

## Electronic supplementary information (ESI)

### Two intensified fluorescence colors switching achieved by branched dyes nano aggregates

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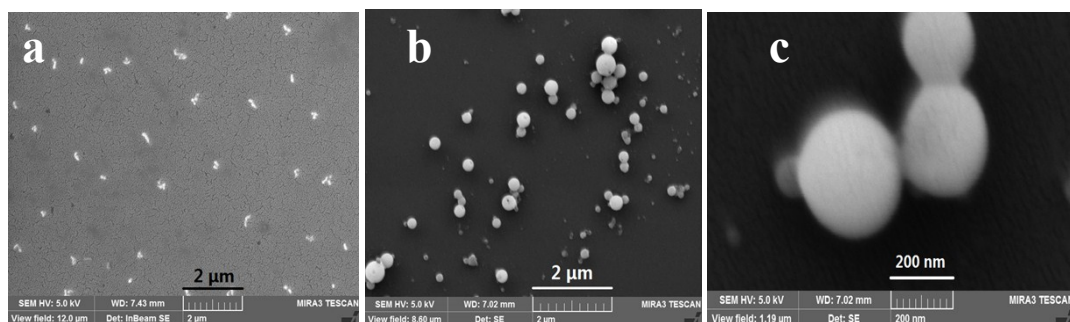
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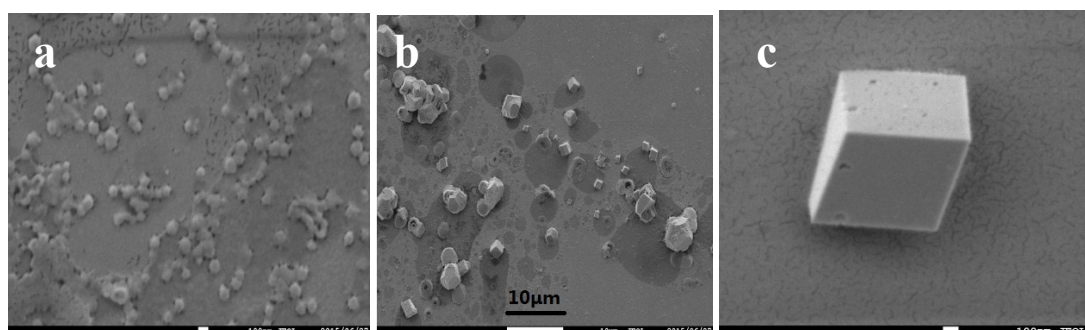
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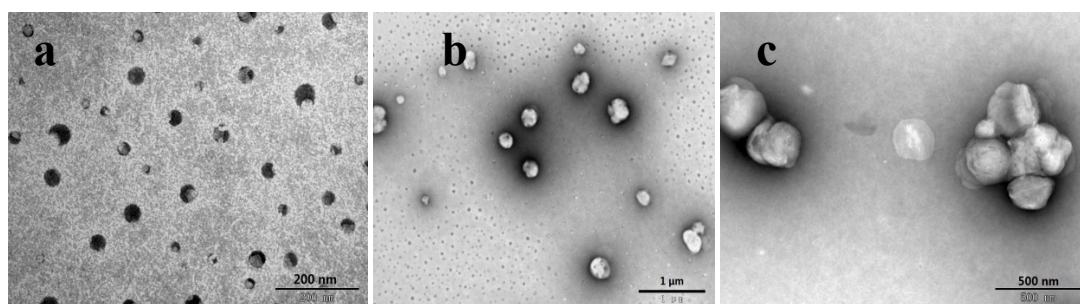
## 1. Supporting Tables and Figures



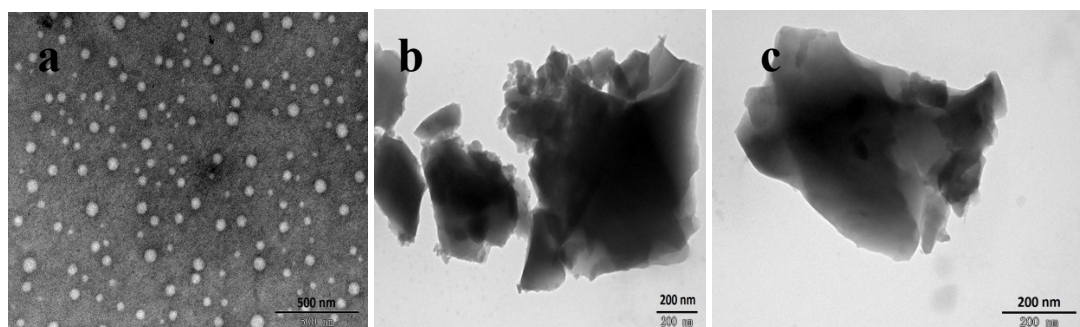
**Figure S1** SEM images of C3 aggregates in DMF/H<sub>2</sub>O (60% water sample, v/v) solution ( $1 \times 10^{-5}$  mol/L) at different aggregation time courses of 30 min (a) and 12 h (b, c), (c) is the magnified image at 12 h.



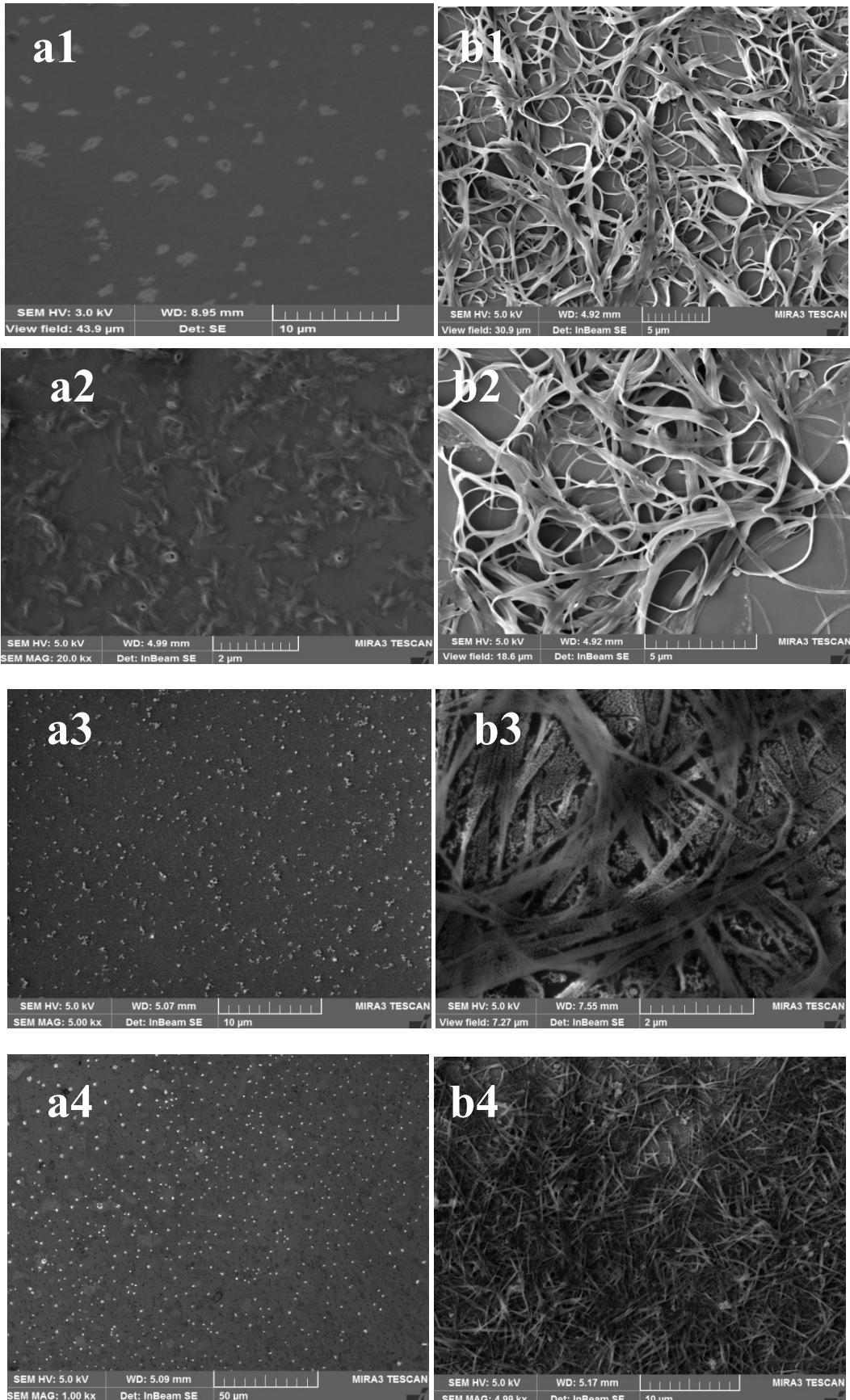
**Figure S2** SEM images of C5 aggregates in THF/H<sub>2</sub>O (60% water sample, v/v) mixed solution ( $1 \times 10^{-5}$  mol/L) at different aggregation time courses of 30 min (a) and 12 h (b, c), (c) is the magnified image at 12 h.

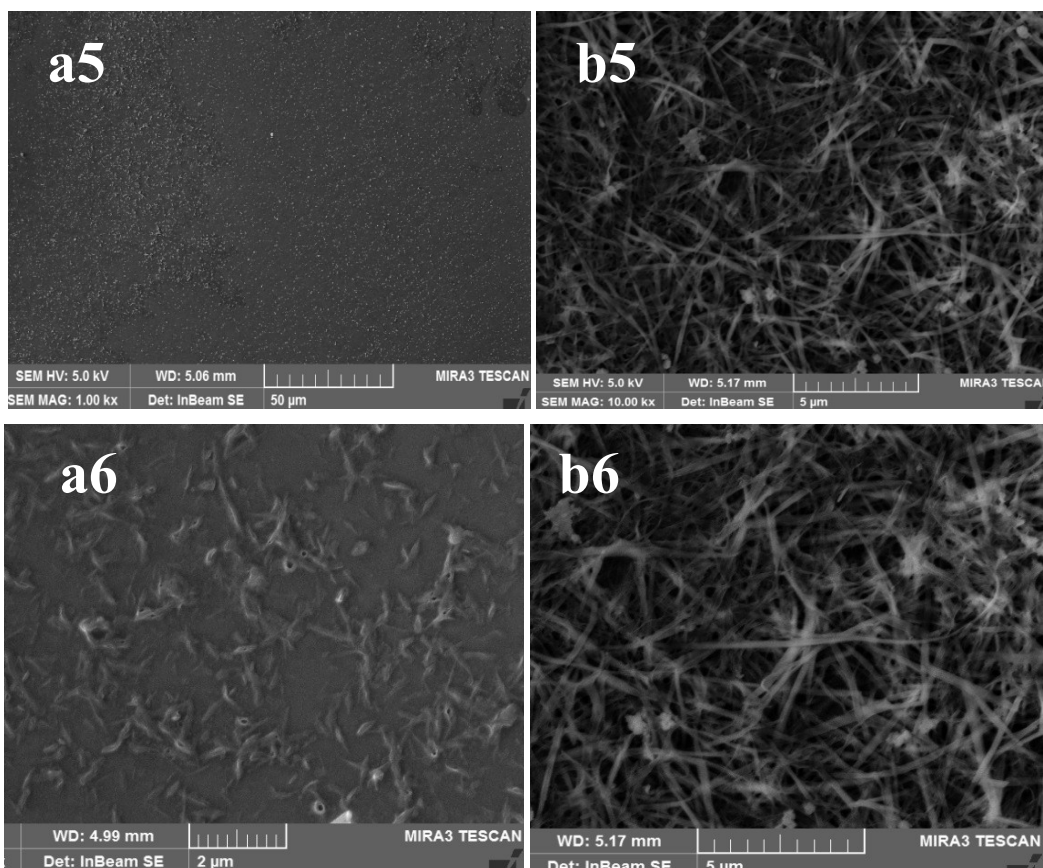


**Figure S3** TEM images of C3 aggregates in DMF/H<sub>2</sub>O (60% water sample, v/v) solution ( $1 \times 10^{-5}$  mol/L) at different aggregation time courses of 30 min (a) and 12 h (b, c), (c) is the magnified image at 12 h.

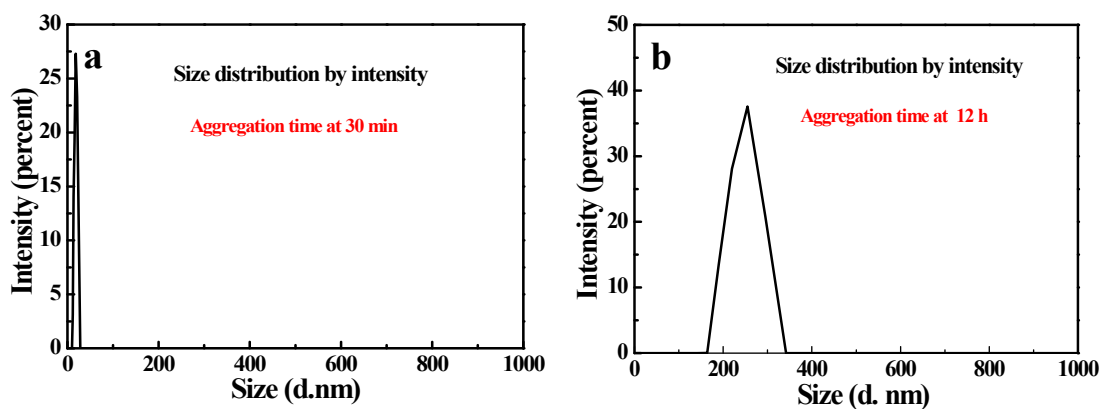


**Figure S4** TEM images of C5 aggregates in THF/H<sub>2</sub>O (60% water fraction, v/v) solution ( $1 \times 10^{-5}$  mol/L) at different aggregation time courses of 30 min (a) and 12 h (b, c), (c) is the magnified image at 12 h.

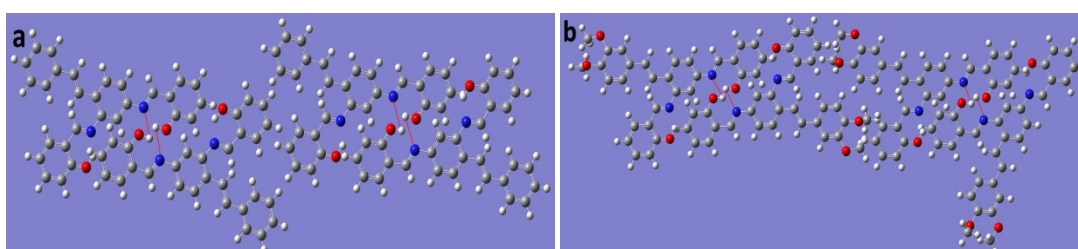




**Figure S5** SEM images of C11 (a1/b1), C12 (a2/b2), C13 (a3/b3), C14 (a4/b4), C15 (a5/b5) and C16 (a6/b6) in mixed DMF/H<sub>2</sub>O (40/60 (v/v)) solution ( $1 \times 10^{-5}$  mol/L), (a1-a4) at the aggregation time course of 30 min and (b1~b4) at aggregation time course of 12 h.

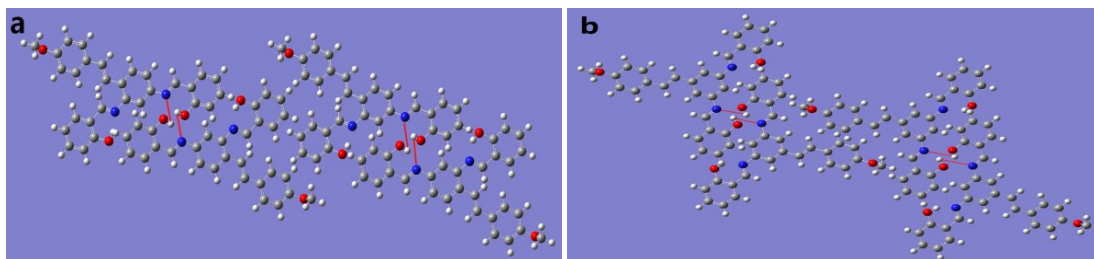


**Figure S6** Size distribution of C1 aggregates (at 30 min (a) and 12 h (b) respectively) in DMF/H<sub>2</sub>O (40/60 (v/v)) mixture solution ( $1 \times 10^{-5}$  mol/L) obtained by DLS.

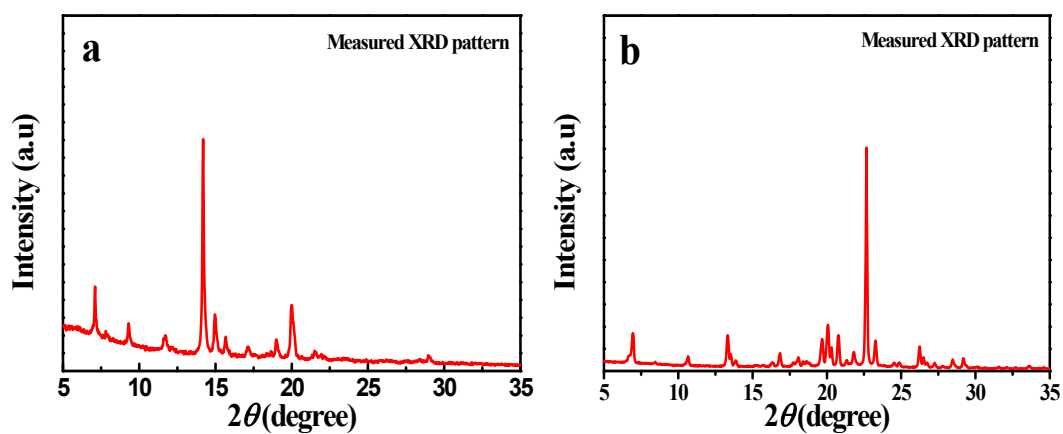




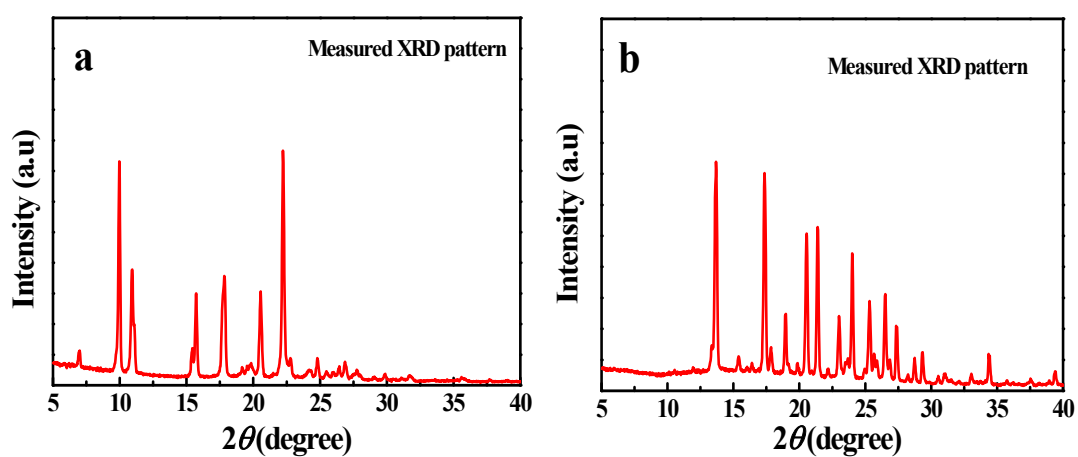
**Figure S7** Simulated stacking modes of **C1** (a) and **C3** (b) molecules utilizing the  $\pi$ - $\pi$  stacking interaction and intermolecular hydrogen bond interaction (O-H $\cdots$ N, red line).



**Figure S8** Simulated stacking modes of **C2** (a) and **C5** (b) molecules utilizing the  $\pi$ - $\pi$  stacking interaction and intermolecular hydrogen bond interaction (O-H $\cdots$ N, red line).



**Figure S9** Measured XRD pattern of powders of **C5** (a) and **C6** (b).



**Figure S10** Measured XRD pattern of powders of **C11** (a) and **C14** (b).

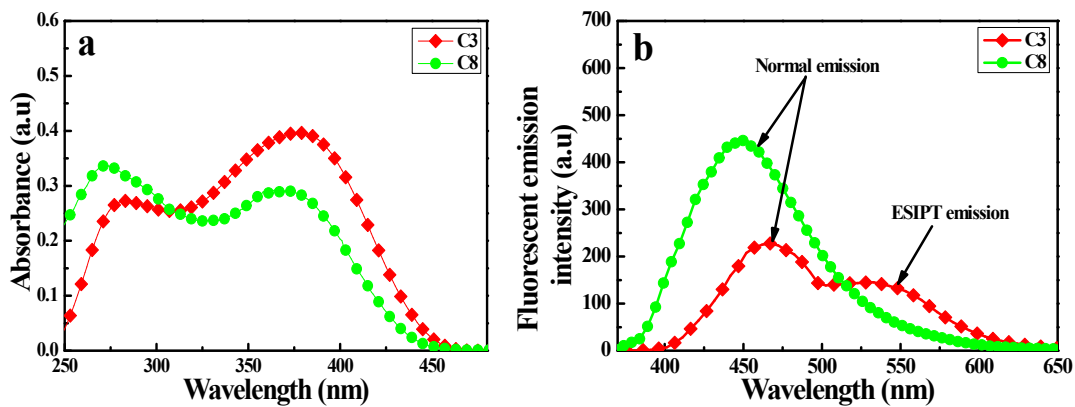


Figure S11 (a) UV absorption spectra and emission spectra of C3 and C8 in DMF solution, Ex: 350 nm, C,  $1 \times 10^{-5}$  mol/L

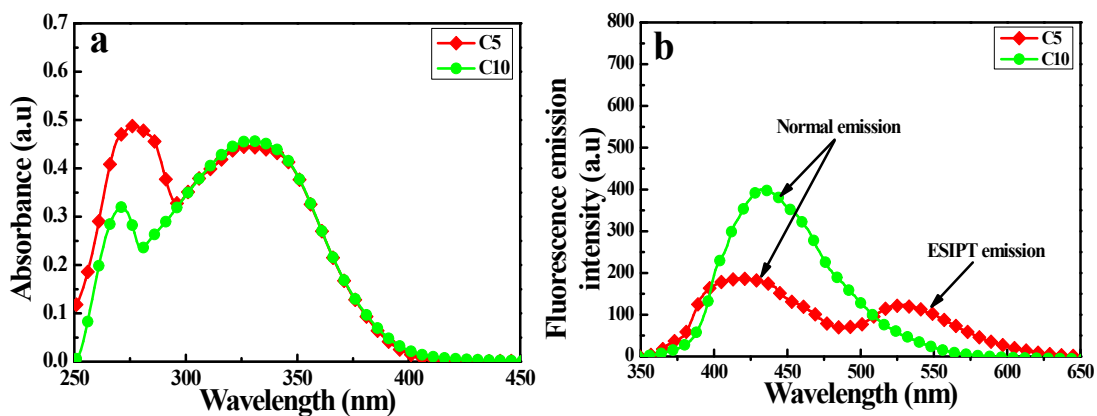


Figure S12 Emission spectra of C5 (a) and C10 (b) in THF solution, Ex: 350 nm, C,  $1 \times 10^{-5}$  mol/L

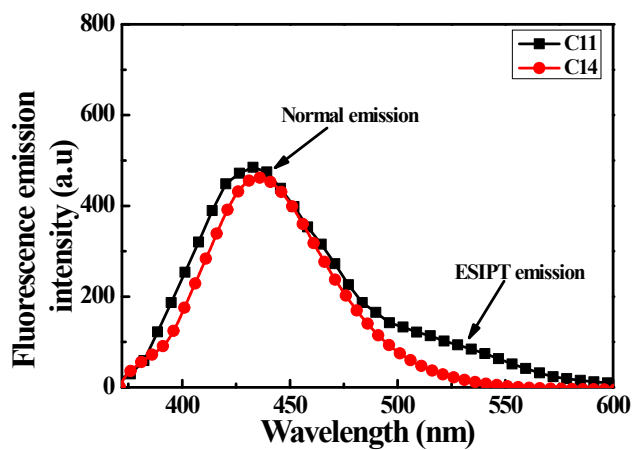


Figure S13 Emission spectra of C11 (a) and C14 (b) in DMF solution, Ex: 350 nm, C,  $1 \times 10^{-5}$  mol/L

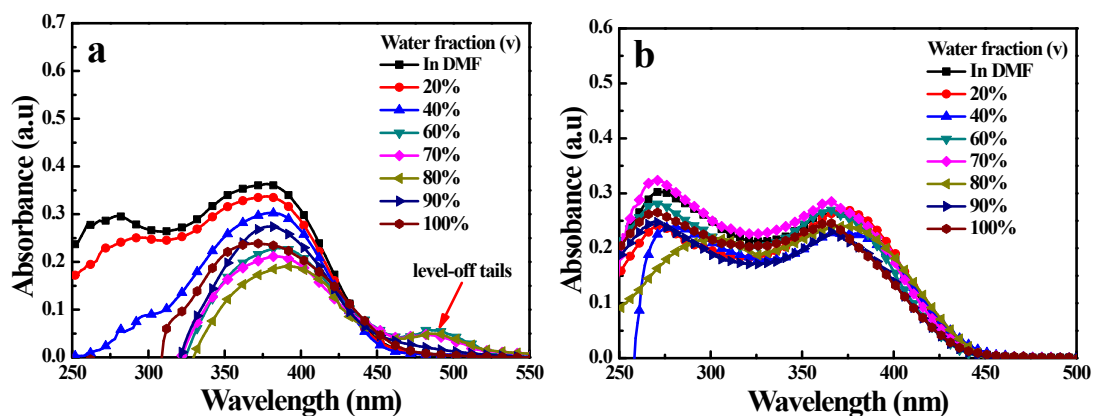


Figure S14 UV-vis absorption spectra of C3 (a) and C8 (b) in DMF/H<sub>2</sub>O mixed solution with different water volume fractions, C,  $1 \times 10^{-5}$  mol/L.

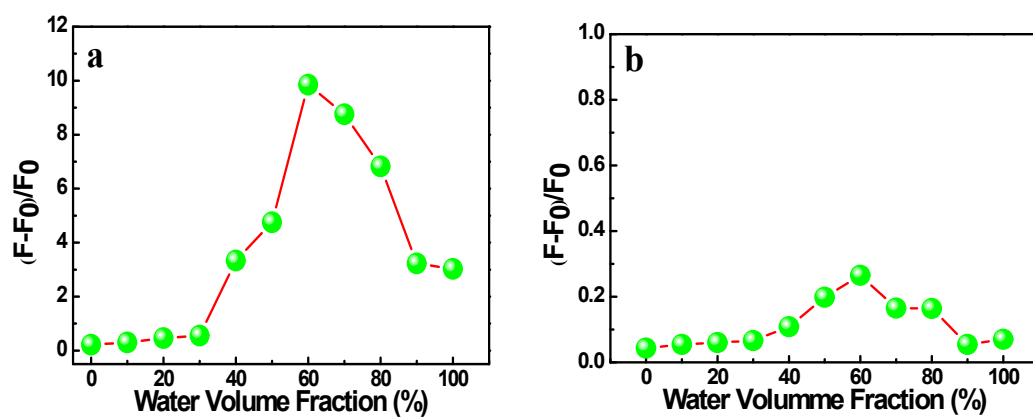


Figure S15 Effect of water volume fraction ( $f_w$ ) of C3 (a) and C8 (b) on the fluorescent intensity in mixed DMF/H<sub>2</sub>O solution at aggregation time course of 12 h, pH, 7.0, C,  $1 \times 10^{-5}$  mol/L.

