Supporting Information

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1. X-ray crystallography

Table S1-1 Selected bond lengths of compound 3a

Bond	Length [Å]	Bond	Length [Å]
N4−N3	1.3563(18)	N7−O4	1.212(2)
N4−C2	1.3244(18)	N2−C5	1.322(2)
N5−C1	1.3252(19)	N2−C3	1.3760(19)
N5−C2	1.3290(18)	N2−C7	1.470(2)
O3−N7	1.2181(19)	N1−C5	1.3208(19)
N6−O1	1.2217(17)	N1−C4	1.3754(19)
N6−C2	1.443(2)	N1−C6	1.462(2)
N6−O2	1.2078(18)	O5−C8	1.412(2)
N3−C1	1.3294(18)	C4−C3	1.338(2)
N7−C1	1.447(2)	C8−C7	1.505(2)

Table S1-2 Bond angles data of compound 3a

Bond	Angle [°]	Bond	Angle [°]
C2−N4−N3	103.83(11)	N4−C2−N6	121.01(12)
C1−N5−C2	97.90(11)	N5−C2−N6	121.75(12)
O1−N6−C2	117.50(13)	C5−N2−C3	108.29(13)
O2−N6−O1	123.74(15)	C5−N2−C7	125.71(13)
O2−N6−C2	118.75(13)	C3−N2−C7	125.56(14)
C1−N3−N4	104.32(12)	C5−N1−C4	108.28(13)
O3−N7−C1	117.76(15)	C5−N1−C6	125.71(13)
O4−N7−O3	124.33(16)	C4−N1−C6	125.97(14)
O4−N7−C1	117.89(14)	N1−C5−N2	109.02(12)
N5−C1−N3	116.75(13)	C3−C4−N1	107.28(13)
N5−C1−N7	121.74(13)	C4−C3−N2	107.13(14)
N3−C1−N7	121.51(14)	O5−C8−C7	111.73(13)
N4−C2−N5	117.21(13)	N2−C7−C8	111.43(13)

Table S1-3 Torsion angles data of compound 3a

Bond	Angle [°]	Bond	Angle [°]
N4−N3−C1−N5	-0.03(17)	O2−N6−C2−N4	-179.74(15)
N4−N3−C1−N7	179.05(13)	O2−N6−C2−N5	2.1(2)
O3−N7−C1−N5	2.5(2)	N1−C4−C3−N2	0.13(18)
O3−N7−C1−N3	-176.55(14)	O5−C8−C7−N2	62.58(17)
N3−N4−C2−N5	-0.08(17)	C5−N2−C3−C4	-0.45(18)
N3−N4−C2−N6	-178.34(12)	C5−N2−C7−C8	-99.63(18)

Bond	Angle [°]	Bond	Angle [°]
O1−N6−C2−N4	1.3(2)	C5−N1−C4−C3	0.24(18)
O1−N6−C2−N5	-176.86(14)	C4−N1−C5−N2	-0.53(17)
C1−N5−C2−N4	0.06(16)	C3−N2−C5−N1	0.61(17)
C1−N5−C2−N6	178.31(13)	C3−N2−C7−C8	71.83(19)
C2−N4−N3−C1	0.06(14)	C7−N2−C5−N1	173.30(13)
C2−N5−C1−N3	-0.02(16)	C7−N2−C3−C4	-173.16(14)
C2−N5−C1−N7	-179.09(13)	C6−N1−C5−N2	-178.23(14)
O4−N7−C1−N5	-179.04(15)	C6−N1−C4−C3	177.94(14)
O4−N7−C1−N3	1.9(2)		

Table S1-4 Hydrogen bonds data of compound 3a

Bond	d(D-H) [Å]	d(H-A) [Å]	d(D-A) [Å]	D-H-A [°]
O5−H5−N3	0.82	2.07	2.8809(17)	171.0
C5−H5A−N4[1]	0.93	2.68	3.5232(19)	151.6
C5−H5A−O1[1]	0.93	2.49	3.2834(19)	143.4
C4−H4−N5[2]	0.93	2.45	3.3579(19)	164.1
C4−H4−O2[2]	0.93	2.64	3.160(2)	115.7
C8−H8A−O1[3]	0.97	2.57	3.322(2)	134.3
C7−H7A−O1[4]	0.97	2.56	3.396(2)	144.8
C7−H7B−O1[1]	0.97	2.56	3.446(2)	151.2

[1]-X, 1-Y, 1-Z; [2]-X, 1-Y, 2-Z; [3]1+X, 1+Y, +Z; [4]+X, 1+Y, +Z

Table S1-5 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) of compound 3a

Atom	*x*	*y*	*z*	U_{eq}
H5	4562	7771	6584	90
Atom	*x*	*y*	*z*	U_{eq}
H5A	-512	6886	4992	54
H4	-1689	6482	8604	62
H3	903	9014	8609	64
H8A	5539	10592	6399	64
H8B	4761	9767	7589	64
H7A	2183	10608	6565	64
H7B	2033	9598	5256	64
H6A	-3087	4373	5250	88
H6B	-4448	4483	6345	88
H6C	-2532	3935	6632	88

Table S1-6 Fractional atomic coordinates (Å×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) of compound 3a.

Atom	*x*	*y*	*z*	U_{eq}
N4	2200.3(19)	4852.3(15)	7321.3(11)	45.7(3)
N5	2422.9(19)	4905.4(14)	9519.4(11)	44.4(3)
O3	4948(2)	7328.9(16)	11270.8(12)	75.2(4)
N6	201(2)	2578.0(15)	8135.8(12)	50.9(4)
N3	3544(2)	6248.2(15)	7884.8(12)	48.5(3)
O1	-396(2)	1938.2(15)	7011.4(11)	67.3(4)
N7	4902(2)	7483.3(16)	10116.9(14)	56.0(4)
C1	3597(2)	6196.9(16)	9163.0(13)	42.5(4)
C2	1613(2)	4137.9(16)	8329.6(13)	40.8(4)
O4	5911(3)	8632.6(16)	9715.0(15)	87.5(5)
O2	-298(3)	1973.3(16)	9083.7(13)	88.1(5)
N2	671(2)	8395.4(15)	6623.6(12)	47.0(3)
N1	-1608.2(19)	6162.7(15)	6620.2(11)	44.5(3)
O5	4796(2)	8403.3(13)	6079.2(11)	60.2(4)
C5	-489(2)	7100.8(17)	5885.2(14)	45.1(4)
C4	-1130(3)	6884(2)	7884.6(14)	51.5(4)
C3	290(3)	8272(2)	7888.0(15)	53.6(4)
C8	4507(3)	9702.3(17)	6642.6(16)	53.5(4)
C7	2294(3)	9673.0(18)	6203.2(16)	53.5(4)
C6	-3042(3)	4605(2)	6173.6(18)	58.6(5)

U_{eq} is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Table S1-7 Anisotropic Displacement Parameters (Å^2×10^3) of compound 3a.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N4	51.0(7)	55.7(8)	30.1(6)	7.0(5)	5.3(5)	19.0(6)
N5	52.8(7)	50.9(7)	29.6(6)	6.6(5)	4.0(5)	19.7(6)
O3	104.7(11)	71.8(8)	40.9(7)	-7.7(6)	-3.9(7)	30.6(8)
N6	59.8(8)	55.2(8)	32.2(7)	6.1(6)	3.2(6)	15.7(6)
N3	52.4(7)	52.6(7)	39.6(7)	10.5(6)	7.0(5)	17.2(6)
O1	78.1(8)	65.2(8)	39.8(7)	-4.5(5)	-0.9(6)	9.0(6)
N7	65.6(8)	52.3(8)	47.5(8)	-0.4(6)	-0.7(6)	23.3(7)
C1	46.5(8)	48.4(8)	34.6(8)	5.1(6)	2.8(6)	21.0(6)
C2	45.8(7)	48.8(8)	28.9(7)	6.2(6)	4.3(5)	18.9(6)
O4	101.1(11)	56.5(8)	76.2(10)	5.4(7)	-0.5(8)	-1.0(7)
O2	123.8(13)	65.5(8)	44.9(8)	15.8(6)	10.9(7)	-3.4(8)
N2	55.6(7)	52.9(7)	31.6(6)	5.5(5)	7.2(5)	18.9(6)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	46.1(7)	54.1(7)	34.0(6)	6.7(5)	6.8(5)	18.9(5)
O5	78.5(8)	56.5(7)	48.9(7)	12.3(5)	21.5(6)	24.0(6)
C5	52.5(8)	56.0(9)	27.9(7)	4.2(6)	6.2(6)	21.5(7)
C4	54.1(9)	72.6(11)	30.7(8)	10.0(7)	13.3(6)	23.7(8)
C3	62.7(9)	64.9(10)	30.7(8)	-0.9(7)	8.0(7)	21.6(8)
C8	64(1)	45.1(8)	41.9(8)	4.8(6)	9.4(7)	8.2(7)
C7	70.4(10)	46.0(8)	41.9(9)	9.6(7)	10.0(7)	17.3(7)
C6	53.1(9)	58.6(10)	57.9(10)	7.2(8)	4.1(8)	14.6(8)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a\times^2U_{11}+...+2hka\times b\times U_{12}]$.

Table S2-1 Selected bond lengths of compound 3b

Bond	Length [Å]	Bond	Length [Å]
O1−C1	1.241(2)	C2−N3	1.451(3)
C4−C5	1.381(3)	N3−O7	1.206(3)
C4−N4	1.443(2)	N3−O6	1.211(3)
C4−C3	1.386(3)	O8−C12	1.408(2)
C6−C1	1.454(3)	N2−C11	1.474(2)
C6−N5	1.444(2)	N2−C7	1.323(2)
C6−C5	1.372(3)	N2−C9	1.369(3)
C1−C2	1.451(2)	N1−C7	1.324(2)
N5−O3	1.216(2)	N1−C8	1.361(3)
N5−O2	1.209(2)	N1−C10	1.465(2)
N4−O4	1.230(2)	C12−C11	1.503(3)
N4−O5	1.225(3)	C8−C9	1.344(3)
C3−C2	1.365(3)		

Table S2-2 Bond angles data of compound 3b

Bond	Angle [°]	Bond	Angle [°]
C5−C4−N4	119.23(17)	C1−C2−N3	117.92(15)
C5−C4−C3	121.08(16)	C3−C2−C1	125.22(17)
C3−C4−N4	119.64(17)	C3−C2−N3	116.84(16)
N5−C6−C1	119.12(15)	O7−N3−C2	118.7(2)
C5−C6−C1	124.55(16)	O7−N3−O6	123.6(2)
C5−C6−N5	116.27(16)	O6−N3−C2	117.67(19)
O1−C1−C6	125.45(17)	C7−N2−C11	125.79(16)
O1−C1−C2	123.57(17)	C7−N2−C9	107.78(16)
C2−C1−C6	110.91(15)	C9−N2−C11	126.34(17)
O3−N5−C6	119.32(16)	C7−N1−C8	108.63(16)

Bond	Angle [°]	Bond	Angle [°]
O2−N5−C6	119.31(16)	C7−N1−C10	126.15(17)
O2−N5−O3	121.36(17)	C8−N1−C10	125.22(17)
C6−C5−C4	119.26(17)	O8−C12−C11	111.94(17)
O4−N4−C4	118.18(18)	N2−C11−C12	112.00(15)
O5−N4−C4	118.68(18)	N2−C7−N1	109.01(16)
O5−N4−O4	123.13(17)	C9−C8−N1	106.94(18)
C2−C3−C4	118.93(16)	C8−C9−N2	107.63(19)

Table S2-3 Torsion angles data of compound 3b

Bond	Angle [°]	Bond	Angle [°]
O1−C1−C2−C3	178.02(18)	C5−C6−N5−O2	-153.0(2)
O1−C1−C2−N3	-0.3(3)	N4−C4−C5−C6	179.97(15)
C4−C3−C2−C1	0.7(3)	N4−C4−C3−C2	-179.94(16)
C4−C3−C2−N3	179.04(18)	C3−C4−C5−C6	2.5(3)
C6−C1−C2−C3	0.9(3)	C3−C4−N4−O4	179.38(17)
C6−C1−C2−N3	-177.43(17)	C3−C4−N4−O5	0.8(3)
C1−C6−N5−O3	-151.0(2)	C3−C2−N3−O7	139.3(2)
C1−C6−N5−O2	29.7(3)	C3−C2−N3−O6	-41.3(3)
C1−C6−C5−C4	-0.7(3)	O8−C12−C11−N2	-67.4(2)
C1−C2−N3−O7	-42.2(3)	N1−C8−C9−N2	0.2(3)
C1−C2−N3−O6	137.2(2)	C11−N2−C7−N1	-175.81(16)
N5−C6−C1−O1	-0.9(3)	C11−N2−C9−C8	175.93(19)
N5−C6−C1−C2	176.12(15)	C7−N2−C11−C12	86.1(2)
N5−C6−C5−C4	-177.80(15)	C7−N2−C9−C8	-0.6(3)
C5−C4−N4−O4	1.8(3)	C7−N1−C8−C9	0.2(3)
C5−C4−N4−O5	-176.75(17)	C8−N1−C7−N2	-0.6(2)
C5−C4−C3−C2	-2.4(3)	C10−N1−C7−N2	-179.96(17)
C5−C6−C1−O1	-177.93(18)	C10−N1−C8−C9	179.56(19)
C5−C6−C1−C2	-0.9(2)	C9−N2−C11−C12	-89.9(2)
C5−C6−N5−O3	26.2(3)	C9−N2−C7−N1	0.8(2)

Table S2-4 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) of compound 3b

Atom	*x*	*y*	*z*	U_{eq}
H5	-51	2242	-917	39
H3	1069	3874	1722	41
H8	6513	4627	997	72
H12A	6537	6046	2157	50
H12B	5540	5076	2120	50

Atom	*x*	*y*	*z*	U_{eq}
H11A	4658	6840	808	51
H11B	5127	8010	1701	51
H7	5478	7162	-458	43
H8A	7329	11223	595	60
H10A	6353	8383	-1488	73
H10B	7413	9193	-934	73
H10C	6488	10483	-1356	73
H9	6603	10254	1740	62

Table S2-5 Fractional atomic coordinates ($Å \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of compound 3b.

Atom	*x*	*y*	*z*	U_{eq}
O1	2723(1)	5483(2)	-69.9(10)	46.6(4)
C4	404.3(13)	2877(2)	434.3(13)	31.8(4)
C6	1224.1(13)	3686(2)	-612.9(12)	31.1(4)
C1	2027.6(13)	4667(2)	75.0(12)	30.8(4)
N5	1198.7(12)	3646(3)	-1554.1(11)	44.2(5)
C5	444.7(13)	2837(2)	-444.7(13)	32.6(4)
N4	-415.7(12)	1986(2)	610.6(13)	43.0(4)
O4	-1040.2(12)	1177(2)	-29.2(13)	60.0(5)
C3	1115.6(14)	3816(3)	1137.8(13)	34.5(4)
C2	1886.3(13)	4653(2)	959.7(12)	32.8(4)
O5	-469.0(13)	2099(3)	1382.2(13)	71.7(6)
N3	2602.5(15)	5642(3)	1714.6(12)	56.7(6)
O3	394.6(12)	3504(3)	-2177.9(11)	71.2(6)
O2	1978.6(13)	3737(4)	-1705.0(11)	89.7(8)
O7	3483.6(15)	5541(4)	1819.2(15)	109.3(10)
O6	2275.4(18)	6541(4)	2201.5(15)	103.1(9)
O8	6015.9(11)	4360.8(19)	1125.0(11)	48.1(4)
N2	5837.5(11)	8336(2)	788.3(11)	36.0(4)
N1	6475.2(11)	9202(2)	-220.2(11)	35.6(4)
C12	5884.0(15)	5643(3)	1747.0(14)	41.6(5)
C11	5286.5(15)	7253(3)	1257.8(15)	42.5(5)
C7	5849.3(13)	8042(2)	-51.4(13)	36.0(5)
C8	6870.5(17)	10288(3)	529.7(16)	50.2(6)
C10	6701.8(17)	9326(3)	-1072.9(15)	49.0(6)
C9	6471.7(18)	9753(3)	1158.5(16)	51.8(6)

U_{eq} is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Table S2-6 Anisotropic Displacement Parameters ($Å^2×10^3$) of compound 3b.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	44.6(8)	50.4(9)	55.8(9)	-3.1(7)	31.5(7)	-12.8(7)
C4	28.9(9)	22.1(9)	49.2(10)	8.8(7)	19.9(8)	3.4(7)
C6	31.4(9)	30.4(9)	34.4(9)	2.0(7)	15.1(7)	6.6(7)
C1	30.6(9)	26.9(9)	39.8(9)	4.1(7)	18.2(7)	3.7(7)
N5	37.9(9)	59.0(11)	37.8(9)	-0.5(8)	16.0(7)	3.9(8)
C5	29.4(9)	23.3(9)	44.7(10)	-0.9(7)	12.3(8)	3.9(7)
N4	35.7(9)	31.5(9)	66.8(12)	14.3(8)	23.8(8)	1.7(7)
O4	44.9(9)	46.0(9)	92.4(13)	-5.7(8)	28.0(9)	-17.0(7)
C3	35.9(10)	35(1)	38.3(9)	7.3(8)	20.3(8)	3.8(8)
C2	30.2(9)	32.8(10)	37.1(9)	-1.0(7)	13.7(7)	-1.3(7)
O5	61.4(10)	97.7(15)	68.2(11)	24.8(10)	38.1(9)	-14.3(10)
N3	51.3(11)	80.3(15)	43.6(10)	-13.3(9)	22.8(9)	-26.9(10)
O3	48.4(9)	119.9(17)	40.0(8)	-11.3(9)	8.5(7)	-6.2(10)
O2	49.2(10)	183(2)	45.2(9)	-11.1(12)	27.5(8)	-11.7(12)
O7	48.0(11)	203(3)	76.0(13)	-42.7(16)	20.6(10)	-49.6(14)
O6	99.4(16)	142(2)	81.0(14)	-68.1(15)	48.3(13)	-44.1(15)
O8	48.5(8)	40.1(8)	67.4(9)	-5.5(7)	34.9(7)	-7.1(6)
N2	34.0(8)	30.2(8)	47.9(9)	-2.1(7)	19.4(7)	-2.8(7)
N1	34.0(8)	31.3(8)	43.6(9)	2.1(7)	16.2(7)	0.5(6)
C12	41.7(10)	46.6(12)	43.5(10)	1.5(9)	23.8(9)	-4.1(9)
C11	37.2(10)	42.8(12)	57.2(12)	-0.9(9)	28.5(9)	-3.8(9)
C7	32.8(9)	29.3(9)	44.4(10)	-4.4(8)	11.4(8)	-3.1(8)
C8	52.8(13)	41.3(12)	62.7(13)	-13.8(10)	27.9(11)	-22.8(10)
C10	48.5(12)	56.5(14)	46.4(11)	10.1(10)	22.3(10)	5.6(10)
C9	58.6(13)	47.7(13)	54.9(12)	-19(1)	27.2(11)	-18.6(11)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a\times^2U_{11}+...+2hka\times b\times U_{12}]$.

