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Characterization of anti-BCG benz[α]anthraquinones and new siderophores from a Xinjiang-desert-isolated rare actinomycete, *Nocardia* sp. XJ31

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Table S1 Selective isolation media for rare Actinomycetes

Media	Component
HV agar [83]	Humic acid 1 g, Na_2HPO_4 0.5 g, KCl 1.7 g, $MgSO_4·7H_2O$ 0.05 g, $FeSO_4·7H_2O$ 0.01 g, $CaCl_2$ 1 g, mixed vitamin 3.7 mg, agar 20 g, distilled water 1 L, pH 7.0-7.2, autoclave at 121°C, 20 min, then add 100 mg of cycloheximide and 20 mg of nalidixic acid.
SM3 agar [84]	Tryptone 3 g, peptone 5 g, NaCl 5 g, glucose 10 g, agar 20 g, distilled water 1 L, pH 7.0, autoclave at 121°C, 20 min, then add 10 mg of nalidixic acid, 50 mg of nystatin and 50 mg of cycloheximide.
MOPS agar	MOPS 5 g, proline 1 g, $(NH_4)_2SO_4$ 1 g, NaCl 1 g, $CaCl_2$ 2 g, K_2HPO_4 1 g, $MgSO_4·7H_2O$ 1 g, agar 20 g, distilled water 1 L, pH 7.2, autoclave at 121°C, 20 min, then add 10 mg of nalidixic acid and 50 mg of Cycloheximide.
starch-Casein-Nitrate agar (SCN) [85]	Starch 10 g, casein vitamin free 0.3 g, KNO_3 2 g, K_2HPO_4 2 g, $MgSO_4·7H_2O$ 0.05 g, $FeSO_4·7H_2O$ 0.01 g, $CaCO_3$ 0.02 g, agar 20 g, distilled water 1 L, pH 7.0-7.2, autoclave at 121°C, 20 min, then add 25 mg of novobiocin, 50 mg of nystatin and 50 mg of cycloheximide.
AV (arginine vitamine) agar [86]	L-arginine 0.3 g, glycerol 1 g, K_2HPO_4 0.3 g, $MgSO_4·7H_2O$ 0.2 g, NaCl 0.3 g, trace solution 1 mL, agar 20 g, distilled water 1 L, pH 7.3, autoclave at 121°C, 20 min, then add 10 mg of nalidixic acid and 50 mg of cycloheximide. Trace solution: $FeSO_4·7H_2O$ 0.1g, $MnCl_2·4H_2O$ 0.1g, $ZnSO_4·7H_2O$ 0.1g, H_2O 100 mL.

Table S2 Components of 21 fermentation media for OSMAC strategy

Media	Component
P2	Yeast extract 4 g, malt extract 10 g, dextrose 4 g, distilled water 1 L, pH 7.2
Sa	soluble starch 10 g, yeast extract 4 g, peptone 2 g, $Fe_2(SO_4)_3·4H_2O$ 0.04 g, KBr 0.1 g, distilled water 1 L
GT	Soluble starch 20 g, L-Asparagine 0.5 g, KNO_3 1 g, K_2HPO_4 0.5 g, NaCl 0.5 g, $MgSO_4·7H_2O$ 0.5 g, $CaCO_3$ 1 g, distilled water 1 L, pH 7.5
VER01	Soluble starch 10 g, dextrose 10 g, glycerin 10 g, corn syrup powder 2.5 g, peptone 5 g, yeast extract 2 g, NaCl 1 g, $CaCO_3$ 3 g, distilled water 1 L, pH 7.5
AM1	Soluble starch 20 g, dextrose 4 g, K_2HPO_4 0.5 g, KNO_3 1.0 g, $MgSO_4·7H_2O$ 0.5 g, $FeSO_4·7H_2O$ 0.01 g, pH 7.0-7.2
AM2	Soluble starch 5 g, dextrose 20 g, Soy flour 10 g, peptone 2 g, yeast extract 2 g, NaCl 4 g, K_2HPO_4 0.5 g, $MgSO_4·7H_2O$ 0.5 g, $CaCO_3$ 2 g, distilled water 1 L, pH 7.8
AM3	yeast extract 4 g, malt extract 10 g, dextrose 4 g, distilled water 1 L, pH 7.2
NM	Dextrose 5 g, soluble starch 10 g, peptone10 g, soybean peptone10 g, yeast extract 3 g, KNO_3 1.0 g, one-fold Trace element solution 0.2 mL, $CaCO_3$ 1 g, distilled water 1 L, pH 7.0. Trace element solution (1 fold): $FeSO_4$ 4 g, $MnSO_4$ 5 g, $ZnSO_4·7H_2O$ 2.5 g, Borax 1.4 g, $CoCl_2·6H_2O$ 0.2 g, $CuSO_4·5H_2O$ 0.5 g, $MgSO_4·2H_2O$ 0.2 g, distilled water 1 L, pH 7.2
NM2	Dextrose 1 g, lactose 10 g, glycerin 20 mL, soybean peptone 5 g, NH_4NO_3 1.5 g, yeast extract 1 g, one-fold Trace element solution 0.2 mL, distilled water 1 L, pH 6.0
MM1	Dextrose 10 g, soluble starch 10 g, Soy flour 15 g, NaCl 3 g, K_2HPO_4 1 g, $MgSO_4·7H_2O$ 1 g, $FeSO_4·7H_2O$ 0.001 g, $CuSO_4·5H_2O$ 0.007 g, $MnCl_2·4H_2O$ 0.008 g, $ZnSO_4·5H_2O$ 0.002 g, distilled water 1 L, pH 7.0
M001	Soluble starch 20 g, yeast extract 8.0 g, peptone 4.0 g, $CaCO_3$ 1.0 g, distilled water 1 L, pH 7.2
M1	Soluble starch 10 g, yeast extract 4 g, peptone 2 g, distilled water 1 L, pH 7.2
M6	Beef extract 4 g, peptone 4 g, yeast extract 1 g, dextrose 10 g, distilled water 1 L, pH 7.2
M8	Soluble starch 15 g, yeast extract 4 g, K_2HPO_4 1 g, $MgSO_4$ 0.5 g, distilled water 1 L, pH 7.2
M9	Soluble starch 20 g, KNO_3 1.0 g, K_2HPO_4 0.5 g, $MgSO_4$ 0.5 g, $FeSO_4$ 0.01 g, distilled

	water 1 L, pH 7.2
M10	Yeast extract 24 g, K_2HPO_4 9.4 g, KH_2PO_4 2.2 g, distilled water 1 L, pH 7.2
M11	NaCl 5 g, Enzymatic hydrolysis of casein 15 g, Soy flour papain 5 g, distilled water 1 L, pH 7.2
M12	Peptone 5 g, yeast extract 1 g, sodium citrate 0.2 g, NaCl 19.45 g, $MnCl_2$ 5.9 g, $MgSO_4$ 3.24 g, $CaCl_2$ 1.8 g, KCl 0.55 g, $NaHCO_3$ 0.5 g, KBr 0.08 g, $SrCl_2$ 0.034 g, boric acid 0.022 g, sodium silicate 0.004 g, NaF 0.002 g, ammonium nitrate 0.0016 g, Na_2PO_4 0.008 g, distilled water 1 L, pH 7.2
Noc02	Sucrose 20 g, tryptone 10 g, K_2HPO_4 0.5 g, NaCl 0.5 g, $FeSO_4 \cdot 7H_2O$ 0.01 g, distilled water 1 L, pH 6.5
Noc03	Starch 5.0 g, soybean flour 20.0 g, peptone 2.0 g, glucose 20.0 g, yeast extract 2.0 g, NaCl 4.0 g, K_2HPO_4 0.5 g, $MgSO_4 \cdot 7H_2O$ 0.5 g, $CaCO_3$ 2.0 g, distilled water 1 L
Noc05	Starch 10 g, glucose 10 g, glycerol 10 g, corn steep powder 2.5 g, peptone 5 g, yeast extract 2 g, $NaNO_3$ 1 g, $CaCO_3$ 3 g, distilled water 1 L, pH 7.2

Table S3 Detailed information of sampling sites

Sample ID	Environment	Sample description	Coordinate	Altitude	Temperature
1#	Plateau river	River sediment	38°41.406 N 74°58.391 E	3368 m	19.4°C
2#	Desert highway	Saline and alkali soil	39°51.924 N 80°57.832 E	1057 m	28.2°C
3#	Tianshan mountain	Red mineral soil	42°21.736 N 88°40.162 E	1639 m	44.5°C
4#	Desert river	Soil on plant root, 10 cm below surface	40°36.804 N 79°41.260 E	1058 m	30.0°C
5#	Desert river	Red sediment, 10 cm below surface	40°36.804 N 79°41.260 E	1058 m	30.0°C
6#	Desert river	Saline and alkali soil	40°36.804 N 79°41.260 E	1058 m	30.0°C
7#	Desert land	Saline and alkali soil, 30 cm below surface	39°51.901 N 77°47.002 E	1154 m	38.7°C
8#	Plateau lake	Lake sediment	38°22.681 N 75°02.775 E	3655 m	17.1°C
9#	Arid land	Soil, 20 cm below surface	42°04.680 N 87°10.059 E	1063 m	36.0°C
10#	Flaming mountain	Soil	42°55.476 N 89°30.779 E	< 0 m	51.5°C
11#	Flaming mountain	Red soil	42°55.476 N 89°30.779 E	< 0 m	51.5°C
12#	Flaming mountain	Soil	42°55.476 N 89°30.779 E	< 0 m	51.5°C
13#	Aydingkol Lake	Saline and alkali sand soil	42°42.677 N 89°02.695 E	-150 m	42.0°C
14#	Kanerjing	River sediment	43° 38.61 N 90°39.411 E	< 0 m	31.9°C
15#	Desert highway	Soil on plant root	40°11.443 N 81°1.201 E	1029 m	22.4°C

16#	Plateau river	River sediment	-	-	-
17#	Plateau river	River sediment	-	-	-

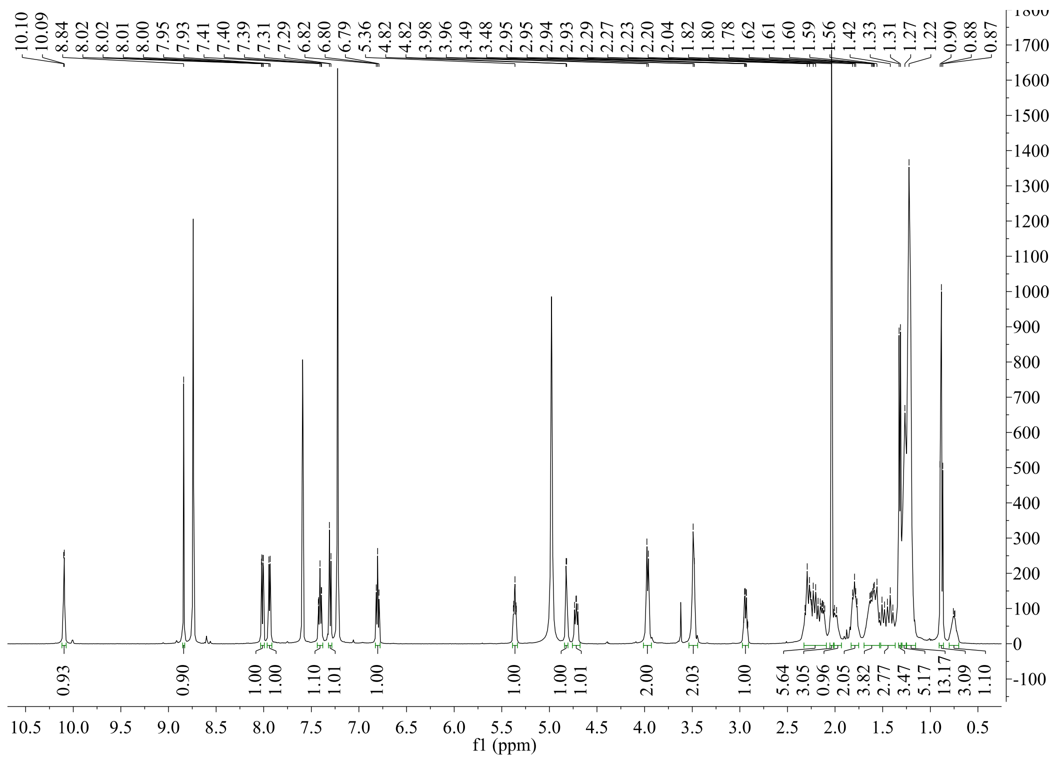

Fig. S1a ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **1a**

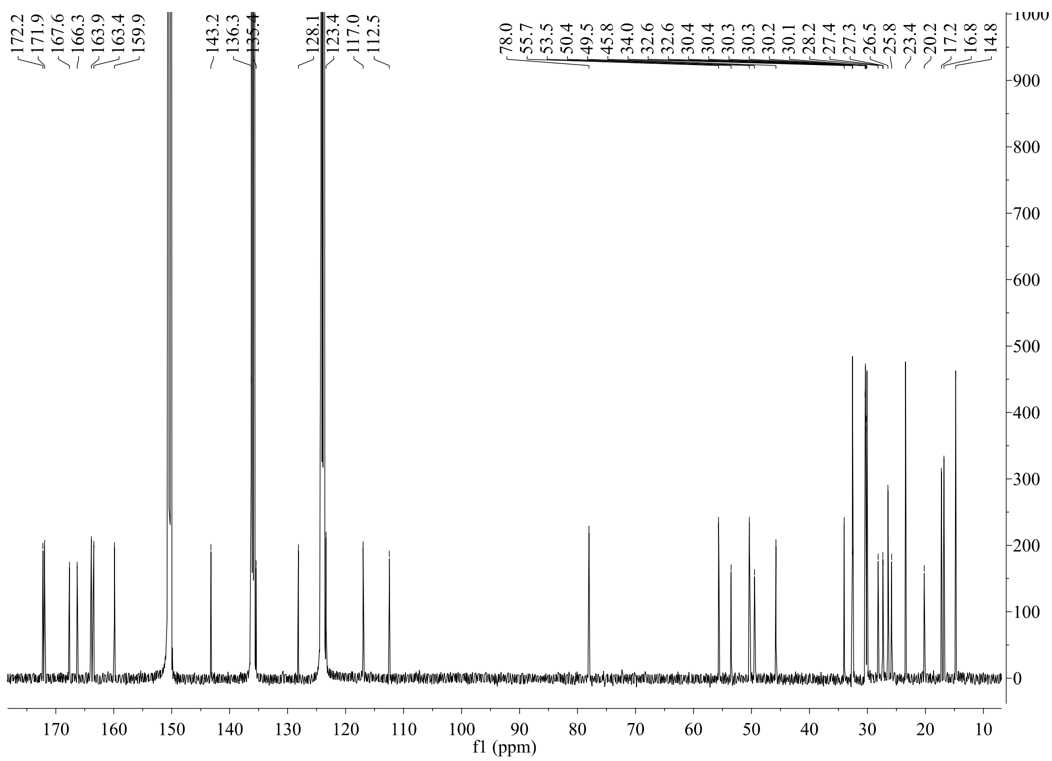

Fig. S1b ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **1a**

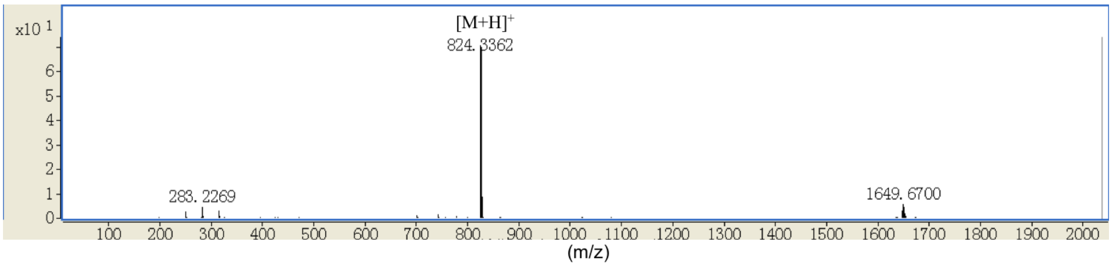

Fig. S1c HR-ESI-MS spectrum of **1a**

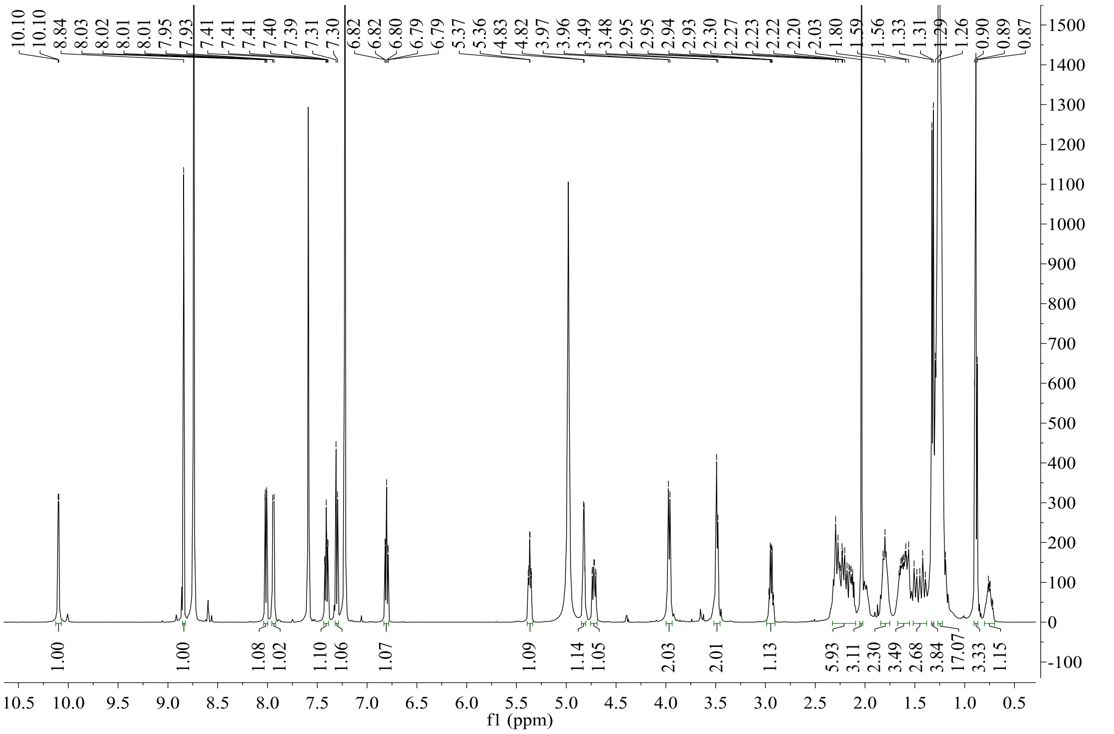

Fig. S2a ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **2a**

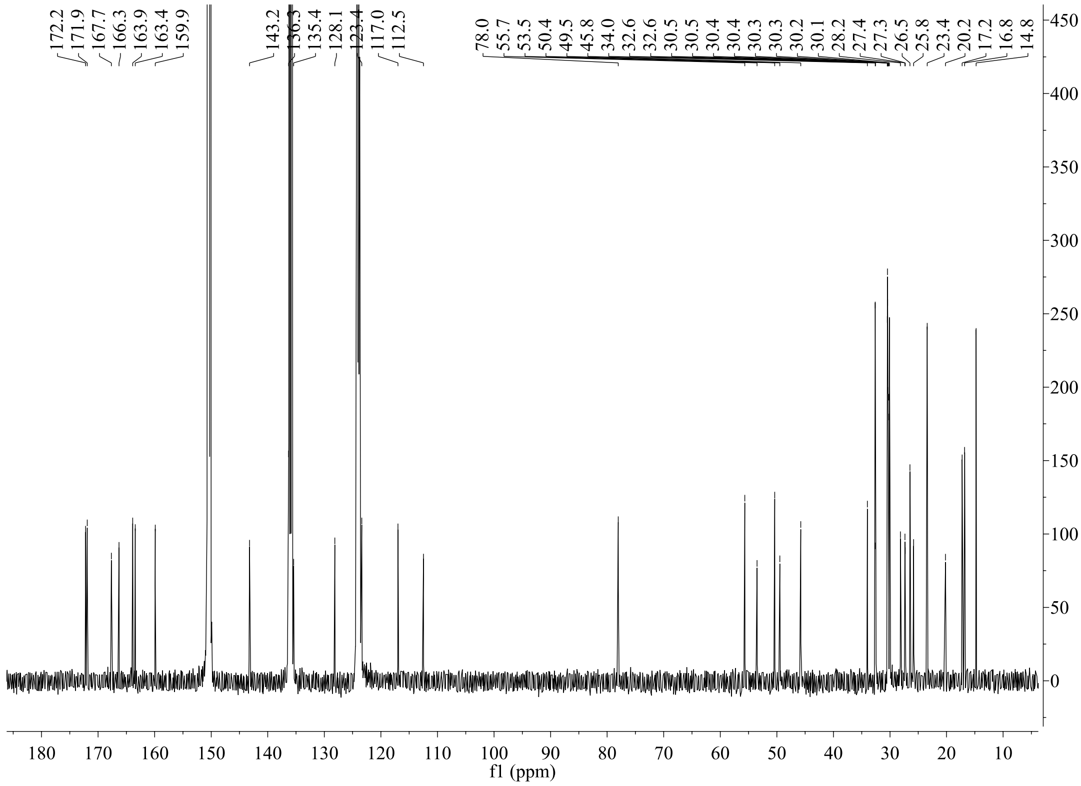

Fig. S2b ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **2a**

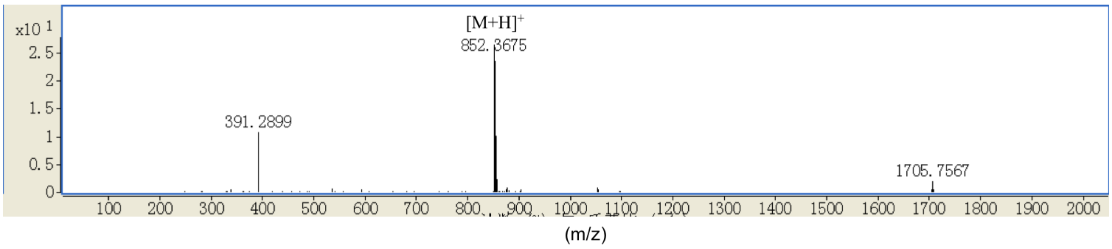

Fig. S2c HR-ESI-MS spectrum of **2a**

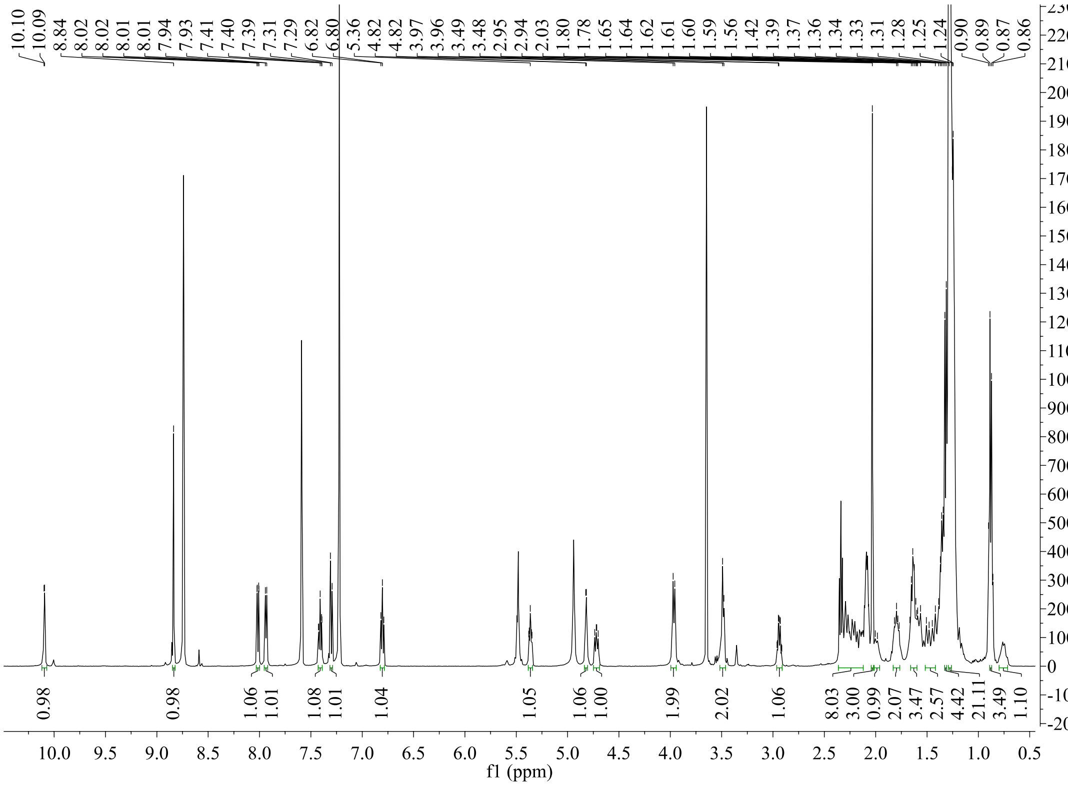

Fig. S3a ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **3a**

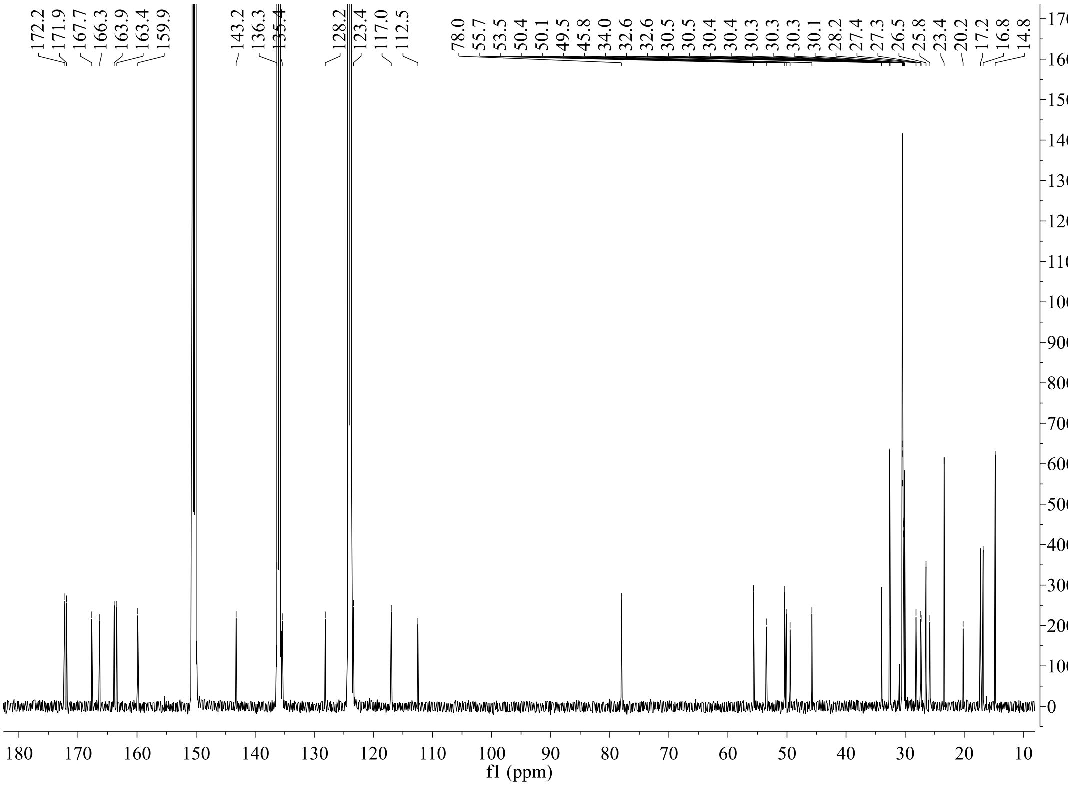

Fig. S3b ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **3a**

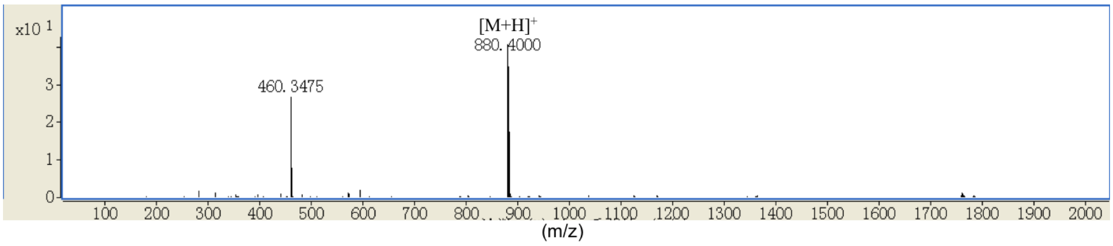

Fig. S3c HR-ESI-MS spectrum of **3a**

Table S4 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **4a**

Pos.	δ_C	δ_H, mult (*J* in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			
2	167.6			
3	123.4	7.30, br d (*8.4*)	4	1, 2, 5, 6
4	135.4	7.39, dq (*1.6*, *7.0*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *6.8*)	4, 6	1, 2, 3, 4, 6
6	128.1	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4, 7
7	166.3			
9	143.2	8.84, s		7, 10, 12
10	136.4			
12	159.9			
13	NH	10.11, d (*3.0*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.36, m	18, 35a, 35b	15, 18, 19, 35, 36, 54
18	45.8	2.95, m	17, 54	19, 54
19	172.2			
20	NH	7.94, d (*6.9*)	21	19, 21, 22
21	50.4	4.65, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.9	1.32-1.25, m	24, 25b, 26a, 26b	22, 24
		0.74, m	24, 25a, 26b	
26	28.2	1.69-1.53, m	25a, 27a	
		1.52-1.41, m	25a, 25b, 27b	
27	32.5	2.30-2.10, m	21, 26a, 27b	
		1.25-1.17, m	27a	
28	27.4	2.37-2.30, m	14, 28b, 29a, 29b	
		2.30-2.10, m	14, 28a, 29a. 29b	15, 30
29	20.2	2.30-2.10, m	29b, 30b	14, 30
		1.86-1.76, m	28a, 28b, 29a	
30	27.5	2.02-1.94, m	30b, 31	
		1.52-1.41, m	29a, 30a, 31	
31	49.3	4.00, m	30a	29, 30, 33
33	166.8			
34	23.5	2.37-2.30, m	52	33, 52
35	34.0	2.30-2.10, m	17, 35b, 36	17, 18, 36, 37