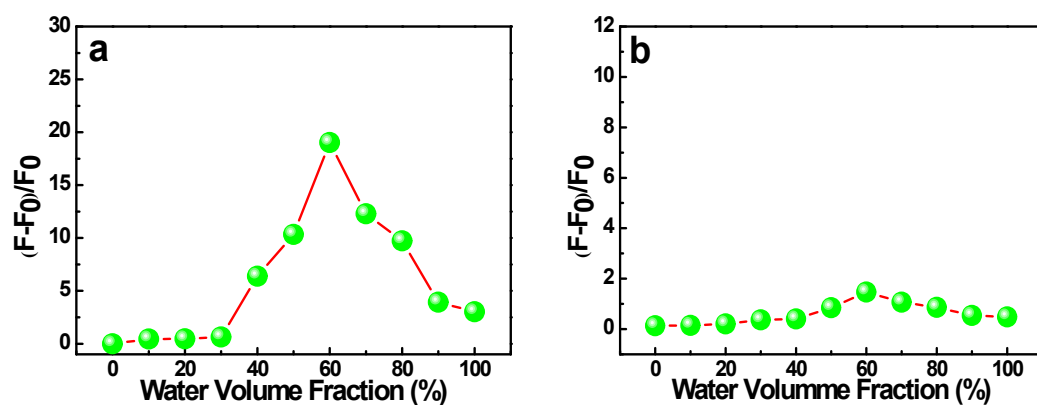
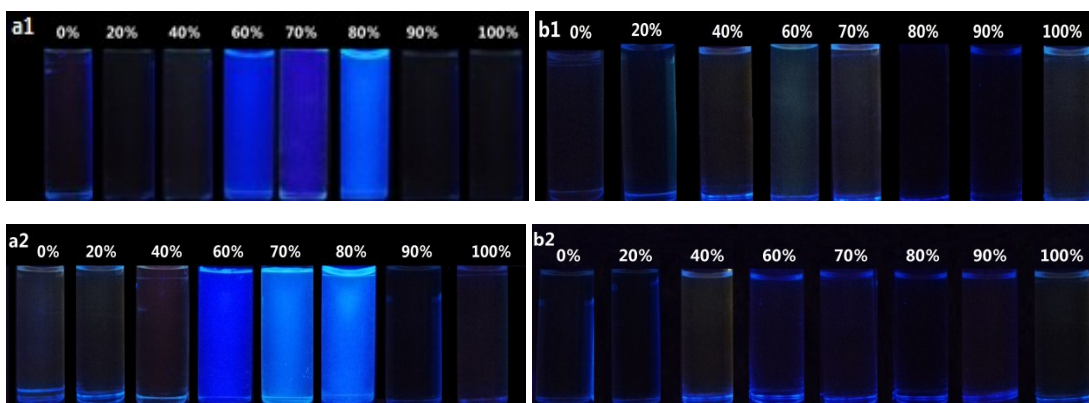
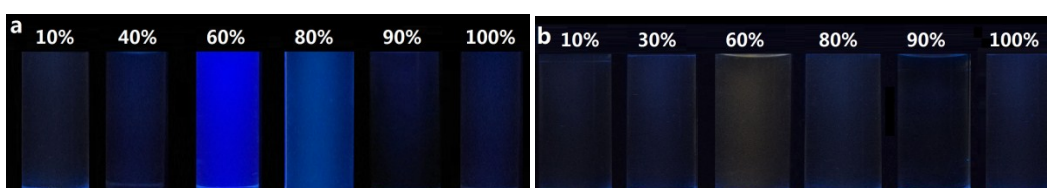


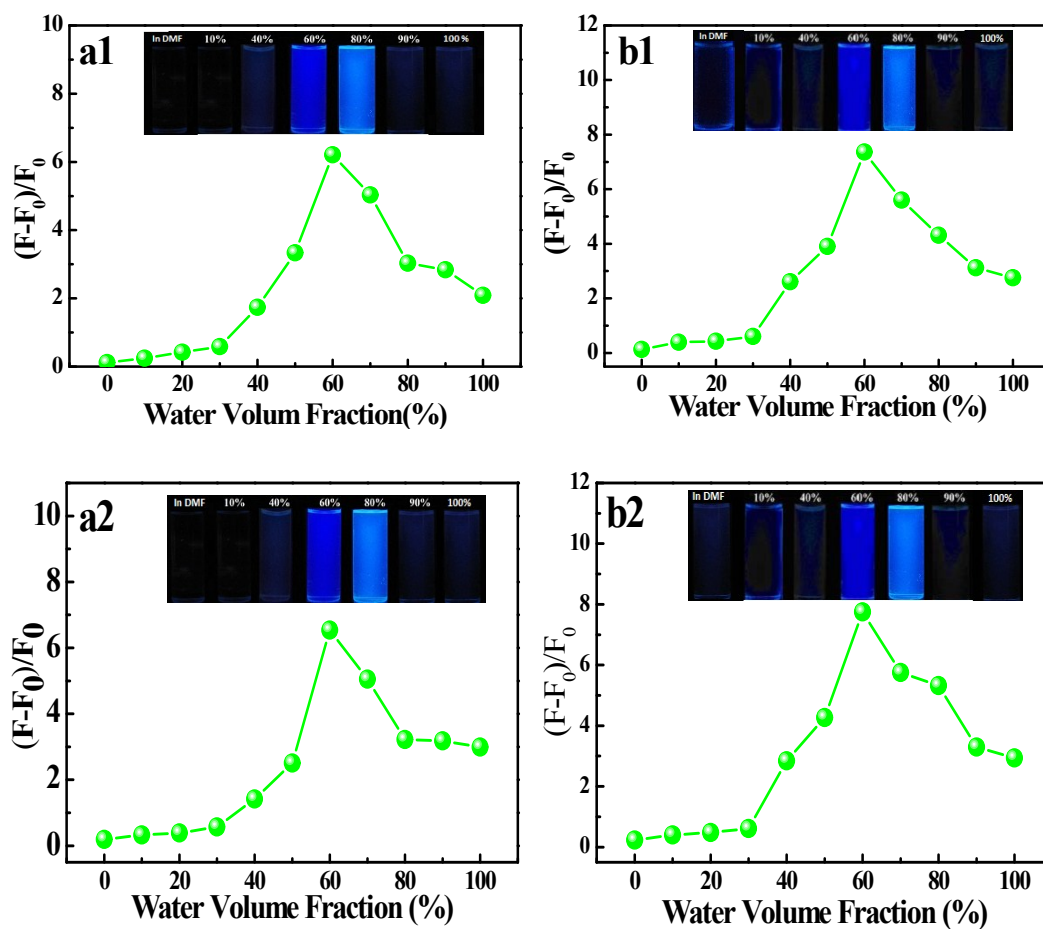
Figure S16 Effect of water volume fraction ( $f_w$ ) of C5 (a) and C10 (b) on fluorescent intensity in THF/H<sub>2</sub>O mixed solvents at the time course of 12 h, pH, 7.0, C,  $1 \times 10^{-5}$  mol/L.



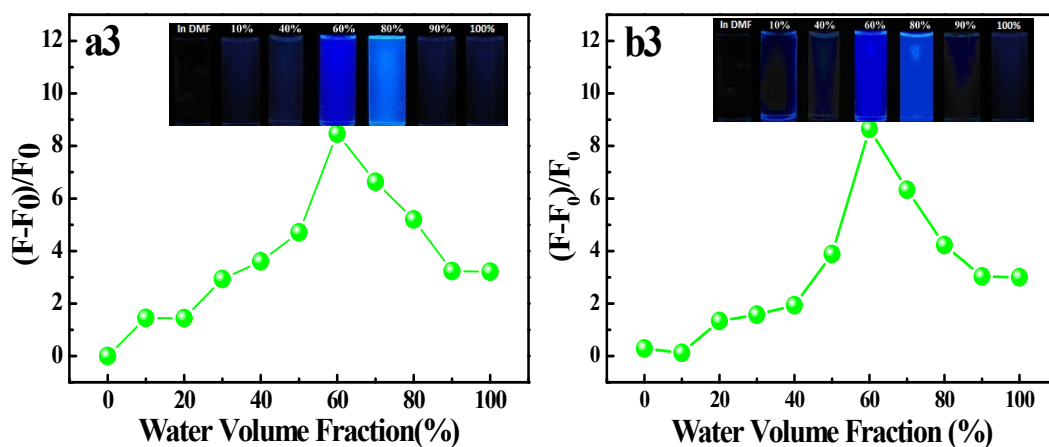
**Figure S17** Optical photographs recorded under 365 nm UV lamp irradiation of C1(a1), C6 (b1), C3 (a2) and C8 (b2) in DMF/H<sub>2</sub>O mixtures with various volume fractions of water at aggregation time of 12 h. C,  $1 \times 10^{-5}$  mol/L.



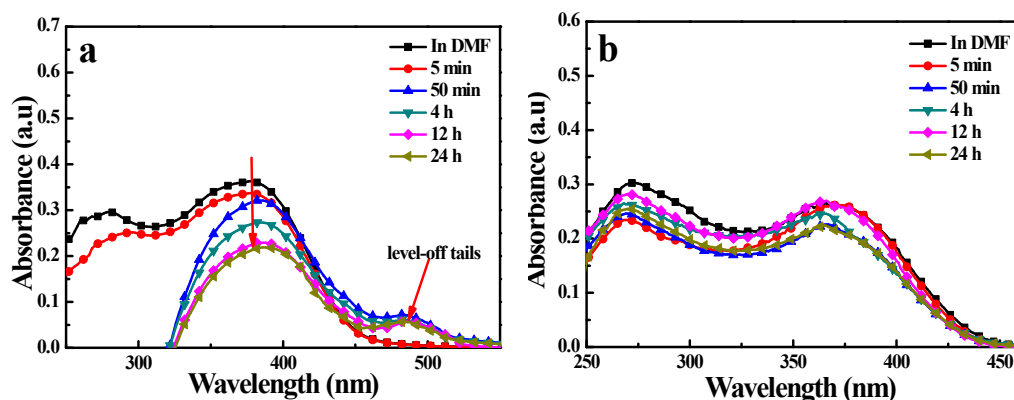
**Figure S18** Optical photographs recorded under 365 nm UV lamp irradiation of C5 (a) and C10 (b) in THF/H<sub>2</sub>O mixture solution with various volume fractions of water at aggregation time of 12 h. C,  $1 \times 10^{-5}$  mol/L.



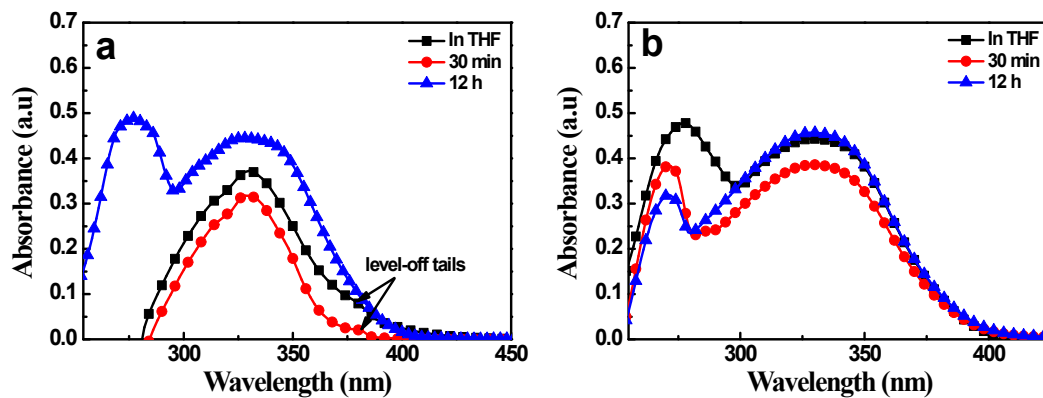




**Figure S19** (a1/a2/a3) Effect of water volume fractions ( $f_w$ ) of C11, C12, C13 and (b1/b2/b3) effect of water volume fractions ( $f_w$ ) of C14, C15, C16 on fluorescent intensity in mixed DMF/H<sub>2</sub>O solution at aggregation time course of 12 h, pH, 7.0, C,  $1 \times 10^{-5}$  mol/L respectively, the insert images in H<sub>2</sub>O fraction with DMF under 365 nm UV illumination.



**Figure S20** Time-dependent evolution of UV-visible absorption spectra of C3 (a) and C8 (b) in mixed DMF/H<sub>2</sub>O solvent (DMF/H<sub>2</sub>O =40/60 (v/v)), C,  $1 \times 10^{-5}$  mol/L.



**Figure S21** Time-dependent absorption spectra of C5 (a) and C10 (b) in mixed THF/H<sub>2</sub>O solvent (60% water sample (v/v)), C,  $1 \times 10^{-5}$  mol/L respectively

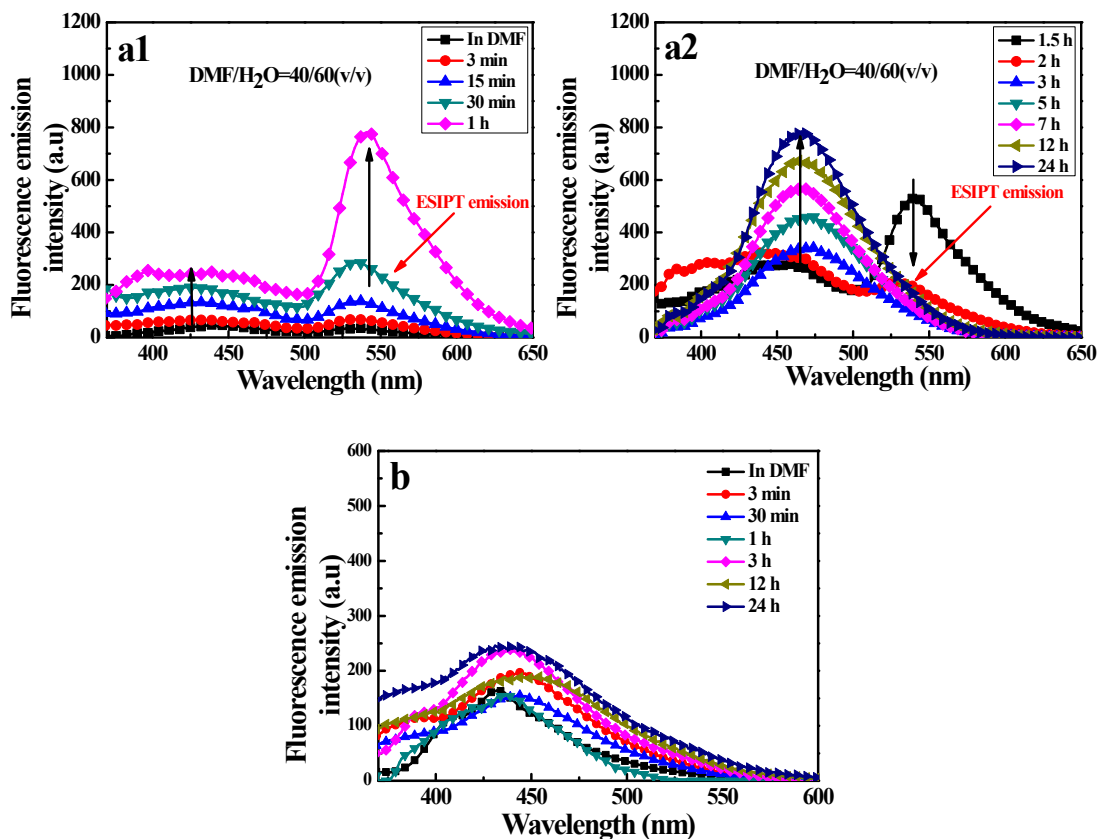


Figure S22 Time-dependent evolution of the emission spectra of C3 (a1/a2) and C8 (b) in mixed DMF/H<sub>2</sub>O (60% water fraction, v/v) solution, C,  $1 \times 10^{-5}$  mol/L, Ex: 350 nm.

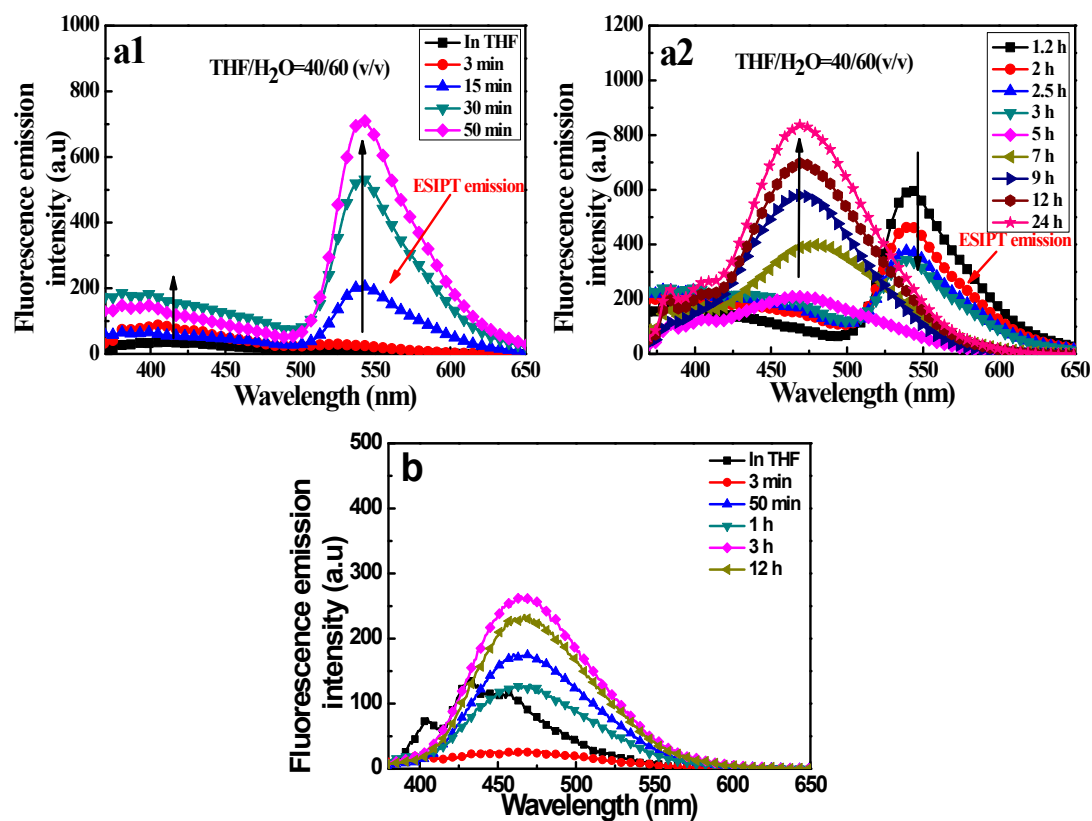


Figure S23 Time-dependent evolution of the emission spectra of C5 (a1/a2) and C10 (b) in mixed THF/H<sub>2</sub>O

(60% water fraction, v/v) solution, C,  $1 \times 10^{-5}$  mol/L, Ex: 350 nm.

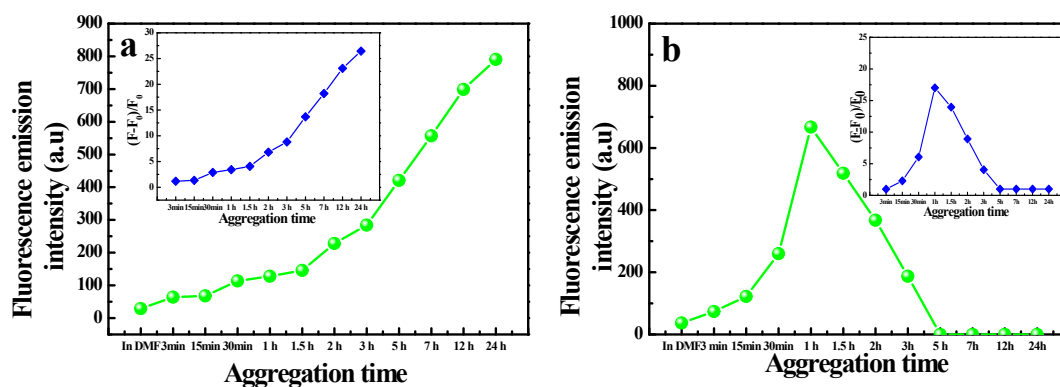


Figure S24 Plots of the fluorescence emission intensities of enol and keto tautomers of the target branched dyes

C1 (peaked at 470 nm (a) and 535 nm (b) respectively) to different aggregation time.

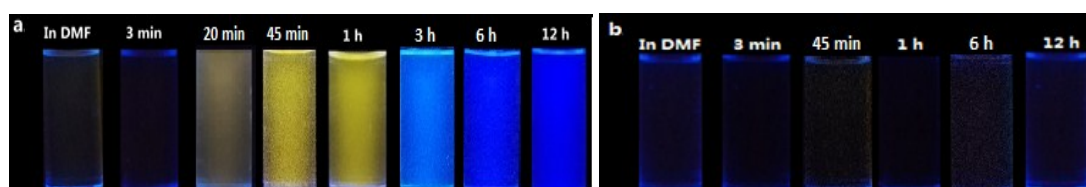


Figure S25 Images under different aggregation time intervals of C3 (a) and C8 (b) under UV lamp at 365 nm in

DMF/H<sub>2</sub>O mixture (60% water fraction (v)), C,  $1 \times 10^{-5}$  mol/L.

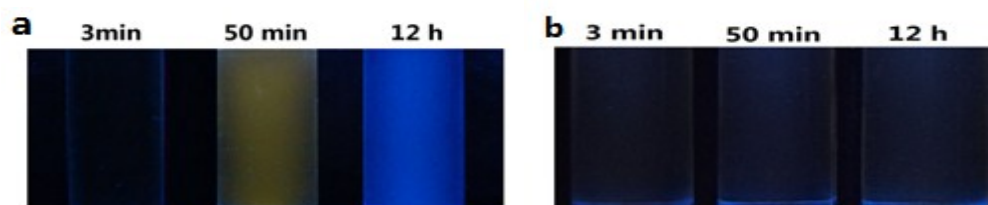


Figure S26 The images under different aggregation time intervals of C5 (a) and C10 (b) under UV lamp at 365

nm in THF/H<sub>2</sub>O mixture (60% water fraction (v)), C,  $1 \times 10^{-5}$  mol/L.

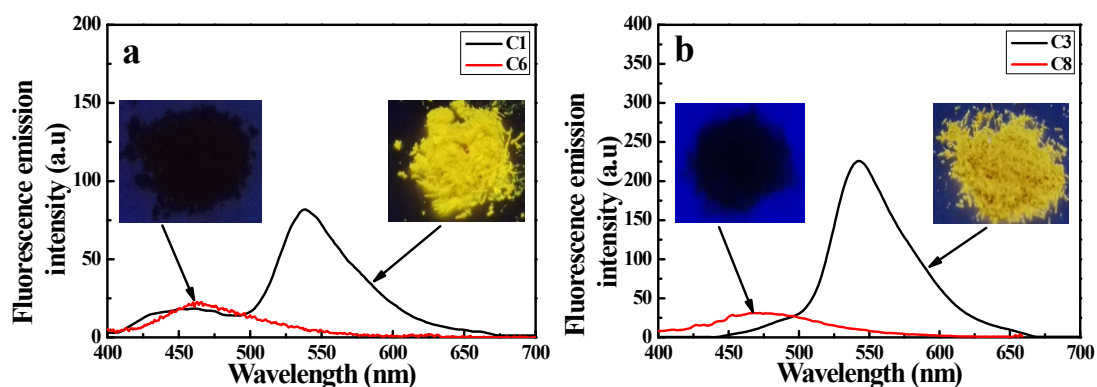


Figure S27 Emission spectra of C1/C6 (a) and emission spectra of C3/C8 (b) in solid state, Ex: 350 nm, the insert

images are solid state of C1/C6 and C3/C8 under 365 nm UV lamp respectively.