Table S3-1 Selected bond lengths of compound 4b

Bond	Length [Å]	Bond	Length [Å]
O1−C6	1.443(3)	O7−N6	1.214(4)
O1−N3	1.382(4)	O9−N5	1.185(4)
O4−C7	1.235(3)	N5−C8	1.452(3)
N2−C1	1.322(3)	C7−C12	1.445(4)
N2−C2	1.370(3)	C7−C8	1.459(4)
N2−C5	1.465(4)	C12−C11	1.369(4)
O6−N4	1.182(4)	C8−C9	1.358(4)
O10−N5	1.180(3)	O3−N3	1.192(4)

Bond	Length [Å]	Bond	Length [Å]
N1−C1	1.316(3)	N6−C10	1.437(4)
N1−C3	1.380(4)	C6−C5	1.488(4)
N1−C4	1.464(4)	O2−N3	1.195(4)
O5−N4	1.181(3)	C9−C10	1.386(4)
O8−N6	1.221(4)	C10−C11	1.373(4)
N4−C12	1.451(4)	C2−C3	1.325(5)

Table S3-2 Bond angles data of compound 4b

Bond	Angle [°]	Bond	Angle [°]
N3−O1−C6	113.8(2)	N5−C8−C7	118.9(2)
C1−N2−C2	108.8(2)	C9−C8−N5	117.0(2)
C1−N2−C5	125.0(2)	C9−C8−C7	124.1(2)
C2−N2−C5	126.3(2)	O8−N6−C10	118.1(3)
C1−N1−C3	108.2(2)	O7−N6−O8	122.5(3)
C1−N1−C4	125.4(2)	O7−N6−C10	119.4(3)
C3−N1−C4	126.3(3)	N1−C1−N2	108.5(2)
O6−N4−C12	118.2(3)	O1−C6−C5	105.8(2)
O5−N4−O6	120.6(3)	C8−C9−C10	119.4(3)
O5−N4−C12	121.2(2)	C9−C10−N6	120.0(3)
O10−N5−O9	120.1(3)	C11−C10−N6	119.1(3)
O10−N5−C8	119.8(3)	C11−C10−C9	120.9(2)
O9−N5−C8	120.0(3)	C12−C11−C10	119.9(3)
O4−C7−C12	125.0(2)	O3−N3−O1	118.0(3)
O4−C7−C8	123.2(2)	O3−N3−O2	129.9(4)
C12−C7−C8	111.7(2)	O2−N3−O1	112.1(3)
C7−C12−N4	120.0(2)	C3−C2−N2	107.1(3)
C11−C12−N4	116.1(2)	C2−C3−N1	107.4(3)
C11−C12−C7	123.8(2)	N2−C5−C6	112.4(2)

Table S3-3 Torsion angles data of compound 4b

Bond	Angle [°]	Bond	Angle [°]
O1−C6−C5−N2	65.4(3)	C12−C7−C8−N5	176.6(2)
O4−C7−C12−N4	4.8(4)	C12−C7−C8−C9	-3.9(4)
O4−C7−C12−C11	-173.3(3)	C8−C7−C12−N4	-177.6(2)
O4−C7−C8−N5	-5.8(4)	C8−C7−C12−C11	4.3(4)
O4−C7−C8−C9	173.8(3)	C8−C9−C10−N6	179.3(3)
N2−C2−C3−N1	-0.1(3)	C8−C9−C10−C11	0.1(4)
O6−N4−C12−C7	-173.0(3)	N6−C10−C11−C12	-178.9(2)
O6−N4−C12−C11	5.2(4)	C1−N2−C2−C3	-0.1(3)

Bond	Angle [°]	Bond	Angle [°]
O10−N5−C8−C7	-26.7(5)	C1−N2−C5−C6	80.2(3)
O10−N5−C8−C9	153.7(4)	C1−N1−C3−C2	0.3(3)
O5−N4−C12−C7	6.4(4)	C6−O1−N3−O3	-1.0(4)
O5−N4−C12−C11	-175.3(3)	C6−O1−N3−O2	179.6(3)
O8−N6−C10−C9	-0.1(5)	C9−C10−C11−C12	0.4(4)
O8−N6−C10−C11	179.1(3)	N3−O1−C6−C5	177.0(2)
N4−C12−C11−C10	179.0(2)	C2−N2−C1−N1	0.3(3)
O7−N6−C10−C9	179.8(3)	C2−N2−C5−C6	-97.3(3)
O7−N6−C10−C11	-0.9(5)	C3−N1−C1−N2	-0.4(3)
O9−N5−C8−C7	156.8(3)	C5−N2−C1−N1	-177.6(2)
O9−N5−C8−C9	-22.8(5)	C5−N2−C2−C3	177.8(3)
N5−C8−C9−C10	-178.5(2)	C4−N1−C1−N2	179.5(3)
C7−C12−C11−C10	-2.8(4)	C4−N1−C3−C2	-179.6(3)
C7−C8−C9−C10	1.9(4)		

Table S3-4 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) of compound 4b

Atom	*x*	*y*	*z*	U_{eq}
H1	3636	9088	5012	68
H6A	2245	7853	2793	78
H6B	2344	7415	3681	78
H9	7239	4769	3363	71
H11	7707	5128	5693	69
H2	699	11435	4089	82
H3	888	11583	5499	85
H5A	3372	9707	3511	80
H5B	2103	10406	3136	80
H4A	2511	9134	6549	119
H4B	2710	10875	6658	119
H4C	3773	9860	6447	119

Table S3-5 Fractional atomic coordinates (Å×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) of compound 4b.

Atom	*x*	*y*	*z*	U_{eq}
O1	692.7(18)	8248(2)	3218.4(13)	74.6(7)
O4	4749(2)	7770(3)	4335.4(12)	79.1(7)
N2	2262(2)	10116(2)	4292.8(13)	56.7(6)
O6	6613(4)	6540(5)	6458.4(16)	154.2(17)
O10	4312(3)	6764(5)	2866.7(17)	154.3(19)

Atom	*x*	*y*	*z*	U_{eq}
N1	2435(2)	10238(3)	5537.6(14)	59.8(6)
O5	5068(3)	7600(4)	5881.5(15)	102.8(9)
O8	8950(3)	3276(4)	4022.1(18)	118.0(11)
N4	5955(2)	6856(3)	5871.3(14)	63.2(7)
O7	9210(3)	3481(3)	5263.6(16)	106(1)
O9	5873(3)	6268(5)	2418.1(15)	127.8(13)
N5	5362(2)	6422(3)	2961.8(15)	67.4(7)
C7	5579(2)	6820(3)	4407.2(15)	51.9(6)
C12	6276(2)	6320(3)	5142.1(15)	52.0(6)
C8	6009(2)	6109(3)	3744.1(15)	52.9(6)
O3	687(3)	5879(3)	2830.2(17)	105.0(9)
N6	8660(3)	3791(3)	4617.7(18)	81.1(8)
C1	2932(2)	9684(3)	4959.7(16)	56.3(7)
C6	2015(3)	8149(3)	3286.9(17)	64.9(8)
O2	-1007(3)	7046(4)	2924(2)	128.4(13)
C9	6993(3)	5166(3)	3808.0(17)	59.4(7)
C10	7626(2)	4800(3)	4541.9(17)	59.8(7)
C11	7272(3)	5377(3)	5203.7(17)	57.8(7)
N3	84(3)	6929(4)	2969.8(17)	87.0(9)
C2	1306(3)	10985(3)	4452(2)	68.2(8)
C3	1410(3)	11065(3)	5222(2)	70.6(8)
C5	2492(3)	9681(4)	3516.4(17)	66.5(8)
C4	2897(4)	10007(4)	6369.6(18)	79.1(9)

U_{eq} is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Table S3-6 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) of compound 4b.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	58.0(12)	84.7(14)	76.3(14)	-17.8(11)	-3(1)	4.9(10)
O4	74.8(14)	98.4(15)	60.9(12)	-6.9(11)	2.1(10)	40.1(12)
N2	47.9(12)	57.9(12)	63.3(13)	3.5(10)	6.7(10)	3.3(9)
O6	172(3)	232(4)	50.9(15)	-8.0(19)	-5.9(16)	110(3)
O10	102(2)	273(5)	76.0(18)	-49(2)	-19.9(15)	89(3)
N1	54.6(13)	60.6(12)	65.9(14)	-5.8(10)	14.8(10)	-0.2(10)
O5	112(2)	131(2)	68.8(15)	-3.4(14)	24.9(14)	54.7(18)
O8	115(2)	134(2)	102(2)	-19.7(17)	10.0(17)	69.9(19)
N4	72.9(16)	62.2(13)	52.7(13)	-0.4(10)	5.3(11)	3.6(11)
O7	96.6(19)	126(2)	91.6(19)	20.7(15)	5.5(14)	59.8(17)
O9	102(2)	226(4)	56.2(15)	7.7(19)	13.6(14)	36(2)
N5	56.5(14)	79.6(16)	61.3(15)	-15.3(12)	-4.4(11)	10.6(11)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C7	46.7(13)	51.2(12)	55.9(14)	-4.4(10)	2.4(11)	0.6(10)
C12	53.4(14)	46.4(12)	55.3(15)	-3.6(10)	6.8(11)	-4.1(10)
C8	49.1(14)	54.1(13)	53.7(14)	-6.4(11)	3.7(11)	-1(1)
O3	116(2)	94.3(18)	107(2)	-33.9(15)	24.4(17)	-5.7(16)
N6	77.6(18)	77.4(16)	86(2)	-1.1(14)	8.1(15)	29.3(14)
C1	52.3(14)	57.4(14)	58.7(16)	1.2(11)	7.8(12)	8.2(11)
C6	55.6(16)	83.5(19)	52.0(15)	-2.4(13)	-1.1(12)	14.6(13)
O2	70.5(18)	162(3)	150(3)	-63(2)	10.9(17)	-19.0(17)
C9	54.4(15)	57.6(14)	66.4(17)	-11.0(12)	11.0(12)	3.0(11)
C10	52.8(15)	55.6(14)	69.3(17)	-1.4(12)	4.8(12)	7.7(11)
C11	57.8(15)	52.9(13)	60.1(15)	5.1(11)	2.4(12)	2.9(11)
N3	79(2)	107(2)	73.7(18)	-27.5(16)	7.6(14)	-4.5(16)
C2	48.7(15)	62.3(15)	91(2)	1.5(14)	3.5(14)	6.4(12)
C3	53.7(16)	63.3(16)	97(2)	-12.7(15)	18.4(15)	4.8(12)
C5	59.5(16)	81.4(18)	56.7(16)	13.2(14)	3.8(13)	4.5(14)
C4	92(2)	87(2)	60.9(18)	-3.8(15)	20.7(16)	0.0(17)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a\times^2U_{11}+...+2hka\times b\times U_{12}]$.

2. Differential scanning calorimetry (DSC) and thermogravimetric analysis (TG-DTG) curves

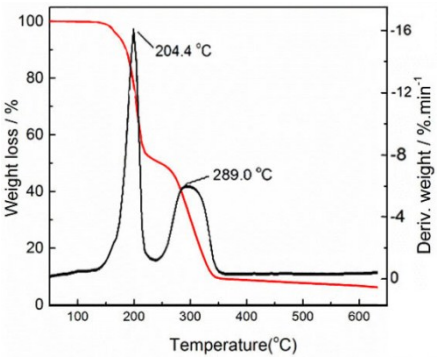

Figure S1 TG curves and DTG curves of compound 2a in argon atmosphere

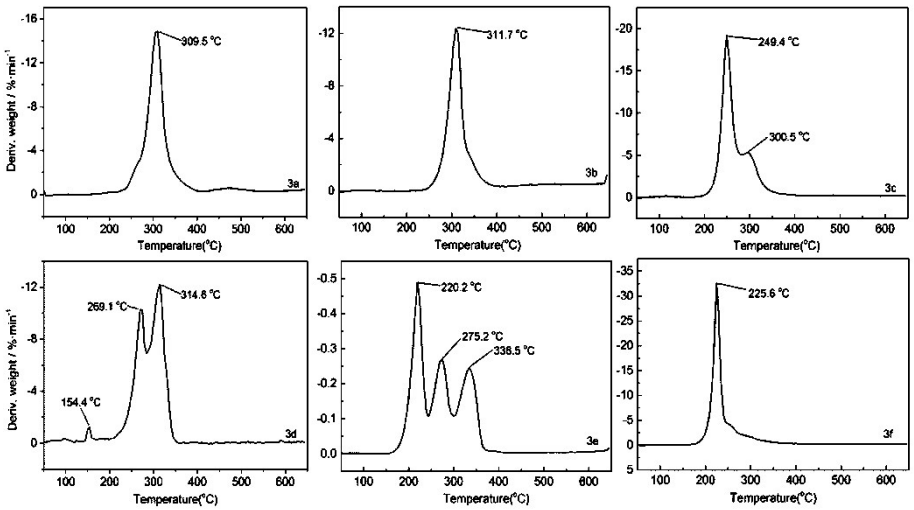

Figure S2 DTG curves of compounds 3a-f

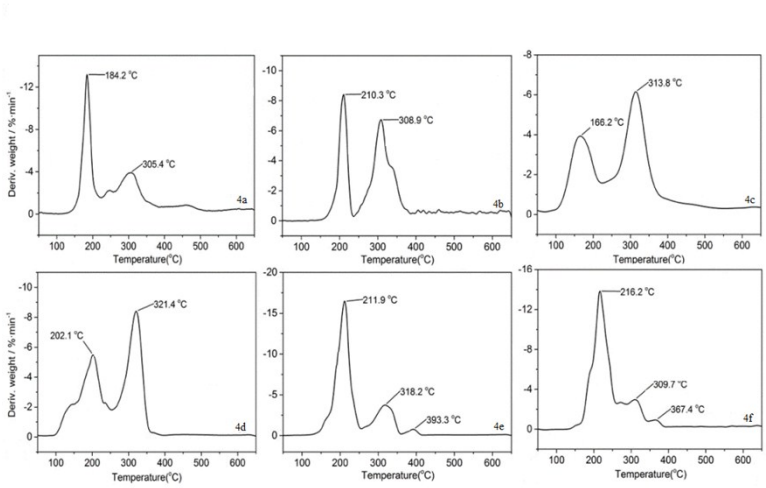

Figure S3 DTG curves of compounds 4a-f in argon atmosphere.

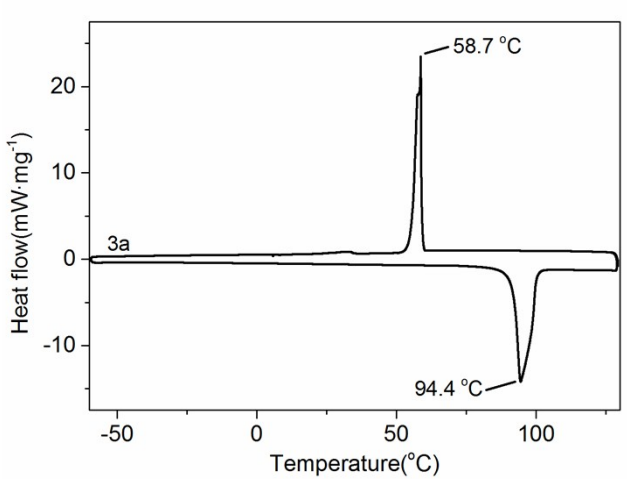

Figure S4 Secondary heating and cooling DSC curves of compound 3a.

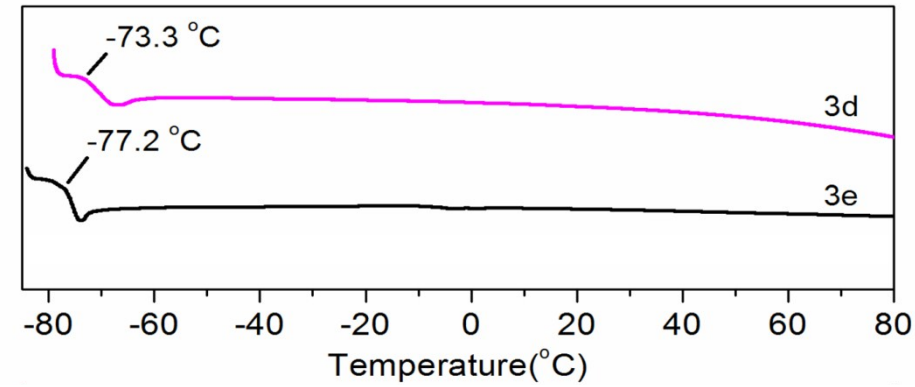

Figure S5 Secondary heating DSC curves of compounds 3d and 3e.

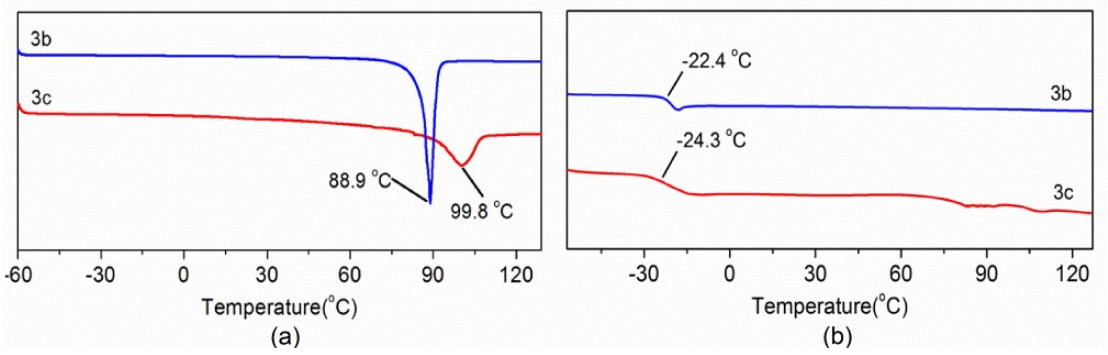

Figure S6 First heating (a) and secondary heating (b) DSC curves of compound 3b and 3c.