		1.86-1.76, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.69-1.53, m	35a, 35b	17, 38
37	30.4-30.1[a]	1.25-1.17, m		
38	30.4-30.1[a]	1.25-1.17, m		
39	30.4-30.1[a]	1.25-1.17, m		
40	30.4-30.1[a]	1.25-1.17, m		
41	30.4-30.1[a]	1.25-1.17, m		
42	30.4-30.1[a]	1.25-1.17, m		44
43	32.6	1.32-1.25, m	37-42, 44	41
44	23.4	1.32-1.25, m	43, 45	43
45	14.8	0.88, t (*6.8*)	44	43, 44
52	10.1	1.03, t (*7.4*)	34	33, 34
54	17.2	1.35, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

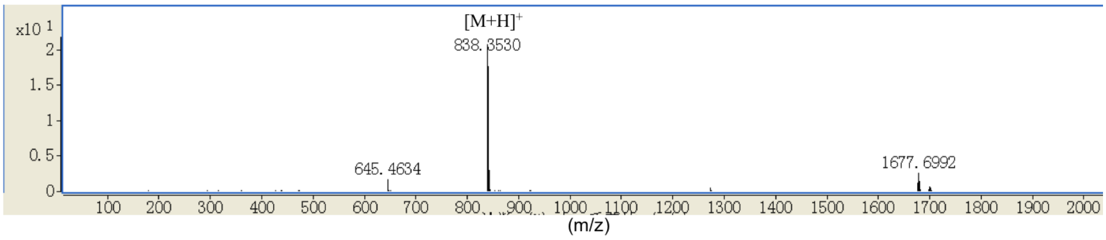

Fig. S4a HR-ESI-MS spectrum of **4a**

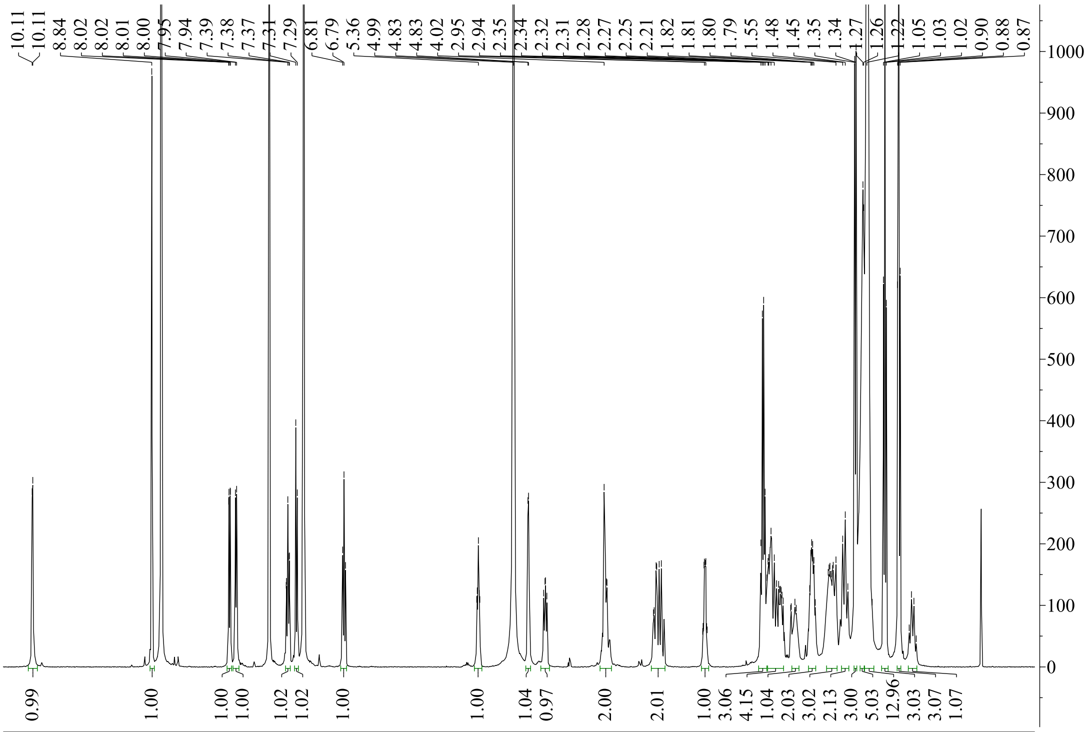

Fig. S4b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **4a**

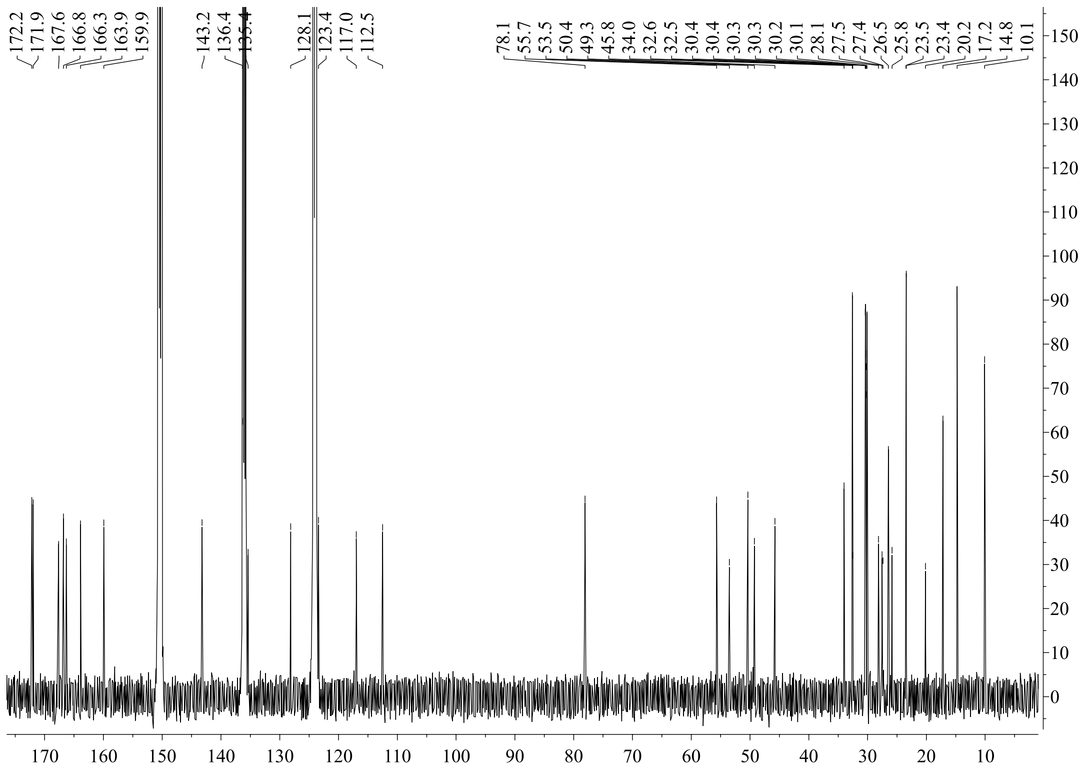

Fig. S4c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **4a**

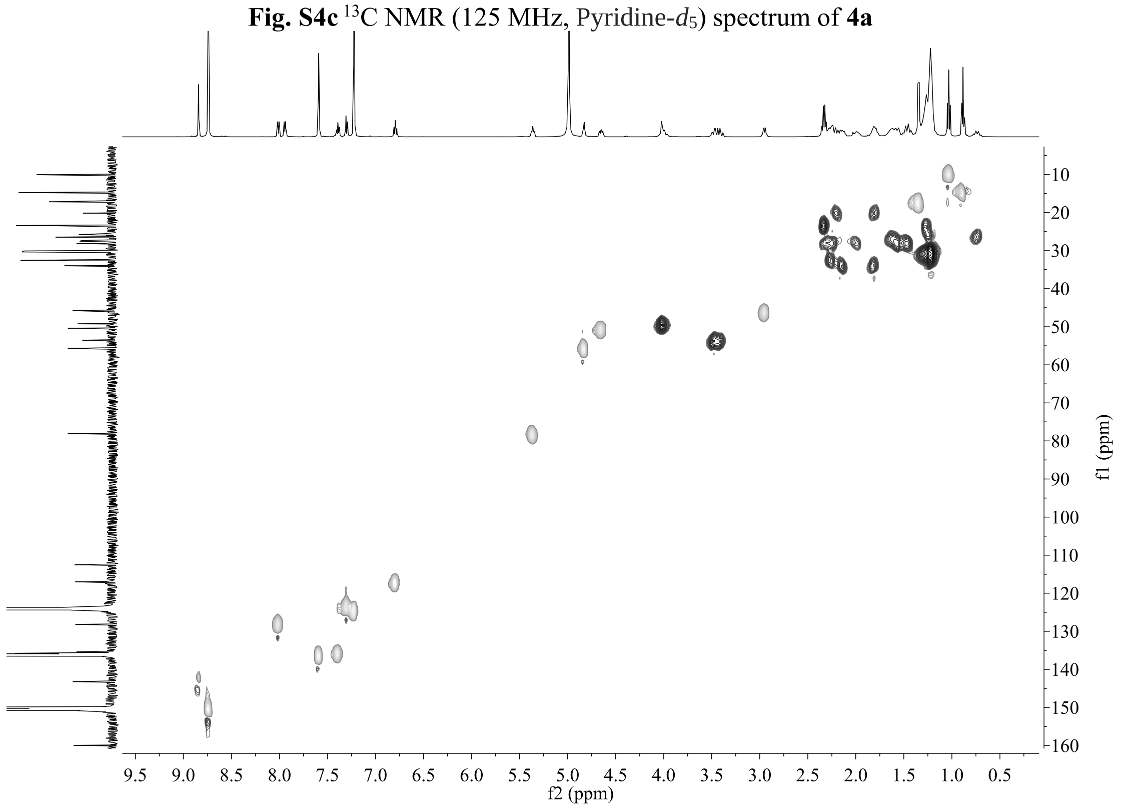

Fig. S4d HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **4a**

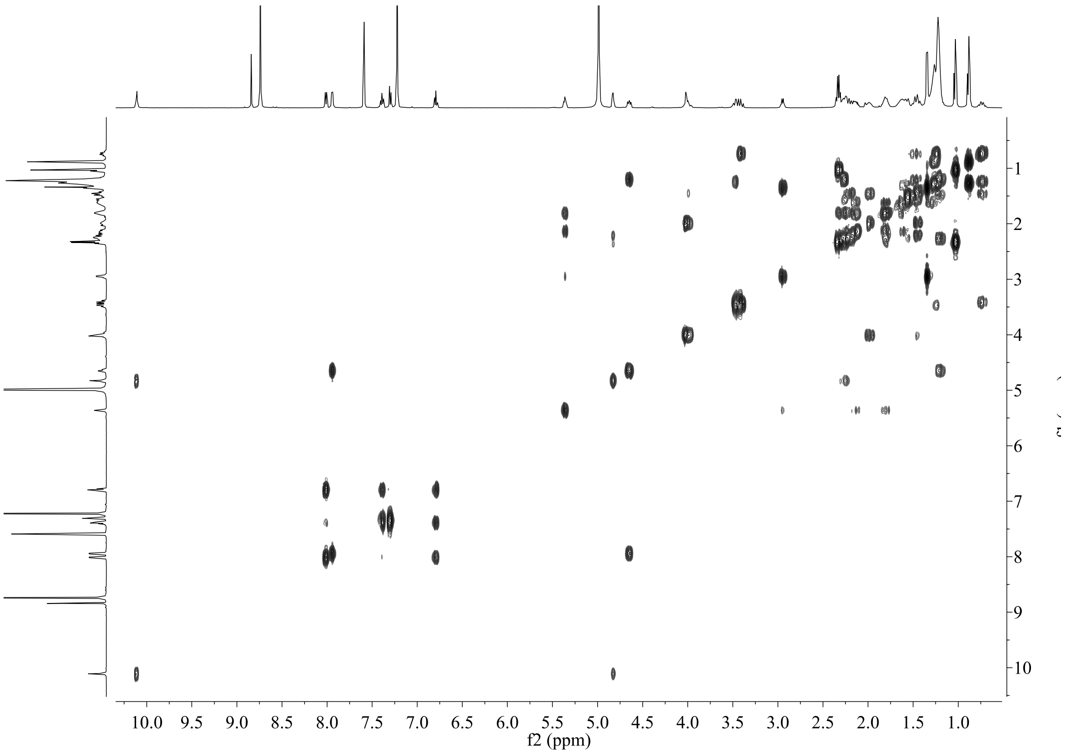

Fig. S4e ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **4a**

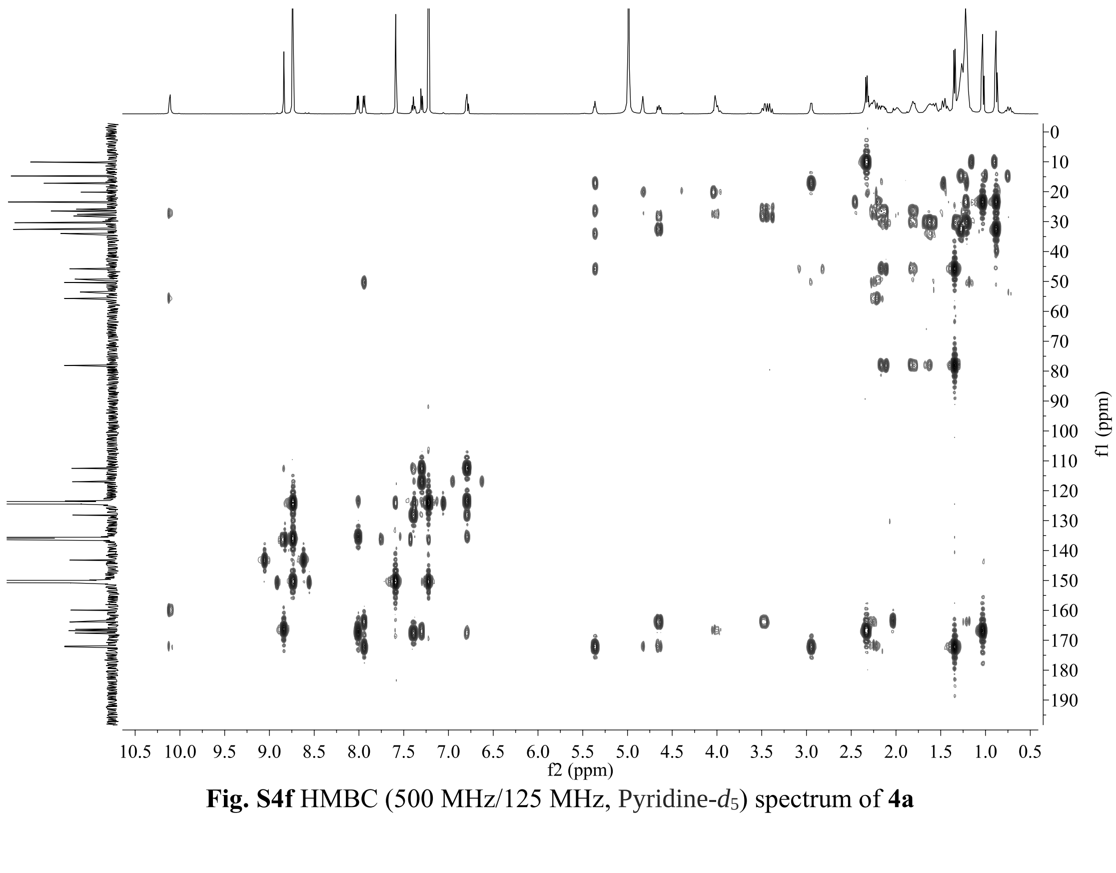

Fig. S4f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **4a**

Table S5 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **5a**

Pos.	δ_C	δ_H, mult (*J* in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			

2	167.6			
3	123.4	7.31, br d (*8.2*)	4	1, 2, 5, 6
4	135.4	7.40, dq (*1.7*, *7.1*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *7.4*)	4, 6	1, 2, 3, 4, 6
6	128.2	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	160.0			
13	NH	10.10, d (*3.1*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.37, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.7	2.96, m	17, 54	19, 54
19	172.2			
20	NH	7.97, d (*7.0*)	21	19, 21, 22
21	50.4	4.73, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.8	1.32-1.25, m	24, 25b, 26a, 26b	22, 24
		0.73, m	24, 25a, 26b	
26	28.2	1.66-1.56, m	25a, 27a	
		1.50-1.43, m	25a, 25b, 27b	
27	32.5	2.39-2.10, m	21, 26a, 27b	
		1.25-1.17, m	27a	
28	27.5	2.39-2.10, m	14, 28b, 29a, 29b	15, 30
29	20.2	2.39-2.10, m	29b, 30b	14, 30
		1.85-1.77, m	28a, 28b, 29a	
30	27.8	2.02-1.95, m	30b, 31	
		1.50-1.43, m	29a, 30a, 31	
31	49.5	4.09, m	30a	29, 30, 33
33	166.8			
34	31.5	2.39-2.10, m	52	33, 52
35	34.0	2.39-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.85-1.77, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.66-1.56, m	35a, 35b	17, 38
37	30.4-30.1[a]	1.25-1.17, m		
38	30.4-30.1[a]	1.25-1.17, m		
39	30.4-30.1[a]	1.25-1.17, m		
40	30.4-30.1[a]	1.25-1.17, m		
41	30.4-30.1[a]	1.25-1.17, m		
42	30.4-30.1[a]	1.25-1.17, m		44
43	32.6	1.32-1.25, m	37-42, 44	41
44	23.4	1.32-1.25, m	43, 45	43
45	14.8	0.88, t (*6.8*)	44	43, 44
52	19.4	1.66-1.56, m	34, 53	33, 34, 53

53	13.8	0.79, t (*7.3*)	52	34, 52
54	17.1	1.37, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