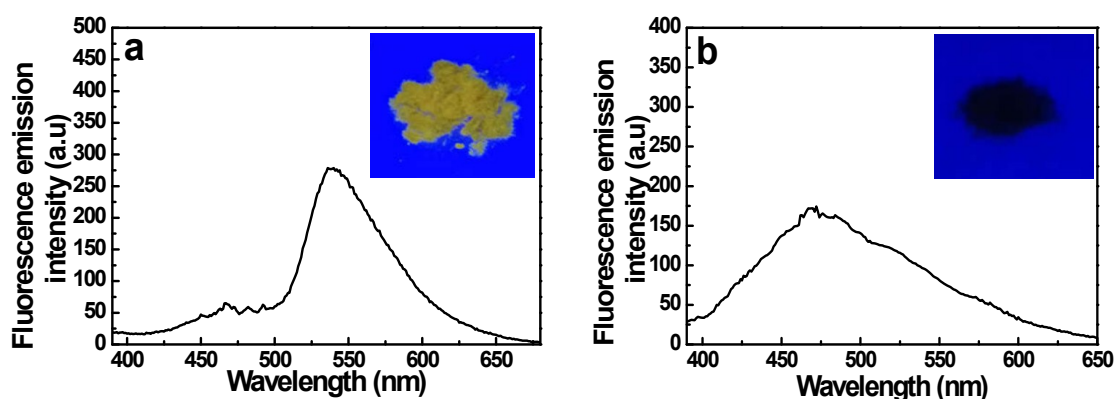
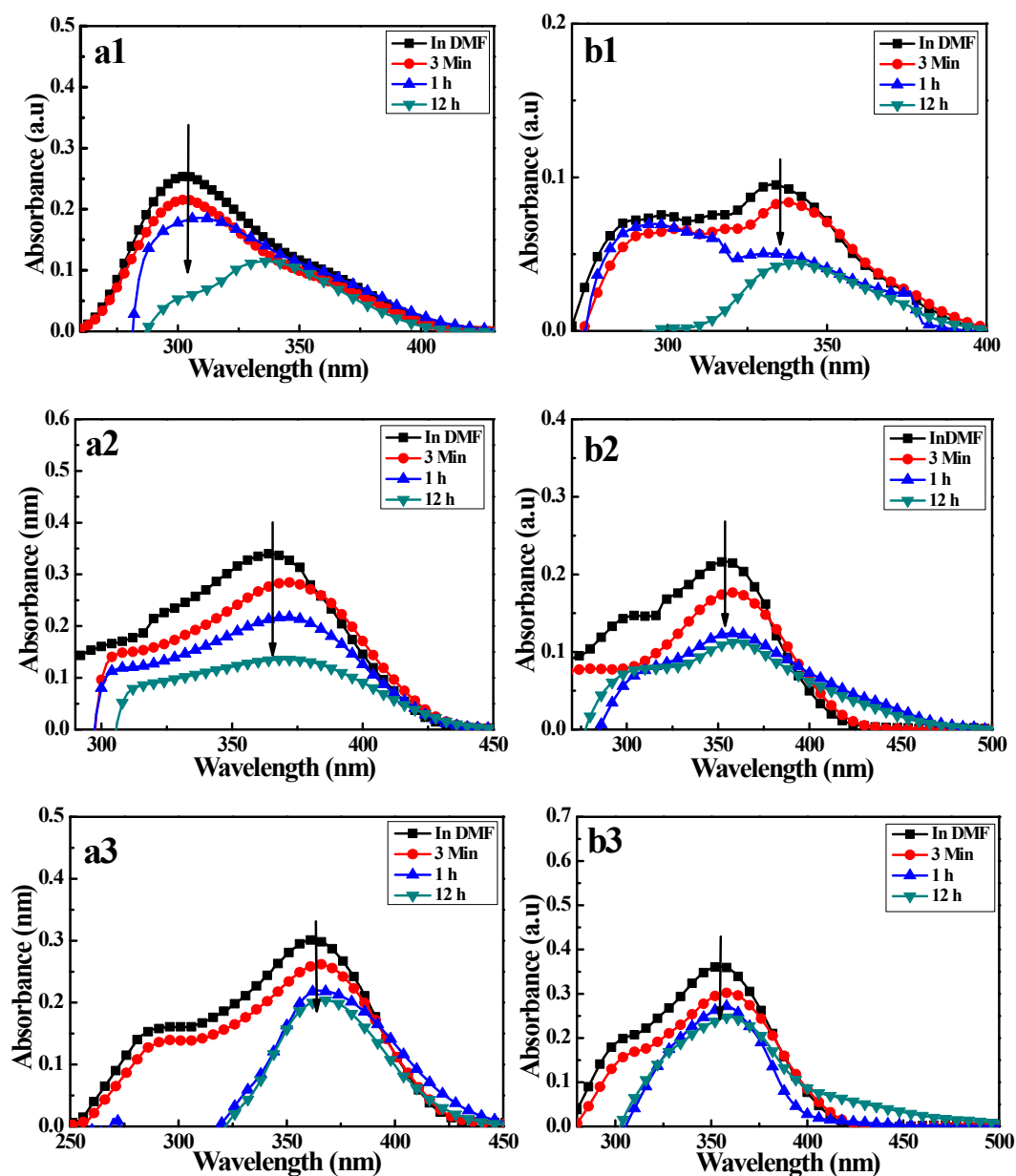
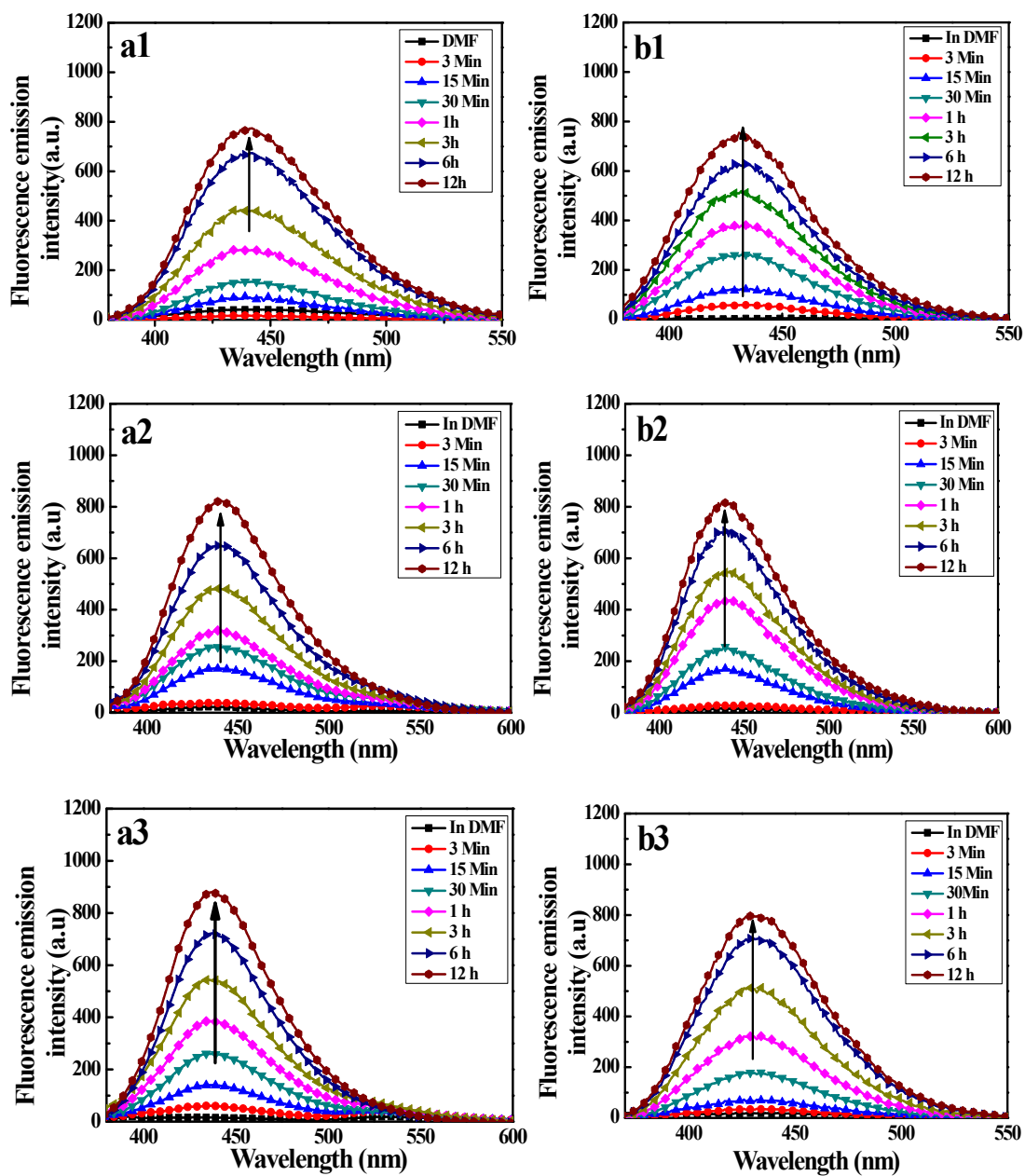


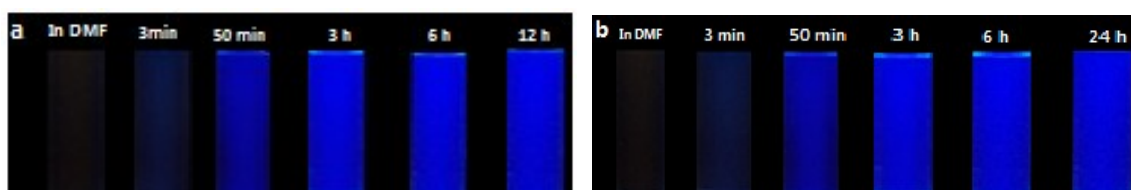
Figure S28 Emission spectra of C5 (a) and C10 (b) in solid state, EX: 350 nm, the images are solid state C5 and C10 under 365 nm UV lamp respectively.



**Figure S29** (a1/a2/a3) Time-dependent evolution of UV-visible absorption spectra of **C11**, **C12**, **C13** and (b1/b2/b3) time-dependent evolution of UV-visible absorption spectra of **C14**, **C15**, **C16** in mixed DMF/H<sub>2</sub>O solvent (DMF/H<sub>2</sub>O =40/60 (v/v)), C, 1×10<sup>-5</sup> mol/L.

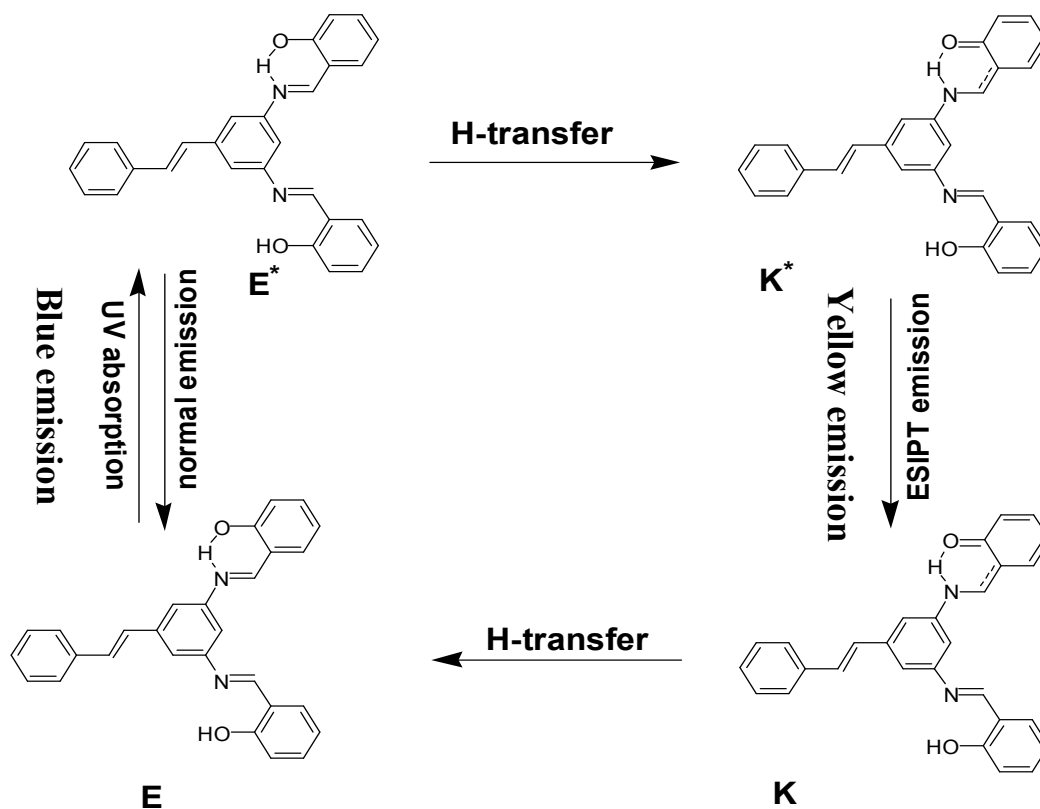


**Figure S30** (a1/a2/a3) Time-dependent evolution of fluorescence spectra of **C11**, **C12**, **C13** and (b1/b2/b3) time-dependent evolution of the fluorescence spectra of **C14**, **C15**, **C16** in mixed DMF/H<sub>2</sub>O solvent (DMF/H<sub>2</sub>O =40/60 (v/v)), C, 1×10<sup>-5</sup> mol/L, Ex: 350 nm.





**Figure S31** Images under different aggregation time internals of linear dyes **C11** (a) and linear reference **C14** (b) under 365 nm UV lamp in DMF/H<sub>2</sub>O mixture (60% water volume fraction), C, 1×10<sup>-5</sup> mol/L



**Scheme S1** A typical four-level cycle of enol-keto phototautomerization during internal proton transfer in the excited state of **C4**

## 2. X-ray single crystal diffraction data of target C1

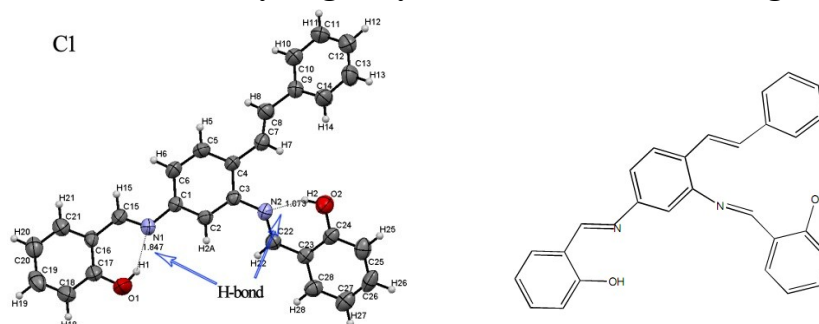


Table S1 Atomic coordinates of compound C1

Number	Label	Charge	SybylType	Xfrac + ESD	Yfrac + ESD	Zfrac + ESD	Symm. op.
1	N1	0	N.2	1.4625(7)	0.46275(11)	0.6672(3)	x,y,z
2	N2	0	N.2	0.7605(6)	0.38220(9)	0.5350(3)	x,y,z
3	O1	0	O.3	1.6120(7)	0.51227(11)	0.5211(3)	x,y,z
4	H1	0	H	1.5221	0.4962	0.5464	x,y,z
5	O2	0	O.3	0.3509(6)	0.34877(9)	0.4657(3)	x,y,z
6	H2	0	H	0.454	0.3606	0.5107	x,y,z
7	C1	0	C.2	1.2954(8)	0.43346(12)	0.6948(3)	x,y,z
8	C2	0	C.2	1.1156(7)	0.42284(12)	0.6081(3)	x,y,z
9	H2A	0	H	1.1076	0.4351	0.5351	x,y,z
10	C3	0	C.2	0.9446(7)	0.39432(12)	0.6255(3)	x,y,z
11	C4	0	C.2	0.9514(8)	0.37568(12)	0.7359(3)	x,y,z
12	C5	0	C.2	1.1363(9)	0.38742(14)	0.8232(3)	x,y,z
13	H5	0	H	1.1453	0.3756	0.8969	x,y,z
14	C6	0	C.2	1.3037(8)	0.41540(14)	0.8052(4)	x,y,z
15	H6	0	H	1.4229	0.4225	0.8658	x,y,z
16	C7	0	C.2	0.7776(8)	0.34495(14)	0.7565(3)	x,y,z
17	H7	0	H	0.6414	0.3432	0.7014	x,y,z
18	C8	0	C.2	0.7953(8)	0.31958(14)	0.8452(4)	x,y,z
19	H8	0	H	0.9327	0.3213	0.8994	x,y,z
20	C9	0	C.2	0.6198(8)	0.28851(13)	0.8684(4)	x,y,z
21	C10	0	C.2	0.6704(9)	0.26526(14)	0.9709(4)	x,y,z
22	H10	0	H	0.8136	0.2689	1.02	x,y,z
23	C11	0	C.2	0.5109(10)	0.23715(15)	0.9997(4)	x,y,z
24	H11	0	H	0.5468	0.222	1.0682	x,y,z
25	C12	0	C.2	0.3046(10)	0.23138(15)	0.9304(4)	x,y,z
26	H12	0	H	0.1969	0.2125	0.9513	x,y,z

27	C13	0	C.2	0.2512(10)	0.25319(17)	0.8288(4)	x,y,z
28	H13	0	H	0.1085	0.2488	0.78	x,y,z
29	C14	0	C.2	0.4089(9)	0.28157(16)	0.7991(4)	x,y,z
30	H14	0	H	0.3708	0.2964	0.7301	x,y,z
31	C15	0	C.2	1.6361(9)	0.47453(13)	0.7421(4)	x,y,z
32	H15	0	H	1.6535	0.4635	0.817	x,y,z
33	C16	0	C.2	1.8053(8)	0.50400(13)	0.7164(3)	x,y,z
34	C17	0	C.2	1.7919(9)	0.52143(14)	0.6060(4)	x,y,z
35	C18	0	C.2	1.9675(10)	0.54830(15)	0.5837(4)	x,y,z
36	H18	0	H	1.9586	0.5599	0.5098	x,y,z
37	C19	0	C.2	2.1525(10)	0.55801(15)	0.6680(5)	x,y,z
38	H19	0	H	2.2684	0.576	0.6512	x,y,z
39	C20	0	C.2	2.1683(10)	0.54125(15)	0.7776(5)	x,y,z
40	H20	0	H	2.2936	0.5478	0.8358	x,y,z
41	C21	0	C.2	1.9953(9)	0.51477(14)	0.7992(4)	x,y,z
42	H21	0	H	2.0061	0.5034	0.8735	x,y,z
43	C22	0	C.2	0.7918(8)	0.38280(12)	0.4277(3)	x,y,z
44	H22	0	H	0.9328	0.3931	0.4095	x,y,z
45	C23	0	C.2	0.6166(7)	0.36805(12)	0.3351(3)	x,y,z
46	C24	0	C.2	0.4073(8)	0.34928(13)	0.3571(3)	x,y,z
47	C25	0	C.2	0.2580(8)	0.33096(14)	0.2685(4)	x,y,z
48	H25	0	H	0.1203	0.3184	0.2835	x,y,z
49	C26	0	C.2	0.3120(10)	0.33121(14)	0.1570(4)	x,y,z
50	H26	0	H	0.2106	0.3184	0.0973	x,y,z
51	C27	0	C.2	0.5132(10)	0.35009(16)	0.1317(4)	x,y,z
52	H27	0	H	0.5467	0.3505	0.0557	x,y,z
53	C28	0	C.2	0.6623(8)	0.36817(14)	0.2206(4)	x,y,z
54	H28	0	H	0.7984	0.3809	0.2041	x,y,z

**Table S2** Bond lengths of compound **C1** (Å)

Number	Atom1	Atom2	Type	Polymeric	Length	SybylType
1	N1	C1	Unknown	No	1.423(6)	un
2	N1	C15	Unknown	No	1.273(6)	un
3	N2	C3	Unknown	No	1.423(5)	un
4	N2	C22	Unknown	No	1.284(5)	un
5	O1	H1	Unknown	No	0.820(4)	1
6	O1	C17	Unknown	No	1.343(6)	1
7	O2	H2	Unknown	No	0.821(3)	1
8	O2	C24	Unknown	No	1.347(5)	1
9	C1	C2	Unknown	No	1.367(5)	un
10	C1	C6	Unknown	No	1.402(6)	un
11	C2	H2A	Unknown	No	0.930(4)	1
12	C2	C3	Unknown	No	1.388(6)	un
13	C3	C4	Unknown	No	1.411(5)	un

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14	C4	C5	Unknown	No	1.400(6)	un
15	C4	C7	Unknown	No	1.458(6)	un
16	C5	H5	Unknown	No	0.931(4)	1
17	C5	C6	Unknown	No	1.363(7)	un
18	C6	H6	Unknown	No	0.929(4)	1
19	C7	H7	Unknown	No	0.930(4)	1
20	C7	C8	Unknown	No	1.310(6)	un
21	C8	H8	Unknown	No	0.929(4)	1
22	C8	C9	Unknown	No	1.481(7)	un
23	C9	C10	Unknown	No	1.400(6)	un
24	C9	C14	Unknown	No	1.362(6)	un
25	C10	H10	Unknown	No	0.931(5)	1
26	C10	C11	Unknown	No	1.372(7)	un
27	C11	H11	Unknown	No	0.930(5)	1
28	C11	C12	Unknown	No	1.335(7)	un
29	C12	H12	Unknown	No	0.930(5)	1
30	C12	C13	Unknown	No	1.368(7)	un
31	C13	H13	Unknown	No	0.930(5)	1
32	C13	C14	Unknown	No	1.374(8)	un
33	C14	H14	Unknown	No	0.930(5)	1
34	C15	H15	Unknown	No	0.930(5)	1
35	C15	C16	Unknown	No	1.429(7)	un
36	C16	C17	Unknown	No	1.390(6)	un
37	C16	C21	Unknown	No	1.380(6)	un
38	C17	C18	Unknown	No	1.388(7)	un
39	C18	H18	Unknown	No	0.930(5)	1
40	C18	C19	Unknown	No	1.362(7)	un
41	C19	H19	Unknown	No	0.929(6)	1
42	C19	C20	Unknown	No	1.372(8)	un
43	C20	H20	Unknown	No	0.930(5)	1
44	C20	C21	Unknown	No	1.367(8)	un
45	C21	H21	Unknown	No	0.930(5)	1
46	C22	H22	Unknown	No	0.930(5)	1
47	C22	C23	Unknown	No	1.433(5)	un
48	C23	C24	Unknown	No	1.405(6)	un
49	C23	C28	Unknown	No	1.392(6)	un
50	C24	C25	Unknown	No	1.367(6)	un
51	C25	H25	Unknown	No	0.930(5)	1
52	C25	C26	Unknown	No	1.375(7)	un
53	C26	H26	Unknown	No	0.930(5)	1
54	C26	C27	Unknown	No	1.379(8)	un
55	C27	H27	Unknown	No	0.930(5)	1
56	C27	C28	Unknown	No	1.365(6)	un
57	C28	H28	Unknown	No	0.930(5)	1

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**Table S3** Bond angles of compound **C1** (°)

Number	Atom1	Atom2	Atom3	Angle	Number	Atom1	Atom2	Atom3	Angle
1	C1	N1	C15	122.1(4)	45	C9	C14	H14	119.2(5)
2	C3	N2	C22	120.6(3)	46	C13	C14	H14	119.3(5)
3	H1	O1	C17	109.5(4)	47	N1	C15	H15	118.6(5)
4	H2	O2	C24	109.5(4)	48	N1	C15	C16	123.0(4)
5	N1	C1	C2	117.5(4)	49	H15	C15	C16	118.5(4)
6	N1	C1	C6	123.9(4)	50	C15	C16	C17	121.6(4)
7	C2	C1	C6	118.6(4)	51	C15	C16	C21	120.9(4)
8	C1	C2	H2A	119.0(4)	52	C17	C16	C21	117.4(4)
9	C1	C2	C3	122.1(4)	53	O1	C17	C16	120.6(4)
10	H2A	C2	C3	118.9(4)	54	O1	C17	C18	120.0(4)
11	N2	C3	C2	122.6(3)	55	C16	C17	C18	119.4(4)
12	N2	C3	C4	117.5(3)	56	C17	C18	H18	119.4(5)
13	C2	C3	C4	120.0(4)	57	C17	C18	C19	121.3(5)
14	C3	C4	C5	116.6(4)	58	H18	C18	C19	119.4(5)
15	C3	C4	C7	121.4(4)	59	C18	C19	H19	119.9(5)
16	C5	C4	C7	122.0(4)	60	C18	C19	C20	120.2(5)
17	C4	C5	H5	118.5(4)	61	H19	C19	C20	119.9(5)
18	C4	C5	C6	123.0(4)	62	C19	C20	H20	120.8(5)
19	H5	C5	C6	118.5(4)	63	C19	C20	C21	118.4(5)
20	C1	C6	C5	119.7(4)	64	H20	C20	C21	120.8(5)
21	C1	C6	H6	120.1(4)	65	C16	C21	C20	123.4(5)
22	C5	C6	H6	120.2(5)	66	C16	C21	H21	118.3(5)
23	C4	C7	H7	116.9(4)	67	C20	C21	H21	118.4(5)
24	C4	C7	C8	126.2(4)	68	N2	C22	H22	118.9(4)
25	H7	C7	C8	117.0(4)	69	N2	C22	C23	122.1(4)
26	C7	C8	H8	116.5(5)	70	H22	C22	C23	119.0(4)
27	C7	C8	C9	127.0(4)	71	C22	C23	C24	121.9(4)
28	H8	C8	C9	116.6(4)	72	C22	C23	C28	119.9(4)
29	C8	C9	C10	117.8(4)	73	C24	C23	C28	117.9(4)
30	C8	C9	C14	124.9(4)	74	O2	C24	C23	120.7(4)
31	C10	C9	C14	117.2(4)	75	O2	C24	C25	118.8(4)
32	C9	C10	H10	119.7(5)	76	C23	C24	C25	120.4(4)
33	C9	C10	C11	120.6(4)	77	C24	C25	H25	120.2(4)
34	H10	C10	C11	119.6(5)	78	C24	C25	C26	119.8(4)
35	C10	C11	H11	119.6(5)	79	H25	C25	C26	120.1(5)
36	C10	C11	C12	120.6(5)	80	C25	C26	H26	119.3(5)



37	H11	C11	C12	119.7(5)	81	C25	C26	C27	121.4(5)
38	C11	C12	H12	119.9(5)	82	H26	C26	C27	119.3(5)
39	C11	C12	C13	120.2(5)	83	C26	C27	H27	120.7(5)
40	H12	C12	C13	119.9(5)	84	C26	C27	C28	118.6(5)
41	C12	C13	H13	120.0(5)	85	H27	C27	C28	120.7(5)
42	C12	C13	C14	119.8(5)	86	C23	C28	C27	121.9(4)
43	H13	C13	C14	120.1(5)	87	C23	C28	H28	119.1(4)
44	C9	C14	C13	121.5(5)	88	C27	C28	H28	119.0(5)

**Table S4** Torsion angles of compound **C1** (°)

Number	Atom1	Atom2	Atom3	Atom4	Torsion	Number	Atom1	Atom2	Atom3	Atom4	Torsion
1	C15	N1	C1	C2	-179.9(4)	65	C11	C12	C13	H13	178.9(5)
2	C15	N1	C1	C6	0.7(7)	66	C11	C12	C13	C14	-1.1(8)
3	C1	N1	C15	H15	0.1(7)	67	H12	C12	C13	H13	-1.1(9)
4	C1	N1	C15	C16	-179.8(4)	68	H12	C12	C13	C14	178.9(5)
5	C22	N2	C3	C2	29.0(6)	69	C12	C13	C14	C9	0.4(8)
6	C22	N2	C3	C4	-150.0(4)	70	C12	C13	C14	H14	-179.6(5)
7	C3	N2	C22	H22	-4.5(6)	71	H13	C13	C14	C9	-179.6(5)
8	C3	N2	C22	C23	175.4(4)	72	H13	C13	C14	H14	0.4(9)
9	H1	O1	C17	C16	0.5(6)	73	N1	C15	C16	C17	-0.8(7)
10	H1	O1	C17	C18	-179.9(4)	74	N1	C15	C16	C21	-177.7(4)
11	H2	O2	C24	C23	0.2(6)	75	H15	C15	C16	C17	179.3(4)
12	H2	O2	C24	C25	179.8(4)	76	H15	C15	C16	C21	2.4(7)
13	N1	C1	C2	H2A	-0.5(6)	77	C15	C16	C17	O1	2.9(7)
14	N1	C1	C2	C3	179.4(4)	78	C15	C16	C17	C18	-176.6(4)
15	C6	C1	C2	H2A	178.8(4)	79	C21	C16	C17	O1	179.9(4)
16	C6	C1	C2	C3	-1.2(6)	80	C21	C16	C17	C18	0.3(7)
17	N1	C1	C6	C5	-179.6(4)	81	C15	C16	C21	C20	176.7(5)
18	N1	C1	C6	H6	0.4(7)	82	C15	C16	C21	H21	-3.2(7)
19	C2	C1	C6	C5	1.0(6)	83	C17	C16	C21	C20	-0.2(7)
20	C2	C1	C6	H6	-179.0(4)	84	C17	C16	C21	H21	179.8(4)
21	C1	C2	C3	N2	-178.2(4)	85	O1	C17	C18	H18	0.3(8)
22	C1	C2	C3	C4	0.8(6)	86	O1	C17	C18	C19	-179.7(5)
23	H2A	C2	C3	N2	1.7(6)	87	C16	C17	C18	H18	179.9(5)
24	H2A	C2	C3	C4	-179.2(4)	88	C16	C17	C18	C19	-0.2(8)
25	N2	C3	C4	C5	178.8(4)	89	C17	C18	C19	H19	179.8(5)
26	N2	C3	C4	C7	0.4(6)	90	C17	C18	C19	C20	-0.1(8)
27	C2	C3	C4	C5	-0.2(6)	91	H18	C18	C19	H19	-0.2(9)
28	C2	C3	C4	C7	-178.7(4)	92	H18	C18	C19	C20	179.9(5)
29	C3	C4	C5	H5	-179.9(4)	93	C18	C19	C20	H20	-179.7(5)
30	C3	C4	C5	C6	0.1(6)	94	C18	C19	C20	C21	0.2(8)
31	C7	C4	C5	H5	-1.5(7)	95	H19	C19	C20	H20	0.4(9)
32	C7	C4	C5	C6	178.5(4)	96	H19	C19	C20	C21	-179.7(5)
33	C3	C4	C7	H7	-15.8(6)	97	C19	C20	C21	C16	-0.0(8)

34	C3	C4	C7	C8	164.1(4)	98	C19	C20	C21	H21	180.0(5)
35	C5	C4	C7	H7	165.8(4)	99	H20	C20	C21	C16	179.9(5)
36	C5	C4	C7	C8	-14.2(7)	100	H20	C20	C21	H21	-0.2(9)
37	C4	C5	C6	C1	-0.5(7)	101	N2	C22	C23	C24	-4.8(6)
38	C4	C5	C6	H6	179.5(4)	102	N2	C22	C23	C28	-178.0(4)
39	H5	C5	C6	C1	179.5(4)	103	H22	C22	C23	C24	175.1(4)
40	H5	C5	C6	H6	-0.5(8)	104	H22	C22	C23	C28	1.9(6)
41	C4	C7	C8	H8	-0.7(7)	105	C22	C23	C24	O2	7.8(6)
42	C4	C7	C8	C9	179.2(4)	106	C22	C23	C24	C25	-171.7(4)
43	H7	C7	C8	H8	179.3(4)	107	C28	C23	C24	O2	-178.8(4)
44	H7	C7	C8	C9	-0.8(7)	108	C28	C23	C24	C25	1.6(6)
45	C7	C8	C9	C10	-178.0(5)	109	C22	C23	C28	C27	172.2(4)
46	C7	C8	C9	C14	0.0(8)	110	C22	C23	C28	H28	-7.7(7)
47	H8	C8	C9	C10	1.9(7)	111	C24	C23	C28	C27	-1.3(7)
48	H8	C8	C9	C14	180.0(5)	112	C24	C23	C28	H28	178.8(4)
49	C8	C9	C10	H10	-2.6(7)	113	O2	C24	C25	H25	-0.1(7)
50	C8	C9	C10	C11	177.4(4)	114	O2	C24	C25	C26	179.9(4)
51	C14	C9	C10	H10	179.2(5)	115	C23	C24	C25	H25	179.5(4)
52	C14	C9	C10	C11	-0.8(7)	116	C23	C24	C25	C26	-0.6(7)
53	C8	C9	C14	C13	-177.5(5)	117	C24	C25	C26	H26	179.2(5)
54	C8	C9	C14	H14	2.5(8)	118	C24	C25	C26	C27	-0.8(7)
55	C10	C9	C14	C13	0.5(7)	119	H25	C25	C26	H26	-0.9(8)
56	C10	C9	C14	H14	-179.5(5)	120	H25	C25	C26	C27	179.1(5)
57	C9	C10	C11	H11	-179.8(5)	121	C25	C26	C27	H27	-178.9(5)
58	C9	C10	C11	C12	0.1(8)	122	C25	C26	C27	C28	1.1(8)
59	H10	C10	C11	H11	0.2(8)	123	H26	C26	C27	H27	1.1(9)
60	H10	C10	C11	C12	-179.9(5)	124	H26	C26	C27	C28	-178.9(5)
61	C10	C11	C12	H12	-179.2(5)	125	C26	C27	C28	C23	-0.1(7)
62	C10	C11	C12	C13	0.8(8)	126	C26	C27	C28	H28	179.9(5)
63	H11	C11	C12	H12	0.8(9)	127	H27	C27	C28	C23	180.0(5)
64	H11	C11	C12	C13	-179.3(5)	128	H27	C27	C28	H28	-0.1(8)

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### 3. Synthesis of the intermediates and the final compounds

#### Synthesis of Intermediates

##### **Intermediate 1, 1, 2-dinitro-4-styrylbenzene**

The known **intermediate 1** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: the desired product as the yellow needle solid (yield, 50%, m.p. 140.8-142.0 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.532-7.517 (d, *J*=7.5 Hz, Ar-H, 2H), 7.304-7.273 (t, *J*=7.75 Hz, Ar-H, 2H; -CH=CH-, 1H), 7.175-7.158 (d, *J*=8.5 Hz, Ar-H, 1H), 7.140-7.111 (d, *J*=7.5 Hz, Ar-H, 1H), 6.693-6.661 (d, *J*=16.0 Hz, CH=CH, 1H), 5.899-5.863 (m, Ar-H, 2H), 5.026 (s, -NH<sub>2</sub>, 4H). Elementary analysis, Anal. Calcd for C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>: C, 62.22; H, 3.73; N, 10.37. Found: C, 62.29; H, 3.65; N, 10.41.

