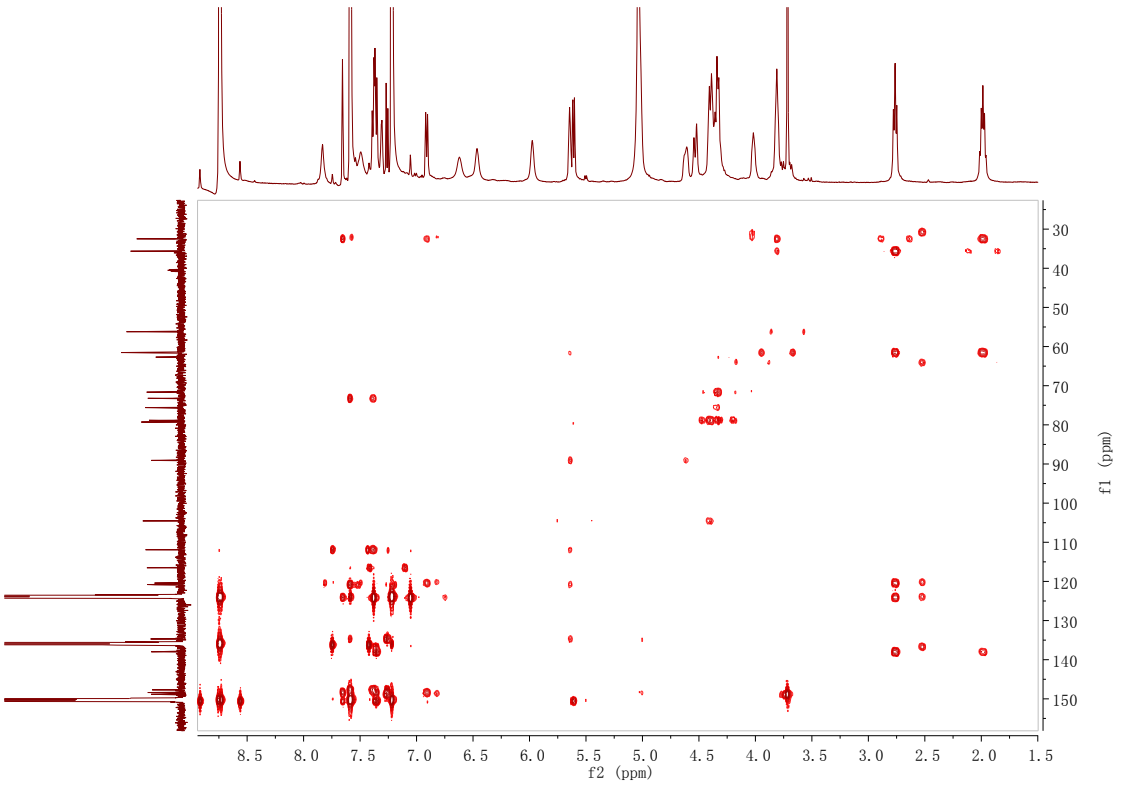


Figure S189. The HMBC spectrum of B-1 in C_5D_5N

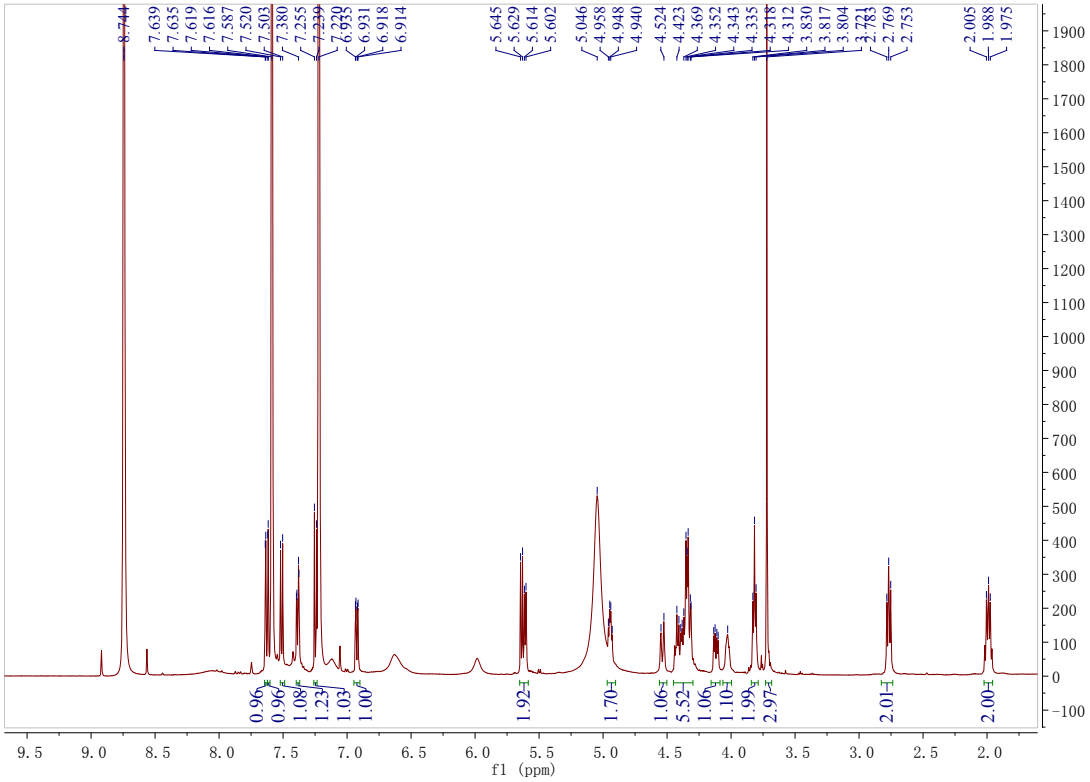


Figure S190. The ^{1}H-NMR spectrum of B-2 in C_5D_5N

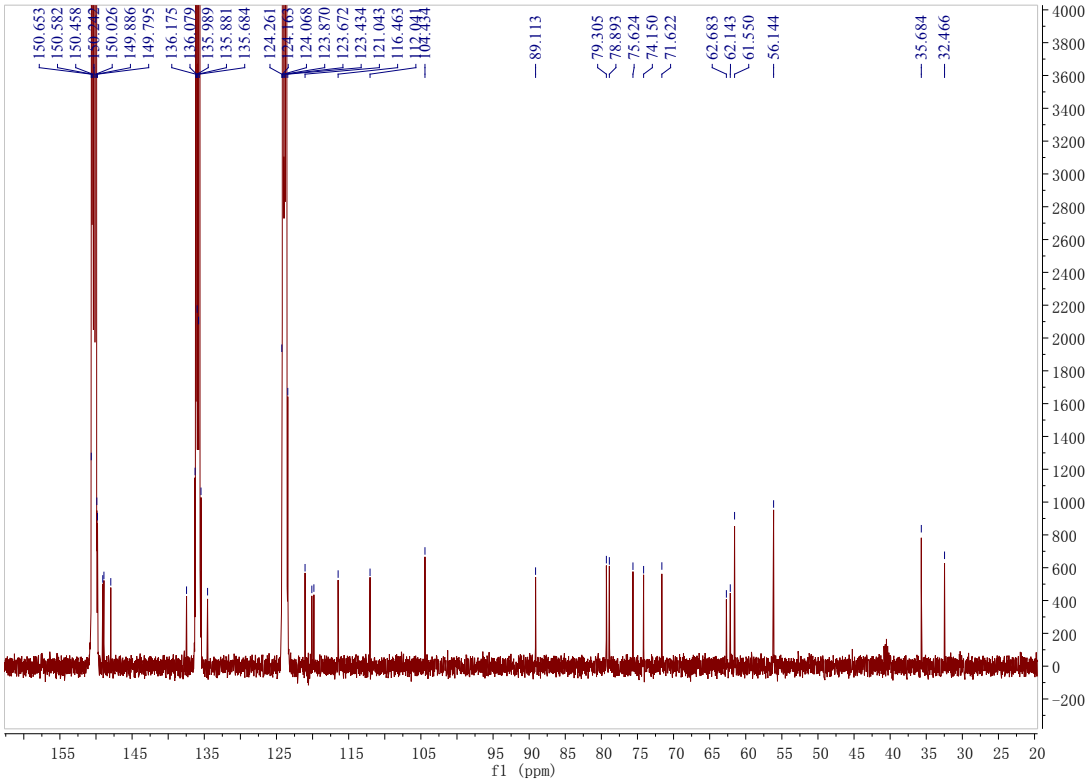


Figure S191. The ^{13}C-NMR spectrum of B-2 in C_5D_5N

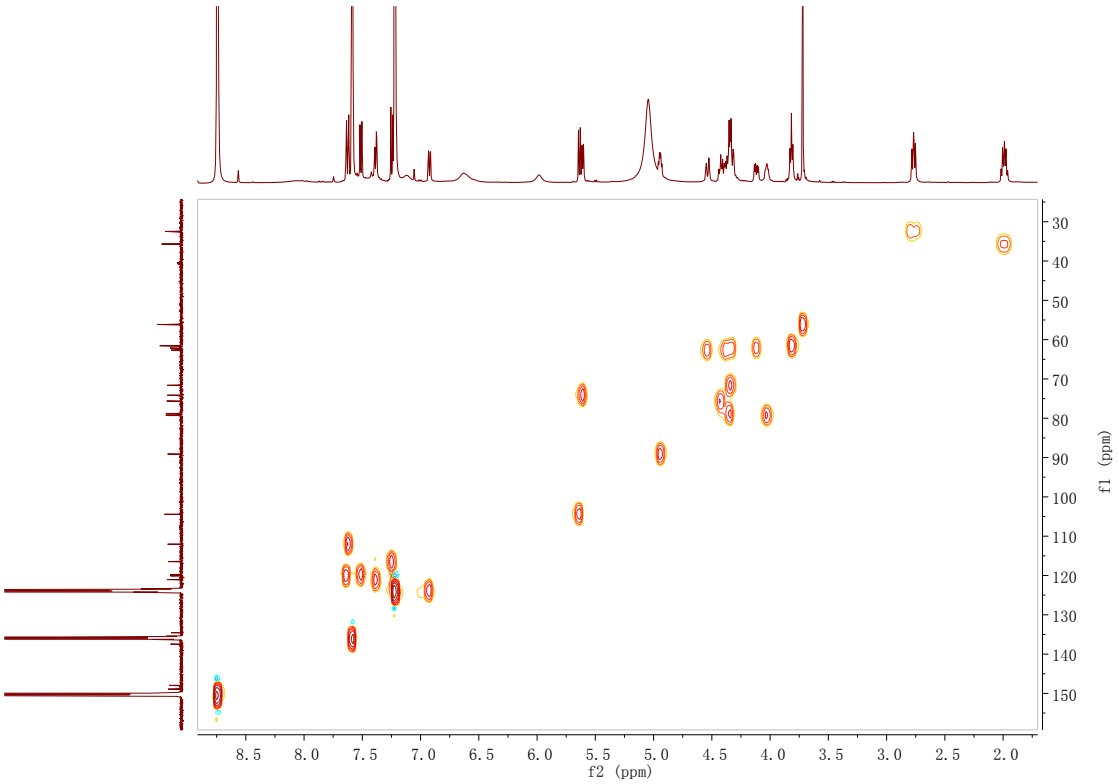


Figure S192. The HSQC spectrum of B-2 in C_5D_5N

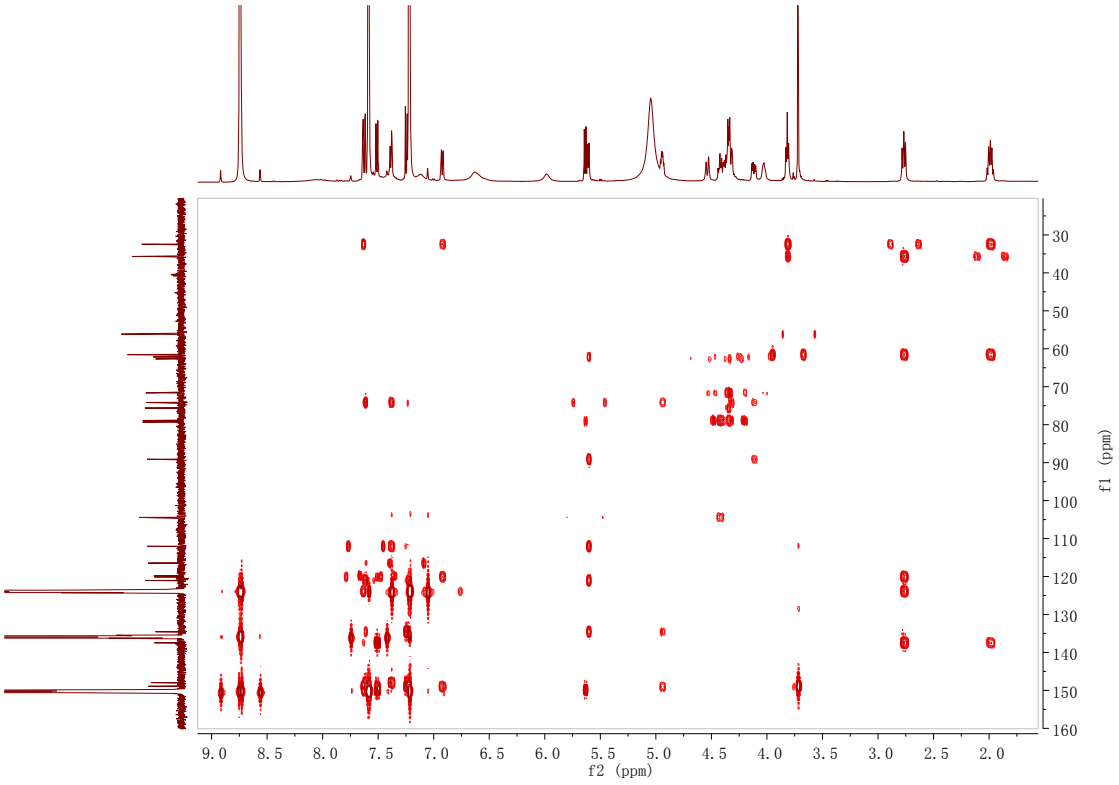


Figure S193. The HMBC spectrum of B-2 in C_5D_5N

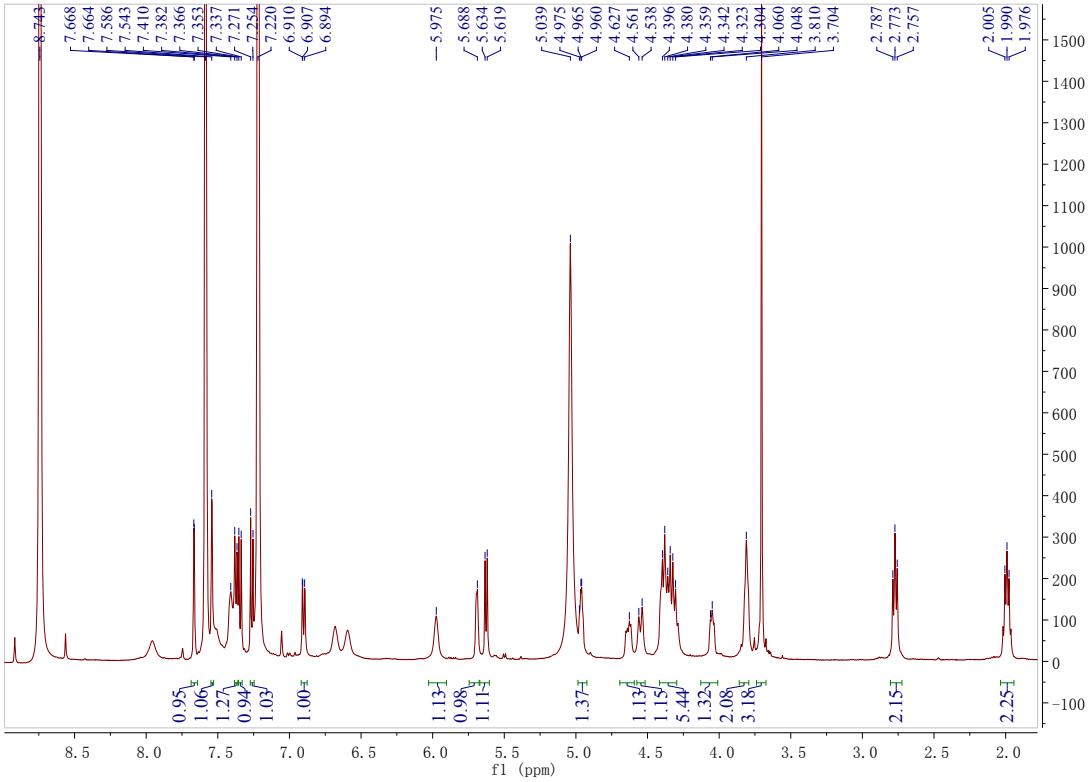


Figure S194. The ^{1}H-NMR spectrum of B-3 in C_5D_5N

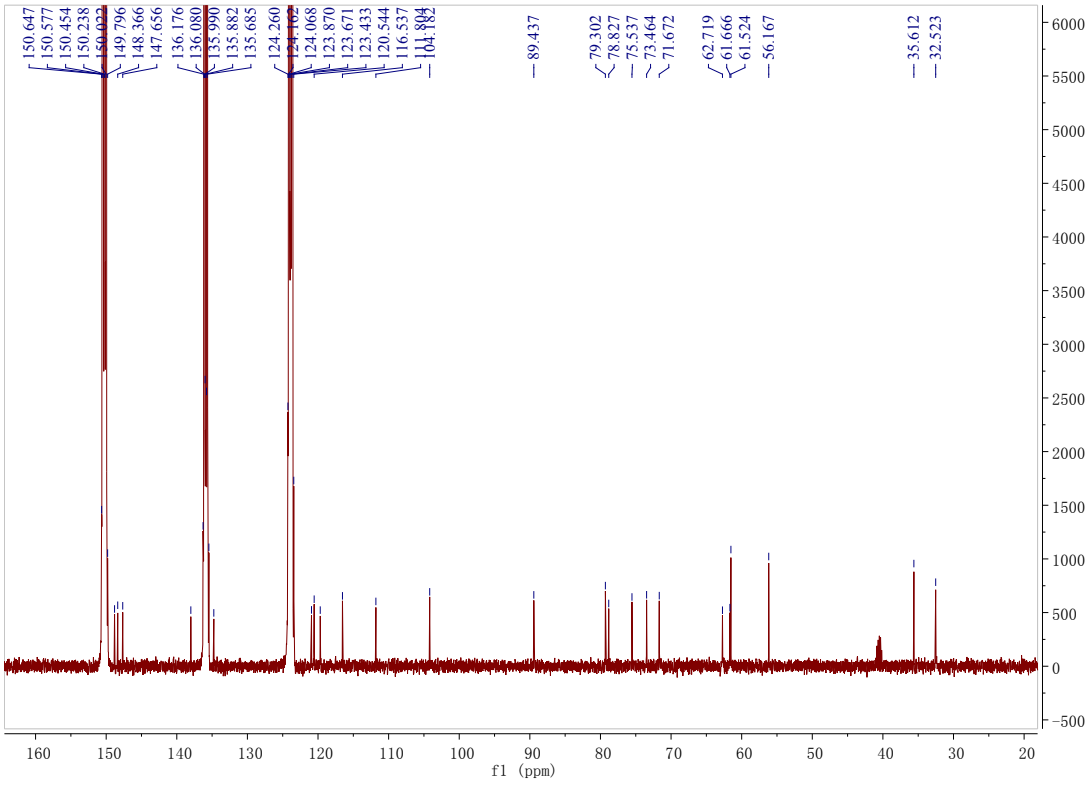


Figure S195. The ^{13}C-NMR spectrum of B-3 in C_5D_5N

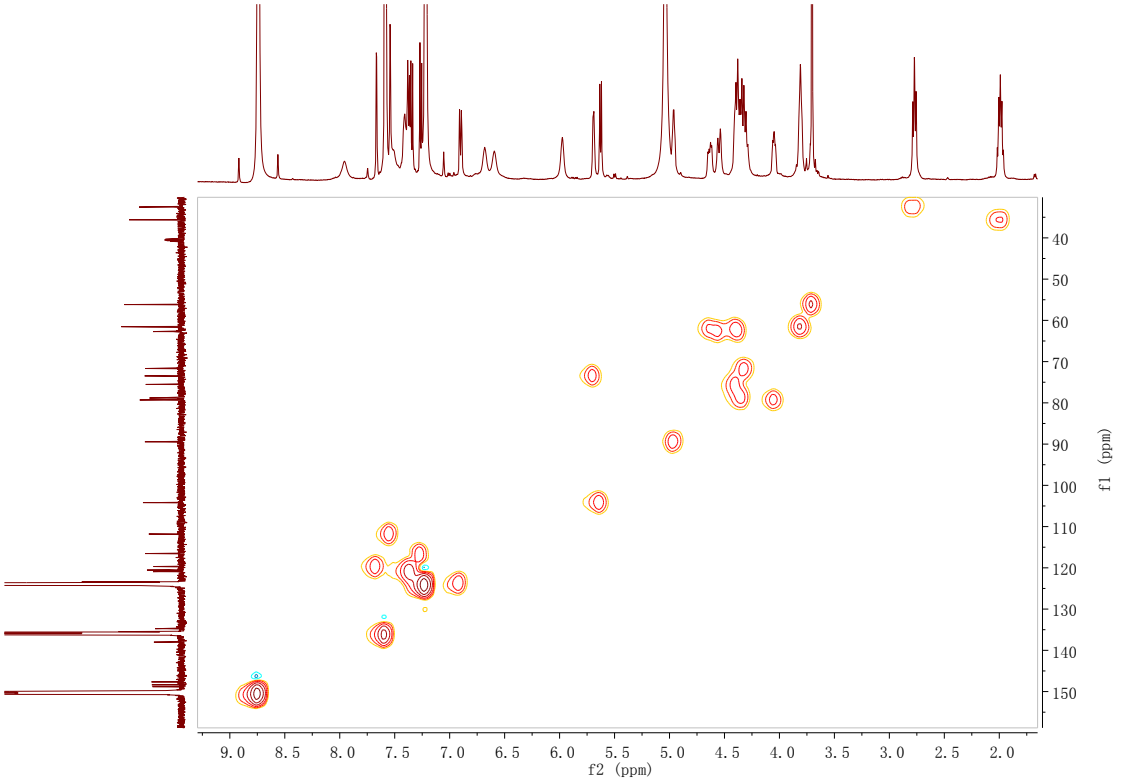


Figure S196. The HSQC spectrum of B-3 in C_5D_5N

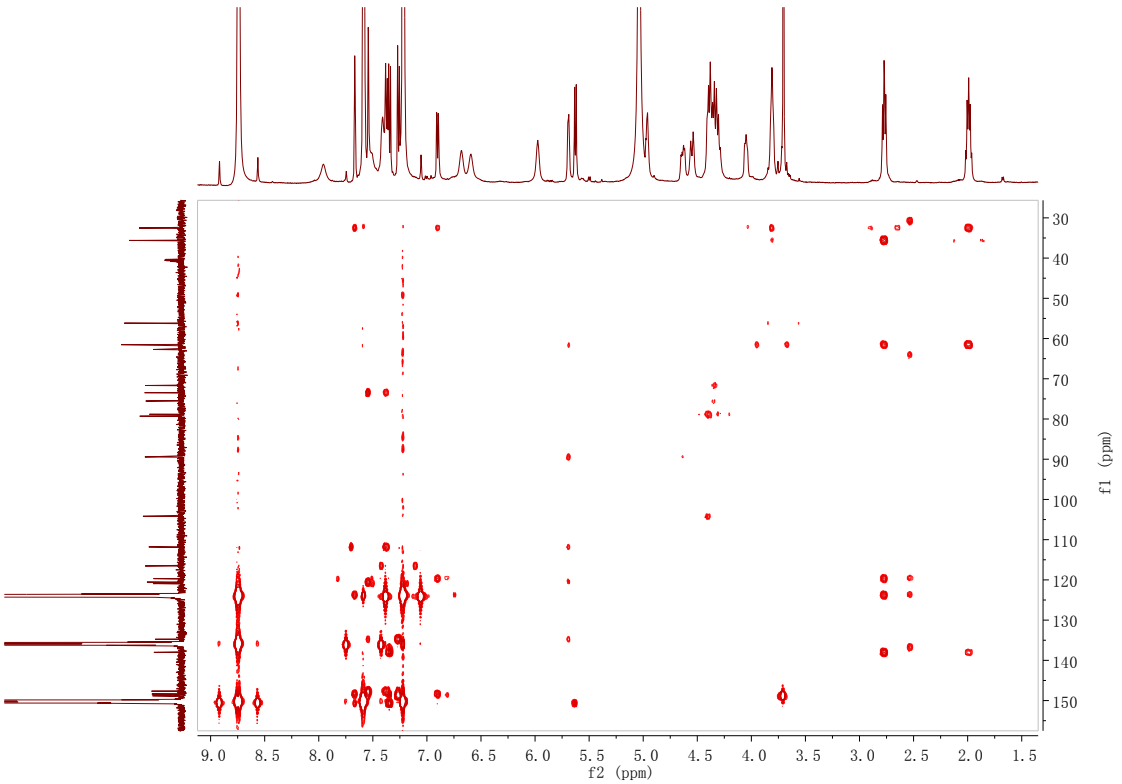


Figure S197. The HMBC spectrum of B-3 in C_5D_5N