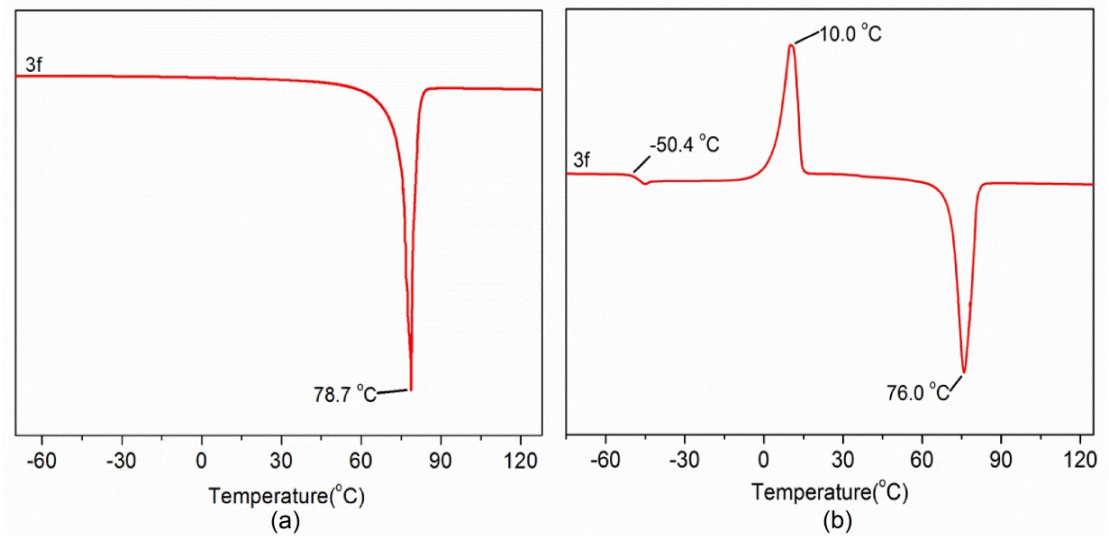

Figure S7 First heating (a) and secondary heating (b) DSC curves of compound 3f.

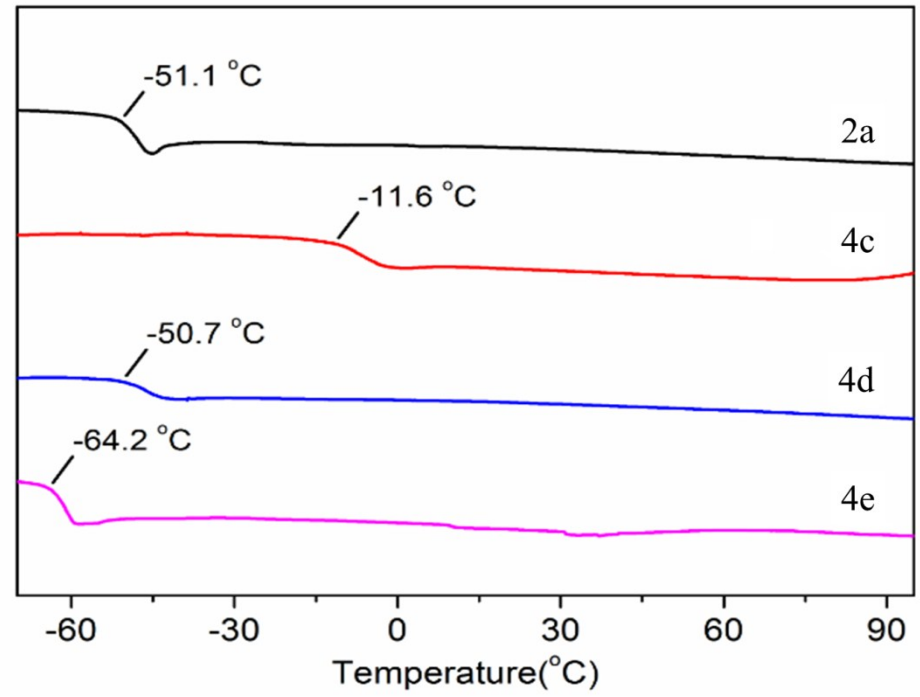

Figure S8 Secondary heating DSC curves of compounds 2a, 4c, 4d and 4e.

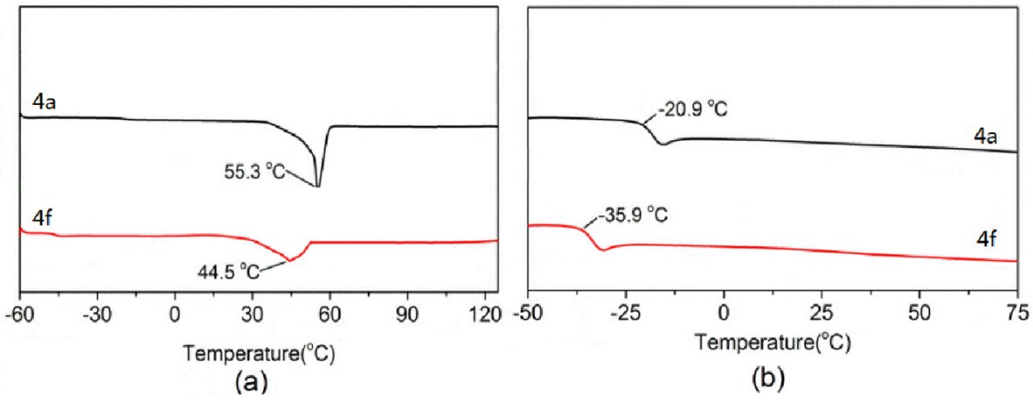

Figure S9 First heating (a) and secondary heating (b) DSC curves of compounds 4a and 4f.

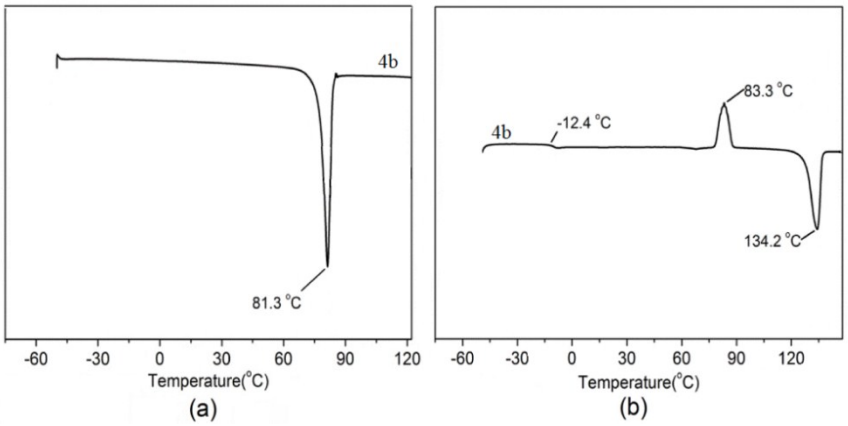

Figure S10 First heating (a) and secondary heating (b) DSC curves of compound 4b.

3. Structure characterization

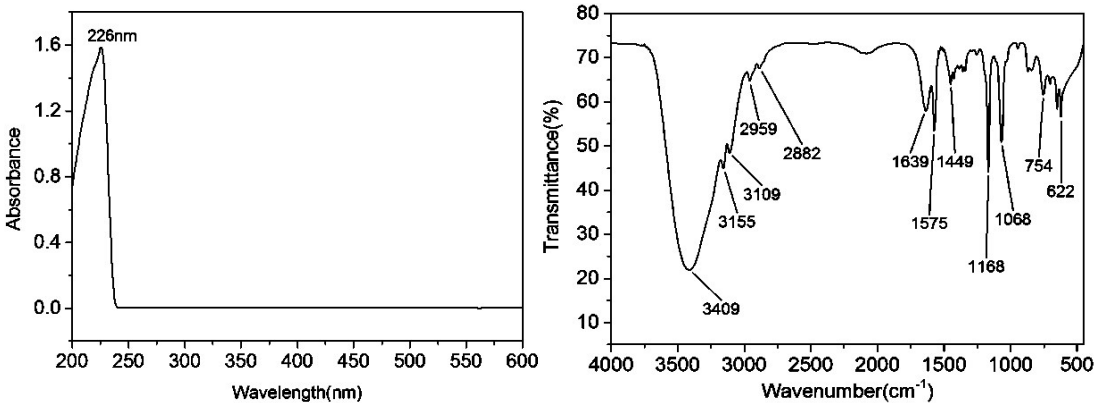

Figure S11 UV-Vis and FT-IR spectra of compound 1.

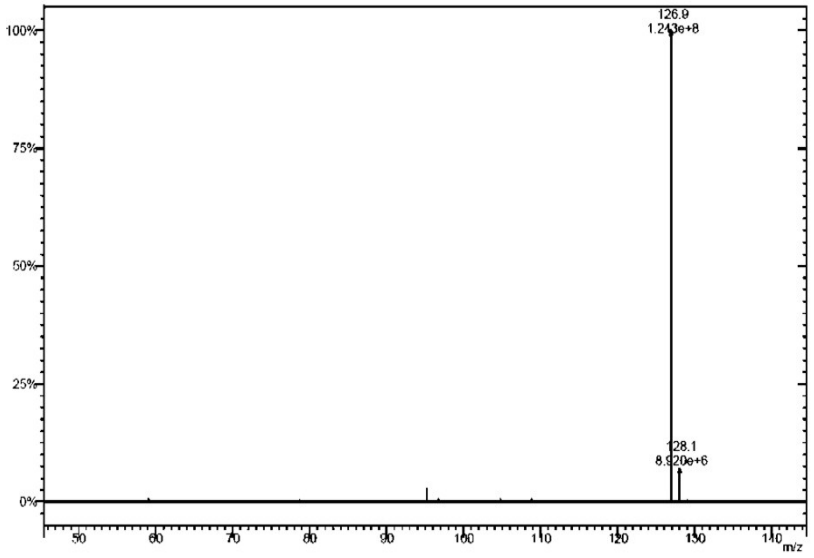

Figure S12 ESI-MS (+) spectrum of compound 1.

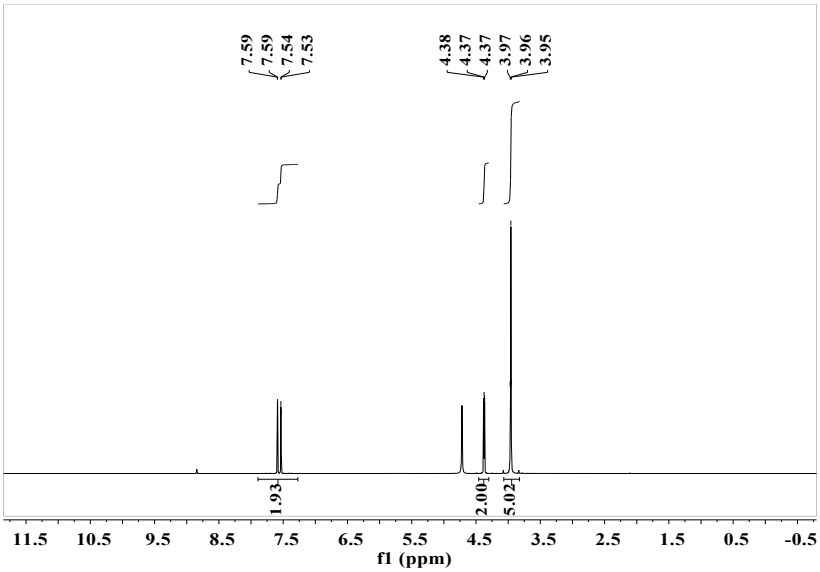

Figure S13 ^{1}H-NMR spectrum of compound 1 in D_2O.

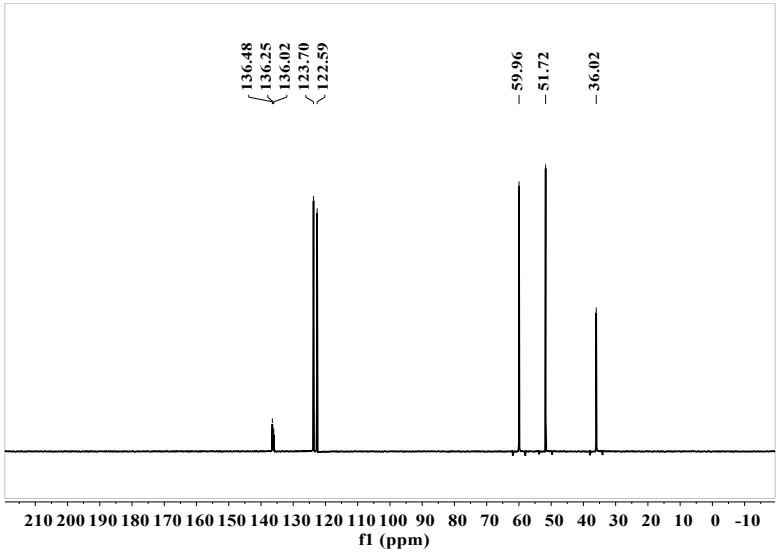

Figure S14 ^{13}C-NMR spectrum of compound 1 in D_2O.

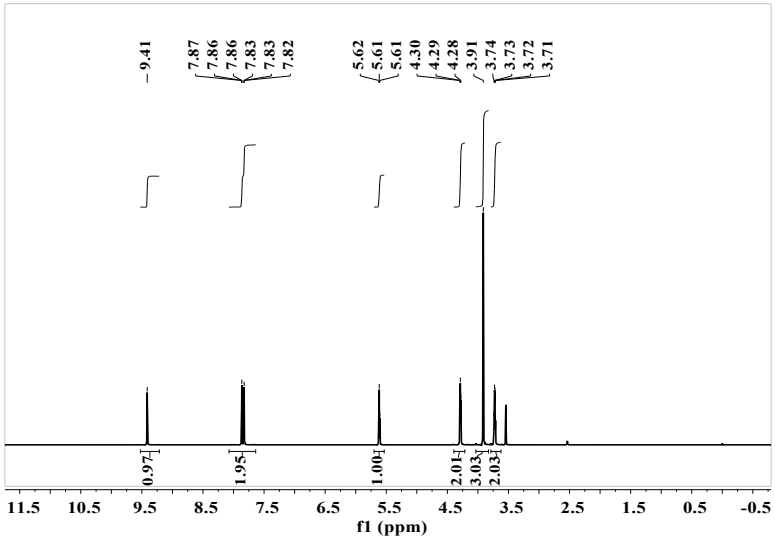

Figure S15 ^{1}H-NMR spectrum of compound 1 in DMSO-d_6.

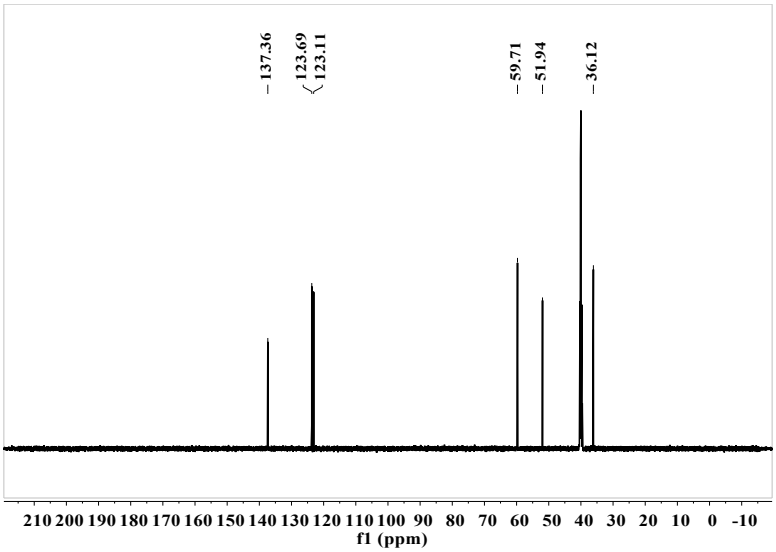

Figure S16 ^{13}C-NMR spectrum of compound 1 in DMSO-d_6.

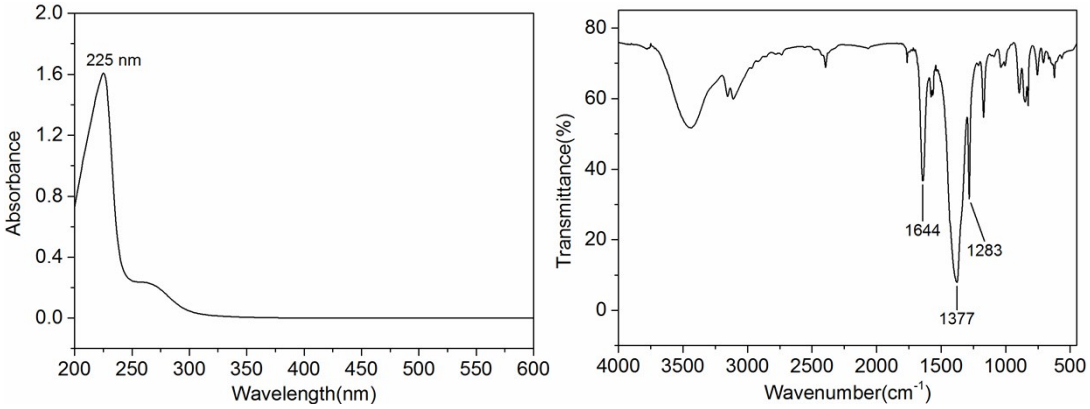

Figure S17 UV-Vis and FT-IR spectra of compound 2a.

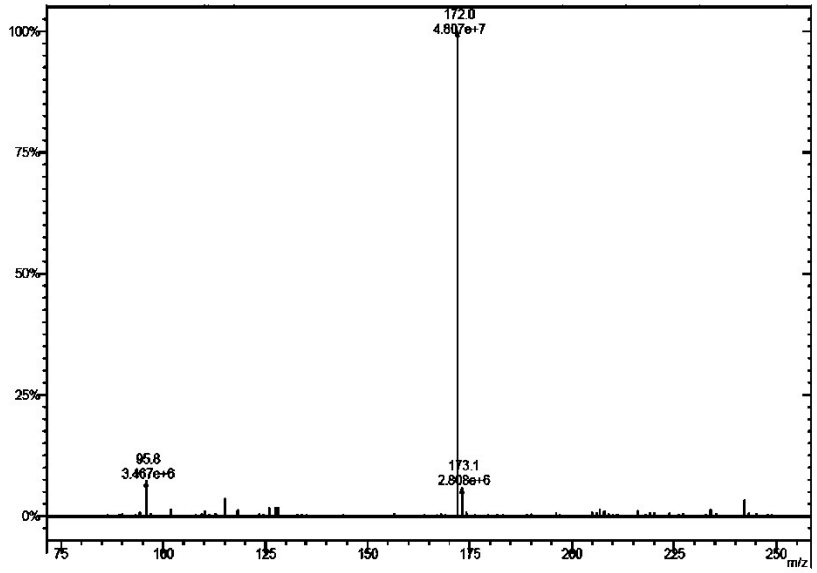

Figure S18 ESI-MS (+) spectrum of compound 2a.

