

## An Organic White Light-Emitting Fluorophore

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**Compounds 4 and 5.** 1,6-Dimethoxynaphthalene (5 g) was lithiated according to a known procedure<sup>1</sup> in a 100 ml three-neck round bottom flask. The lithiated 1,6-dimethoxynaphthalene was cooled to -78 °C. Methyl benzoate (1.7 g) in 20 mL THF was added dropwise over 20 min. The mixture was allowed to warm to rt over 6 h. The reaction mixture was quenched with deionized water and neutralized with 2 N HCl. THF was removed *in vacuo*. The resulting mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 50 mL). The combined extracts were dried over MgSO<sub>4</sub> and filtered, and evaporated to dryness. The residue was purified via flash chromatography (silica gel; EtOAc:hexane, 20:80) to afford 4.5 g (71%) of **4** and 0.77 g (11%) of **5**. Data for compound **4**: <sup>1</sup>H NMR (CDCl<sub>3</sub>, 250 MHz) δ (ppm): 8.06 (s, 2H), 7.32-7.40 (m, 7H), 7.22 – 7.17 (m, 4H), 6.68 (dd, *J* = 6.3, 2.3 Hz, 2H), 5.38 (s, 1H), 3.88 (s, 6H), 3.69 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ (ppm): 156.8, 156.0, 146.7, 135.3, 134.0, 127.9, 126.6, 126.4, 123.3, 120.2, 118.4, 106.8, 102.1, 81.4, 55.4, 55.3. ESI [M-OH]<sup>+</sup> calcd 463.1904, found 463.3515. Data for compound **5**: <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ (ppm): 8.30 (d, *J* = 9.2 Hz, 1H), 7.94 (d, *J* = 9.2 Hz, 1H), 7.49 (s, 2H), 7.34 – 7.28 (m, 7H), 7.14 – 7.06 (m, 4H), 6.61 (dd, *J* = 7.8, 2.9 Hz, 2H), 5.38 (s, 1H), 3.97 (s, 3H), 3.76 (s, 3H), 3.68 (s, 3H), 3.14 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75MHz) δ (ppm): 156.7, 155.8, 155.4, 155.2, 146.4, 138.5, 134.3, 127.7, 126.7, 126.3, 124.9, 123.7, 122.7, 121.4, 121.1, 120.2, 118.3, 113.9, 105.4, 101.3, 101.3, 81.7, 56.5, 55.4, 55.3, 55.2. ESI [M-OH]<sup>+</sup> calcd 463.1904, found 463.1664.

**Compound 6.** The preparation procedure is practically the same as for compounds **4** and **5** with the exception that phthalic anhydride (1.96 g) is used instead of methyl benzoate. After the reaction is quenched with distilled water, THF is removed by steam distillation. The resulting precipitate is collected by suction filtration. The resulting residue is washed with cold EtOH (20 × 3 mL) to afford 3.7 g (55%) of **6**. Data for compound **6**: <sup>1</sup>H NMR (CDCl<sub>3</sub>, 250 MHz) δ (ppm): 7.97 (s, 2H), 7.93 (d, *J* = 7.5 Hz, 1H), 7.83 – 7.74 (m, 2H), 7.64 (td, *J* = 13.9, 1.9 Hz), 7.39 (d, *J* = 2.38 Hz,

<sup>1</sup> Johansson, A. M.; Mellin, C.; Hacksell, U. *J. Org. Chem.* **1986**, *51*, 5252.

2H), 7.36 (d,  $J = 3.7$  Hz, 4H), 6.80 (dd,  $J = 5.5, 3.2$  Hz, 2H), 3.83 (s, 3H), 3.53 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  (ppm): 169.5, 155.6, 155.0, 152.6, 135.3, 134.4, 129.6, 128.6, 127.5, 125.2, 124.3, 120.4, 119.1, 118.5, 107.3, 102.9, 90.0, 55.5. ESI  $[\text{M}+\text{H}]^+$  calcd 507.1802, found 507.1638.

**Compounds 7, 8 and 9.** The preparation procedure is the same as for compounds **4** and **5** except that 2, 4-dimethoxybenzophenone is used instead of methyl benzoate. The crude product is purified via flash chromatography (silica gel; EtOAc:hexane, 20:80) to afford 0.52 g (11%) of **7**, 3.43 g (71%) of **8** and 27 mg (<1%) of **9**. Data for compound **7**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  (ppm): 8.31 (d,  $J = 9.3$  Hz, 1H), 7.92 (d,  $J = 8.9$  Hz, 1H), 7.45-7.09 (m, 7H), 6.63 (d,  $J = 7.6$  Hz, 1H), 6.52 (d,  $J = 2.4$  Hz, 1H), 6.46 (d,  $J = 8.6$  Hz, 1H), 6.33 (dd,  $J = 8.6, 2.4$  Hz, 1H), 5.38 (s, 1H), 3.97 (s, 3H), 3.81 (s, 3H), 3.56 (s, 3H), 3.28 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  (ppm): 159.5, 158.0, 155.2, 147.3, 130.4, 129.3, 128.2, 127.6, 126.6, 124.8, 123.7, 122.6, 121.0, 114.3, 103.4, 101.4, 99.4, 81.4, 56.7, 55.4, 55.3. ESI  $[\text{M}-\text{OH}]^+$  calcd 413.1753, found 413.1223. Data for compound **8**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  (ppm): 8.06 (s, 1H), 7.27-7.38 (m, 7H), 7.14 (s, 1H), 6.84 (d,  $J = 8.6$  Hz, 1H), 6.68 (d,  $J = 5.1$  Hz, 1H), 6.55 (d,  $J = 2.0$  Hz, 1H), 6.40 (dd,  $J = 8.6, 2.0$  Hz, 1H), 5.29 (s, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.63 (s, 3H), 3.56 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  (ppm): 160.1, 158.6, 156.7, 156.0, 146.9, 135.2, 134.3, 130.5, 127.8, 127.1, 126.7, 126.6, 126.4, 122.9, 120.1, 118.4, 106.8, 103.6, 102.2, 100.0, 81.0, 55.6, 55.3, 55.2. ESI  $[\text{M}-\text{OH}]^+$  calcd 413.1753, found 413.1549. Data for compound **9**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  (ppm): 9.04 (s, 1H), 7.33 – 7.22 (m, 8H), 6.68 (d,  $J = 5$  Hz, 1H), 6.55 (s, 1H), 6.27 (s, 1H), 6.10 (s, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.80 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  (ppm): 160.6, 157.6, 156.0, 155.8, 144.7, 135.3, 132.3, 130.0, 127.8, 127.6, 127.4, 123.9, 121.8, 118.4, 107.2, 104.8, 102.9, 102.5, 84.5, 55.4, 55.2, 55.2. ESI  $[\text{M}-\text{OH}]^+$  calcd 399.1591, found 399.1506.

**Compound 10.** To a stirred solution of **4** (0.200 g) in 30 mL anhydrous  $\text{CH}_2\text{Cl}_2$  at  $-78$  °C,  $\text{BBr}_3$  (1.5 mL) is added dropwise. The mixture is warmed to rt slowly before quenching with 20 mL

distilled H<sub>2</sub>O. After stirring for 20 min and filtration, a red precipitate is collected. The red precipitate is washed and transferred into a round bottom flask with acetone and dried *in vacuo*. The resulting red powder is purified by flash chromatography (silica gel, Hexane: EtOAc 6:4) to give 107 mg (61%) of compound **10**. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz) δ (ppm): 10.24 (s, 2H), 8.07 (s, 2H), 7.70 (s, 2H), 7.36 – 7.12 (m, 10 H), 6.72 (d, *J* = 7 Hz, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 62.9 MHz) δ (ppm): 154.1, 150.7, 150.4, 149.6, 135.9, 135.5, 130.8, 129.1, 128.9, 128.3, 127.5, 126.2, 125.9, 124.4, 124.3, 122.6, 119.2, 118.2, 112.0, 111.7, 107.3 77.2. MALDI-TOF [M-OMe]<sup>+</sup> calcd 339.117, found 338.982.

**Compound 12** was prepared with the same method as compound **10** except that 500 mg of compound **7** are used and the temperature is raised to 50 °C before adding BBr<sub>3</sub> affording 390 mg (99%) of **12**. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz) δ (ppm): 9.97 (s, 1H), 8.17 (d, *J* = 9.2 Hz), 7.77 (d, *J* = 9.0 Hz), 7.36 – 7.25 (m, 5H), 7.19 (t, *J* = 7.5 Hz, 2H), 7.04 (t, *J* = 6.6 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 1H), 6.70 (d, *J* = 2.1 Hz, 1H), 6.63 (dd, *J* = 7.0, 3.4 Hz, 2H), 3.75 (s, 3H). HRMS [M+H]<sup>+</sup> calcd 353.1172, found 353.1171.

**Compound 13**. To a stirred solution of **8** (0.500 g) in 30 mL anhydrous CH<sub>2</sub>Cl<sub>2</sub> at -78 °C, BBr<sub>3</sub> (4.65 g) is added dropwise. The mixture is warmed to rt slowly before quenching with 20 mL distilled H<sub>2</sub>O. After stirring for 20 min and filtration, a red precipitate is collected. The red precipitate is washed with acetone, transferred into a round bottom flask and dried *in vacuo*. The resulting red powder is purified by flash chromatography (silica gel, EtOAc-MeOH 9:1) to give 60 mg (15%) of compound **13**. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz) δ (ppm): 10.68 (bs, 1H), 7.99 (s, 1H), 7.91 (s, 1H), 7.69-7.40 (m, 7H), 7.03 (d, *J* = 9.8 Hz, 1H), 6.82 (d, *J* = 6.6 Hz, 1H), 6.43 (d, *J* = 9.6 Hz, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ (ppm): 195.7, 158.9, 155.1, 149.5, 149.3, 137.4, 133.5, 132.4, 131.5, 130.5, 130.2, 129.7, 125.5, 122.5, 120.5, 120.4, 118.2, 112.4, 108.3, 106.5. HRMS [M+H]<sup>+</sup> calcd 339.1021, found 339.1016.

**SNAFR-1** was prepared in the same manner as compound **13** except that 25 mg of compound **7** are used and the temperature is raised to 50 °C before the addition of BBr<sub>3</sub> affording 16 mg (56%) of **SNAFR-1**. Both tautomers (see text) are present. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz) δ (ppm): 8.57 (d, *J* = 9.7 Hz), 8.50 (d, *J* = 9.1 Hz), 7.67-7.60 (m), 7.57 (s), 7.53-7.43 (m), 7.3 (dd, *J* = 9.1, 2.3 Hz), 7.22 (d, *J* = 2.3 Hz), 7.07 (d, *J* = 9.3 Hz), 7.02 (d, *J* = 8.7 Hz), 6.83 (d, *J* = 7.9 Hz), 6.53-6.47 (m), 6.46 (d, *J* = 8.26), 6.30 (d, *J* = 2.0 Hz). HRMS [M+H]<sup>+</sup> calcd 339.1021, found 339.1036.

**Compound 16** is observed when MeOH is added into a solution of compound **12** in DMSO. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz) δ (ppm): 10.09 (s, 1H), 8.23 (d, *J* = 9.2 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.37 – 7.31 (m, 4H), 7.25 – 7.17 (m, 4H), 7.09 - 6.96 (m, 3H), 6.78 (d, *J* = 2.5 Hz, 1H), 6.70 (t, *J* = 6.5 Hz, 2H), 3.80 (s, 3H), 2.84 (s, 3H).