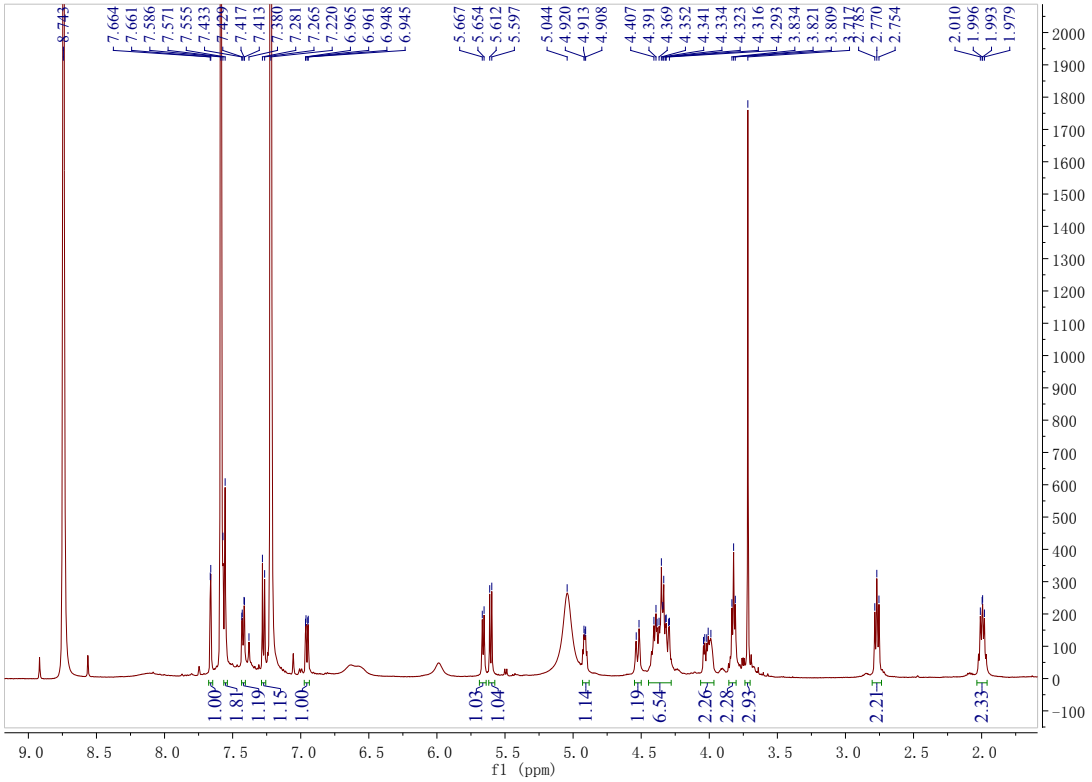


Figure S198. The ^{1}H-NMR spectrum of B-4 in C_5D_5N

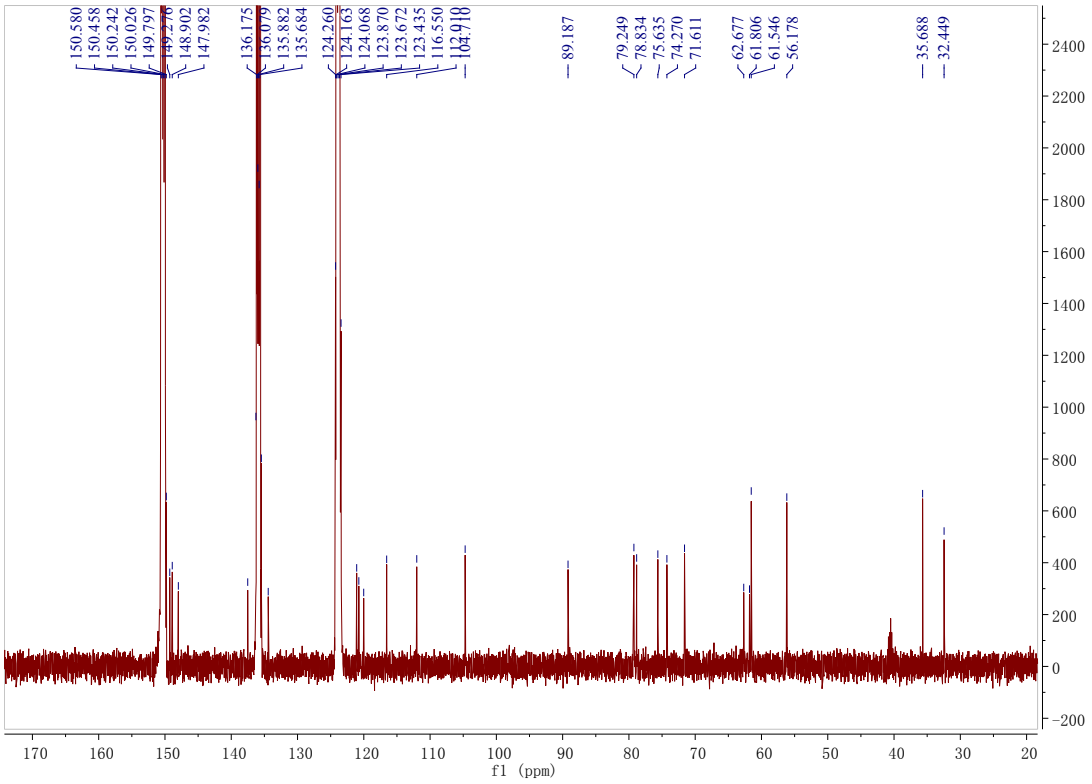


Figure S199. The ^{13}C-NMR spectrum of B-4 in C_5D_5N

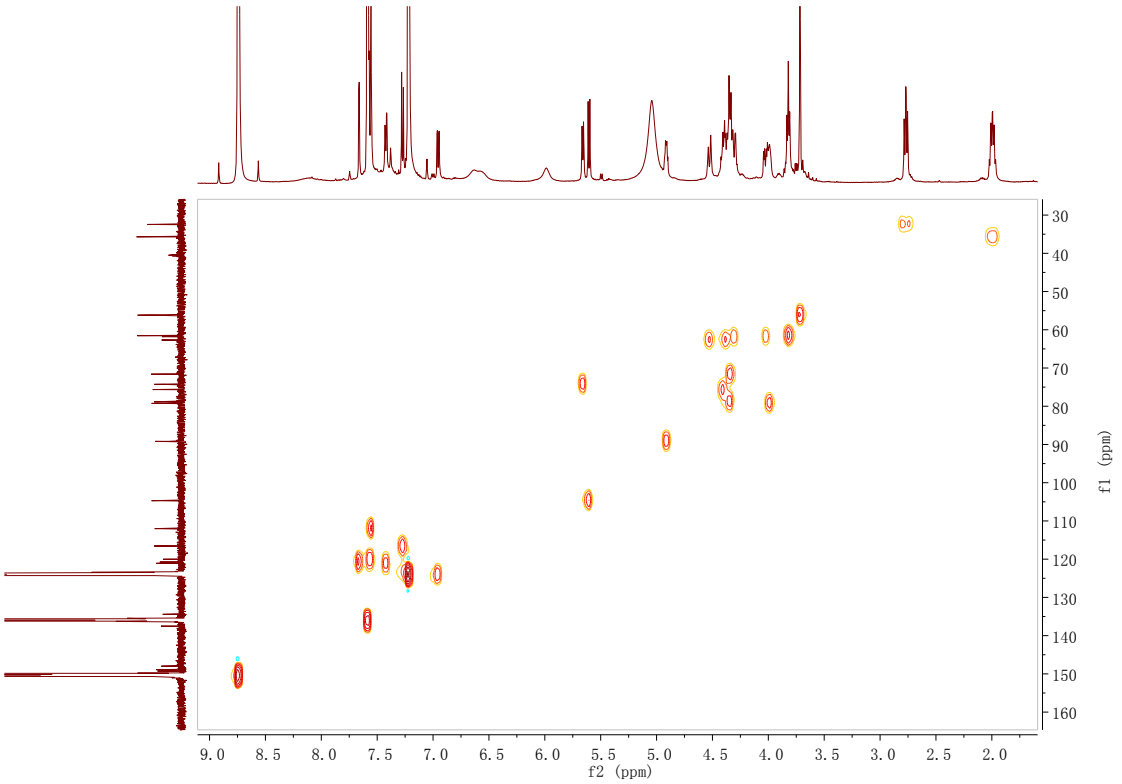


Figure S200. The HSQC spectrum of B-4 in C_5D_5N

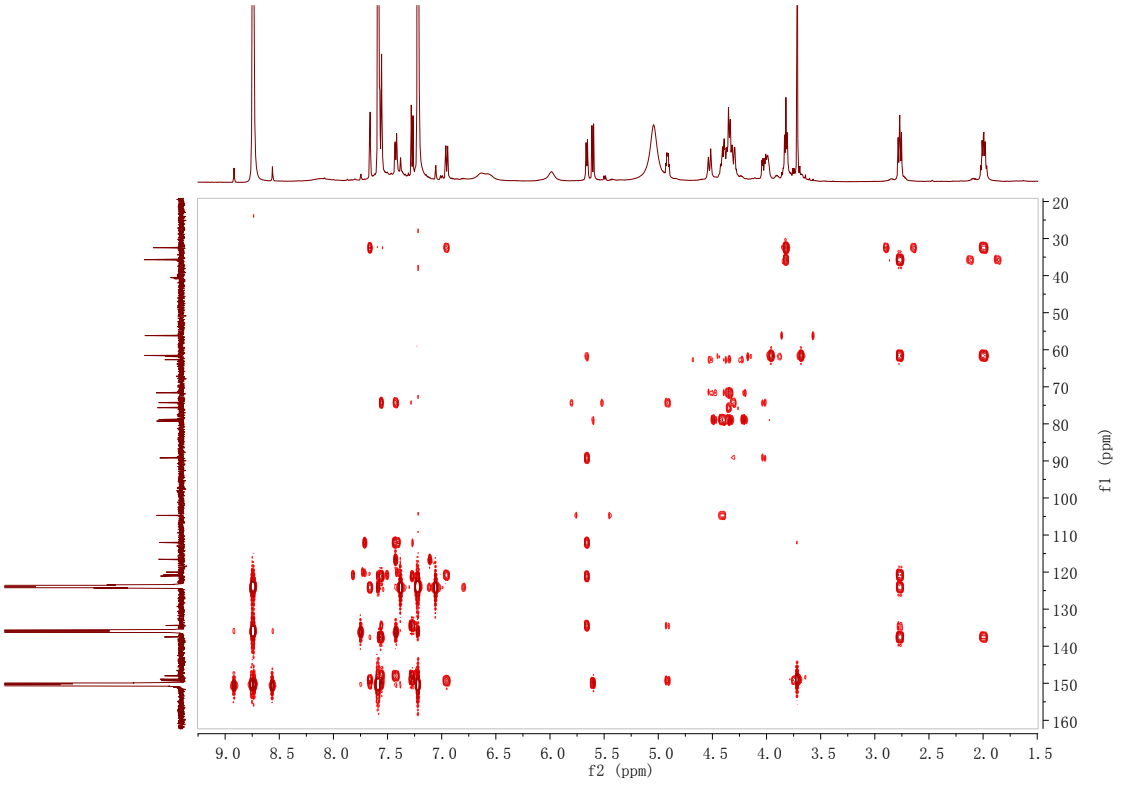


Figure S201. The HMBC spectrum of B-4 in C_5D_5N

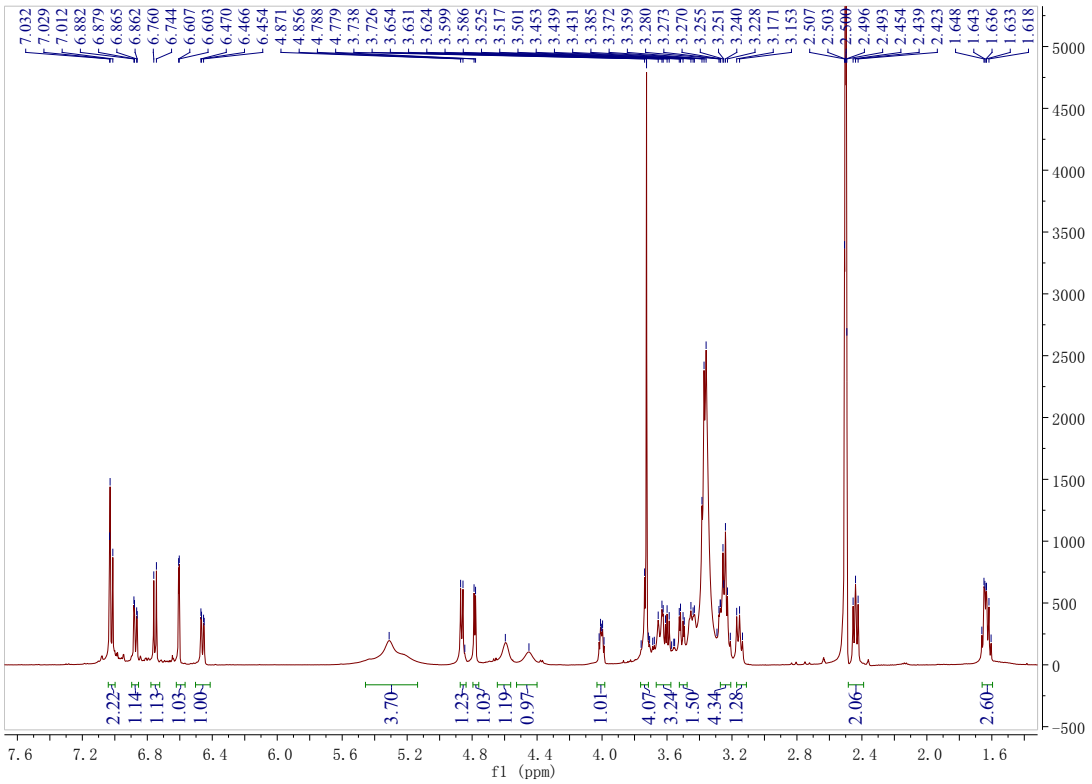


Figure S202. The ^{1}H-NMR spectrum of C-1 in DMSO-d_6

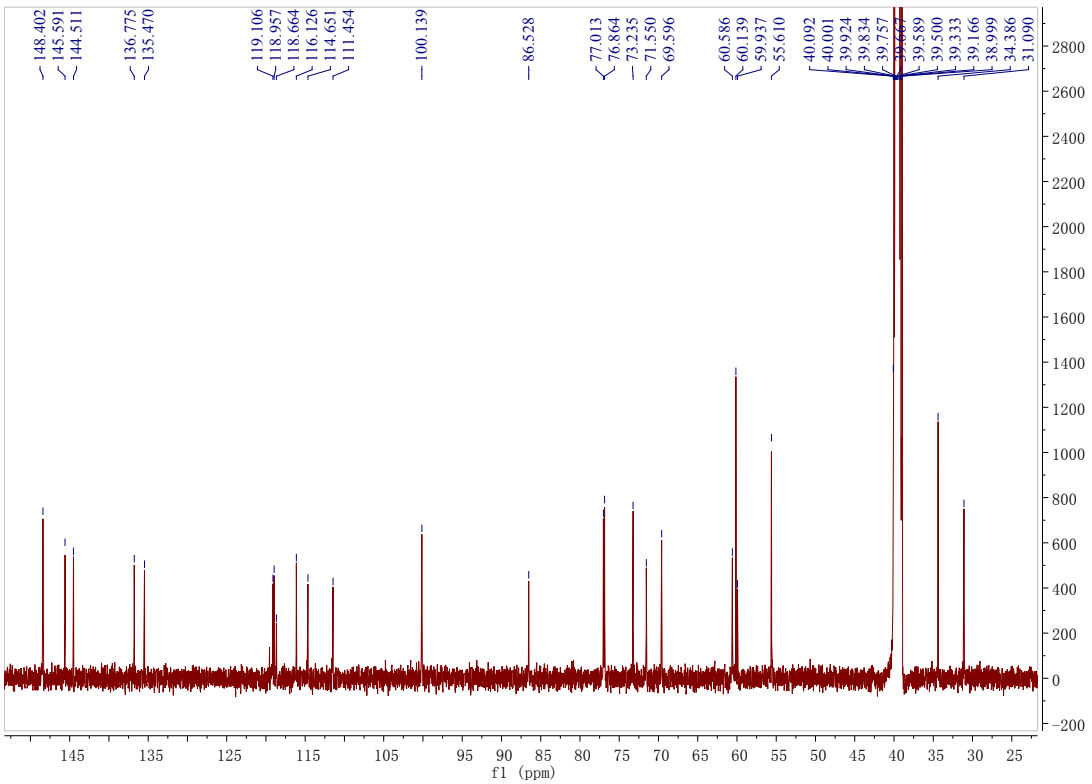


Figure S203. The ^{13}C-NMR spectrum of C-1 in DMSO-d_6

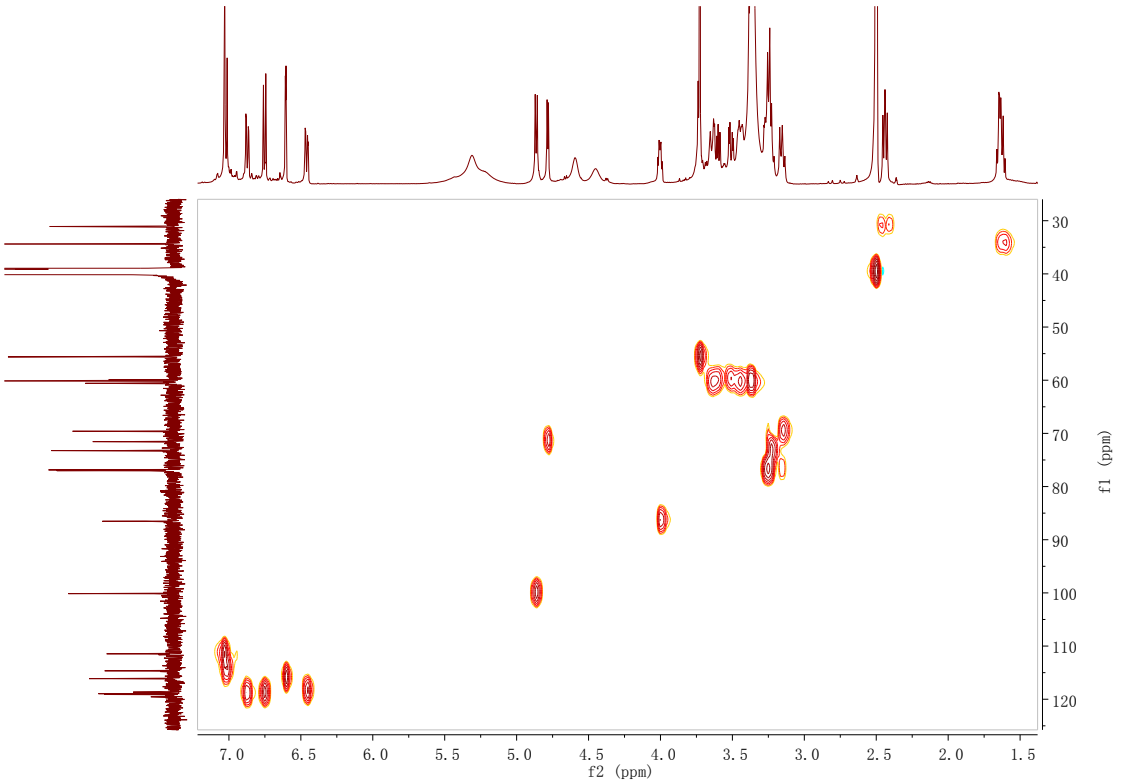


Figure S204. The HSQC spectrum of C-1 in DMSO-d_6

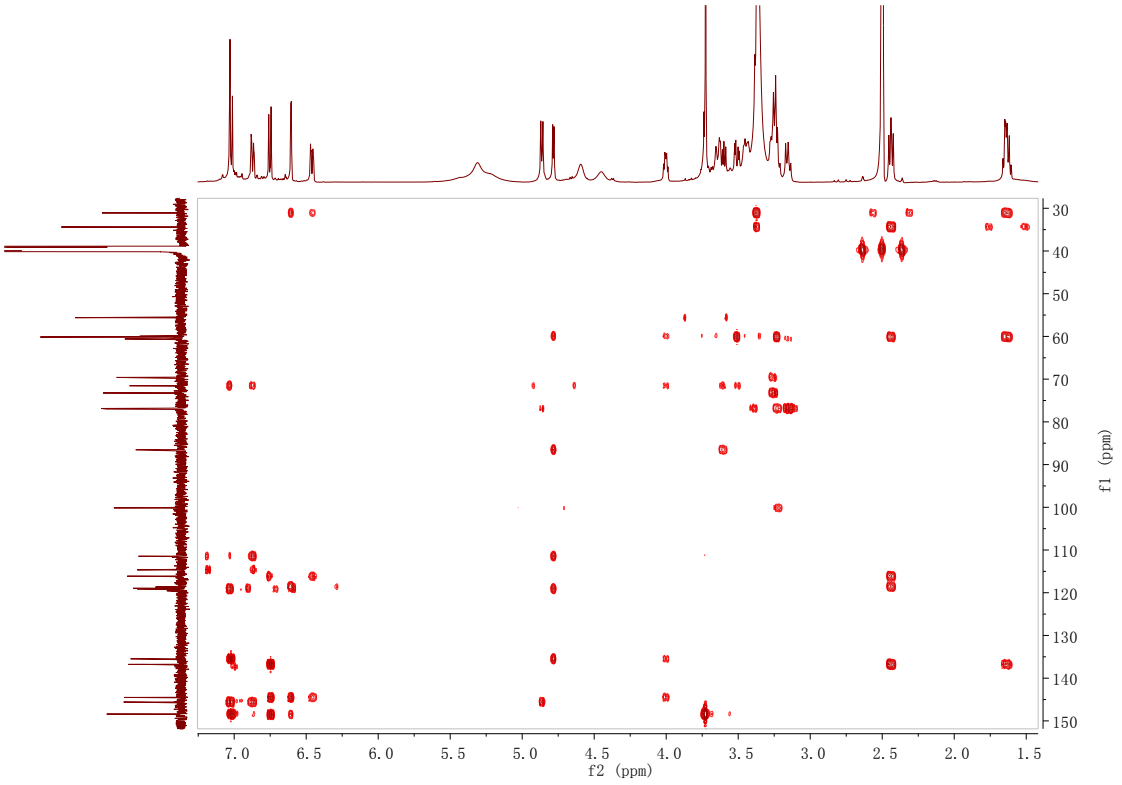


Figure S205. The HMBC spectrum of C-1 in DMSO-d_6

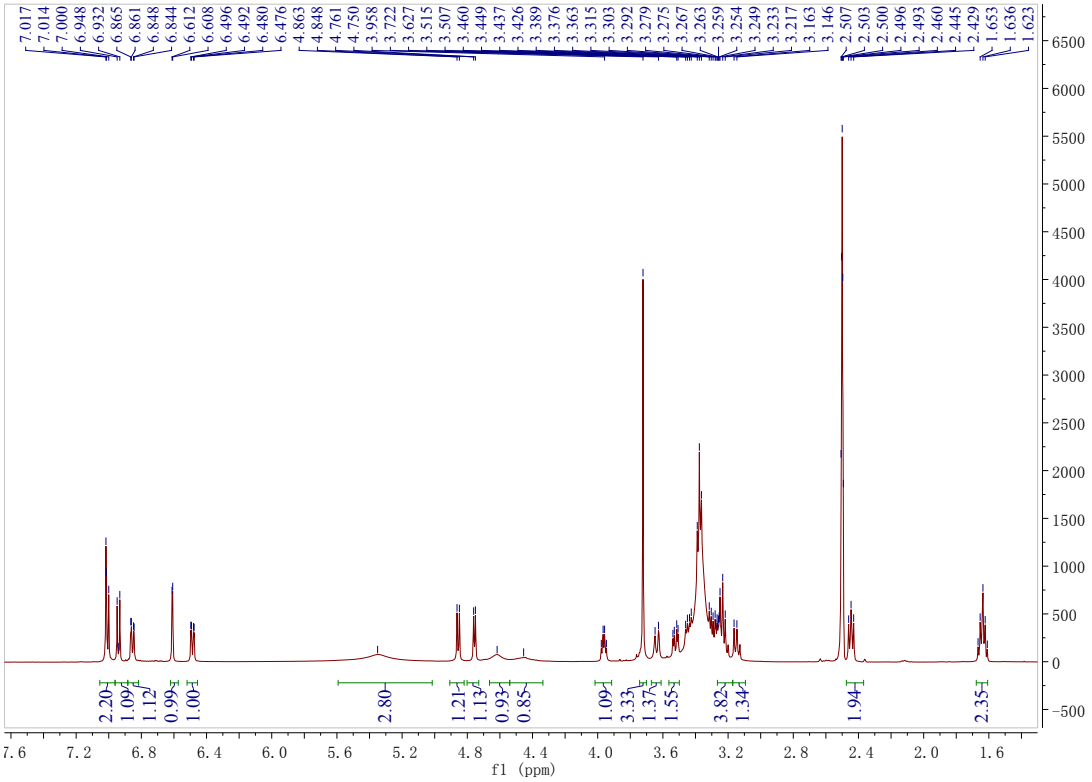


Figure S206. The ^{1}H-NMR spectrum of C-2 in DMSO-d_6