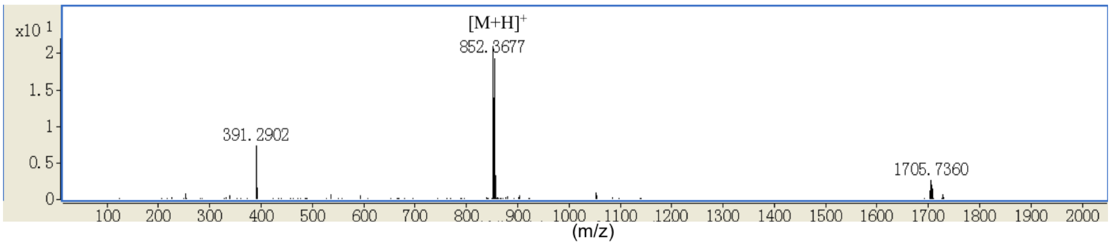

Fig. S5a HR-ESI-MS spectrum of **5a**

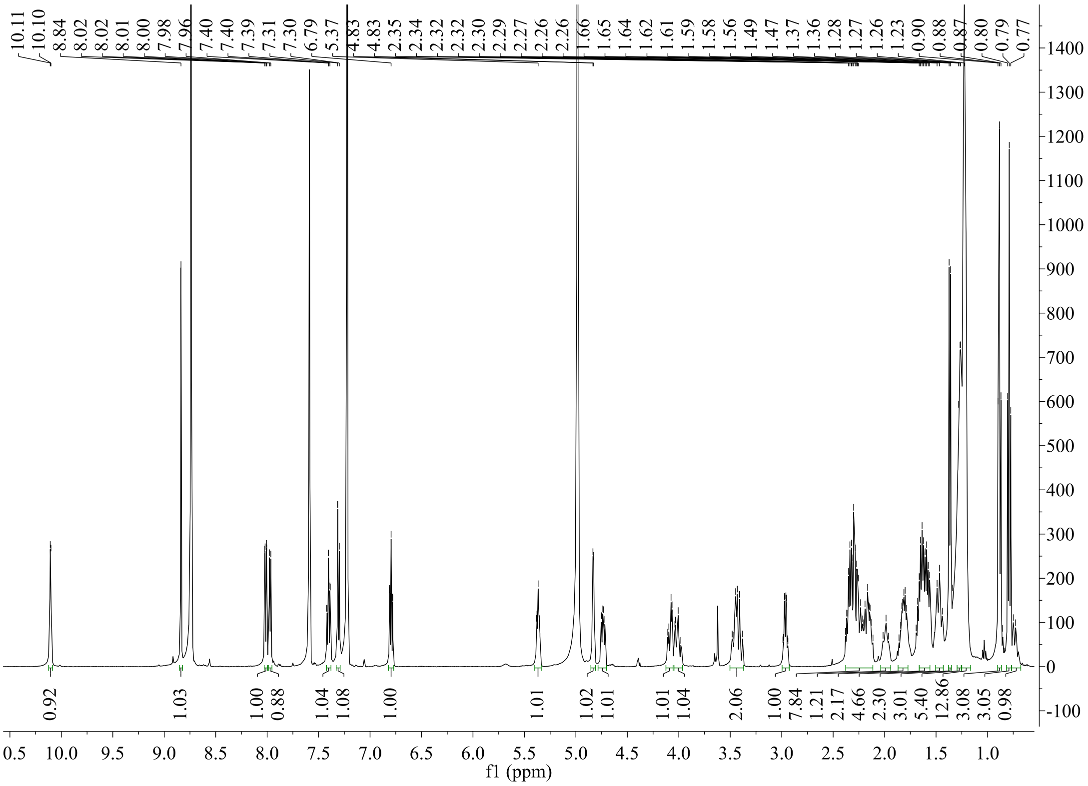

Fig. S5b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **5a**

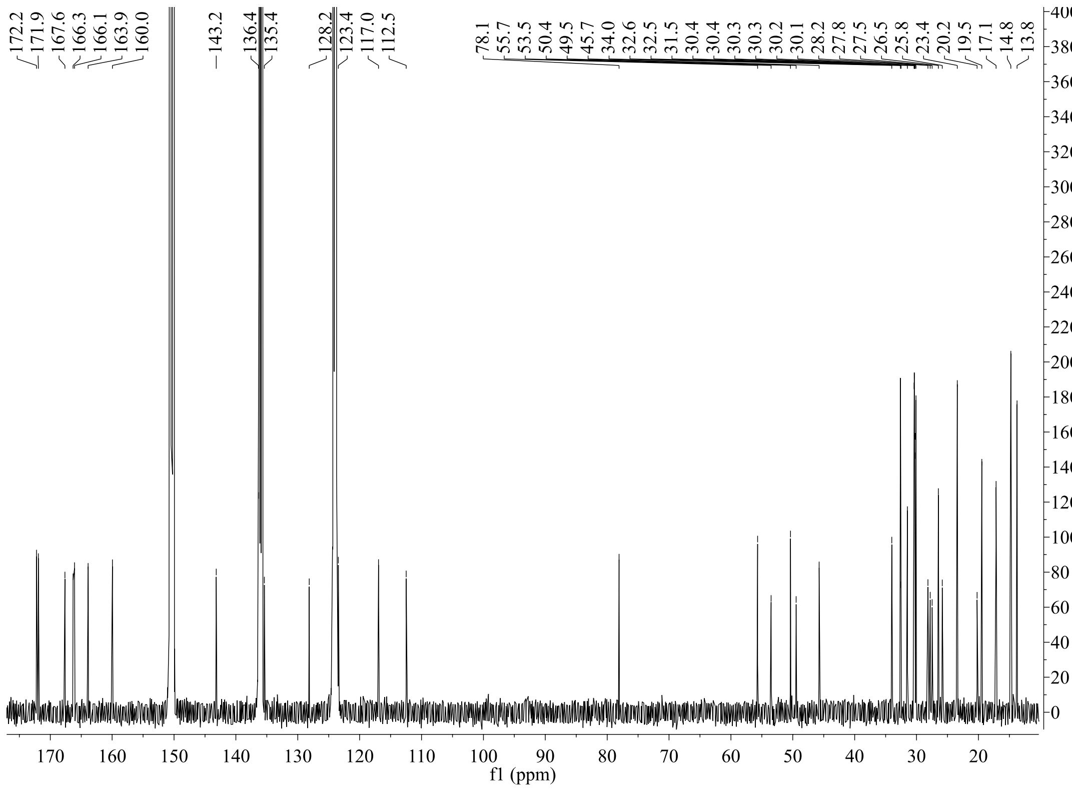

Fig. S5c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **5a**

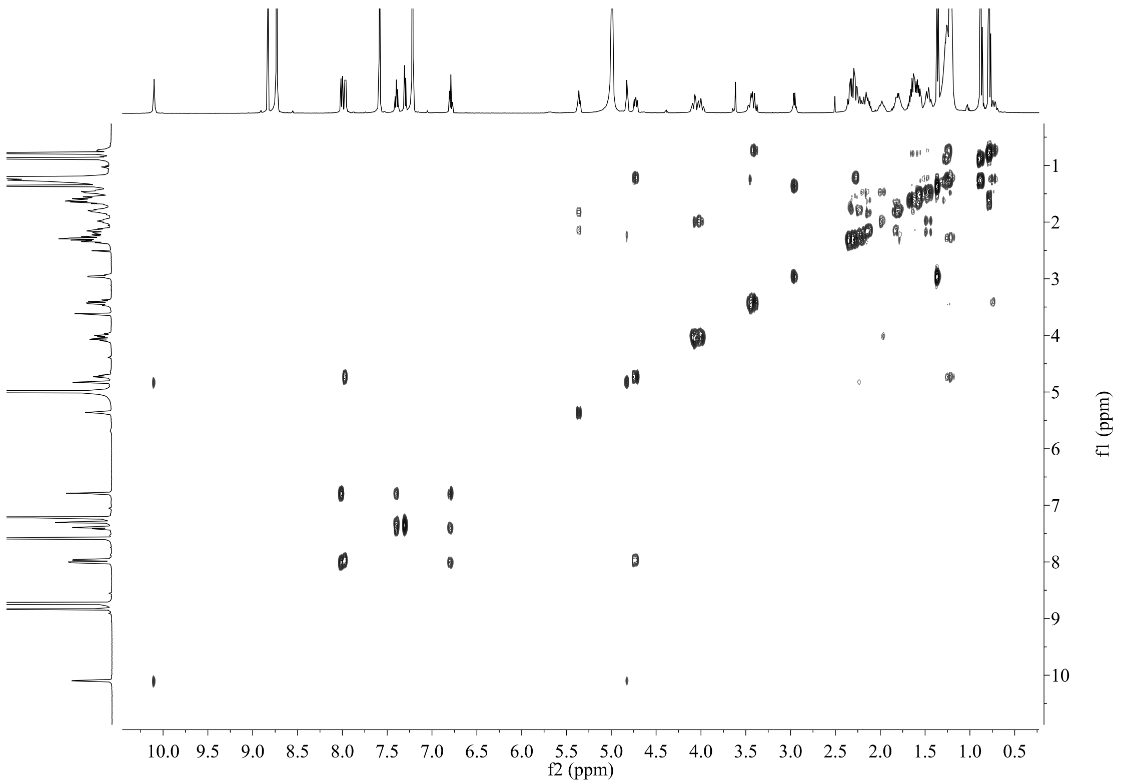

Fig. S5d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **5a**

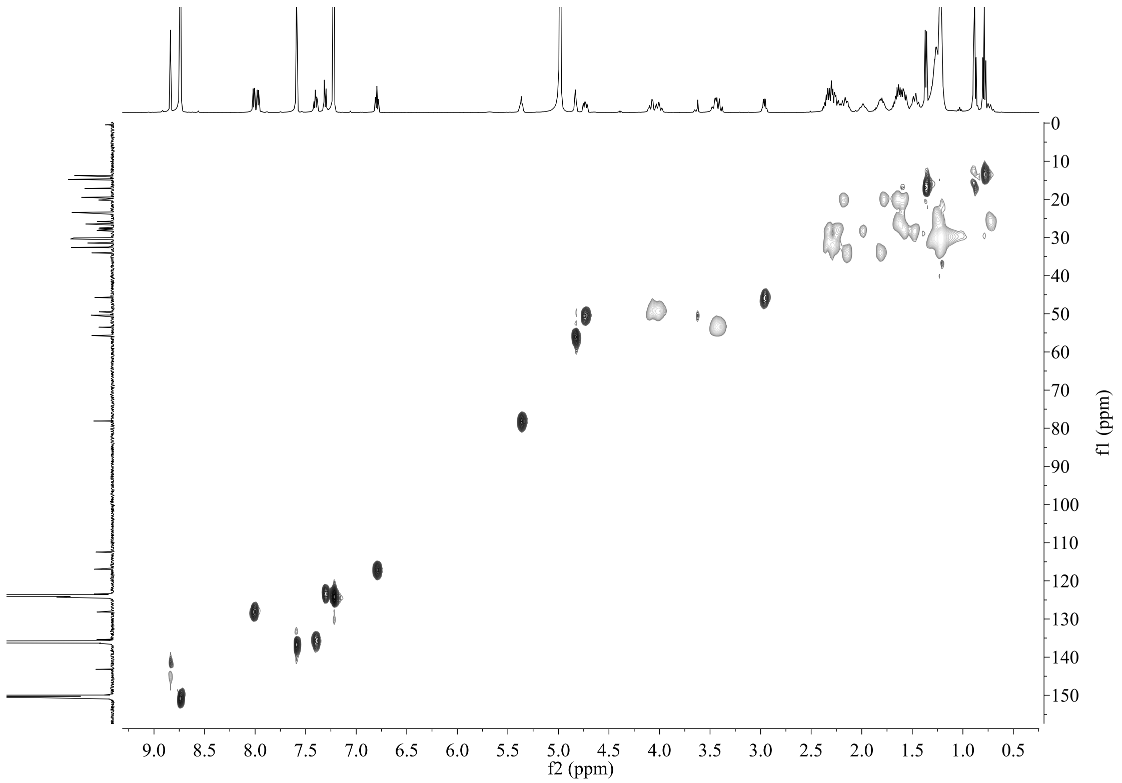

Fig. S5e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **5a**

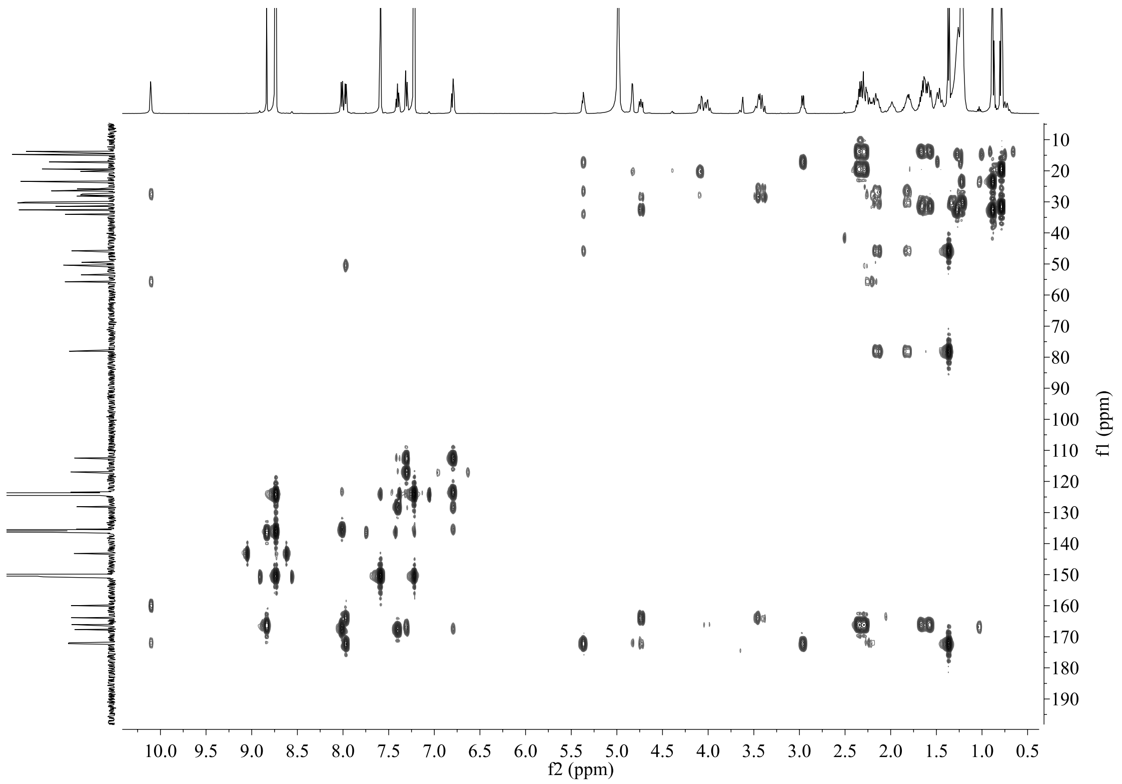

Fig. S5f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **5a**

Table S6 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **6a**

Pos.	δ_C	δ_H, mult (J in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			
2	167.6			

3	123.4	7.30, br d (*8.4*)	4	1, 2, 5, 6
4	135.4	7.39, dq (*1.6*, *7.0*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *6.8*)	4, 6	1, 2, 3, 4, 6
6	128.1	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	159.9			
13	NH	10.11, d (*3.0*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.36, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.8	2.95, m	17, 54	19, 54
19	172.2			
20	NH	7.94, d (*6.9*)	21	19, 21, 22
21	50.4	4.65, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.9	1.30-1.21, m	24, 25b, 26a, 26b	22, 24
		0.74, m	24, 25a, 26b	
26	28.2	1.69-1.53, m	25a, 27a	
		1.52-1.41, m	25a, 25b, 27b	
27	32.5	2.30-2.10, m	21, 26a, 27b	
		1.30-1.21, m	27a	
28	27.4	2.37-2.30, m	14, 28b, 29a, 29b	
		2.30-2.10, m	14, 28a, 29a. 29b	15, 30
29	20.2	2.30-2.10, m	29b, 30b	14, 30
		1.86-1.76, m	28a, 28b, 29a	
30	27.5	2.02-1.94, m	30b, 31	
		1.52-1.41, m	29a, 30a, 31	
31	49.3	4.00, m	30a	29, 30, 33
33	166.8			
34	23.5	2.37-2.30, m	52	33, 52
35	34.0	2.30-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.86-1.76, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.69-1.53, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.30-1.21, m		
38	30.5-30.1[a]	1.30-1.21, m		
39	30.5-30.1[a]	1.30-1.21, m		
40	30.5-30.1[a]	1.30-1.21, m		
41	30.5-30.1[a]	1.30-1.21, m		
42	30.5-30.1[a]	1.30-1.21, m		
43	30.5-30.1[a]	1.30-1.21, m		
44	30.5-30.1[a]	1.30-1.21, m		46
45	32.6	1.30-1.21, m	37-44, 46	43
46	23.4	1.30-1.21, m	45, 47	45

47	14.8	0.88, t (*6.8*)	46	45, 46
52	10.1	1.03, t (*7.4*)	34	33, 34
54	17.2	1.35, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

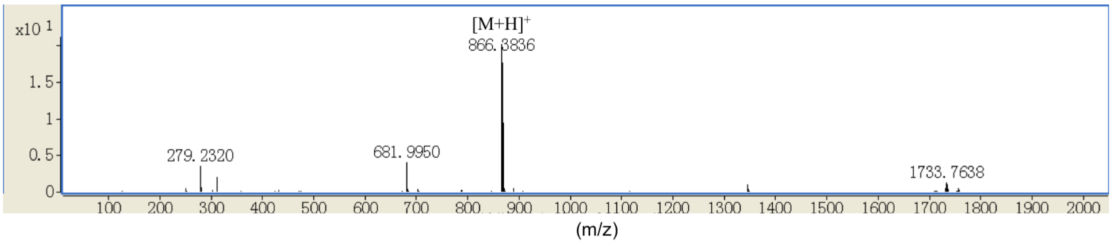

Fig. S6a HR-ESI-MS spectrum of **6a**

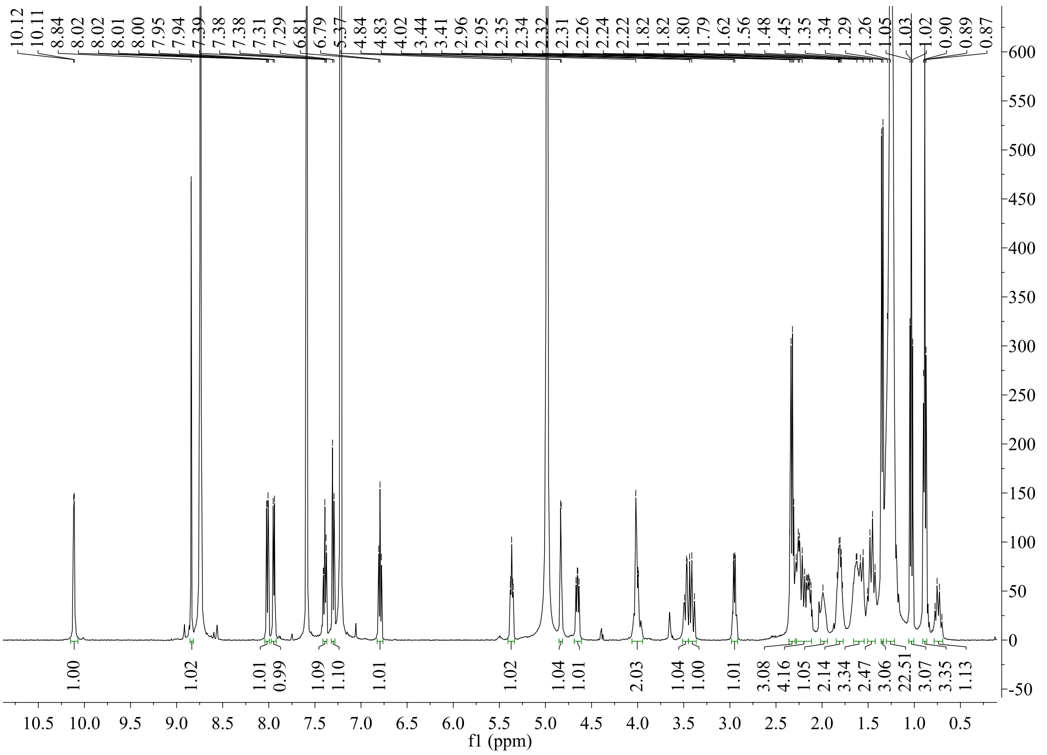

Fig. S6b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **6a**

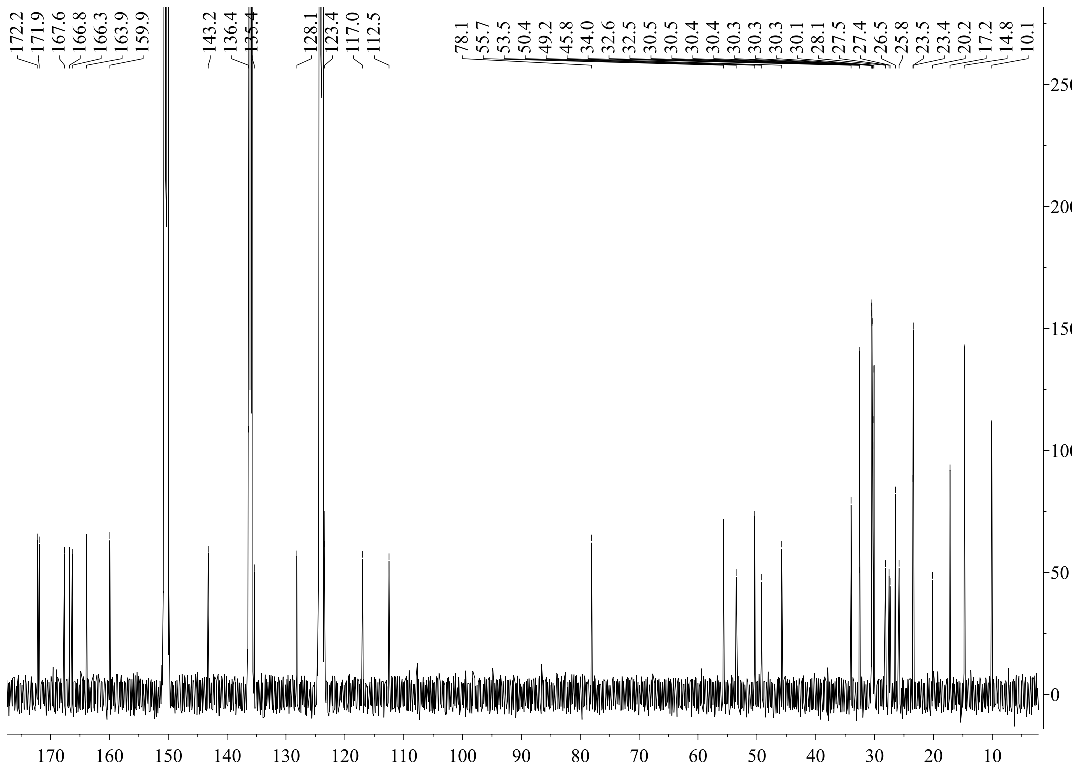

Fig. S6c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **6a**

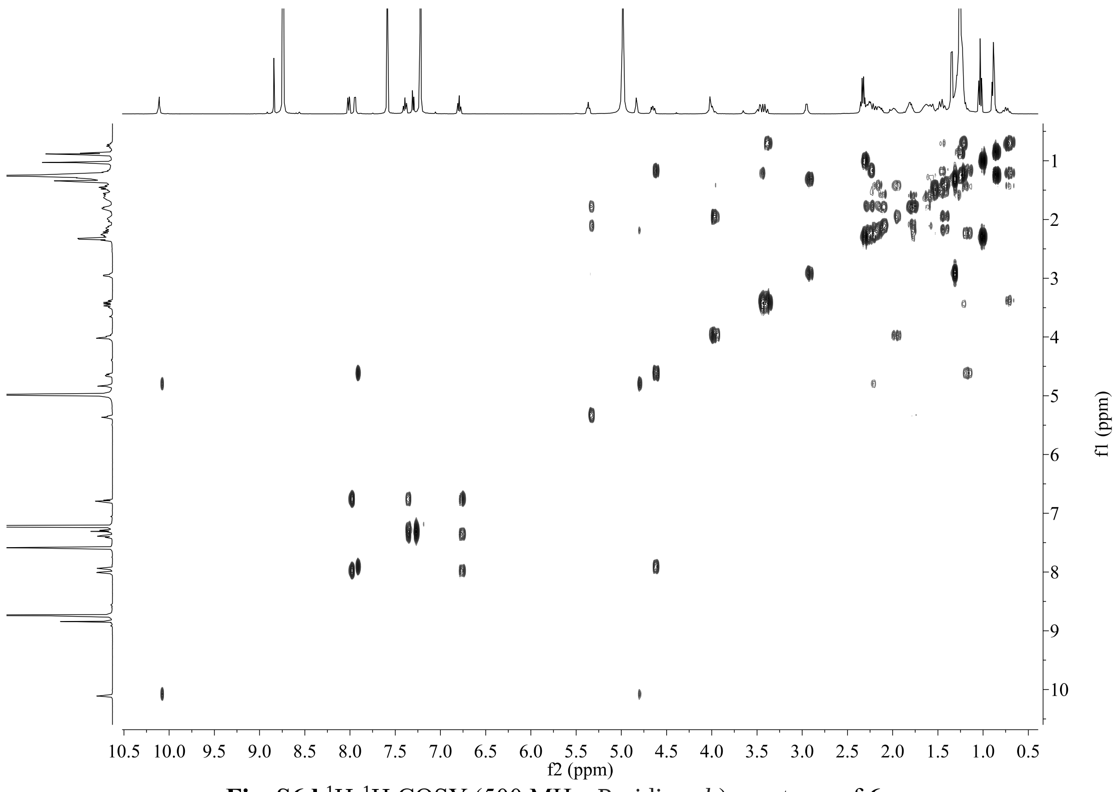

Fig. S6d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **6a**

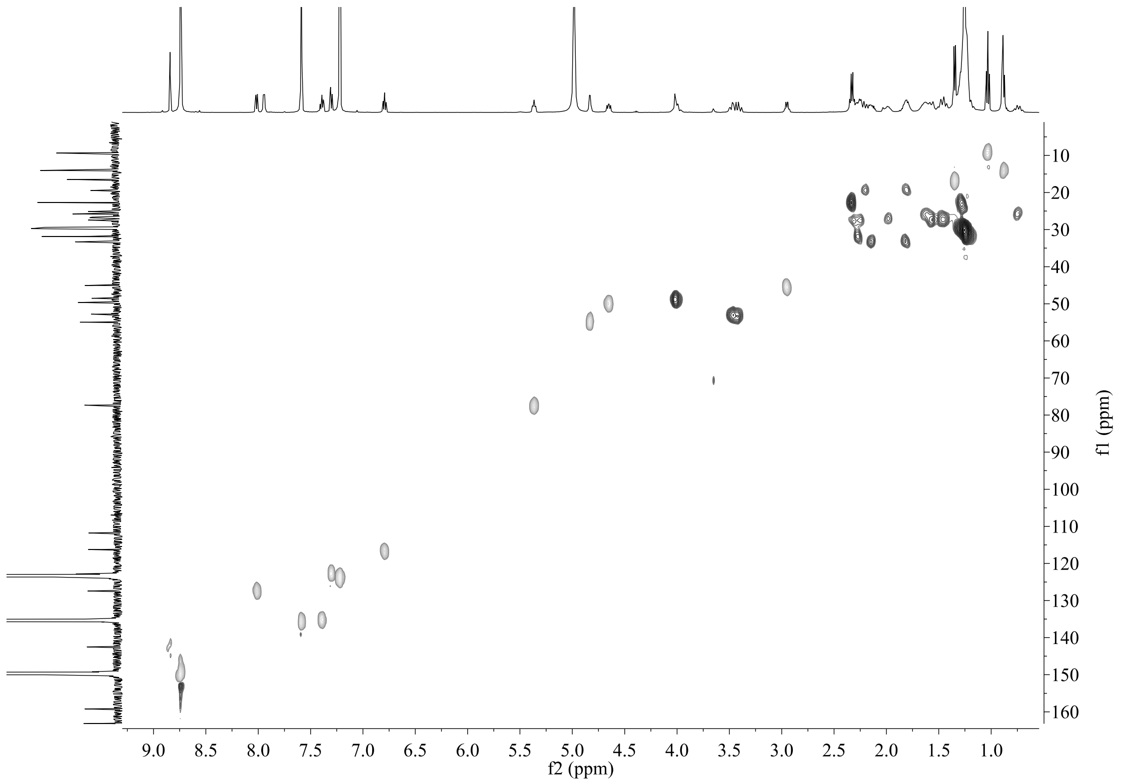

Fig. S6e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **6a**

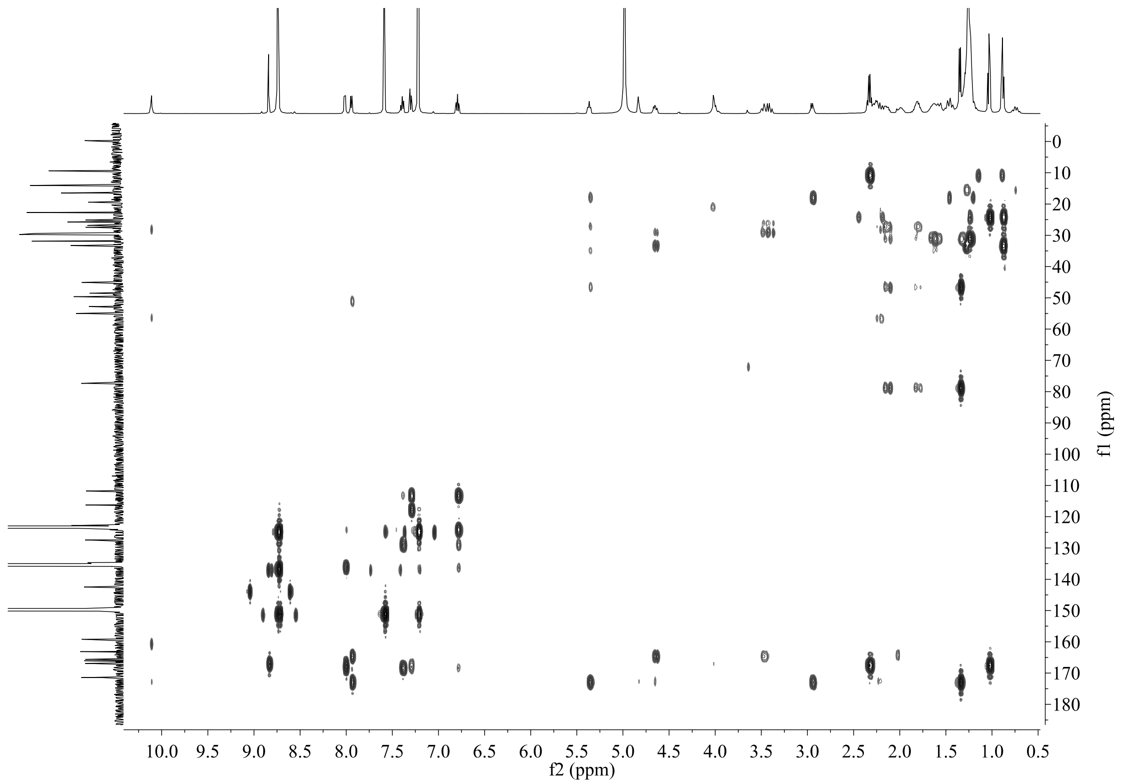

Fig. S6f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **6a**

Table S7 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of compound **7a**

Pos.	δ_C	δ_H, mult (*J* in Hz)	COSY	HMBC
1	112.5			
2	167.6			

3	123.4	7.31, br d (*8.2*)	4	1, 2, 5, 6
4	135.4	7.40, dq (*1.7*, *7.1*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *7.4*)	4, 6	1, 2, 3, 4, 6
6	128.2	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	160.0			
13	NH	10.10, d (*3.1*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.37, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.7	2.96, m	17, 54	19, 54
19	172.2			
20	NH	7.97, d (*7.0*)	21	19, 21, 22
21	50.4	4.73, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.8	1.29-1.21, m	24, 25b, 26a, 26b	22, 24
		0.73, m	24, 25a, 26b	
26	28.2	1.66-1.56, m	25a, 27a	
		1.50-1.43, m	25a, 25b, 27b	
27	32.5	2.39-2.10, m	21, 26a, 27b	
		1.29-1.21, m	27a	
28	27.5	2.39-2.10, m	14, 28b, 29a, 29b	15, 30
29	20.2	2.39-2.10, m	29b, 30b	14, 30
		1.85-1.77, m	28a, 28b, 29a	
30	27.8	2.02-1.95, m	30b, 31	
		1.50-1.43, m	29a, 30a, 31	
31	49.5	4.09, m	30a	29, 30, 33
33	166.8			
34	31.5	2.39-2.10, m	52	33, 52, 53
35	34.0	2.39-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.85-1.77, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.66-1.56, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.29-1.21, m		
38	30.5-30.1[a]	1.29-1.21, m		
39	30.5-30.1[a]	1.29-1.21, m		
40	30.5-30.1[a]	1.29-1.21, m		
41	30.5-30.1[a]	1.29-1.21, m		
42	30.5-30.1[a]	1.29-1.21, m		
43	30.5-30.1[a]	1.29-1.21, m		
44	30.5-30.1[a]	1.29-1.21, m		46
45	32.6	1.29-1.21, m	37-44, 46	43
46	23.4	1.29-1.21, m	45, 47	45
47	14.8	0.88, t (*6.8*)	46	45, 46