# Compound 4

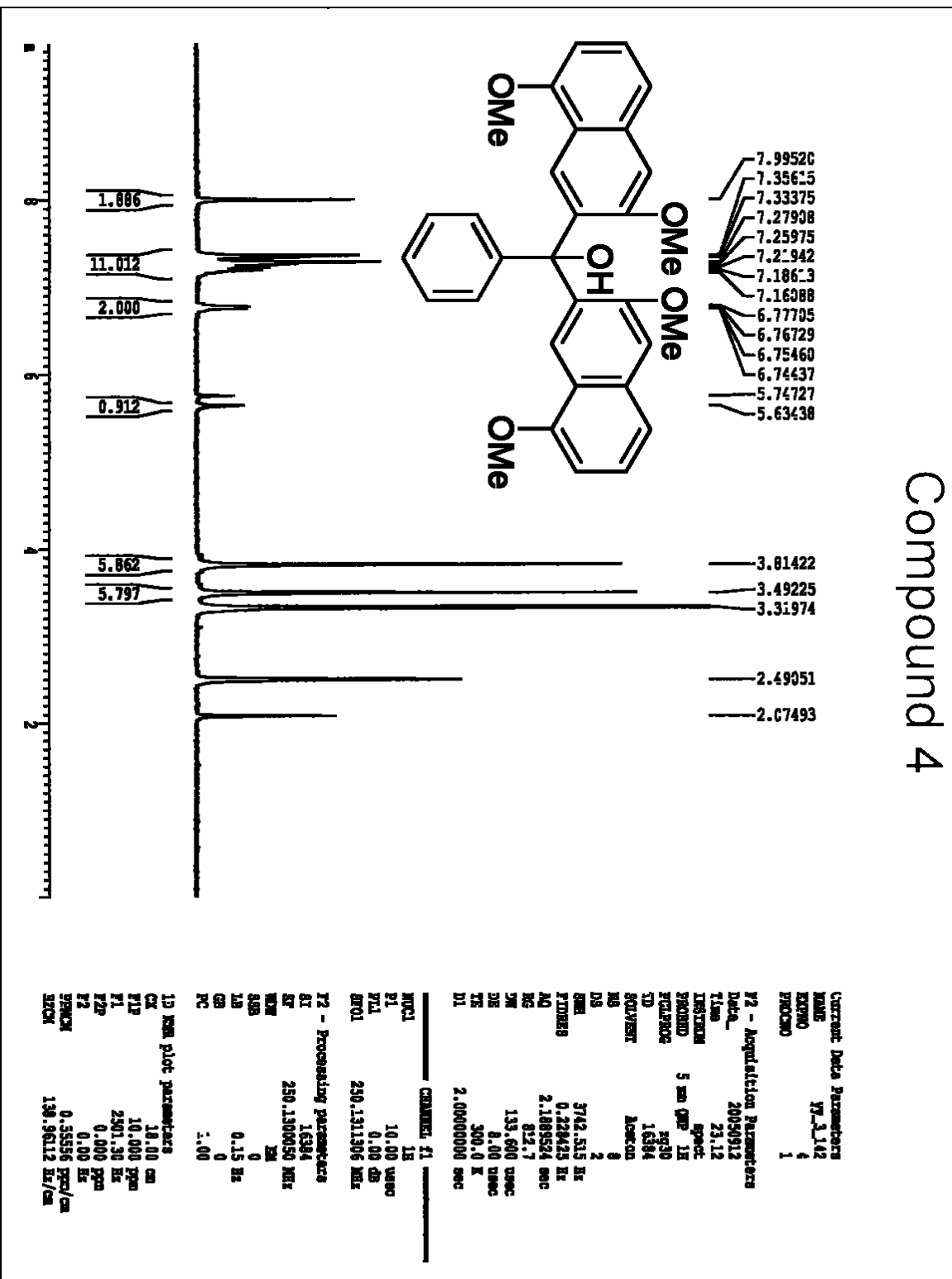


Figure S1. <sup>1</sup>H NMR of compound 4

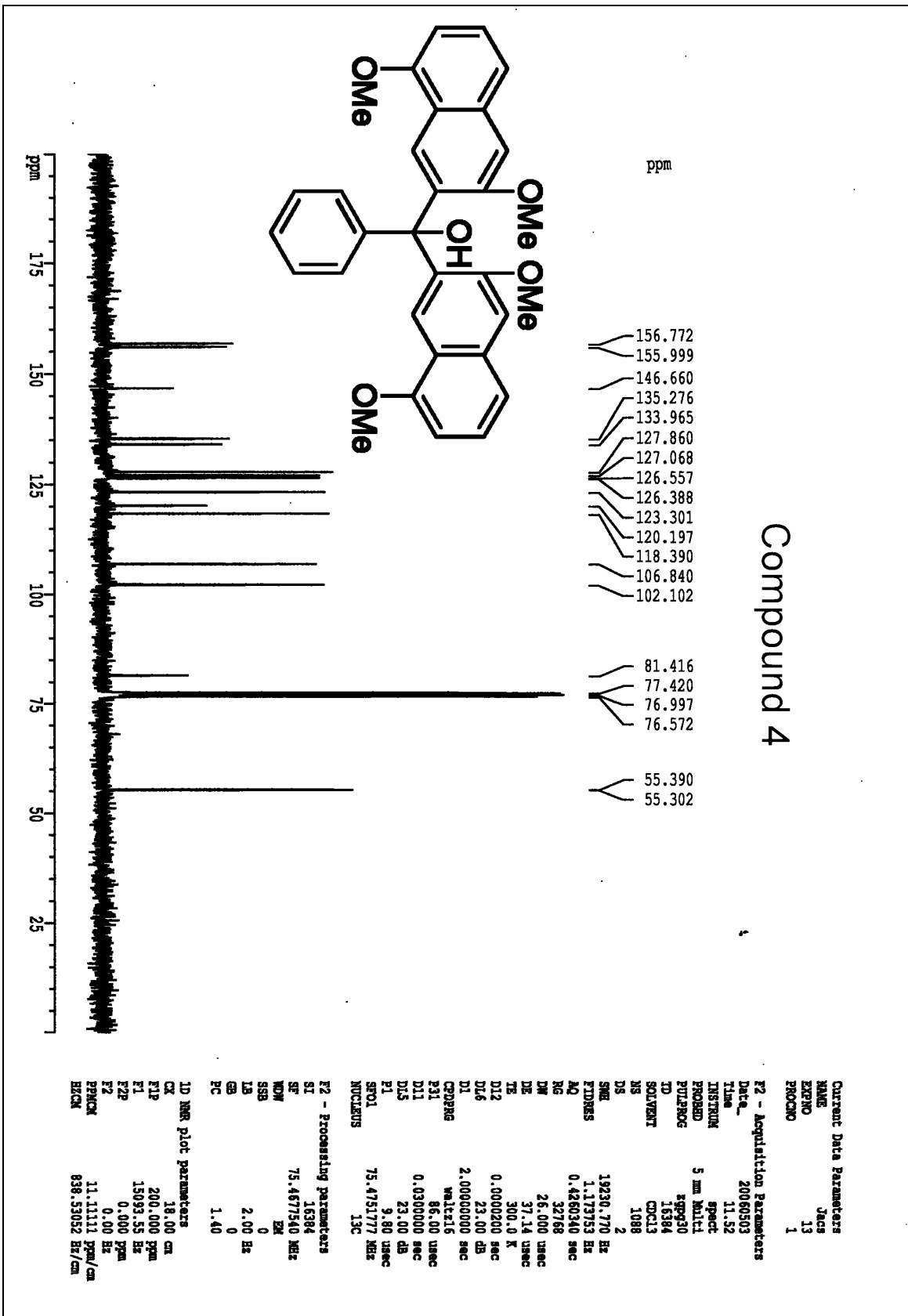


Figure S2. <sup>13</sup>C NMR of 4.



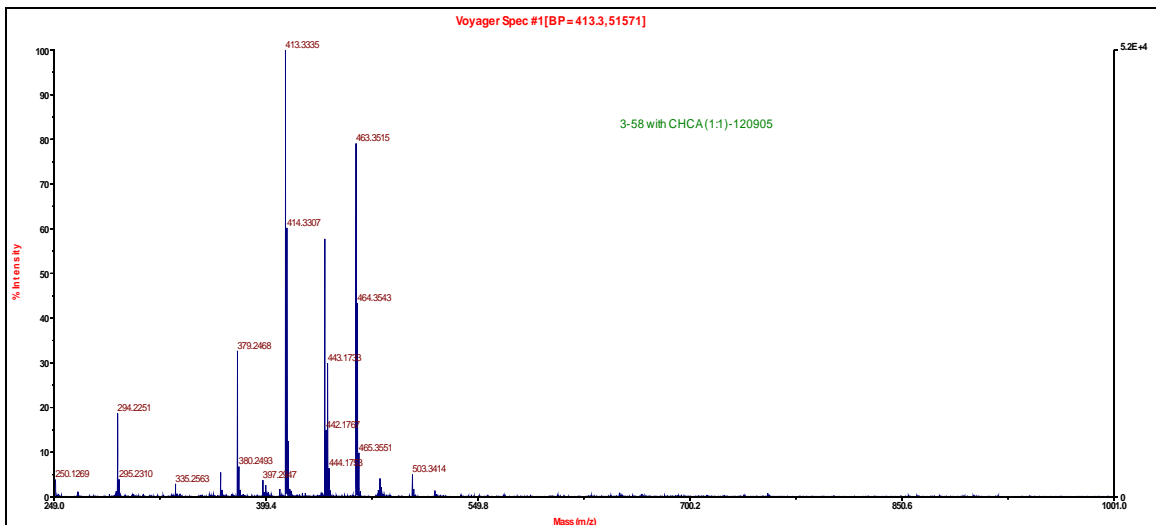


Figure S3. ESI MS of 4.

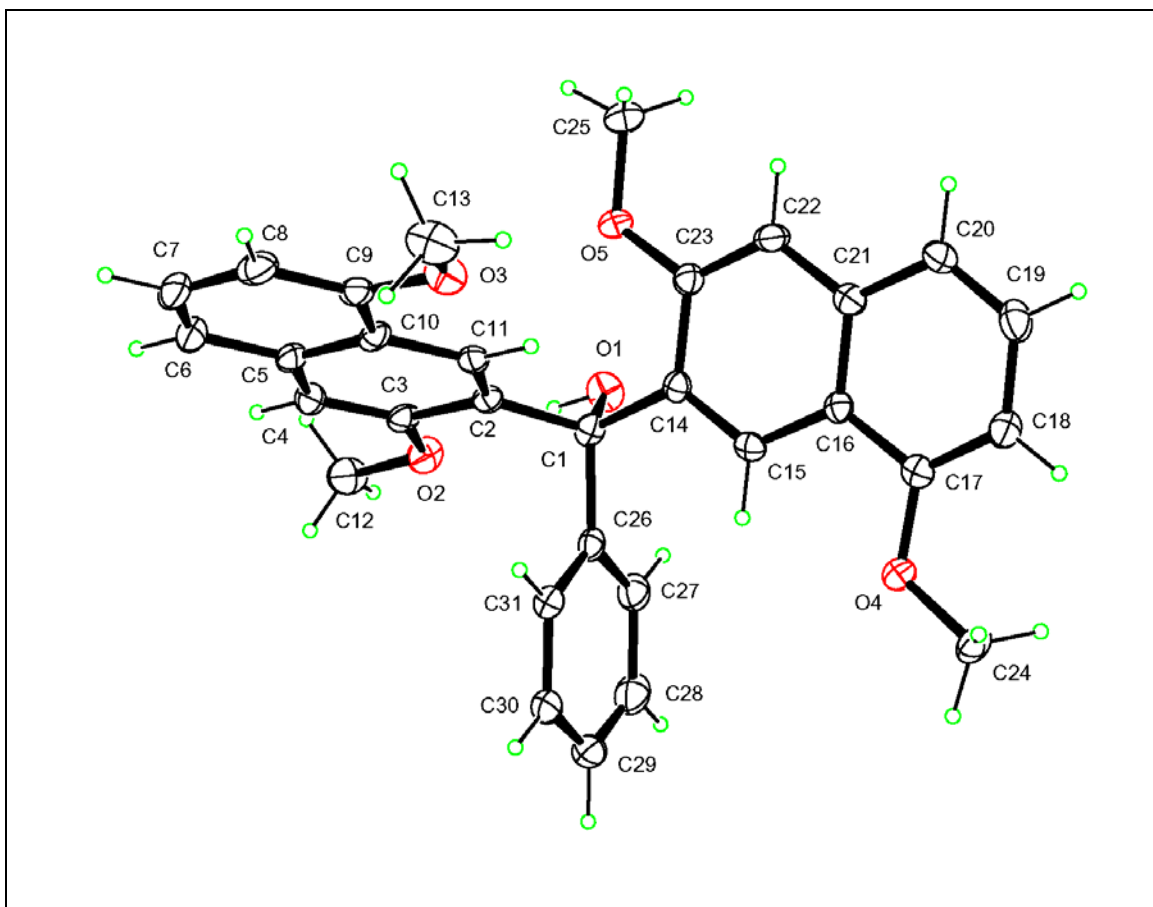


Figure S4. Ortep drawing for 4.