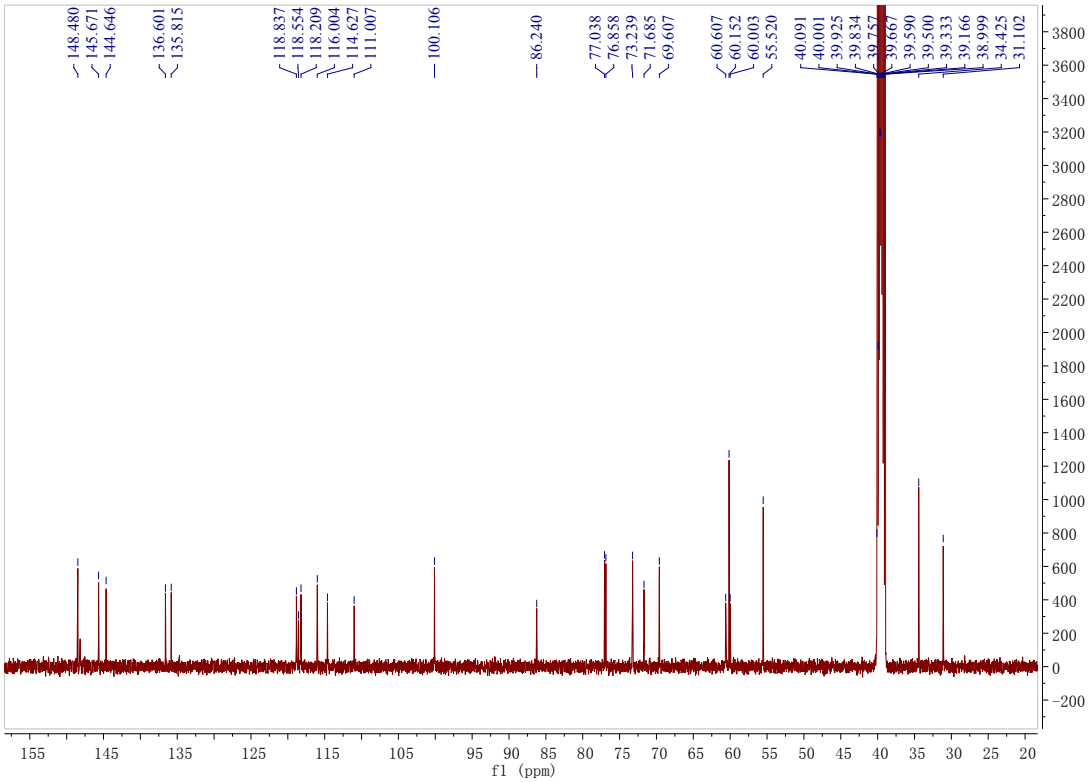


Figure S207. The ^{13}C-NMR spectrum of C-2 in DMSO-d_6

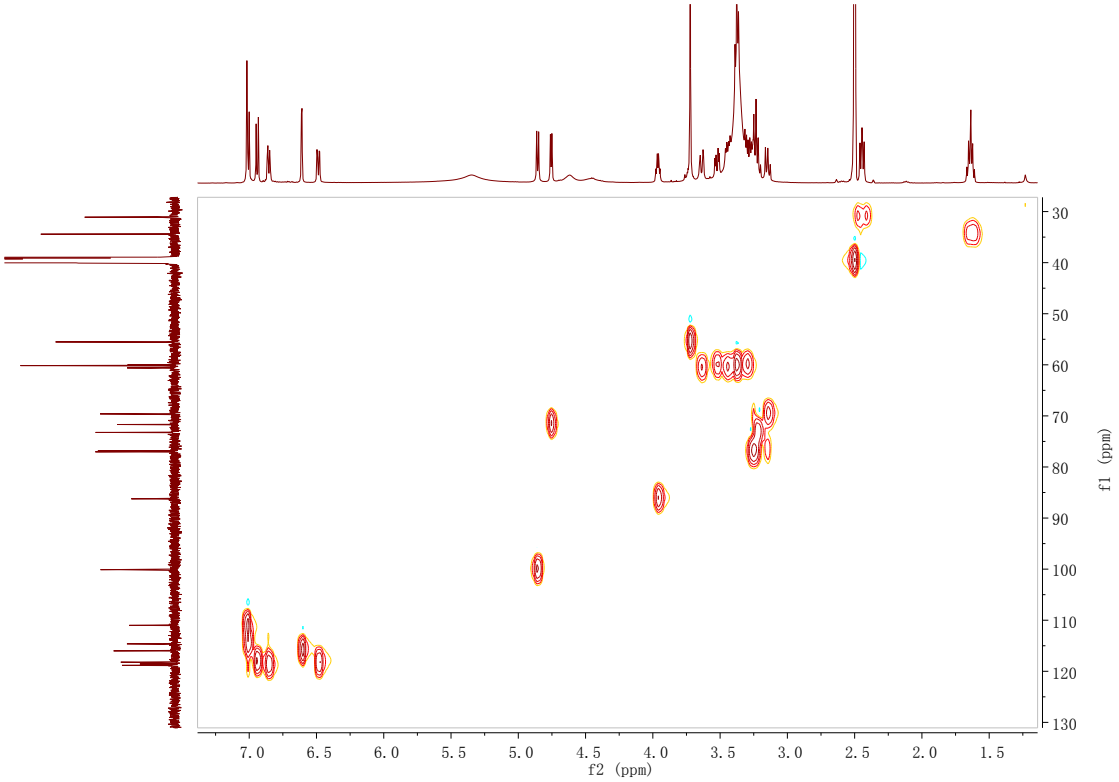


Figure S208. The HSQC spectrum of C-2 in DMSO-d_6

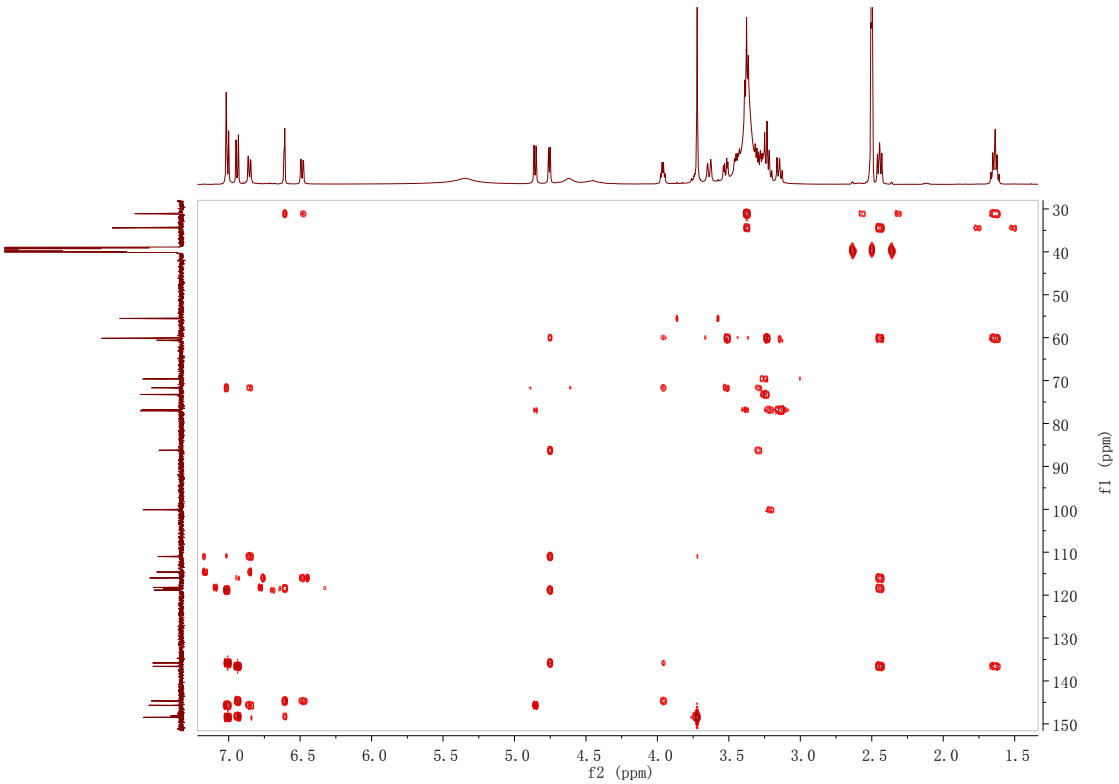


Figure S209. The HMBC spectrum of C-2 in DMSO-d_6

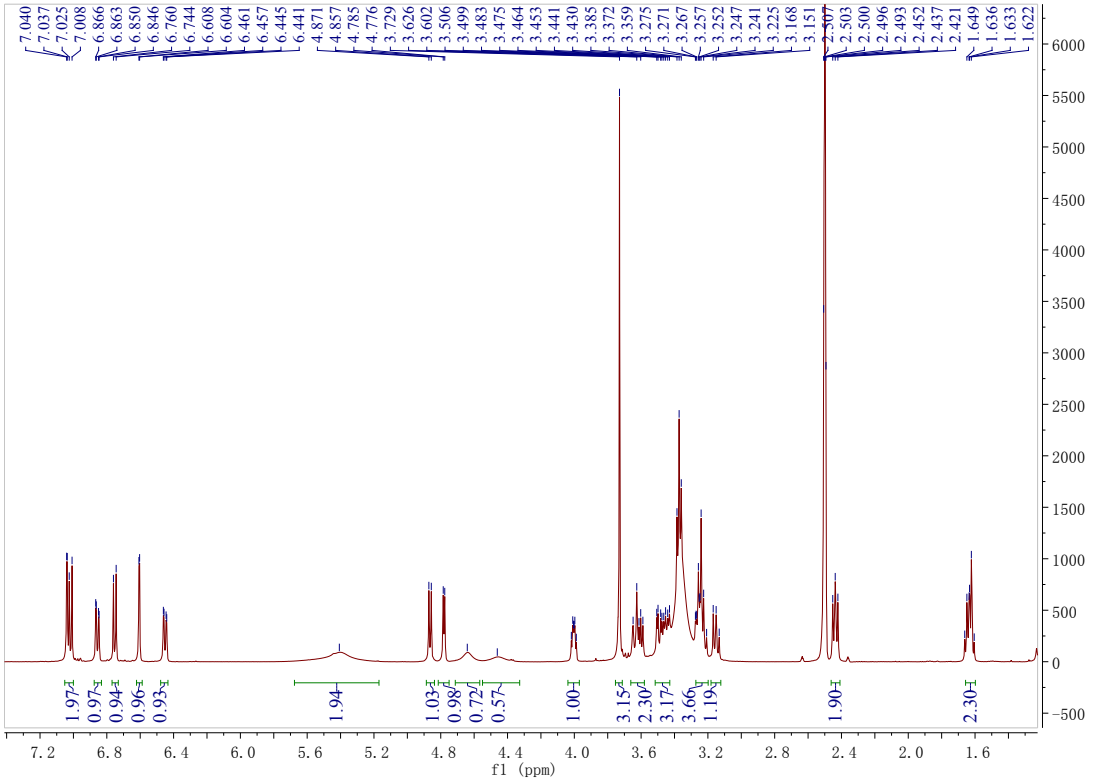


Figure S210. The ^{1}H-NMR spectrum of C-3 in DMSO-d_6

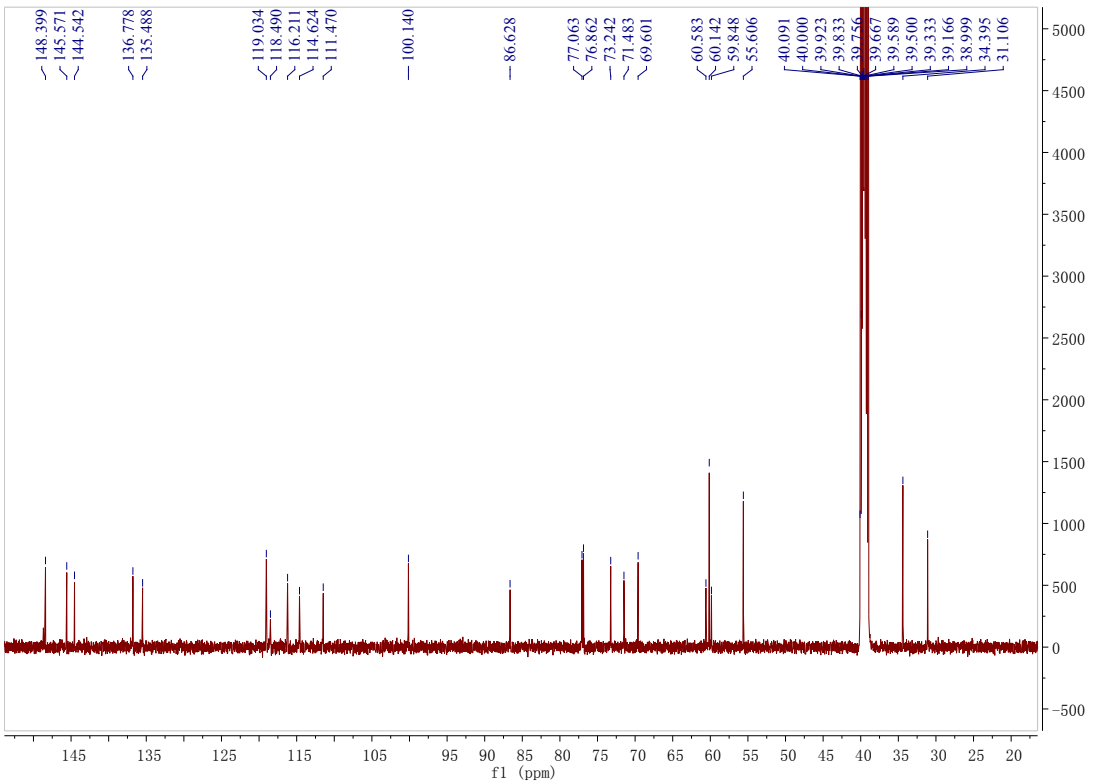


Figure S211. The ^{13}C-NMR spectrum of C-3 in DMSO-d_6

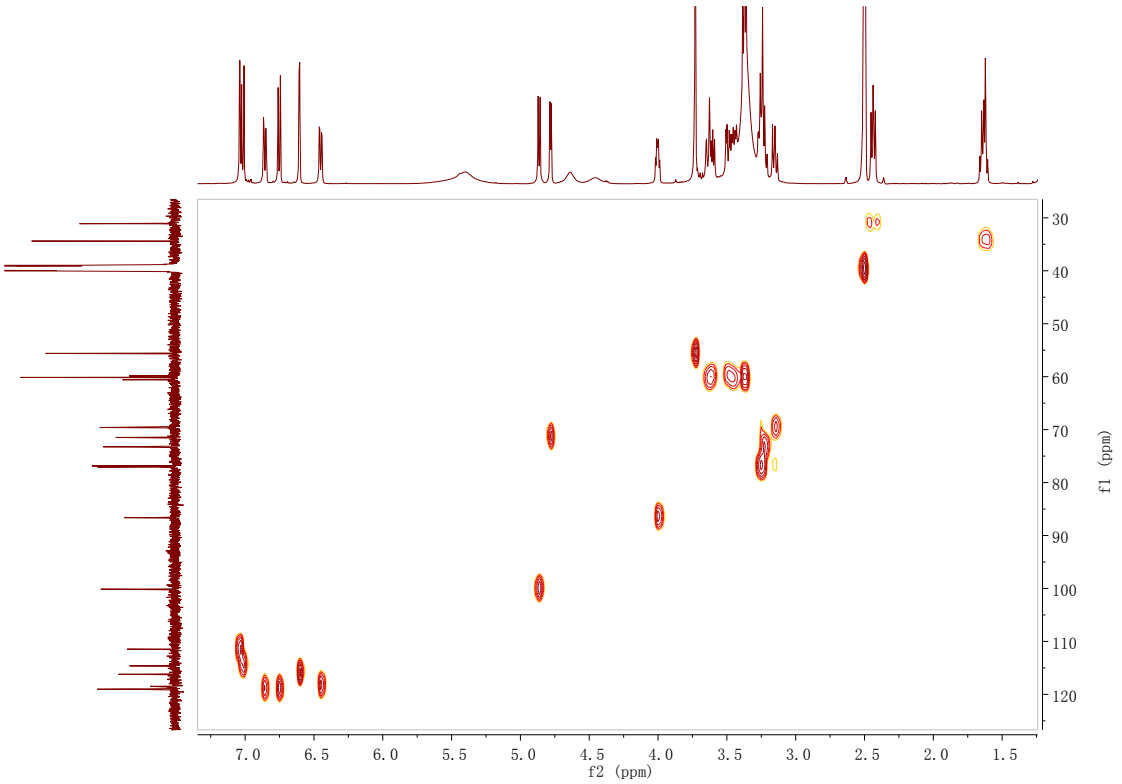


Figure S212. The HSQC spectrum of C-3 in DMSO-d_6

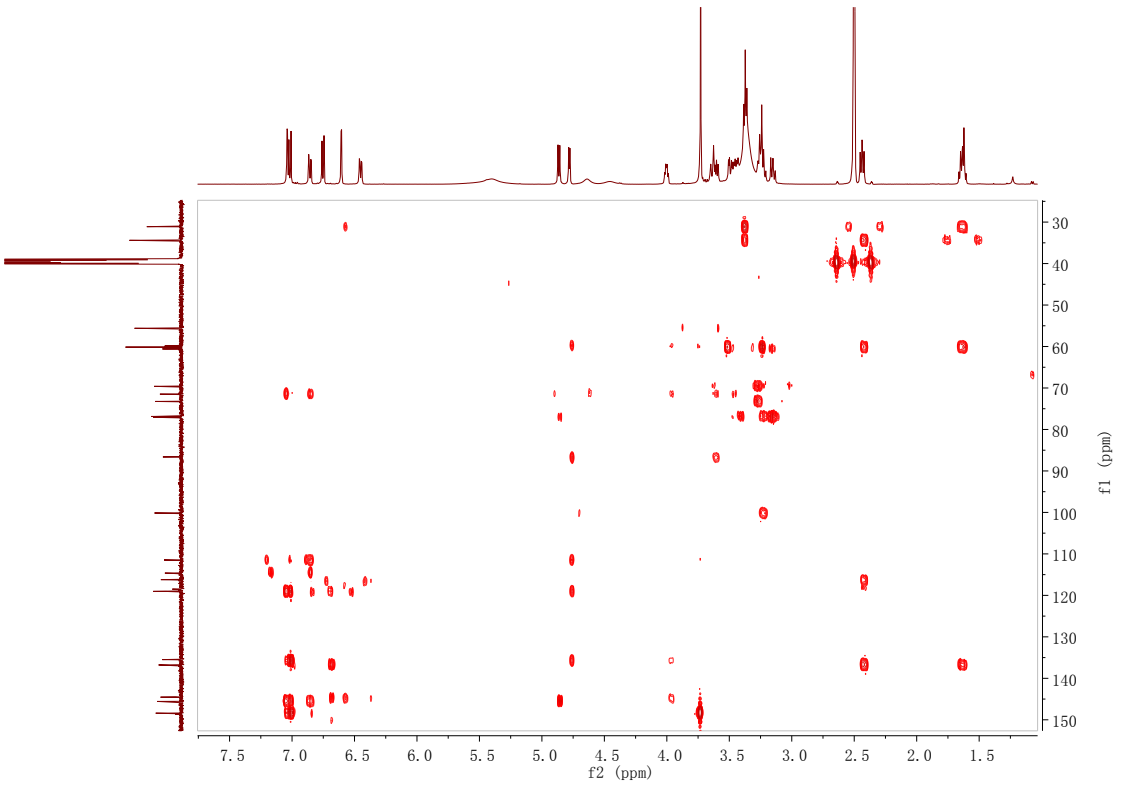


Figure S213. The HMBC spectrum of C-3 in DMSO-d_6

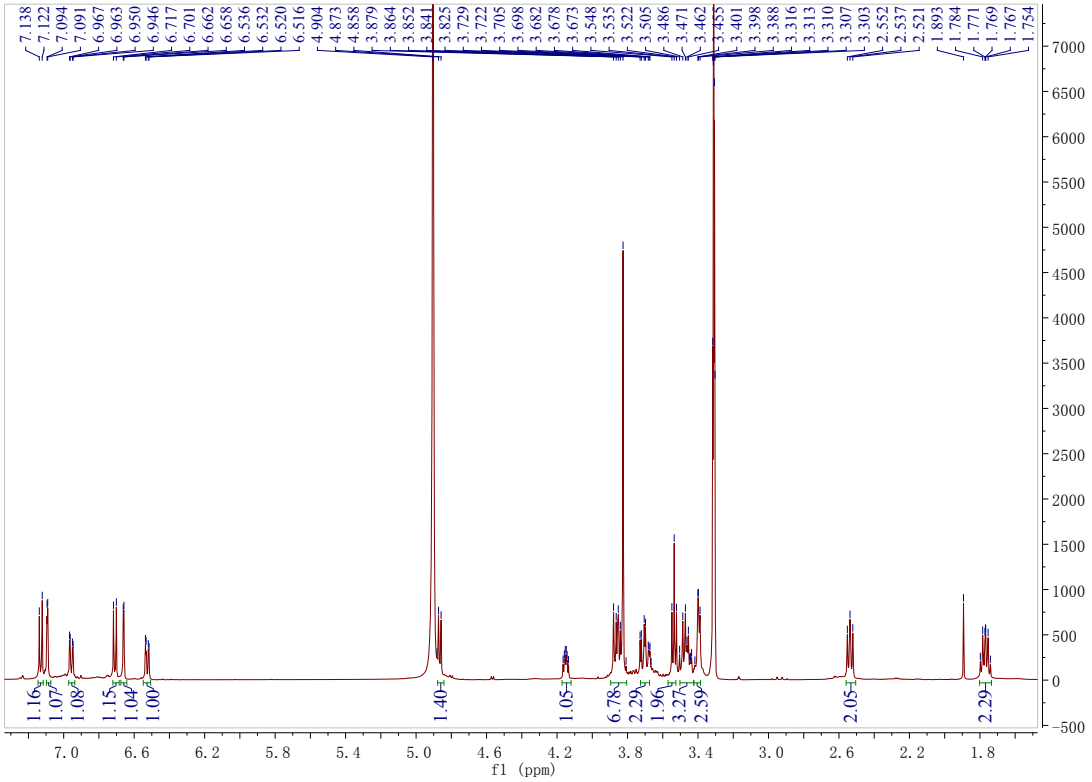


Figure S214. The ^{1}H-NMR spectrum of C-1 in CD_3OD

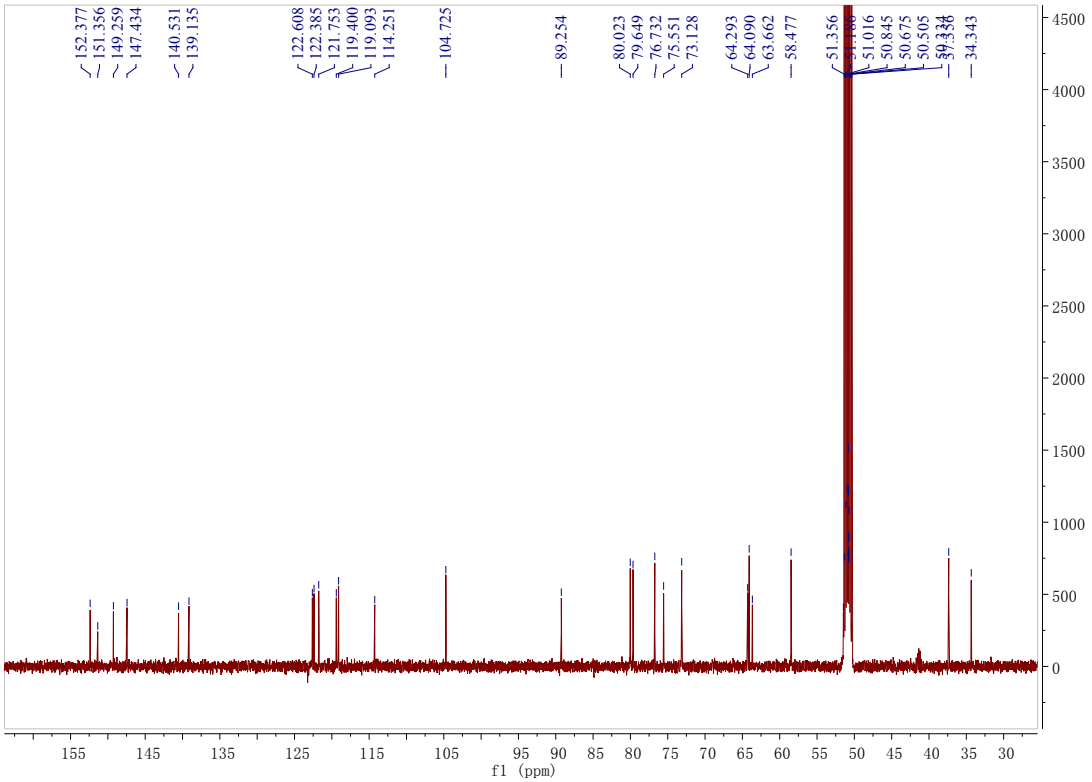


Figure S215. The ^{13}C-NMR spectrum of C-1 in CD_3OD