52	19.4	1.66-1.56, m	34, 53	33, 34, 53
53	13.8	0.79, t (*7.3*)	52	34, 52
54	17.1	1.37, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

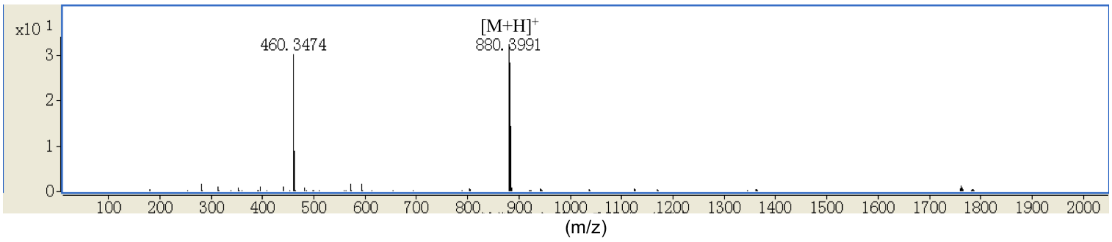

Fig. S7a HR-ESI-MS spectrum of **7a**

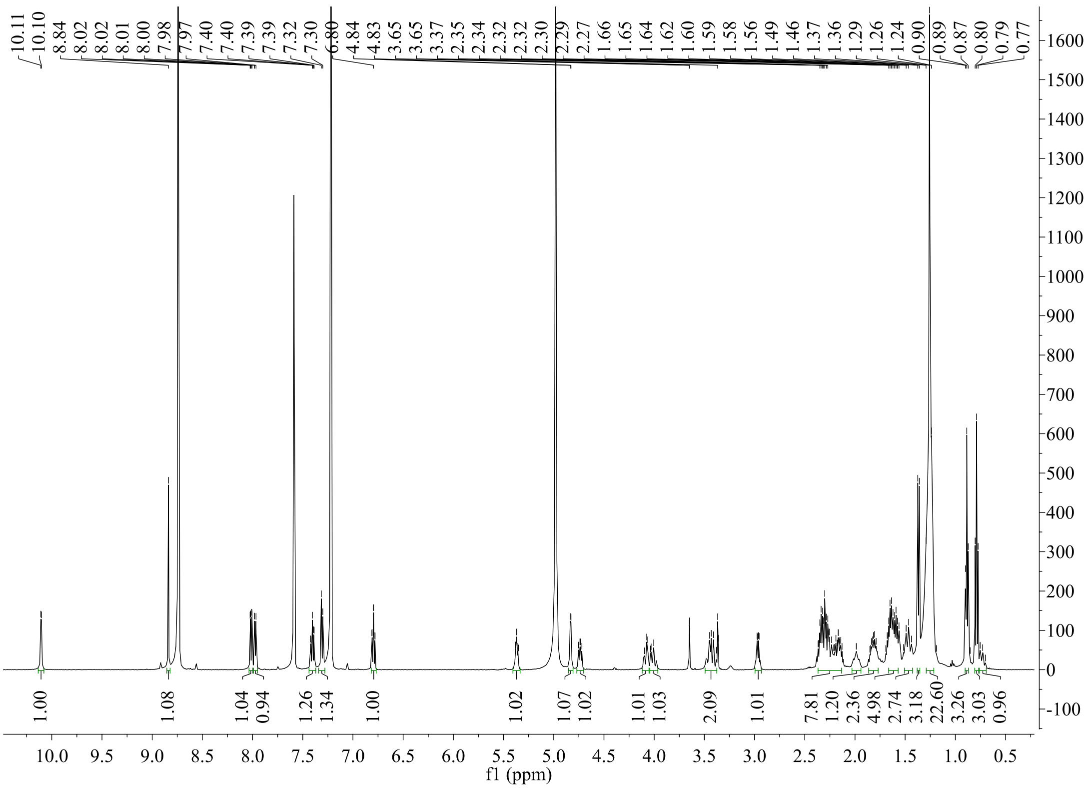

Fig. S7b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **7a**

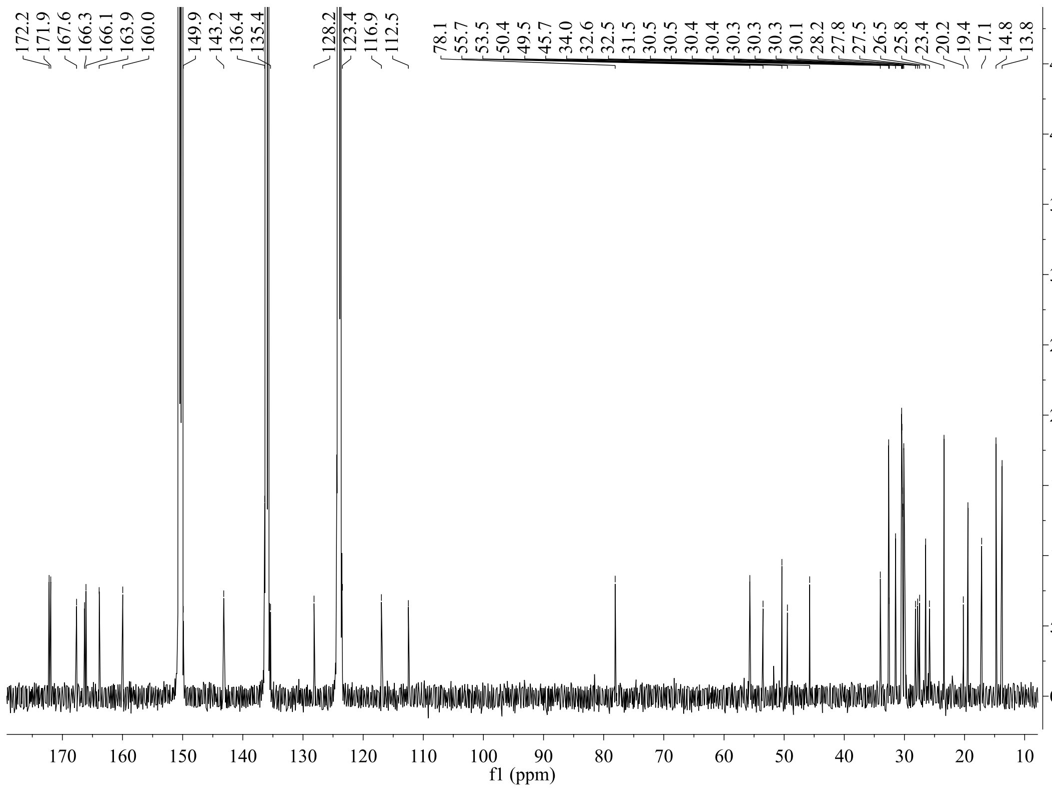

Fig. S7c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **7a**

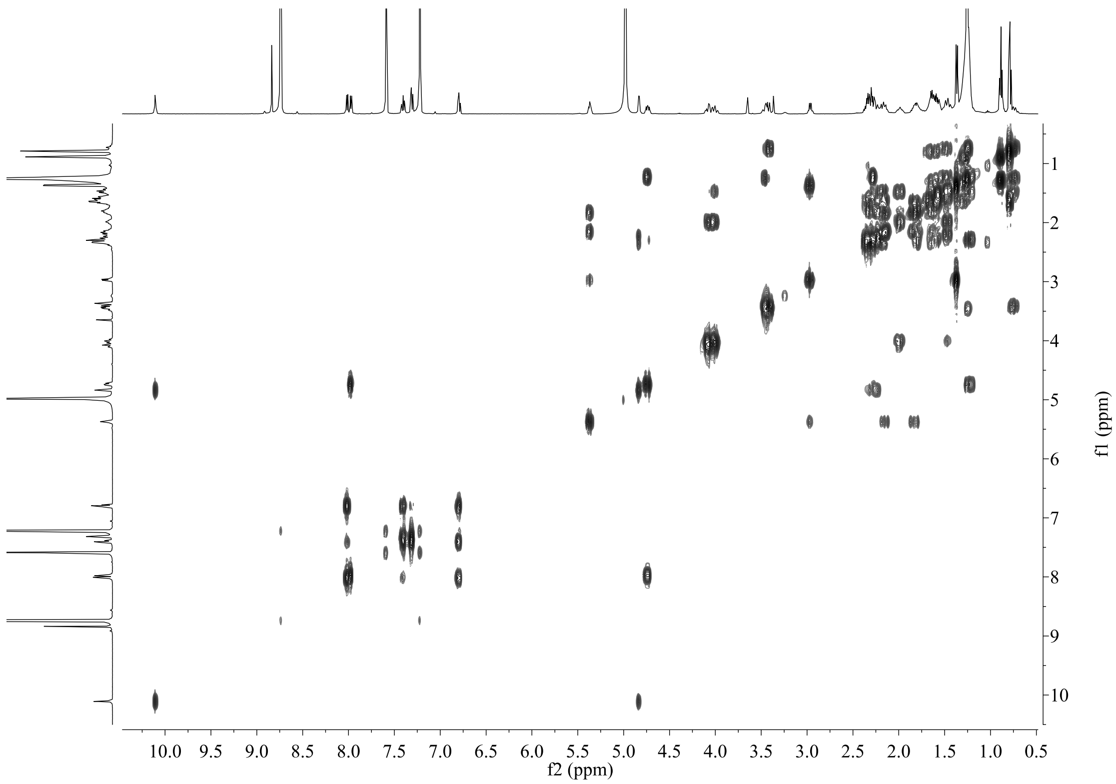

Fig. S7d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **7a**

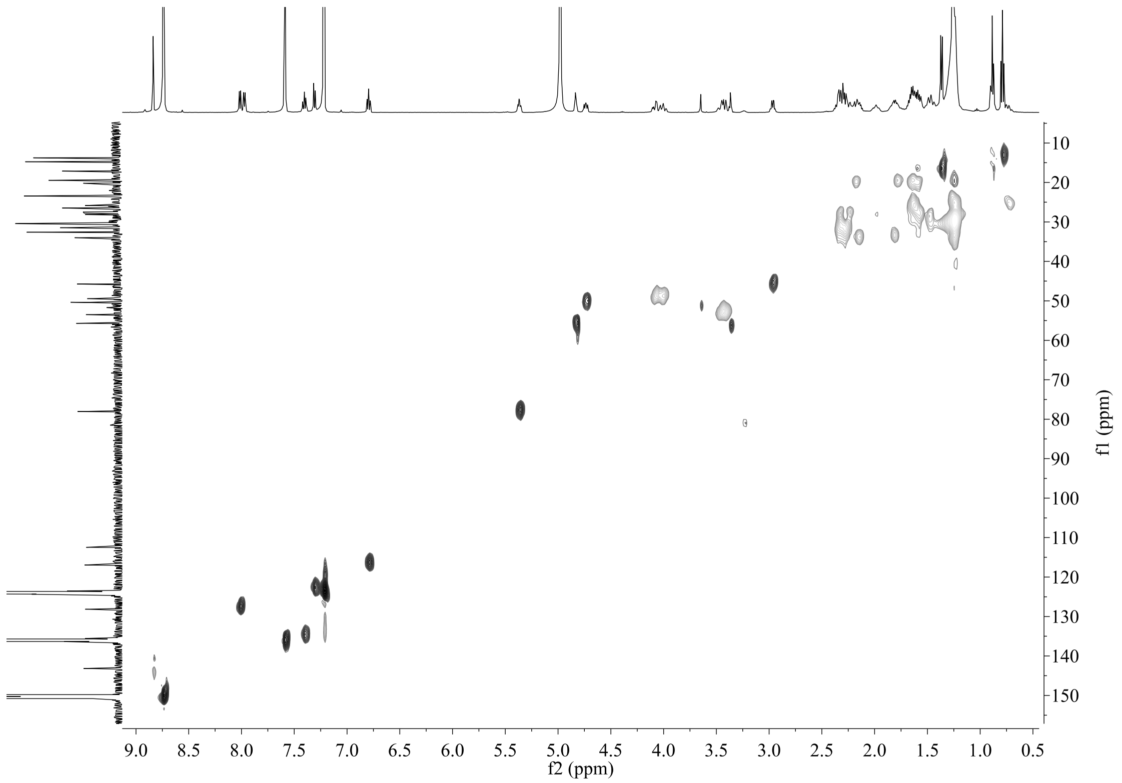

Fig. S7e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **7a**

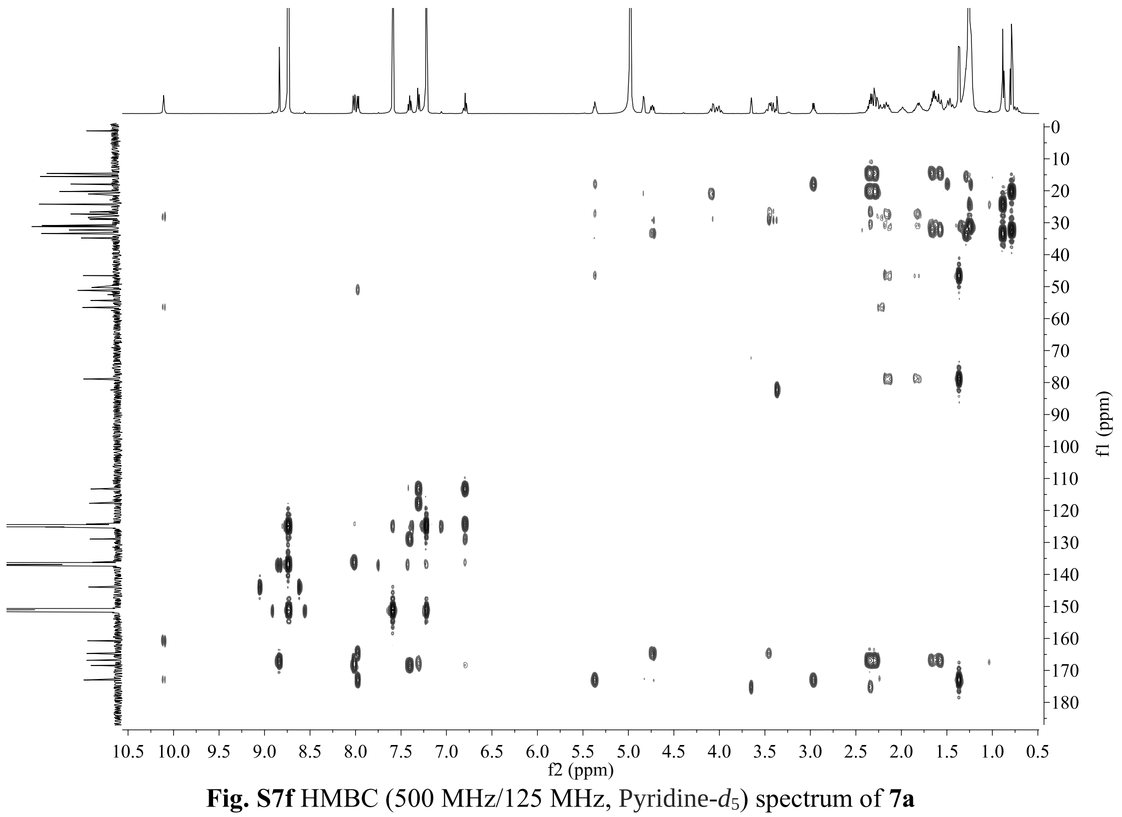

Fig. S7f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **7a**

Table S8 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **8a**

Pos.	δ_C	δ_H, mult (J in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			
2	167.6			

3	123.4	7.30, br d (*8.4*)	4	1, 2, 5, 6
4	135.4	7.39, dq (*1.6*, *7.0*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *6.8*)	4, 6	1, 2, 3, 4, 6
6	128.1	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	159.9			
13	NH	10.11, d (*3.0*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.36, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.8	2.95, m	17, 54	19, 54
19	172.2			
20	NH	7.94, d (*6.9*)	21	19, 21, 22
21	50.4	4.65, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.9	1.33-1.17, m	24, 25b, 26a, 26b	22, 24
		0.74, m	24, 25a, 26b	
26	28.2	1.69-1.53, m	25a, 27a	
		1.52-1.41, m	25a, 25b, 27b	
27	32.5	2.30-2.10, m	21, 26a, 27b	
		1.33-1.17, m	27a	
28	27.4	2.37-2.30, m	14, 28b, 29a, 29b	
		2.30-2.10, m	14, 28a, 29a. 29b	15, 30
29	20.2	2.30-2.10, m	29b, 30b	14, 30
		1.86-1.76, m	28a, 28b, 29a	
30	27.5	2.02-1.94, m	30b, 31	
		1.52-1.41, m	29a, 30a, 31	
31	49.3	4.00, m	30a	29, 30, 33
33	166.8			
34	23.5	2.37-2.30, m	52	33, 52
35	34.0	2.30-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.86-1.76, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.69-1.53, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.33-1.17, m		
38	30.5-30.1[a]	1.33-1.17, m		
39	30.5-30.1[a]	1.33-1.17, m		
40	30.5-30.1[a]	1.33-1.17, m		
41	30.5-30.1[a]	1.33-1.17, m		
42	30.5-30.1[a]	1.33-1.17, m		
43	30.5-30.1[a]	1.33-1.17, m		
44	30.5-30.1[a]	1.33-1.17, m		
45	30.5-30.1[a]	1.33-1.17, m		
46	30.5-30.1[a]	1.33-1.17, m		48

47	32.6	1.33-1.17, m	37-46, 48	45
48	23.4	1.33-1.17, m	47, 49	47
49	14.8	0.88, t (*6.8*)	48	47, 48
52	10.1	1.03, t (*7.4*)	34	33, 34
54	17.2	1.35, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