# Compound 5

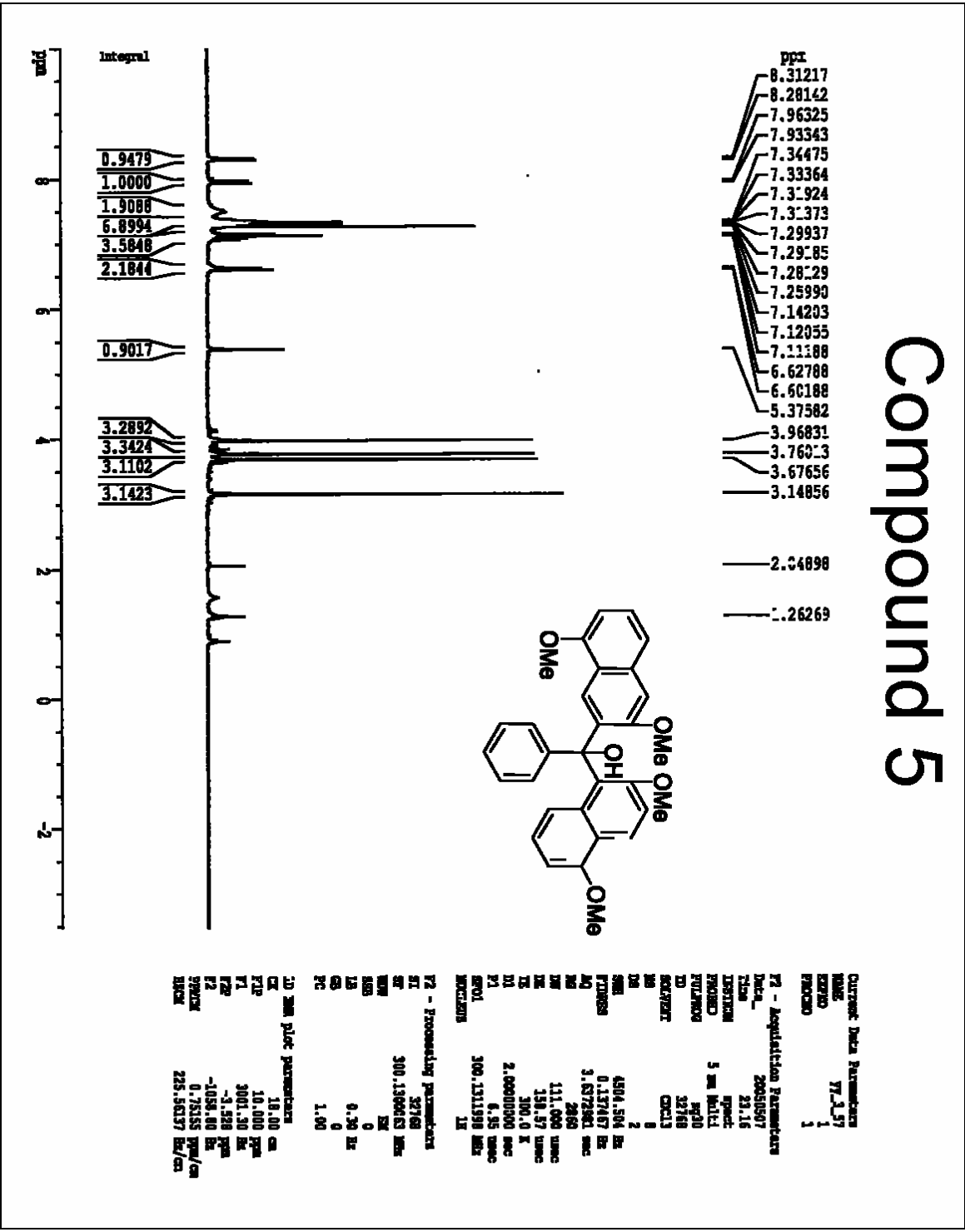
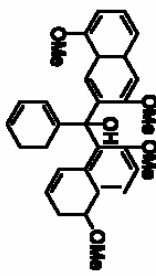
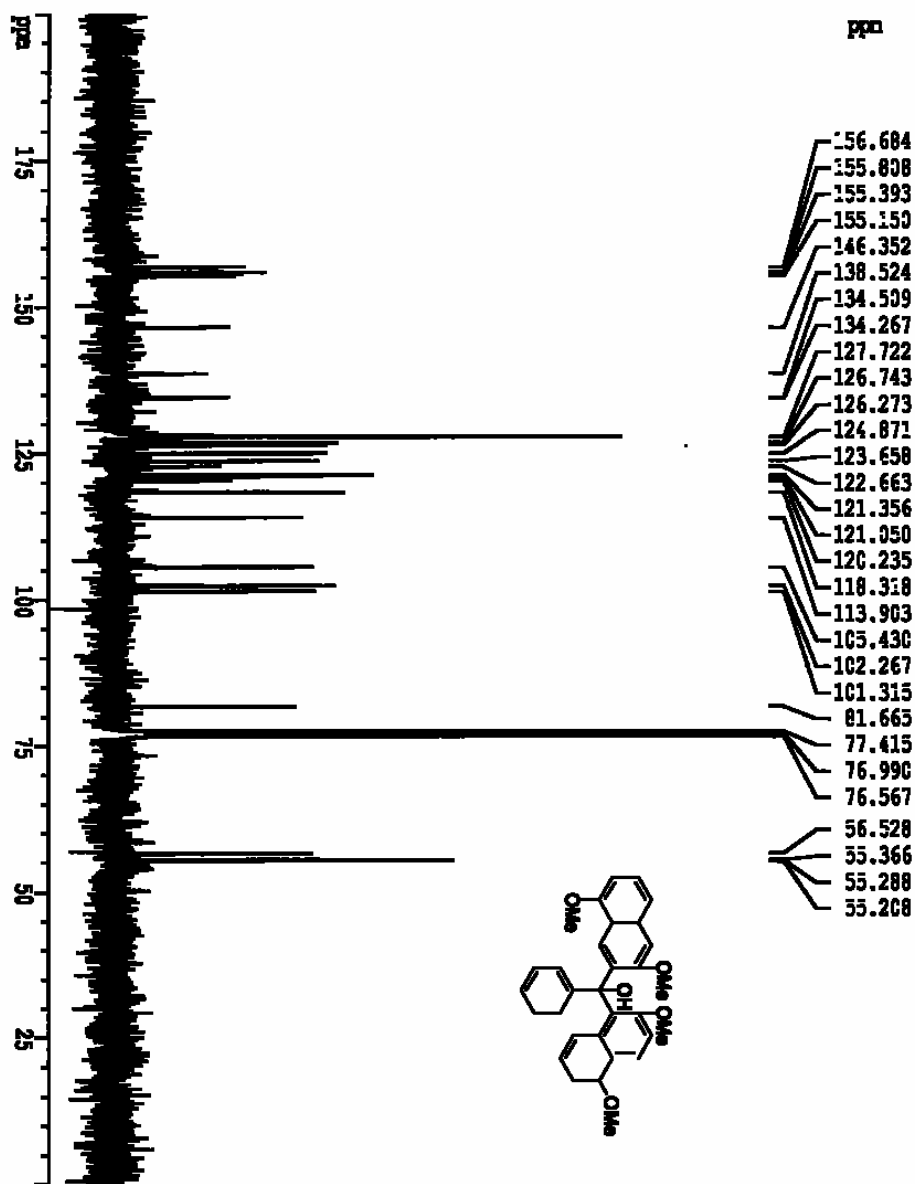


Figure S5. <sup>1</sup>H NMR of 5.

# Compound 5



Current Data Parameters  
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 EXPNO: 6  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20051206  
 Time: 22.24  
 INSTRUM: spect  
 PULPROG: zgpg30  
 TD: 16384  
 SFO: 125.761  
 AQ: 0.4280340 sec  
 RG: 327.68  
 INJ: 25.000 umol  
 DE: 17.14 umol  
 TE: 300.0 K  
 D12: 0.0000000 sec  
 D15: 23.00 sec  
 D1: 2.0000000 sec  
 CENPROG: waltz16  
 P11: 86.00 umol  
 D11: 0.0300000 sec  
 D15: 23.00 sec  
 P1: 5.00 umol  
 SFO1: 75.475177 MHz  
 NUC1: 13C

F2 - Processing parameters  
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 SF: 75.467575 MHz  
 WDM: 64  
 SSB: 0  
 LB: 2.00 Hz  
 GB: 0  
 PC: 1.40

1D NMR plot parameters  
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 FIDP: 260.000 ppm  
 F1: 15053.35 Hz  
 F2: 0.000 ppm  
 FREQM: 11.11111 ppm/cm  
 SFO: 839.53058 Hz/cm

Figure S6. <sup>13</sup>C NMR of 5.

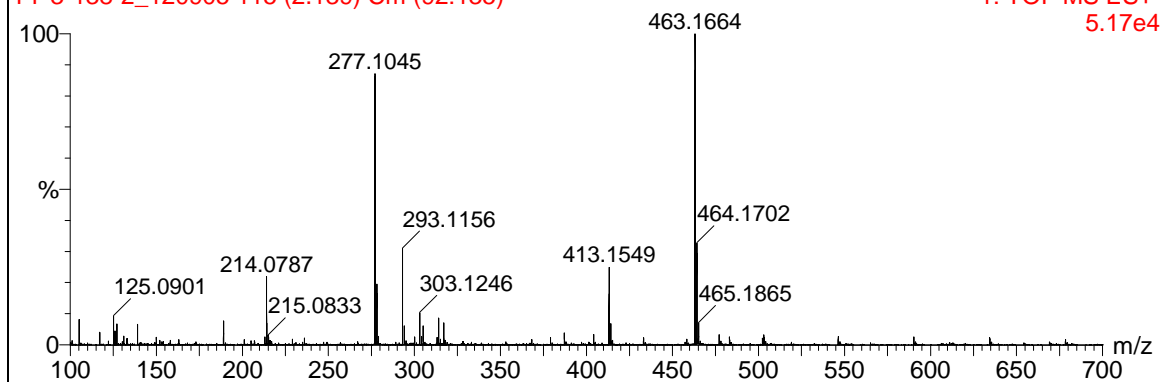


Figure S7. ESI MS of 5.

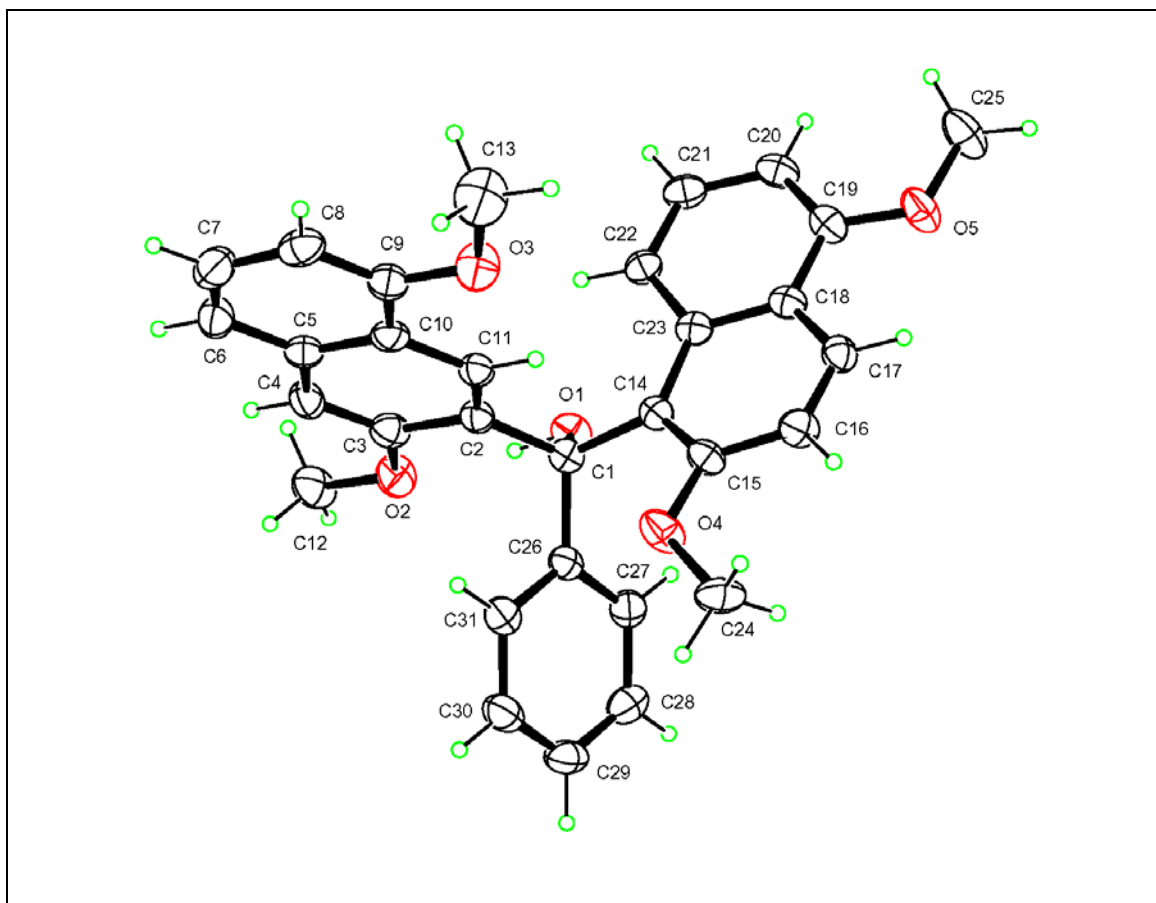


Figure S8. Ortep drawing for 5.