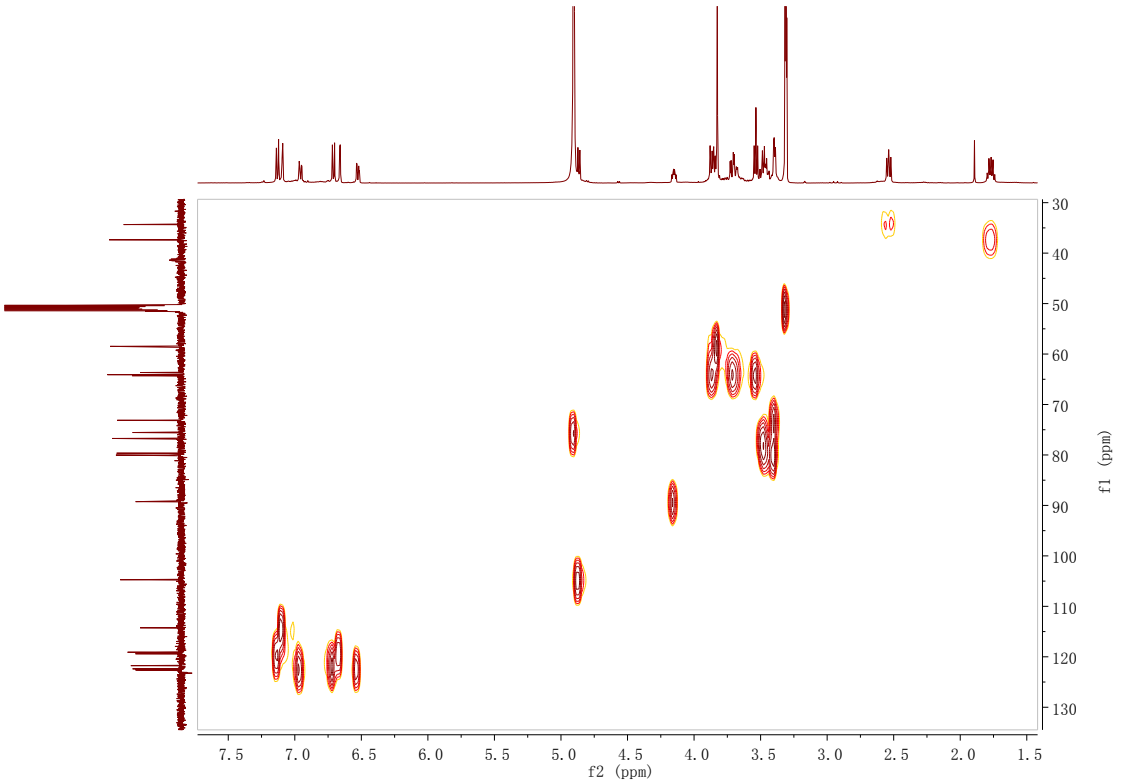


Figure S216. The HSQC spectrum of C-1 in CD_3OD

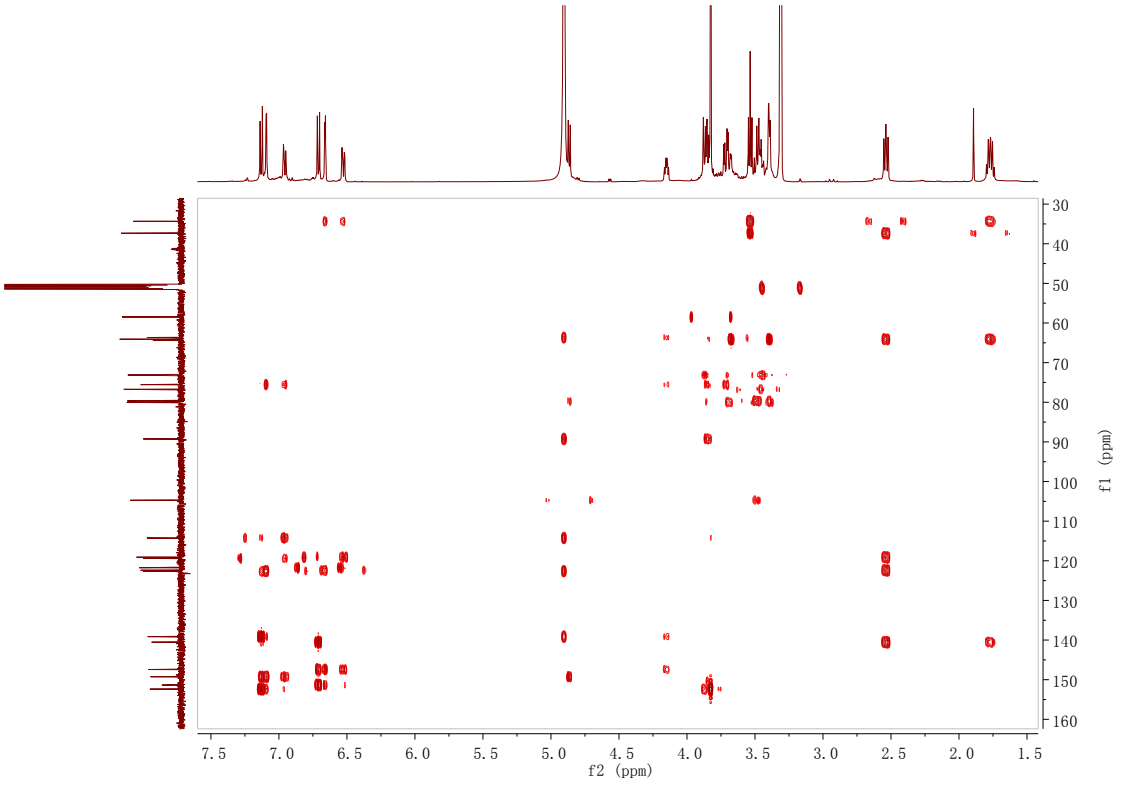


Figure S217. The HMBC spectrum of C-1 in CD_3OD

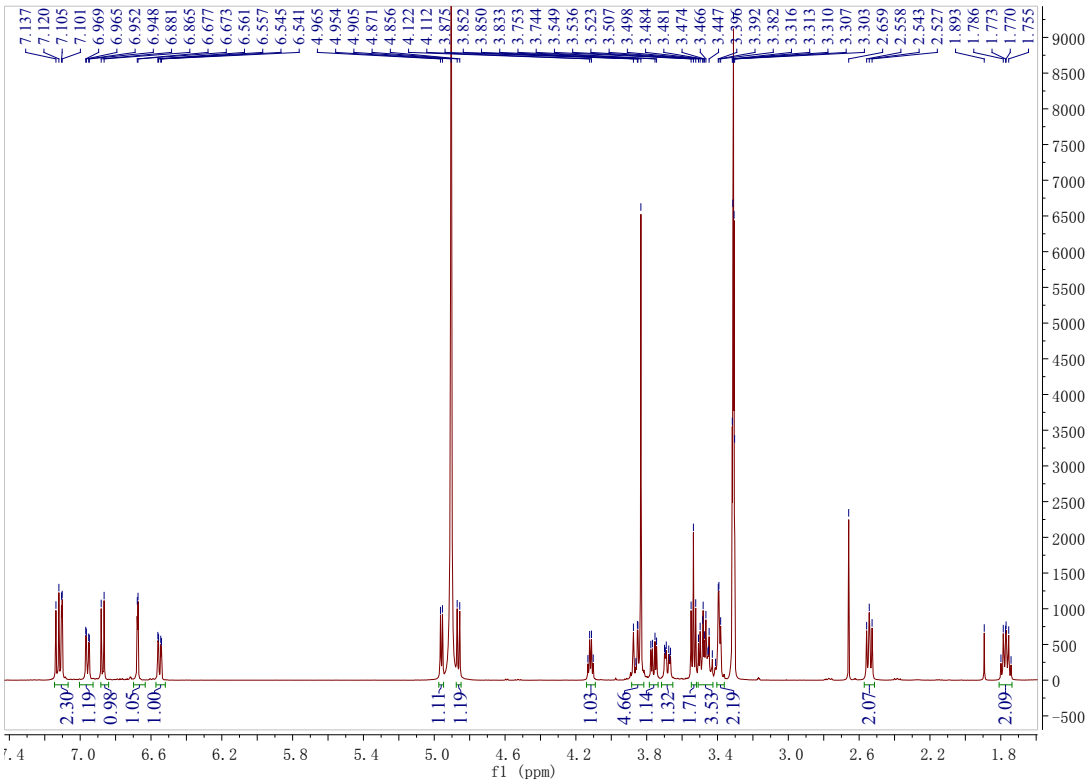


Figure S218. The ^{1}H-NMR spectrum of C-2 in CD_3OD

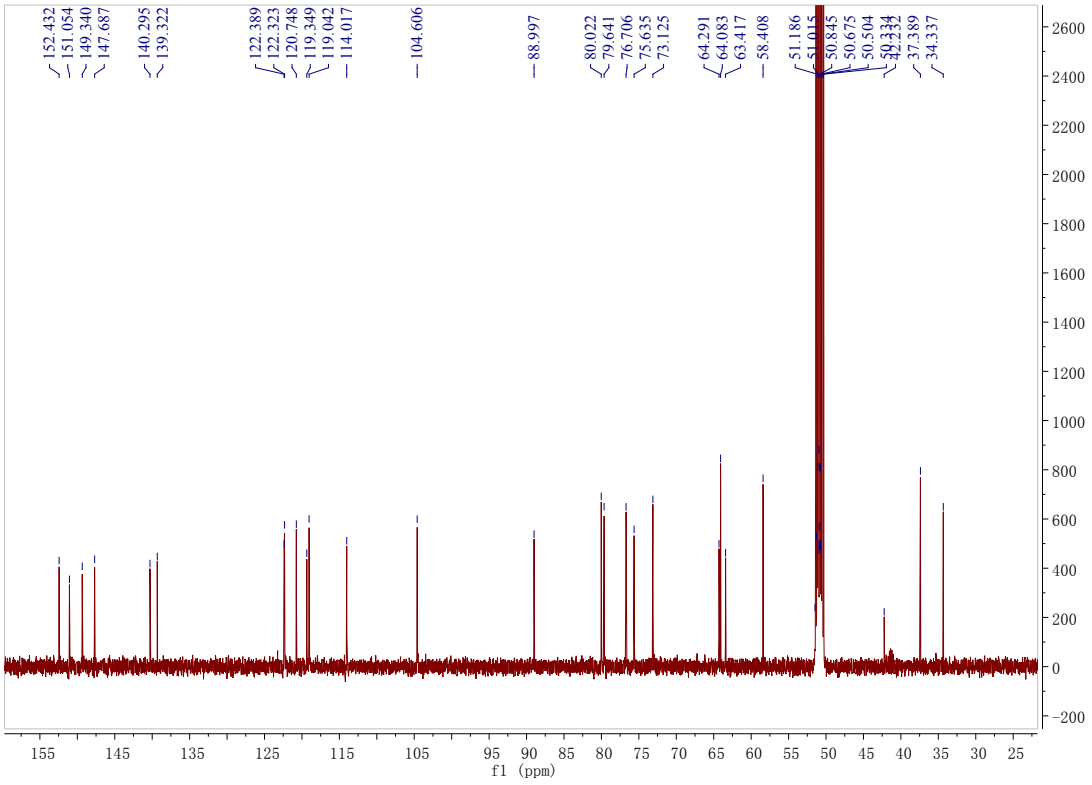


Figure S219. The ^{13}C-NMR spectrum of C-2 in CD_3OD

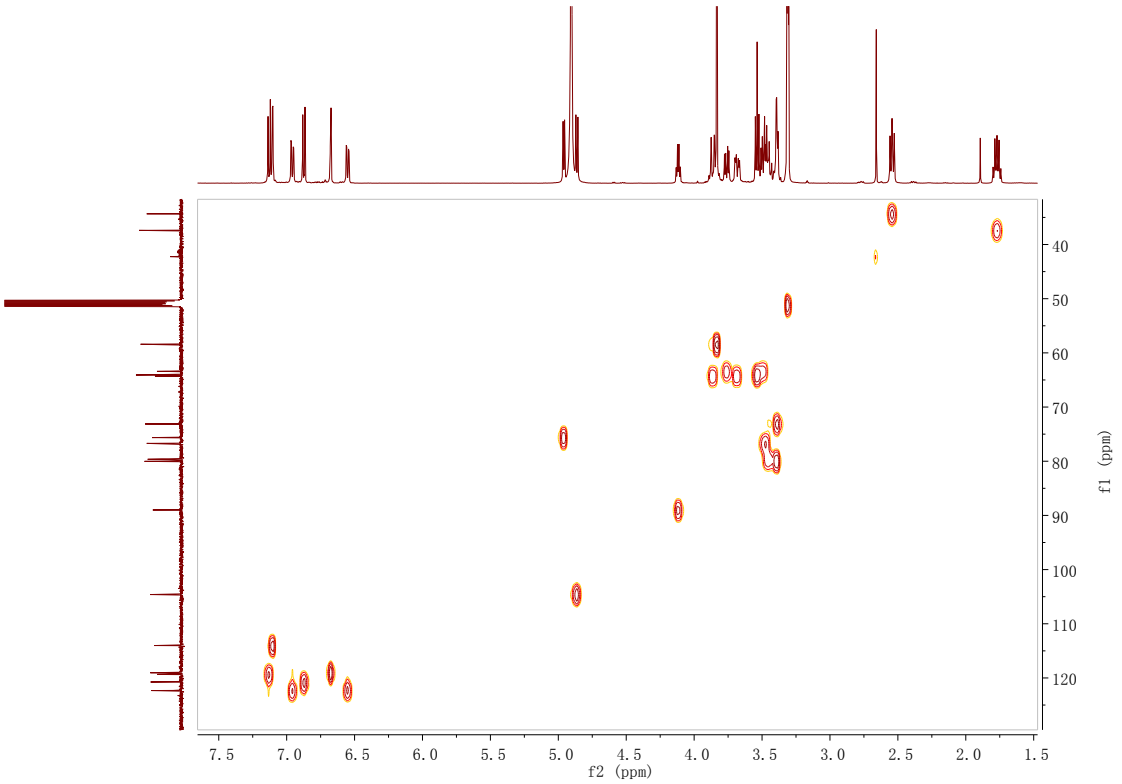


Figure S220. The HSQC spectrum of C-2 in CD_3OD

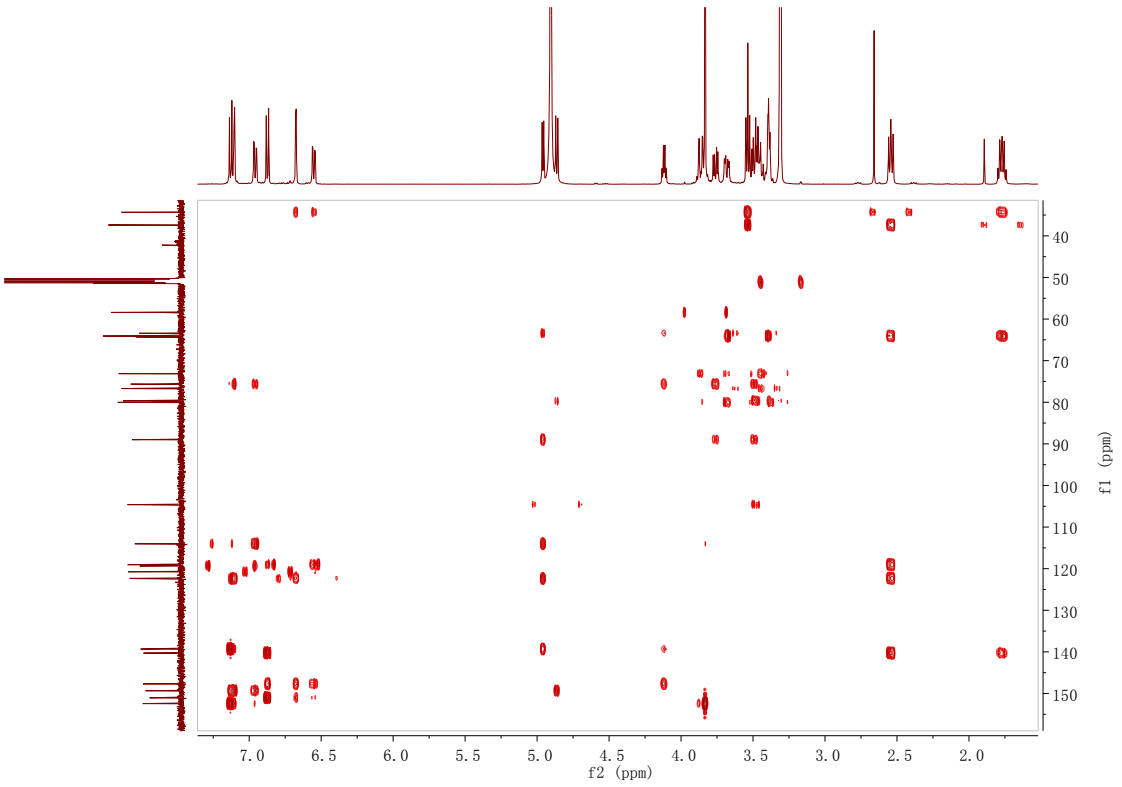


Figure S221. The HMBC spectrum of C-2 in CD_3OD

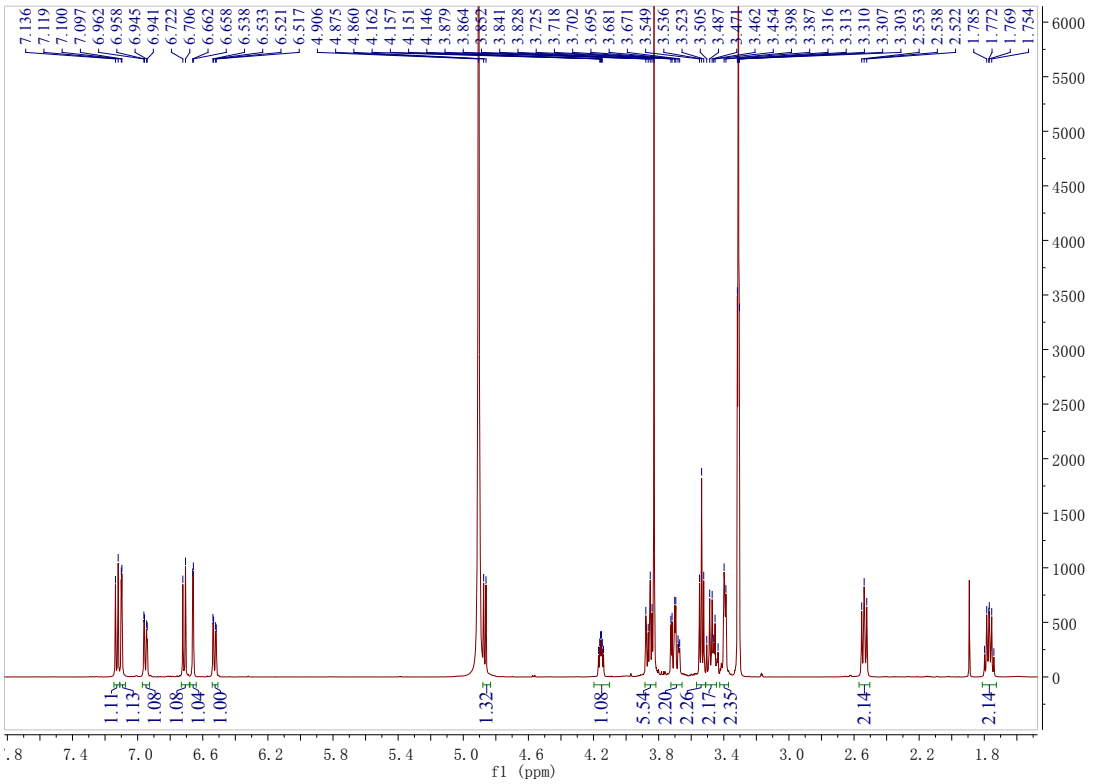


Figure S222. The ^{1}H-NMR spectrum of C-3 in CD_3OD

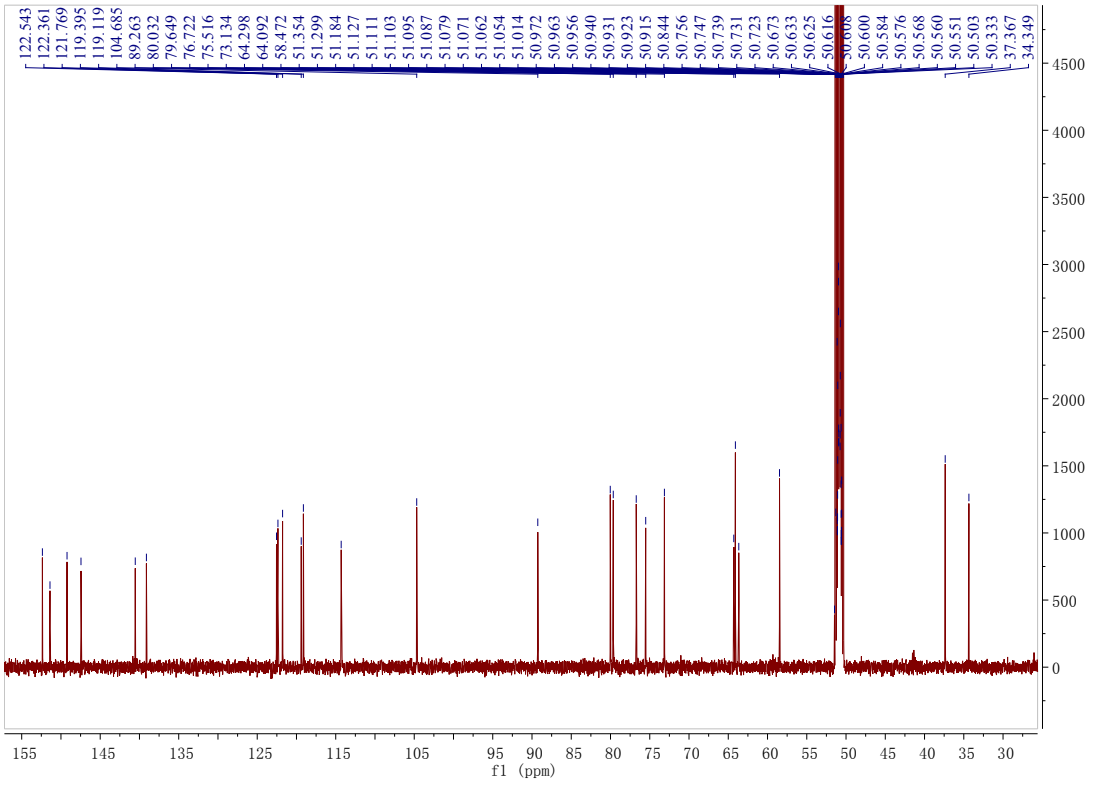


Figure S223. The ^{13}C-NMR spectrum of C-3 in CD_3OD

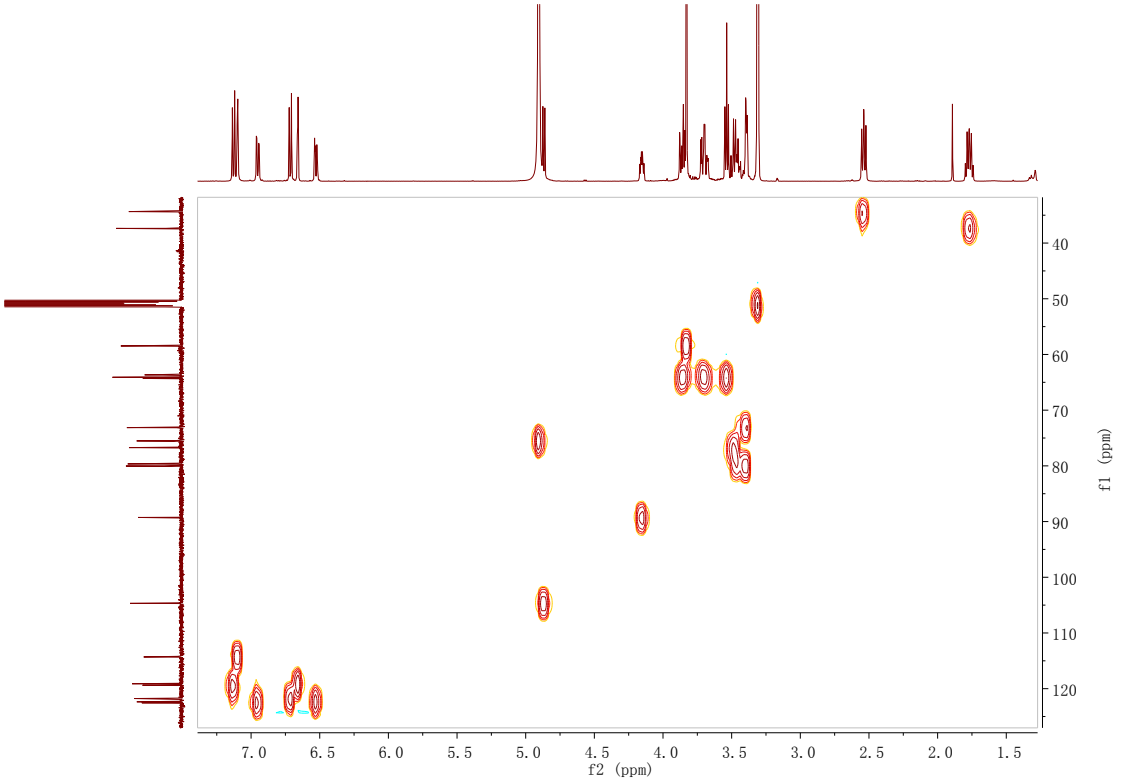


Figure S224. The HSQC spectrum of C-3 in CD_3OD

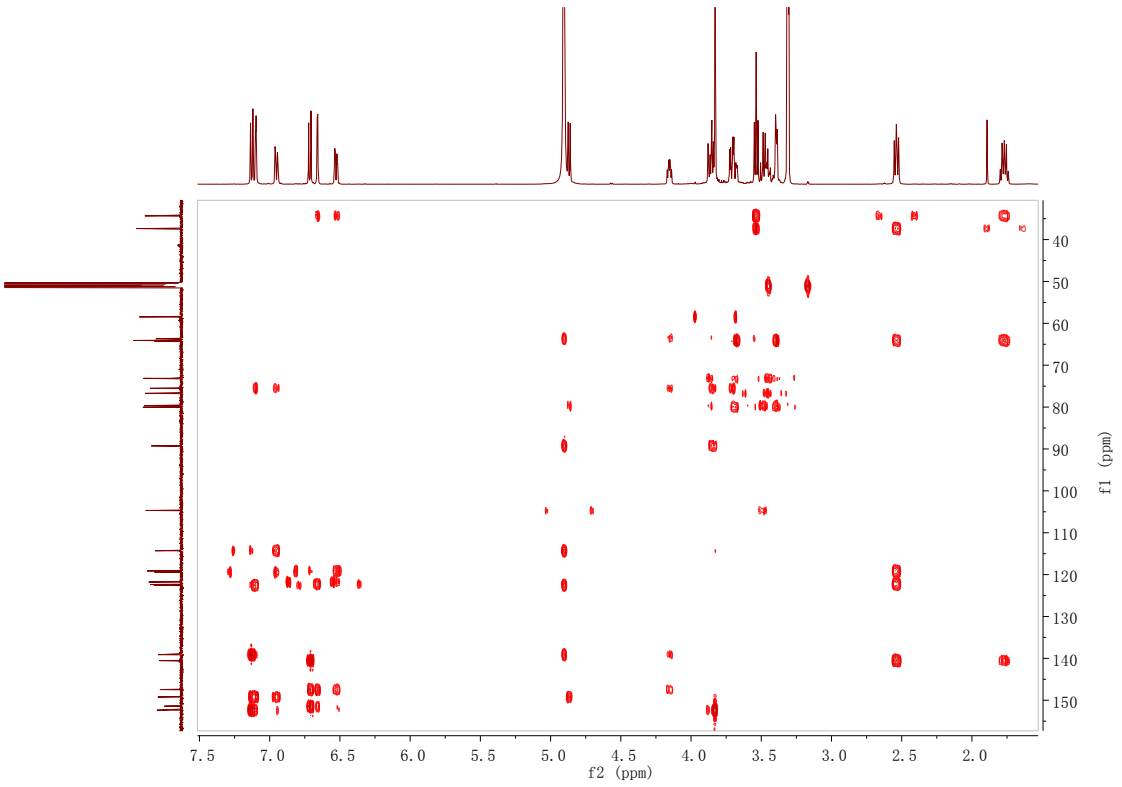