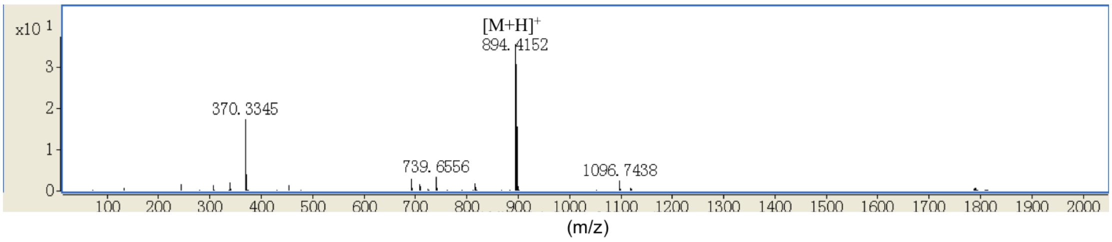

Fig. S8a HR-ESI-MS spectrum of **8a**

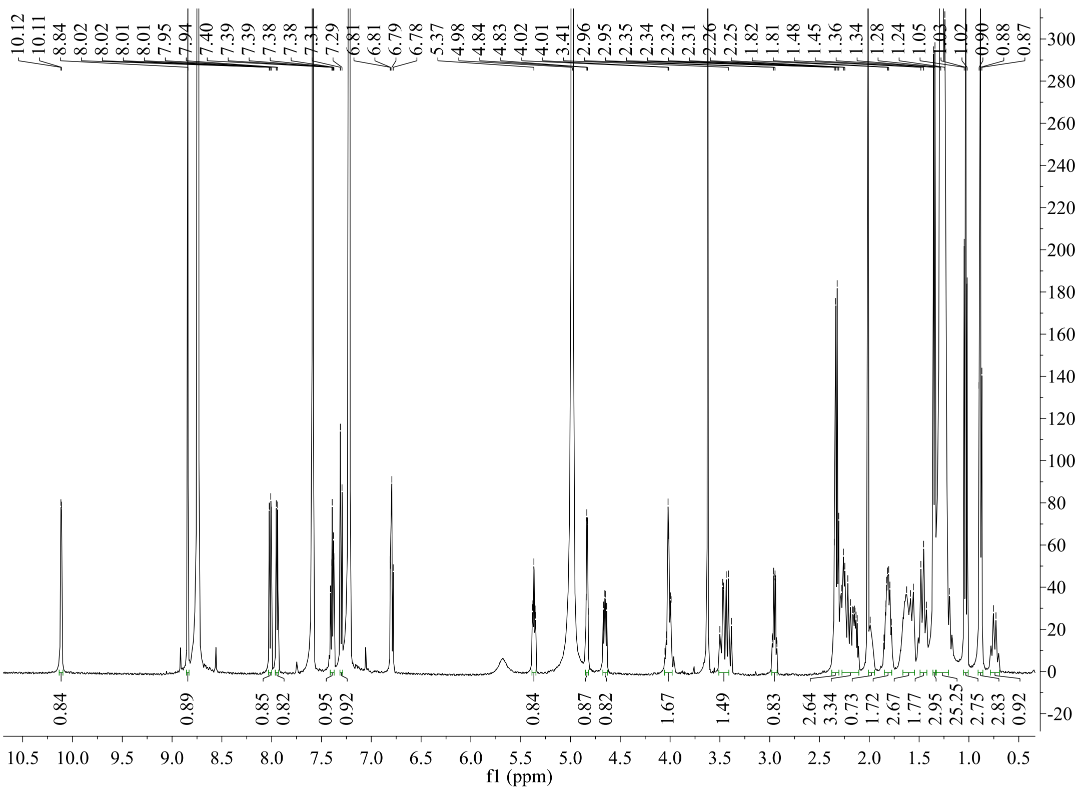

Fig. S8b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **8a**

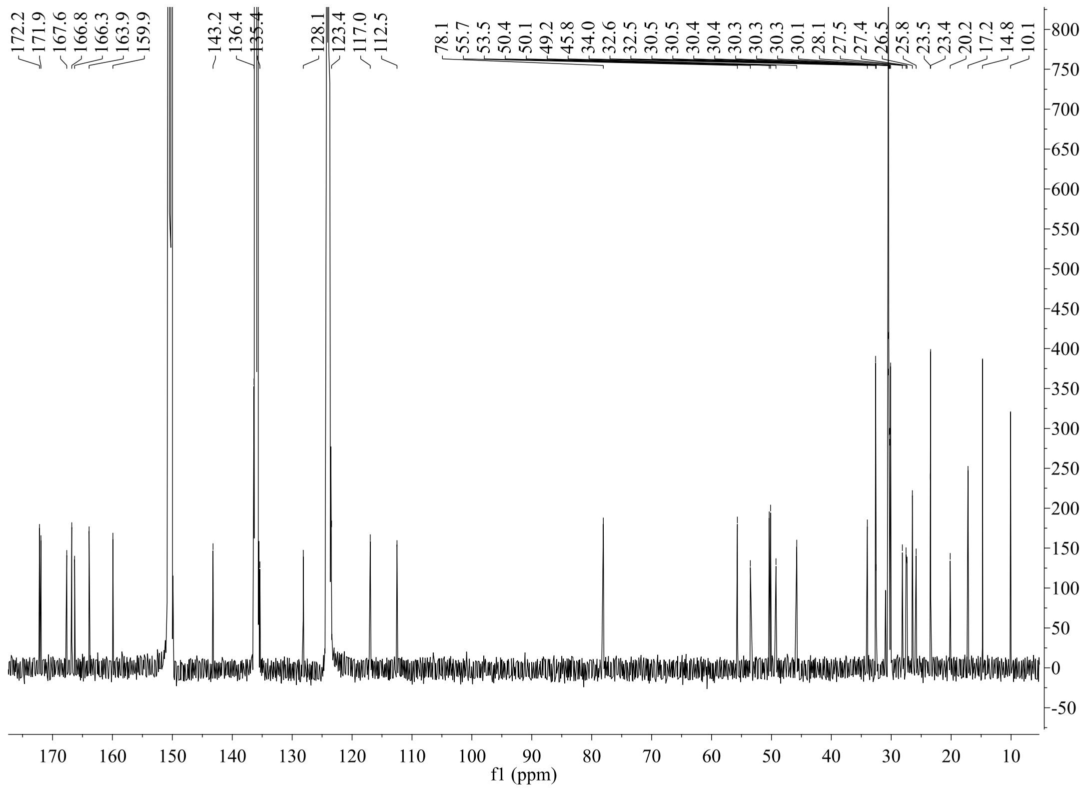

Fig. S8c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **8a**

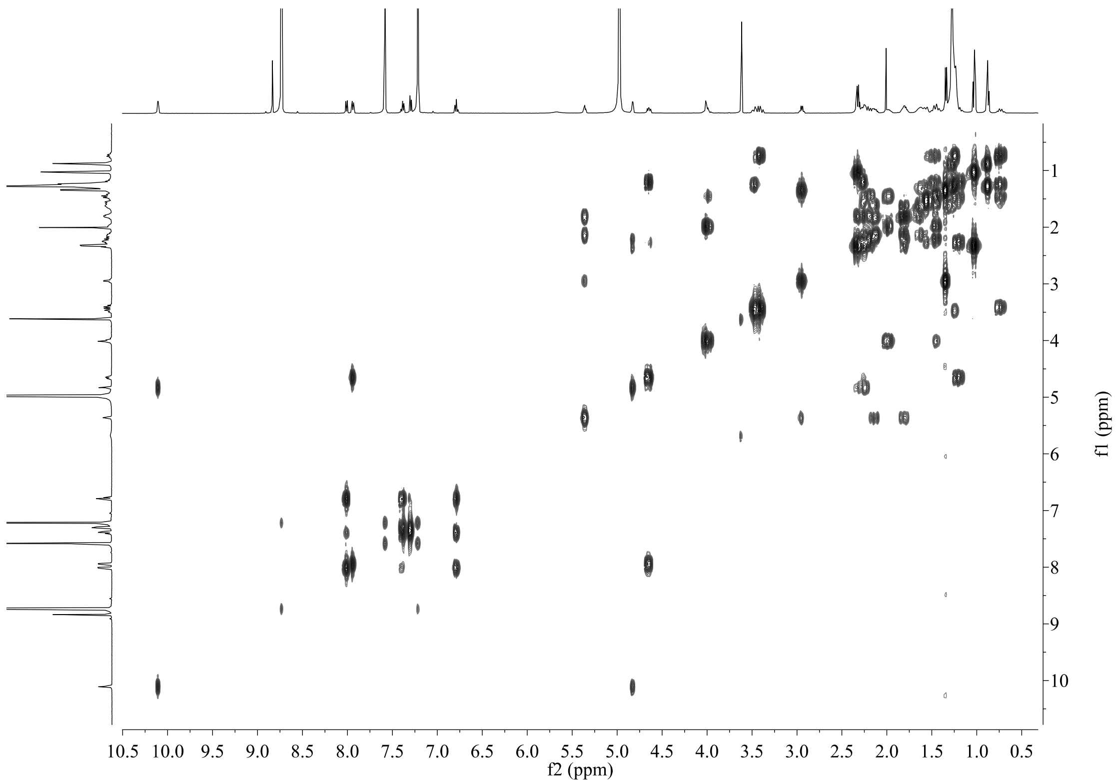

Fig. S8d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **8a**

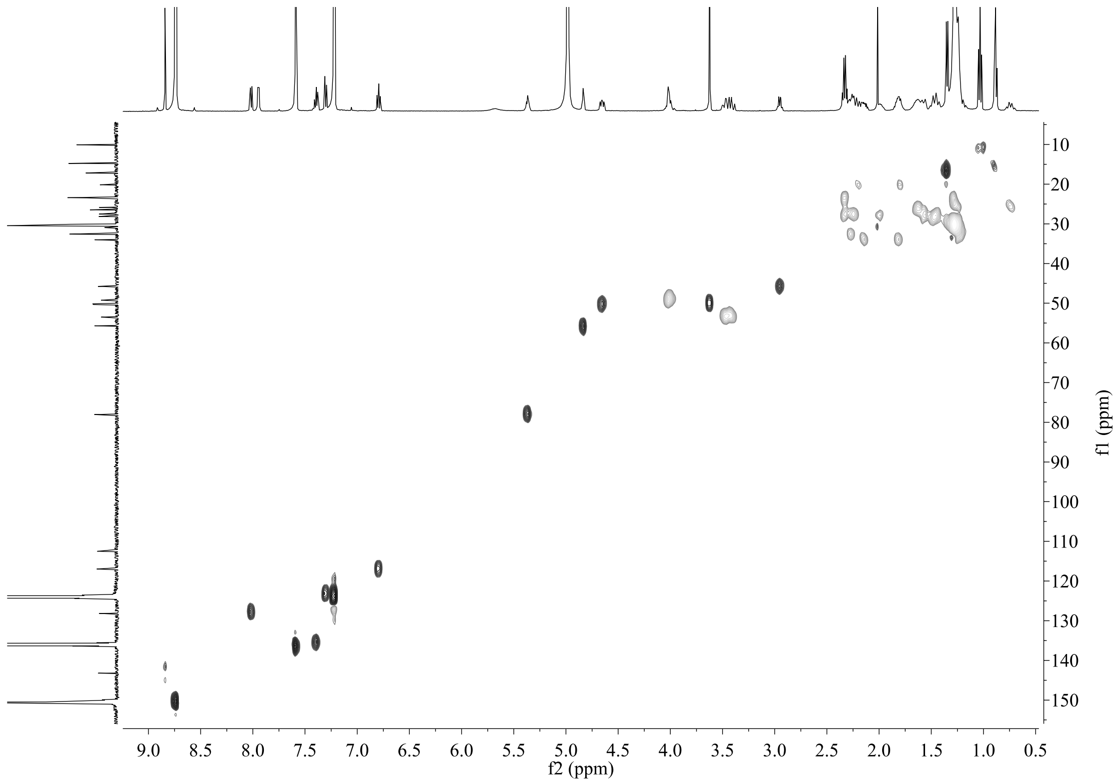

Fig. S8e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **8a**

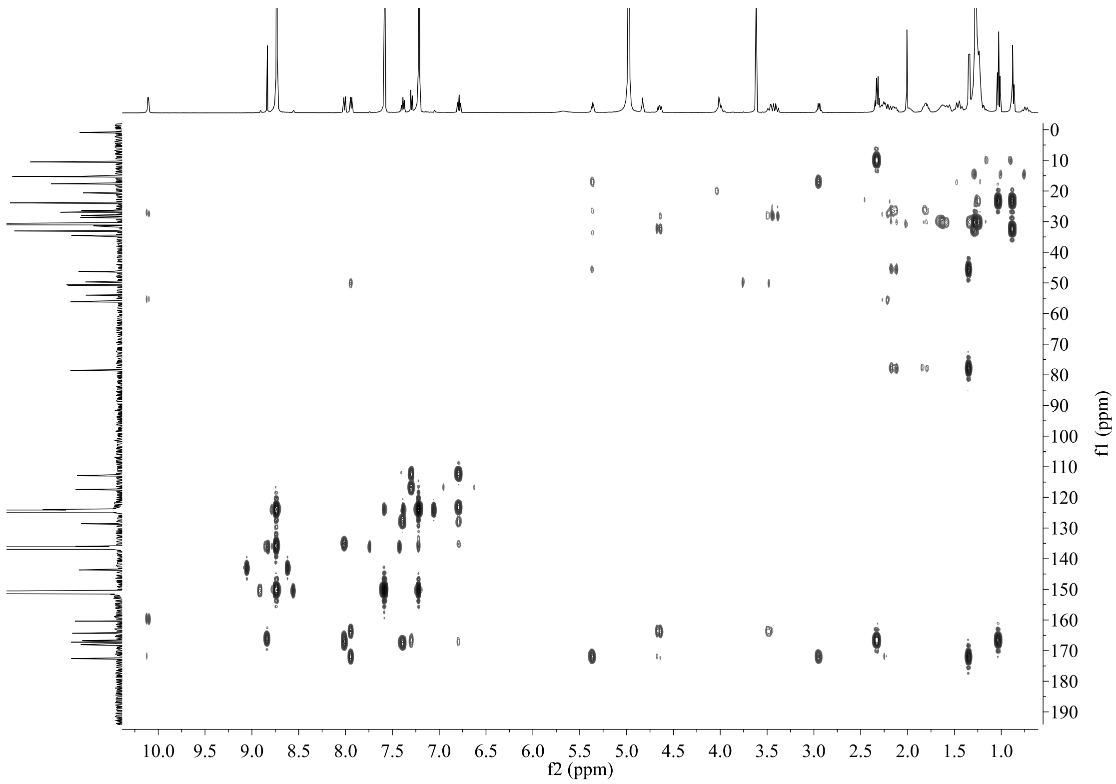

Fig. S8f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **8a**

Table S9 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **9a**

Pos.	δ_C	δ_H, mult (J in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			
2	167.6			

3	123.4	7.31, br d (*8.2*)	4	1, 2, 5, 6
4	135.4	7.40, dq (*1.7*, *7.1*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *7.4*)	4, 6	1, 2, 3, 4, 6
6	128.2	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	160.0			
13	NH	10.10, d (*3.1*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.37, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.7	2.96, m	17, 54	19, 54
19	172.2			
20	NH	7.97, d (*7.0*)	21	19, 21, 22
21	50.4	4.73, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.8	1.30-1.23, m	24, 25b, 26a, 26b	22, 24
		0.73, m	24, 25a, 26b	
26	28.2	1.66-1.56, m	25a, 27a	
		1.50-1.43, m	25a, 25b, 27b	
27	32.5	2.39-2.10, m	21, 26a, 27b	
		1.30-1.23, m	27a	
28	27.5	2.39-2.10, m	14, 28b, 29a, 29b	15, 30
29	20.2	2.39-2.10, m	29b, 30b	14, 30
		1.85-1.77, m	28a, 28b, 29a	
30	27.8	2.02-1.95, m	30b, 31	
		1.50-1.43, m	29a, 30a, 31	
31	49.5	4.09, m	30a	29, 30, 33
33	166.8			
34	31.5	2.39-2.10, m	52	33, 52, 53
35	34.0	2.39-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.85-1.77, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.66-1.56, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.30-1.23, m		
38	30.5-30.1[a]	1.30-1.23, m		
39	30.5-30.1[a]	1.30-1.23, m		
40	30.5-30.1[a]	1.30-1.23, m		
41	30.5-30.1[a]	1.30-1.23, m		
42	30.5-30.1[a]	1.30-1.23, m		
43	30.5-30.1[a]	1.30-1.23, m		
44	30.5-30.1[a]	1.30-1.23, m		
45	30.5-30.1[a]	1.30-1.23, m		
46	30.5-30.1[a]	1.30-1.23, m		48
47	32.6	1.30-1.23, m	37-46, 48	45

48	23.4	1.30-1.23, m	47, 49	47
49	14.8	0.88, t (*6.8*)	48	47, 48
52	19.4	1.66-1.56, m	34, 53	33, 34, 53
53	13.8	0.79, t (*7.3*)	52	34, 52
54	17.1	1.37, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

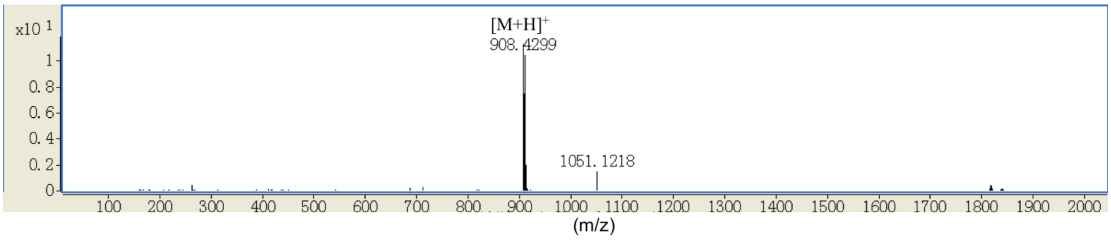

Fig. S9a HR-ESI-MS spectrum of **9a**

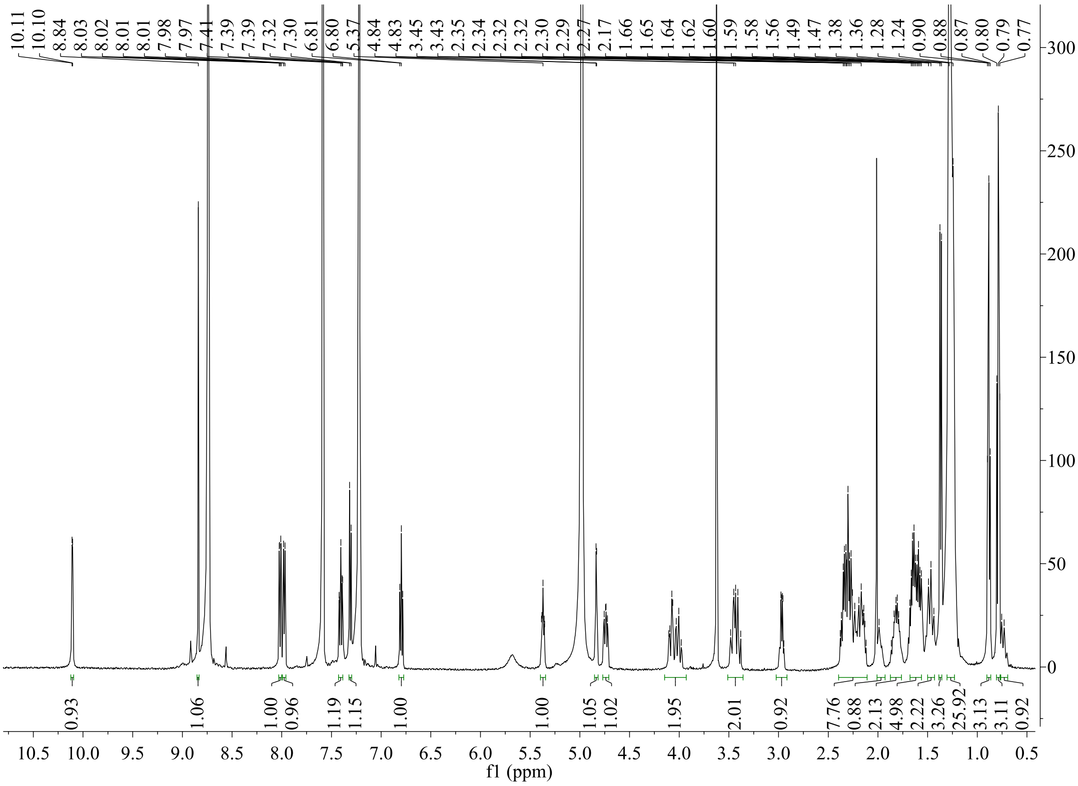

Fig. S9b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **9a**

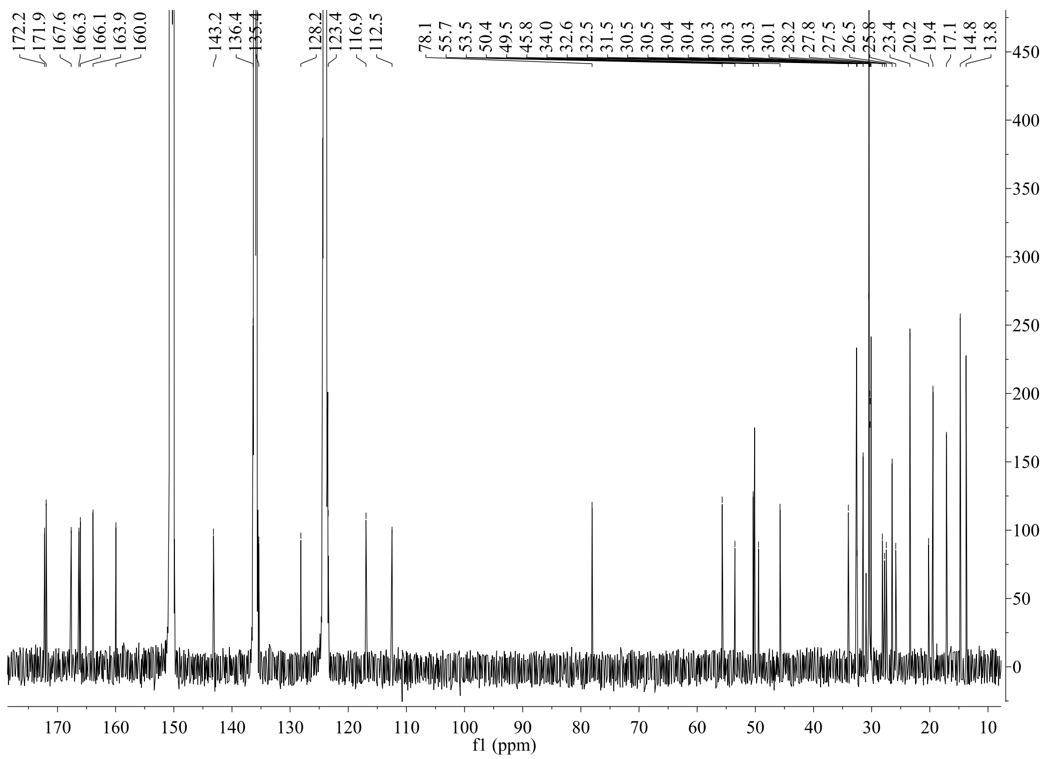

Fig. S9c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **9a**

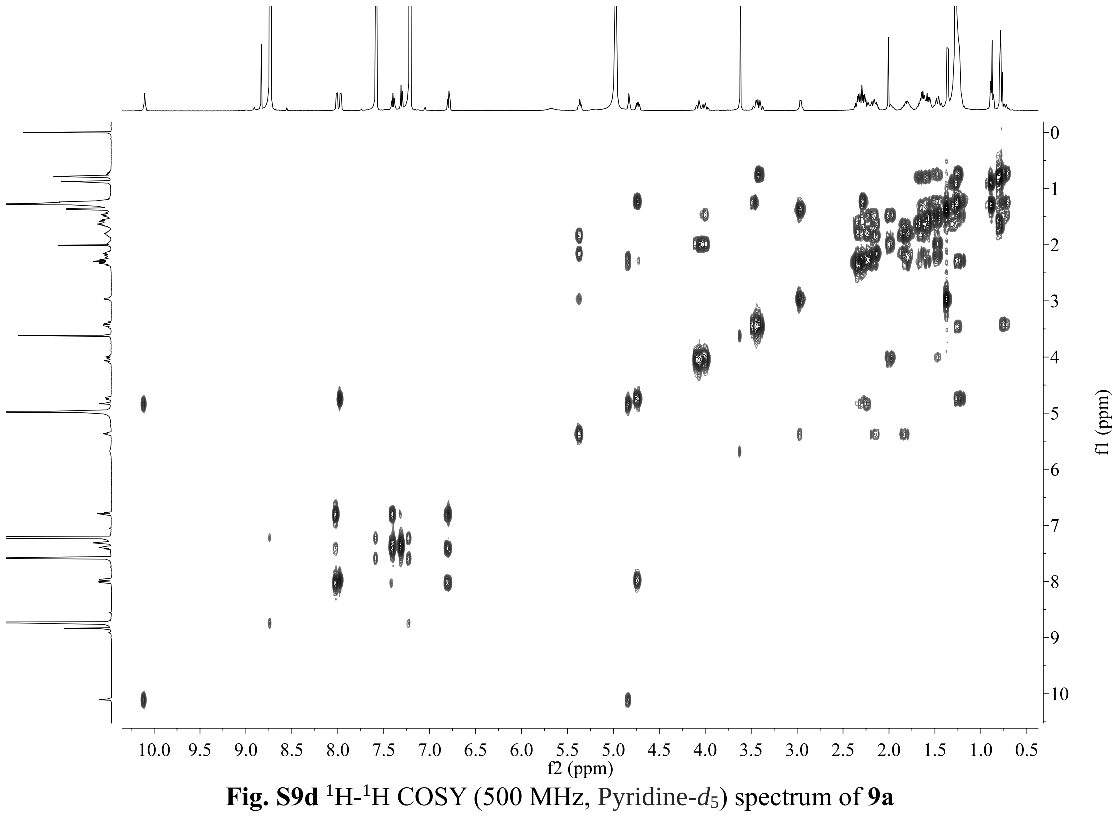

Fig. S9d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **9a**

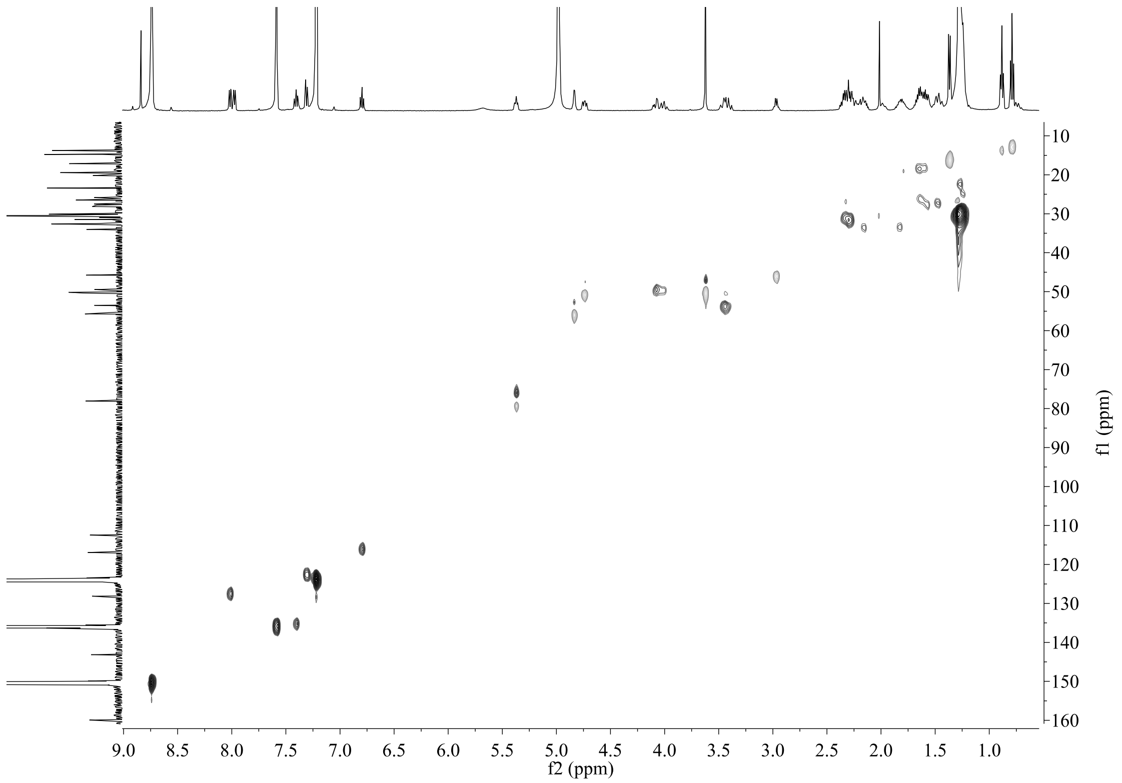

Fig. S9e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **9a**

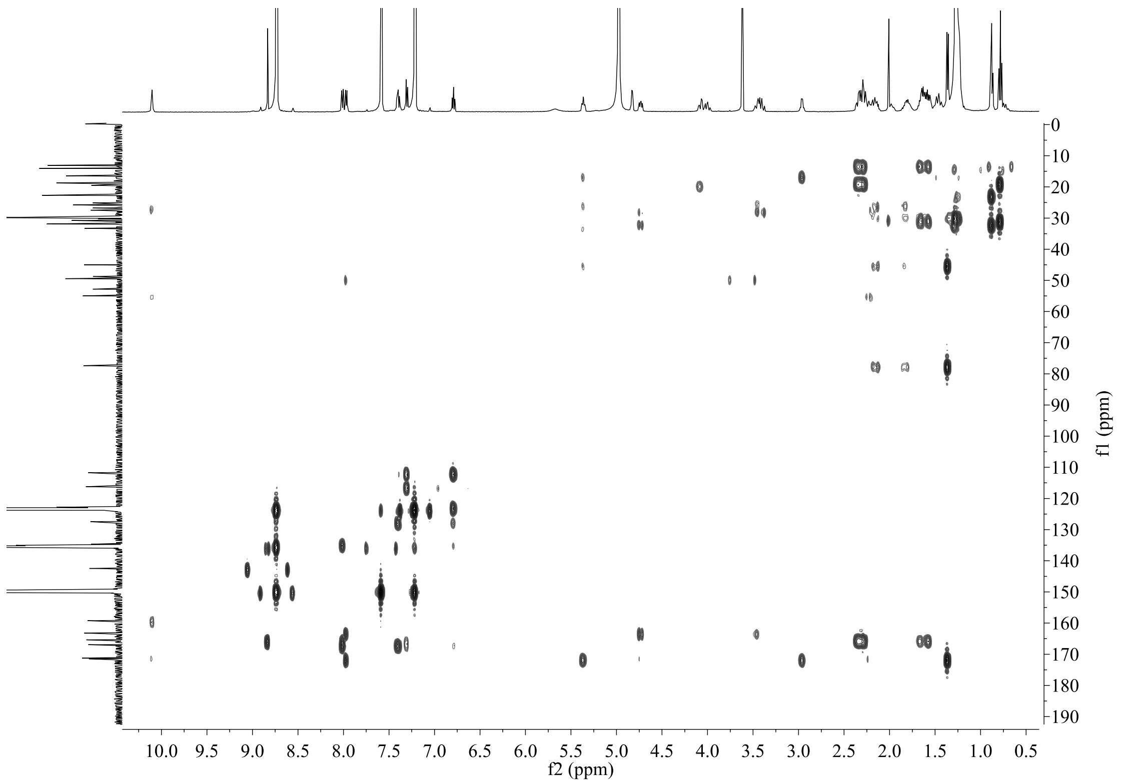

Fig. S9f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **9a**

Table S10 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **10a**

Pos.	δ_C	δ_H, mult (J in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			

2	167.6			
3	123.4	7.30, br d (*8.4*)	4	1, 2, 5, 6
4	135.4	7.39, dq (*1.6*, *7.0*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *6.8*)	4, 6	1, 2, 3, 4, 6
6	128.1	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	159.9			
13	NH	10.11, d (*3.0*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.36, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.8	2.95, m	17, 54	19, 54
19	172.2			
20	NH	7.94, d (*6.9*)	21	19, 21, 22
21	50.4	4.65, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.9	1.31-1.23, m	24, 25b, 26a, 26b	22, 24
		0.74, m	24, 25a, 26b	
26	28.2	1.69-1.53, m	25a, 27a	
		1.52-1.41, m	25a, 25b, 27b	
27	32.5	2.30-2.10, m	21, 26a, 27b	
		1.31-1.23, m	27a	
28	27.4	2.37-2.30, m	14, 28b, 29a, 29b	
		2.30-2.10, m	14, 28a, 29a. 29b	15, 30
29	20.2	2.30-2.10, m	29b, 30b	14, 30
		1.86-1.76, m	28a, 28b, 29a	
30	27.5	2.02-1.94, m	30b, 31	
		1.52-1.41, m	29a, 30a, 31	
31	49.3	4.00, m	30a	29, 30, 33
33	166.8			
34	16.8	2.03, s		33
35	34.0	2.30-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.86-1.76, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.69-1.53, m	35a, 35b	17, 38
37	30.5-30.1	1.31-1.23, m		
38	30.5-30.1	1.31-1.23, m		
39	30.5-30.1	1.31-1.23, m		
40	30.5-30.1	1.31-1.23, m		
41	30.5-30.1	1.31-1.23, m		
42	30.5-30.1	1.31-1.23, m		
43	30.5-30.1	1.31-1.23, m		
44	30.5-30.1	1.31-1.23, m		
45	30.5-30.1	1.31-1.23, m		

46	30.5-30.1	1.31-1.23, m		
47	30.5-30.1	1.31-1.23, m		
48	30.5-30.1	1.31-1.23, m		50
49	32.6	1.31-1.23, m	37-48, 50	47
50	23.4	1.31-1.23, m	49, 51	49
51	14.8	0.88, t (*6.8*)	50	49, 50
54	17.2	1.35, d (*7.3*)	18	17, 18, 19