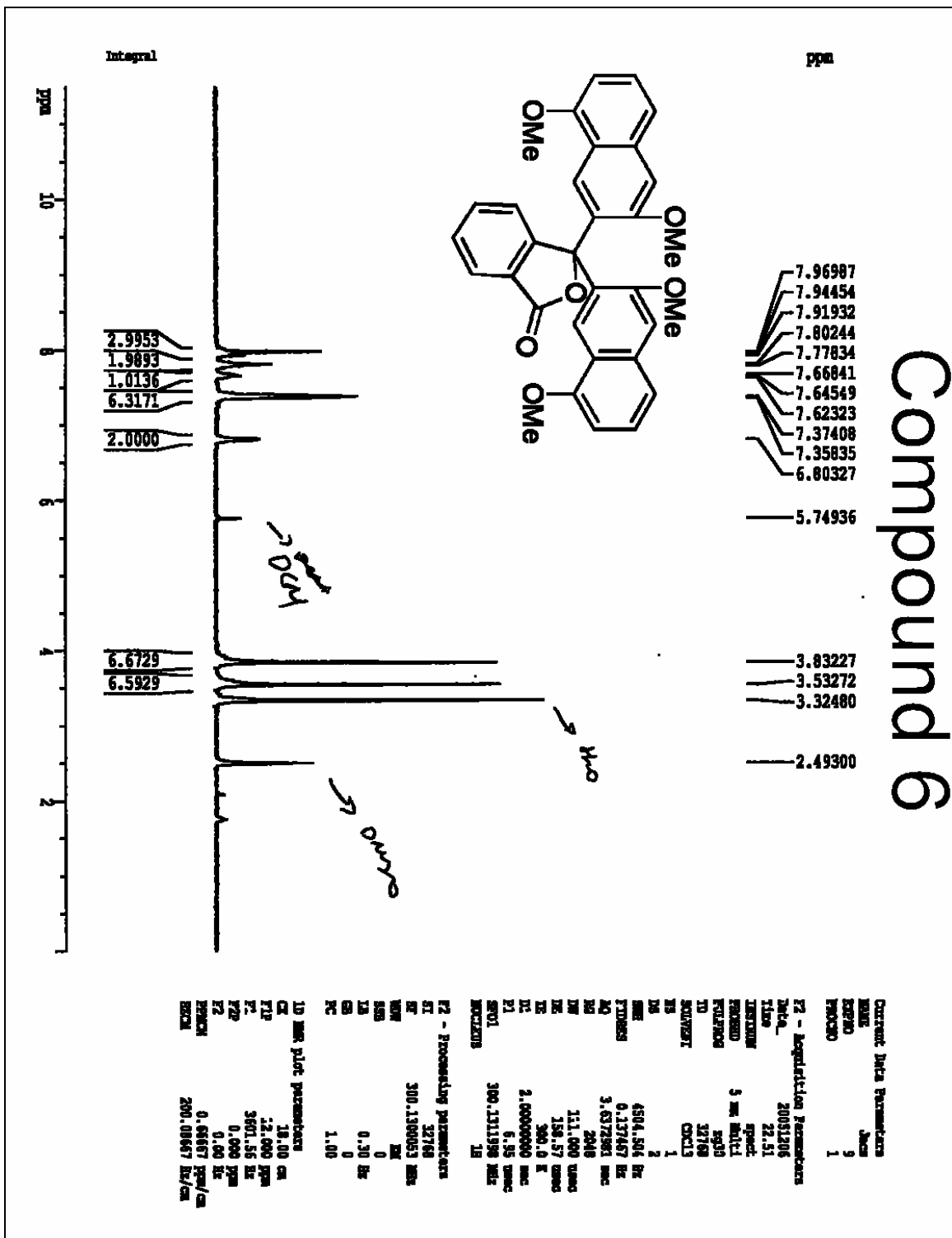
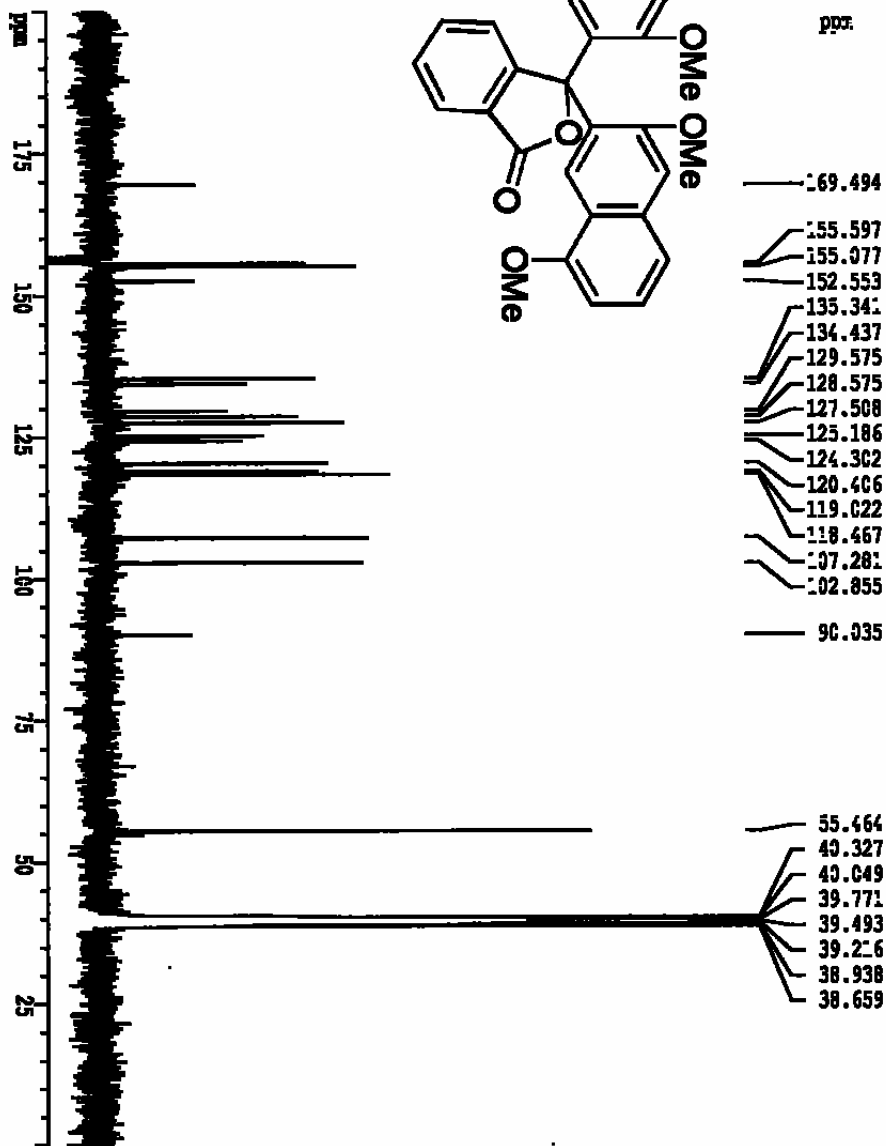
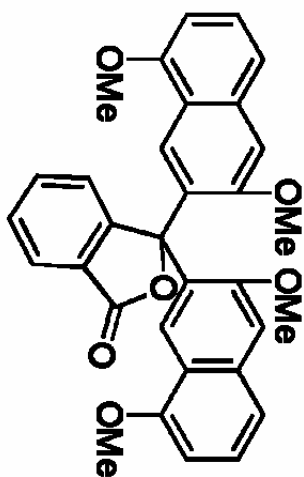


Figure S9. <sup>1</sup>H NMR of 6.

# Compound 6



Parameter	Value
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NAME	Specs
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F2 - Acquisition Parameters	
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INSTRUM	spect
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TD	16384
SOLVENT	DMSO
NS	10240
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F2/FWHZ	1.171793 Hz
AQ	0.4280340 sec
RG	32768
FW	26.000 umsec
RE	37.14 umsec
TE	300.0 K
D12	0.0000200 sec
D16	23.00 dB
D1	2.0000000 sec
CDROMS	66.00 umsec
P31	0.0300000 sec
D11	23.00 dB
D15	9.00 umsec
F1	75.4751777 MHz
SFO1	125
PROCPRG	13C
F2 - Processing parameters	
SI	16384
BF	75.4677801 MHz
WDW	EM
SFB	0
GA	2.00 Hz
GB	0
PC	1.40
1D MR parameters	
CH	10.00 cm
F1P	200.000 ppm
F1	15093.56 Hz
F2P	0.000 ppm
F2	0.00 Hz
FREQC1	13.11111 ppm/cm
RESC1	639.53094 Hz/cm

Figure S10. <sup>13</sup>C NMR of 6.

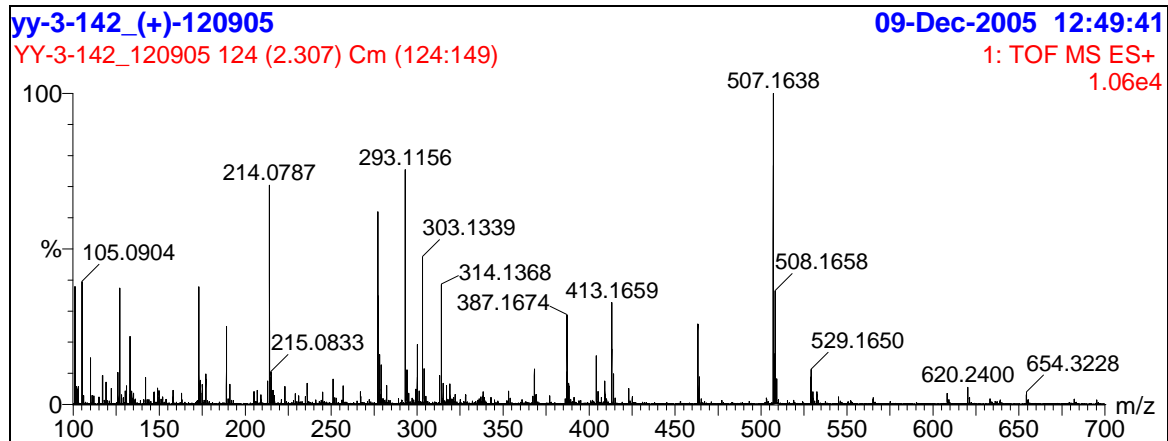


Figure S11. ESI MS of 6.

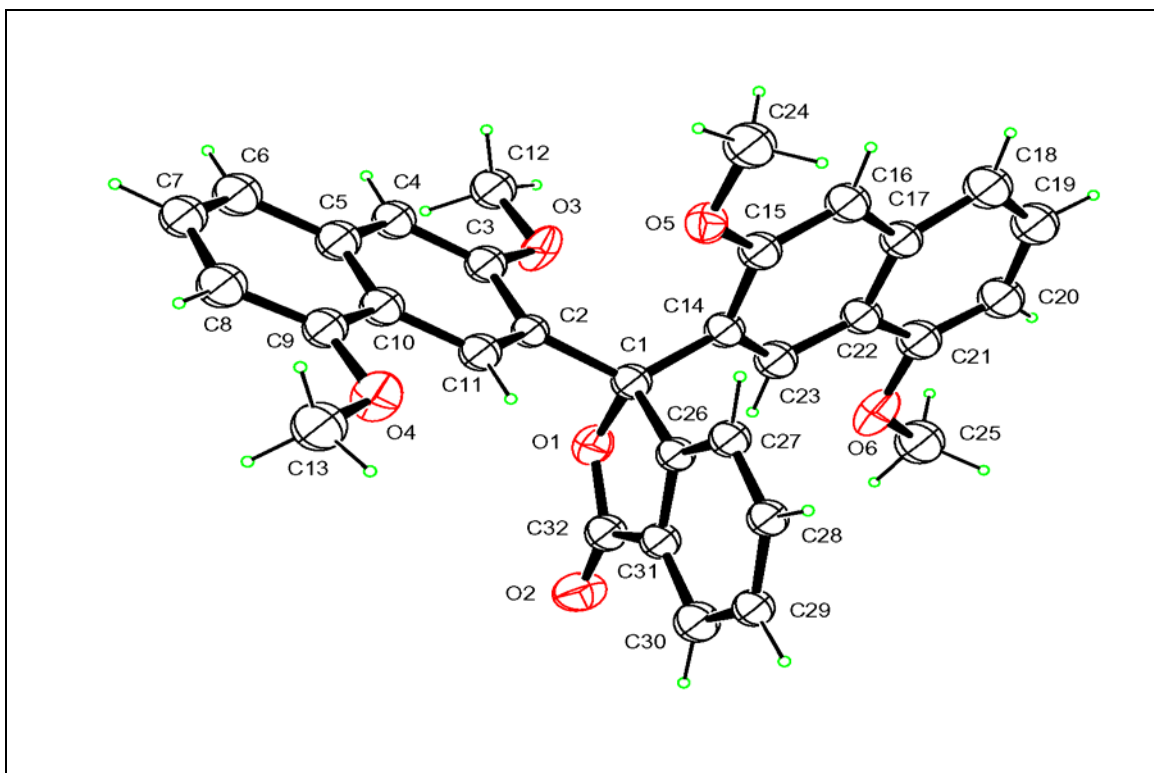


Figure S12. Ortep drawing of 6.