Figure S225. The HMBC spectrum of C-3 in CD_3OD

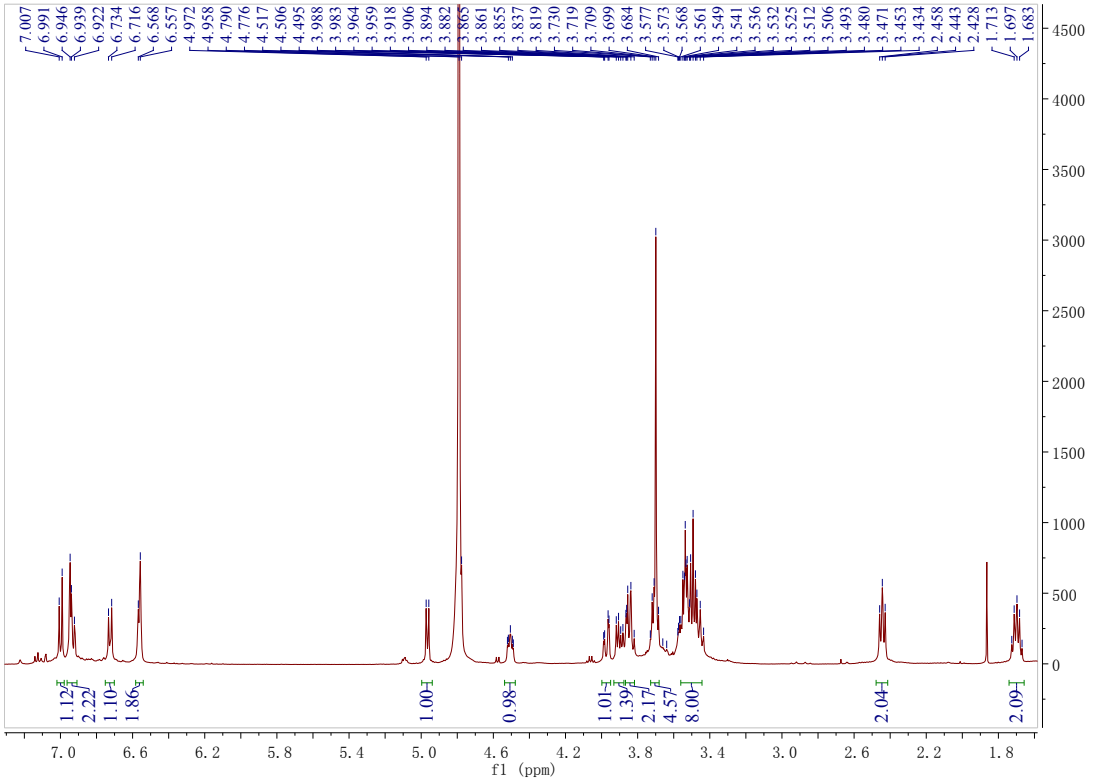


Figure S226. The ^{1}H-NMR spectrum of C-1 in D_2O

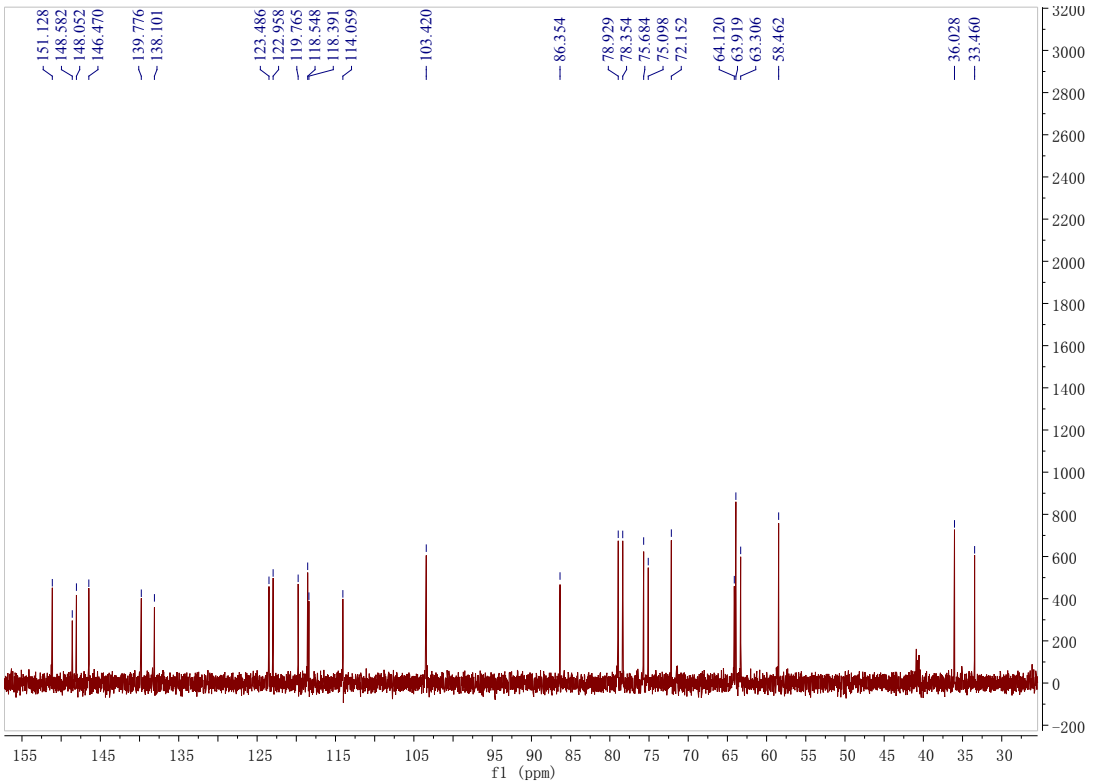


Figure S227. The ^{13}C-NMR spectrum of C-1 in D_2O

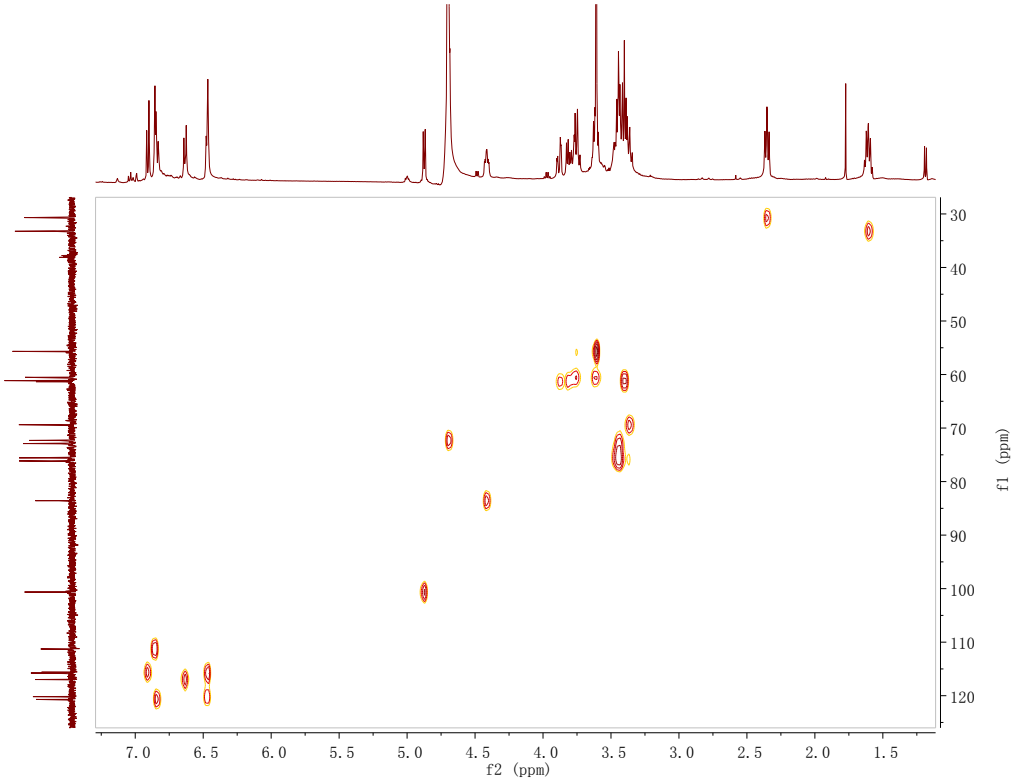


Figure S228. The HSQC spectrum of C-1 in D_2O

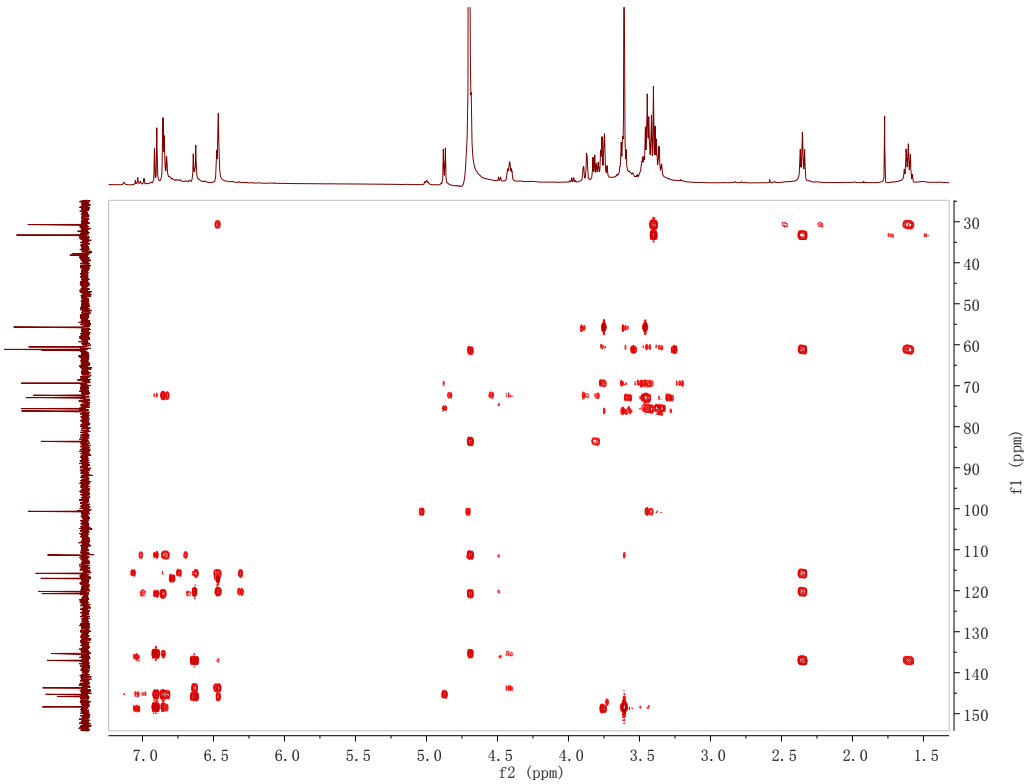


Figure S229. The HMBC spectrum of C-1 in D_2O

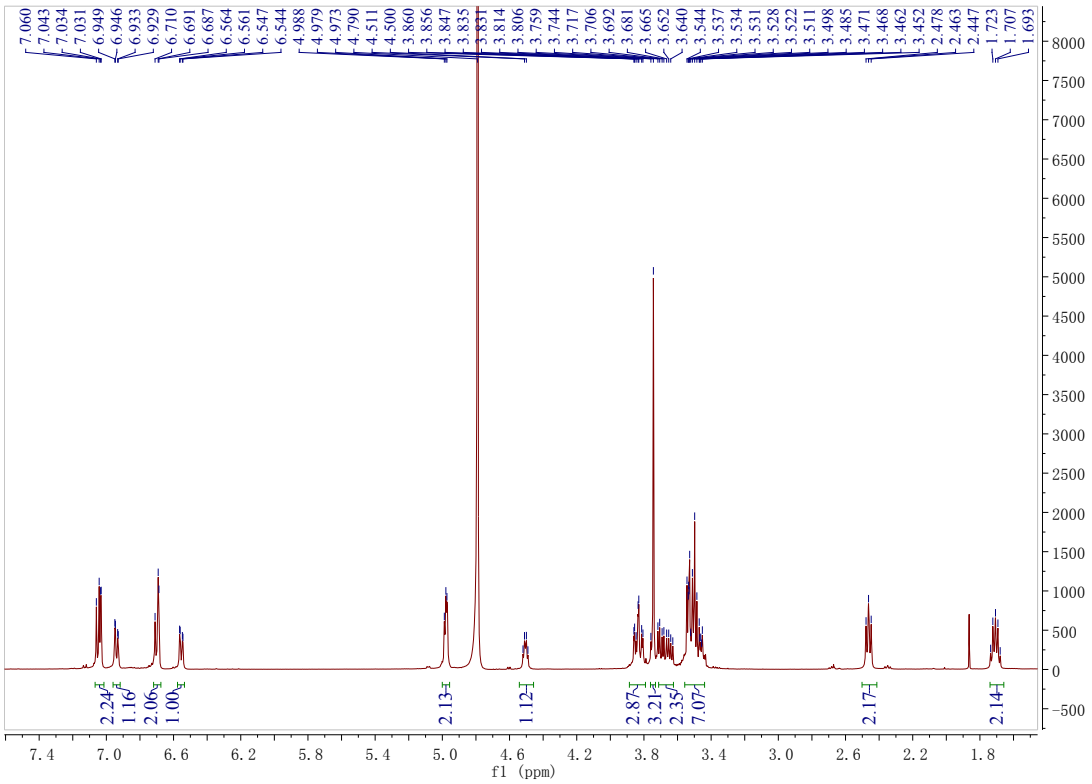


Figure S230. The ^{1}H-NMR spectrum of C-2 in D_2O

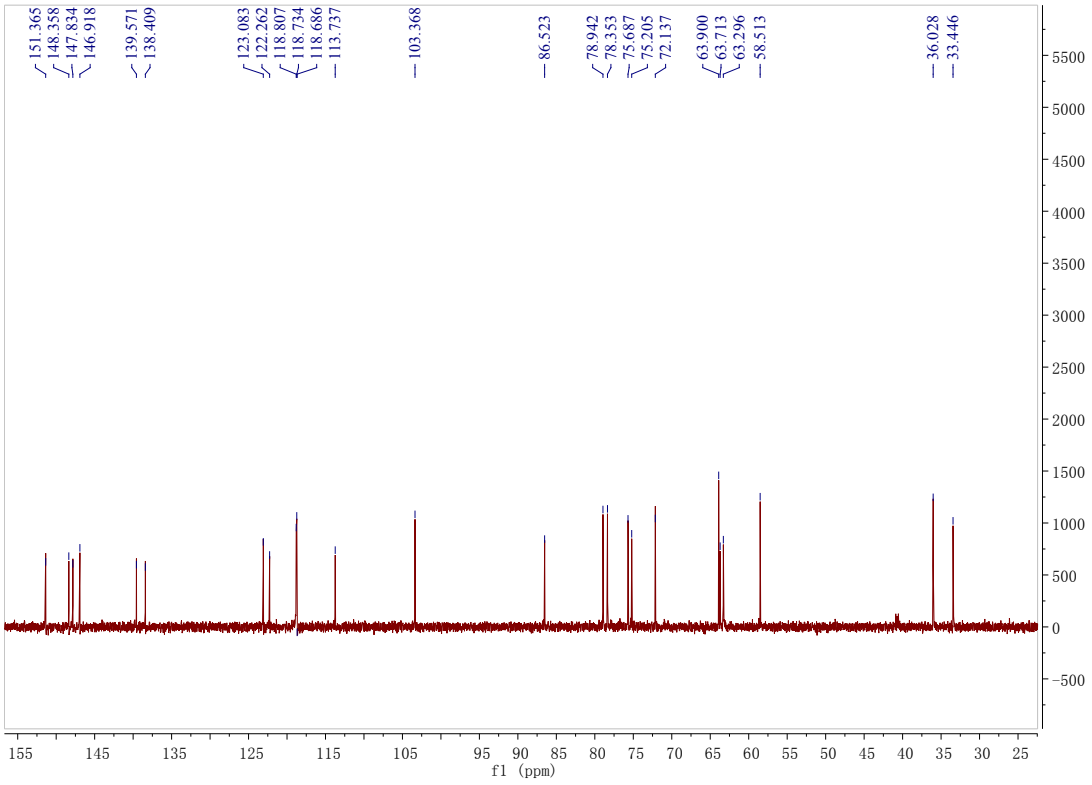


Figure S231. The ^{13}C-NMR spectrum of C-2 in D_2O

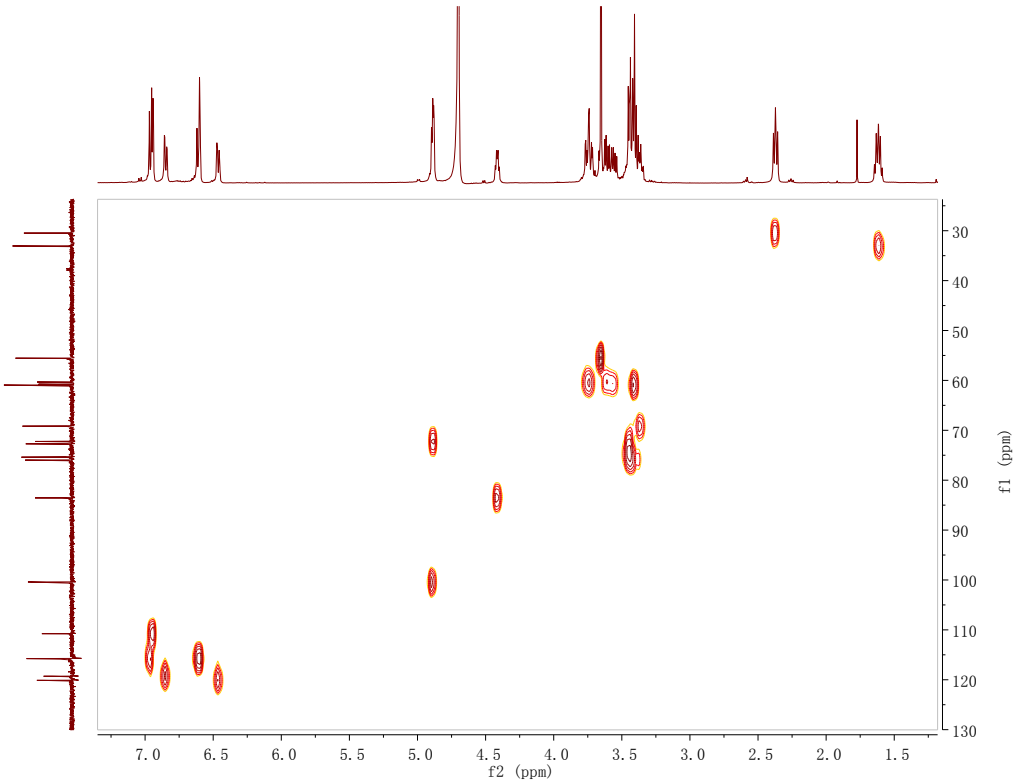


Figure S232. The HSQC spectrum of C-2 in D_2O

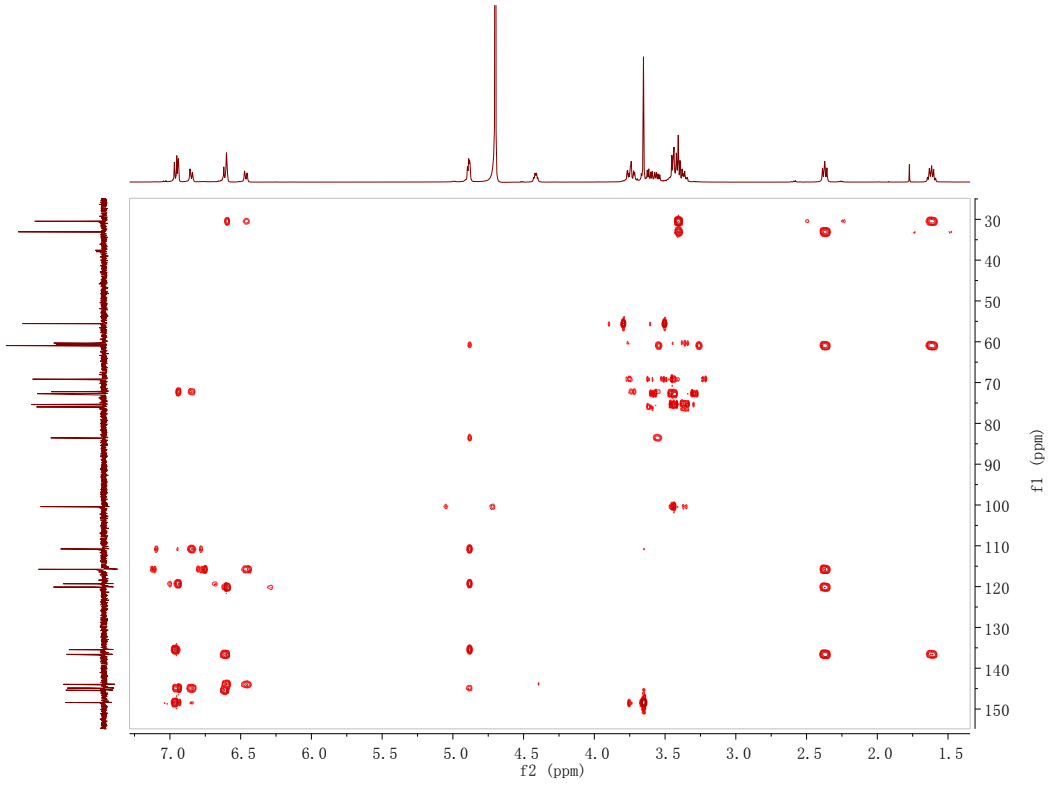


Figure S233. The HMBC spectrum of C-2 in D_2O

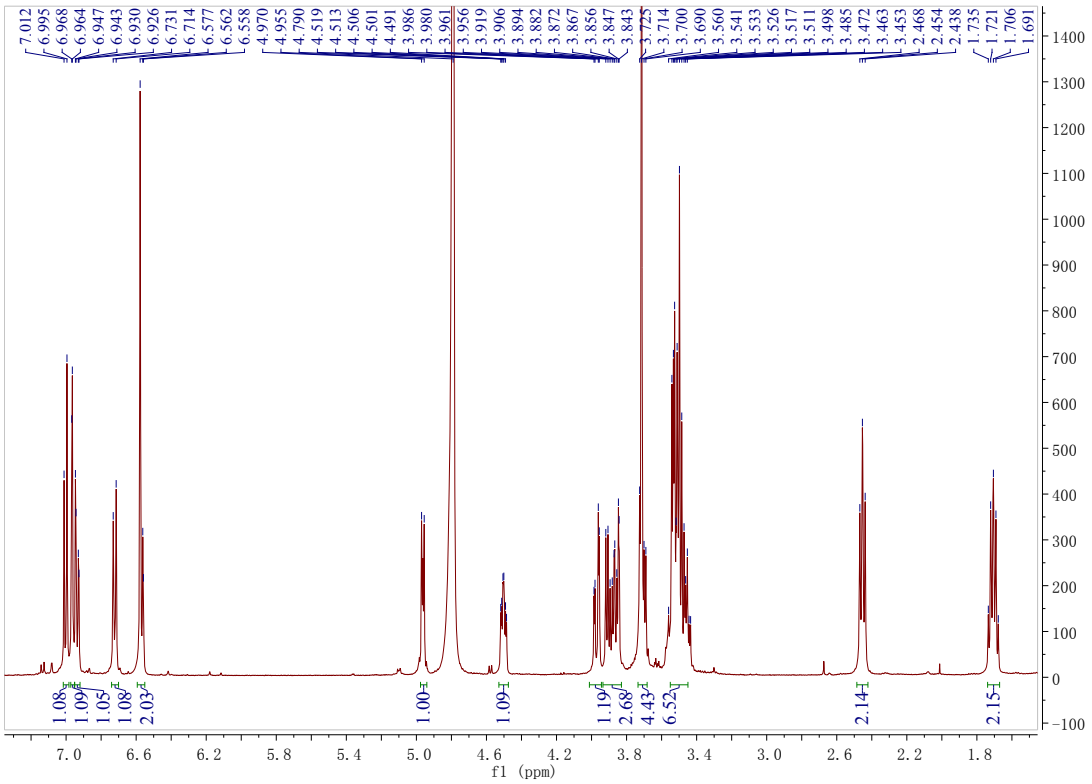