##### **Intermediate 2, 1,2-diamine-4-styrylbenzene**

The known **intermediate 2** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: the desired product as the faint yellow solid (yield, 15%, m.p. 117.6-119.7 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.532-7.517 (d, *J*=7.5 Hz, Ar-H, 2H), 7.304-7.273 (t, *J*=7.75 Hz, Ar-H, 2H; -CH=CH-, 1H), 7.175-7.158 (d, *J*=8.5 Hz, Ar-H, 1H), 7.140-7.111 (d, *J*=7.5 Hz, Ar-H, 1H), 6.693-6.661 (d, *J*=16.0 Hz, CH=CH, 1H), 5.899-5.863 (m, Ar-H, 2H), 5.026 (s, -NH<sub>2</sub>, 4H). Elementary analysis, Anal. Calcd for C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>: C, 79.97; H, 6.71; N, 13.32. Found: C, 80.08; H, 6.60; N, 13.41.

##### **Intermediate 3, 2, 4-(4'-methoxy-cinnameryl)-dinitro-benzene**

The known **intermediate 3** was synthesized as described in our previously work in Ref. 1.

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The characterization data in our report presents as follow: (yield, 50%, m.p. 160.0-162.1 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.805 (s, Ar-H, 1H), 8.409-8.392 (d, *J*=8.5 Hz, Ar-H, 1H), 7.981-7.965 (d, *J*=8.0 Hz, Ar-H, 1H), 7.543-7.526 (d, *J*=8.5 Hz, Ar-H, 2H), 7.493 (s, CH=CH, 1H), 7.289 (s, CH=CH, 1H), 6.958-6.943 (d, *J*=7.5 Hz, Ar-H, 2H), 3.865 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>: C, 60.01; H, 4.02; N, 9.33. Found: C, 60.12; H, 3.89; N, 9.41.

#### **Intermediate 4, 2, 4-(4'-methoxy-cinnameryl)-diaminyl-benzene**

The known **intermediate 4** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the faint yellow solid (yield, 18%, m.p. 141.0-142.9 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.465-7.448 (m, Ar-H, 2H), 7.126-7.096 (m, Ar-H, 2H), 6.883-6.865 (m, Ar-H, 2H), 6.639-6.607 (d, *J*=16.0 Hz, Ar-H, 1H), 5.882-5.885 (m, CH=CH, 2H), 4.946 (s, -NH<sub>2</sub>, 4H), 3.747 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O: C, 74.97; H, 6.71; N, 11.66. Found: C, 75.03; H, 6.65; N, 11.72.

#### **Intermediate 5, 2, 4-(3', 4'-Dimethoxy-cinnameryl)-dinitro-benzene**

The known **intermediate 5** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The red solid product was gained (yield, 55%, m.p. 143.0-144.0 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.732-8.727 (d, *J*=2.5 Hz, CH=CH, 1H), 8.491-8.469 (m, Ar-H, 1H), 8.241-8.223 (d, *J*=9.0 Hz, Ar-H, 1H), 7.586-7.554 (d, *J*=15.0 Hz, Ar-H, 1H), 7.410-7.378 (d, *J*=16.0 Hz, Ar-H, 1H), 7.293-7.290 (d, *J*=1.5 Hz, CH=CH, 1H), 7.248-7.231 (d, *J*=8.5 Hz, Ar-H, 1H), 7.039-7.022 (d, *J*=8.5 Hz, Ar-H, 1H), 3.822 (s, -OCH<sub>3</sub>, 3H), 3.805 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>6</sub>: C, 58.18; H, 4.27;

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N, 8.48. Found: C, 58.27; H, 4.19; N, 8.54.

#### **Intermediate 6, 2, 4-(3', 4'-Dimethoxy-cinnamenyl)-diaminyl-benzene**

The known **intermediate 6** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the faint yellow solid (yield, 20%, m.p. 176.6-177.8 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.216-7.200 (d, *J*=8.0 Hz, Ar-H, 1H), 7.022-7.019 (d, *J*=1.5 Hz, CH=CH, 1H), 7.007-6.990 (d, *J*=8.5 Hz, Ar-H, 1H), 6.955-6.923 (d, *J*=16.0 Hz, Ar-H, 1H), 6.847-6.831 (d, *J*=8.0 Hz, Ar-H, 1H), 6.798-6.766 (d, *J*=16.0 Hz, Ar-H, 1H), 6.191-6.170 (m, Ar-H, 1H), 6.060-6.056 (d, *J*=2.0 Hz, -CH=CH-, 1H), 5.29 (s, -NH<sub>2</sub>, 4H), 3.923 (s, -OCH<sub>3</sub>, 3H), 3.890 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>: C, 71.09; H, 6.71; N, 10.36. Found: C, 71.18; H, 6.62; N, 10.43.

#### **Intermediate 7, 3, 5-(4'-methoxy-cinnamenyl)-dinitro-benzene**

The known **intermediate 7** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the yellow solid (yield, 38%, m.p. 137.2-139.1 °C). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 8.849 (s, Ar-H, 1H), 8.429 (s, Ar-H, 1H), 7.160-7.146 (d, *J*=7.0 Hz, -CH=CH-, 2H), 6.916-6.892 (d, *J*=12.0 Hz, Ar-H, 1H), 6.833-6.819 (d, *J*=7.0 Hz, Ar-H, 2H), 6.566-6.542 (d, *J*=12.0 Hz, Ar-H, 1H), 3.825 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>: C, 60.01; H, 4.02; N, 9.33. Found: C, 60.12; H, 3.94; N, 9.40.

#### **Intermediate 8, 3, 5-(4'-Methoxy-cinnamenyl)-diaminyl-benzene**

The known **intermediate 8** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the



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faint yellow solid (yield, 20%, m.p., 145.6-147.2 °C). <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.45-7.44 (d, *J*=6.0 Hz, Ar-H, 2H), 6.90-6.89 (d, *J*=6.0 Hz, Ar-H, 2H), 6.84-6.82 (d, *J*=12.0 Hz, Ar-H, 1H), 6.76-6.73 (d, *J*=18.0 Hz, Ar-H, 1H), 5.988-5.986 (d, *J*=12.0 Hz, -CH=CH-, 2H), 5.743 (s, Ar-H, 1H), 4.690 (s, -NH<sub>2</sub>, 4H), 3.745 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O: C, 74.97; H, 6.71; N, 11.66. Found: C, 75.03; H, 6.65; N, 11.72.

#### **Intermediate 9, 2-(4'-Methoxy-cinnamenyl)-nitro-benzene**

In a three-necked flask equipped with a magnetic stirrer, 4-methoxy-benzaldehyde, 2-nitrophenyl acetic acid and piperidine were added with the molar ratio of 1:3:3. The mixture was heated to 100 °C for 3 hours with stirring, then the reaction was kept at 130 °C for 5 hours. After the reaction, the product was then extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic layer was dried by anhydrous MgSO<sub>4</sub>. The solvent was removed under reduced pressure to leave the crude product. which was further purified by column chromatography (C<sub>6</sub>H<sub>12</sub>:CH<sub>2</sub>Cl<sub>2</sub>=2:1) to afford the desired product as yellow needle solid (yield, 75%, m.p., 126.4-127.8 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.968-7.927 (m, Ar-H, 2H), 7.723-7.693 (t, *J*=7.5 Hz, Ar-H, 1H), 7.562-7.546 (d, *J*=8.0 Hz, Ar-H, 2H), 7.505-7.474 (t, *J*=7.75 Hz, CH=CH, 1H), 7.335-7.260 (m, Ar-H, CH=CH, 1H), 6.983-6.966 (d, *J*=8.5 Hz, Ar-H, 2H), 3.784 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>: C, 70.58; H, 5.13; N, 5.49. Found: C, 70.63; H, 5.06; N, 5.54.

#### **Intermediate 10, 2-(4'-Methoxy-cinnamenyl)-aminyl-benzene**

The mixed aqueous solution of sodium sulfide hydrate (5.6 g, 23 mmol) and sodium hydroxide (2.2 g, 55 mol) was dropped into a solution of 2-(4'-methoxy-cinnamenyl)-nitro-benzene (5 mmol, 1.4 g) in 100 ml ethanol, the mixed solution was stirred at 60°C for 2-3h. After

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the reaction, the solvent was removed under vacuum and the residue was extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic layer was dried by anhydrous MgSO<sub>4</sub>, and the solvent was removed under reduced pressure to gain the crude product, which was further purified by column chromatography (C<sub>6</sub>H<sub>12</sub>:EtOAc=4:1, v/v) to afford desired product as faint yellow solid (yield, 55 %, m.p., 118.5-120.0 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.574-7.545 (m, Ar-H, 2H), 7.404-7.366 (m, Ar-H, 1H), 7.253-7.220 (d, *J*=16.5 Hz, CH=CH, 1H), 6.947-6.906 (m, Ar-H, 4H), 6.639-6.623 (d, *J*=8.0 Hz, Ar-H, 1H), 6.548-6.518 (t, *J*=7.5 Hz, Ar-H, 1H), 5.290 (s, -NH<sub>2</sub>, 2H), 3.768 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>15</sub>NO: C, 79.97; H, 6.71; N, 6.66. Found: C, 80.04; H, 6.67; N, 6.72.

#### **Intermediate 11, 4-Methoxyl-3'-nitro-diphenylethylene**

The synthesis of **intermediate 11** followed essentially the same procedure as described that of **intermediate 9**, in which 2-nitrophenyl acetic acid was replaced by 3-nitrophenyl acetic acid in synthetic process. (yield, 53%, m.p. 112.2-113.8 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.384 (s, Ar-H, 1H), 8.075-8.021 (m, Ar-H, 2H), 7.649-7.595 (m, Ar-H, 3H), 7.460-7.419 (d, *J*=16.4 Hz, Ar-H, 1H), 7.289-7.247 (d, *J*= 16.8 Hz, Ar-H, 1H), 6.993-6.972 (d, *J*=8.4 Hz, CH=CH, 2H), 3.791 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>: C, 70.58; H, 5.13; N, 5.49. Found: C, 70.64; H, 5.07; N, 5.52.

#### **Intermediate 12, 4-Methoxyl-3'-amine-diphenylethylene**

The synthesis of **intermediate 12** followed essentially the same procedure as described that of **intermediate 10**, in which 2-(4'-methoxy-cinnamenyl)-nitro-benzene was replaced by 3-(4'-methoxy-cinnamenyl)-nitro-benzene in synthetic process (yield, 53%, m.p., 135.1-136.8 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.495-7.473 (d, *J*=8.8 Hz, Ar-H, 2H), 7.012-6.971 (m, Ar-

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H, 2H), 6.923-6.883 (m, Ar-H, 3H), 6.727-6.710 (d,  $J=6.8$  Hz, 2H), 6.462-6.422 (d,  $J=16.0$  Hz, Ar-H, 1H), 5.020 (s, -NH<sub>2</sub>, 2H), 3.746 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>15</sub>NO: C, 79.97; H, 6.71; N, 6.66. Found: C, 80.09, H, 6.65; N, 6.71.

### **Intermediate 13, 4-Methoxyl-4'-nitro-diphenylethylene**

The synthesis of intermediate 13 followed essentially the same procedure as described that of **intermediate 11**, red solid product was gained (yield, 59%, m.p., 158.2-159.6 °C). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.206-8.188 (d,  $J=9.0$  Hz, Ar-H, 2H), 7.599-7.581 (d,  $J=9.0$  Hz, Ar-H, 2H), 7.501-7.484 (d,  $J=8.5$  Hz, Ar-H, 2H), 7.237-7.204 (t,  $J=8.25$  Hz, Ar-H, 1H), 7.018-6.986 (d,  $J=16.0$  Hz, Ar-H, 1H), 6.937-6.919 (d,  $J=9.0$  Hz, CH=CH, 2H), 3.848 (s, -OCH<sub>3</sub>, 3H). Elementary analysis, Anal. Calcd for C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>: C, 70.58; H, 5.13; N, 5.49. Found: C, 70.65; H, 5.04; N, 5.57.

### **Synthesis of target compounds**

#### **Target C1, 2, 2'-(4''-Styryl-1'', 3''-phenylene)-bis(ylidene)-bis-(methyl)diphenol**

The known **target C1** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid (yield, 25%, m.p. 162.6-163.8 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 13.058 (s, -OH, 1H), 13.005 (s, -OH, 1H), 9.110 (s, N=CH, 1H), 9.046 (s, N=CH, 1H), 7.945-7.928 (d,  $J=8.5$  Hz, Ar-H, 1H), 7.751-7.733 (m, Ar-H, 1H), 7.686-7.668 (m, Ar-H, 1H), 7.571-7.502 (m, Ar-H, 4H), 7.485-7.393 (m, Ar-H, 6H), 7.363-7.280 (m, CH=CH, 2H), 7.053-6.986 (m, Ar-H, 4H). <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 164.237, 163.471, 160.330, 148.267, 147.181, 137.082, 133.624, 133.456, 132.548, 130.376, 128.868, 127.929, 126.949, 126.415, 123.056, 120.205, 119.617, 119.332, 119.235, 116.698, 112.134. FT-IR (cm<sup>-1</sup>): 3434.5, 3051.5, 3024.3, 2923.6,

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2853.3, 2727.1, 1613.9, 1589.4, 1565.9, 1492.3, 1481.5, 1456.6, 1281.4, 961.1, 901.4, 875.2, 810.5, 756.2. HRMS (ESI)  $m/z$ : calcd for  $C_{28}H_{22}N_2O_2$   $[M+H]^+$  419.1681, found 419.1685. Elementary analysis, Anal. Calcd for  $C_{28}H_{22}N_2O_2$ : C, 80.36; H, 5.30; N, 6.69. Found: C, 80.42; H, 5.25; N, 6.76.

**Target C2, 2'-(4''-(4''-methoxystyryl)-1'', 3''-phenylene)bis(ylidene)-bis-(methyl)diphenol**

The known **target C2** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid (yield, 15%, m.p. 137.0-139.0 °C).  $^1H$ -NMR (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm): 13.095 (s, -OH, 1H), 13.076 (s, -OH, 1H), 9.111 (s, N=CH, 1H), 9.044 (s, N=CH, 1H), 7.912-7.896 (d,  $J=8.0$  Hz, Ar-H, 1H), 7.746-7.732 (d,  $J=7.0$  Hz, Ar-H, 1H), 7.682-7.669 (d,  $J=6.5$  Hz, Ar-H, 1H), 7.516-7.426 (m, Ar-H, 6H), 7.412-7.226 (m, CH=CH, 2H), 7.054-6.981 (m, Ar-H, 6H), 3.784 (s, -OCH<sub>3</sub>, 3H).  $^{13}C$ -NMR (DMSO, 125 MHz, TMS):  $\delta$ =164.113, 163.261, 160.342, 159.213, 147.783, 146.796, 133.398, 132.534, 130.080, 129.736, 127.761, 126.594, 120.644, 120.209, 119.605, 119.320, 119.222, 116.682, 116.650, 114.363, 112.080, 55.160. FT-IR ( $cm^{-1}$ ): 3431.4, 3057.6, 3029.9, 3001.9, 2951.4, 2924.6, 2852.6, 2836.5, 2831.2, 1609.6, 1569.4, 1550.5, 1511.6, 1479.6, 1456.6, 1282.5, 1251.9, 969.7, 908.2, 855.3, 830.8, 809.3, 754.2. HRMS (ESI)  $m/z$ : calcd for  $C_{29}H_{24}N_2O_3$   $[M-H]^+$  447.1787, found 447.1790. Elementary analysis, Anal. Calcd for  $C_{29}H_{24}N_2O_3$ : C, 77.66; H, 5.39; N, 6.25. Found: C, 77.70; H, 5.27; N, 6.33.

**Target C3**

**2,2'-(4''-(3''',4'''-dimethoxystyryl)-1'',3''-phenylene)bis(ylidene)-bis-(methyl)diphenol**

The known target **C3** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the

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faint yellow solid (yield, 28%, m.p. 153.0-155.0 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 13.191 (s, -OH, 1H), 13.101 (s, -OH, 1H), 9.102 (s, N=CH, 1H), 9.060 (s, N=CH, 1H), 7.893-7.876 (d, *J*=8.5 Hz, Ar-H, 1H), 7.744-7.729 (d, *J*=7.5 Hz, Ar-H, 1H), 7.681-7.666 (d, *J*=7.5 Hz, Ar-H, 1H), 7.526-7.524 (d, *J*=1.0 Hz, CH=CH, 1H), 7.484-7.423 (m, Ar-H, 4H), 7.269-7.236 (d, *J*=16.5 Hz, Ar-H, 1H), 7.197-7.194 (d, *J*=1.5 Hz, CH=CH, 1H), 7.107-7.090 (d, *J*=8.5 Hz, Ar-H, 1H), 7.046-6.982 (m, Ar-H, 5H), 3.827 (s, -OCH<sub>3</sub>, 3H), 3.782 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 163.908, 163.240, 160.452, 160.344, 148.956, 148.907, 133.565, 132.588, 132.535, 130.316, 130.149, 130.085, 126.581, 121.038, 120.242, 119.595, 119.319, 119.289, 119.212, 116.649, 111.941, 109.458, 55.500, 55.319. FT-IR (cm<sup>-1</sup>): 3433.0, 3053.9, 3002.3, 2932.0, 2903.7, 2833.8, 1615.8, 1588.4, 1565.7, 1513.4, 1480.7, 1456.0, 1280.4, 1263.7, 961.6, 901.5, 876.9, 845.5, 806.1, 755.1. HRMS (ESI) *m/z*: calcd for C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub> [M-H]<sup>-</sup> 477.1893, found 477.1896. Elementary analysis, Anal. Calcd for C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>: C, 75.30; H, 5.48; N, 5.85. Found: C, 75.43; H, 5.37; N, 5.92.

**Target C4, 2, 2'-((5-(2-phenylethenyl)-benzene-1, 3-diy)-bis-(nitrile-methylidene))diphenol**

5-Styryl-benzene-1, 3-diamine (0.21 g, 1.00 mmol) and 2-hydroxy-benzaldehyde (0.488 g, 4.00 mmol) in 100 ml dry ethanol were added into three-necked flask. The reaction mixture was stirred at room temperature under argon protection for 12 h. After the reaction, the solvent was evaporated under vacuum. Recrystallization from ethanol and cyclohexane gave the pure product as the yellow solid. Yield, 69%, m.p. 163.0-164.2 °C. <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 12.828 (s, -OH, 2H), 8.902 (s, CH=N, 2H), 7.608-7.587 (d, *J*=8.6 Hz, Ar-H, 3H), 7.425-7.360 (m, Ar-H, 3H), 7.238-7.150 (m, Ar-H, 4H), 6.987-6.939 (m, Ar-H, 4H), 6.869-6.847 (d, *J*=8.8 Hz, -CH=CH-, 2H), 6.691-6.579 (m, Ar-H, 2H). <sup>13</sup>C-NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ



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(ppm):164.499, 160.673, 159.124, 149.794, 139.936, 133.960, 132.922, 131.425, 130.414, 129.168, 127.810, 120.472, 119.646, 117.082, 114.321, 112.978. FT-IR (cm<sup>-1</sup>): 3433.2, 3047.2, 3023.3, 2921.1, 2844.5, 2725.2, 1614.7, 1585.3, 1556.2, 1483.1, 1477.1, 1455.7, 1278.8, 958.9, 907.4, 872.3, 809.5, 758.4. HRMS (ESI) m/z: calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 419.1681, found 419.1687. Elementary analysis, Anal. Calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>: C, 80.36; H, 5.30; N, 6.69. Found: C, 80.44; H, 5.21; N, 6.75.

### **Target C5**

#### **2, 2'-((5-(2-(4-methoxyphenyl)ethenyl)benzene-1, 3-diyl)-bis-(nitrilomethylylidene))-diphenol**

The known target **C5** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as faint yellow solid (yield, 53%, m.p. 170.6-172.8 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 13.006 (s, -OH, 2H), 9.093 (s, CH=N, 2H), 7.688-7.669 (d, J=7.6 Hz, -CH=CH-, 2H), 7.576-7.556 (d, J=8.0 Hz, Ar-H, 4H), 7.449-7.390 (m, Ar-H, 4H), 7.205-7.164 (d, Ar-H, 1H), 7.017-6.957 (m, Ar-H, 6H), 3.773 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 164.666, 160.789, 159.669, 150.032, 140.322, 133.934, 133.066, 130.198, 129.873, 128.401, 125.525, 119.718, 119.671, 118.273, 117.109, 114.722, 112.772, 55.620. FT-IR (cm<sup>-1</sup>): 3435.3, 3052.3, 3030.2, 3010.6, 2959.2, 2933.8, 2850.7, 2839.4, 1611.7, 1571.3, 1560.2, 1518.5, 1481.6, 1450.1, 1279.2, 1243.4, 973.4, 901.1, 862.2, 839.2, 810.3, 759.1. HRMS (ESI) m/z: calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 449.1787, found 449.1789. Elementary analysis, Anal. Calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>: C, 77.66; H, 5.39; N, 6.25. Found: C, 77.72; H, 5.31; N, 6.32.

### **Target C6, 1, 3-dikis(iminyl-methyl)-bistyrene**

The known target **C6** was synthesized as described in our previously work in Ref. 1. The

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characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid (yield, 27%, m.p. 161.3-162.6 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.751 (s, N=CH, 1H), 8.683 (s, N=CH, 1H), 8.037-8.013 (m, Ar-H, 2H), 7.959-7.935 (m, Ar-H, 2H), 7.850-7.829 (d, J=8.4Hz, CH=CH, 1H), 7.645-7.604 (d, J=16.4 Hz, CH=CH,1H), 7.568-7.522 (m, Ar-H, 8H), 7.379-7.341 (t, J=7.6 Hz, Ar-H, 2H), 7.287-7.210 (m, Ar-H, 3H), 7.104-7.099 (d, J=2.0 Hz, Ar-H, 1H). <sup>13</sup>C-NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 161.524, 161.042, 151.863, 150.494, 137.885, 136.548, 136.473, 132.096, 131.979, 129.381, 129.278, 129.227, 129.155, 127.994, 127.036, 126.752, 124.636, 119.806, 111.555. FT-IR (cm<sup>-1</sup>): 2931.3, 2911.8, 1630.1, 1584.5, 1553.9, 1495.7 1451.2, 975.9, 963.5, 896.4, 875.2, 818.2, 757.8. MS(ESI) m/z: calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub> [M+H]<sup>+</sup> 387.1783, found 387.1788. Elementary analysis, Anal. Calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub>: C, 87.01; H, 5.74; N, 7.25. Found: C, 87.11; H, 5.67; N, 7.32.

#### **Target C7, 1, 3-Dikis(iminyl-methyl)-(4''-methoxy)-bistyrene**

The known target **C7** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid (yield, 46%, m.p. 138.5-139.6 °C) <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.737 (s, -N=CH-, 1H), 8.661 (s, -N=CH-, 1H), 8.021-7.998 (m, Ar-H, 2H), 7.944-7.921 (m, Ar-H, 2H), 7.797-7.777 (d, J=8.0 Hz, CH=CH, 1H), 7.554-7.438 (m, Ar-H, 8H), 7.217-7.176 (m, Ar-H, 2H), 7.079-7.075 (d, J=2.0 Hz, Ar-H, 1H), 6.932-6.910 (d, J=8.8 Hz, Ar-H, 2H) 3.736 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 161.384, 160.860, 159.393, 151.387, 150.194, 136.592, 136.516, 132.077, 131.955, 130.575, 129.616, 129.393, 129.299, 129.258, 129.199, 129.128, 129.073, 129.010, 128.943, 128.808, 128.070, 126.772, 126.667, 122.316, 119.844, 114.816, 114.738, 111.524, 55.589, IR(cm<sup>-1</sup>): 2863.4, 2831.0, 1607.1, 1573.7, 1505.3, 1453.2, 1243.9,

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1175.8, 1031.2, 968.0, 834.3, 768.8. HRMS (ESI) m/z: calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O [M-H]<sup>-</sup> 415.1889, found 415.1891. Elementary analysis, Anal. Calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O: C, 83.63; H, 5.81; N, 6.73. Found: C, 83.71; H, 5.76; N, 6.82.

**Target C8, 1, 3-Dikis(iminyl-methyl)-(3'', 4''-dimethoxy)-bistyrene**

The known target **C8** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid the faint yellow solid (yield, 30%, m.p. 157.2-159.1 °C) .C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>, <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.742 (s, N=CH, 1H), 8.669 (s, N=CH, 1H), 8.024-8.006 (m, Ar-H, 2H), 7.941-7.923 (m, Ar-H, 2H), 7.784-7.736 (d, J=19.2 Hz, CH=CH, 1H), 7.549-7.467 (m, Ar-H, 7H), 7.212-7.161 (m, Ar-H, 2H), 7.096-7.041 (m, Ar-H, 3H), 6.942-6.921 (d, J=8.4 Hz, Ar-H, 1H), 3.774 (s, -OCH<sub>3</sub>, 3H), 3.734 (s, -OCH<sub>3</sub>, 3H).<sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 161.282, 160.878, 157.740, 151.388, 150.128, 149.338, 149.150, 136.621, 136.617, 132.083, 131.961, 130.945, 129.790, 129.639, 129.532, 129.380, 129.303, 129.237, 129.129, 126.817, 122.743, 119.844, 119.712, 119.215, 115.647, 112.466, 111.514, 109.984, 55.980, 55.824. FT-IR (cm<sup>-1</sup>): 2821.8, 1635.7, 1573.0, 1516.0, 1463.8, 1451.5, 1438.1, 1270.8, 1229.0, 1126.5, 1025.8, 958.3, 857.7, 830.8, 801.1, 771.0, 749.8. HRMS (ESI) m/z: calcd for C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>447.1994, found 447.1997. Elementary analysis, Anal. Calcd for C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>: C, 80.69; H, 5.87; N, 6.27. Found: C, 80.73; H, 5.77; N, 6.31.