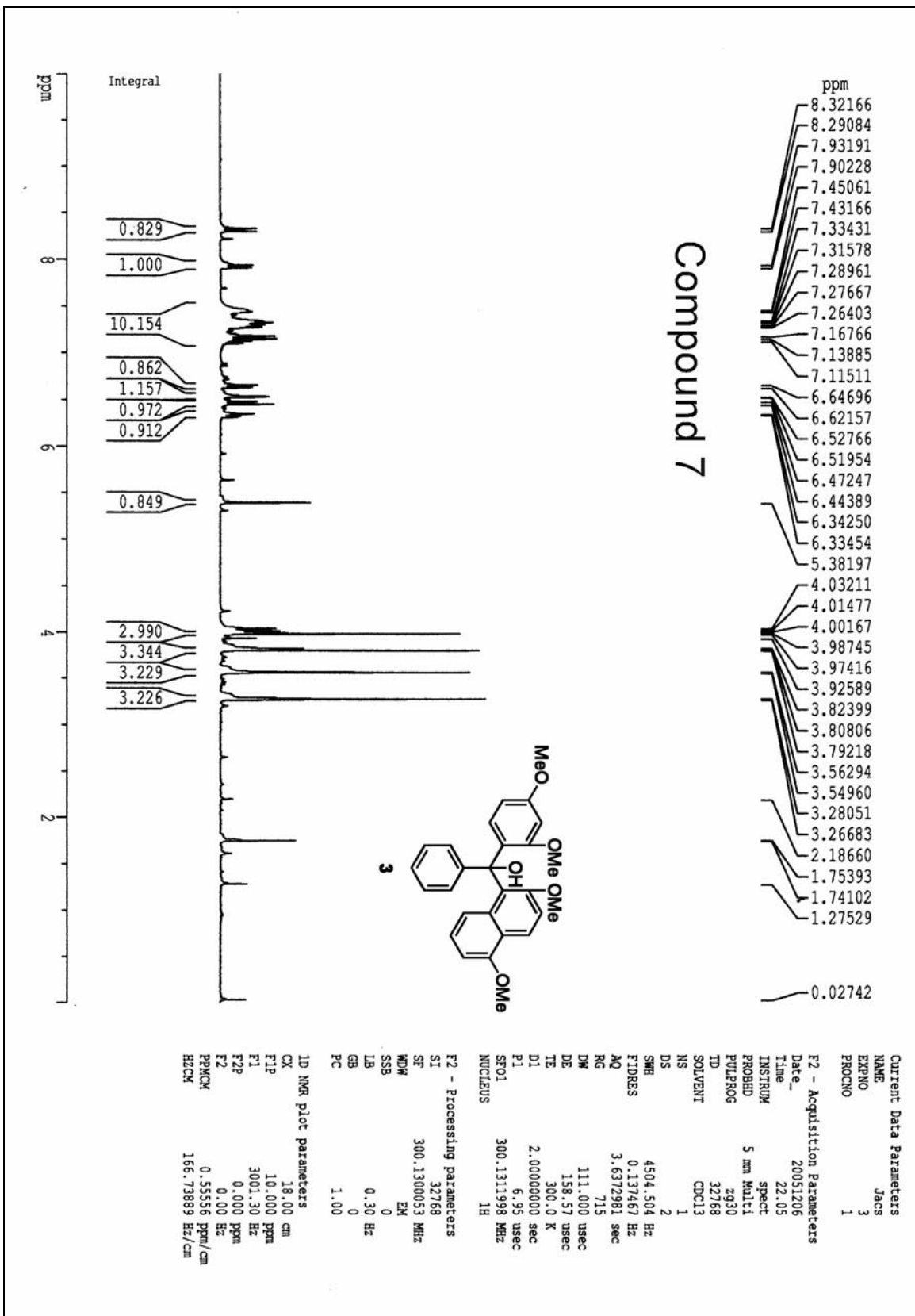


Figure S13. <sup>1</sup>H NMR of 7.



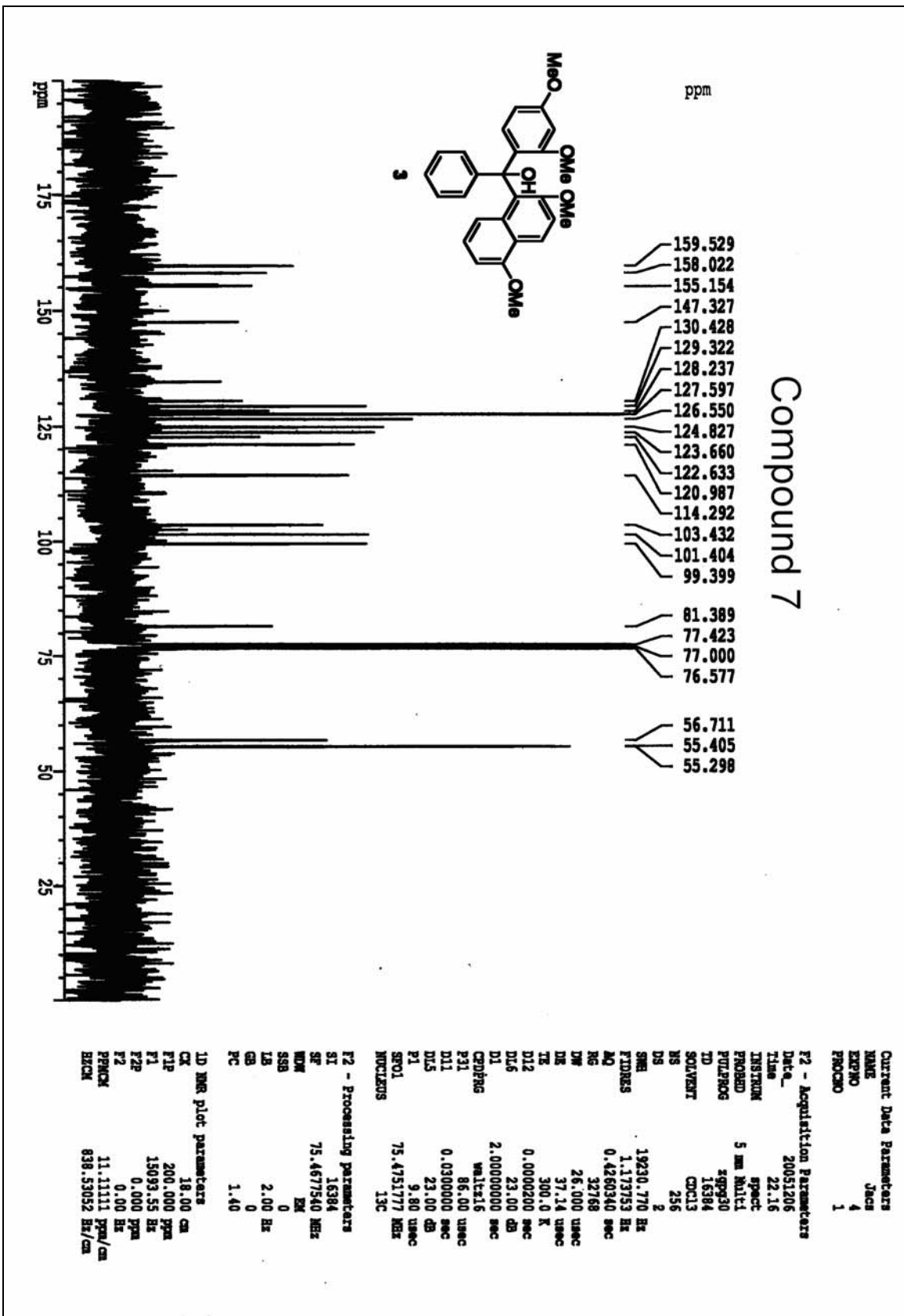


Figure S14. <sup>13</sup>C NMR of 7.

yy-3-183-2\_(+)-120905

09-Dec-2005 12:34:53

YY-3183-2\_120905 121 (2.249) Cm (121:129)

1: TOF MS ES+  
4.19e4

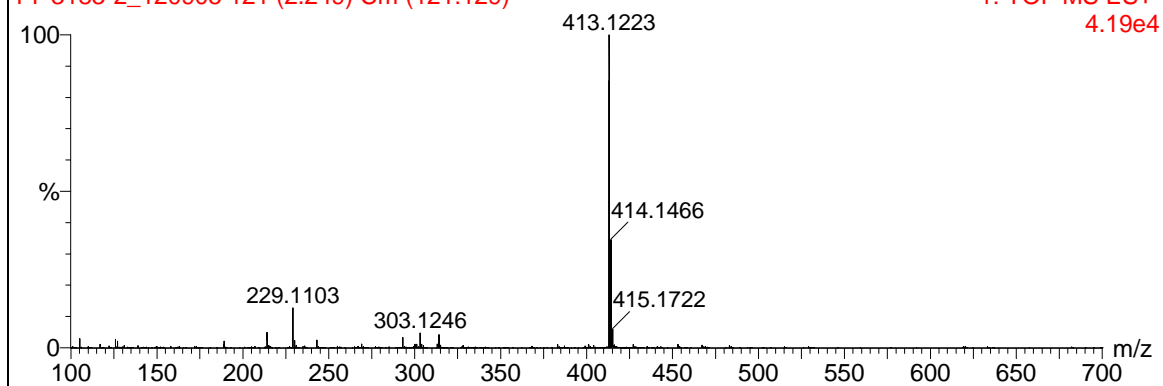


Figure S15. ESI MS of 7.

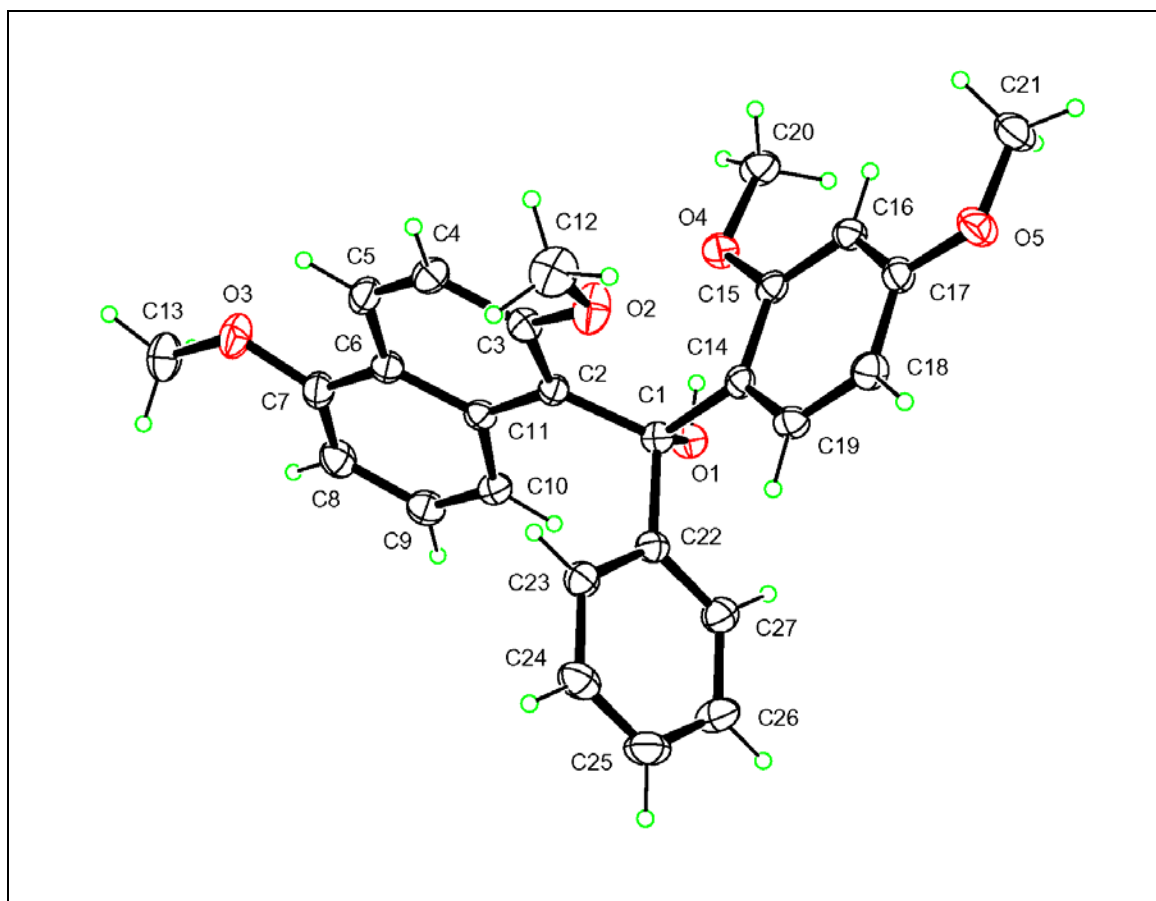


Figure S16. Ortep Drawing of 7.