Figure S234. The ^{1}H-NMR spectrum of C-3 in D_2O

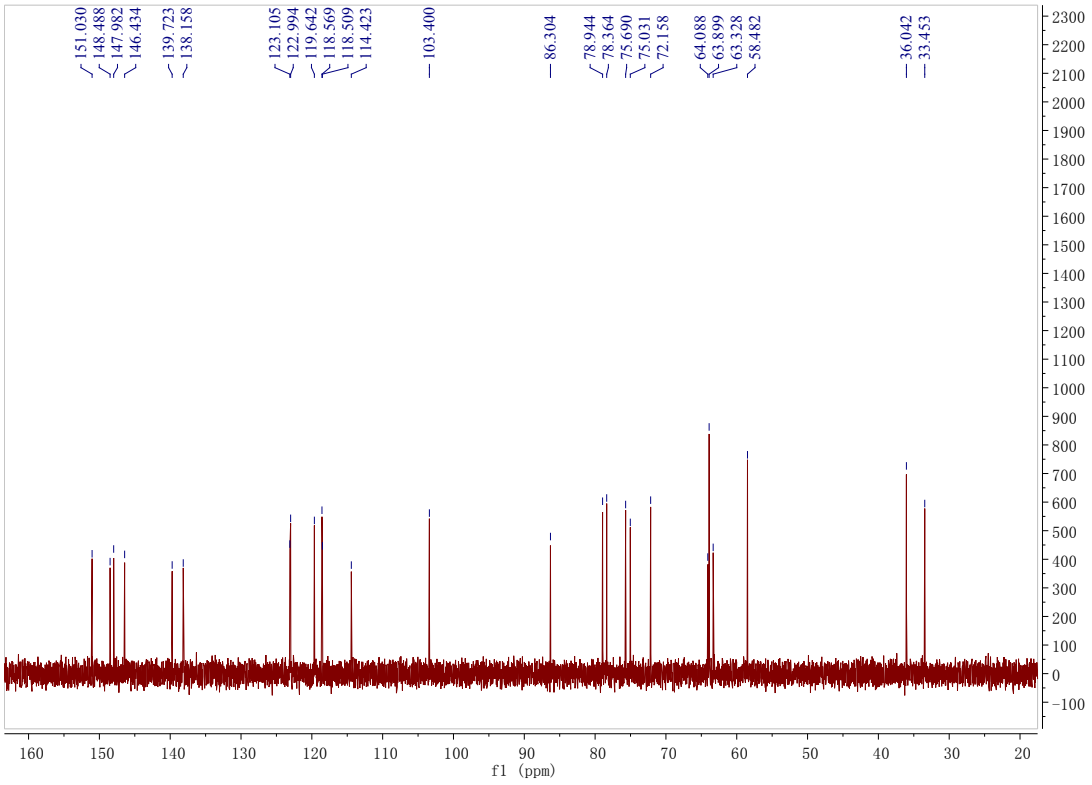


Figure S235. The ^{13}C-NMR spectrum of C-3 in D_2O

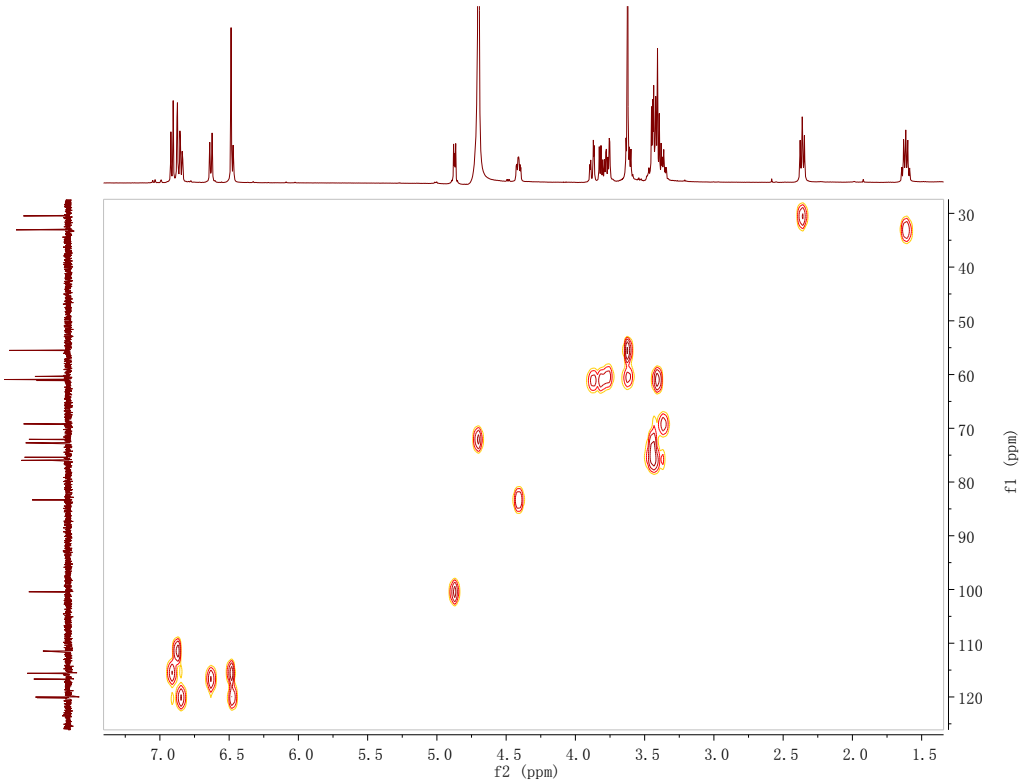


Figure S236. The HSQC spectrum of C-3 in D_2O

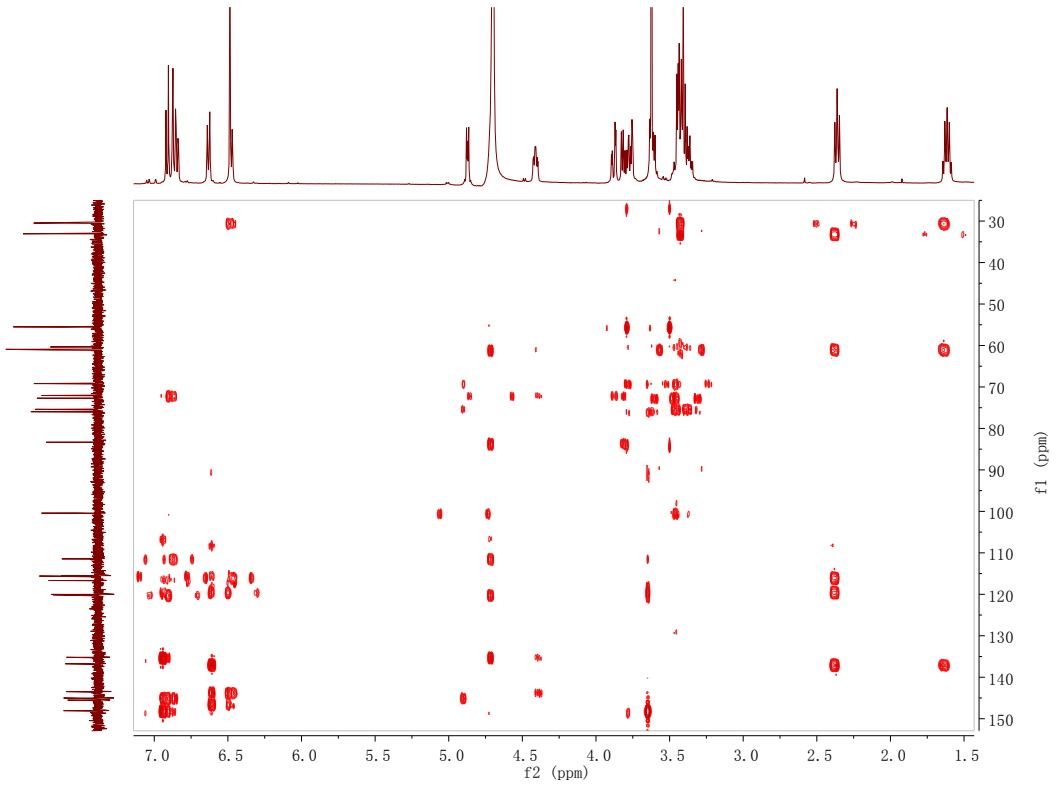


Figure S237. The HMBC spectrum of C-3 in D_2O

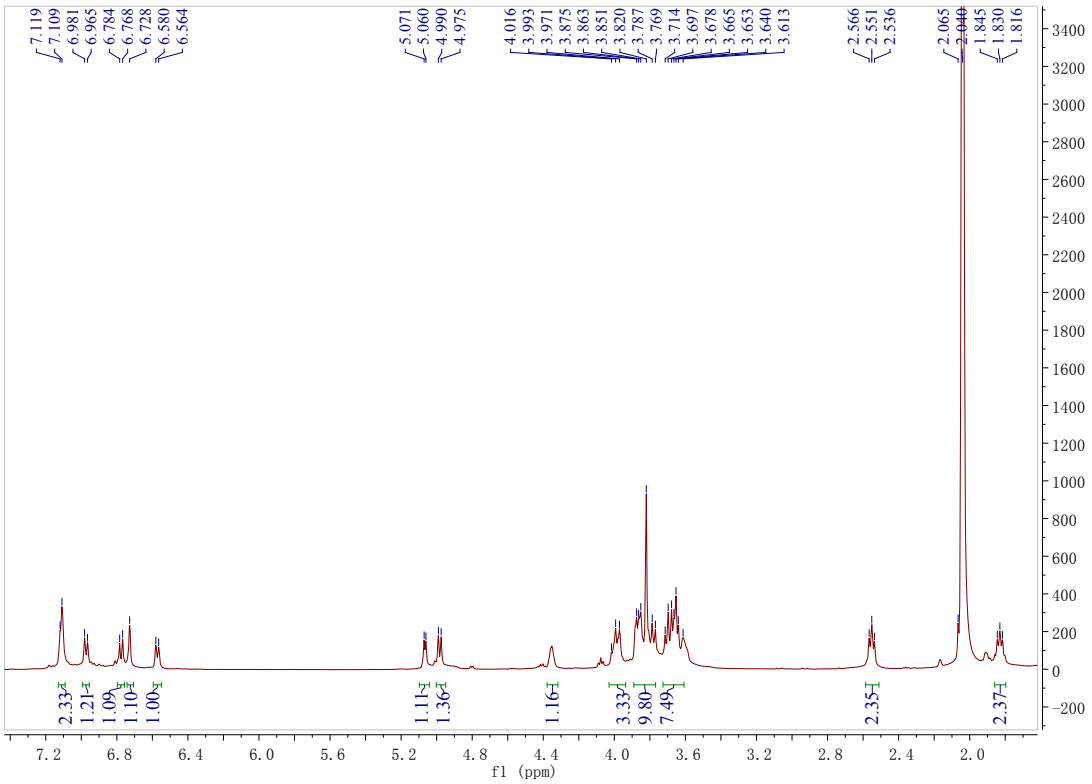


Figure S238. The ^{1}H-NMR spectrum of C-1 in CD_3COOD

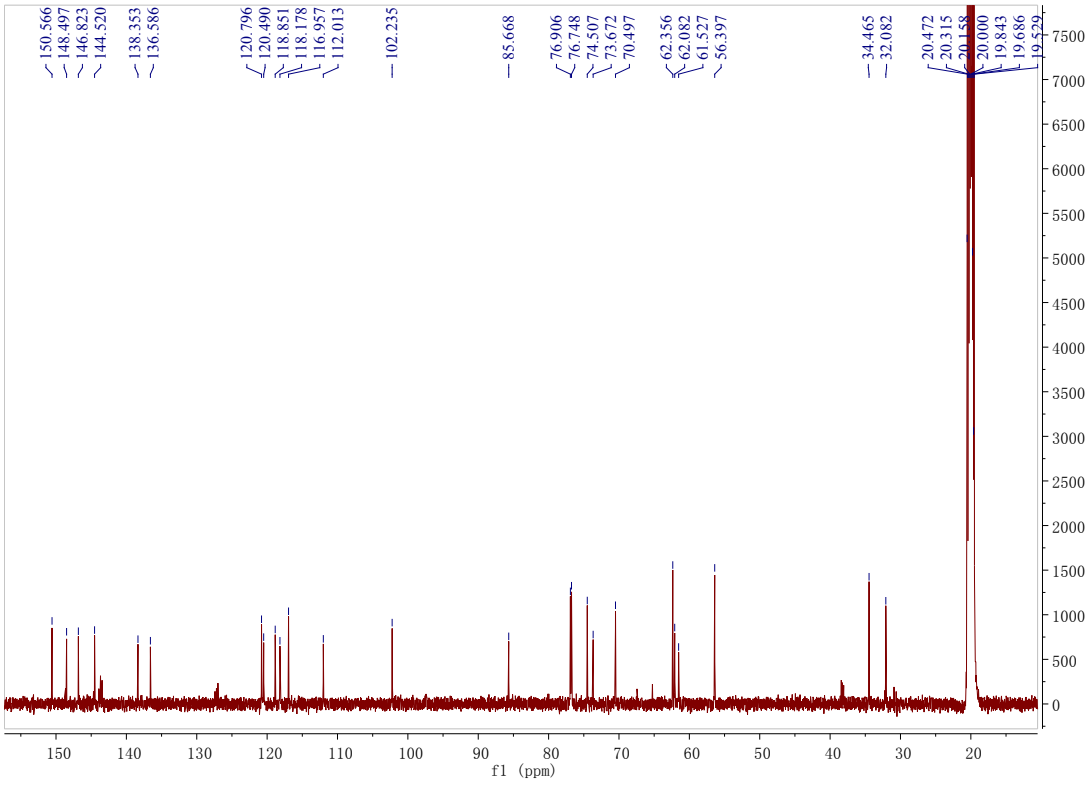


Figure S239. The ^{13}C-NMR spectrum of C-1 in CD_3COOD

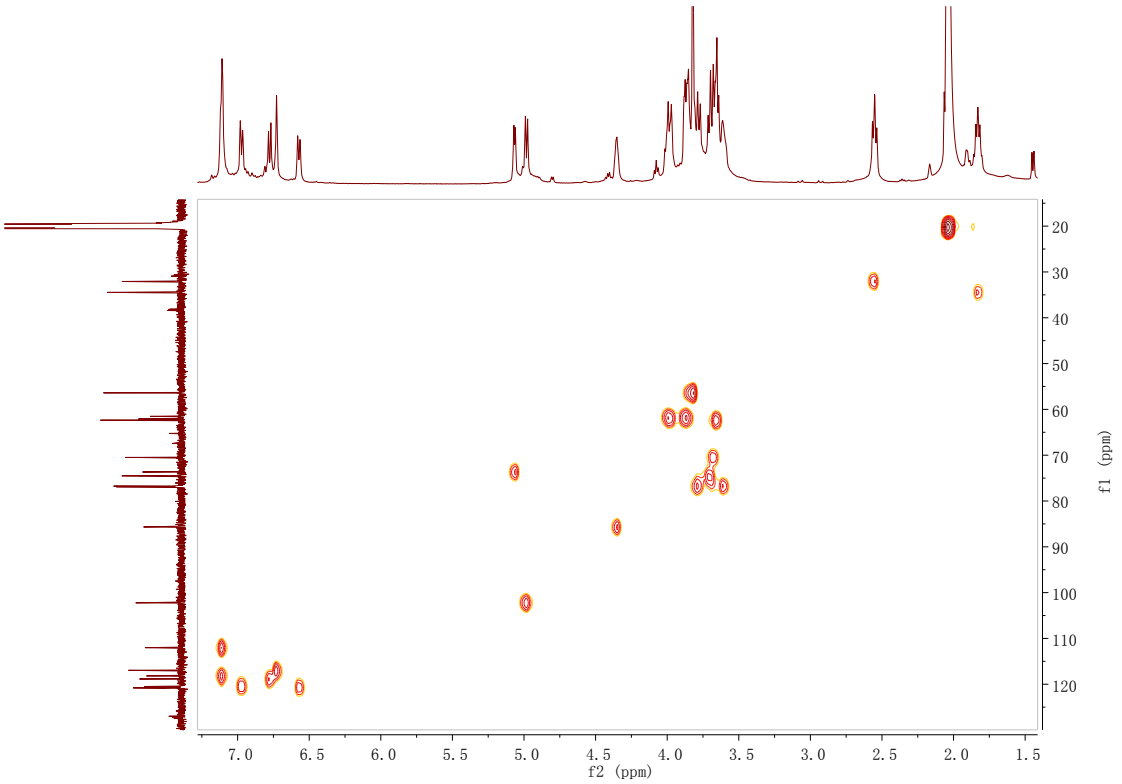


Figure S240. The HSQC spectrum of C-1 in CD_3COOD

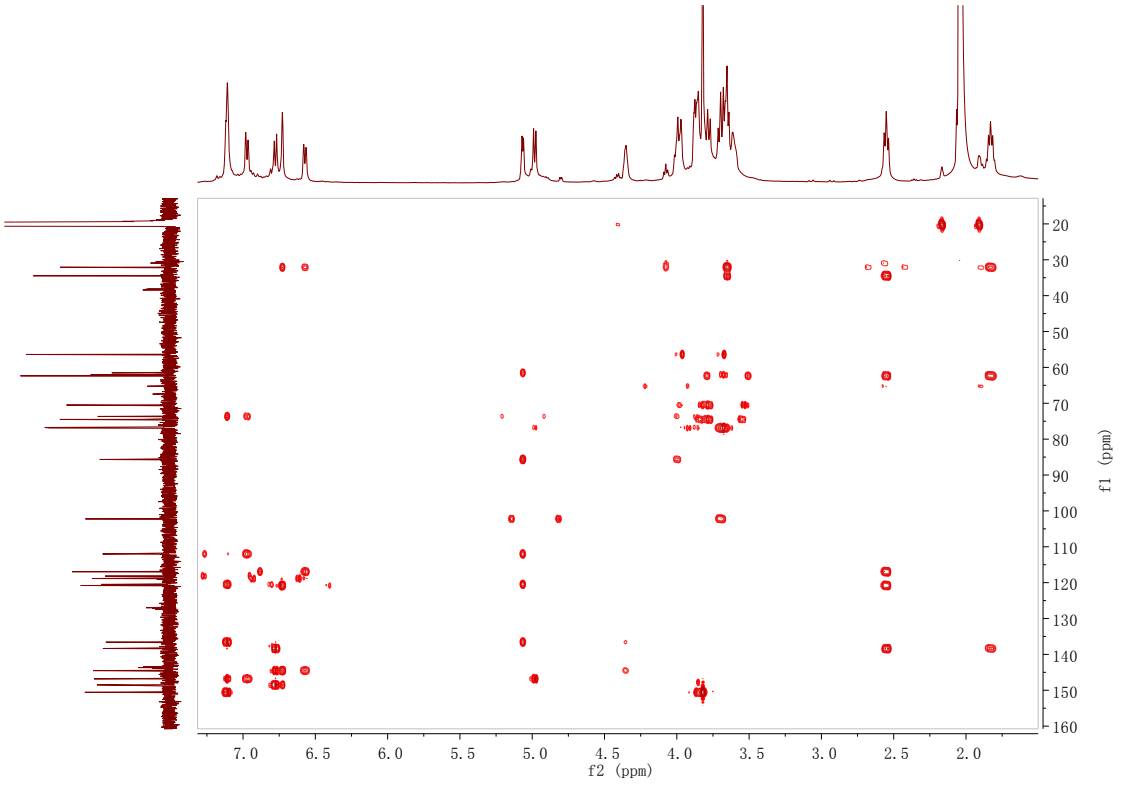


Figure S241. The HMBC spectrum of C-1 in CD_3COOD

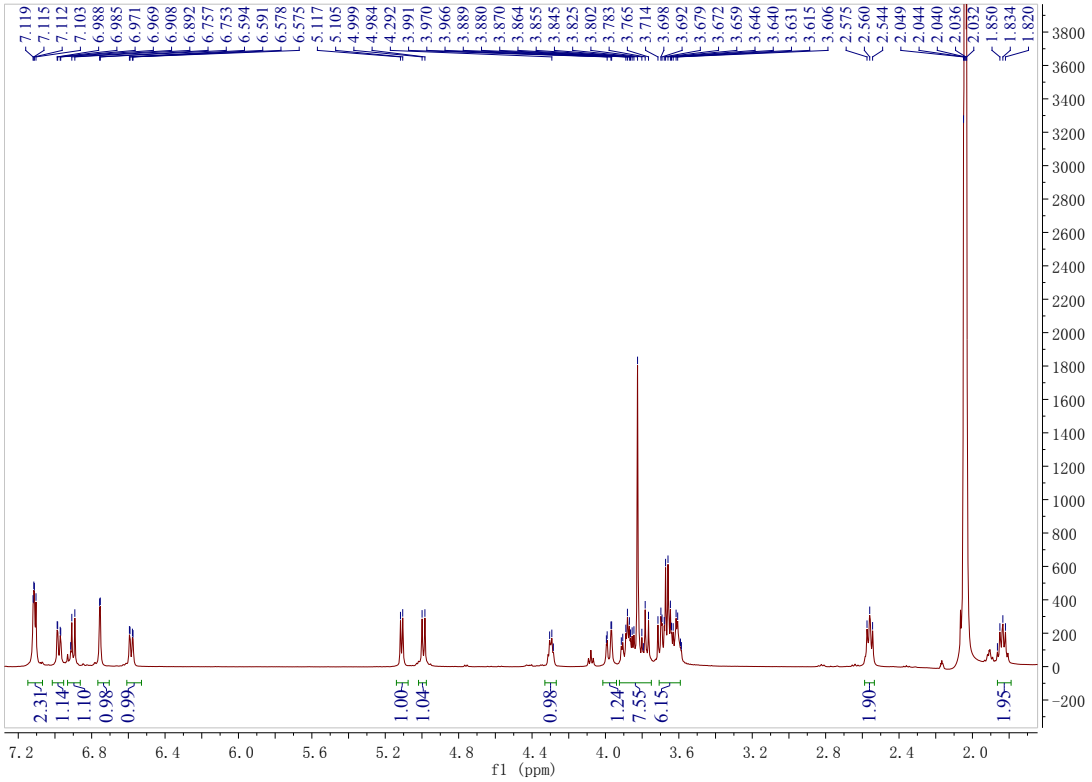


Figure S242. The ^{1}H-NMR spectrum of C-2 in CD_3COOD

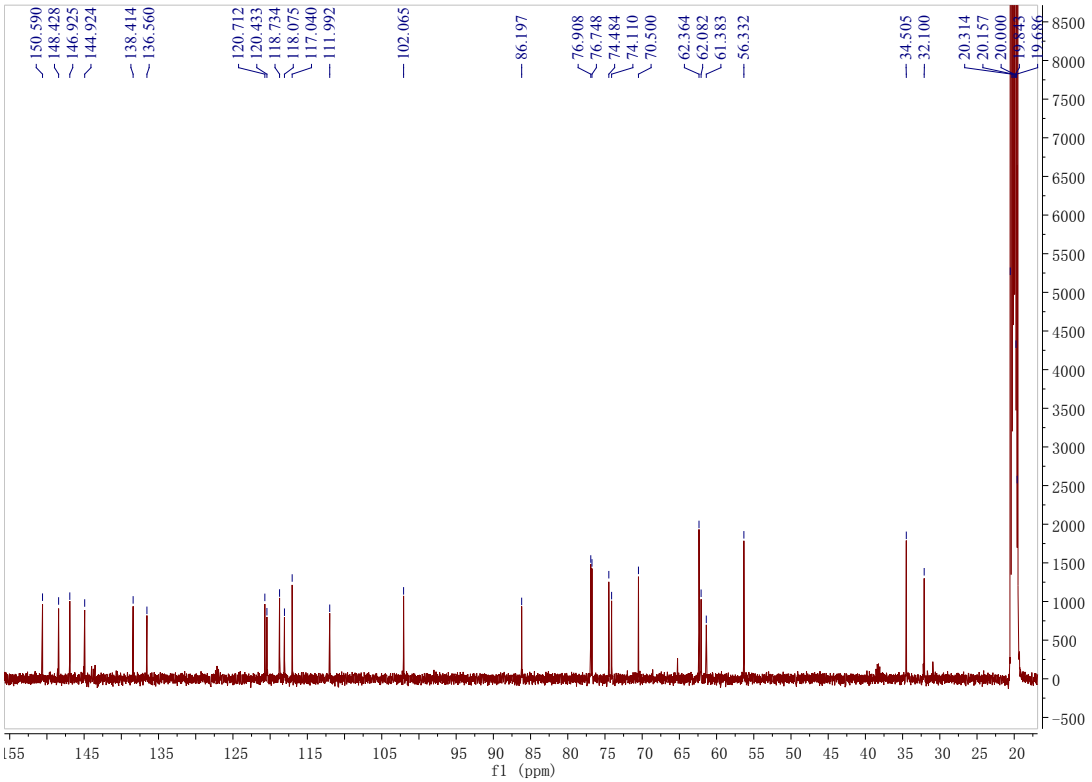


Figure S243. The ^{13}C-NMR spectrum of C-2 in CD_3COOD