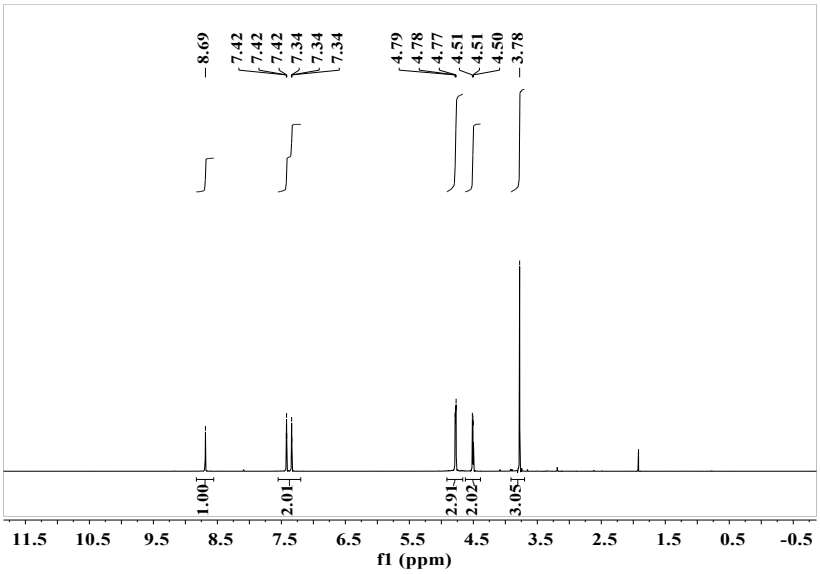

Figure S19 ^{1}H-NMR spectrum of compound 2a in D_2O.

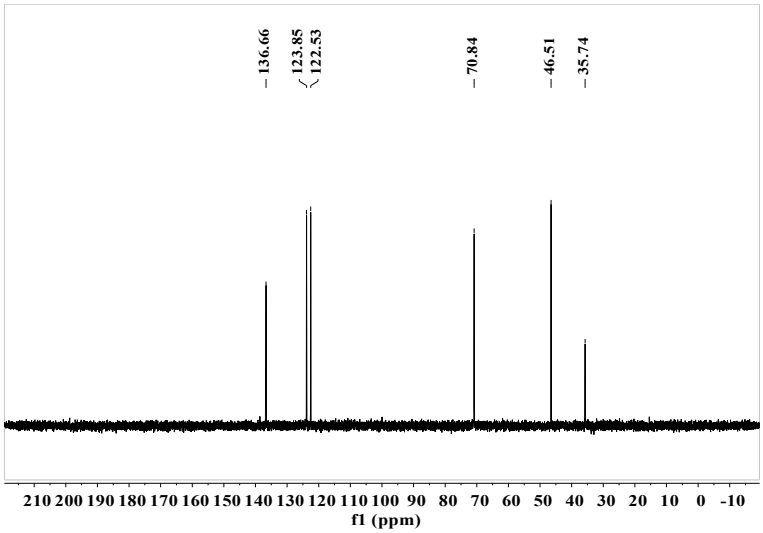

Figure S20 ^{13}C-NMR spectrum of compound 2a in D_2O.

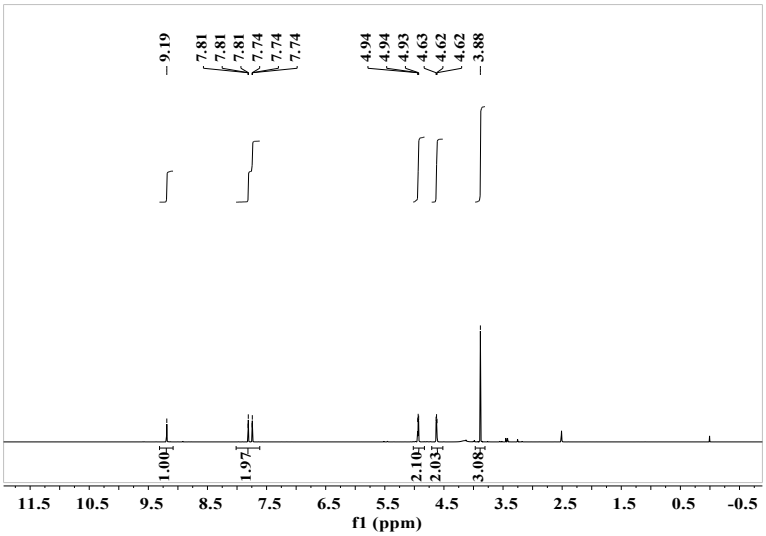

Figure S21 ^{1}H-NMR spectrum of compound 2b in DMSO-d_6.

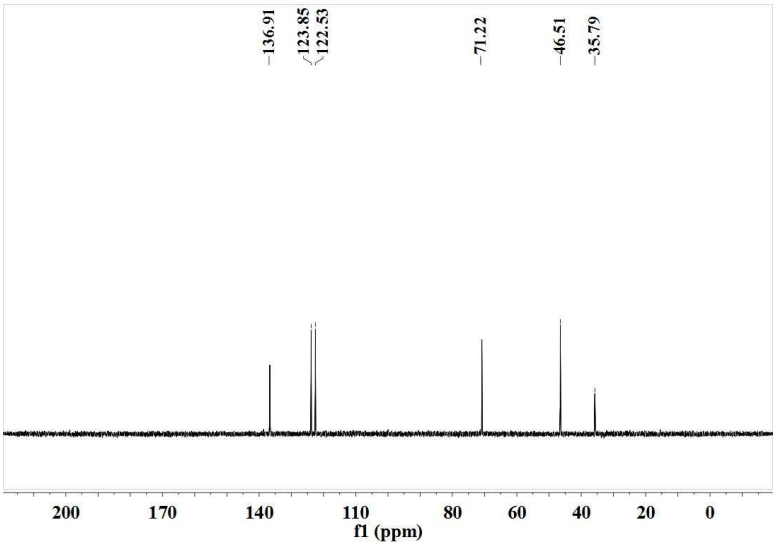

Figure S22 ^{13}C-NMR spectrum of compound 2b in in D_2O.

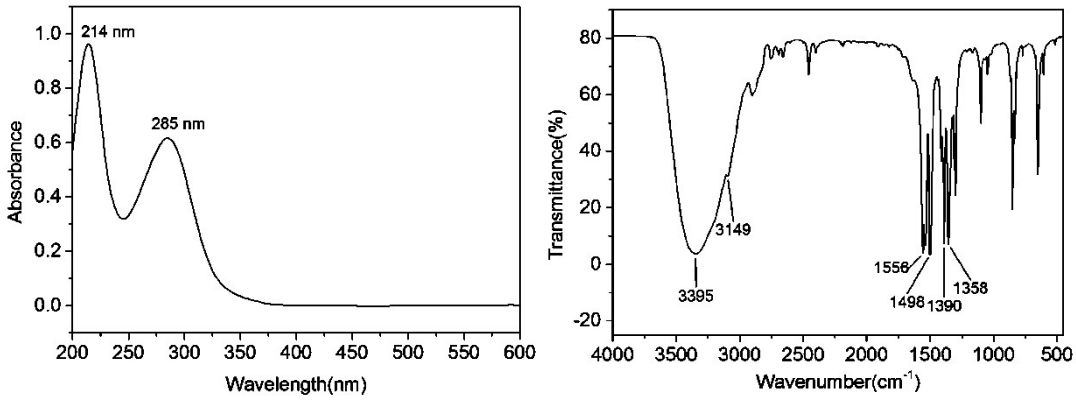

Figure S23 UV-Vis and FT-IR spectra of compound 3a.