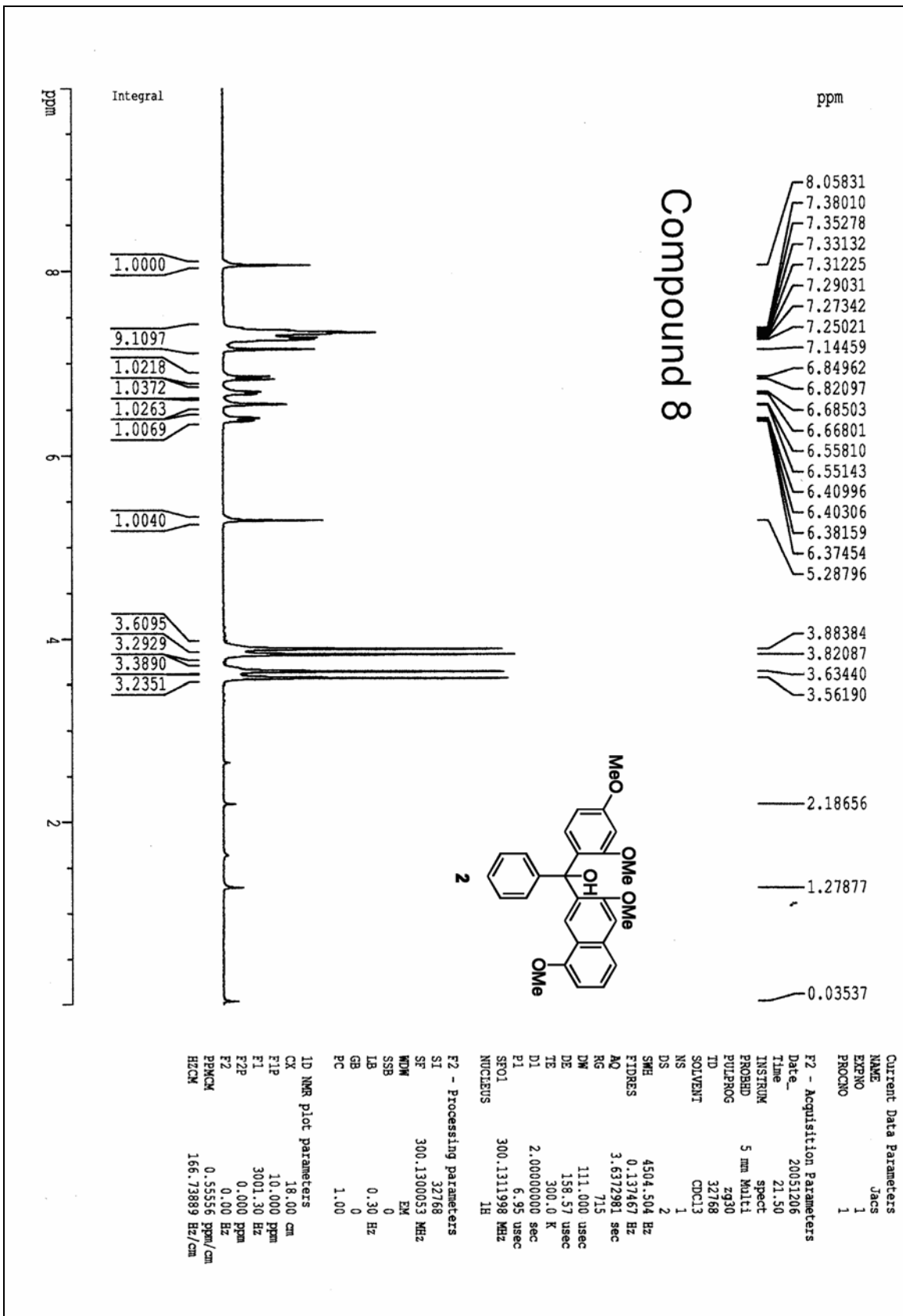


Figure S17. <sup>1</sup>H NMR of 8.

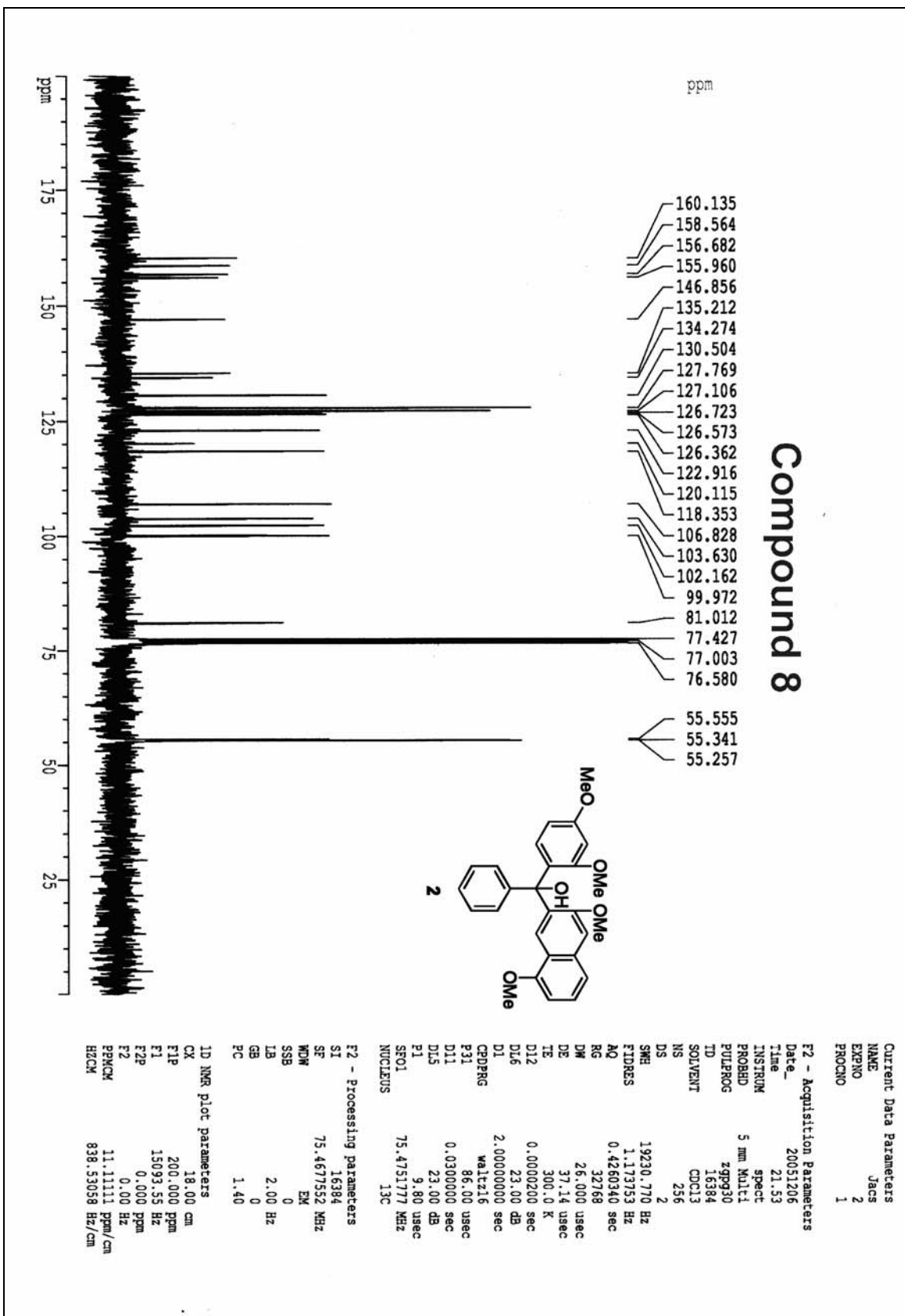


Figure S18. <sup>13</sup>C NMR of 8.