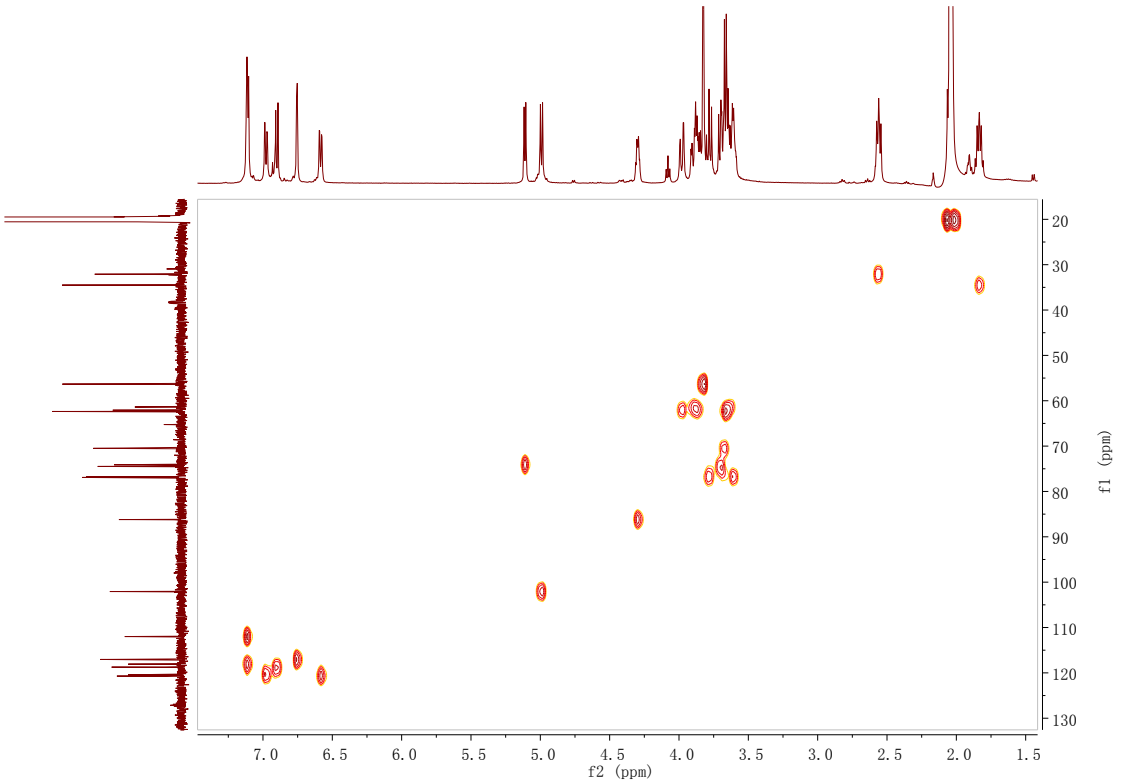


Figure S244. The HSQC spectrum of C-2 in CD_3COOD

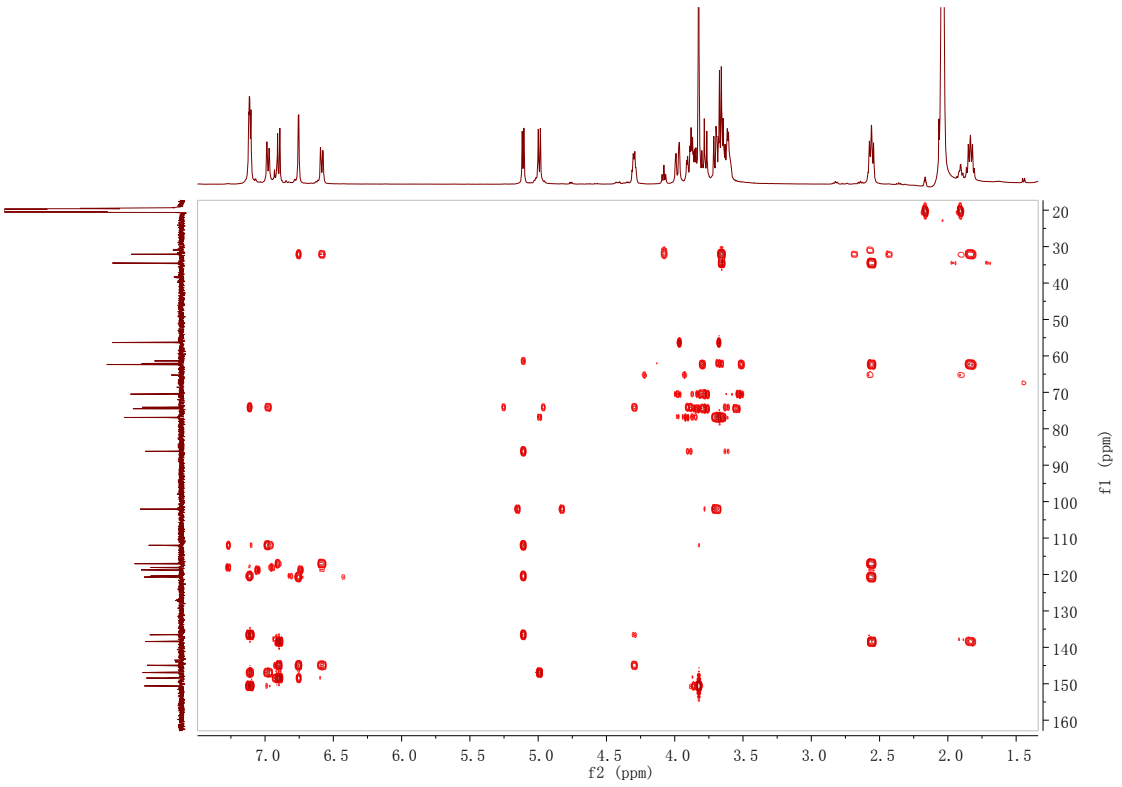


Figure S245. The HMBC spectrum of C-2 in CD_3COOD

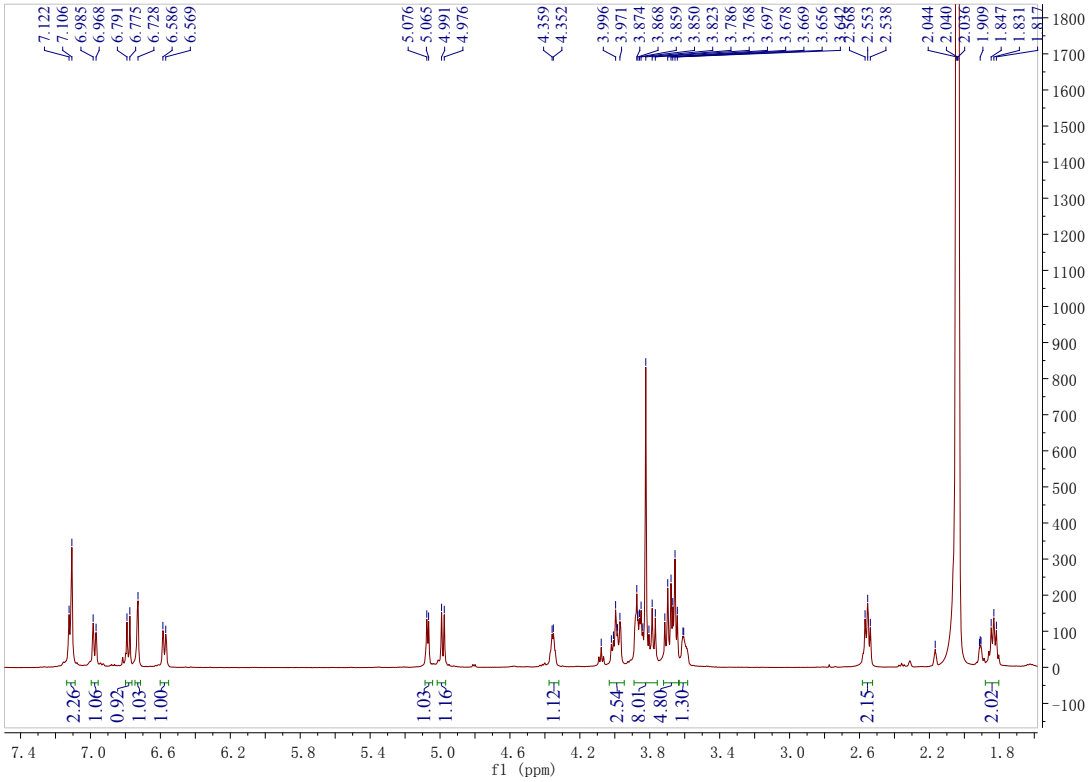


Figure S246. The ^{1}H-NMR spectrum of C-3 in CD_3COOD

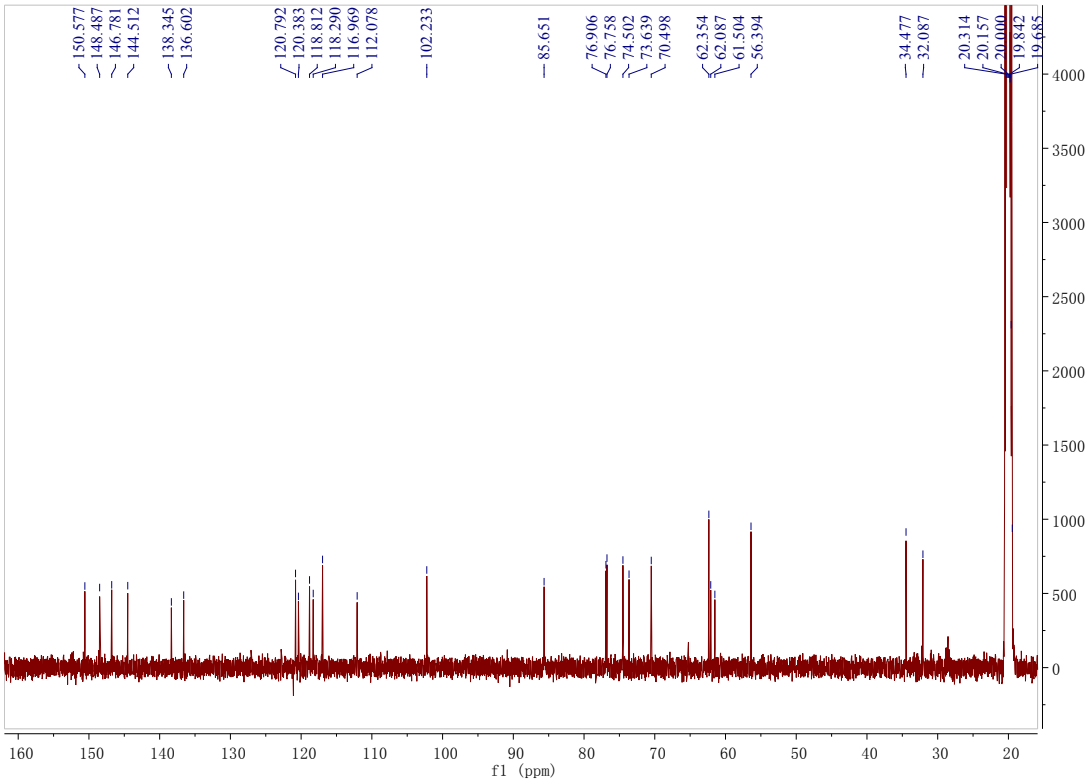


Figure S247. The ^{13}C-NMR spectrum of C-3 in CD_3COOD

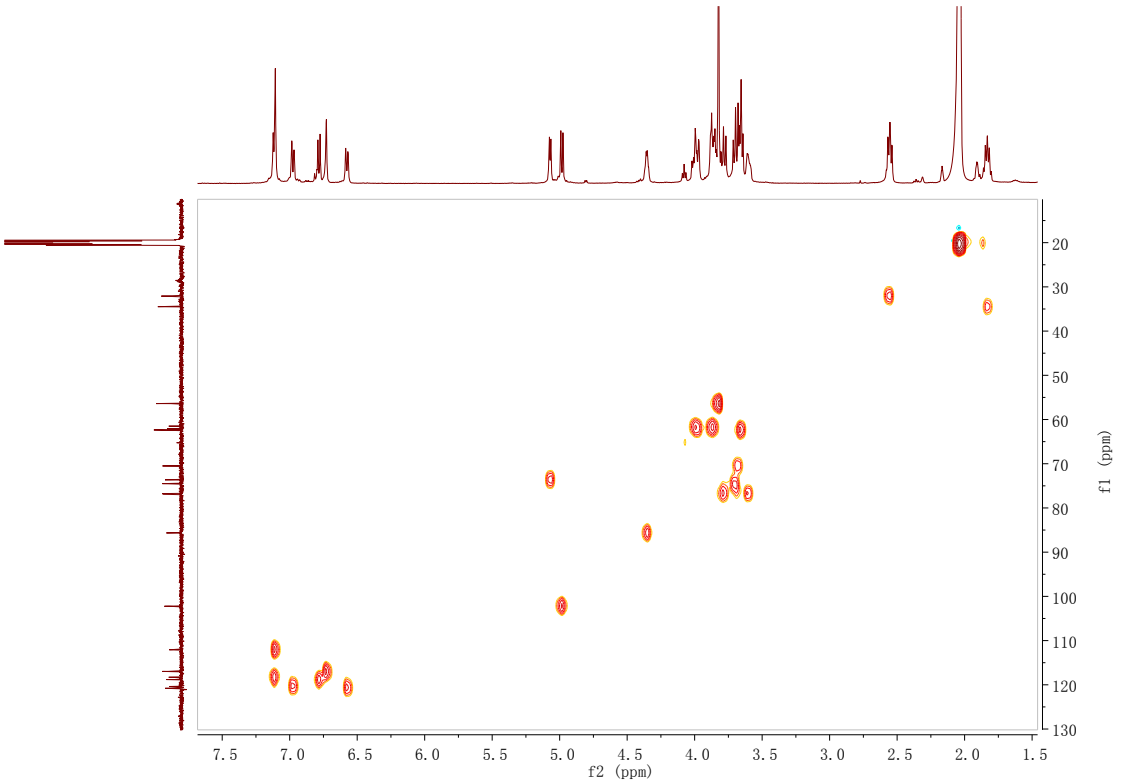


Figure S248. The HSQC spectrum of C-3 in CD_3COOD

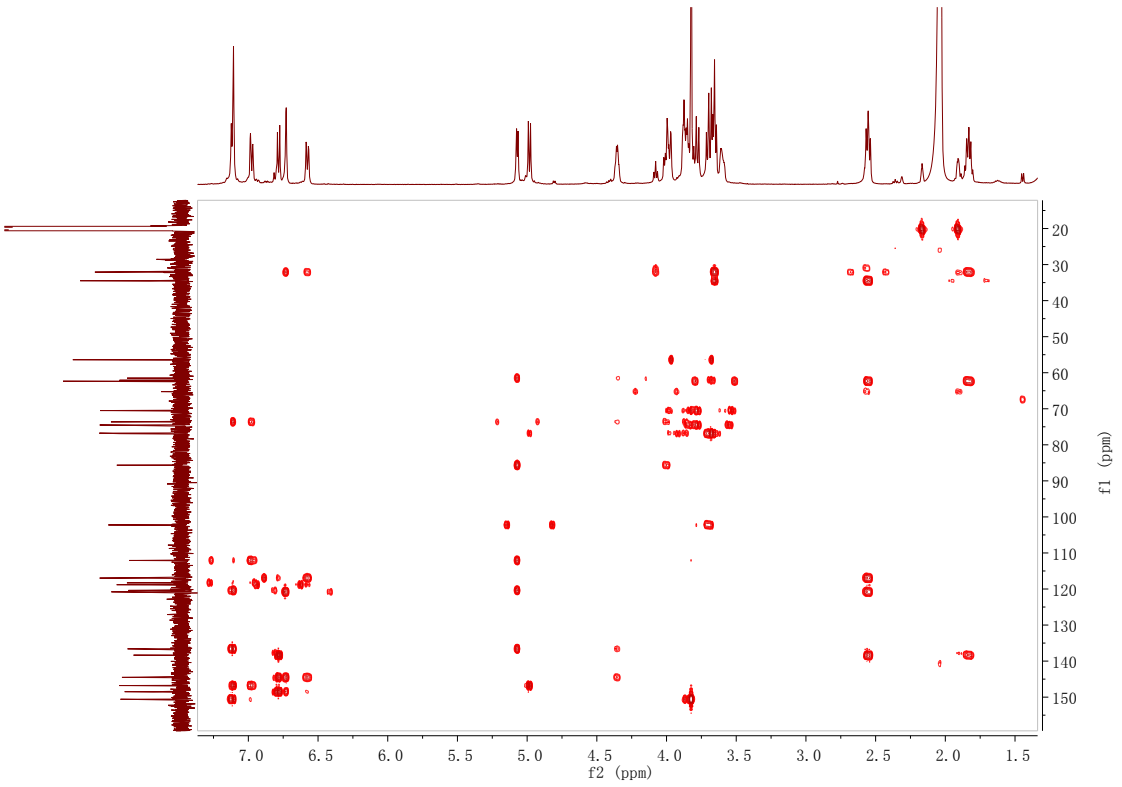


Figure S249. The HMBC spectrum of C-3 in CD_3COOD

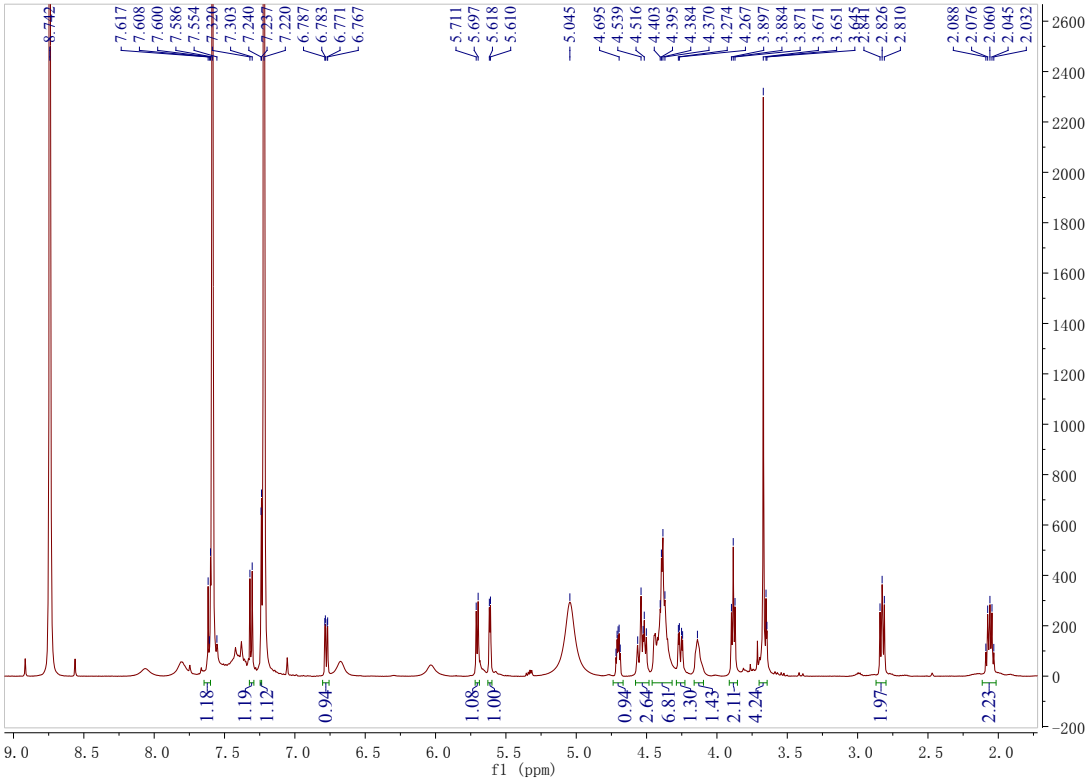


Figure S250. The ^{1}H-NMR spectrum of C-1 in C_5D_5N

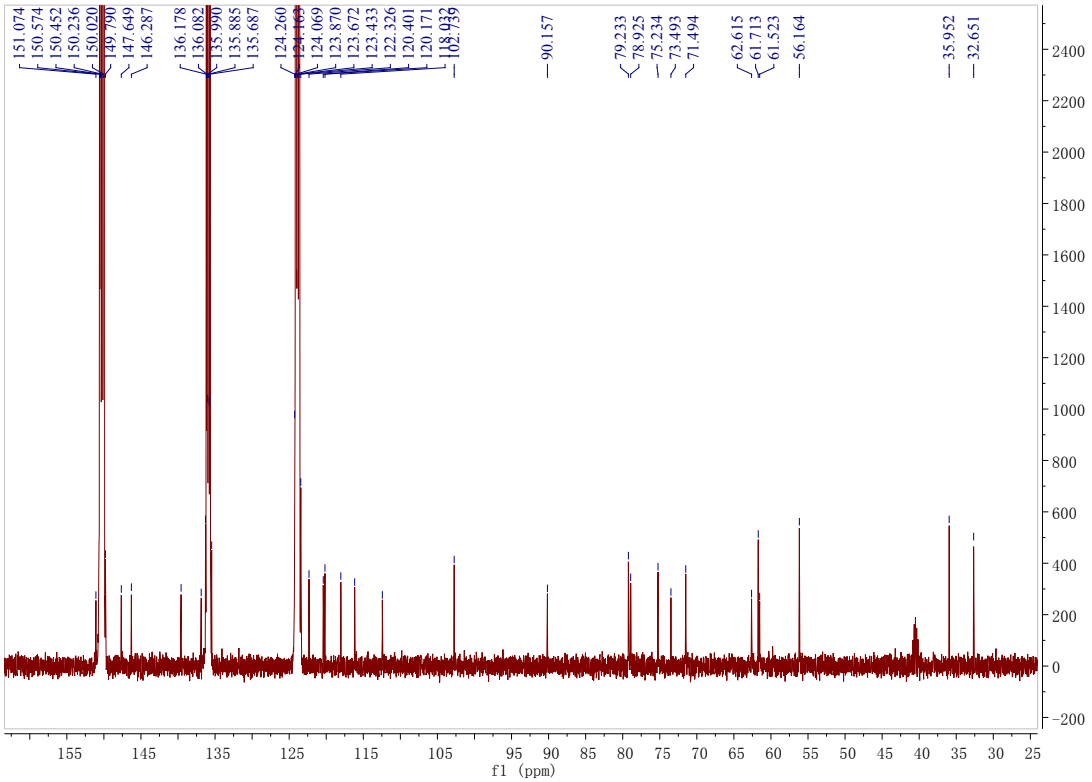


Figure S251. The ^{13}C-NMR spectrum of C-1 in C_5D_5N

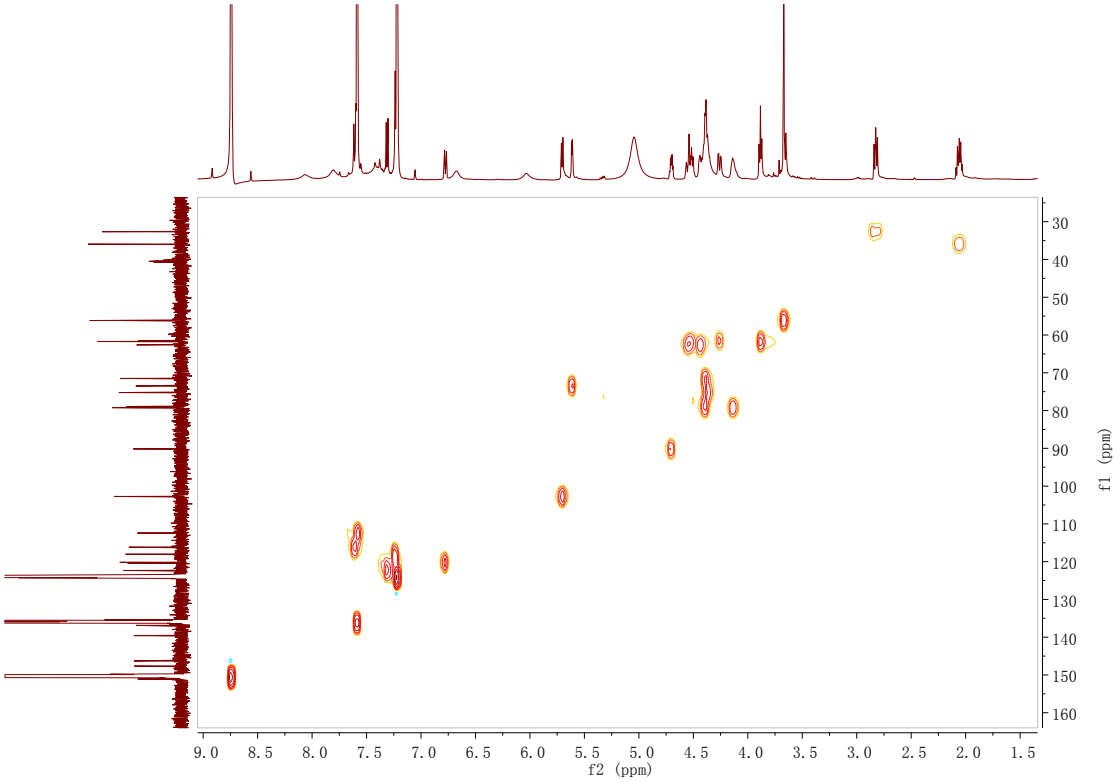


Figure S252. The HSQC spectrum of C-1 in C_5D_5N