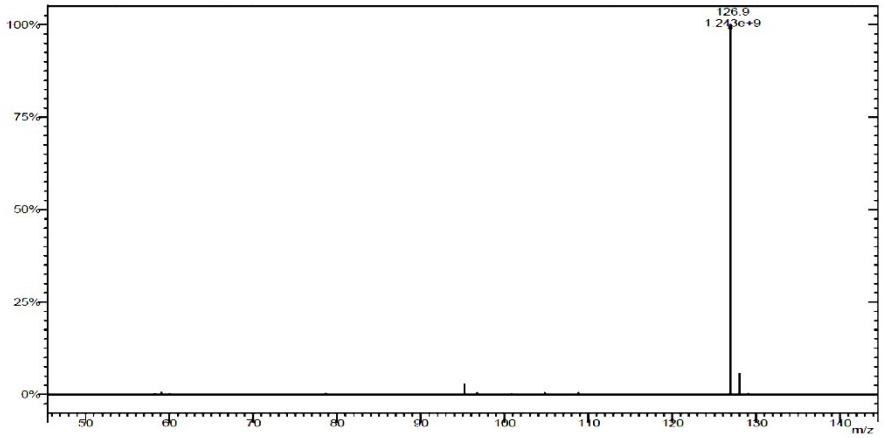

Figure S24 ESI-MS(+) spectrum of compound 3a

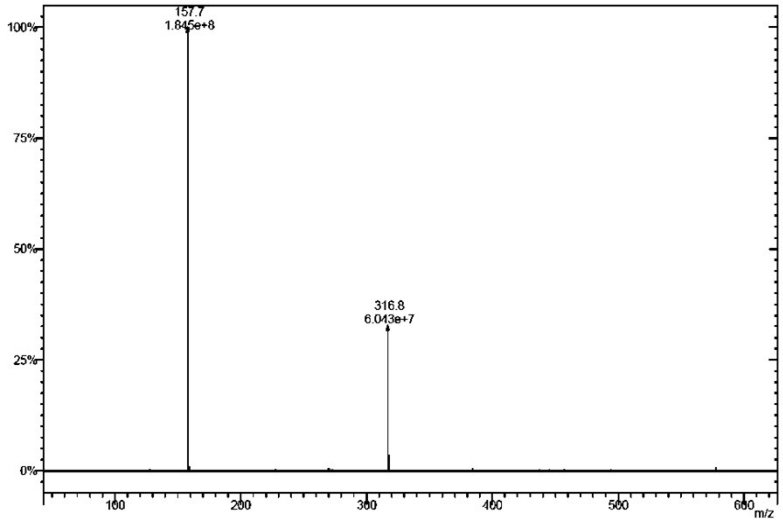

Figure S25 ESI-MS(-) spectrum of compound 3a

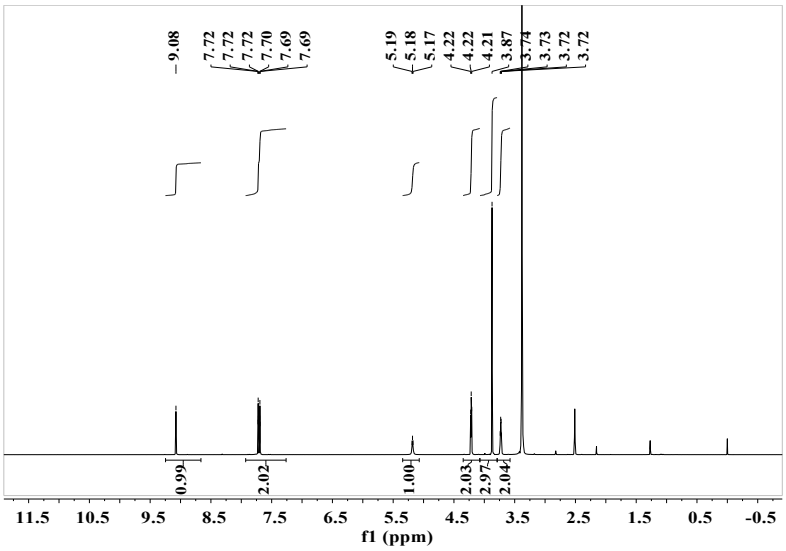

Figure S26 ^{1}H NMR spectrum of compound 3a in DMSO-d_6

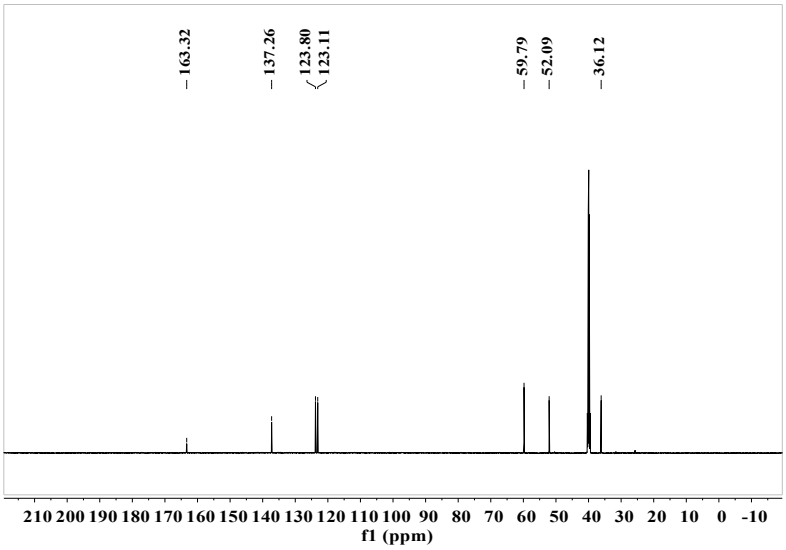

Figure S27 ^{13}C NMR spectrum of compound 3a in DMSO-d_6

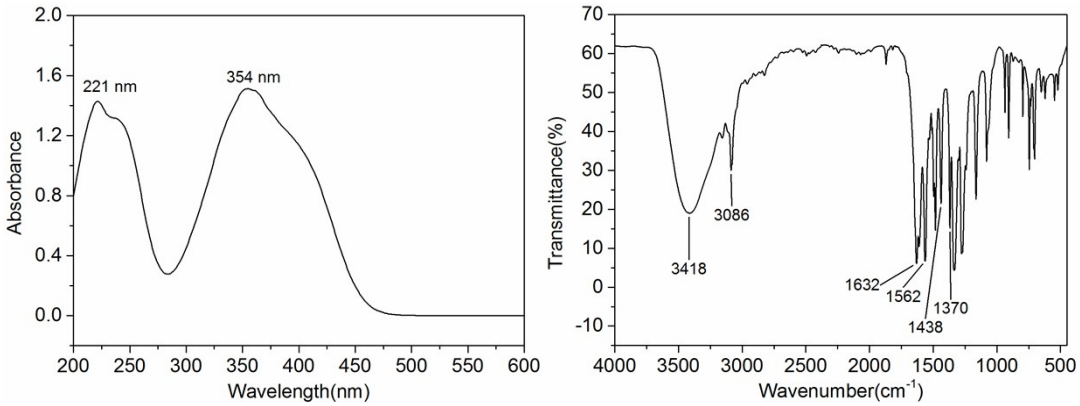

Figure S28 UV-Vis and FT-IR spectra of compound 3b

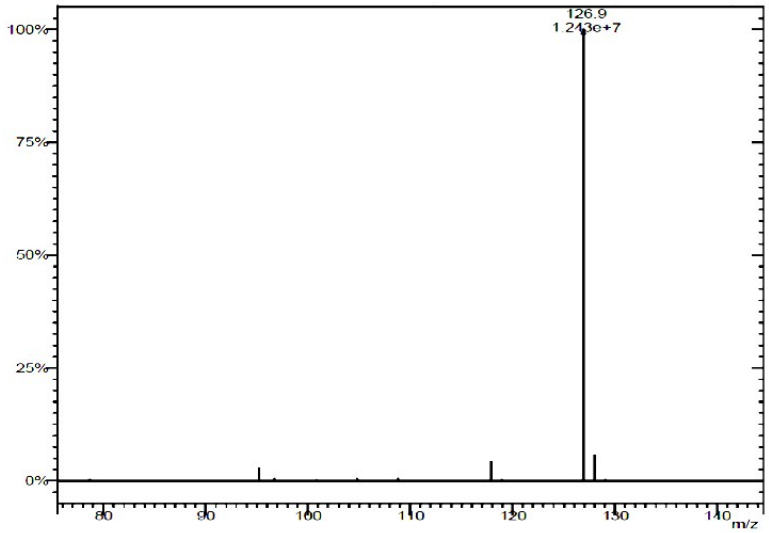

Figure S29 ESI-MS(+) spectrum of compound 3b

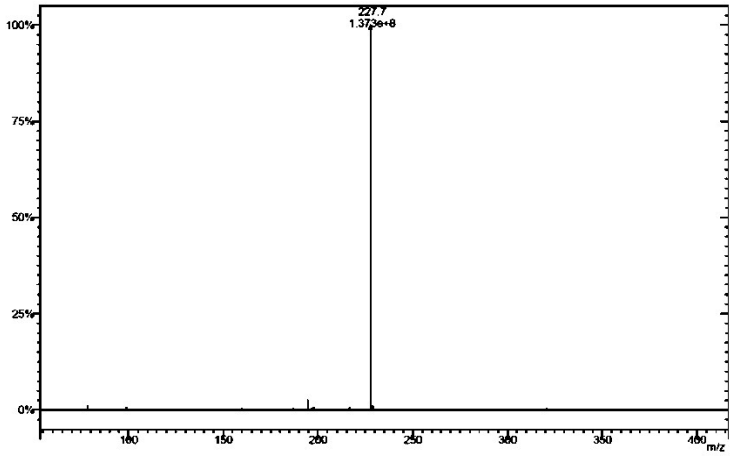

Figure S30 ESI-MS(-) spectrum of compound 3b

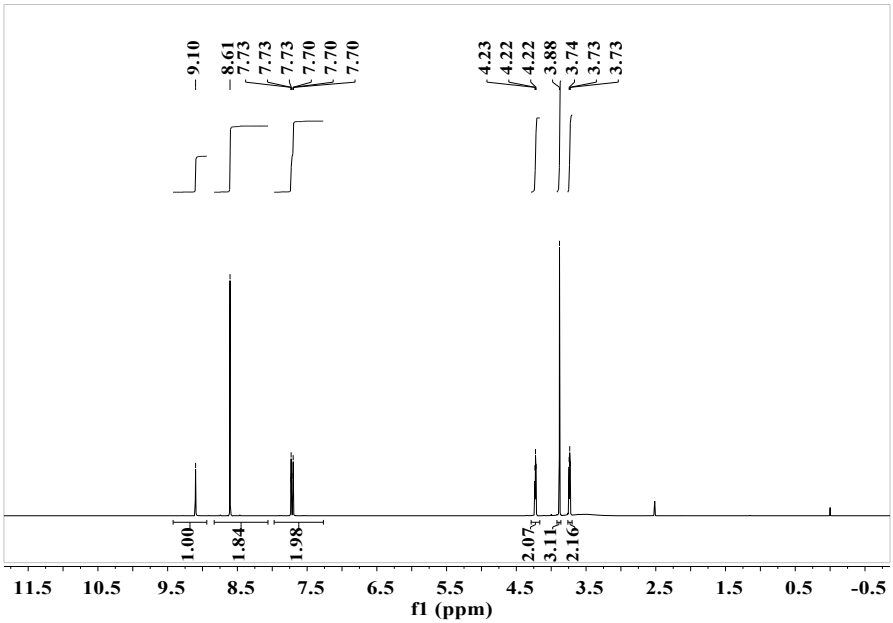

Figure S31 ^{1}H NMR spectrum of compound 3b in DMSO-d_6

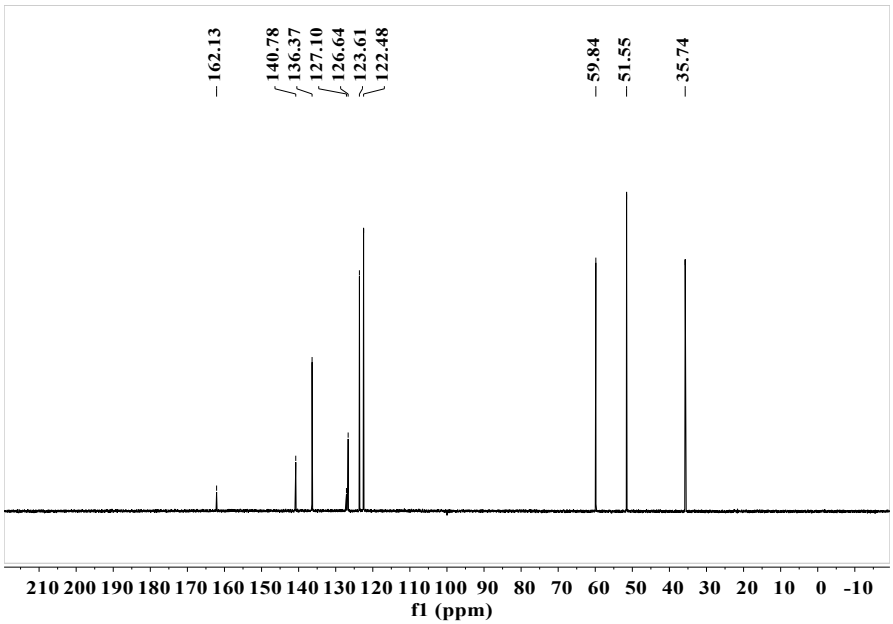

Figure S32 ^{13}C NMR spectrum of compound 3b in D_2O

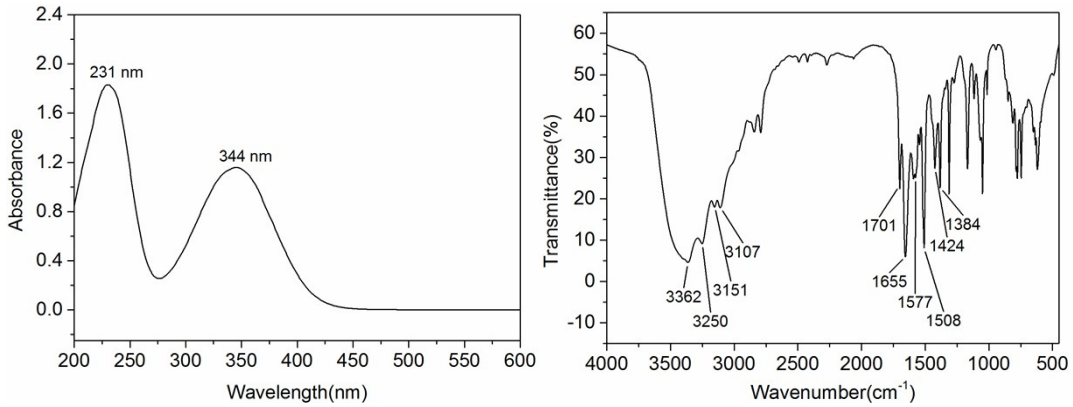

Figure S33 UV-Vis and FT-IR spectra of compound 3c.

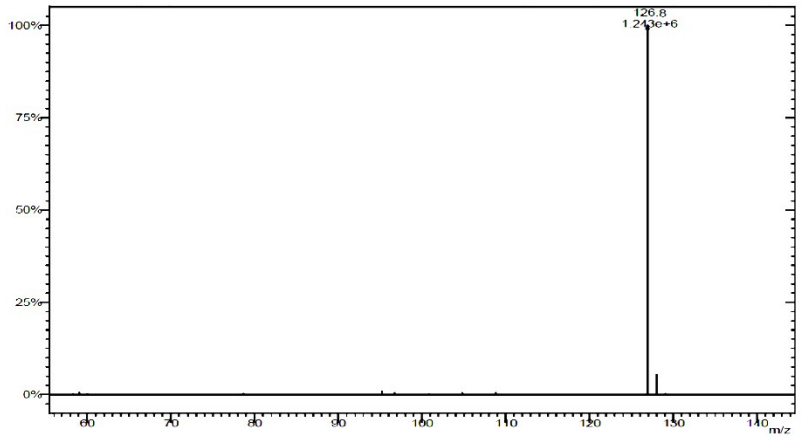

Figure S34 ESI-MS(+) spectrum of compound 3c

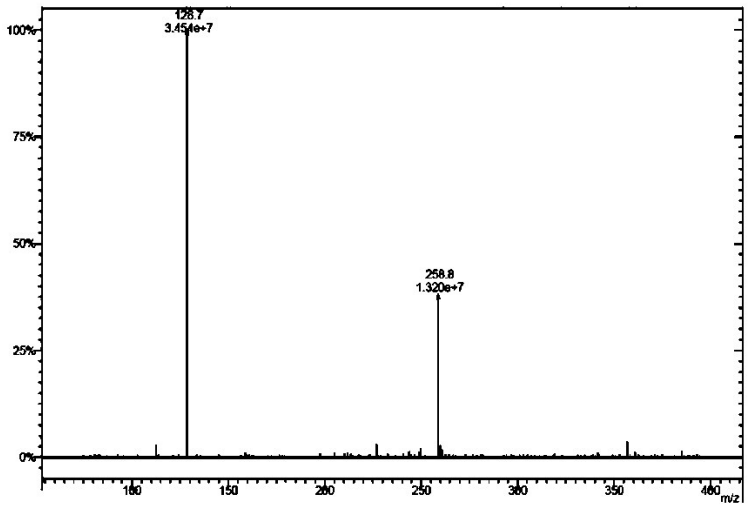

Figure S35 ESI-MS(-) spectrum of compound 3c

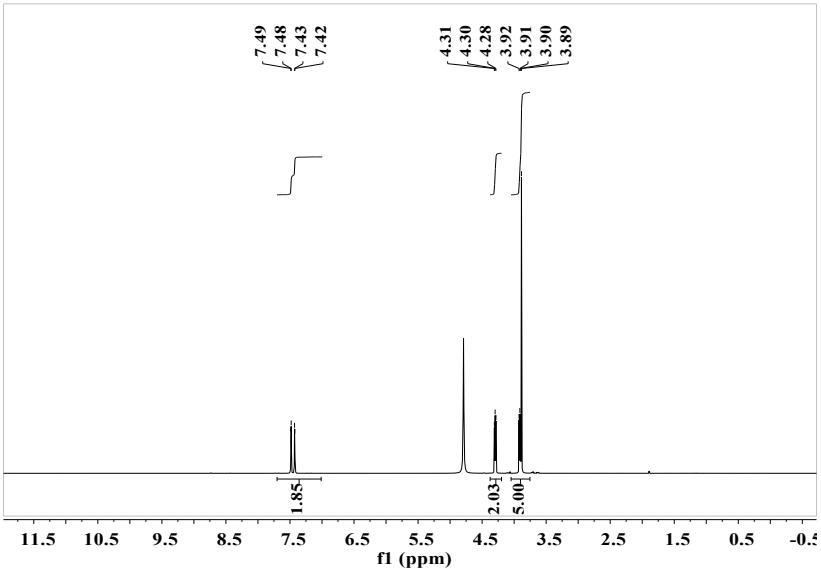

Figure S36 ^{1}H NMR spectrum of compound 3c in D_2O

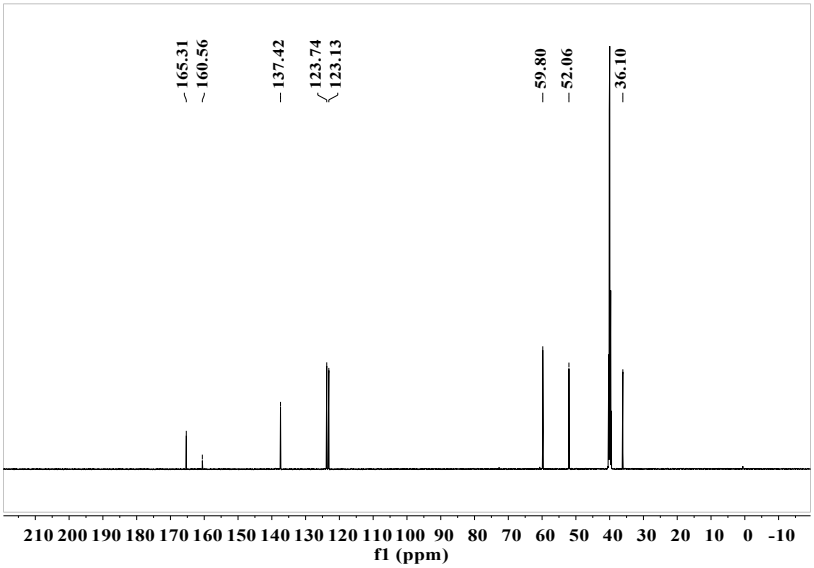

Figure S37 ^{13}C NMR spectrum of compound 3c in DMSO-d_6

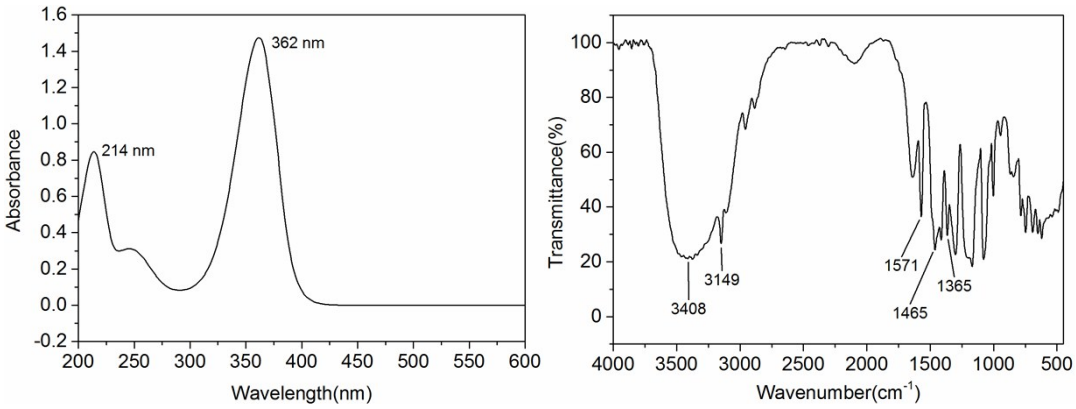

Figure S38 UV-Vis and FT-IR spectra of compound 3d.

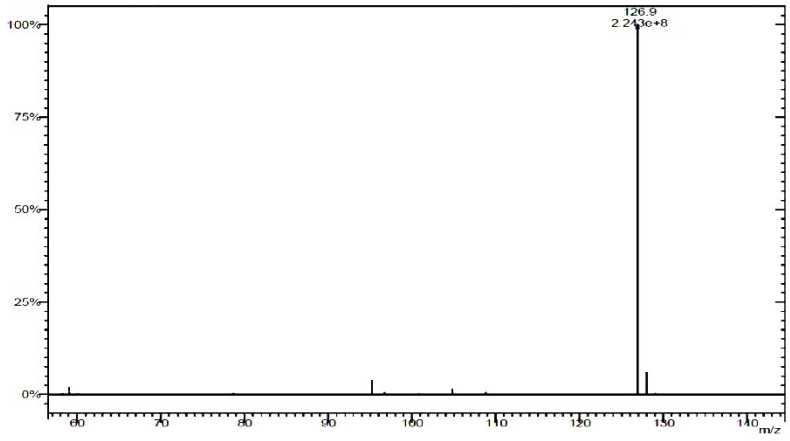

Figure S39 ESI-MS(+) spectrum of compound 3d

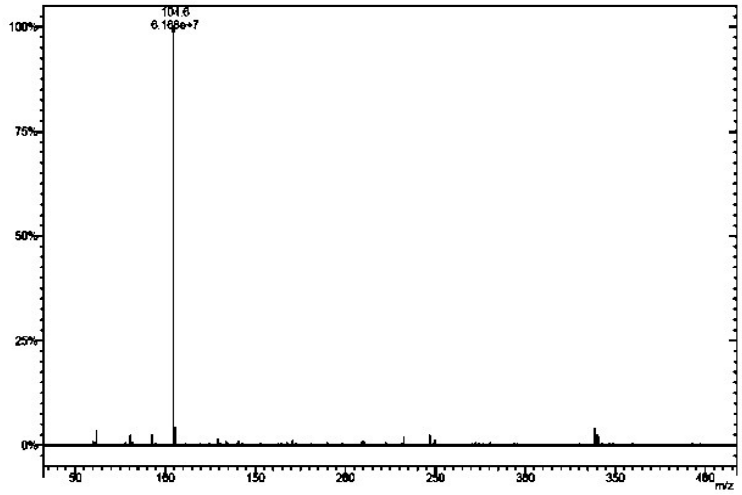

Figure S40 ESI-MS(-) spectrum of compound 3d

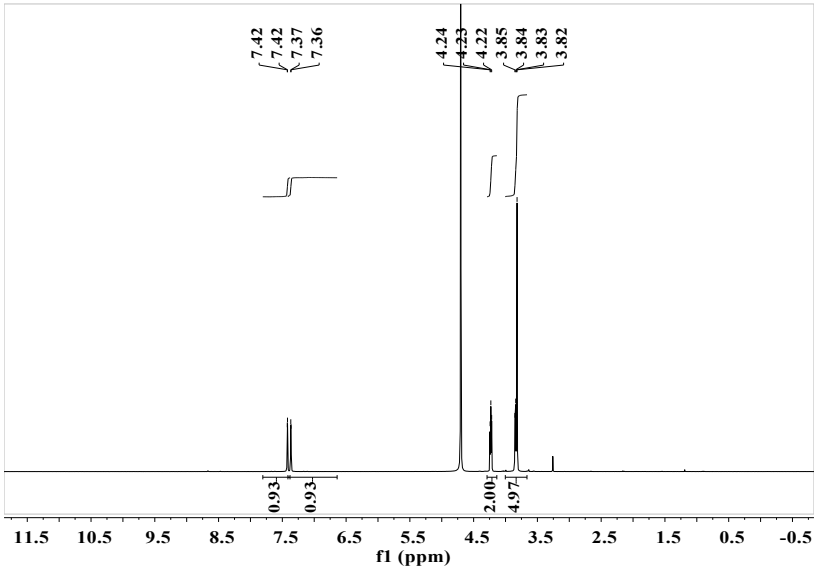

Figure S41 ^{1}H NMR spectrum of compound 3d in D_2O

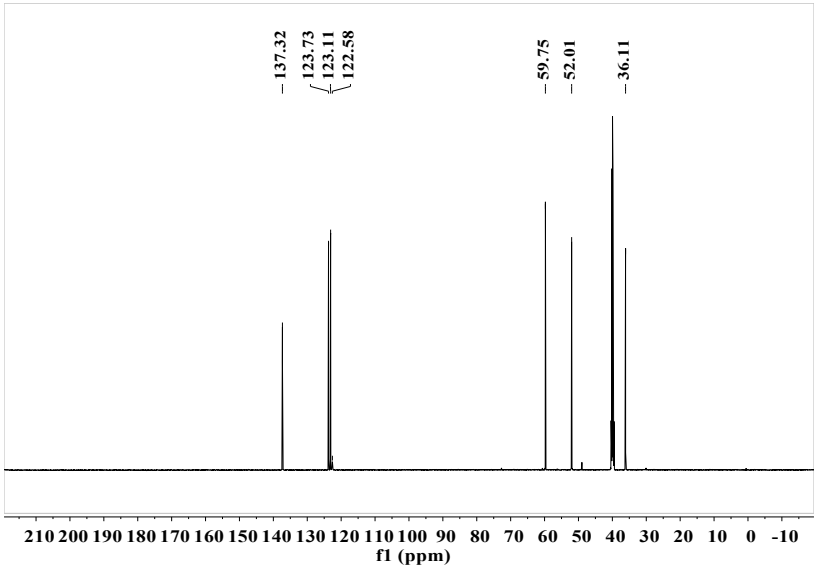

Figure S42 ^{13}C NMR spectrum of compound 3d in DMSO-d_6

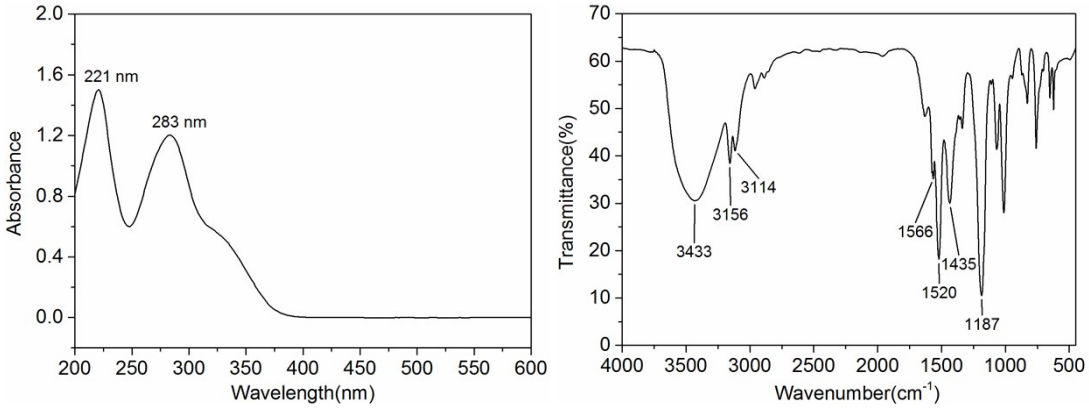

Figure S43 UV-Vis and FT-IR spectra of compound 3e.