**Target C9, N, N'-(5-(2-phenylethenyl)-benzene-1,3-diyl)-bis-(1-phenylmethanimine)**

The synthetic procedure and method were the same as described in the synthetic process of target **C4**, in which 2-hydroxy-benzaldehyde was replaced by benzaldehyde in the synthetic process. Yellow solid was obtained, yield, 61.5%, m.p. 152.0-153.5 °C. <sup>1</sup>H-NMR (400 MHz,

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DMSO-*d*<sub>6</sub>) δ (ppm): 8.545 (s, -CH=N, 2H), 7.782-7.716 (m, Ar-H, 5H), 7.540-7.519 (d, J=8.4 Hz, Ar-H, 3H), 7.329-7.289 (d, J=16.0 Hz, -CH=CH-, 1H), 7.222 (s, Ar-H, 2H), 7.125-7.084 (d, J=16.4 Hz, -CH=CH-, 1H), 6.941-6.859 (m, Ar-H, 8H). <sup>13</sup>C-NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 161.194, 160.803, 158.951, 153.343, 139.166, 132.553, 131.140, 130.858, 130.638, 130.417, 129.474, 129.444, 128.568, 127.762, 118.649, 116.345, 116.105, 116.045, 114.261, 114.029, 112.176. IR(cm<sup>-1</sup>): 2938.2, 2919.5, 1639.2, 1579.9, 1559.8, 1490.3, 1449.6, 969.7, 958.3, 891.3, 869.1, 820.4, 760.2. HRMS (ESI) m/z: calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub> [M+H]<sup>+</sup> 387.1783, found 387.1787. Elementary analysis, Anal. Calcd for C<sub>28</sub>H<sub>22</sub>N<sub>2</sub>: C, 87.01; H, 5.74; N, 7.25. Found: C, 87.12; H, 5.65; N, 7.31.

### Target C10

#### **N, N'-(5-(2-(4-methoxyphenyl)-ethenyl)-benzene-1, 3-diyl)-bis-(1-phenylmethanimine)**

The known target **C10** was synthesized as described in our previously work in Ref. 1. The characterization data in our report presents as follow: The desired product was obtained as the pale yellow solid as the white solid (yield, 47%, m.p. 158.8-159.9 °C) <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.743 (s, -CH=N, 2H), 7.973-7.954 (t, J=7.6 Hz, Ar-H, 4H), 7.567-7.532 (t, J=7.0 Hz, Ar-H, 8H), 7.387-7.356 (d, J=12.4 Hz, Ar-H, 3H), 7.175-7.134 (d, J=16.4 Hz, Ar-H, 1H), 7.049 (s, Ar-H, 1H), 6.964-6.943 (d, J=8.4 Hz, -CH=CH-, 2H), 3.766 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 161.718, 159.556, 153.181, 139.773, 136.428, 132.029, 130.003, 129.602, 129.300, 129.249, 129.232, 129.177, 128.342, 125.957, 117.071, 114.667, 112.186, 55.607. IR(cm<sup>-1</sup>): 2860.2, 2829.9, 1600.3, 1569.2, 1500.8, 1463.0, 1240.1, 1180.3, 1029.0, 970.9, 830.6, 770.5. HRMS (ESI) m/z: calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 417.1889, found 417.1892. Elementary analysis, Anal. Calcd for C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O: C, 83.63; H, 5.81; N, 6.73. Found: C, 83.70; H, 5.73; N,

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6.80.

**Target C11, 2-((4'-Methoxyl-diphenylethylene-2''-ylimino)methyl)phenol**

The synthesis of target **C11** followed essentially the same procedure as described that of target **C1**, in which 1, 2-diamine-4-styrylbenzene was replaced by 2-(4'-methoxy-cinnamenyl)-aminyl-benzene in the synthetic process. Product material was faint yellow solid (yield, 75%, m.p., 110.3-111.0 °C). <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 13.160 (s, -OH, 1H), 8.924 (s, N=CH, 1H), 7.814-7.799 (d, *J*=7.5 Hz, Ar-H, 1H), 7.726-7.708 (m, Ar-H, 1H), 7.503-7.486 (m, Ar-H, 2H), 7.472-7.437 (m, Ar-H, 1H), 7.406-7.367 (m, Ar-H, 3H), 7.356-319 (m, Ar-H, 4H), 7.238-7.206 (d, *J*=16.0 Hz, CH=CH, 1H), 7.037-6.972 (m, CH=CH, 1H), 3.778 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 163.457, 160.315, 159.173, 145.886, 131.317, 130.102, 129.720, 128.441, 127.738, 127.056, 125.677, 121.259, 119.619, 119.248, 119.059, 116.641, 114.331, 55.157. IR (cm<sup>-1</sup>): 3423.0, 3058.0, 3032.7, 3004.6, 2957.2, 2933.6, 2908.3, 2835.2, 1607.0, 1590.2, 1575.5, 1559.8, 1512.0, 1475.6, 1451.2, 1283.6, 1248.1, 961.5, 908.5, 823.5, 755.2. HRMS (ESI) *m/z*: calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 330.1432, found 330.1425. Elementary analysis, Anal. Calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub>: C, 80.23; H, 5.81; N, 4.25. Found: C, 80.34; H, 5.73; N, 4.36.

**Target C12, 3-((4'-Methoxyl-diphenylethylene-2''-ylimino)methyl)phenol**

The synthesis of target **C12** followed essentially the same procedure as described that of target **C11**, in which 2-(4'-methoxy-cinnamenyl)-aminyl-benzene was replaced by 3-(4'-Methoxy-cinnamenyl)-aminyl-benzene in the synthetic process. Product material was faint yellow solid (yield, 60.3%, m.p., 147.0-148.8 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 13.094 (s, -OH, 1H), 9.002 (s, CH=N, 1H), 7.669-7.650 (d, *J*=7.6 Hz, Ar-H, 1H), 7.616 (s, Ar-H, 1H), 7.557-7.535

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(d,  $J=8.8$  Hz, CH=CH, 2H), 7.485-7.466 (d,  $J=7.6$  Hz, Ar-H, 1H), 7.443-7.404 (m, Ar-H, 2H), 7.291-7.260 (t,  $J=6.2$  Hz, Ar-H, 2H), 7.153-7.112 (d,  $J=16.4$  Hz, Ar-H, 1H), 7.000-6.937 (m, Ar-H, 4H), 3.764 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 163.018, 160.754, 149.270, 146.997, 136.856, 133.637, 132.953, 130.407, 129.120, 128.748, 127.609, 125.957, 122.294, 120.500, 119.830, 119.587, 117.021, 112.227, 109.657, 55.949. IR(cm<sup>-1</sup>): 3433.4, 3065.6, 3052.8, 3021.5, 3000.9, 2974.1, 2845.9, 1629.7, 1591.1, 1573.3, 1514.1, 1483.7, 1453.9, 1411.5, 1354.7, 1319.3, 1286.4, 1255.7, 1221.1, 1199.4, 1151.3, 1135.6, 1101.3, 1021.6, 963.1, 916.1, 845.3, 821.0, 803.4, 759.2. HRMS (ESI) *m/z*: calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 330.1271, found 330.1288. Elementary analysis, Anal. Calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub>: C, 80.23; H, 5.81; N, 4.25. Found: C, 80.34; H, 5.73; N, 4.36.

**Target C13, 2-((4'-Methoxyl-diphenylethylene-4''-ylimino)methyl)phenol**

The synthesis of target **C13** followed essentially the same procedure as described that of target **C11**, in which salicylaldehyde was replaced by benzaldehyde in the synthetic process. Product material was faint yellow solid (yield, 75%, m.p., 207.4-209.3°C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 8.655 (s, -N=CH, 1H), 7.930-7.907 (m, Ar-H, 2H), 7.602- 7.581 (d,  $J=8.4$  Hz, Ar-H, 2H), 7.533-7.497 (t,  $J=7.2$  Hz, Ar-H, 5H), 7.283-7.262 (d,  $J=8.4$  Hz, CH=CH, 2H), 7.207 - 7.074 (m, Ar-H, 2H), 6.937-6.915 (d,  $J=8.8$  Hz, Ar-H, 2H), 3.750 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 163.029, 160.741, 159.742, 147.016, 136.832, 133.636, 132.947, 130.870, 130.094, 128.737, 128.273, 128.137, 127.629, 127.436, 125.811, 122.264, 121.883, 119.822, 119.585, 117.016, 114.642, 55.604. IR (cm<sup>-1</sup>): 3448.2, 3057.9, 3021.5, 2957.2, 2934.6, 2909.3, 2838.7, 1621.5, 1604.3, 1571.3, 1490.2, 1456.6, 1407.7, 1384.5, 1363.5, 1283.1, 1266.6, 1254.4, 1190.2, 1178.0, 1149.5, 1110.7, 1031.0, 969.8, 956.5, 911.3, 838.7, 749.4, 741.2. HRMS

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(ESI) m/z: calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 330.1469, found 330.1453. Elementary analysis, Anal.

Calcd for C<sub>22</sub>H<sub>19</sub>NO<sub>2</sub>: C, 80.23; H, 5.81; N, 4.25. Found: C, 80.31; H, 5.72; N, 4.33.

**Target C14, N-benzylidene-2-(4-methoxystyryl)aniline**

The synthesis of target **C14** followed essentially the same procedure as described that of target **C11**, in which salicylaldehyde was replaced by benzaldehyde in the synthetic process. Product material was faint yellow solid (yield, 65%, m.p., 201.0-202.0 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.655 (s, N=CH, 1H), 7.930-7.907 (m, Ar-H, 2H), 7.602-7.581 (d, *J*=8.4 Hz, Ar-H, 2H), 7.533-7.497 (t, *J*=7.2 Hz, Ar-H, 5H), 7.283 -7.262 (d, *J*=8.4 Hz, CH=CH, 2H), 7.207-7.074 (m, Ar-H, 2H), 6.937-6.915 (d, *J*=8.8 Hz, Ar-H, 2H), 3.750 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 160.860, 159.410, 149.482, 136.598, 131.984, 131.426, 130.452, 129.476, 129.363, 129.172, 128.653, 128.089, 126.529, 125.834, 122.702, 119.117, 114.699, 55.565. FT-IR (cm<sup>-1</sup>): 3447.8, 3057.9, 3038.3, 2956.8, 2937.4, 2881.3, 2838.4, 1623.6, 1604.7, 1574.6, 1513.4, 1466.3, 1448.5, 1420.9, 1364.8, 1306.2, 1286.9, 1253.7, 1197.9, 1178.0, 1110.4, 1030.8, 965.1, 887.9, 837.5, 757.4, 730.8, 688.8. HRMS (ESI) m/z: calcd for C<sub>22</sub>H<sub>19</sub>NO [M+H]<sup>+</sup> 314.1544, found 314.1539. Elementary analysis, Anal. Calcd for C<sub>22</sub>H<sub>19</sub>NO: C, 84.33; H, 6.10; N, 4.47. Found: C, 84.43; H, 6.02; N, 4.55.

**Target C15, N-benzylidene-3-(4-methoxystyryl)aniline**

The synthesis of target **C15** followed essentially the same procedure as described that of target **C12**, in which salicylaldehyde was replaced by benzaldehyde in the synthetic process. Product material was faint yellow solid (yield, 43%, m.p. 138.3-139.5°C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 8.657 (s, CH=N, 1H), 7.954-7.931 (m, Ar-H, 2H), 7.548-7.519 (m, Ar-H, 5H), 7.452-7.375 (m, Ar-H, 3H), 7.296-7.256 (d, *J*=16Hz, Ar-H, 1H), 7.134-7.093 (t, *J*=8.2 Hz, Ar-H,

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2H), 6.948-6.927 (d,  $J=8.4$  Hz, CH=CH, 2H), 3.757 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 160.642, 150.949, 137.551, 136.509, 135.507, 131.911, 129.266, 129.143, 129.116, 128.450, 128.339, 128.011, 127.832, 126.869, 122.014, 56.136. FT-IR (cm<sup>-1</sup>): 3437.8, 3034.3, 3026.0, 2972.1, 2933.1, 1611.4, 1583.7, 1572.1, 1545.1, 1494.8, 1446.9, 1451.3, 1269.2, 961.7, 904.2, 852.9, 757.1, 692.3. HRMS (ESI)  $m/z$ : calcd for C<sub>22</sub>H<sub>19</sub>NO [M+H]<sup>+</sup> 314.1563, found 314.1570. Elementary analysis, Anal. Calcd for C<sub>22</sub>H<sub>19</sub>NO: C, 84.33; H, 6.10; N, 4.47. Found: C, 84.42; H, 6.02; N, 4.52

#### **Target C16, Benzylidene-(4-(2-(4-Methoxy-phenyl)-vinyl)-phenyl)-amine**

The synthesis of target **C16** followed essentially the same procedure as described that of target **C13**, in which salicylaldehyde was replaced by benzaldehyde in the synthetic process. Product material was faint yellow solid (yield, 56%, m.p., 201.0-202.0 °C). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 8.655 (s, N=CH, 1H), 7.930-7.907 (m, Ar-H, 2H), 7.602-7.581(d,  $J=8.4$  Hz, Ar-H, 2H), 7.533-7.497(t,  $J=7.2$ Hz, Ar-H, 5H), 7.283-7.262 (d,  $J=8.4$  Hz, CH=CH, 2H), 7.207-7.074 (m, Ar-H, 2H), 6.937-6.915 (d,  $J=8.8$  Hz, Ar-H, 2H), 3.750 (s, -OCH<sub>3</sub>, 3H). <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm): 160.380, 159.377, 150.484, 136.544, 135.927, 131.854, 130.195, 129.257, 129.075, 128.183, 128.154, 127.460, 127.329, 126.035, 122.001, 114.623, 55.596. FT-IR (cm<sup>-1</sup>): 3447.7, 3063.8, 3033.6, 3021.2, 3002.3, 2957.5, 2877.3, 2836.2, 2054.2, 2006.5, 1936.4, 1890.3, 1628.2, 1602.3, 1578.3, 1508.8, 1473.8, 1450.0, 1440.2, 1367.1, 1328.9, 1307.7, 1252.5, 1213.8, 1174.5, 1109.9, 1091.9, 1031.8, 978.6, 884.2, 865.2, 825.3, 761.7, 739.5, 688.0. HRMS (ESI)  $m/z$ : calcd for C<sub>22</sub>H<sub>19</sub>NO [M+H]<sup>+</sup> 314.1341, found 314.1337. Elementary analysis, Anal. Calcd for C<sub>22</sub>H<sub>19</sub>NO: C, 84.33; H, 6.10; N, 4.47. Found: C, 84.46; H, 6.02; N, 4.52.

#### **References and notes**

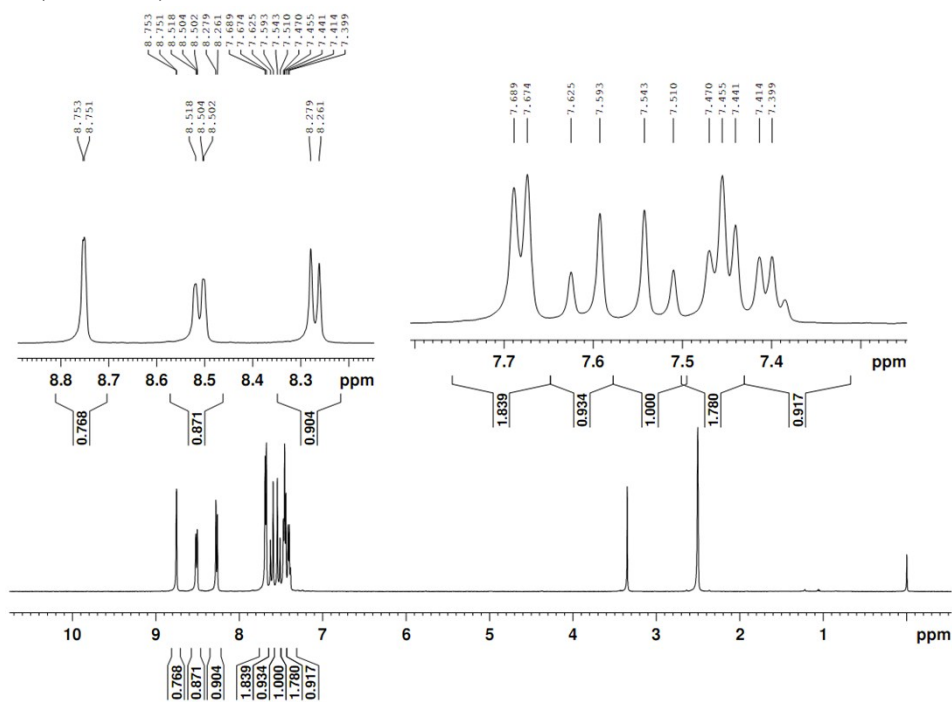


(1). G. Ding, Y. Lu, Y. L. Gong, L. Ma, Z. P. Luo, S. T. Zhang, F. Gao, H. R. Li, *Tetrahedron*, 2016, 72, 3040-3056.

#### 4. The characterization of the intermediates

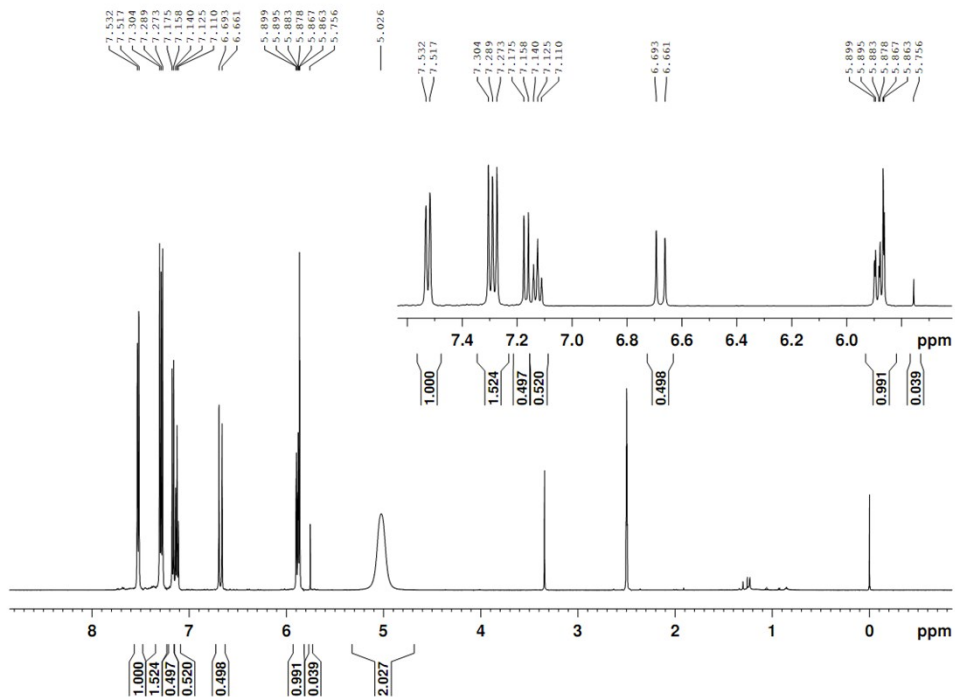
##### Intermediate 1

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



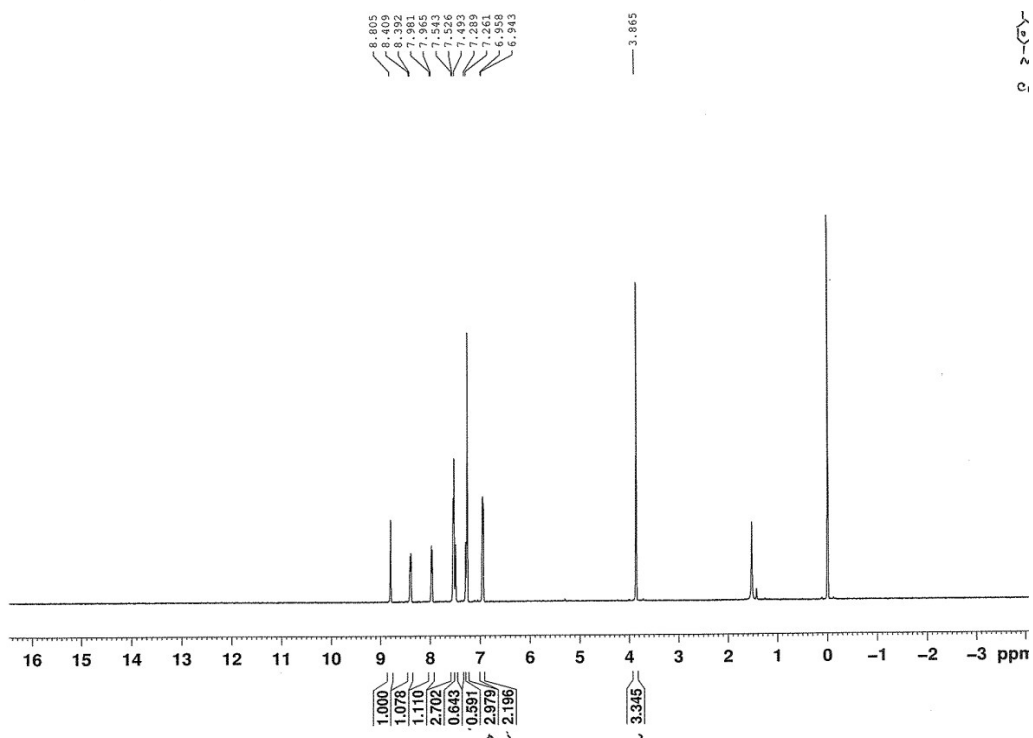
##### Intermediate 2

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



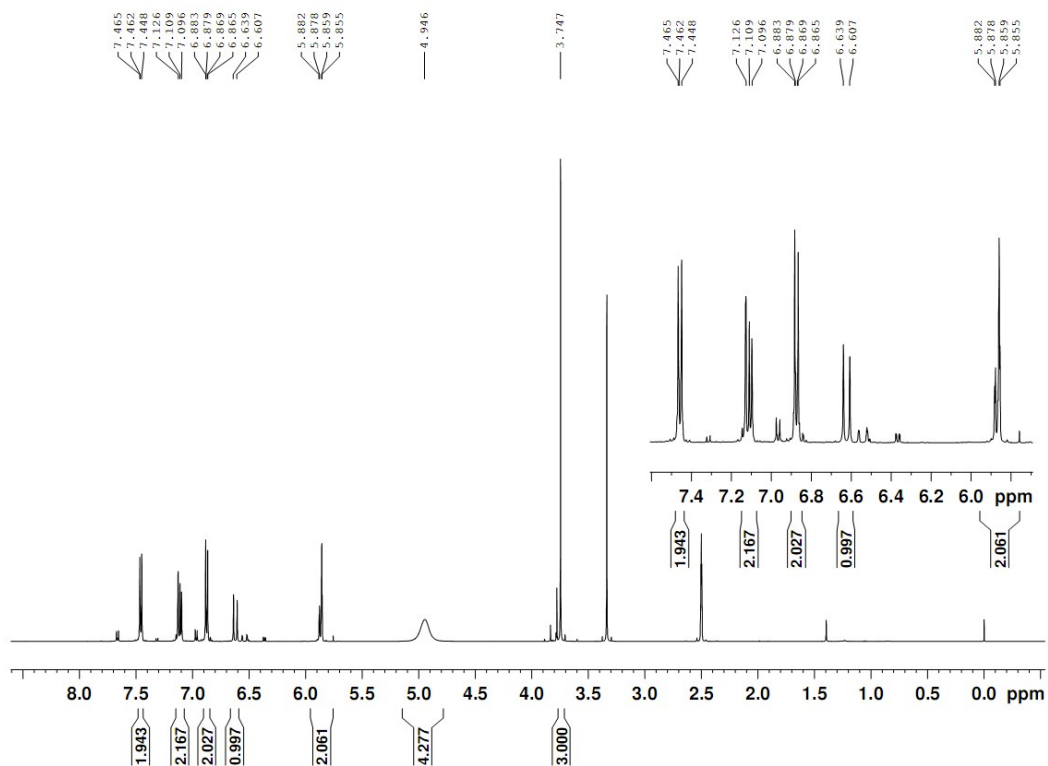
### Intermediate 3

<sup>1</sup>H-NMR (CDCl<sub>3</sub>)



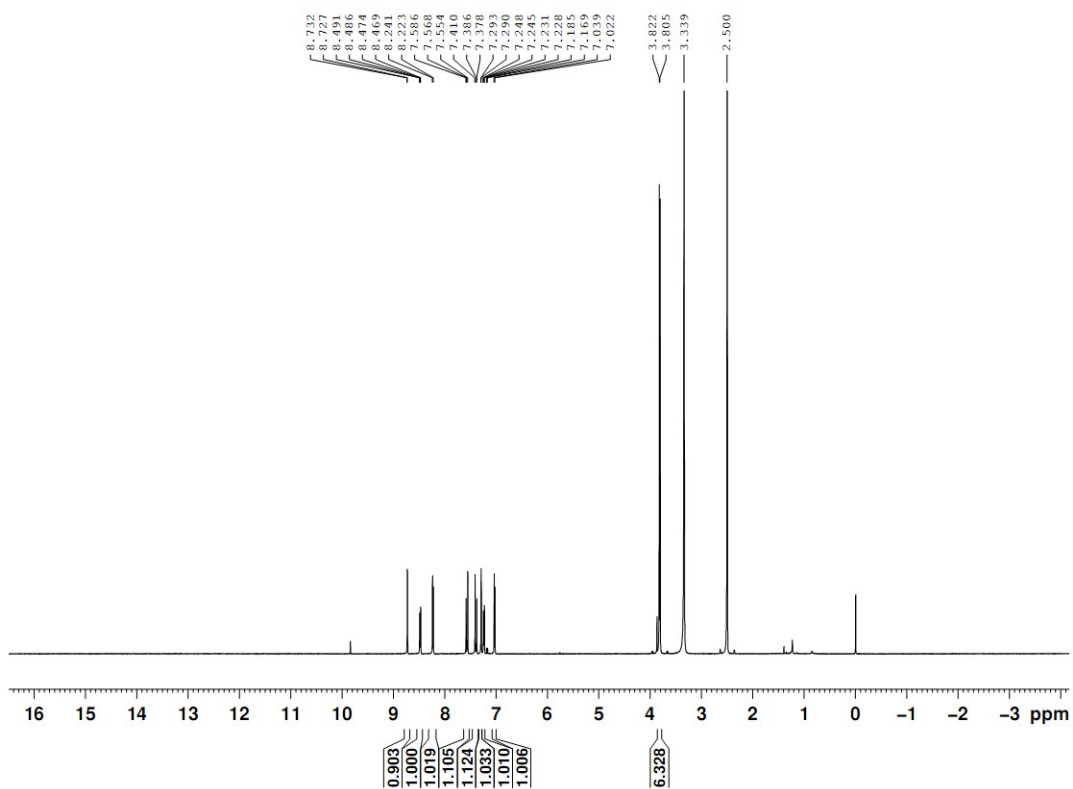
### Intermediate 4

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)