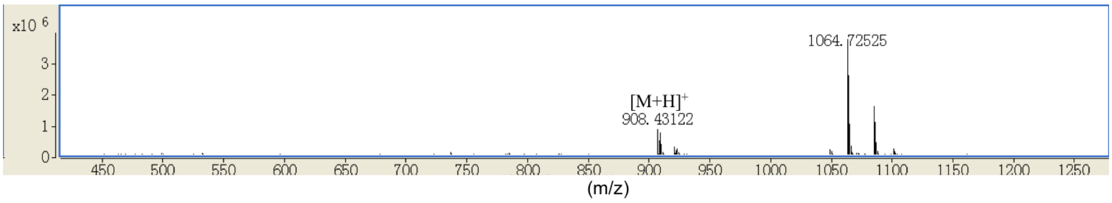

Fig. S10a HR-ESI-MS spectrum of **10a**

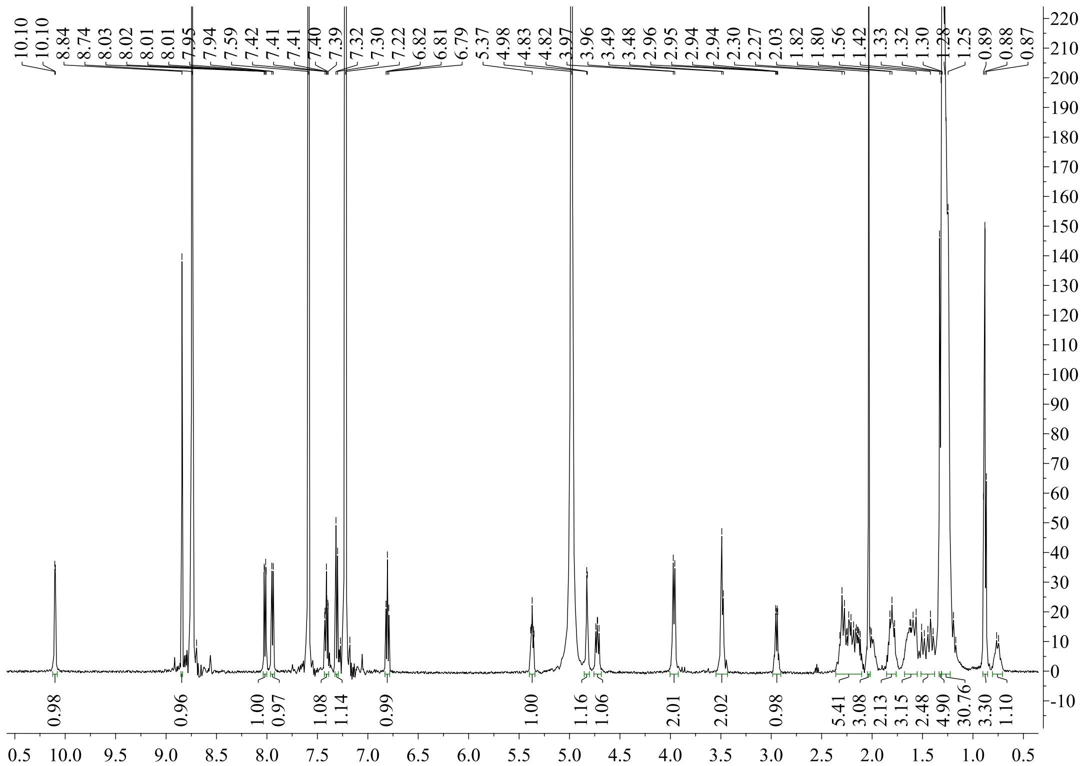

Fig. S10b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **10a**

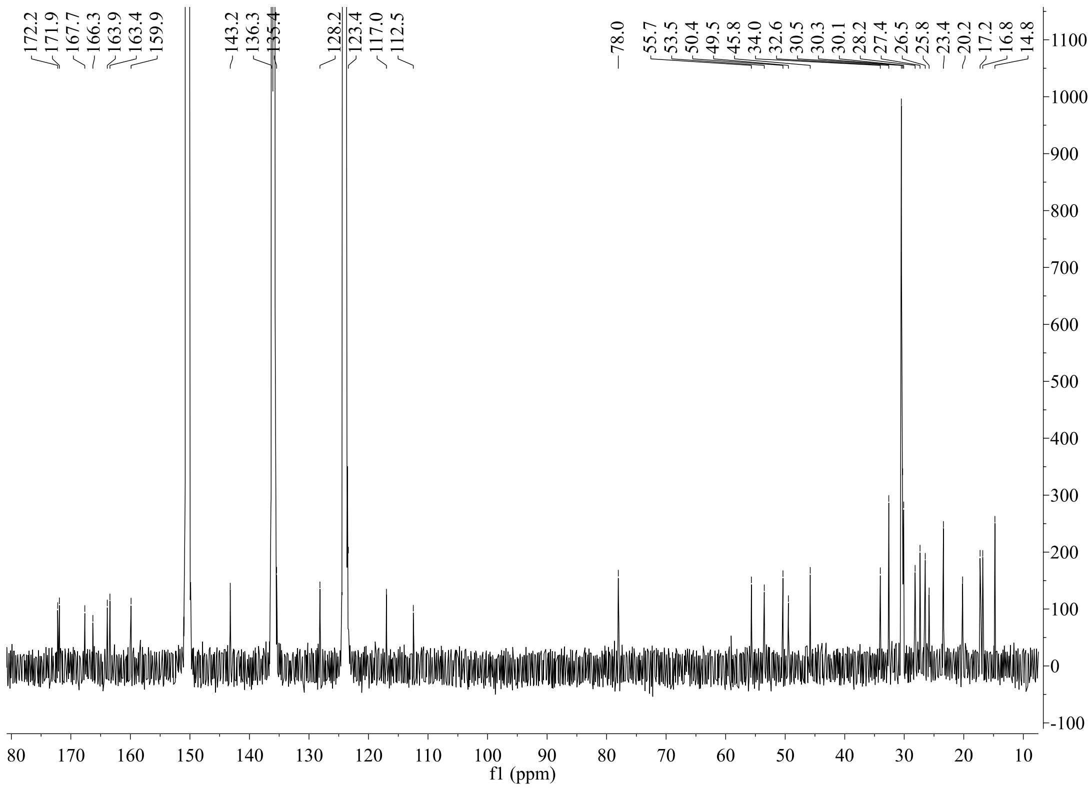

Fig. S10c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **10a**

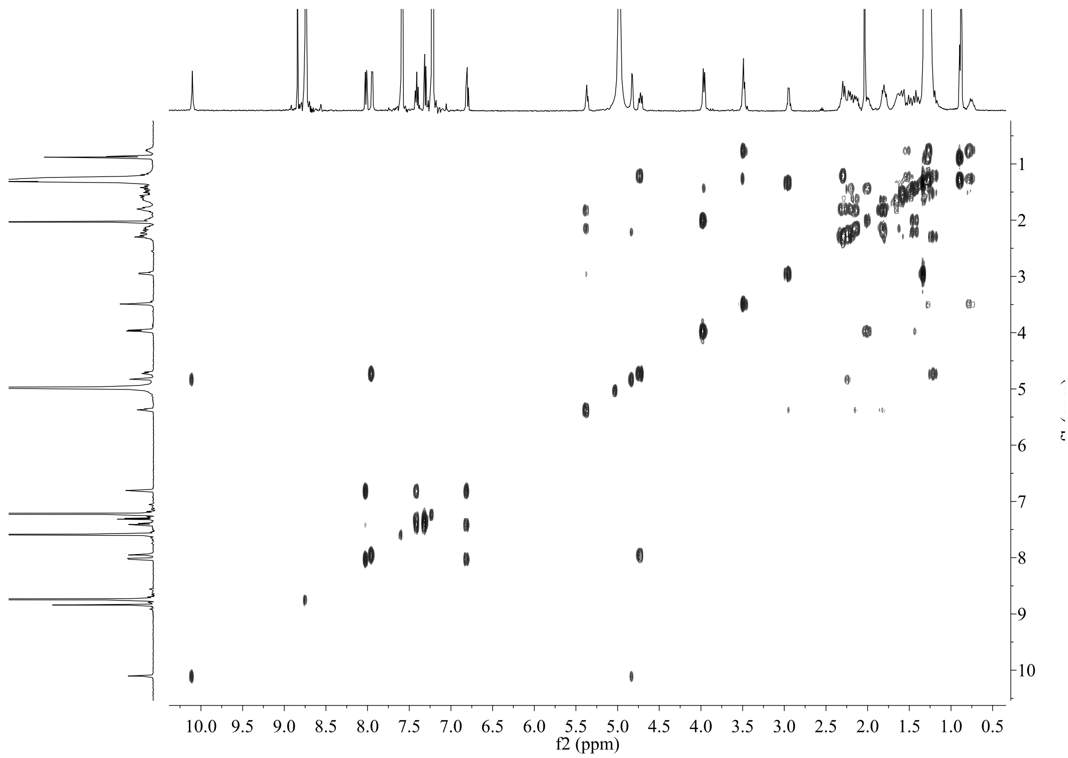

Fig. S10d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **10a**

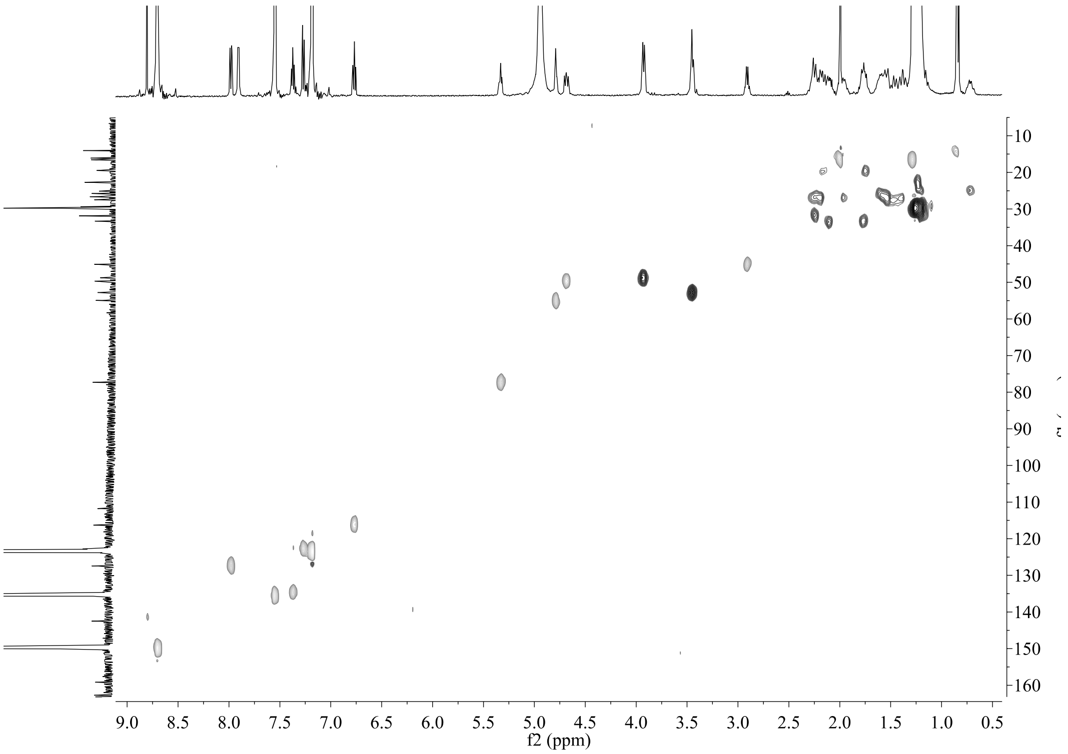

Fig. S10e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **10a**

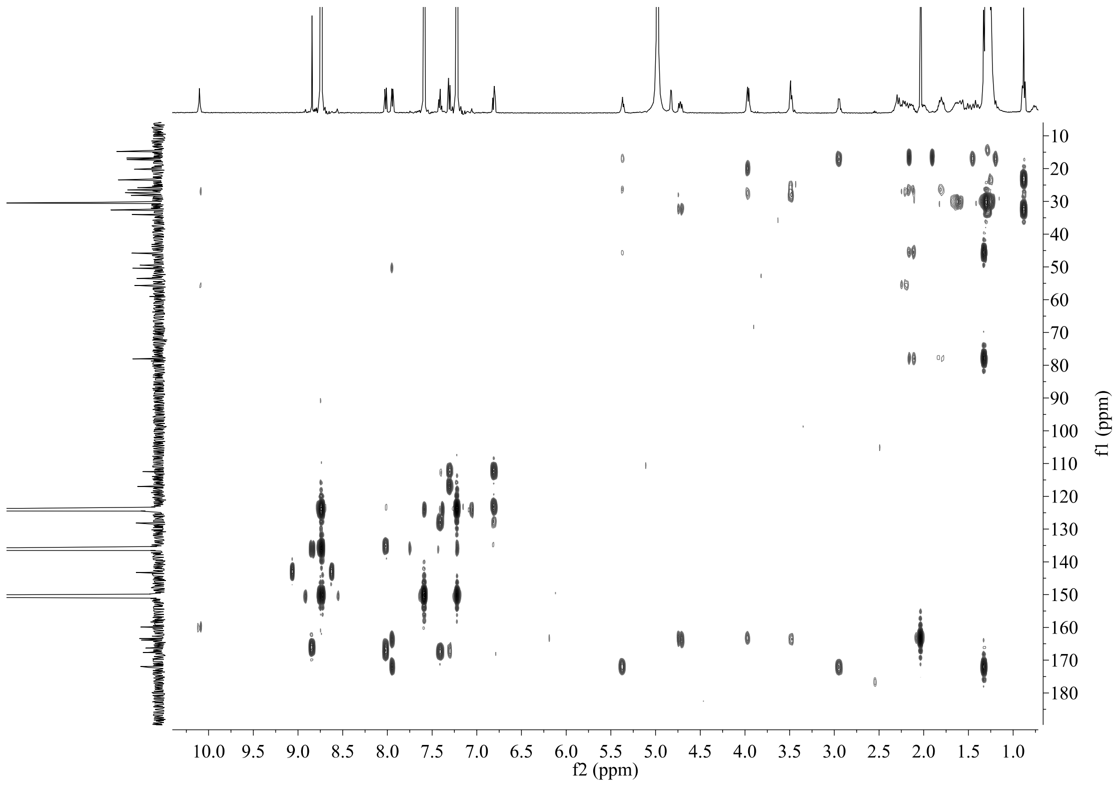

Fig. S10f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **10a**

Table S11 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-d_5) of **11a**

Pos.	δ_C	δ_H, mult (*J* in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			
2	167.6			
3	123.4	7.30, br d (*8.4*)	4	1, 2, 5, 6
4	135.4	7.39, dq (*1.6*, *7.0*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *6.8*)	4, 6	1, 2, 3, 4, 6
6	128.1	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	159.9			
13	NH	10.11, d (*3.0*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.36, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.8	2.95, m	17, 54	19, 54
19	172.2			
20	NH	7.94, d (*6.9*)	21	19, 21, 22
21	50.4	4.65, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.9	1.31-1.23, m	24, 25b, 26a, 26b	22, 24
		0.74, m	24, 25a, 26b	
26	28.2	1.69-1.53, m	25a, 27a	
		1.52-1.41, m	25a, 25b, 27b	
27	32.5	2.30-2.10, m	21, 26a, 27b	
		1.31-1.23, m	27a	
28	27.4	2.37-2.30, m	14, 28b, 29a, 29b	
		2.30-2.10, m	14, 28a, 29a. 29b	15, 30
29	20.2	2.30-2.10, m	29b, 30b	14, 30
		1.86-1.76, m	28a, 28b, 29a	
30	27.5	2.02-1.94, m	30b, 31	
		1.52-1.41, m	29a, 30a, 31	
31	49.3	4.00, m	30a	29, 30, 33
33	166.8			
34	23.5	2.37-2.30, m	52	33, 52
35	34.0	2.30-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.86-1.76, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.69-1.53, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.31-1.23, m		
38	30.5-30.1[a]	1.31-1.23, m		
39	30.5-30.1[a]	1.31-1.23, m		
40	30.5-30.1[a]	1.31-1.23, m		
41	30.5-30.1[a]	1.31-1.23, m		
42	30.5-30.1[a]	1.31-1.23, m		

43	30.5-30.1[a]	1.31-1.23, m		
44	30.5-30.1[a]	1.31-1.23, m		
45	30.5-30.1[a]	1.31-1.23, m		
46	30.5-30.1[a]	1.31-1.23, m		
47	30.5-30.1[a]	1.31-1.23, m		
48	30.5-30.1[a]	1.31-1.23, m		50
49	32.6	1.31-1.23, m	37-48, 50	47
50	23.4	1.31-1.23, m	49, 51	49
51	14.8	0.88, t (*6.8*)	50	49, 50
52	10.1	1.03, t (*7.4*)	34	33, 34
54	17.2	1.35, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

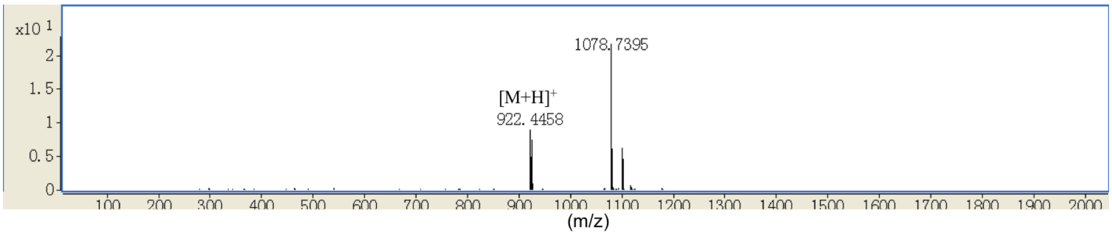

Fig. S11a HR-ESI-MS spectrum of **11a**

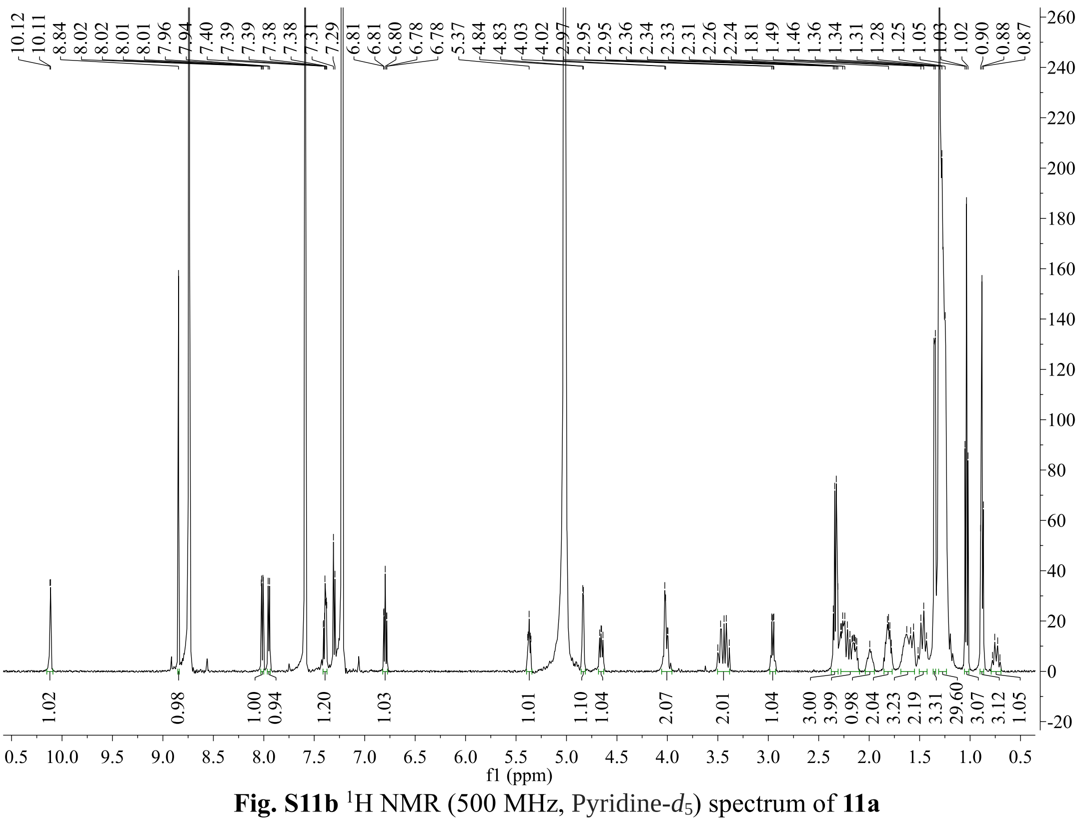

Fig. S11b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **11a**

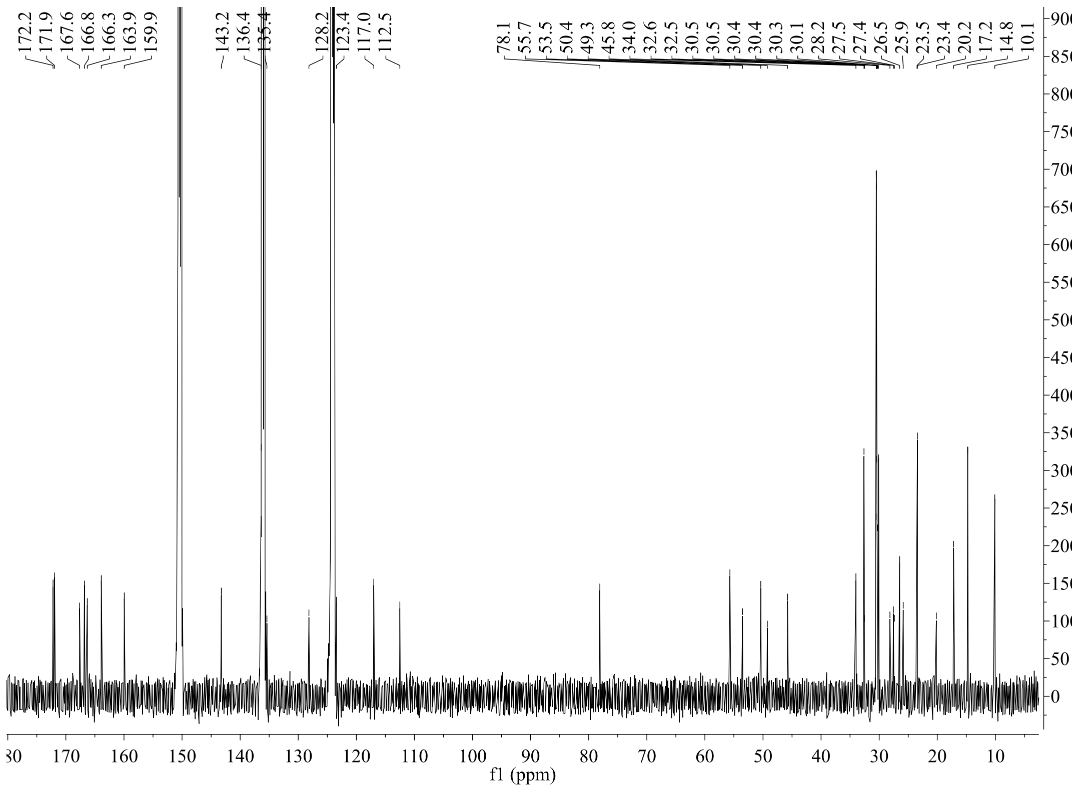

Fig. S11c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **11a**

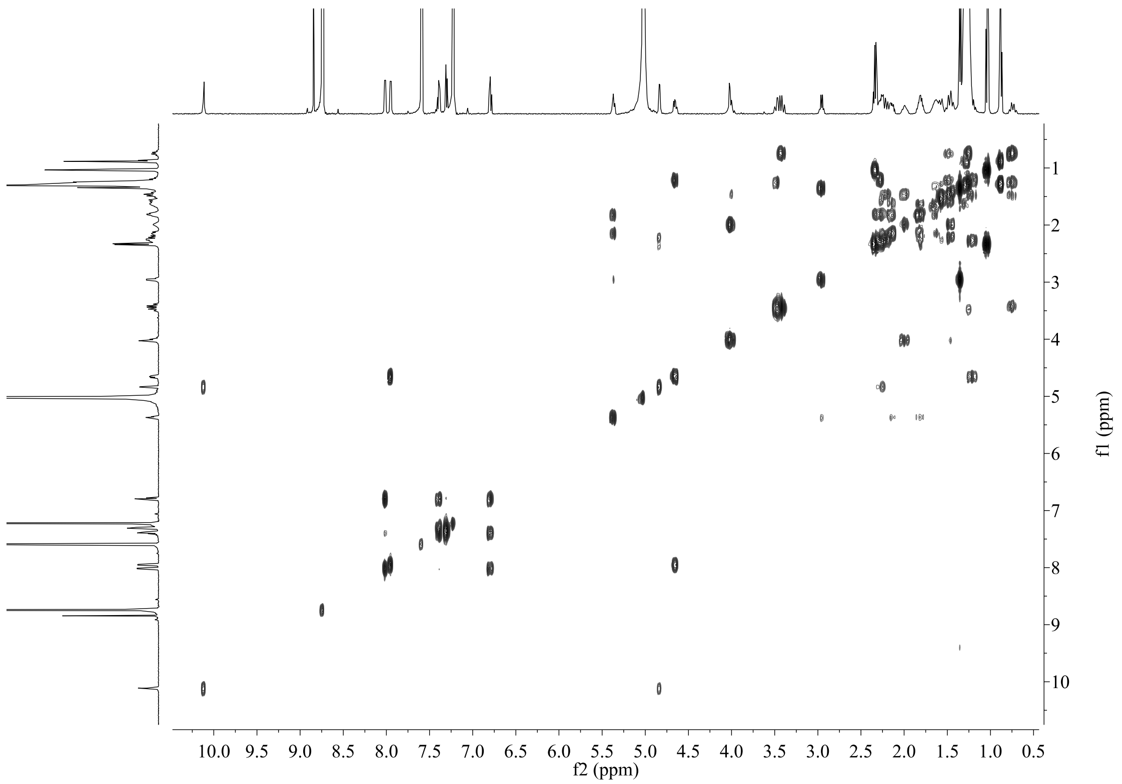

Fig. S11d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **11a**

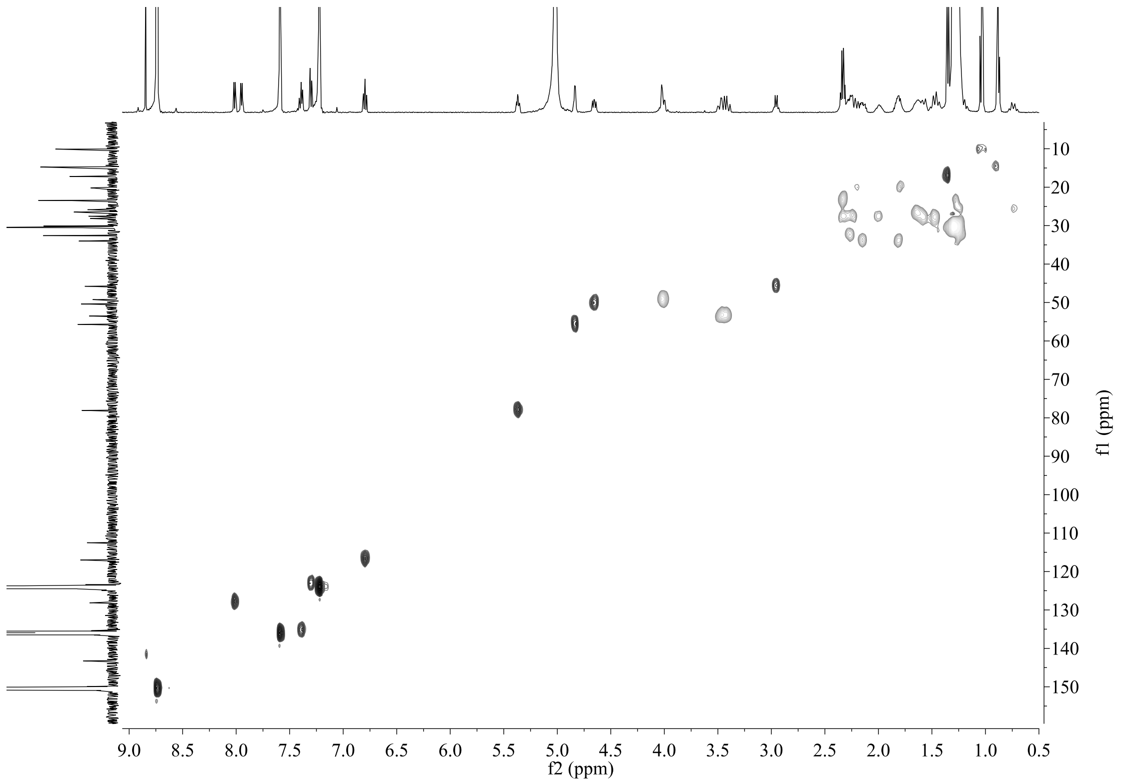

Fig. S11e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **11a**

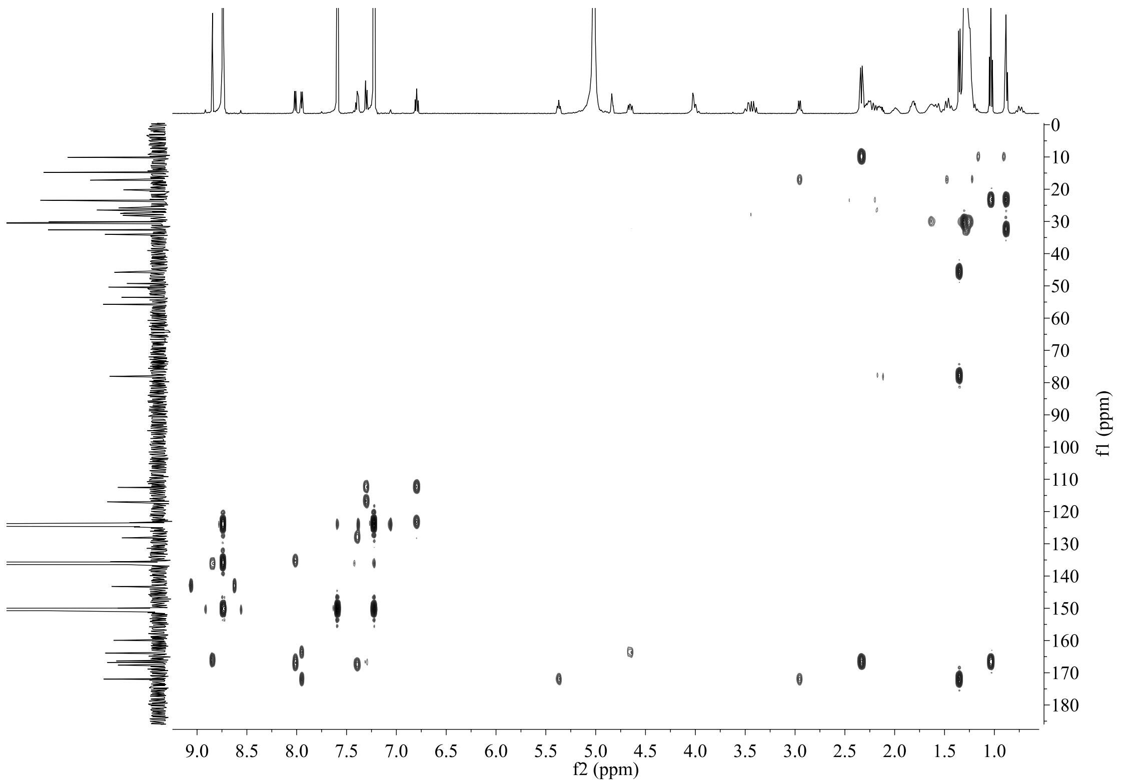

Fig. S11f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **11a**

Table S12 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, Pyridine-*d5*) of **12a**