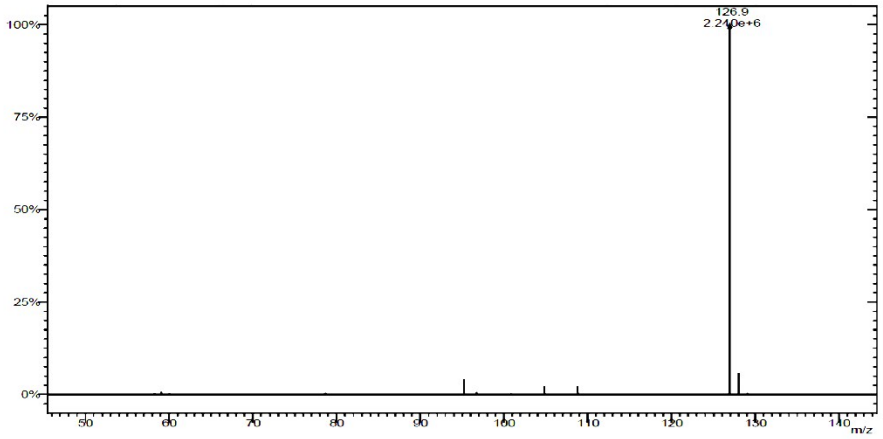

Figure S44 ESI-MS(+) spectrum of compound 3e

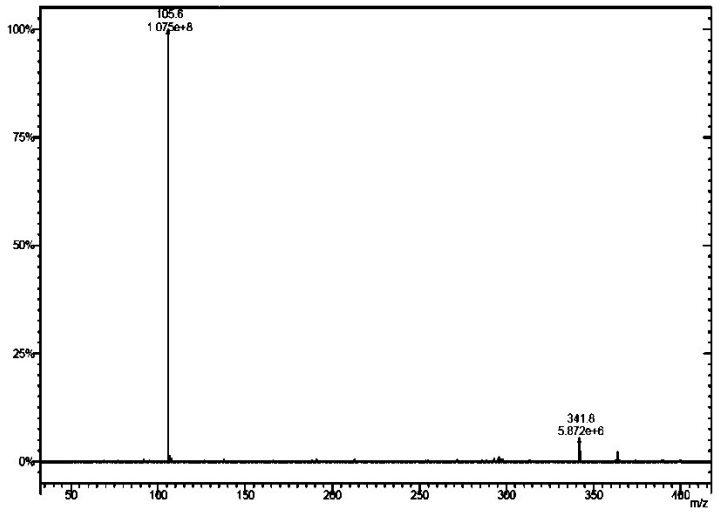

Figure S45 ESI-MS(-) spectrum of compound 3e

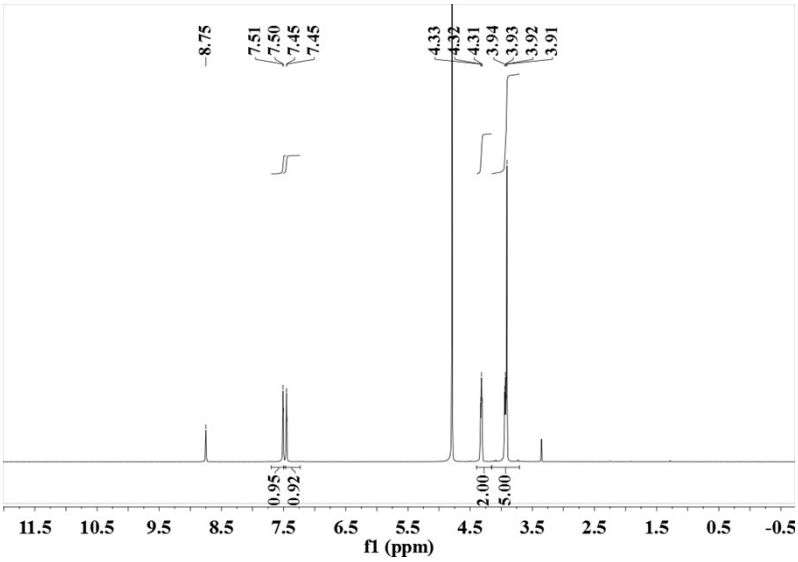

Figure S46 ^{1}H NMR spectrum of compound 3e in D_2O

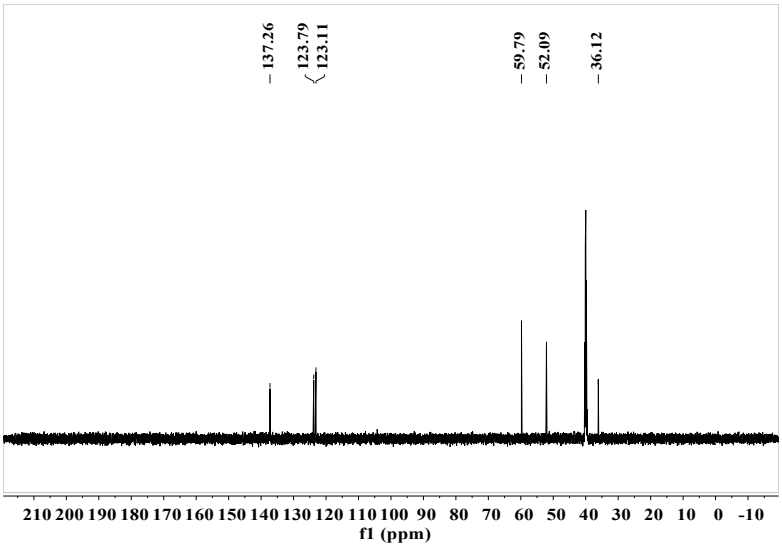

Figure S47 ^{13}C NMR spectrum of compound 3e in DMSO-d_6

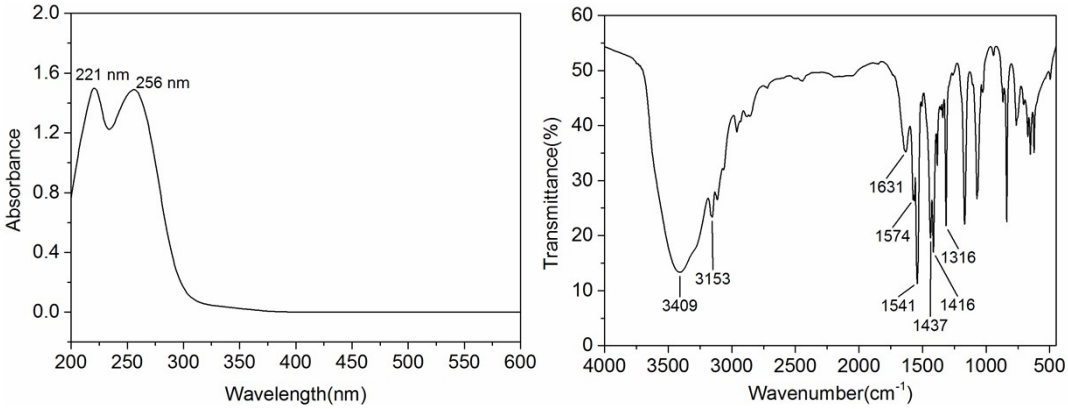

Figure S48 UV-Vis and FT-IR spectra of compound 3f.

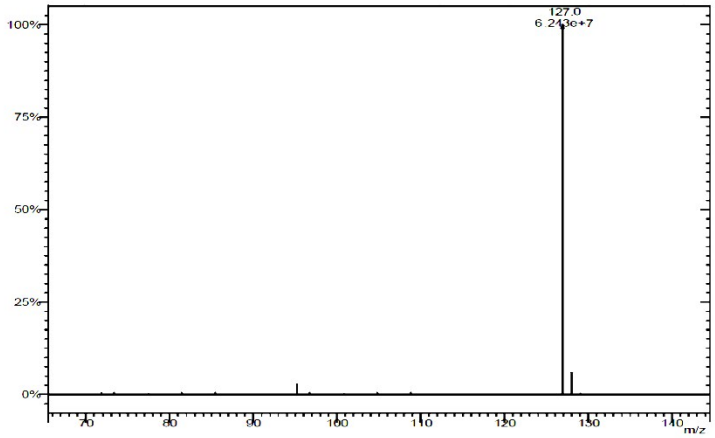

Figure S49 ESI-MS(+) spectrum of compound 3f

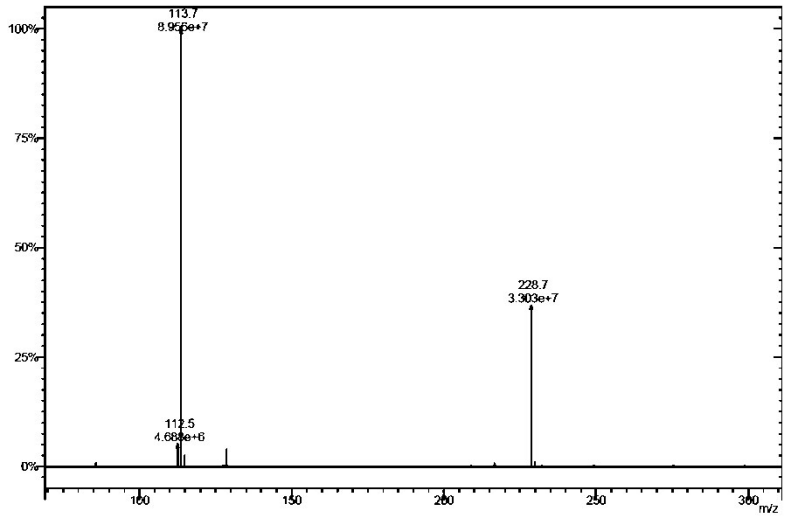

Figure S50 ESI-MS(-) spectrum of compound 3f

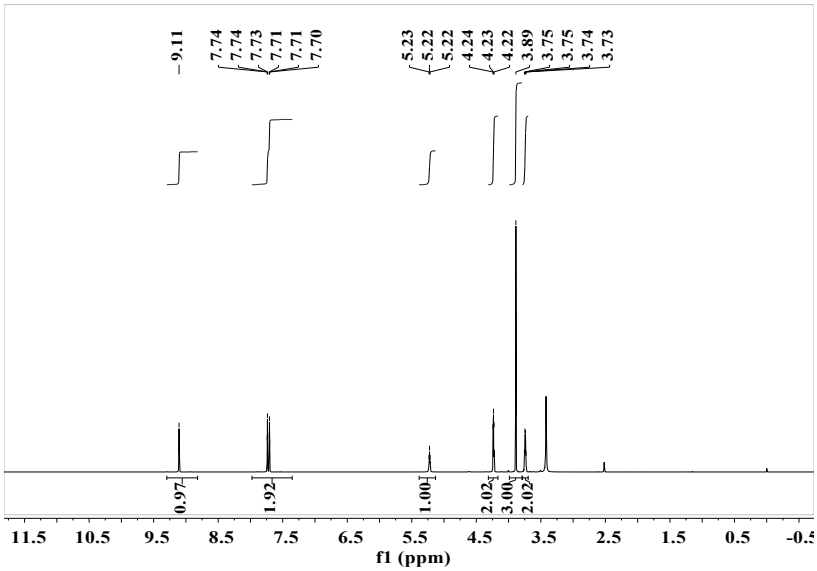

Figure S51 ^{1}H NMR spectrum of compound 3f in DMSO-d_6

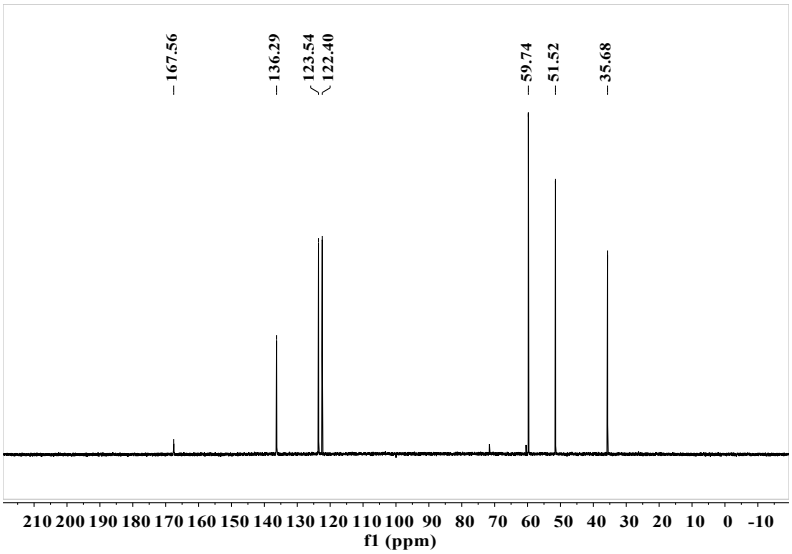

Figure S52 ^{13}C NMR spectrum of compound 3f in D_2O

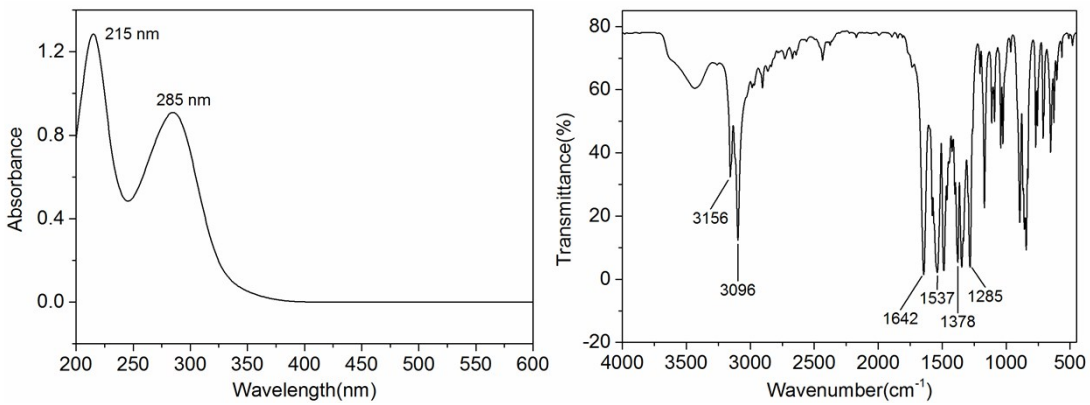

Figure S53 UV-Vis and FT-IR spectra of compound 4a.

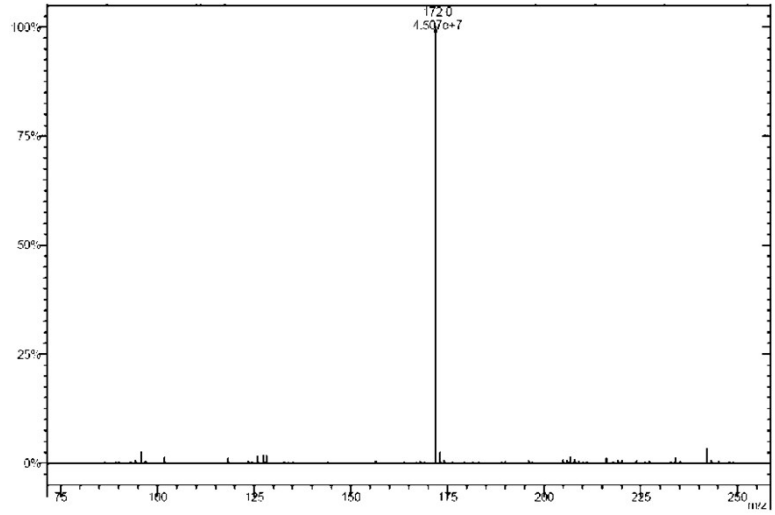

Figure S54 ESI-MS (+) spectrum of compound 4a.

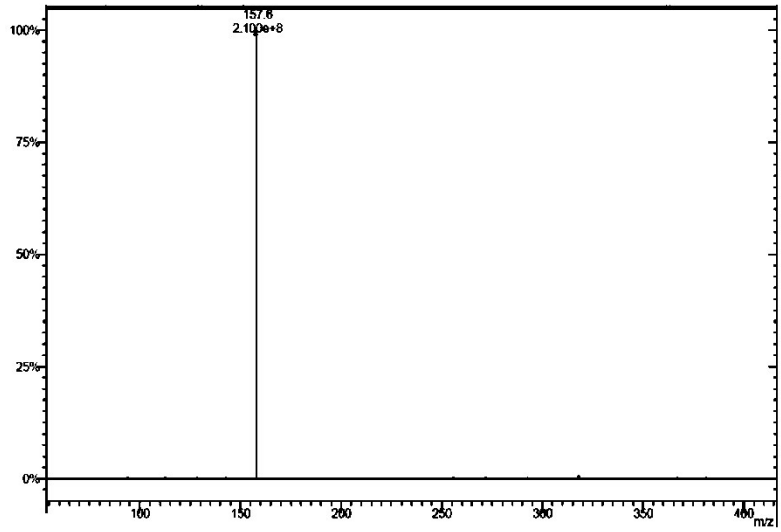

Figure S55 ESI-MS (-) spectrum of compound 4a.

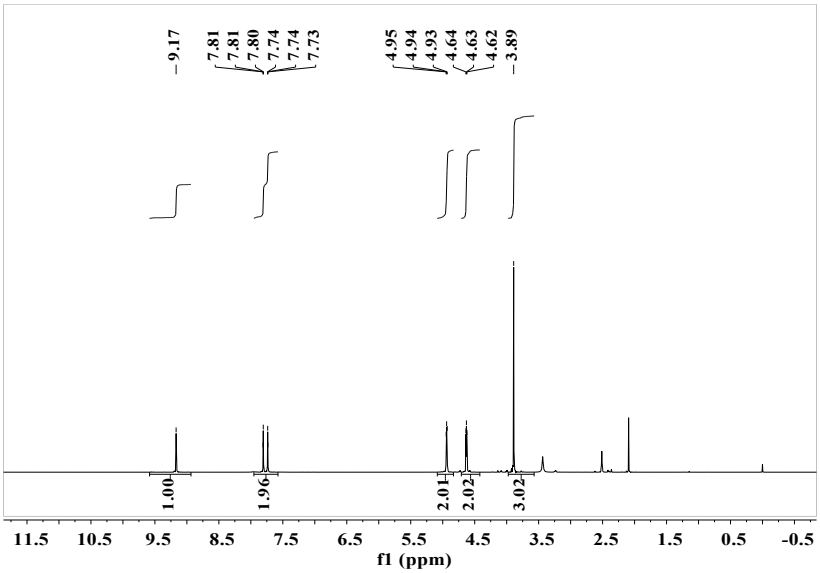

Figure S56 ^{1}H-NMR spectrum of compound 4a in DMSO-d$_6$.

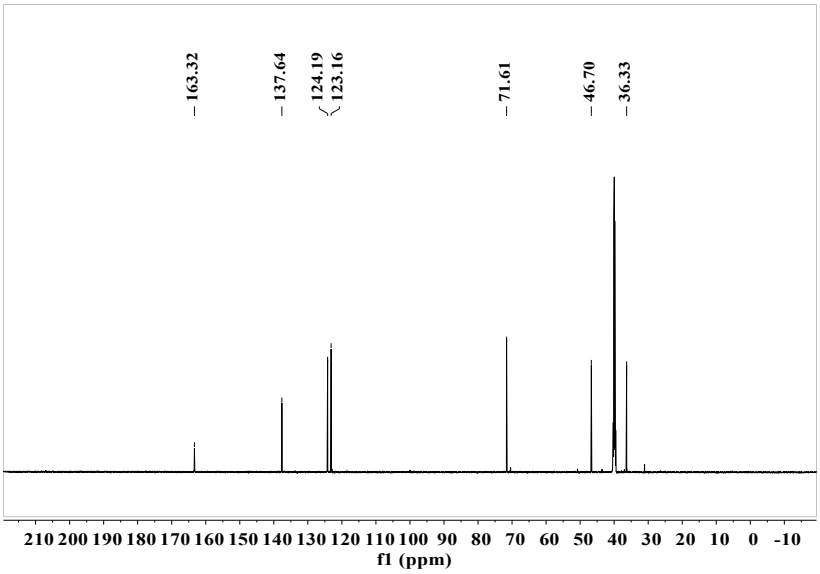

Figure S57 ^{13}C-NMR spectrum of compound 4a in DMSO-d$_6$.