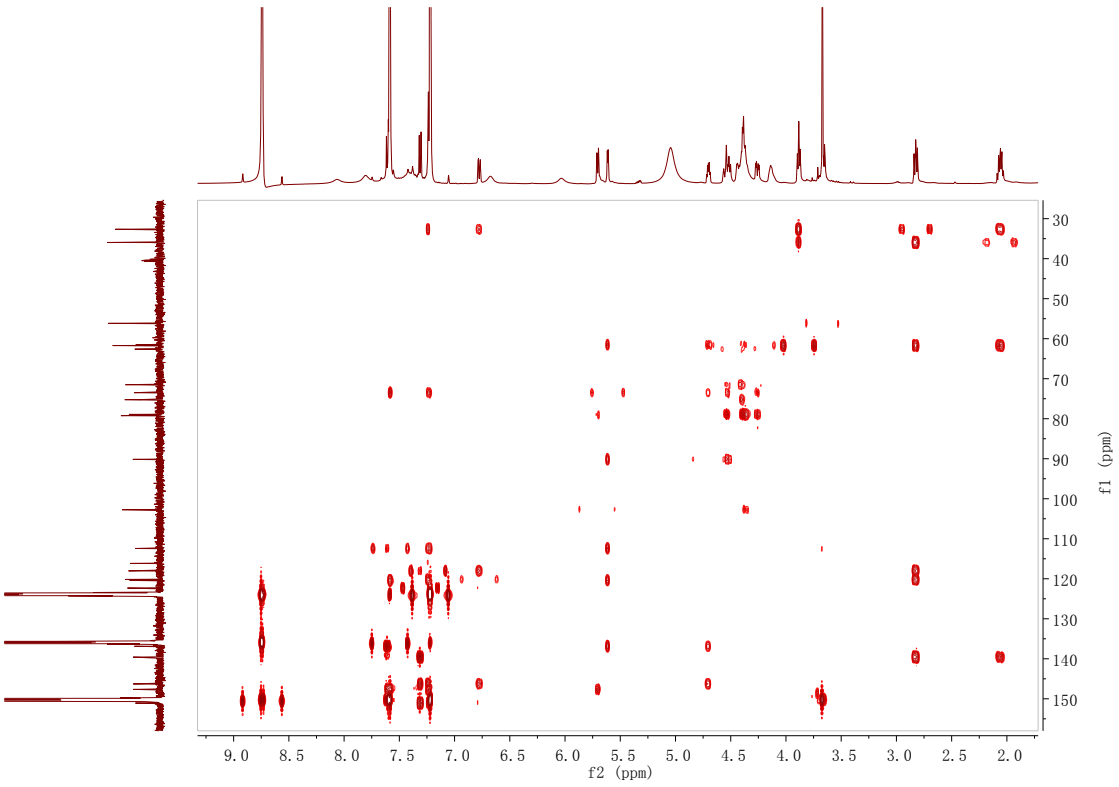


Figure S253. The HMBC spectrum of C-1 in C_5D_5N

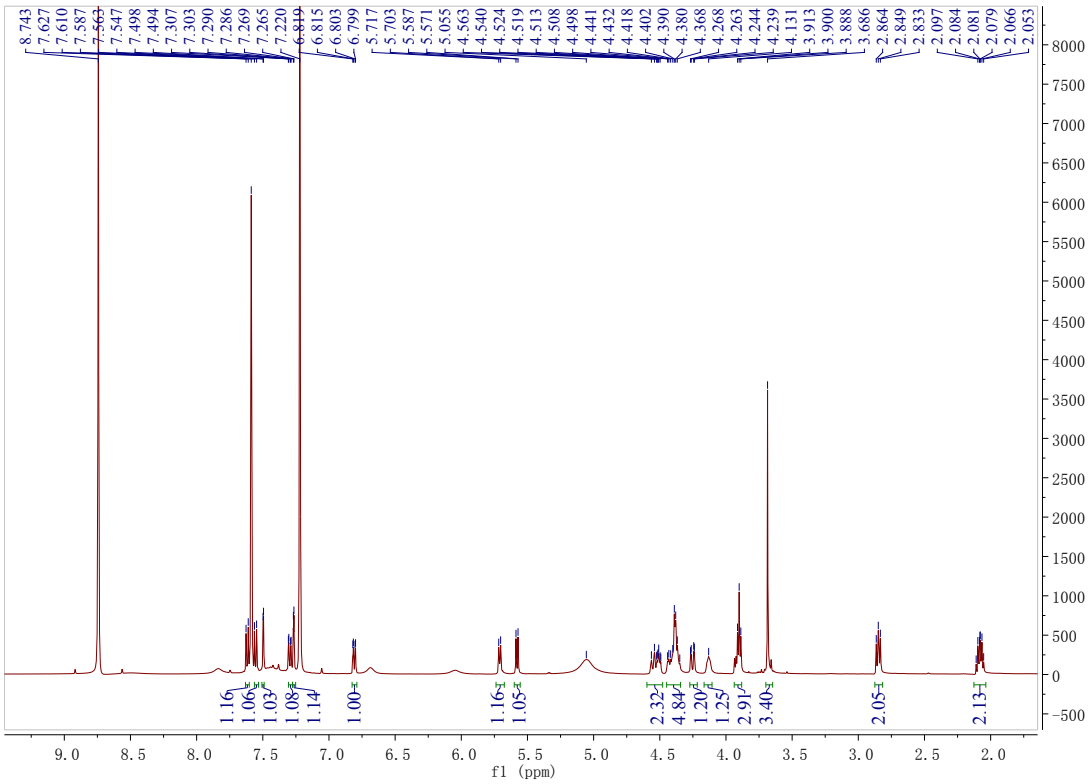


Figure S254. The ^{1}H-NMR spectrum of C-2 in C_5D_5N

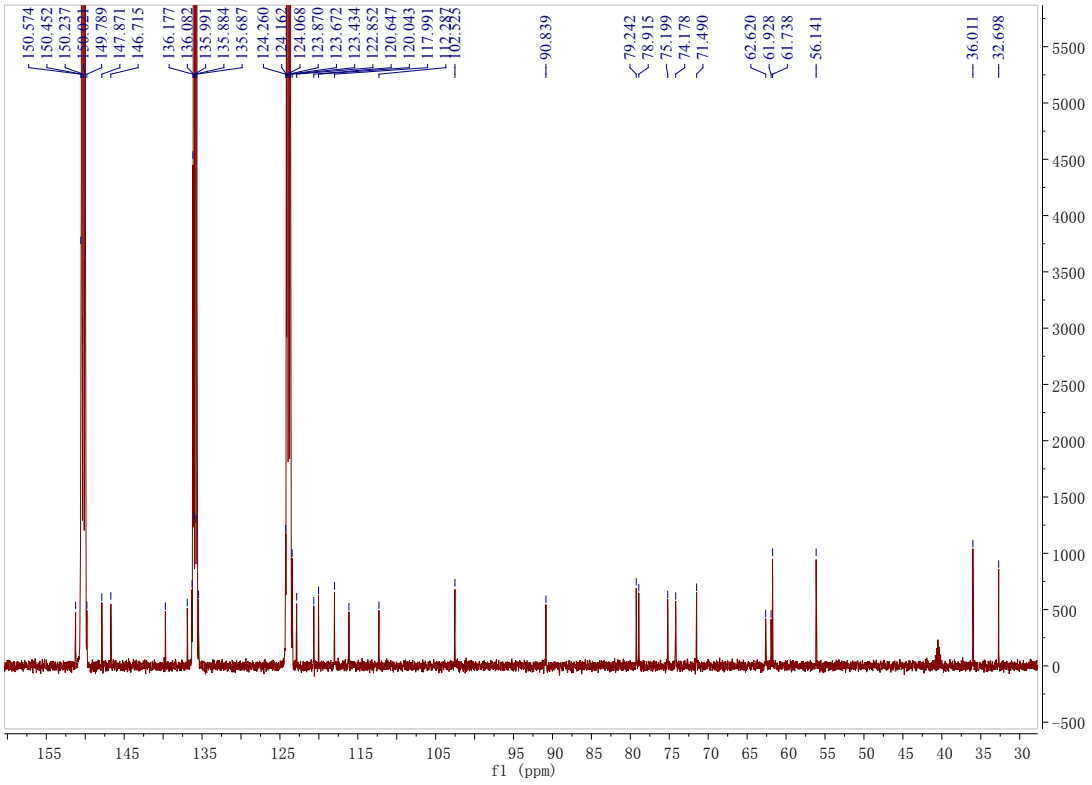


Figure S255. The ^{13}C-NMR spectrum of C-2 in C_5D_5N

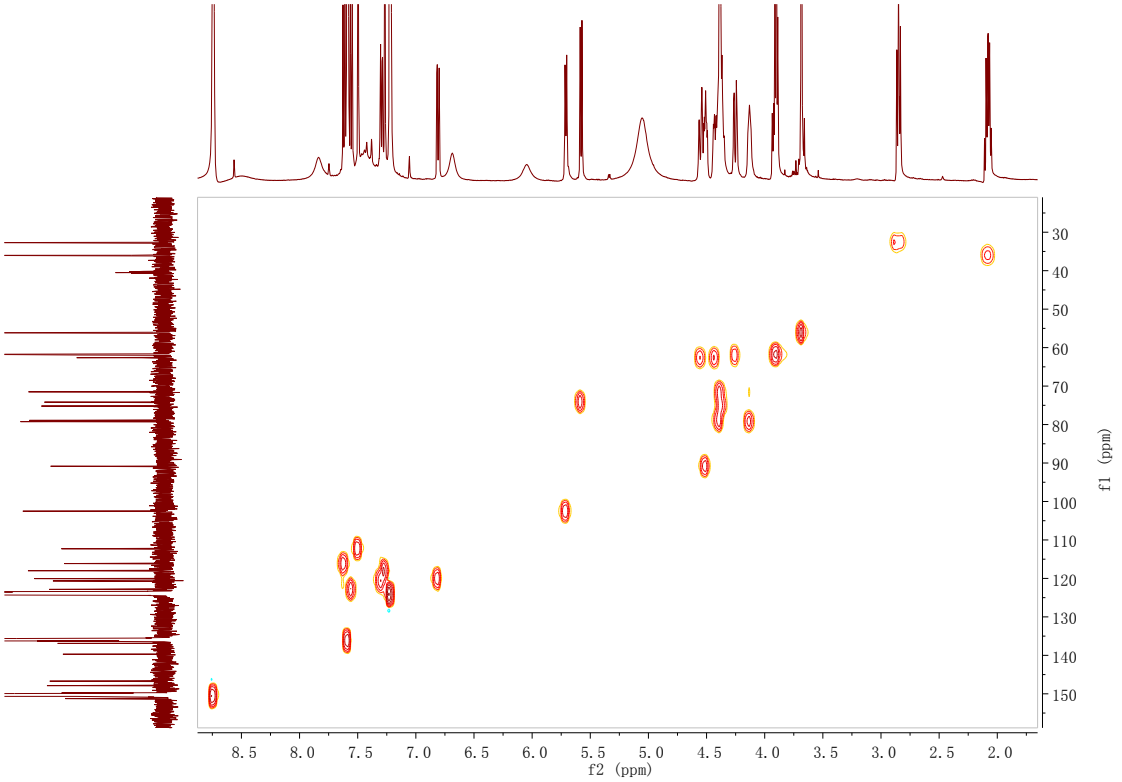


Figure S256. The HSQC spectrum of C-2 in C_5D_5N

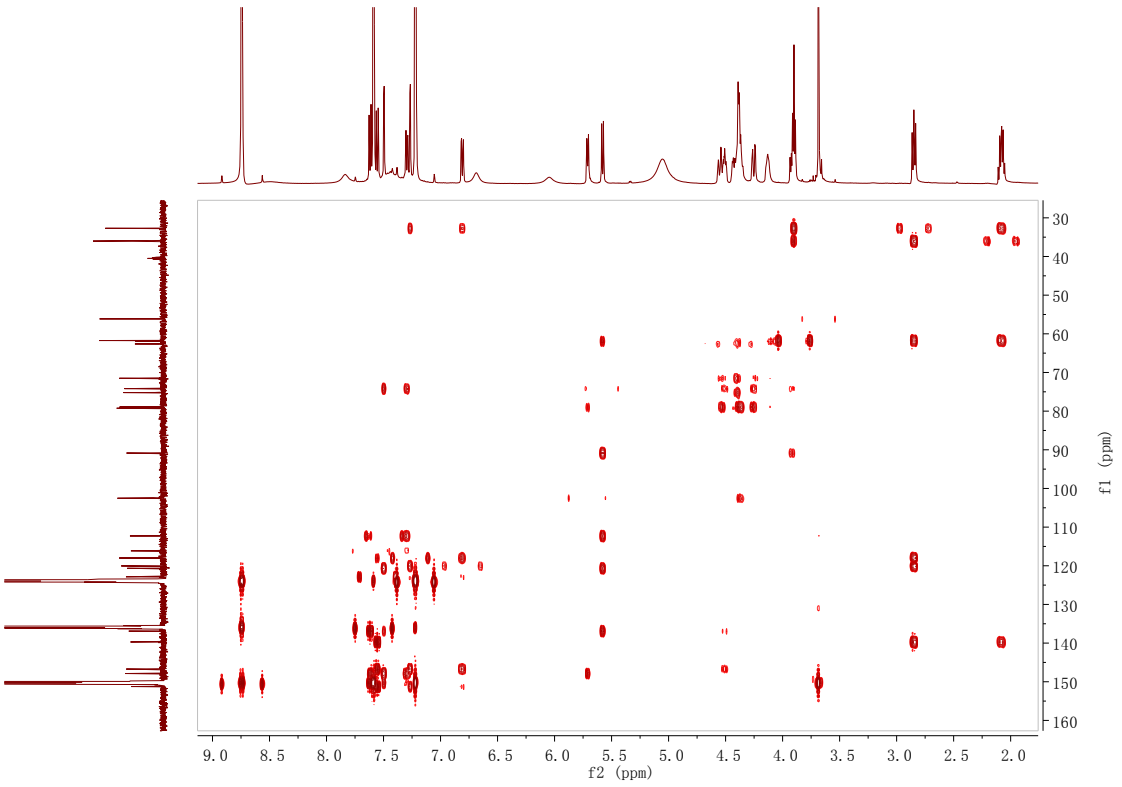


Figure S257. The HMBC spectrum of C-2 in C_5D_5N

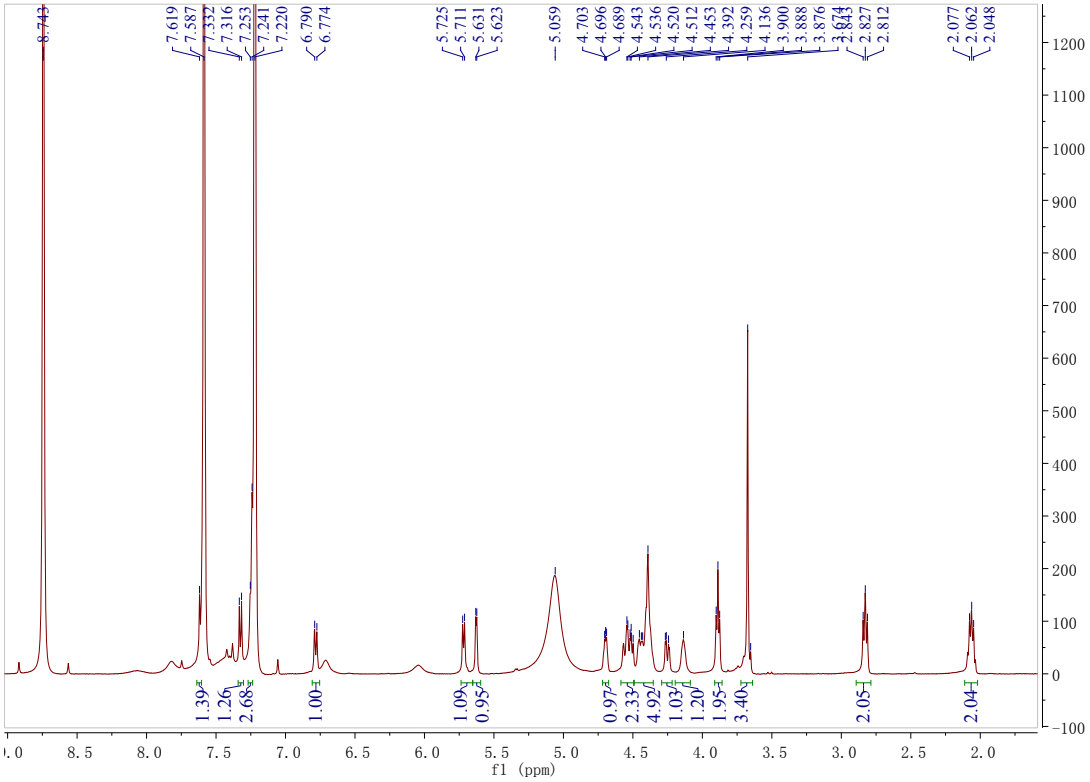


Figure S258. The ^{1}H-NMR spectrum of C-3 in C_5D_5N

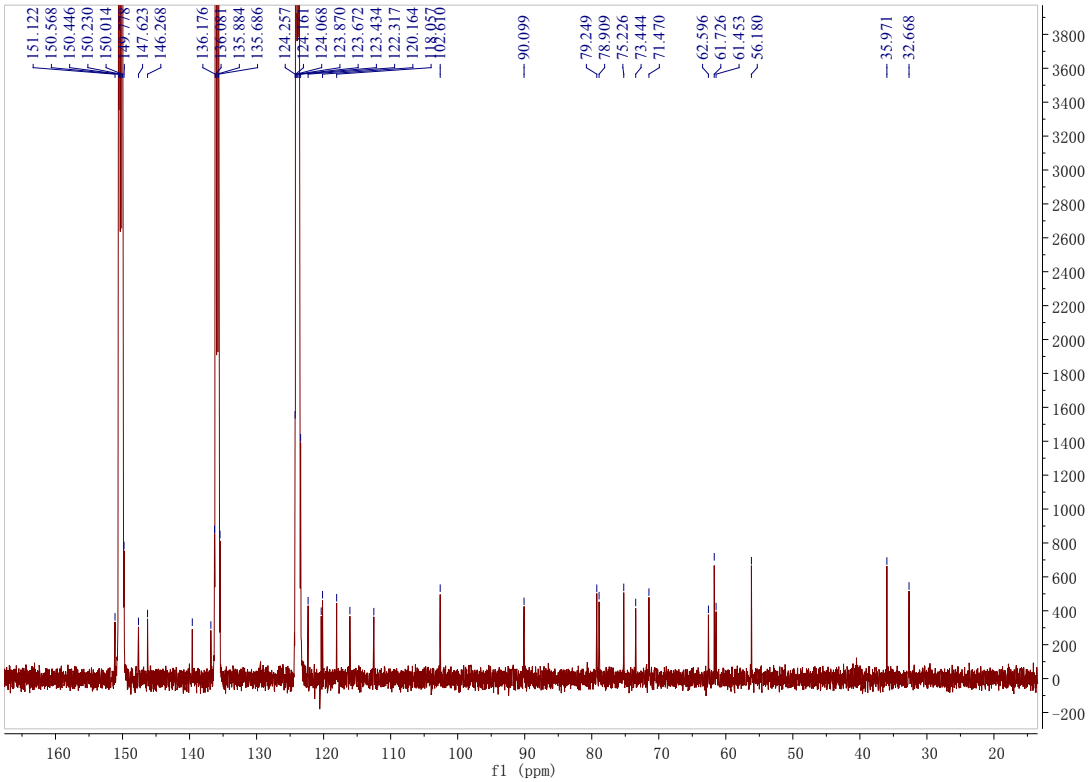


Figure S259. The ^{13}C-NMR spectrum of C-3 in C_5D_5N

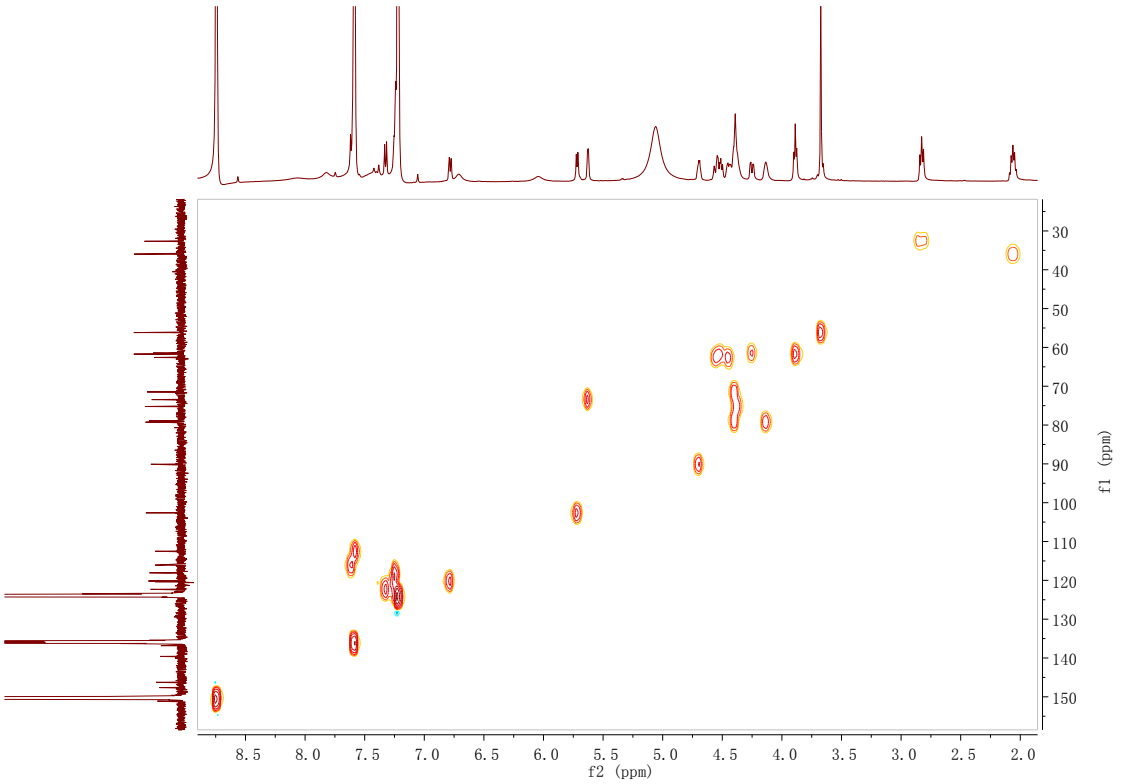


Figure S260. The HSQC spectrum of C-3 in C_5D_5N

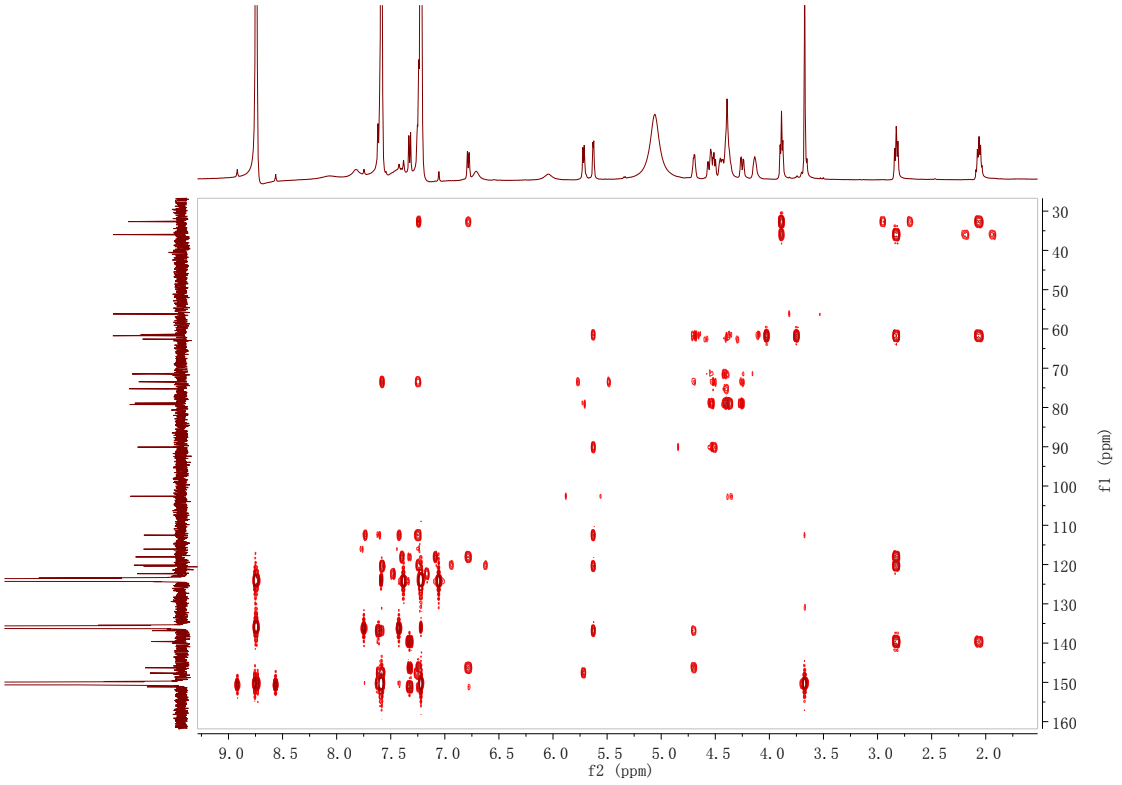


Figure S261. The HMBC spectrum of C-3 in C_5D_5N