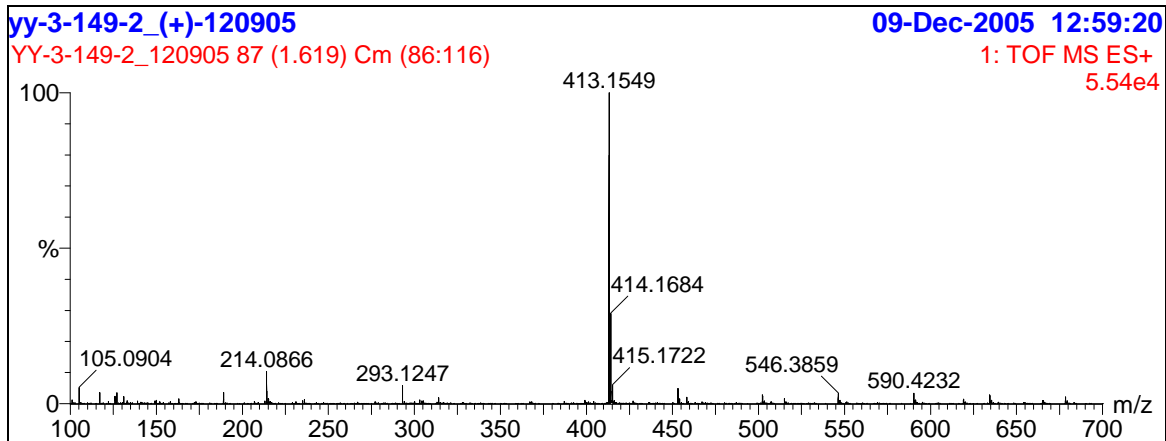


Figure S19. ES MS of 8

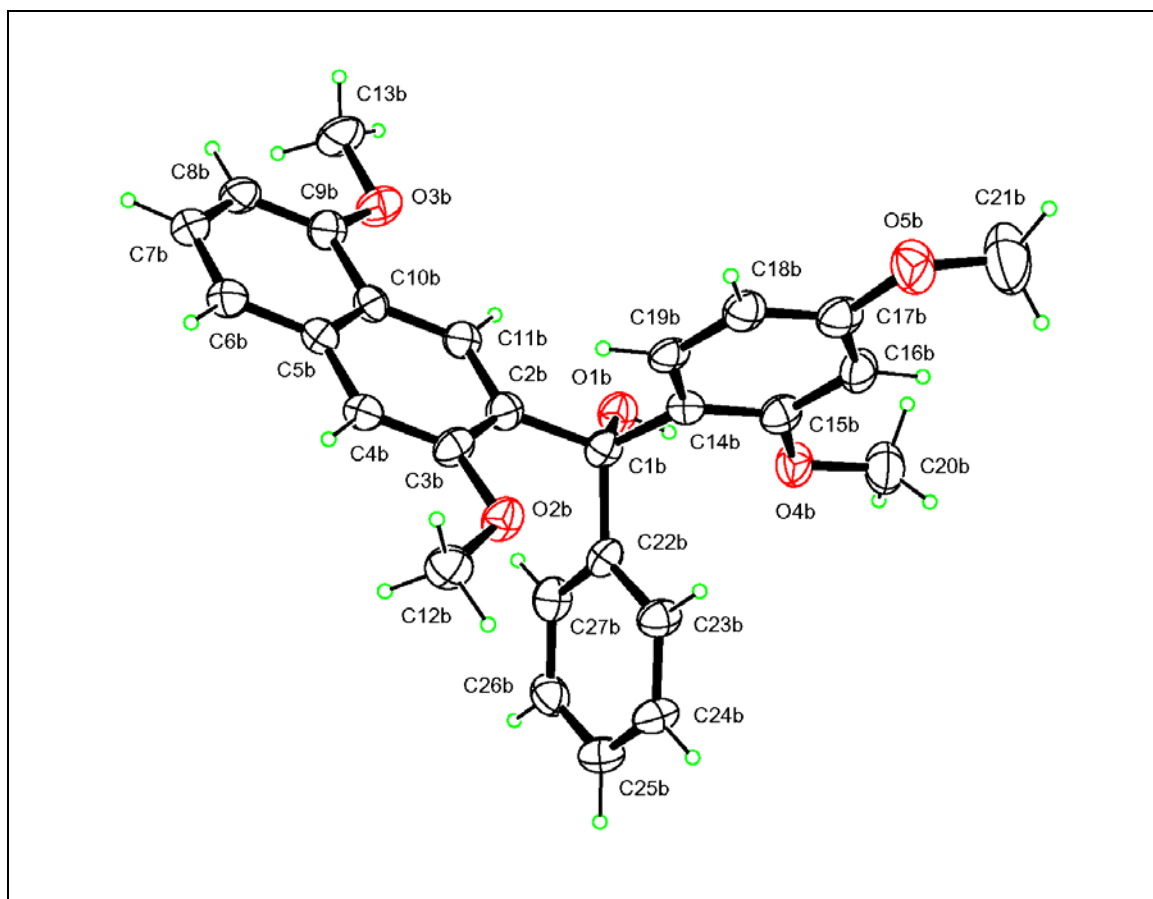
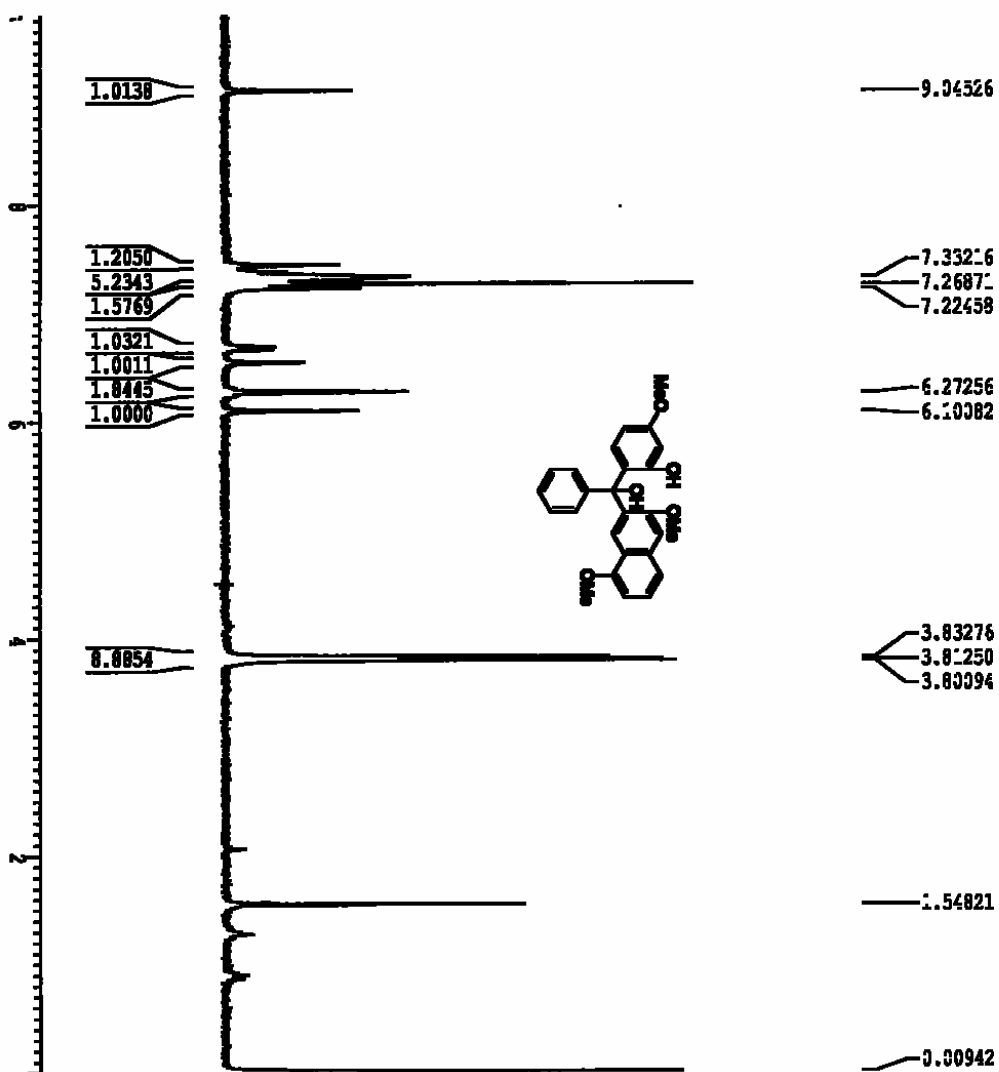


Figure S20. Ortep drawing of 8.

# Compound 9



```

Current Data Parameters
NAME          F2_3_159
EXPNO        4
PROCNO       1
F2 - Acquisition Parameters
Date_        20051026
Time         23.09
INSTRUM      spect
PROBHD       5 mm QNP 1H
PULPROG      zg30
TD           16384
SOLVENT      CDCl3
NS           8
DS           2
SWH          3742.515 Hz
FIDRES       0.228425 Hz
AQ           2.1889524 sec
RG           1024
DM           133.680 uSsec
DE           8.00 uSsec
TE           300.0 K
D1           2.00000000 sec

----- CHANNEL f1 -----
NUC1          1H
P1           10.00 uSsec
PAL          0.00 dB
SFO1         250.1311986 MHz

F2 - Processing parameters
SI           16384
SF           250.1300950 MHz
WDW          EM
SSB          0
GB           0
PC           0.15 Hz
RG           0
PC           1.00

1D NMR plot parameters
CX           18.00 cm
F1P          10.000 ppm
F1          2501.30 Hz
F2P          0.000 ppm
F2           0.00 Hz
FREQCCK      0.555556 ppm/cm
XZCCK        138.96112 Hz/cm
  
```

Figure S21. <sup>1</sup>H NMR of 9.

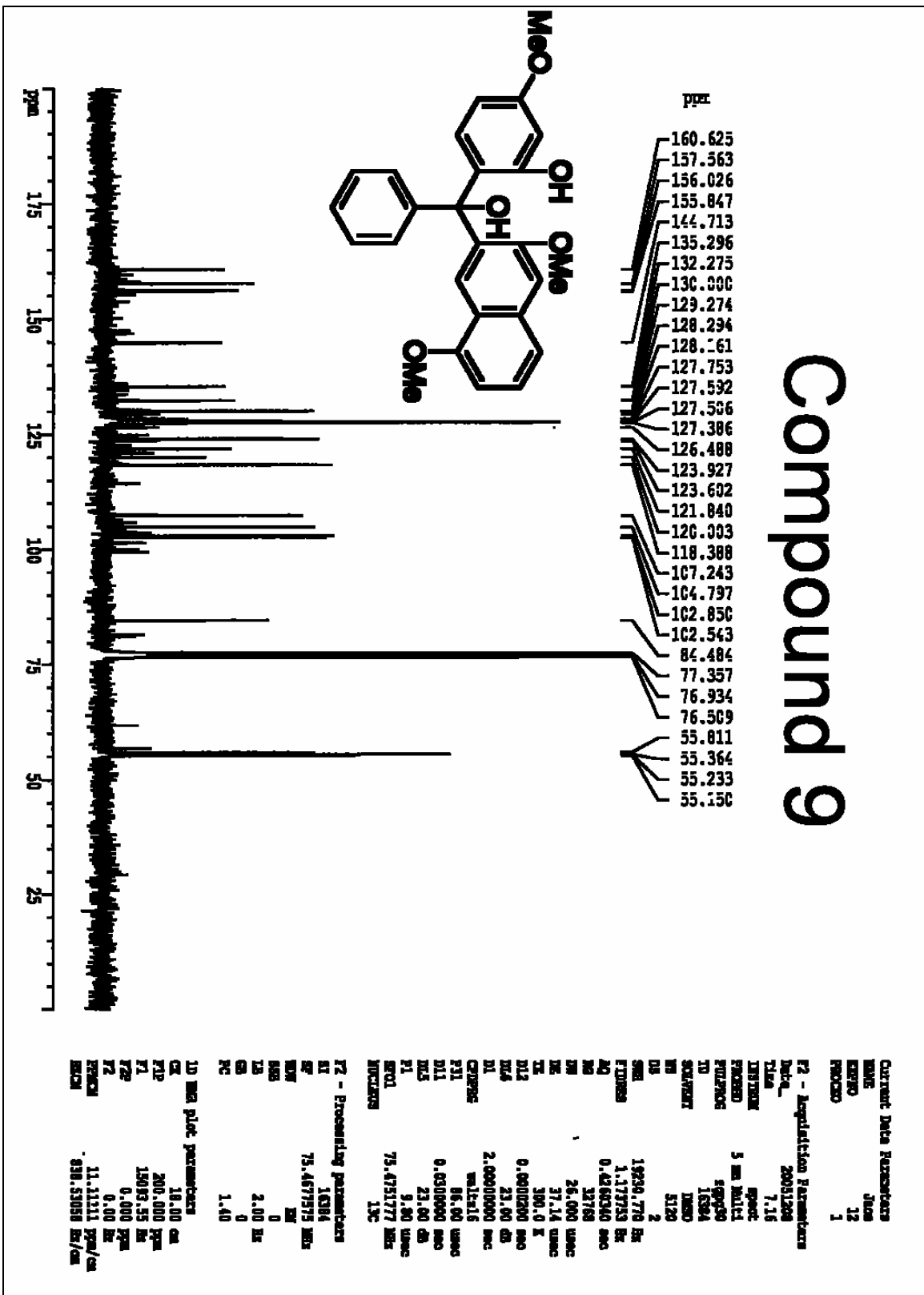


Figure S22. <sup>13</sup>C NMR of 9.

yy-3-169-3\_(+)-120905

09-Dec-2005 13:05:59

YY-3-169-3\_120905 110 (2.048) Cm (77:111)