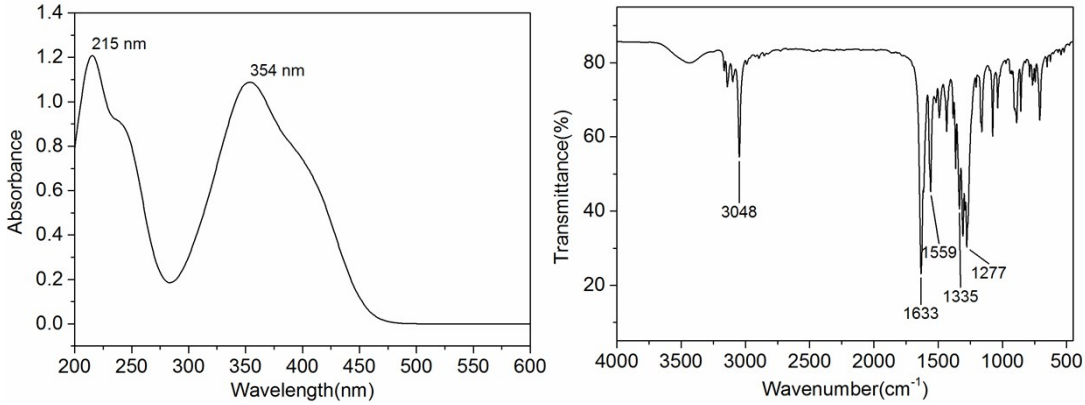

Figure S58 UV-Vis and FT-IR spectra of compound 4b.

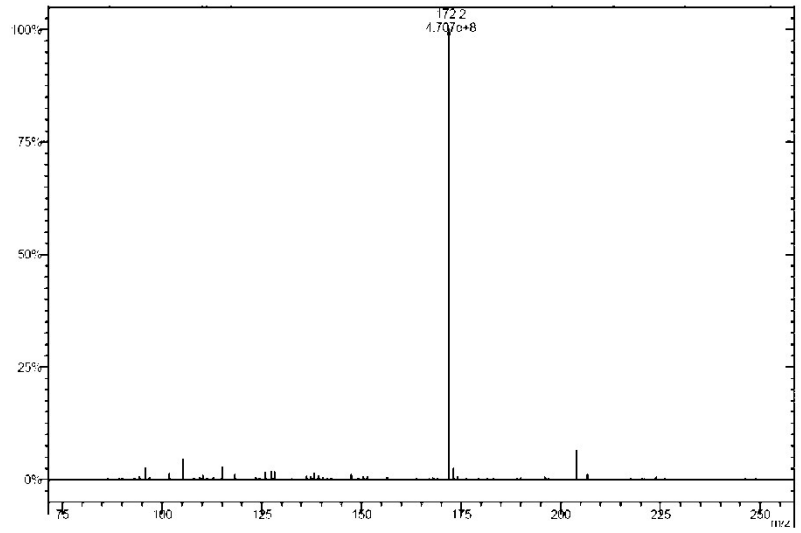

Figure S59 ESI-MS (+) spectrum of compound 4b.

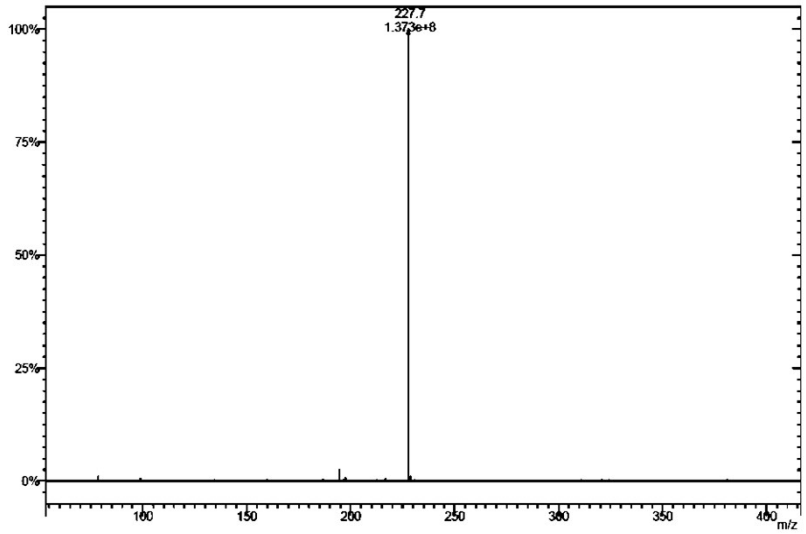

Figure S60 ESI-MS (-) spectrum of compound 4b.

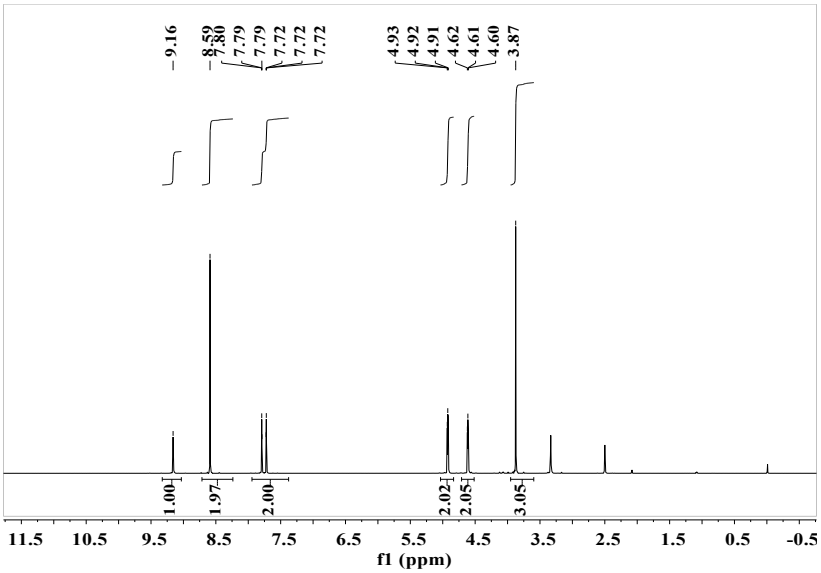

Figure S61 ^{1}H-NMR spectrum of compound 4b in DMSO-d_6.

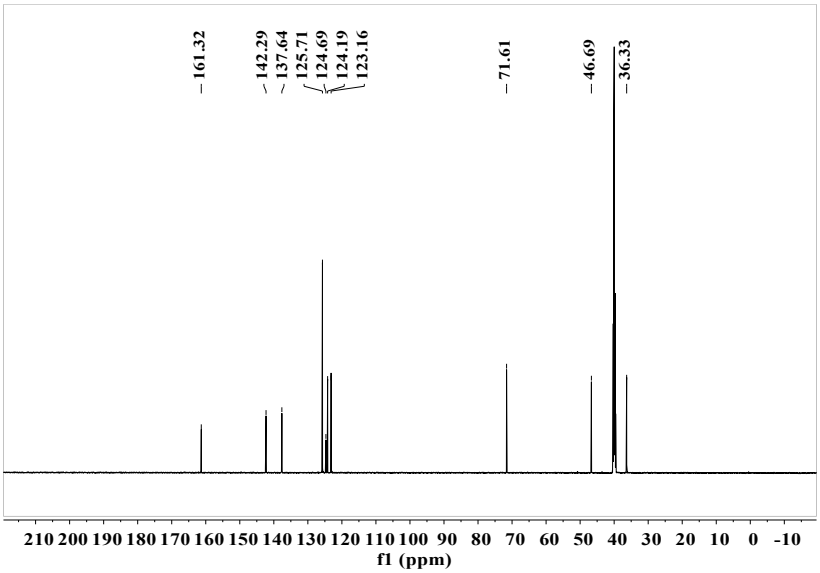

Figure S62 ^{13}C-NMR spectrum of compound 4b in DMSO-d$_6$.

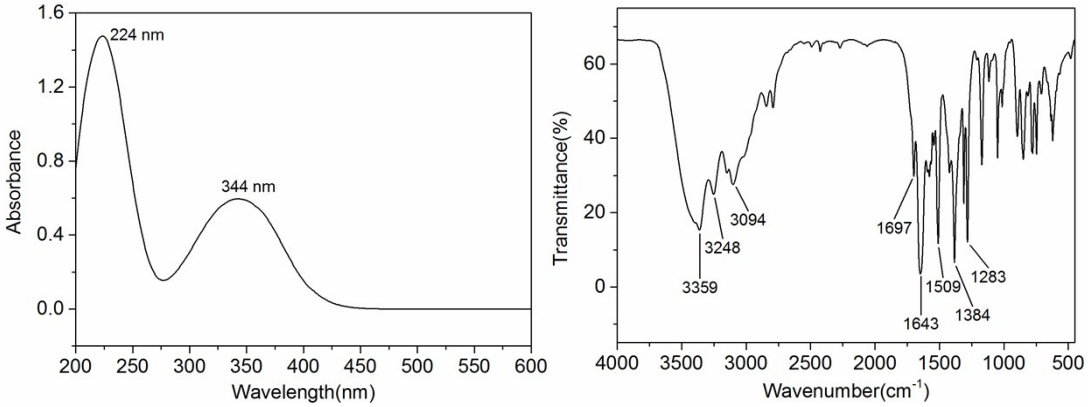

Figure S63 UV-Vis and FT-IR spectra of compound 4c.

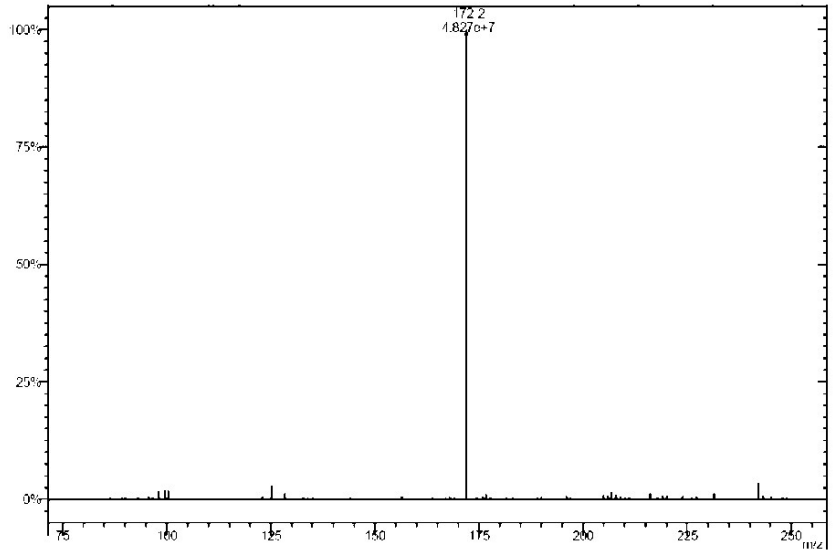

Figure S64 ESI-MS (+) spectrum of compound 4c.

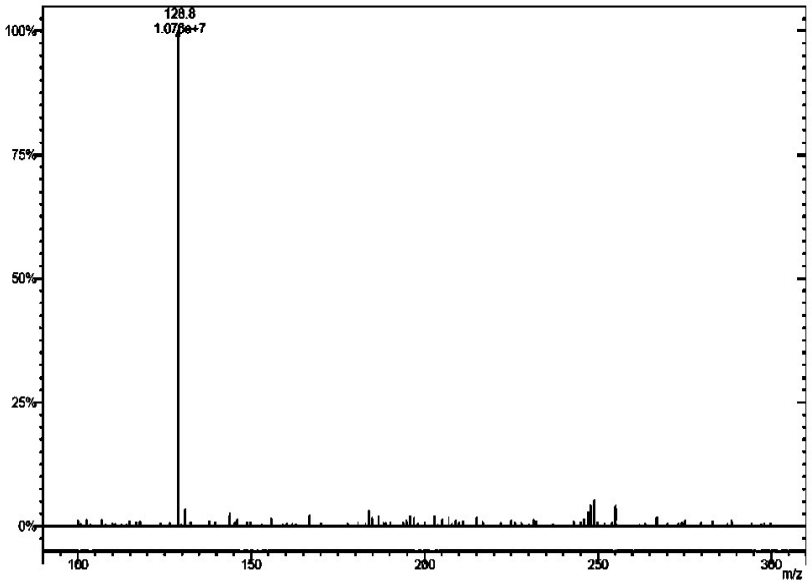

Figure S65 ESI-MS (-) spectrum of compound 4c.

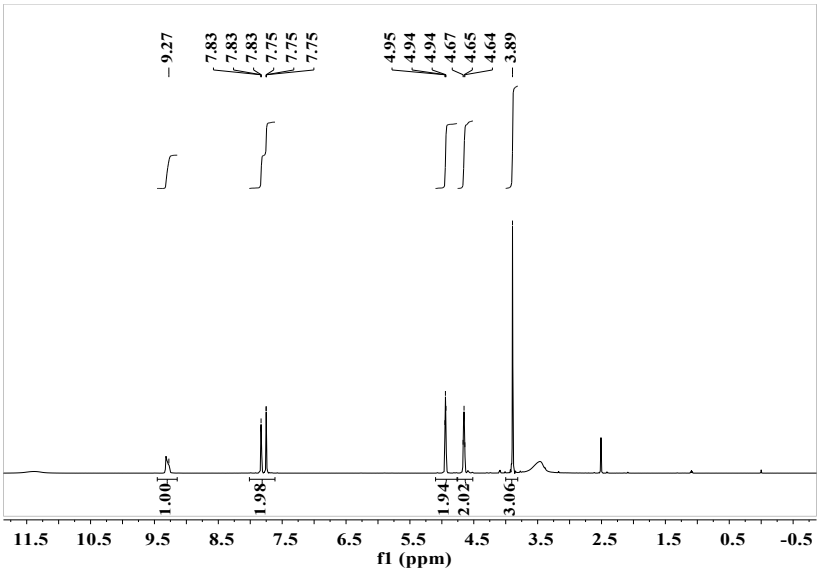

Figure S66 ^{1}H-NMR spectrum of compound 4c in DMSO-d_6.

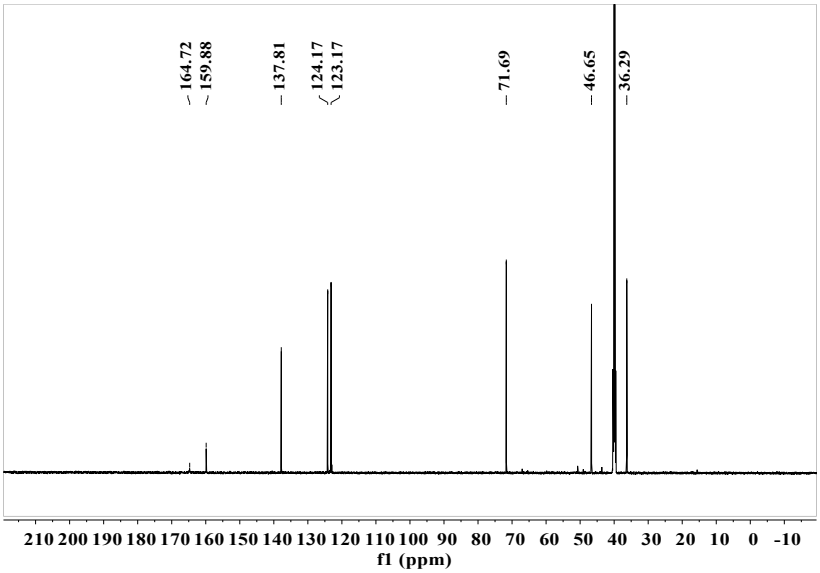

Figure S67 ^{13}C-NMR spectrum of compound 4c in DMSO-d$_6$.

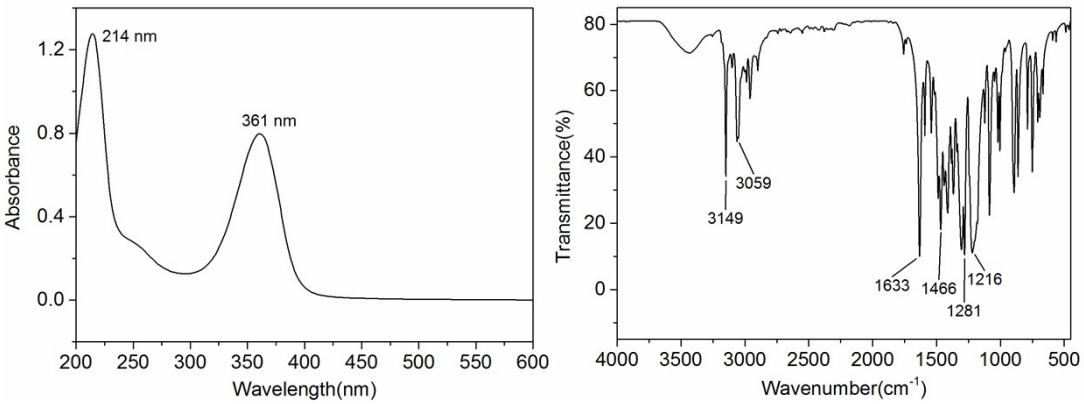

Figure S68 UV-Vis and FT-IR spectra of compound 4d.

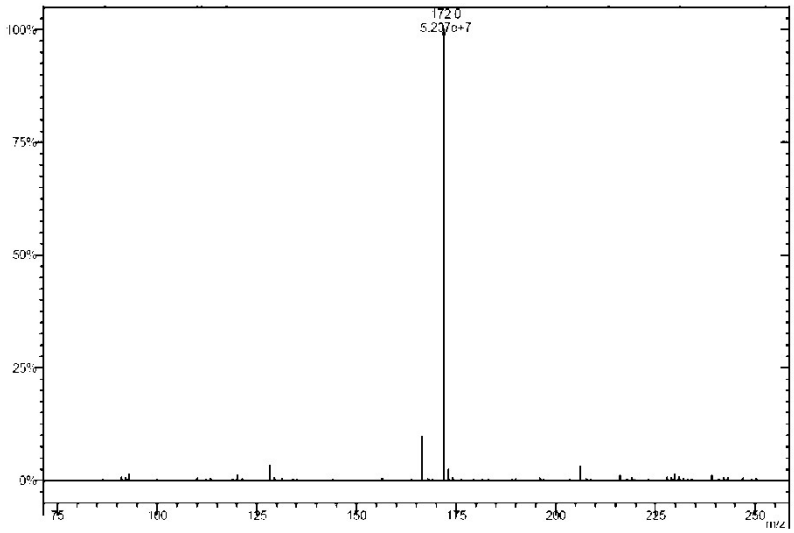

Figure S69 ESI-MS (+) spectrum of compound 4d.

Figure S70 ESI-MS (-) spectrum of compound 4d.