Pos.	δ_C	δ_H, mult (J in Hz)	^{1}H-^{1}H COSY	HMBC
1	112.5			

2	167.6			
3	123.4	7.31, br d (*8.2*)	4	1, 2, 5, 6
4	135.4	7.40, dq (*1.7*, *7.1*)	3, 5, 6	1, 2, 3, 5, 6
5	117.0	6.79, dq (*0.8*, *7.4*)	4, 6	1, 2, 3, 4, 6
6	128.2	8.01, dd (*1.5*, *8.0*)	4, 5	2, 3, 4
7	166.3			
9	143.2	8.84, s		7, 10
10	136.4			
12	160.0			
13	NH	10.10, d (*3.1*)	14	12, 14, 15, 28
14	55.7	4.83, m	13, 28b	15, 29
15	171.9			
17	78.1	5.37, m	18, 35a, 35b	18, 19, 35, 36, 54
18	45.7	2.96, m	17, 54	19, 54
19	172.2			
20	NH	7.97, d (*7.0*)	21	19, 21, 22
21	50.4	4.73, m	20, 27b	19, 22, 26, 27
22	163.9			
24	53.5	3.45, m	25a, 25b	22, 25, 26
25	25.8	1.32-1.23, m	24, 25b, 26a, 26b	22, 24
		0.73, m	24, 25a, 26b	
26	28.2	1.66-1.56, m	25a, 27a	
		1.50-1.43, m	25a, 25b, 27b	
27	32.5	2.39-2.10, m	21, 26a, 27b	
		1.32-1.23, m	27a	
28	27.5	2.39-2.10, m	14, 28b, 29a, 29b	15, 30
29	20.2	2.39-2.10, m	29b, 30b	14, 30
		1.85-1.77, m	28a, 28b, 29a	
30	27.8	2.02-1.95, m	30b, 31	
		1.50-1.43, m	29a, 30a, 31	
31	49.5	4.09, m	30a	29, 30, 33
33	166.8			
34	31.5	2.39-2.10, m	52	33, 52, 53
35	34.0	2.39-2.10, m	17, 35b, 36	17, 18, 36, 37
		1.85-1.77, m	17, 35a, 36	17, 18, 36, 37
36	26.5	1.66-1.56, m	35a, 35b	17, 38
37	30.5-30.1[a]	1.32-1.23, m		
38	30.5-30.1[a]	1.32-1.23, m		
39	30.5-30.1[a]	1.32-1.23, m		
40	30.5-30.1[a]	1.32-1.23, m		
41	30.5-30.1[a]	1.32-1.23, m		
42	30.5-30.1[a]	1.32-1.23, m		
43	30.5-30.1[a]	1.32-1.23, m		
44	30.5-30.1[a]	1.32-1.23, m		
45	30.5-30.1[a]	1.32-1.23, m		
46	30.5-30.1[a]	1.32-1.23, m		

47	30.5-30.1[a]	1.32-1.23, m		
48	30.5-30.1[a]	1.32-1.23, m		50
49	32.6	1.32-1.23, m	37-48, 50	47
50	23.4	1.32-1.23, m	49, 51	49
51	14.8	0.88, t (*6.8*)	50	49, 50
52	19.4	1.66-1.56, m	34, 53	33, 34, 53
53	13.8	0.79, t (*7.3*)	52	34, 52
54	17.1	1.37, d (*7.3*)	18	17, 18, 19

[a] Overlapped each other.

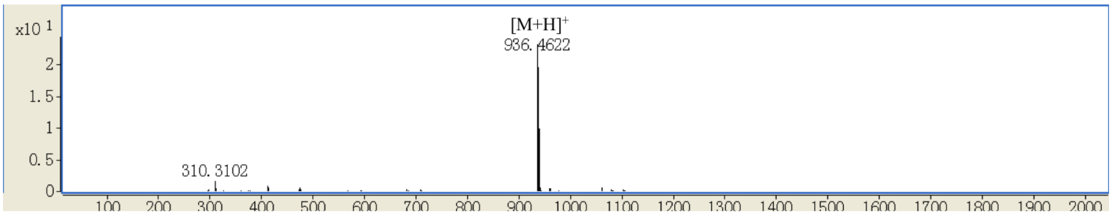

Fig. S12a HR-ESI-MS spectrum of **12a**

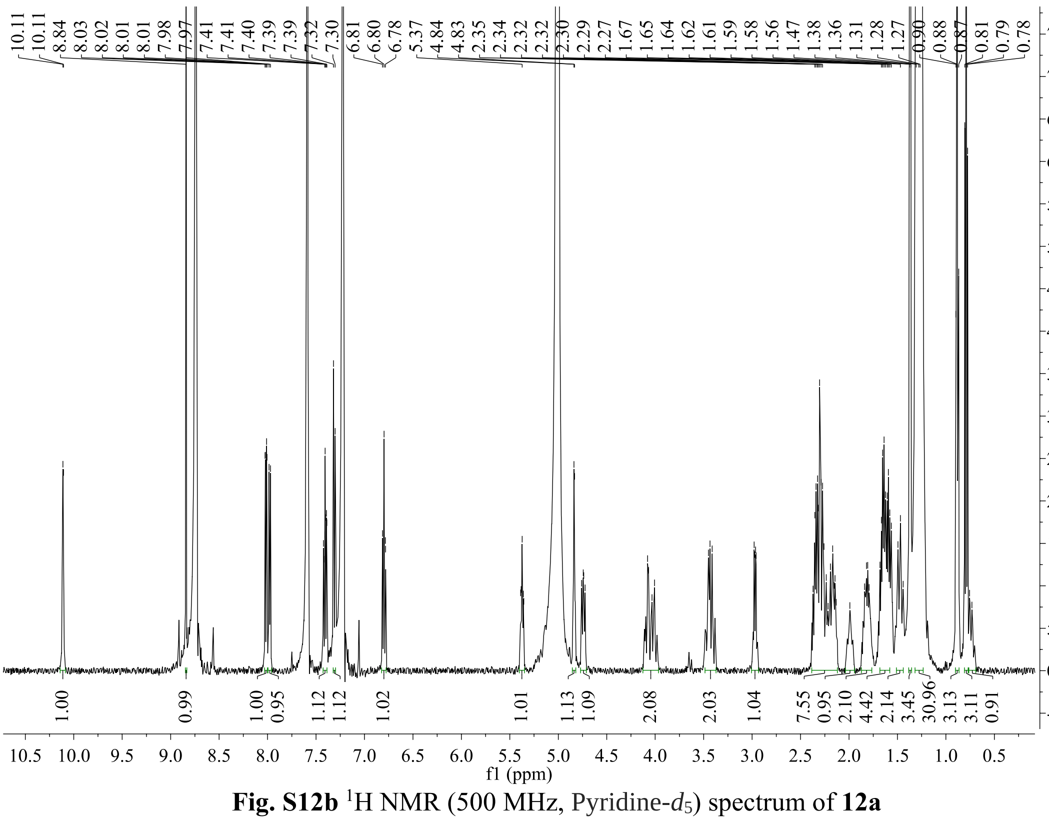

Fig. S12b ^{1}H NMR (500 MHz, Pyridine-d_5) spectrum of **12a**

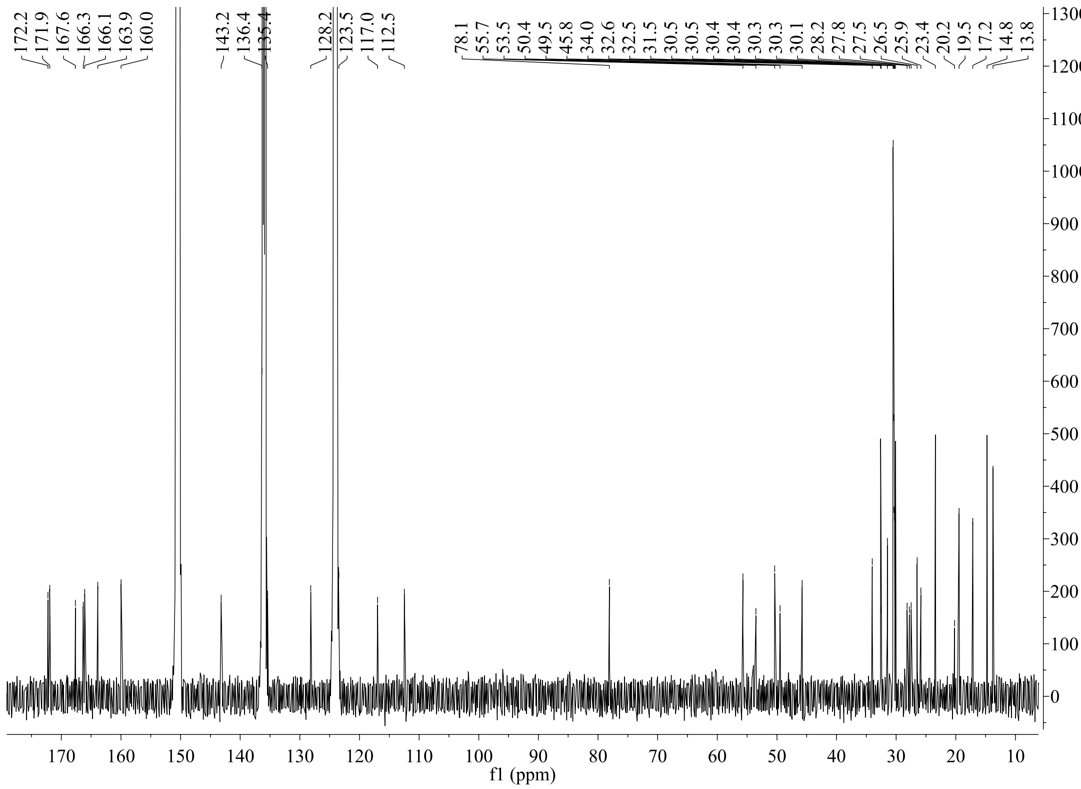

Fig. S12c ^{13}C NMR (125 MHz, Pyridine-d_5) spectrum of **12a**

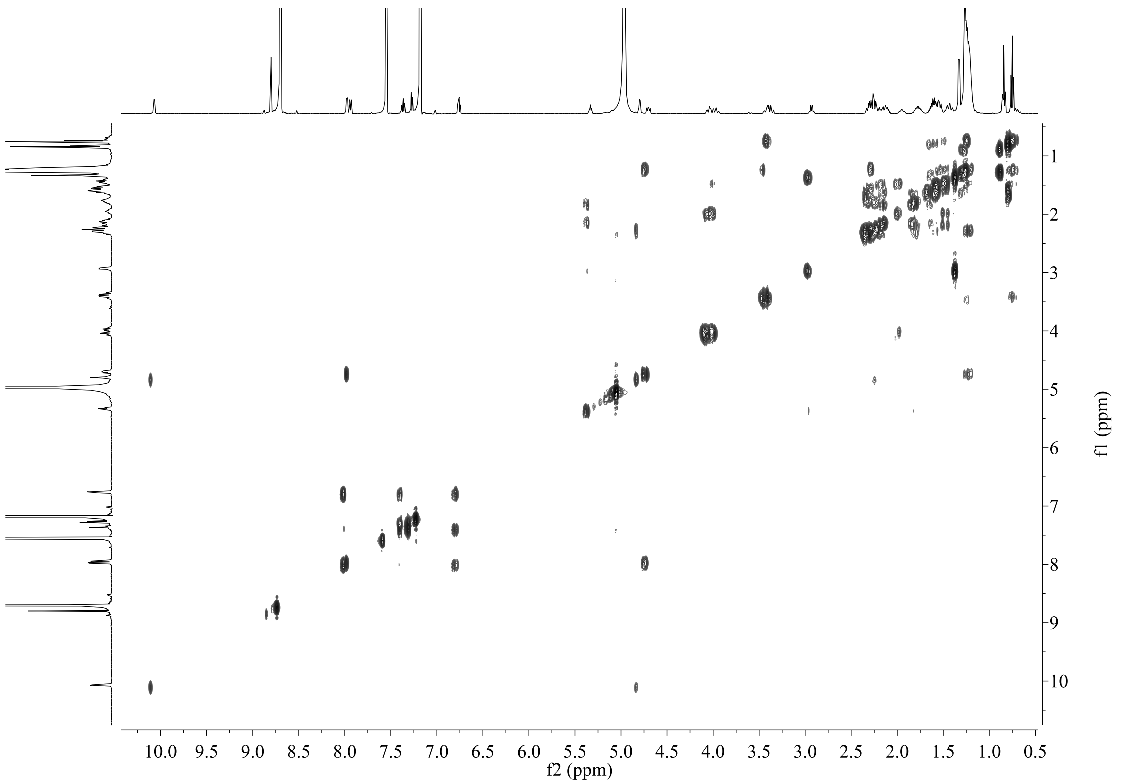

Fig. S12d ^{1}H-^{1}H COSY (500 MHz, Pyridine-d_5) spectrum of **12a**

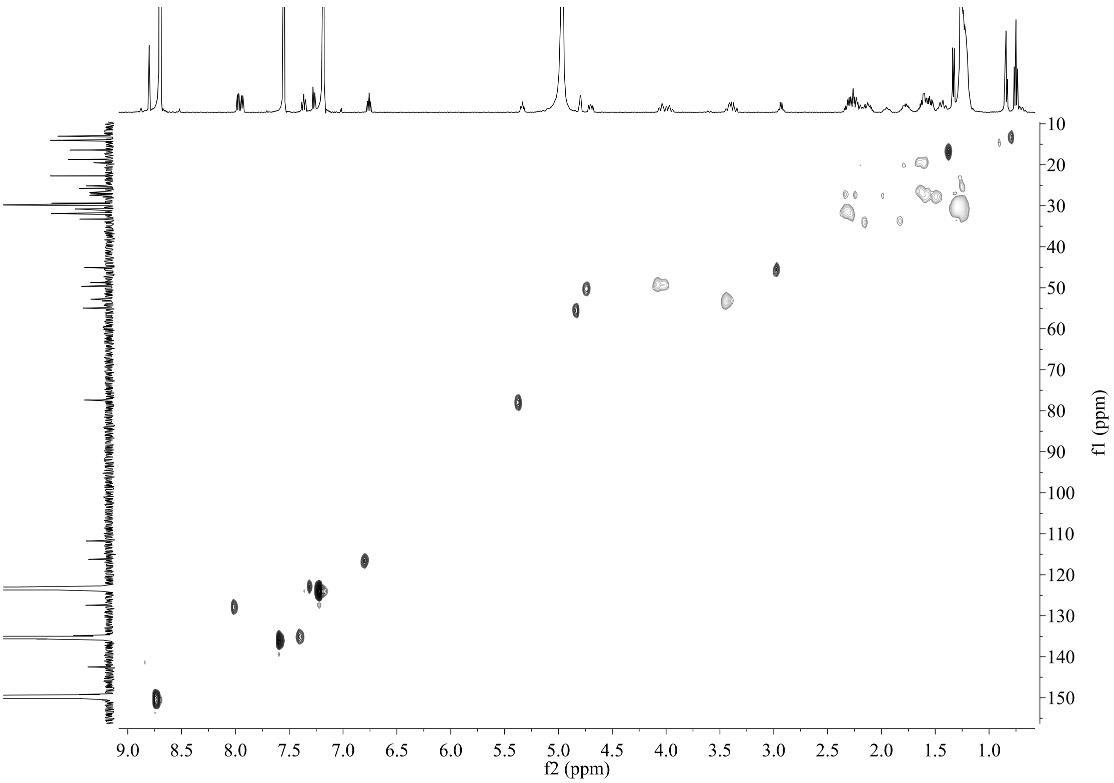

Fig. S12e HSQC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **12a**

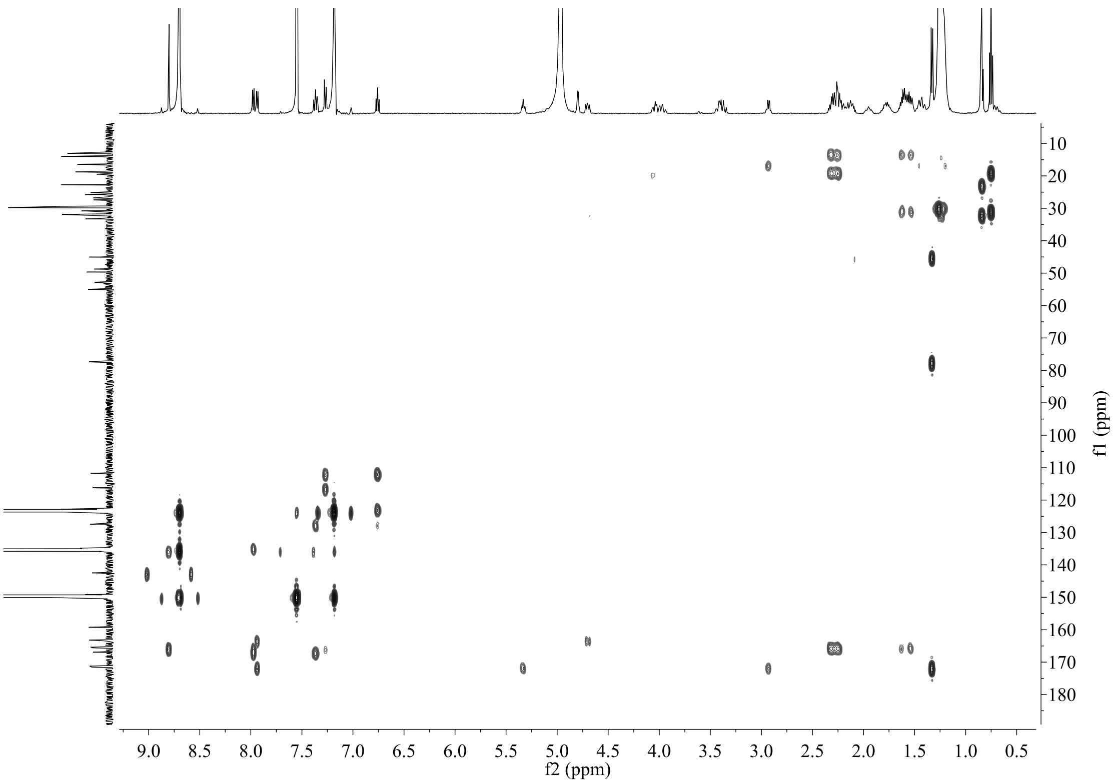

Fig. S12f HMBC (500 MHz/125 MHz, Pyridine-d_5) spectrum of **12a**

Table S13 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, $CDCl_3$) of **13**

Pos.	δ_C	δ_H, mult (*J* in Hz)

1	198.3	
2	45.9	2.93, dd (*16.0*, *4.9*)
		2.18, m
3	37.2	2.55, dd (*15.4*, *11.3*)
4	36.6	2.98, br dd (*17.4, 3.5*)
		2.66, dd (*16.4*, *10.9*)
4a	153.0	
5	121.5	6.99, s
6	163.7	
6a	117.6	
7	189.5	
7a	119.6	
8	157.2	
9	120.4	7.66, d (*8.5*)
10	137.1	7.76, t (*8.4*)
11	121.4	7.84, d (*7.5*)
11a	137.7	
12	184.1	
12a	137.5	
12b	129.3	
13	29.0	1.53, m
14	11.3	1.00, t (*7.4*)
1'	95.8	5.75, br d (*3.0*)
2'	33.4	2.24, br dd (*15.0*, *1.6*)
		2.35, dt (*15.1*, *4.1*)
3'	47.3	4.67, m
4'	74.7	3.60, dd (*9.9, 2.5*)
5'	66.2	3.86, m
6'	17.5	1.25, d (*6.2*)
3'-NAc	174.5	
3'-NAc	23.1	2.27, s
6-OH		12.96, s
3-NH		8.53, br d (*6.5*)