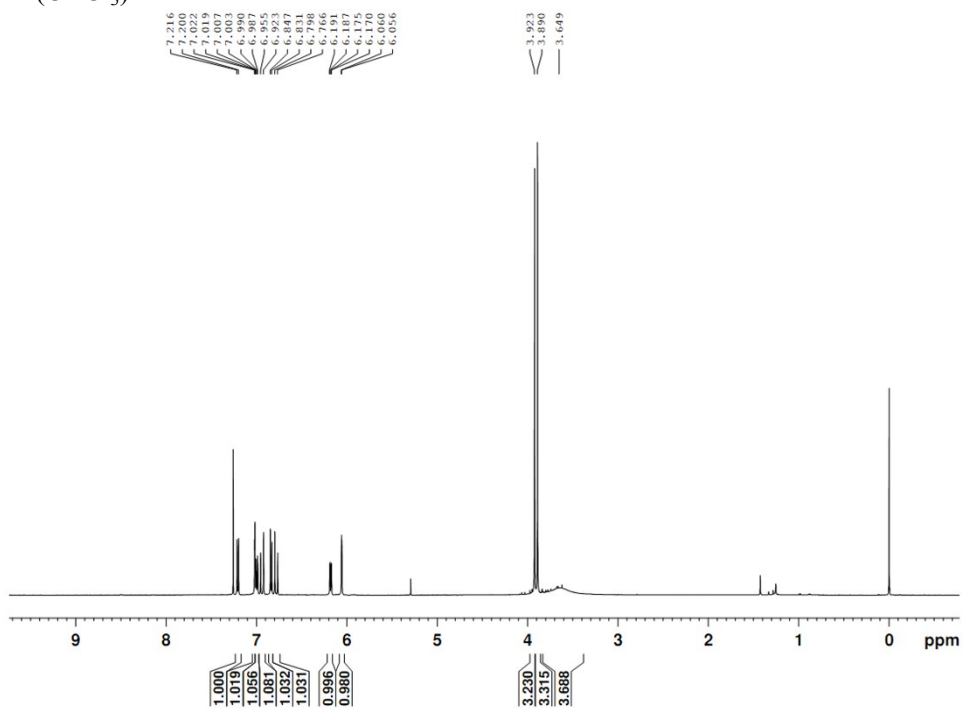
### Intermediate 5

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)



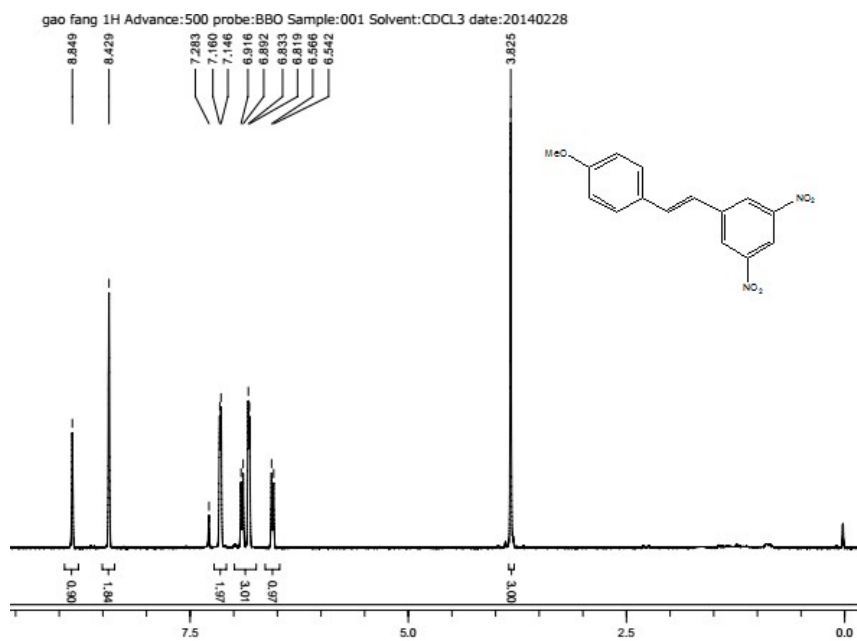
### Intermediate 6

$^1\text{H-NMR}$  ( $\text{CDCl}_3$ )



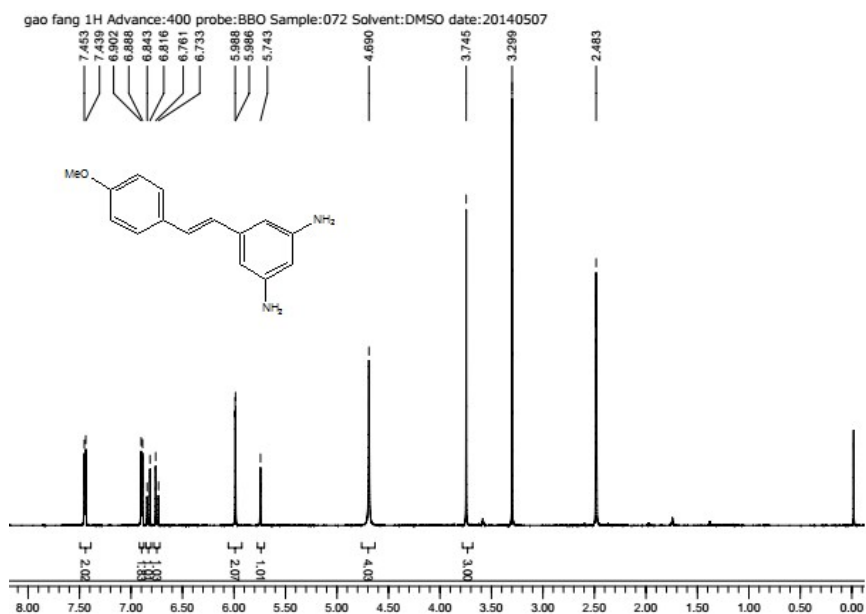
**Intermediate 7**

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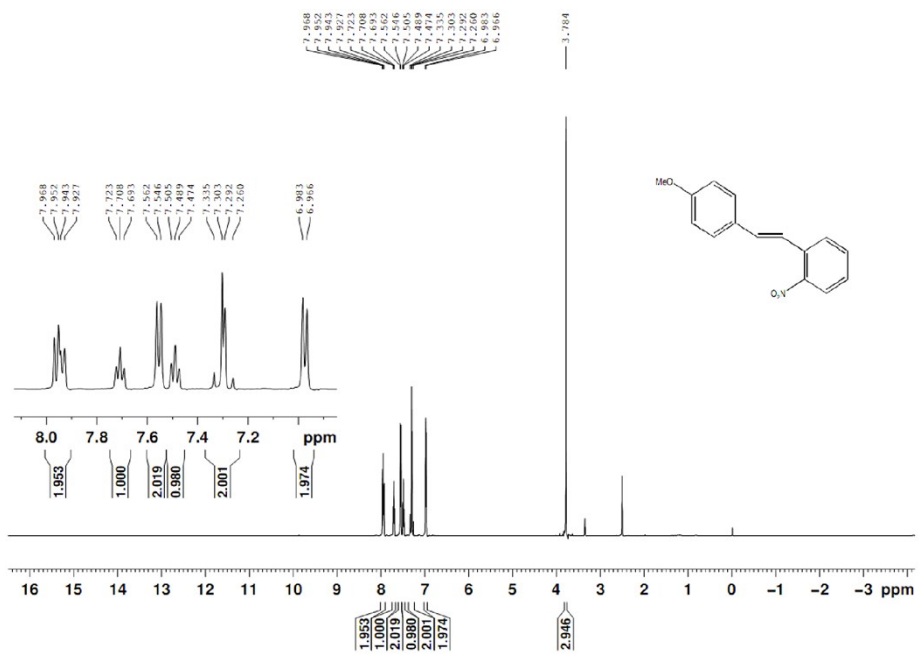
**Intermediate 8**

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



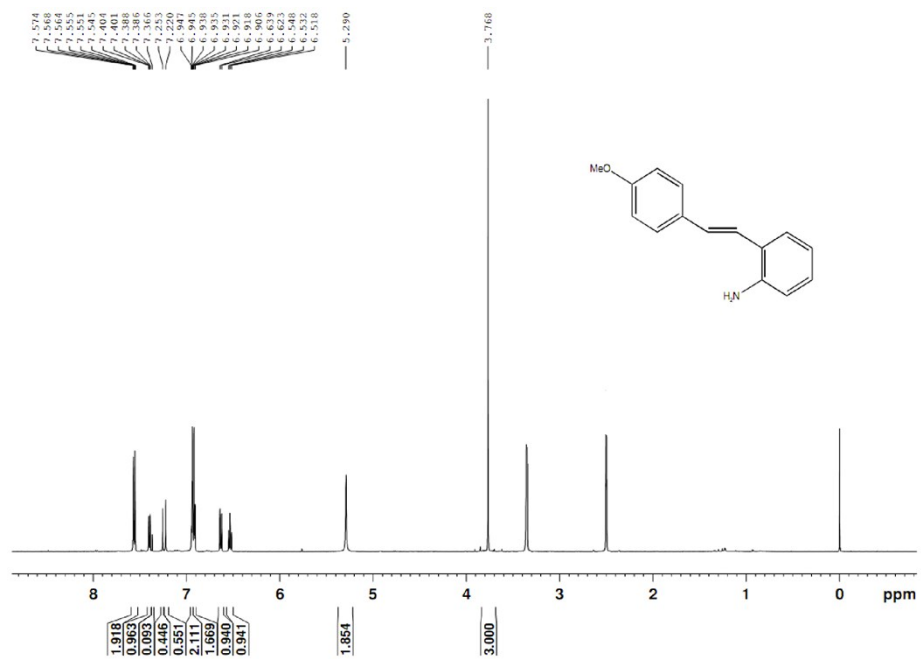
### Intermediate 9

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)



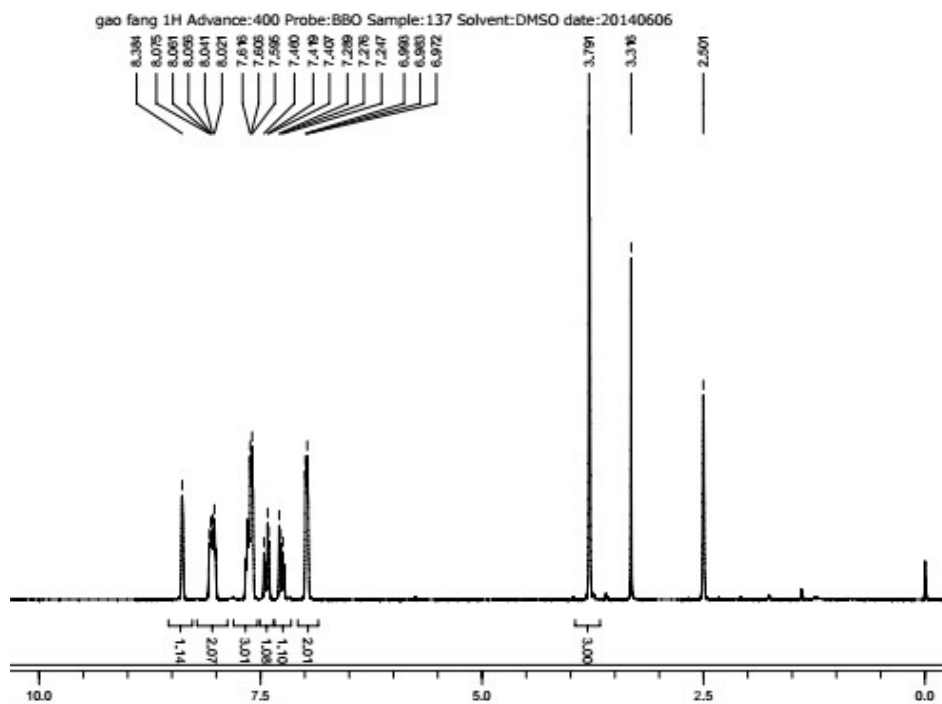
### Intermediate 10

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)



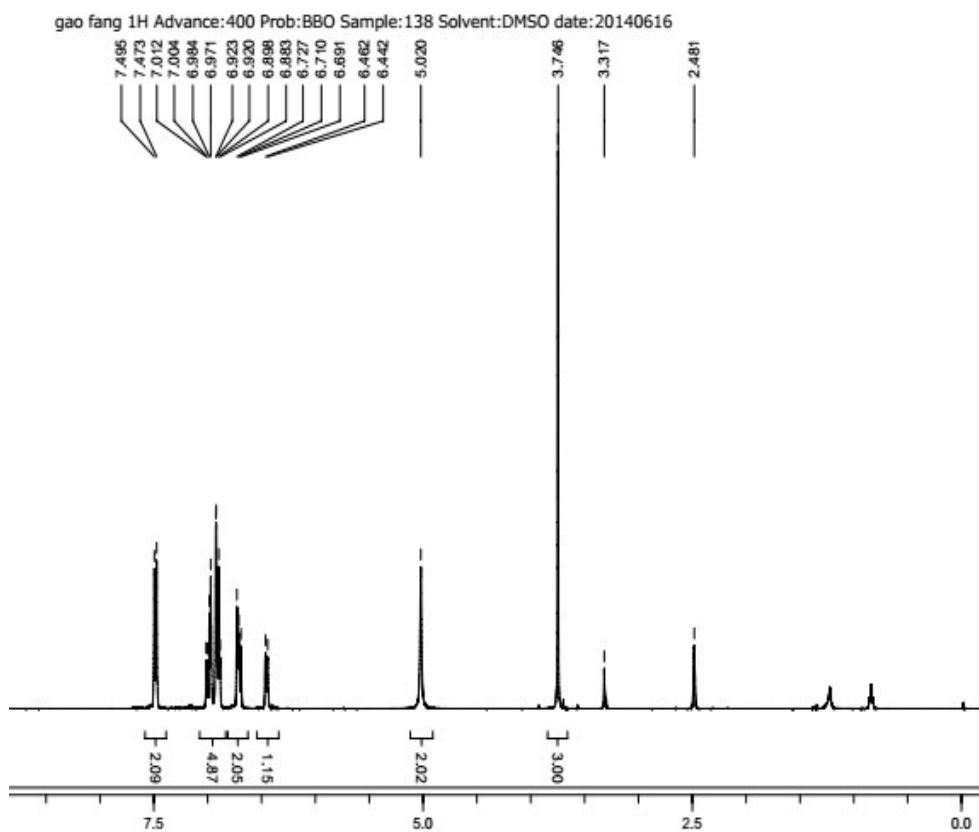
### Intermediate 11

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



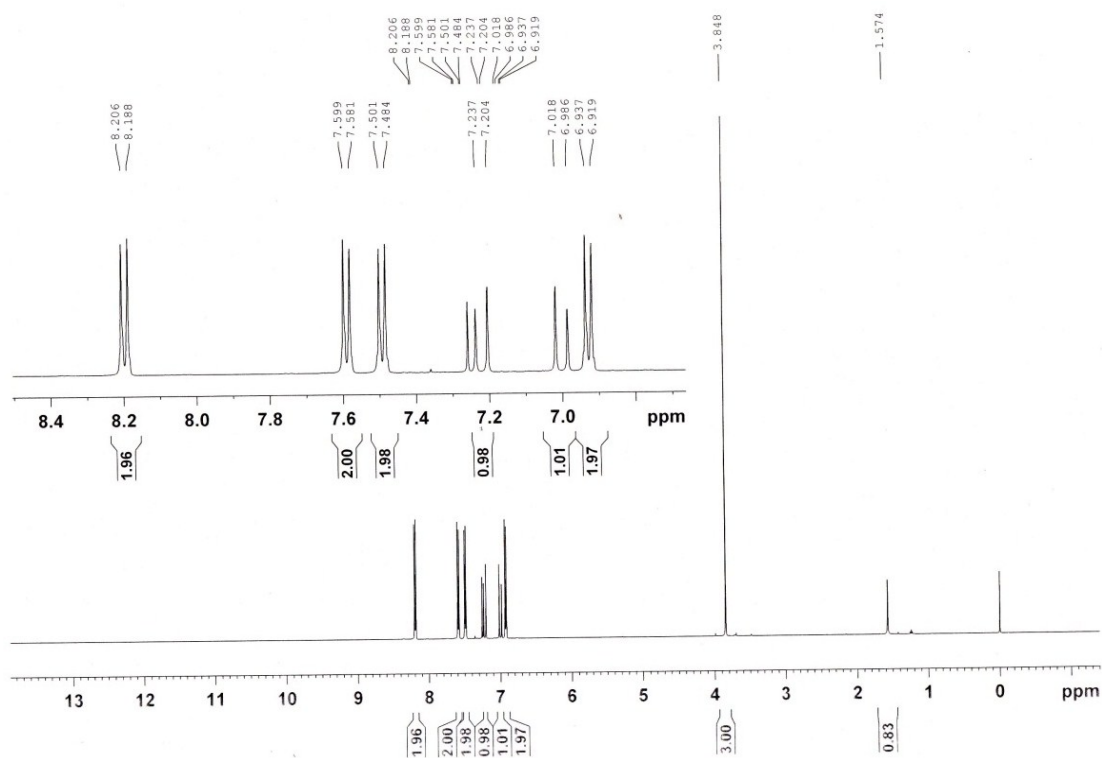
### Intermediate 12

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



### Intermediate 13

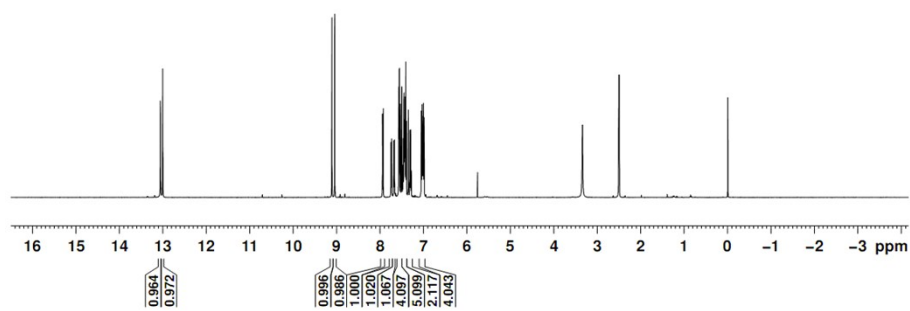
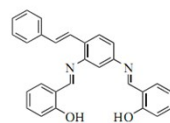
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ )



## 5. The characterization of the final compounds

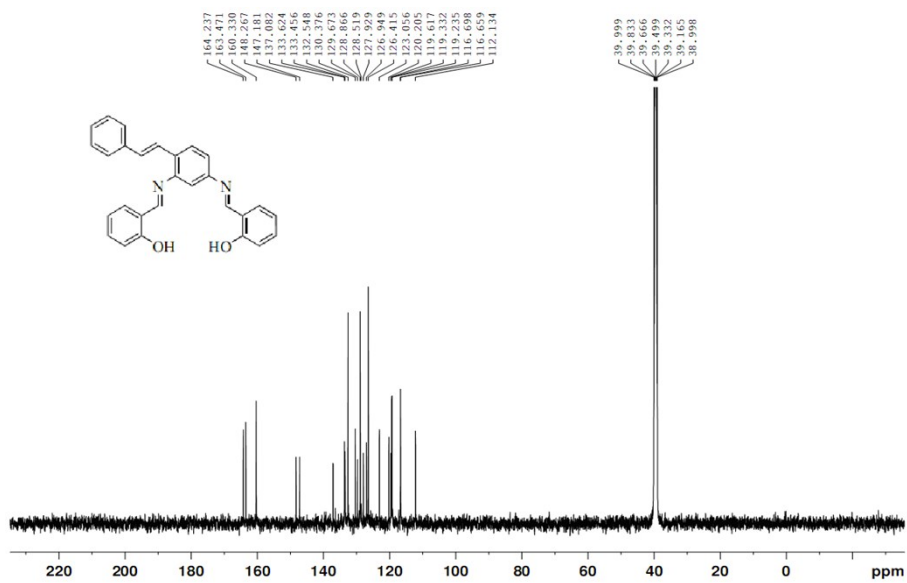
### Target molecule C1

$^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ )



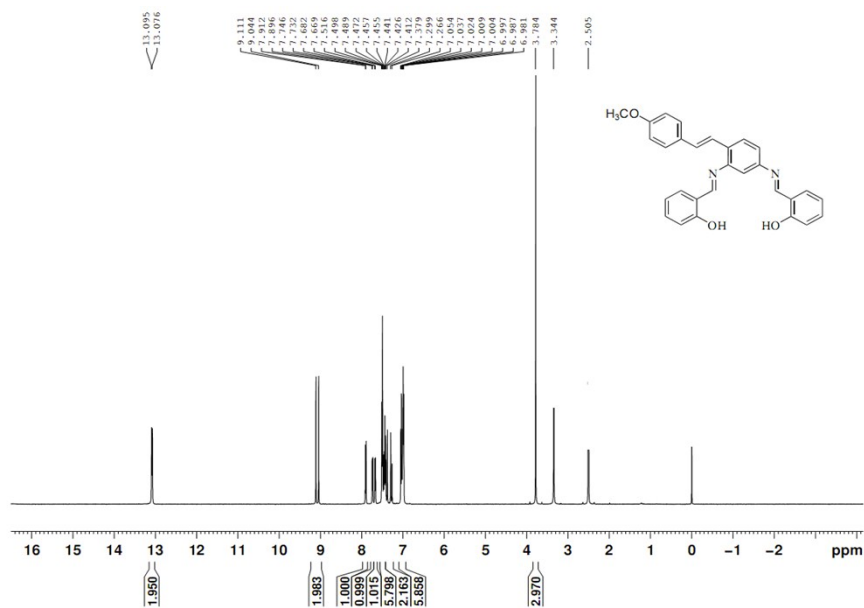
$^{13}\text{C-NMR}$  ( $\text{DMSO-}d_6$ )



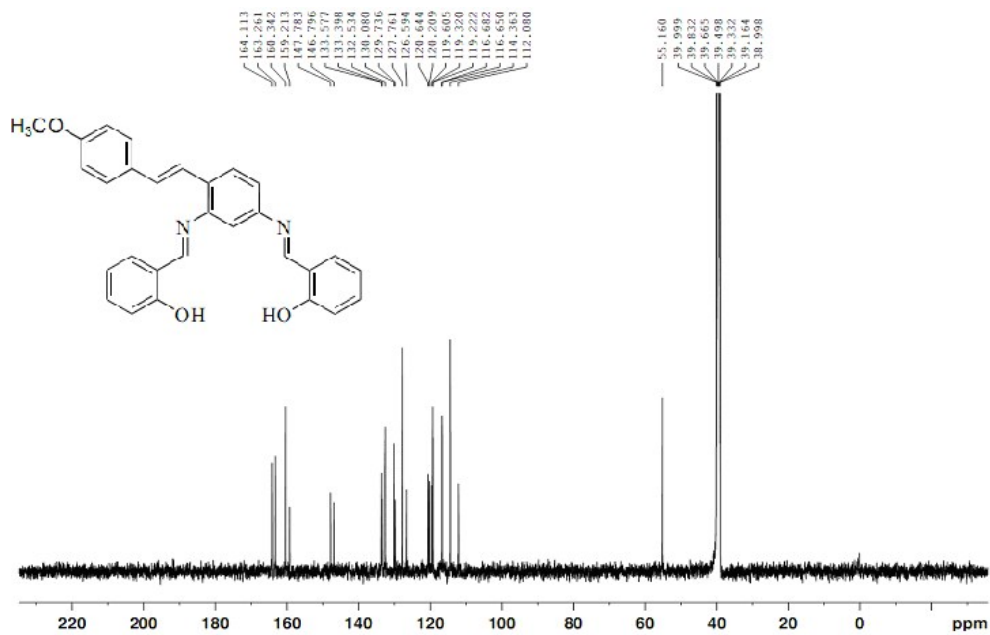


**Target molecule C2**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

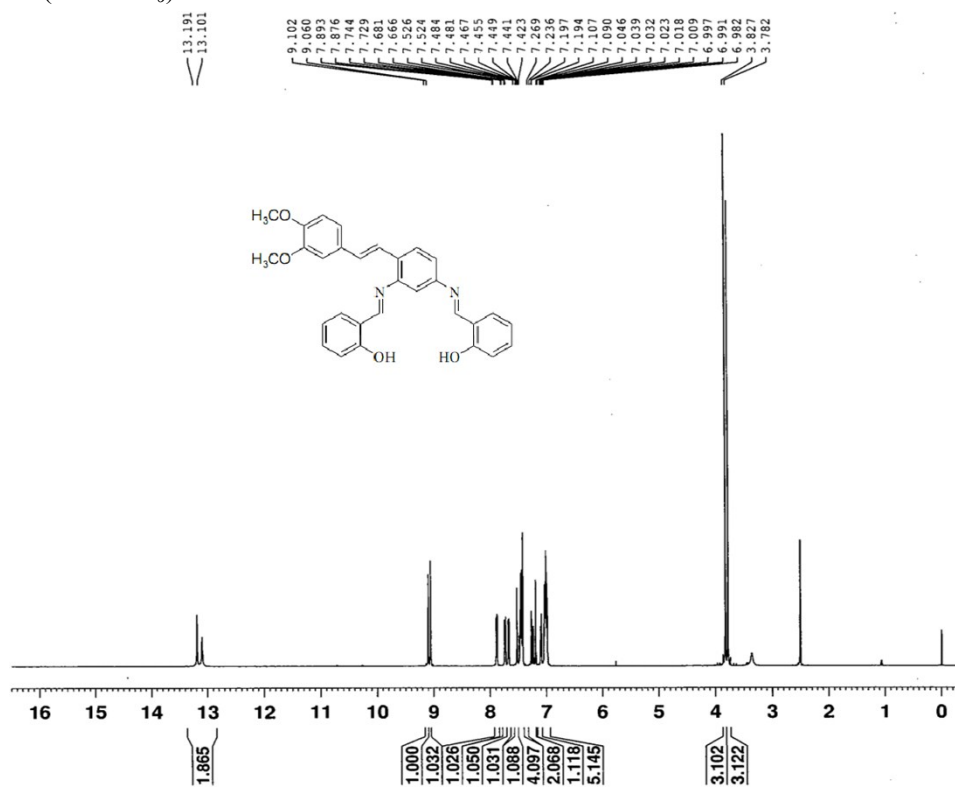


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)