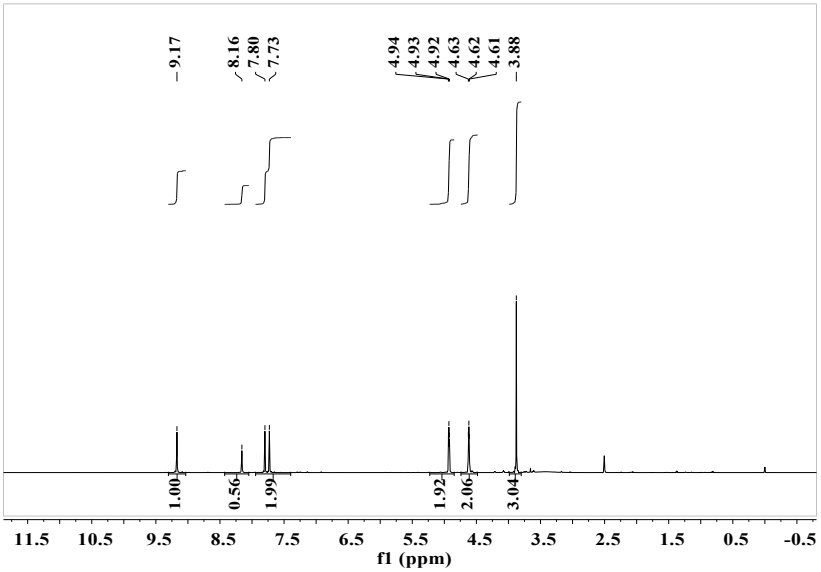

Figure S71 ^{1}H-NMR spectrum of compound 4d in DMSO-d$_6$.

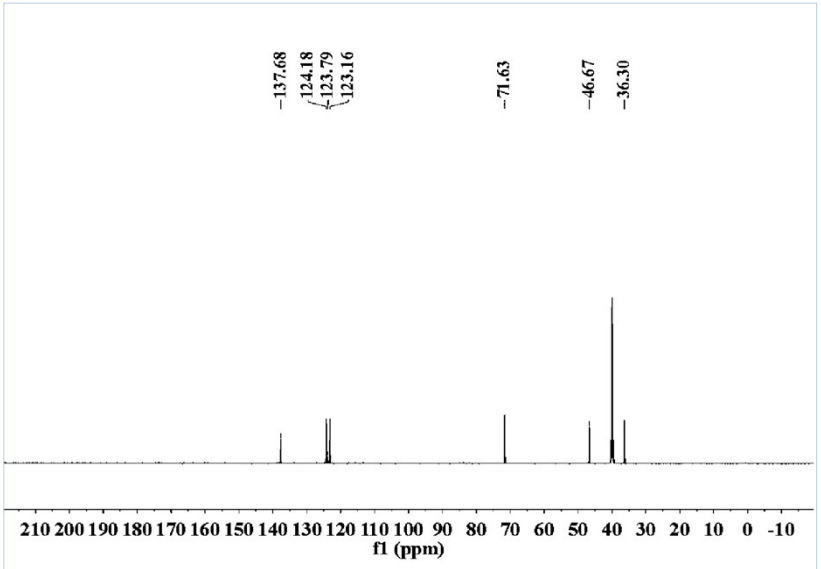

Figure S72 ^{13}C-NMR spectrum of compound 4d in DMSO-d$_6$.

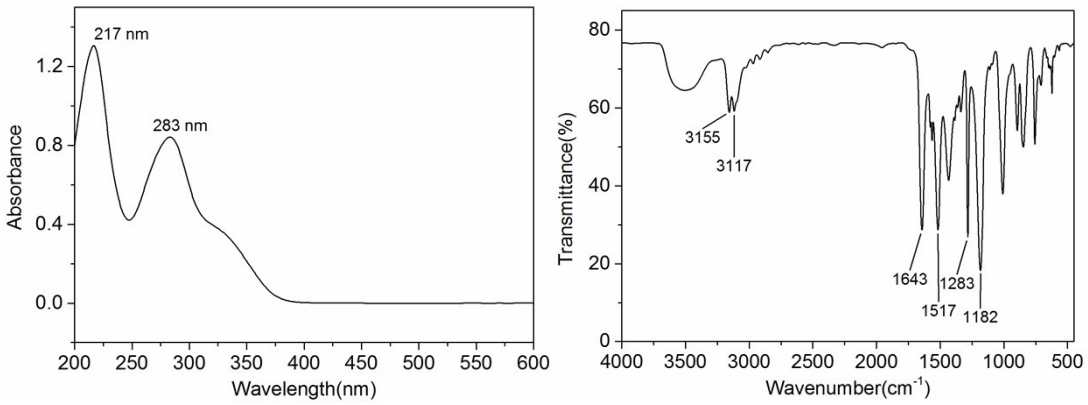

Figure S73 UV-Vis and FT-IR spectra of compound 4e.

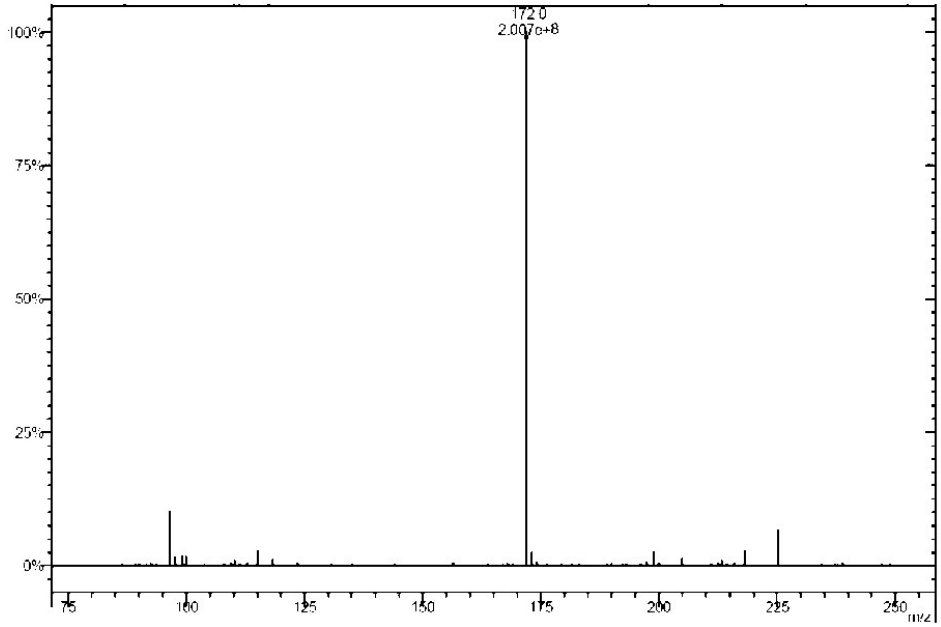

Figure S74 ESI-MS (+) spectrum of compound 4e.

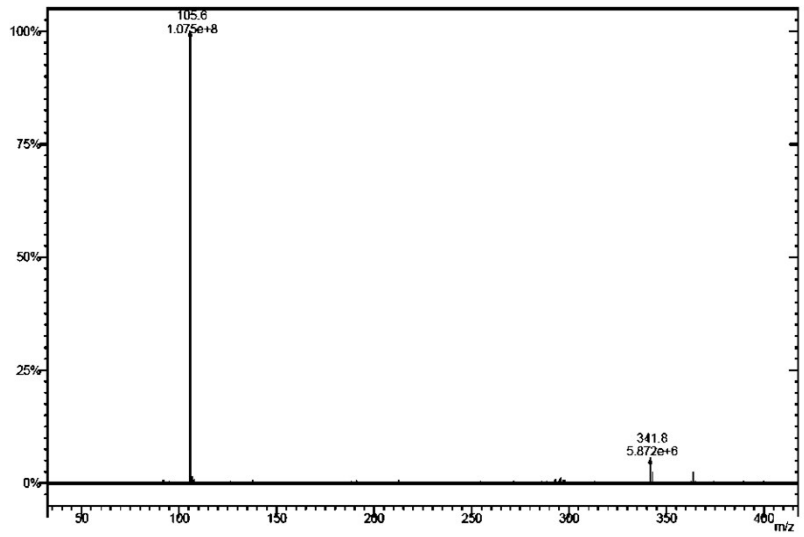

Figure S75 ESI-MS (-) spectrum of compound 4e.

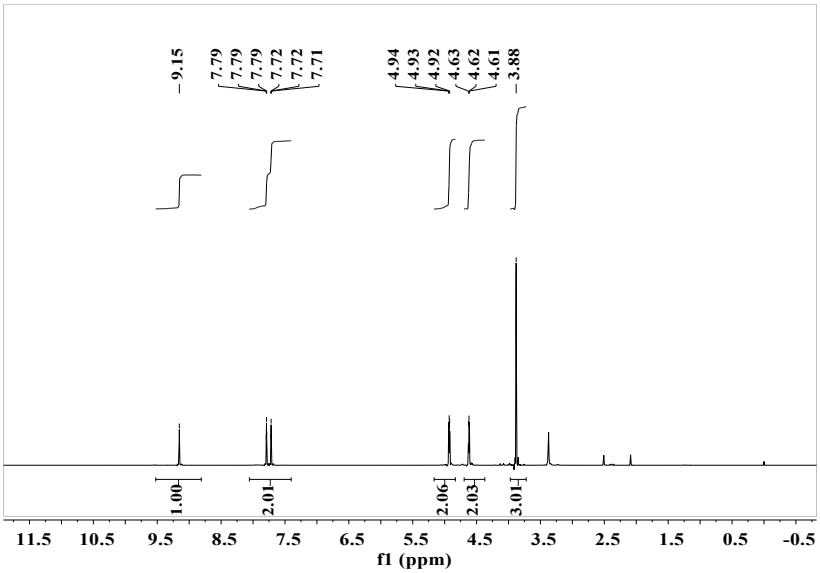

Figure S76 ^{1}H-NMR spectrum of compound 4e in DMSO-d$_6$.

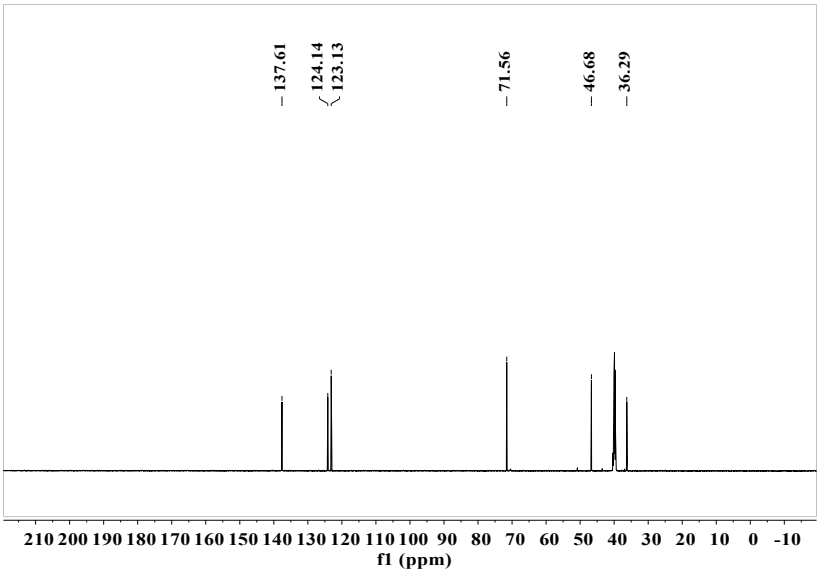

Figure S77 ^{13}C-NMR spectrum of compound 4e in DMSO-d$_6$.

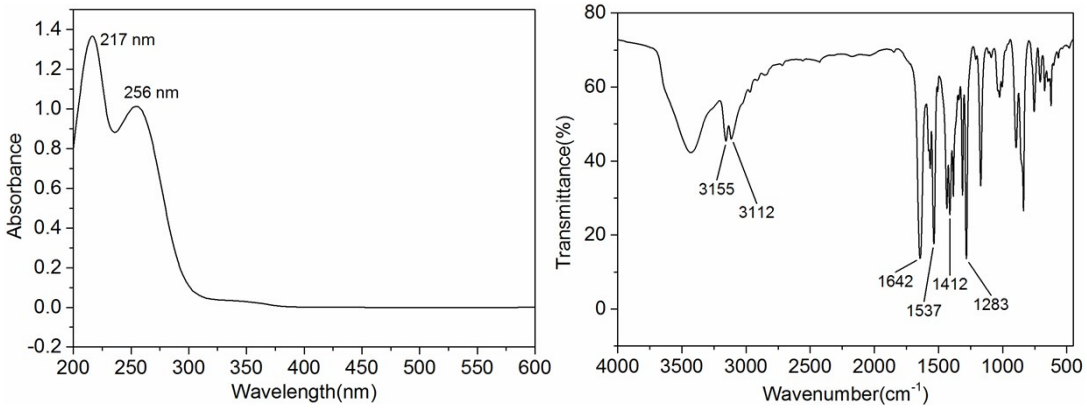

Figure S78 UV-Vis and FT-IR spectra of compound 4f.

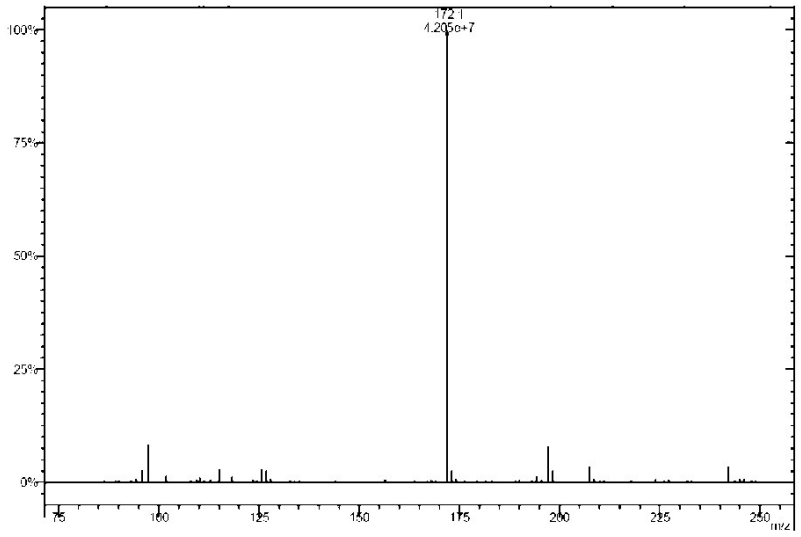

Figure S79 ESI-MS (+) spectrum of compound 4f.

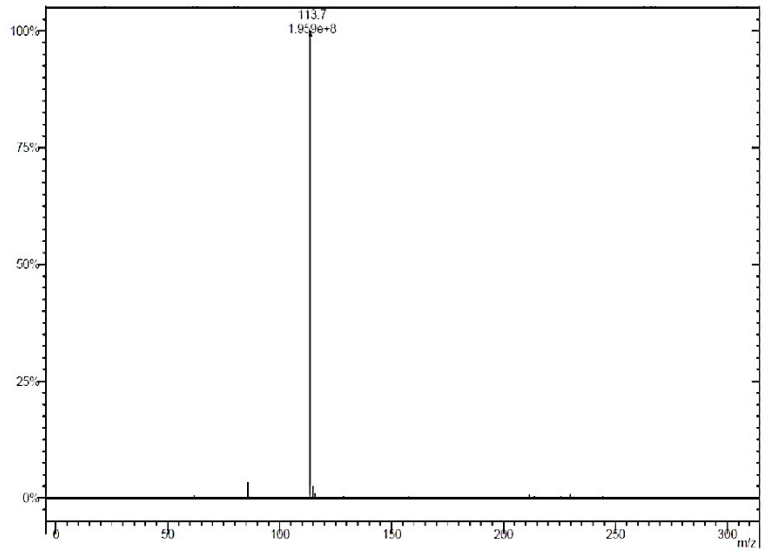

Figure S80 ESI-MS (-) spectrum of compound 4f.

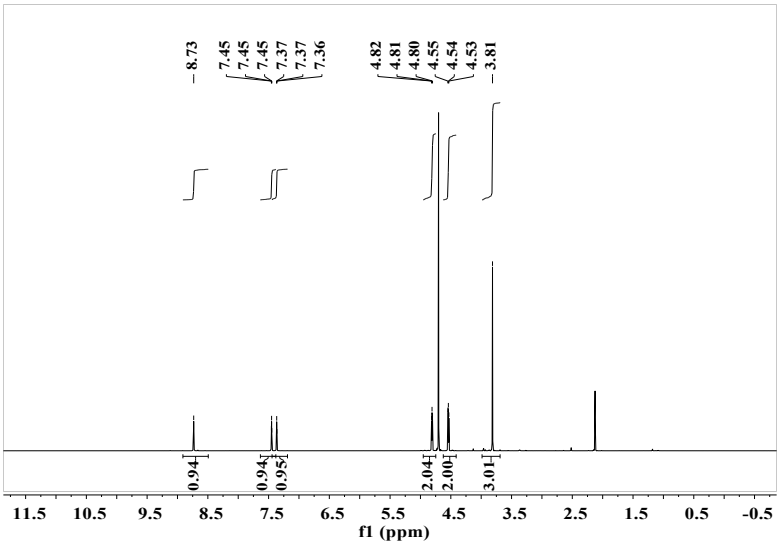

Figure S81 ^{1}H-NMR spectrum of compound 4f in D_2O.

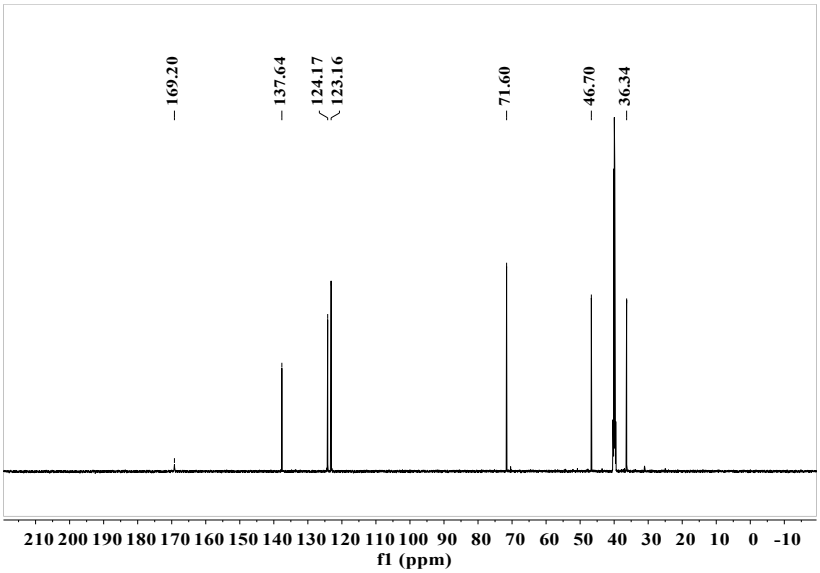

Figure S82 ^{13}C-NMR spectrum of compound 4f in DMSO-d_6.