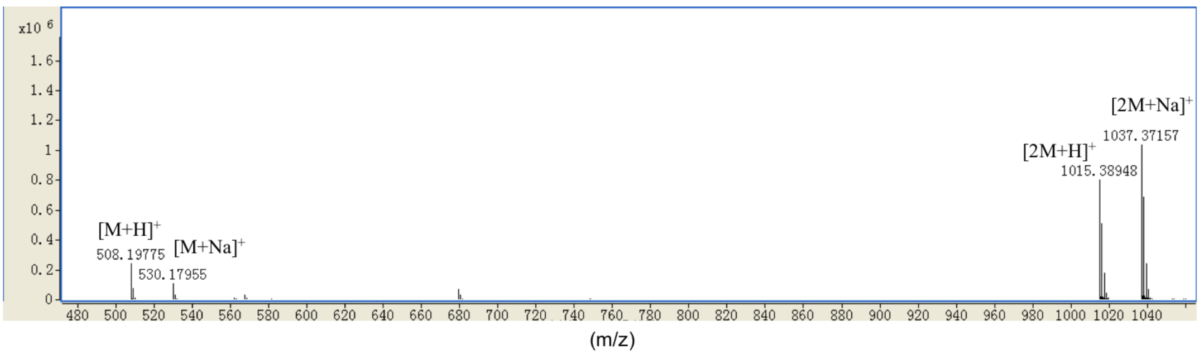

Fig. S13a HR-ESI-MS spectrum of **13**

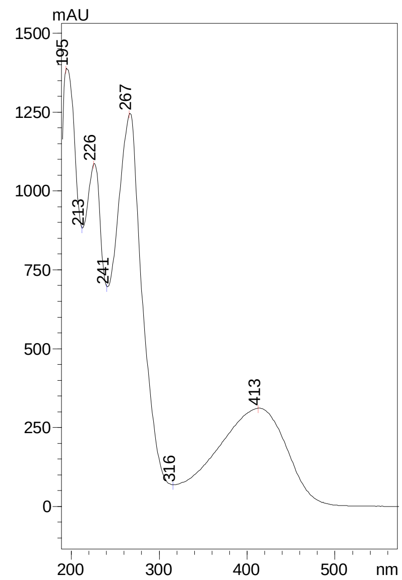

Fig. S13b UV-vis spectrum of **13**

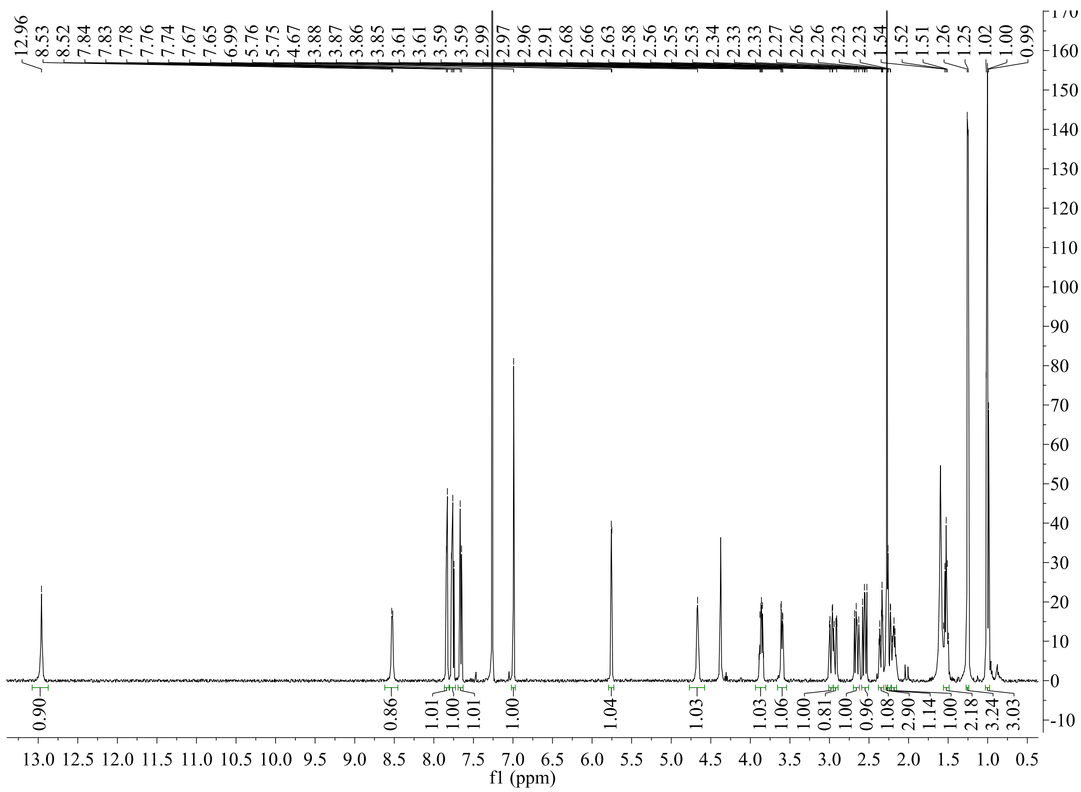

Fig. S13c ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **13**

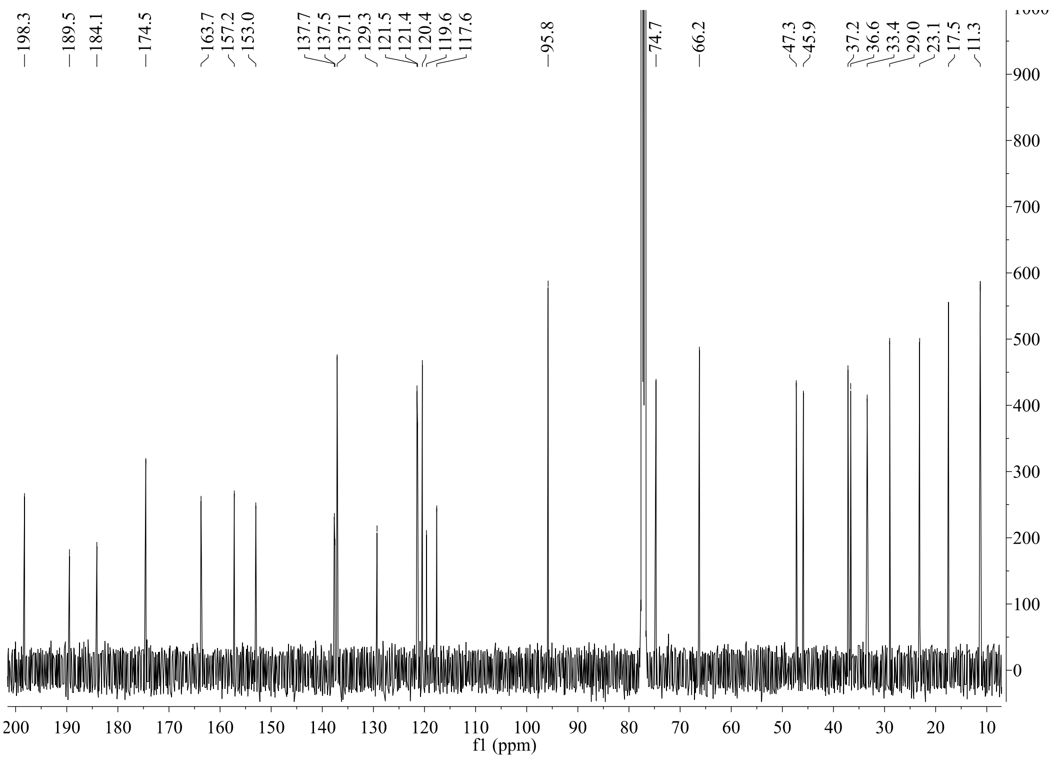

Fig. S13d ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **13**

Table S14 NMR data (^{1}H NMR 500 MHz, ^{13}C NMR 125 MHz, CD_3OD) of **14**

Pos.	δ_C	δ_H, mult (*J* in Hz)	COSY	HMBC
1	200.3			
2	49.1	2.83, dd (*15.5*, *4.7*)	2b, 3	1
		2.53, m	3	1, 3, 13
3	31.9	2.38, m		
4	39.2	3.02, dd (*16.7*, *3.9*)	3, 4b	4a, 12b
		2.7, dd (*16.7*, *10.6*)	3	2, 3, 4a, 5, 12b, 13
4a	154.6			
5	122.1	7.08, s		4, 6, 6a, 12b
6	164.8			
6a	119.0			
7	190.2			
7a	122.1			
8	158.4			
9	121.7	7.75, d (*9.0*)		11
10	137.8	7.83, t (*8.0*)		8, 11a
11	121.2	7.73, d (*7.7*)		8, 12
11a	138.8			
12	185.6			
12a	139.0			
12b	129.3			
13	21.6	1.18, d (*6.6*)		2, 3, 4
1'	96.8	5.97, d (*3.2*)	2'a	3', 5'

2'	34.4	2.35, m	2'b	
		2.22, dd (*15.0*, *1.4*)		1', 3', 4'
3'	47.4	4.65, m	2'a, 4'	
4'	73.7	3.52, dd (*10.0*, *4.3*)		5', 6'
5'	66.9	3.83, m	4', 6'	
6'	18.1	1.19, d (*6.2*)		4', 5'
3'-NAc	174.5			
3'-NAc	23.4	2.25, s		3'-NAc

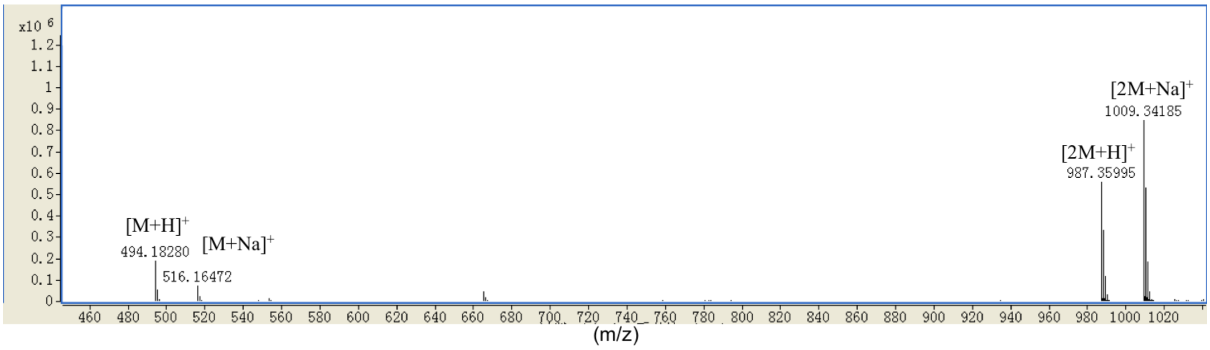

Fig. S14a HR-ESI-MS spectrum of **14**

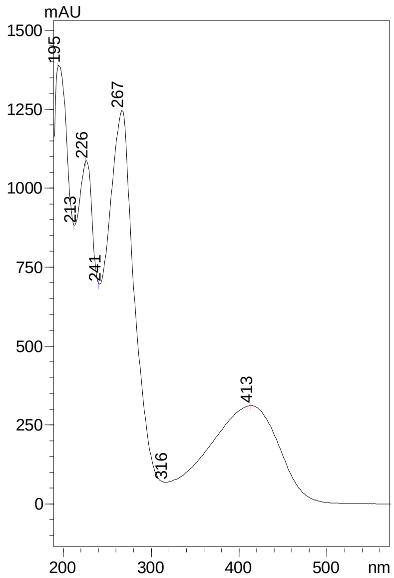

Fig. S14b UV-vis spectrum of **14**

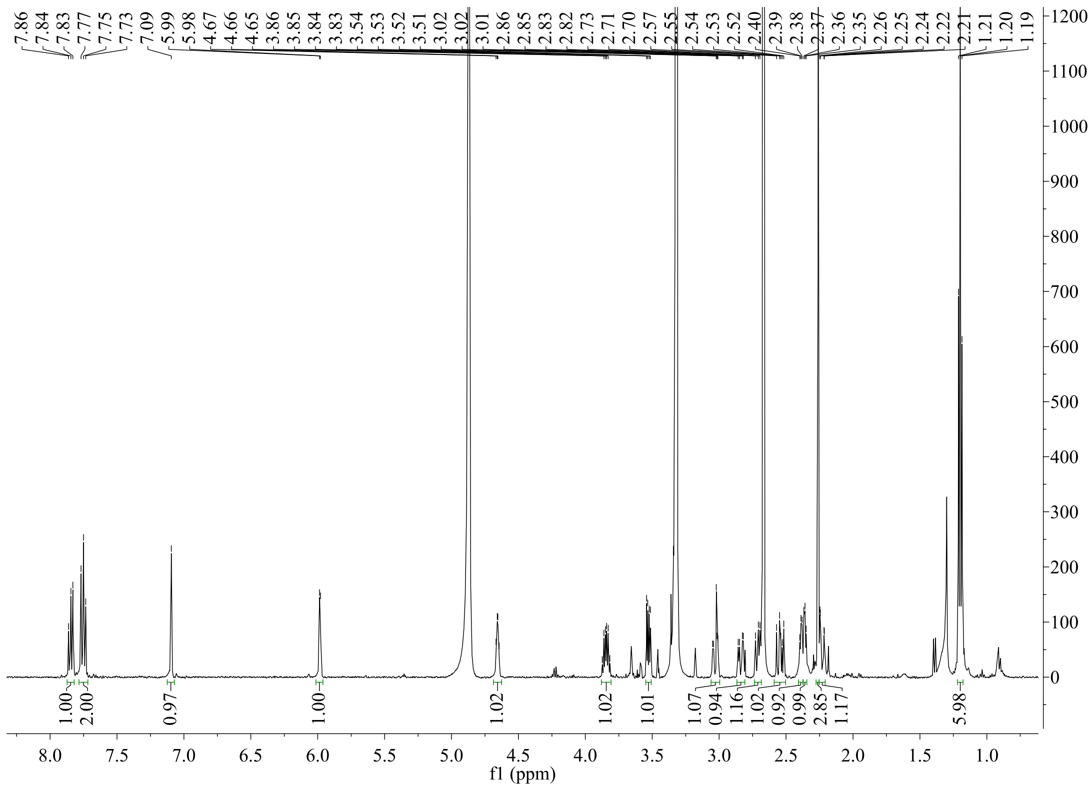

Fig. S14c ^{1}H NMR (500 MHz, CD_3OD) spectrum of **14**

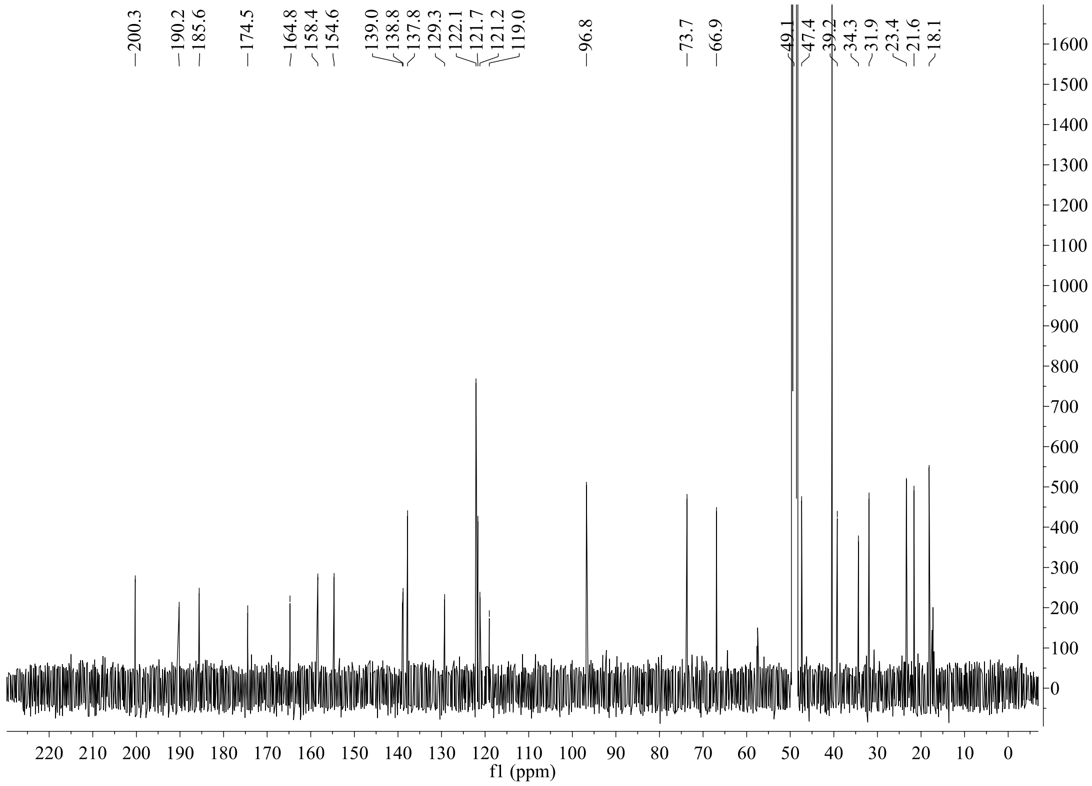

Fig. S14d ^{13}C NMR (125 MHz, CD_3OD) spectrum of **14**

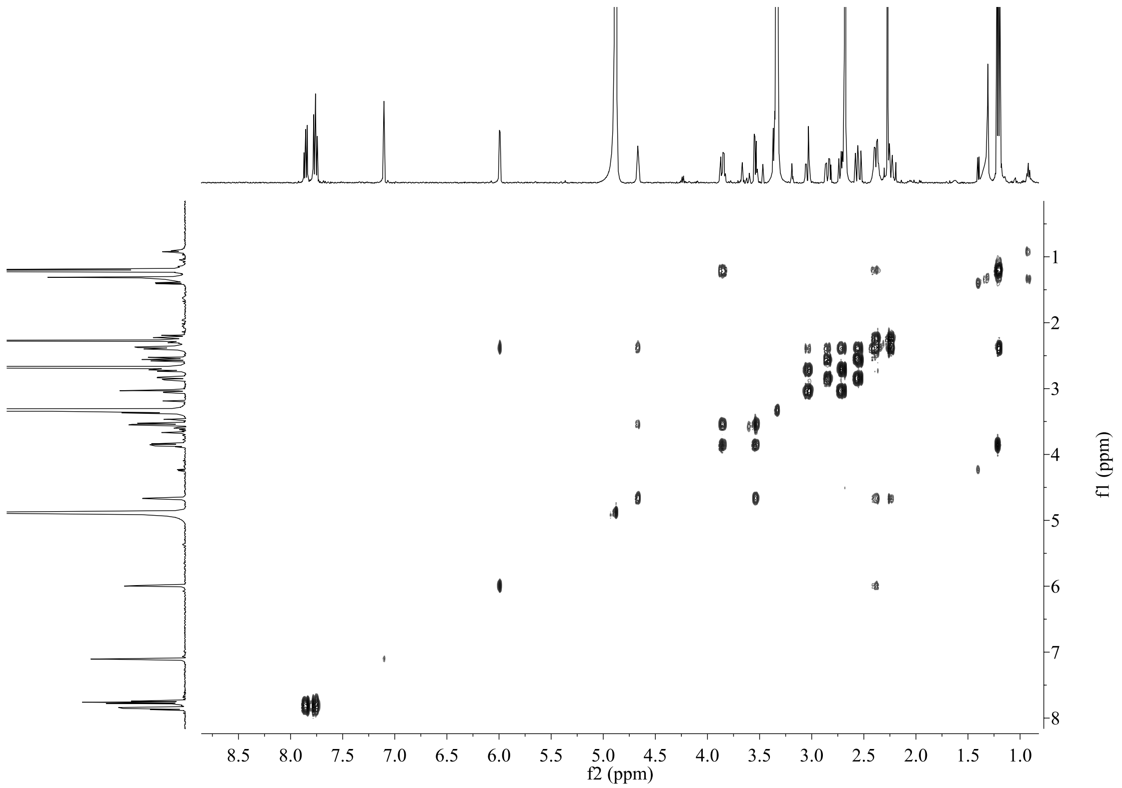

Fig. S14e ^{1}H-^{1}H COSY (500 MHz, CD_3OD) spectrum of **14**

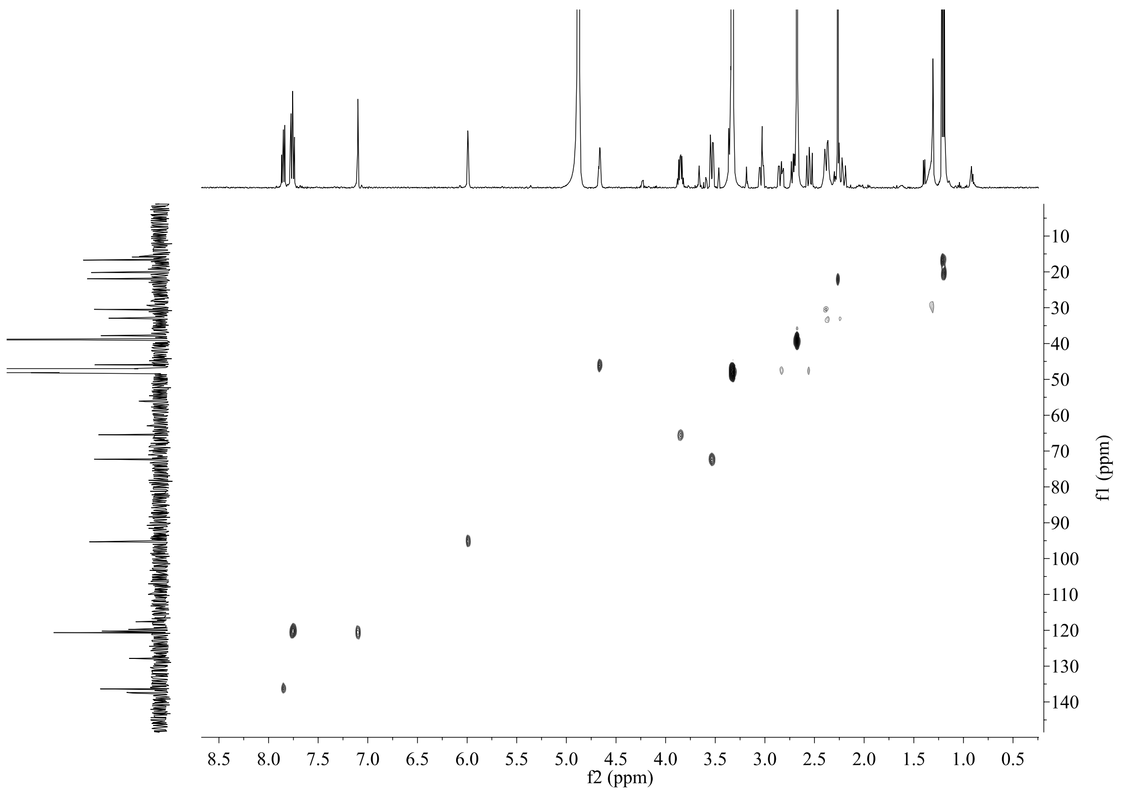

Fig. S14f HSQC (500 MHz/125 MHz, CD_3OD) spectrum of **14**

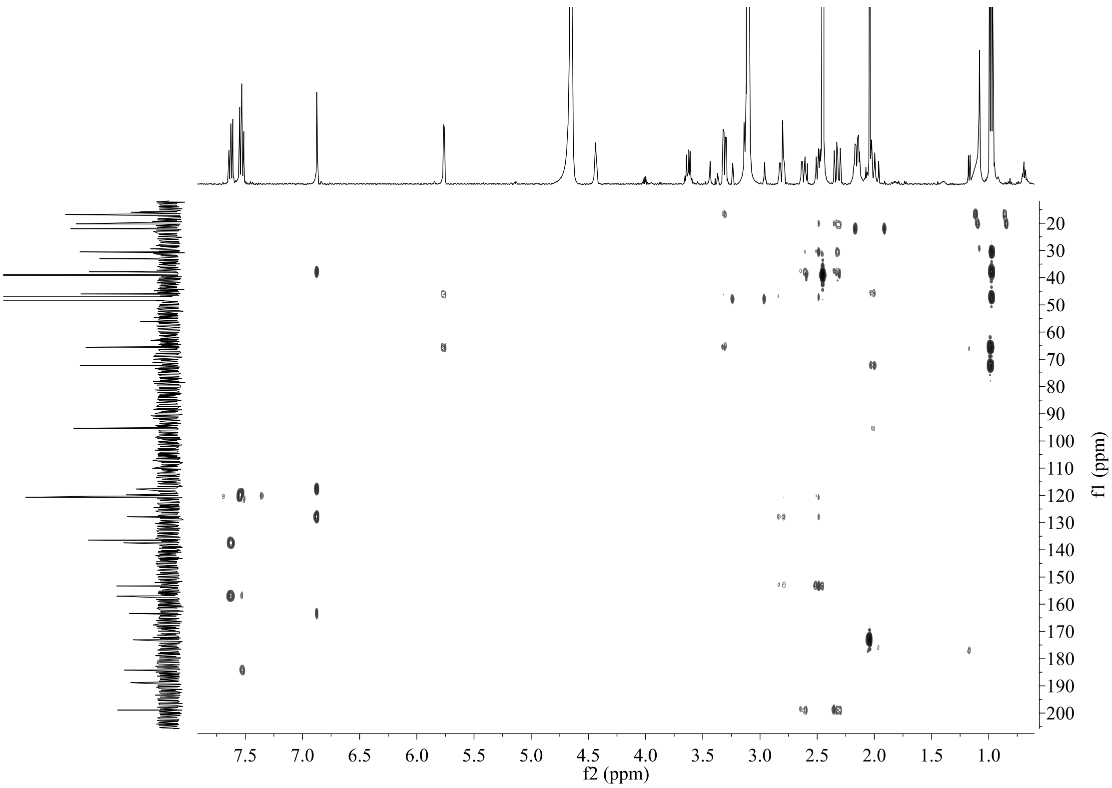

Fig. S14g HMBC (500 MHz/125 MHz, CD_3OD) spectrum of **14**

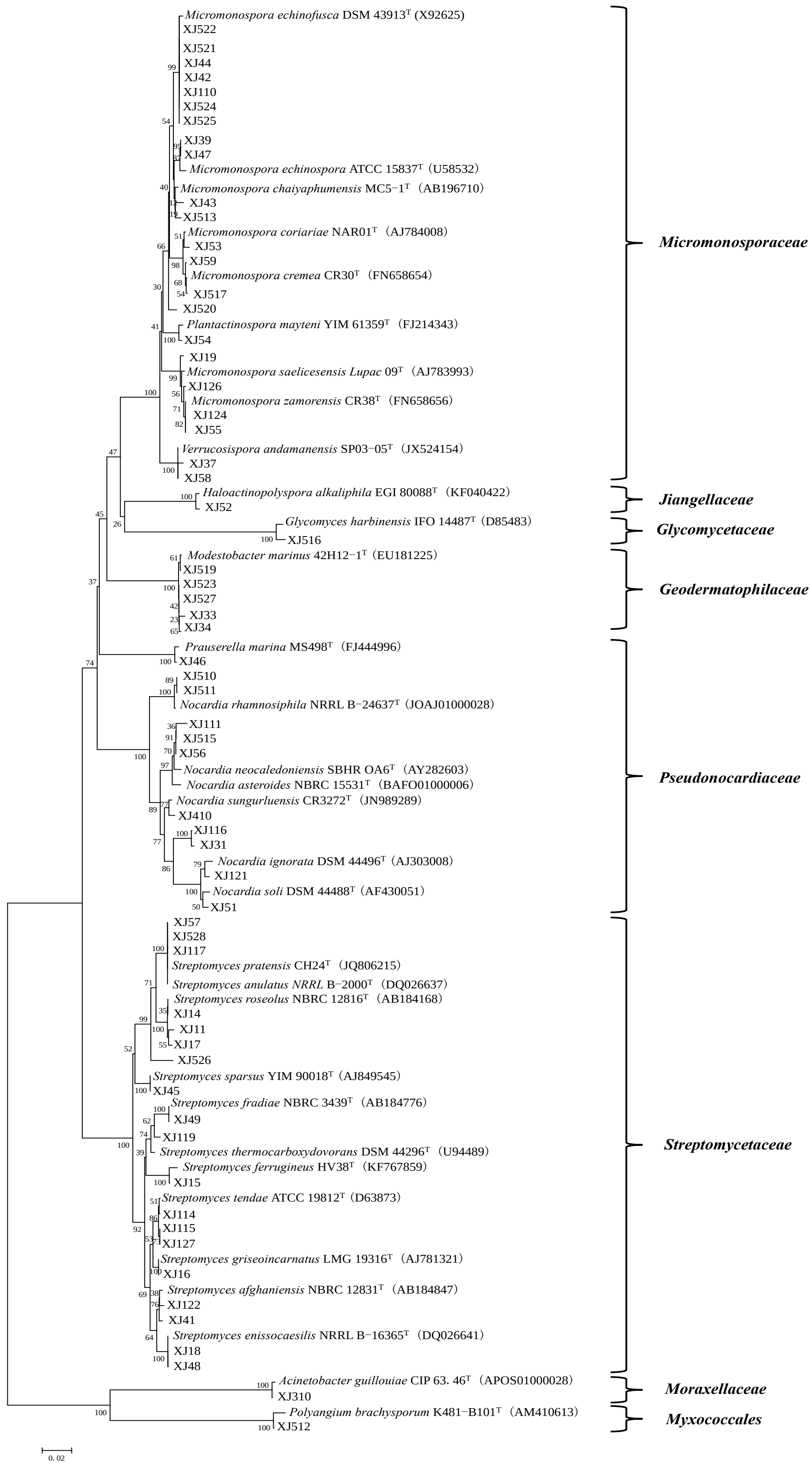

Fig. S15 Neighbor-joining phylogenetic tree of 16S rRNA gene sequences of 59 actinomycetes (including 19 strains *Streptomyces* and 40 strains rare actinomycetes) and related species constructed by MEGA 7.0. Numbers at nodes indicate levels of bootstrap support (%) based on a neighbor-joining analysis of 1000 resampled datasets. NCBI accession numbers are given. Bar, 0.02 nucleotide substitutions per site.

Virtual screen of isolated compounds 1–12 for potential virus polymerase inhibitor

For molecular docking, the 3'-RNA pocket of Lassa virus polymerase (PDB ID: 6KLC), Machupo virus polymerase (PDB ID: 6KLE), Influenza A virus polymerase (PDB ID: 6QX3), and Influenza D virus polymerase (PDB ID: 6KUJ) was extracted as the receptors. The compounds were initially cleaned by the Lipinski's rule of five (Structures violating more than three of Lipinski's rules were discarded). The remaining compounds were docked into the 3'-RNA pockets of four virus polymerases using GOLD16 program. The parameter files for docking was prepared using Hermes. The box dimension for docking calculation was set to 10 Å to allow enough space for orientation sampling.

Table S13 The binding affinities of isolated compounds **1–12 and** via virtual docking approach

	Binding affinities (%)				
Compound	6klc	6kle	6kuj	6qx3	average
1	86.64	87.85	104.48	93.14	93.02
2	92.41	92.86	98.32	101.77	96.34
3	95.4	93.3	99.7	103.55	97.98
4	92.98	90.38	100.29	98.06	95.42
5	97.5	87.09	103.38	98.16	96.53
6	98.99	84.8	100.26	102.26	96.57
7	96.16	93.86	108.25	102.73	100.25
8	94.47	85.17	101.26	99.66	95.14
9	98.51	83.4	99.53	97.96	94.85
10	93.57	93.14	100.6	104.64	97.98
11	105.58	93.15	98.95	101.89	99.89
12	101.15	89.34	95.7	97.3	95.87