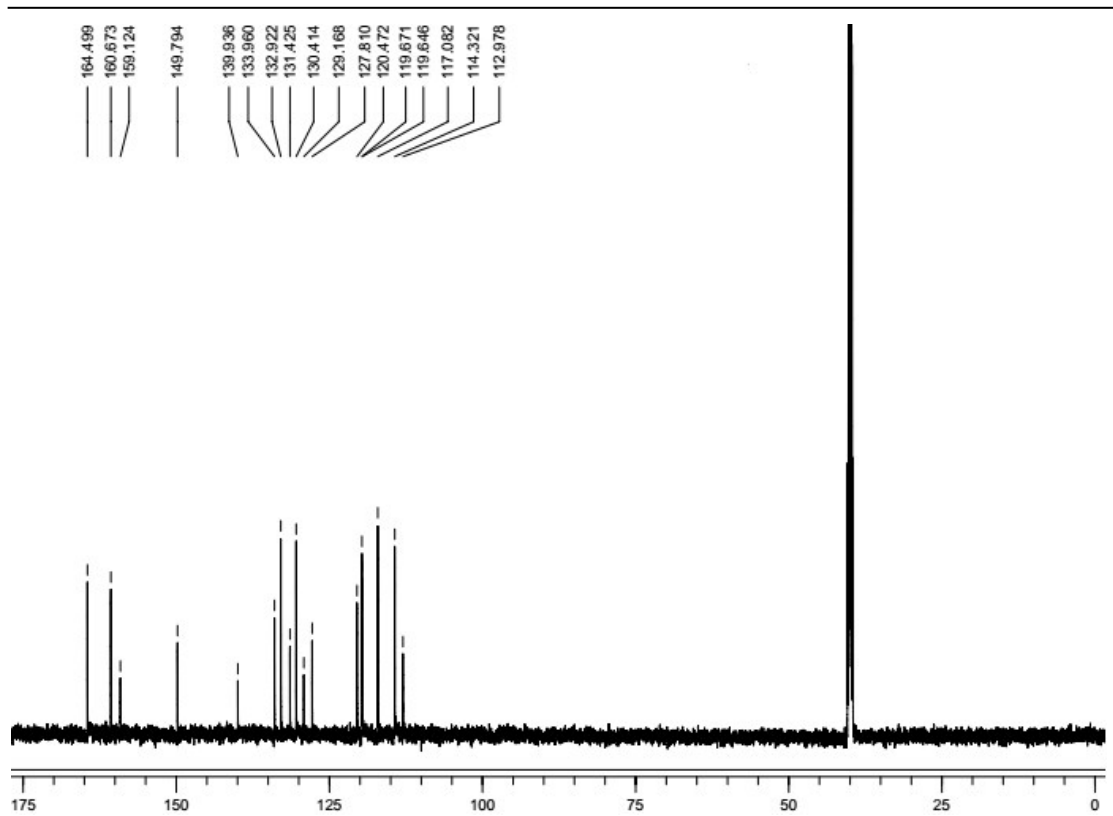
**Target molecule C3**

**<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)**



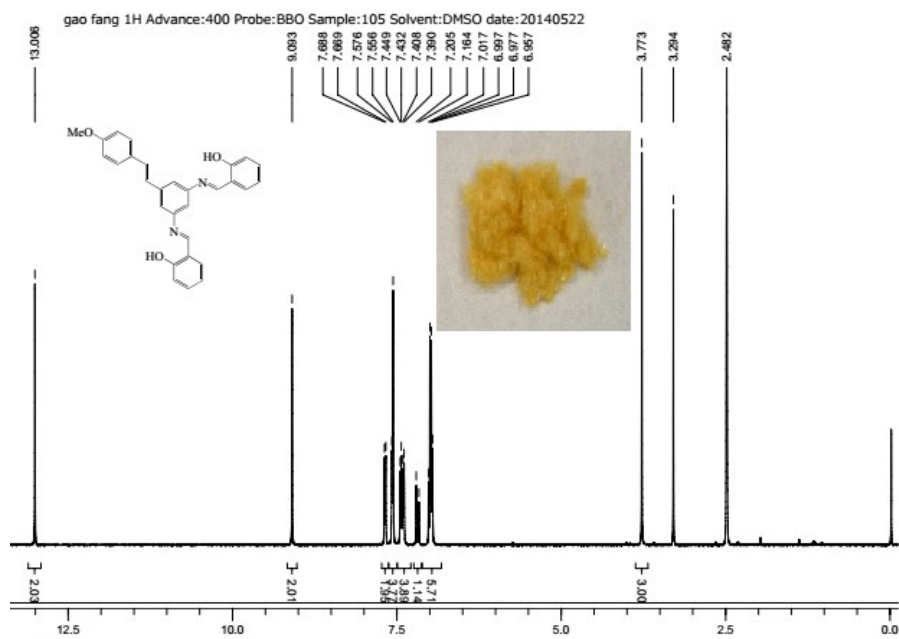
**<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)**



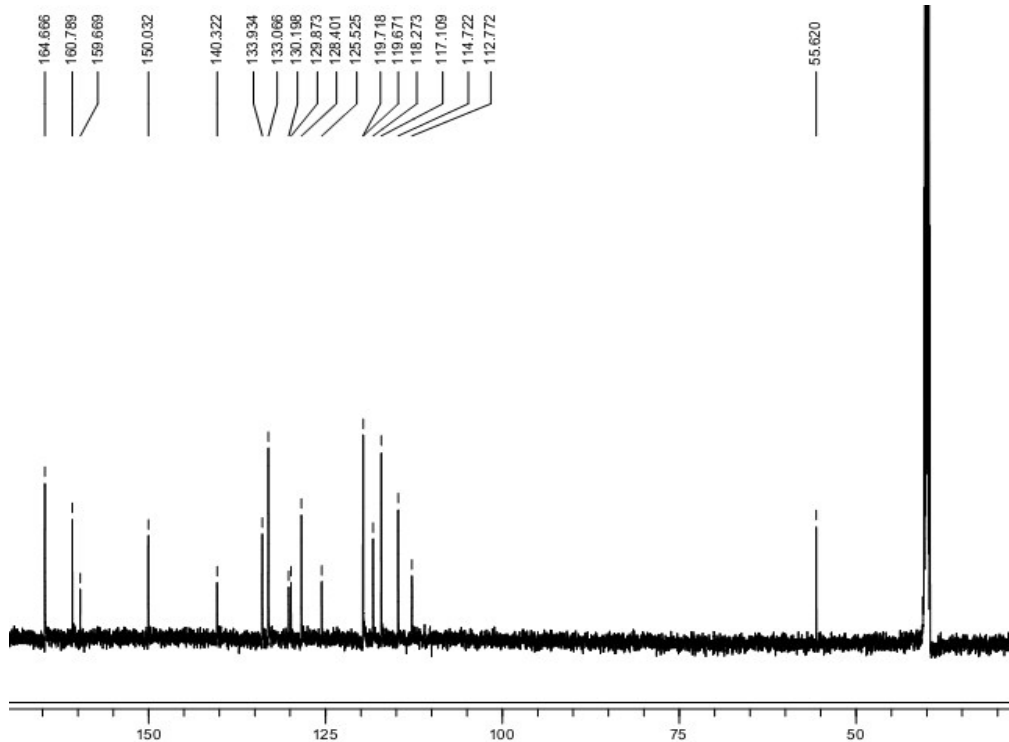


**Target molecule C5**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

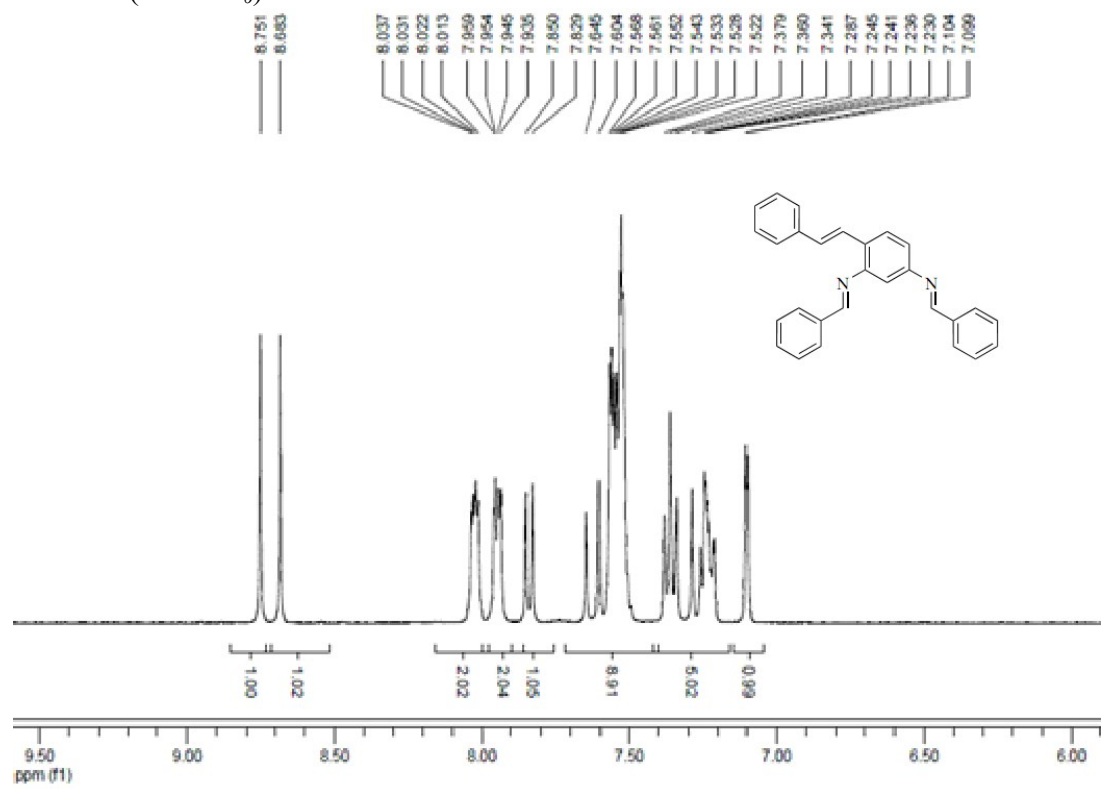


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

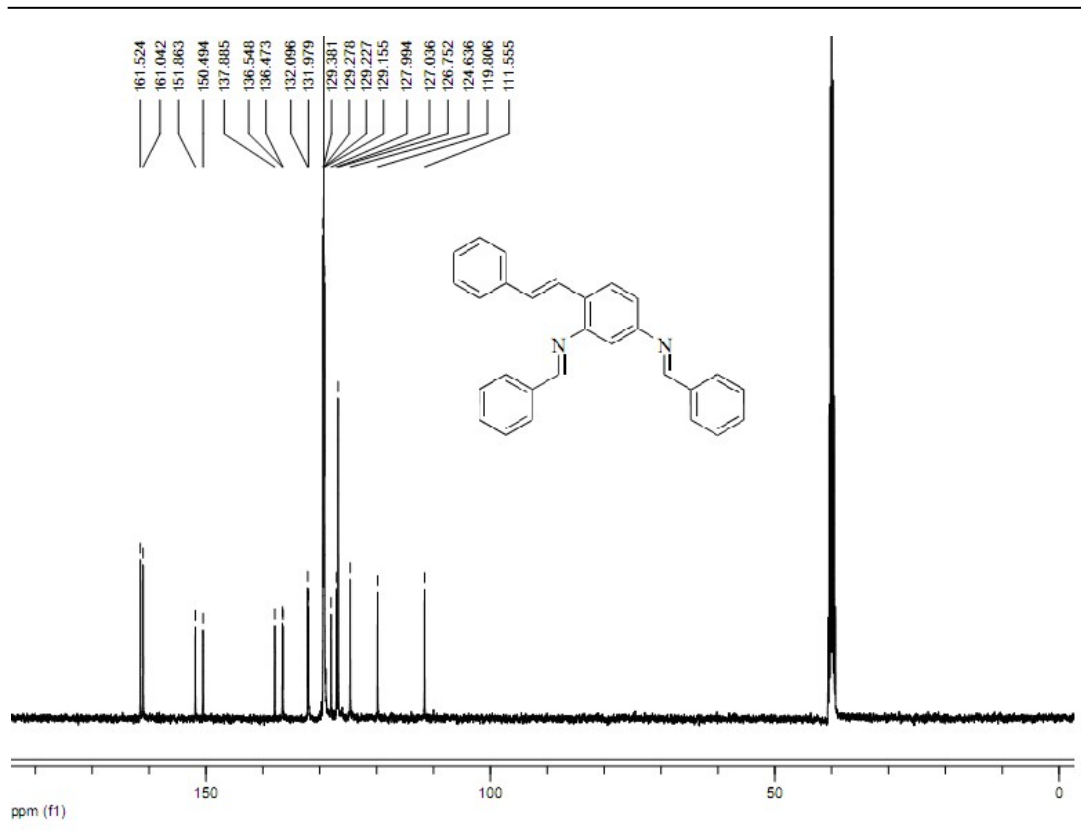


**Target molecule C6**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

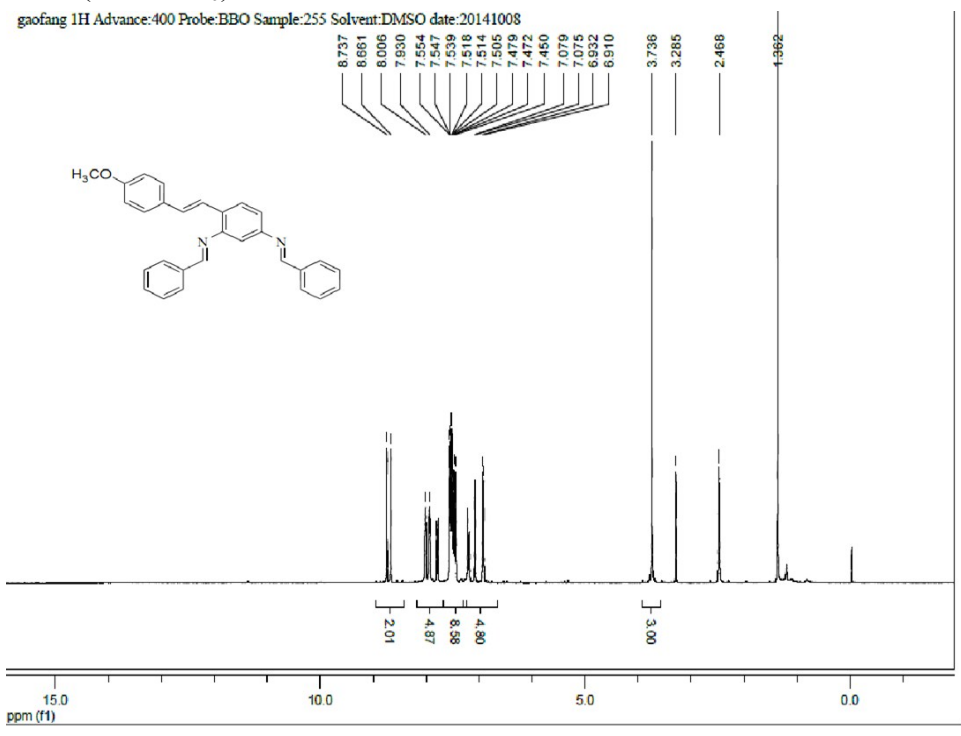


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

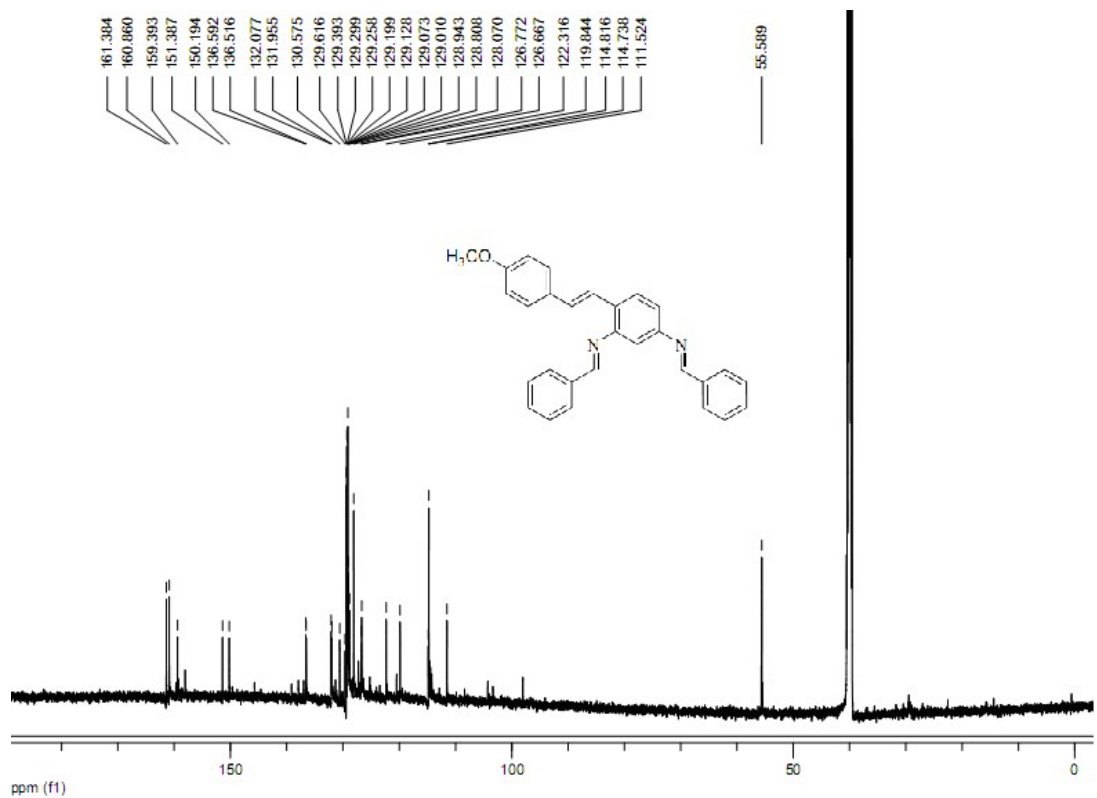


**Target molecule C7**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

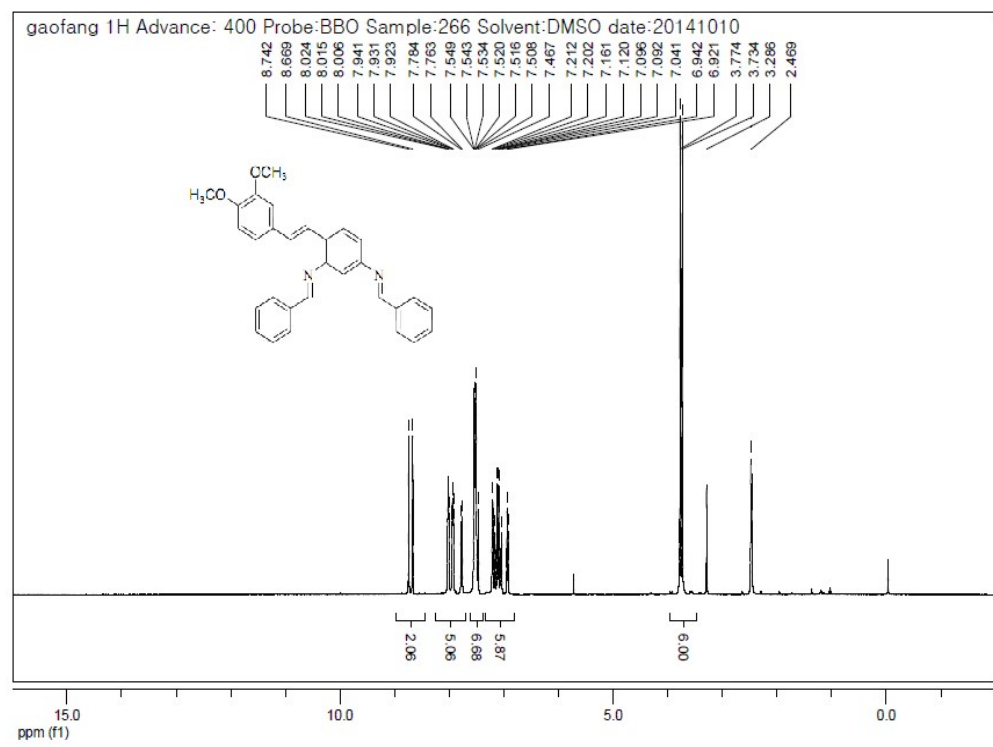


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

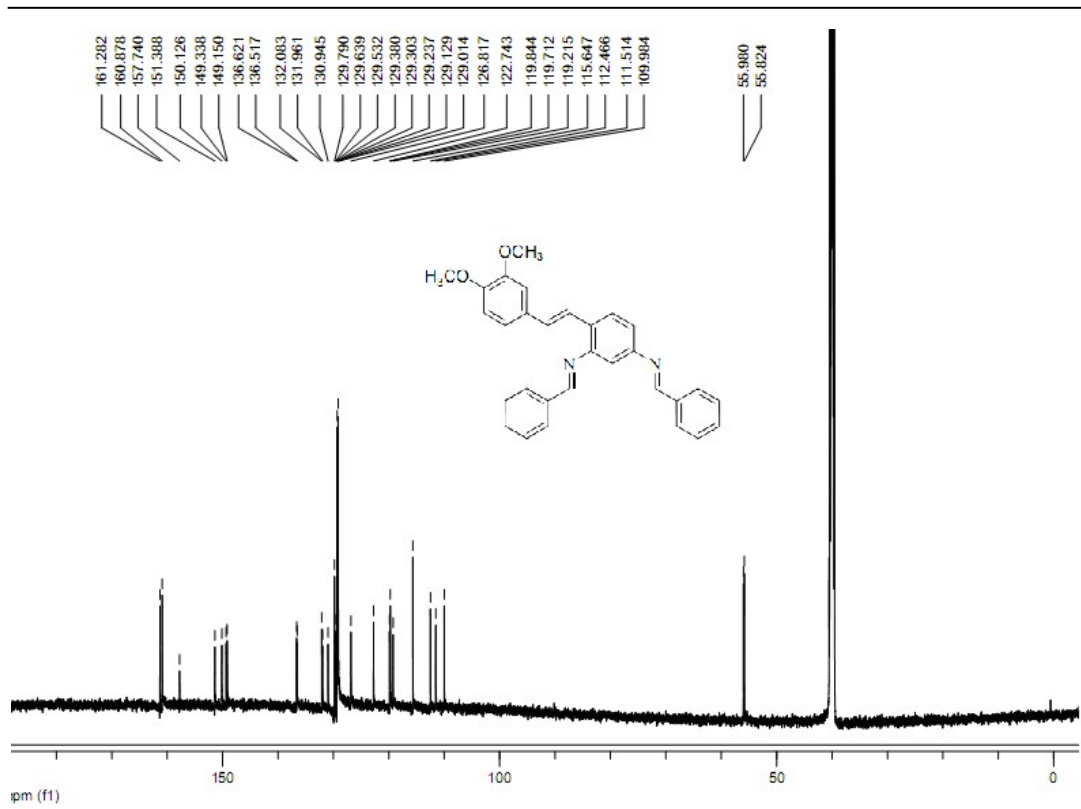


**Target molecule C8**

<sup>1</sup>H-NMR (DMSO-d<sub>6</sub>)

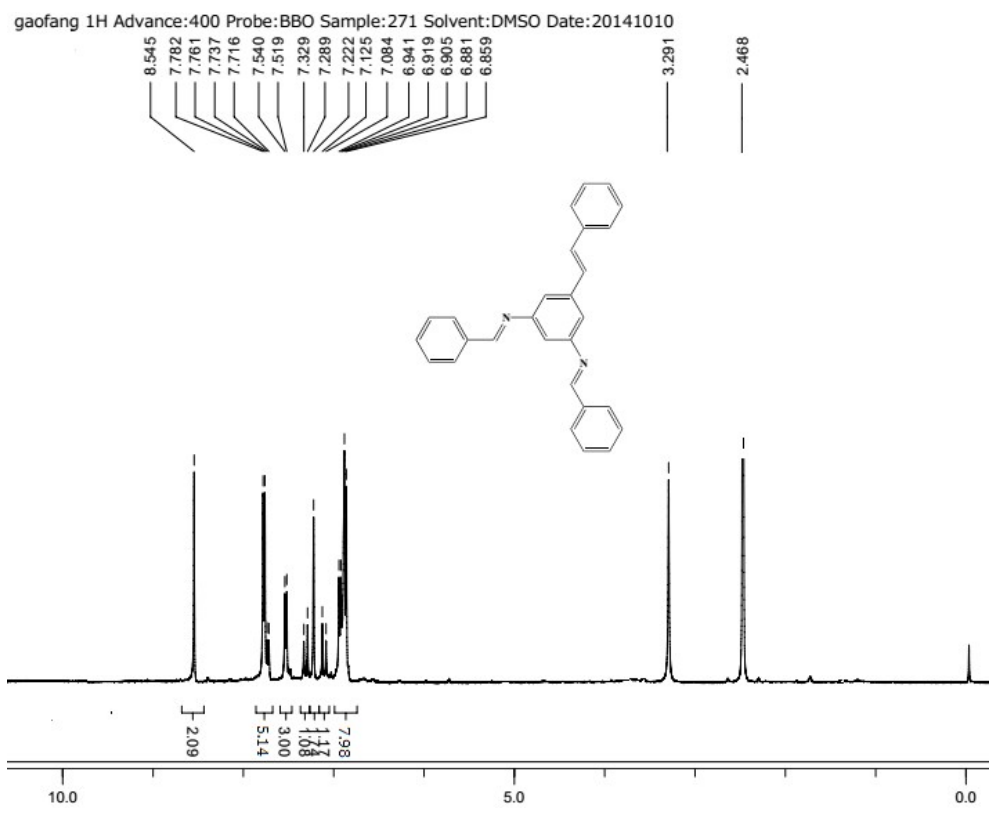


<sup>13</sup>C-NMR (DMSO-d<sub>6</sub>)



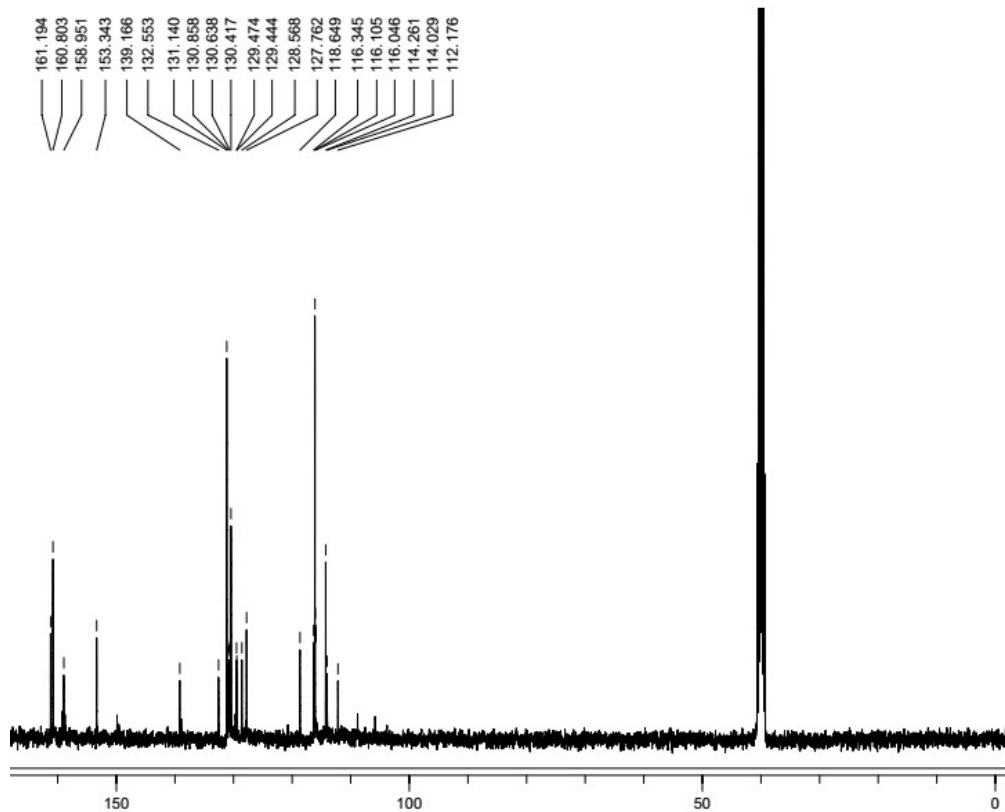
**Target molecule C9**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)



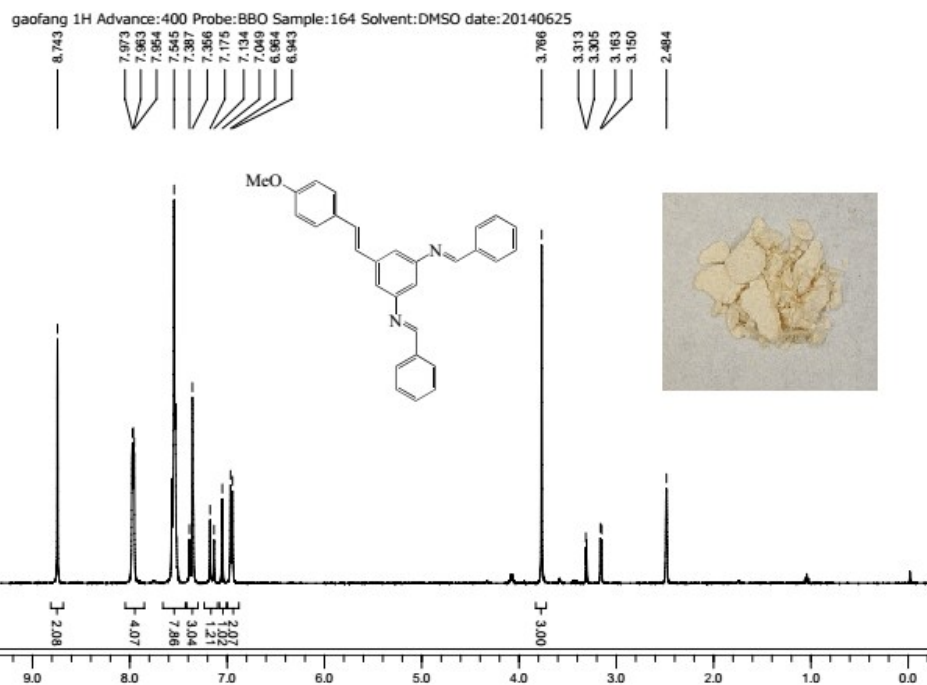
<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)



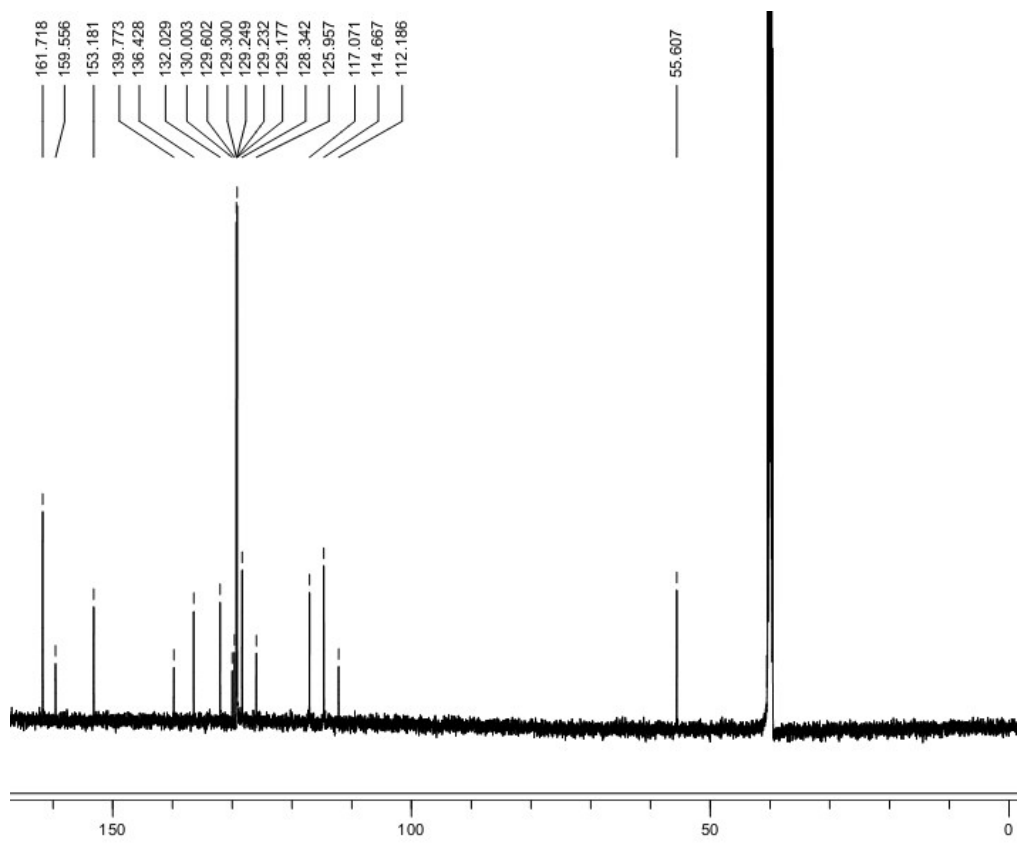


**Target molecule C10**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

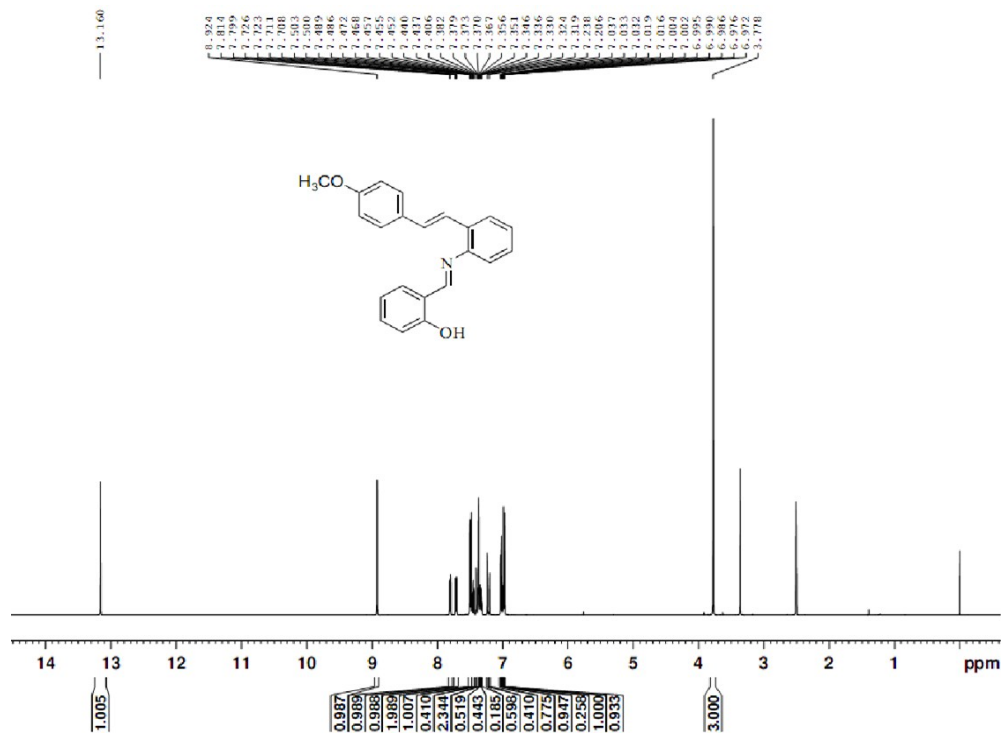


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

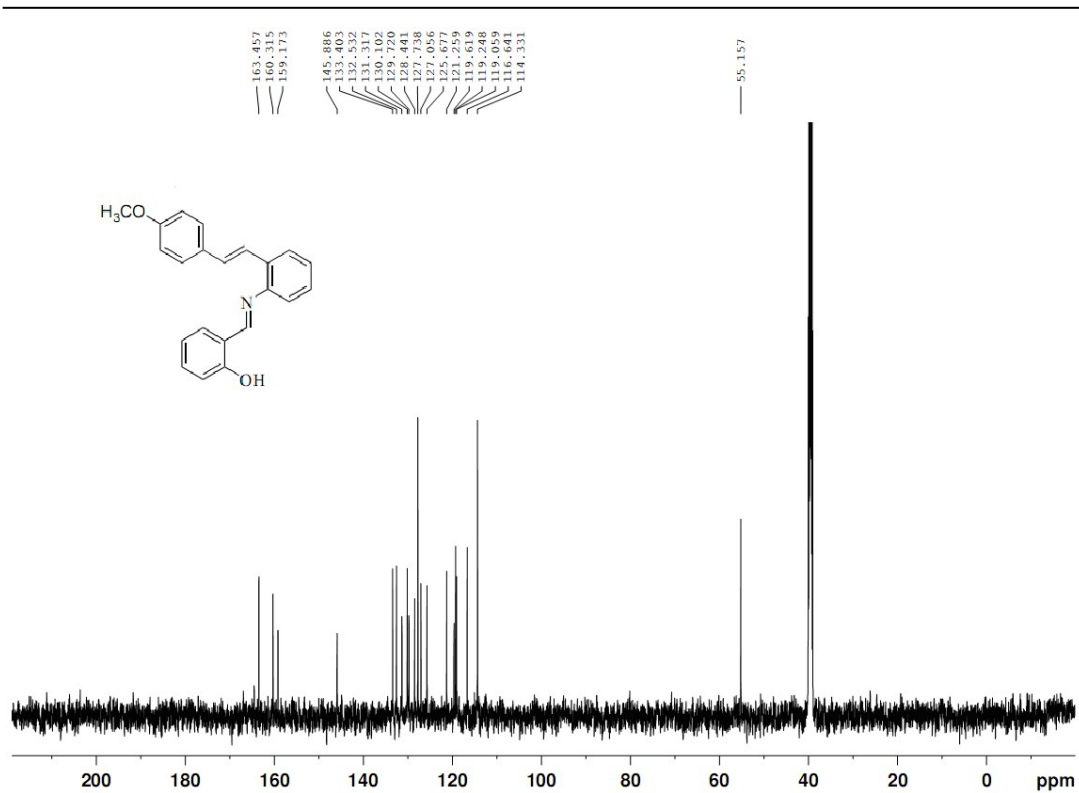


**Target molecule C11**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

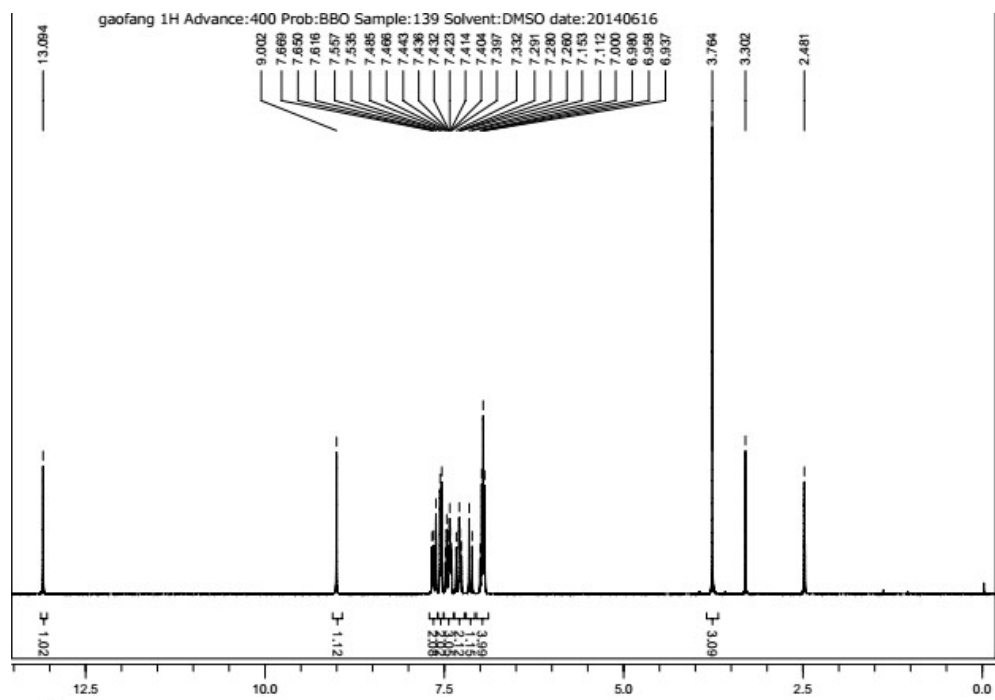


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

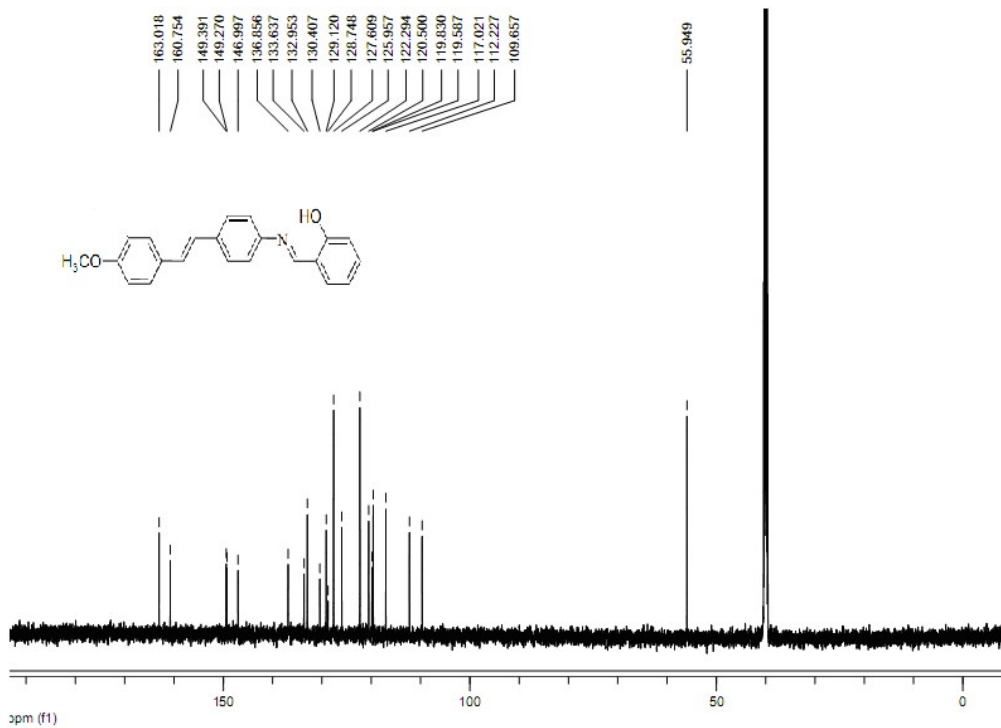


**Target molecule C12**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

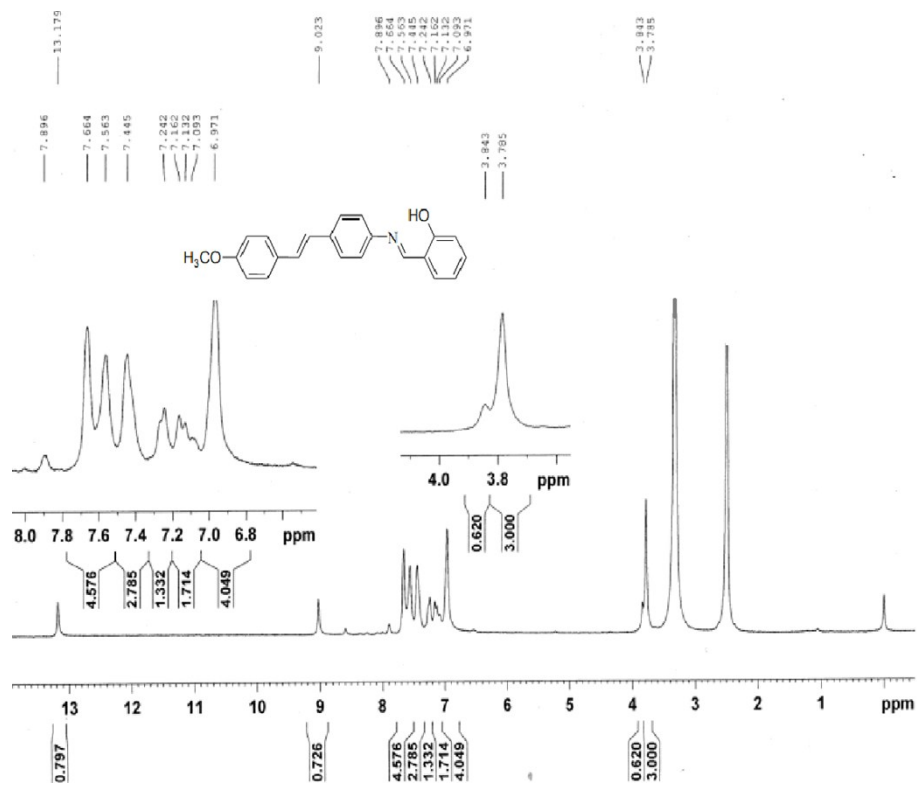


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)

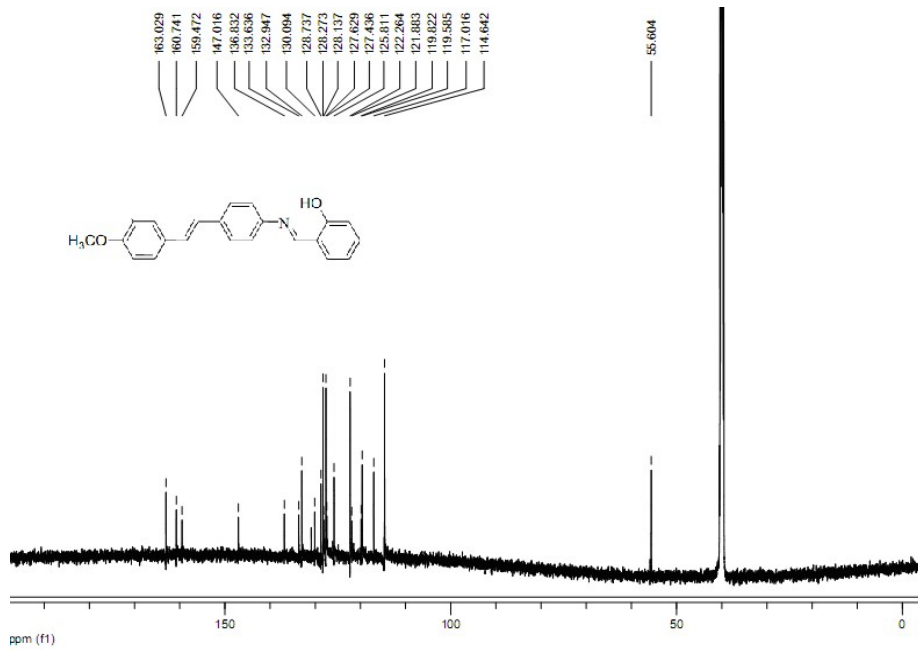


***Target molecule C13***

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

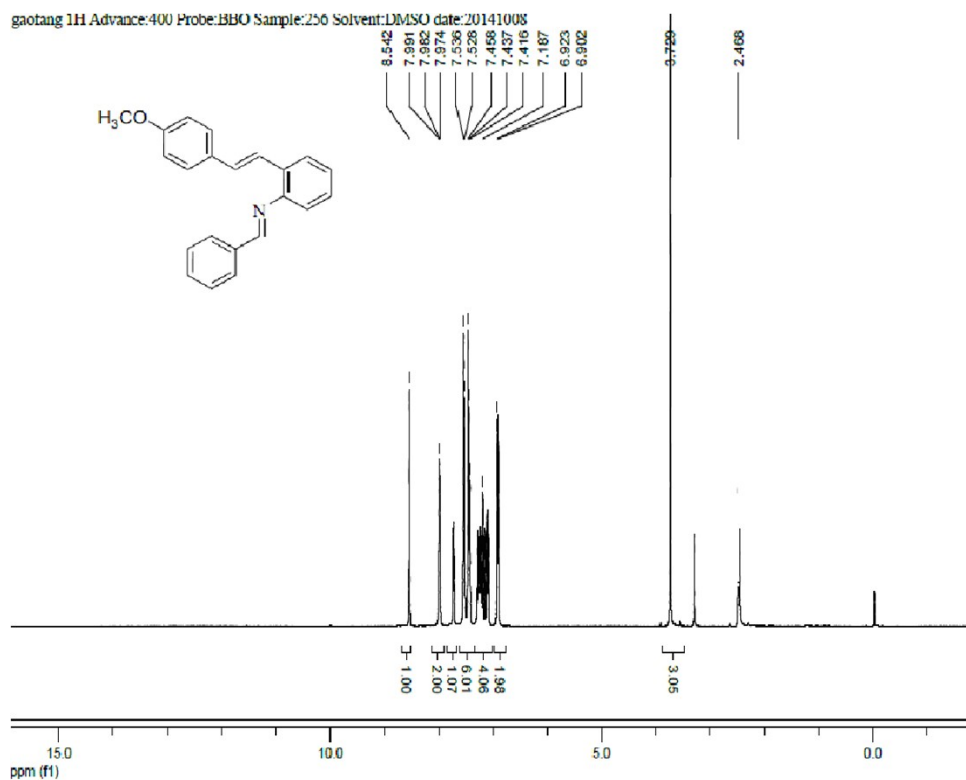


**<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)**

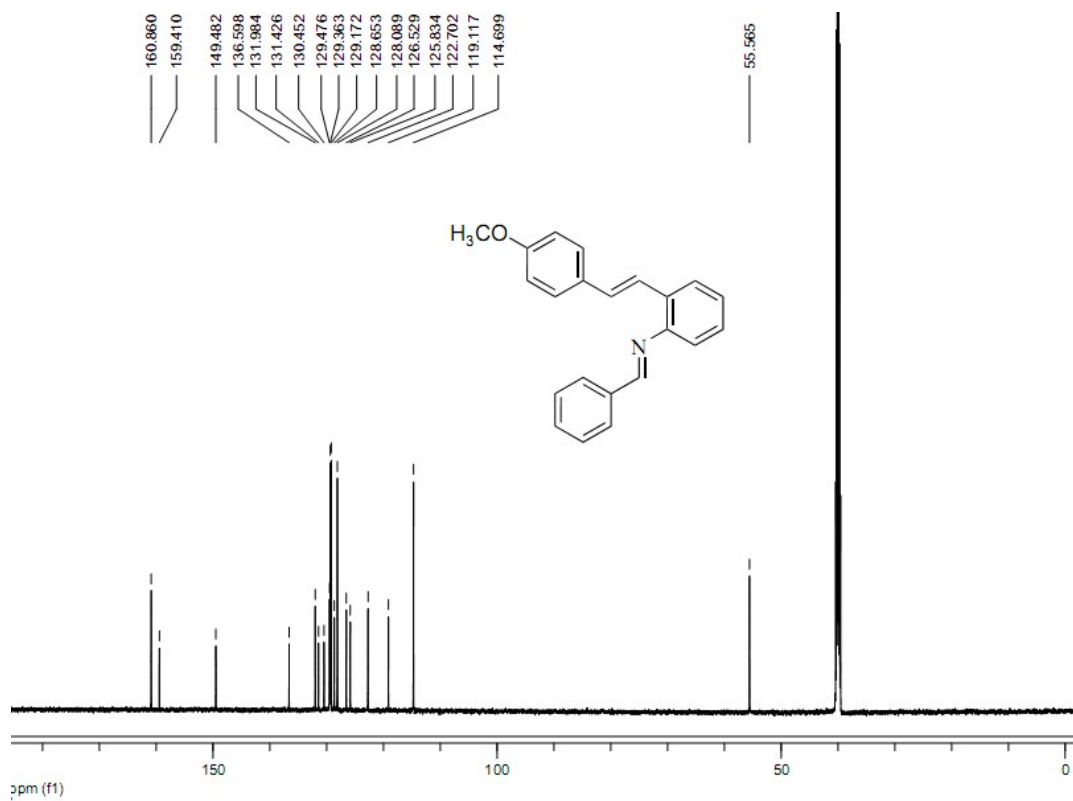


**Target molecule C14**

**<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)**

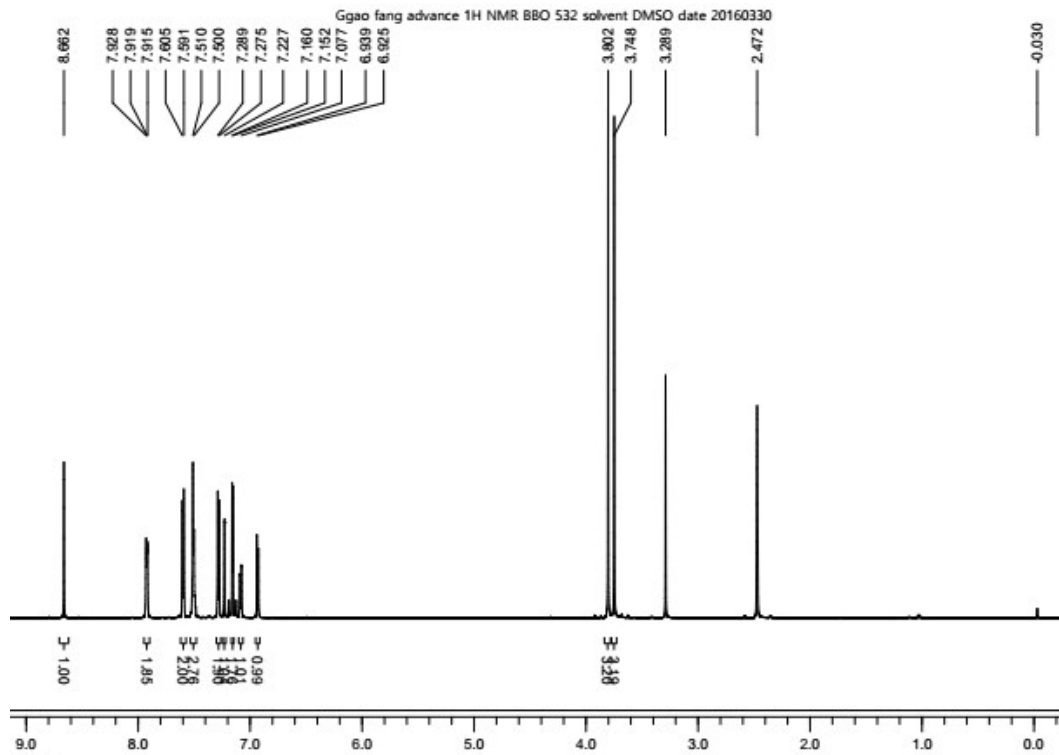


<sup>13</sup>C-NMR (DMSO-d<sub>6</sub>)

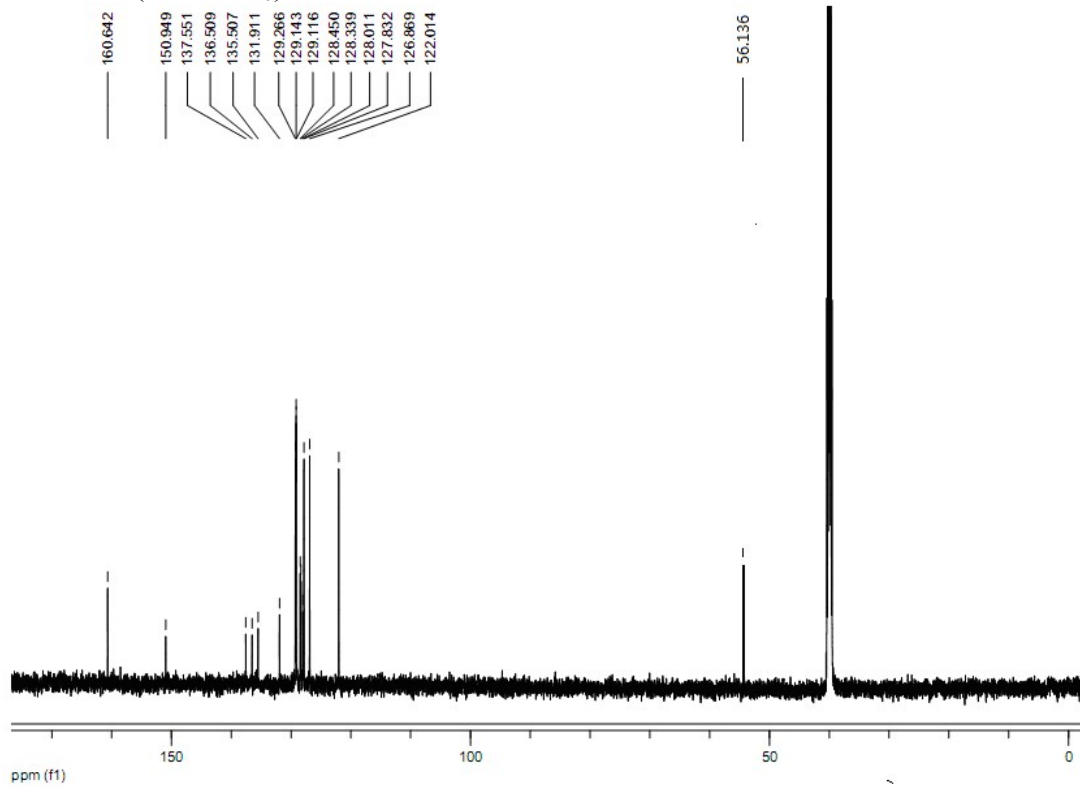


**Target molecule C15**

<sup>1</sup>H-NMR (DMSO-d<sub>6</sub>)



<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)



**Target molecule C16**

<sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>)