1: TOF MS ES+  
1.29e5

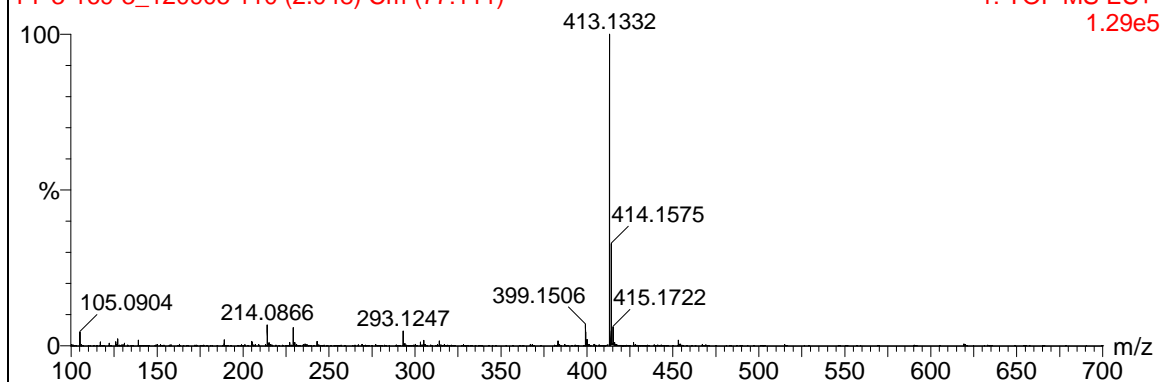


Figure S23. ES MS of 9

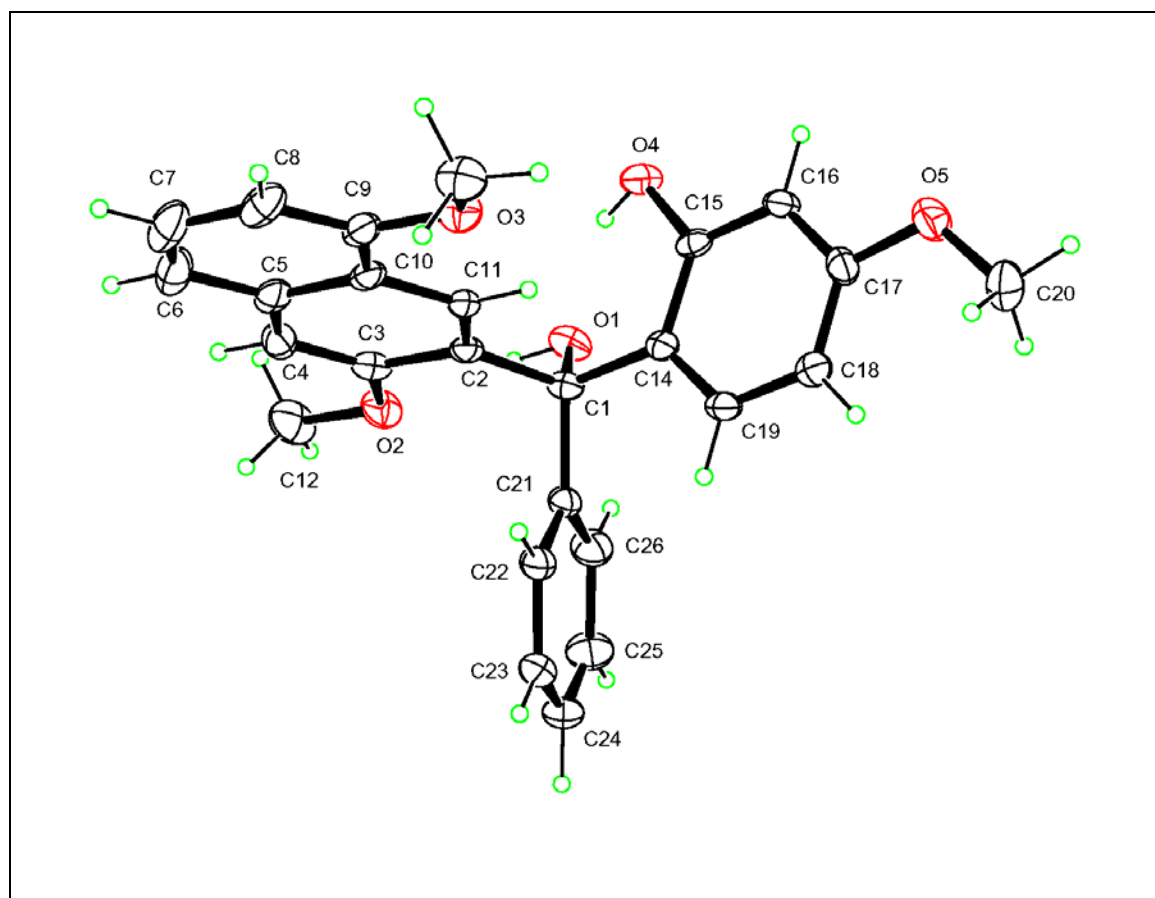


Figure S24. Ortep drawing of 9.



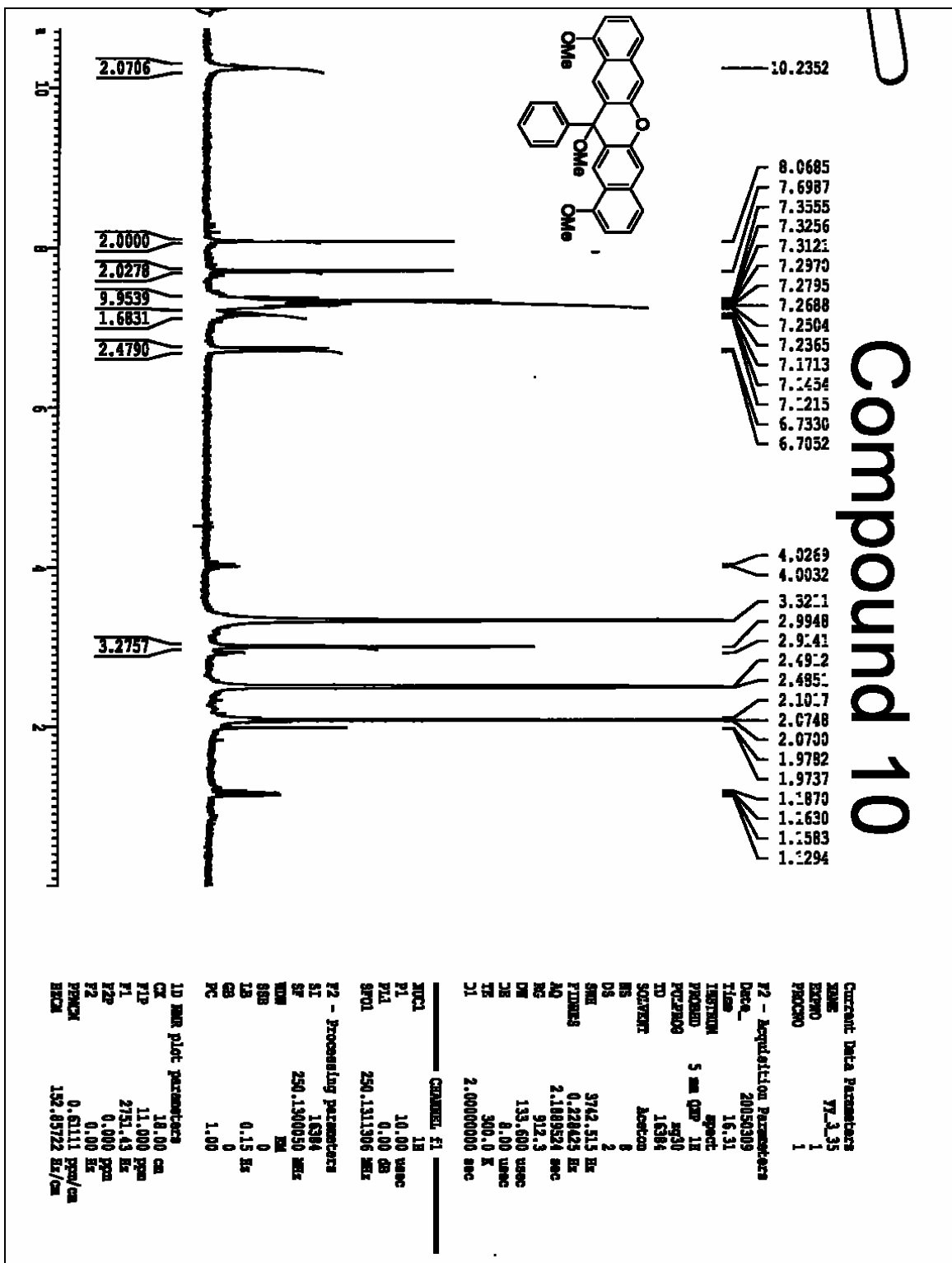
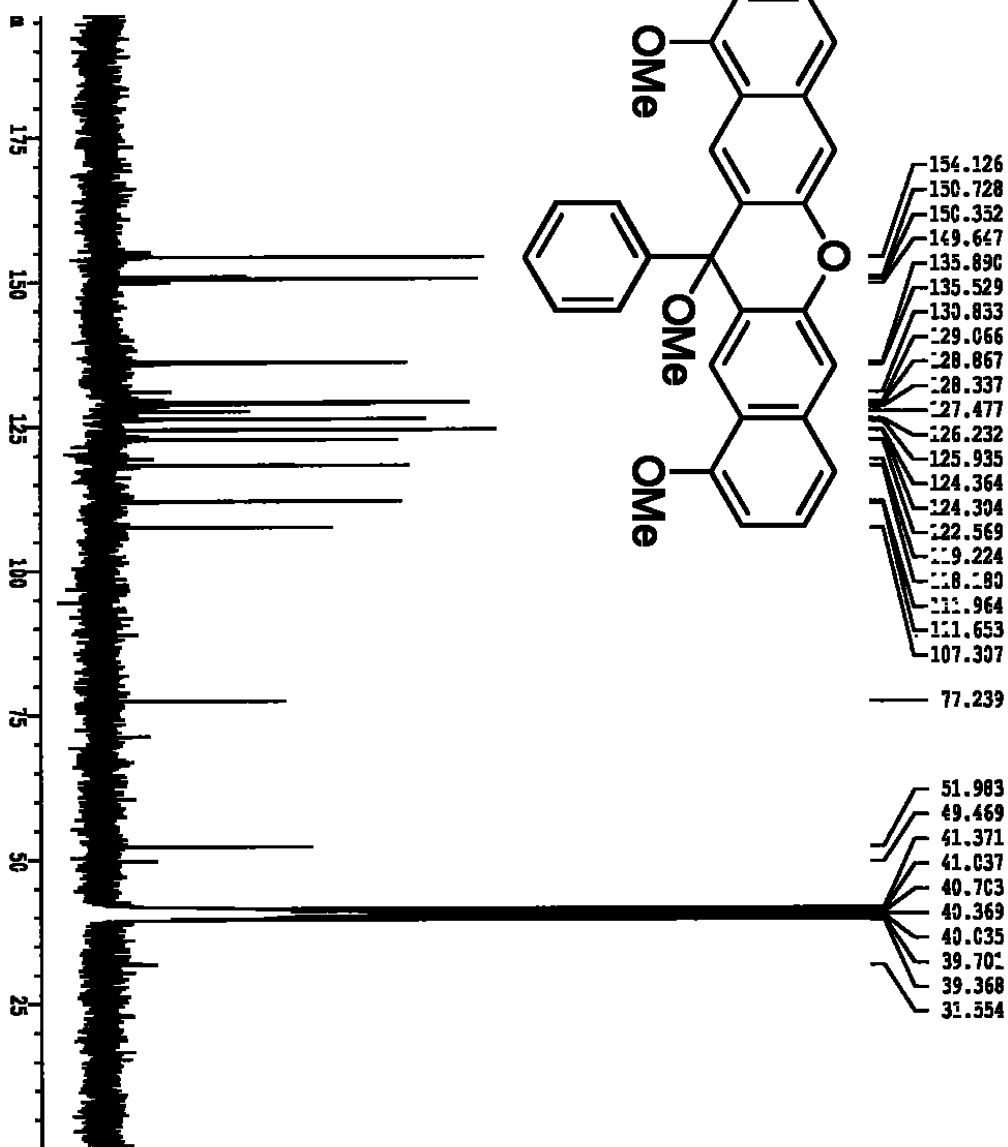
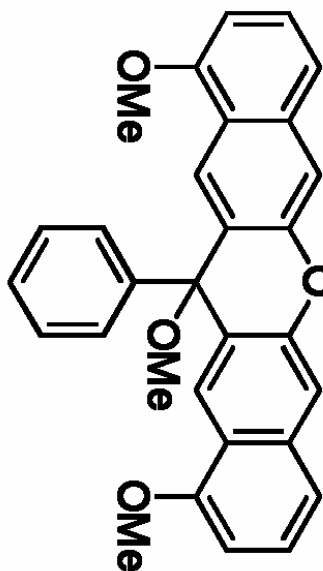


Figure S25. <sup>1</sup>H NMR of 10.

# Compound 10



Current Data Parameters	
NAME	10_3_35
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters	
Date_	20050309
Time	21.57
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	16384
TD0	16384
ACQINSTR	Acquisition
NS	5120
DS	2
SWH	15723.471 Hz
F2	0.455672 Hz
F2RES	0.531812 Hz
AQ	6.682
RG	31.800
IN	0.000000
TE	301.0 K
D1	2.00000000 sec
D11	0.03000000 sec
d12	0.00020000 sec

CHANNEL F1	
NUC1	13C
P1	0.000000
PL1	0.000000
PRG1	g2.pwpr13c139 MHz

CHANNEL F2	
CPDPRG2	waltz16
NUC2	1H
FREQ2	400.140000 MHz
YF2	120.000000
YAL2	22.000000
YAL3	22.000000
SWH2	250.1310005 MHz

F2 - Processing parameters	
SI	16384
SF	62.685140 MHz
WDW	EM
SSB	0
CB	1.00 Hz
CS	0
YC	1.40

1D NMR plot parameters	
SI	16384
CF	200.1000 MHz
F1	125.71904 Hz
F2	6.000000 MHz
PRGPR1	10_3_35322 ppm/cm
SCALE	662.85487 Hz/cm

Figure S26. <sup>13</sup>C NMR of 10.

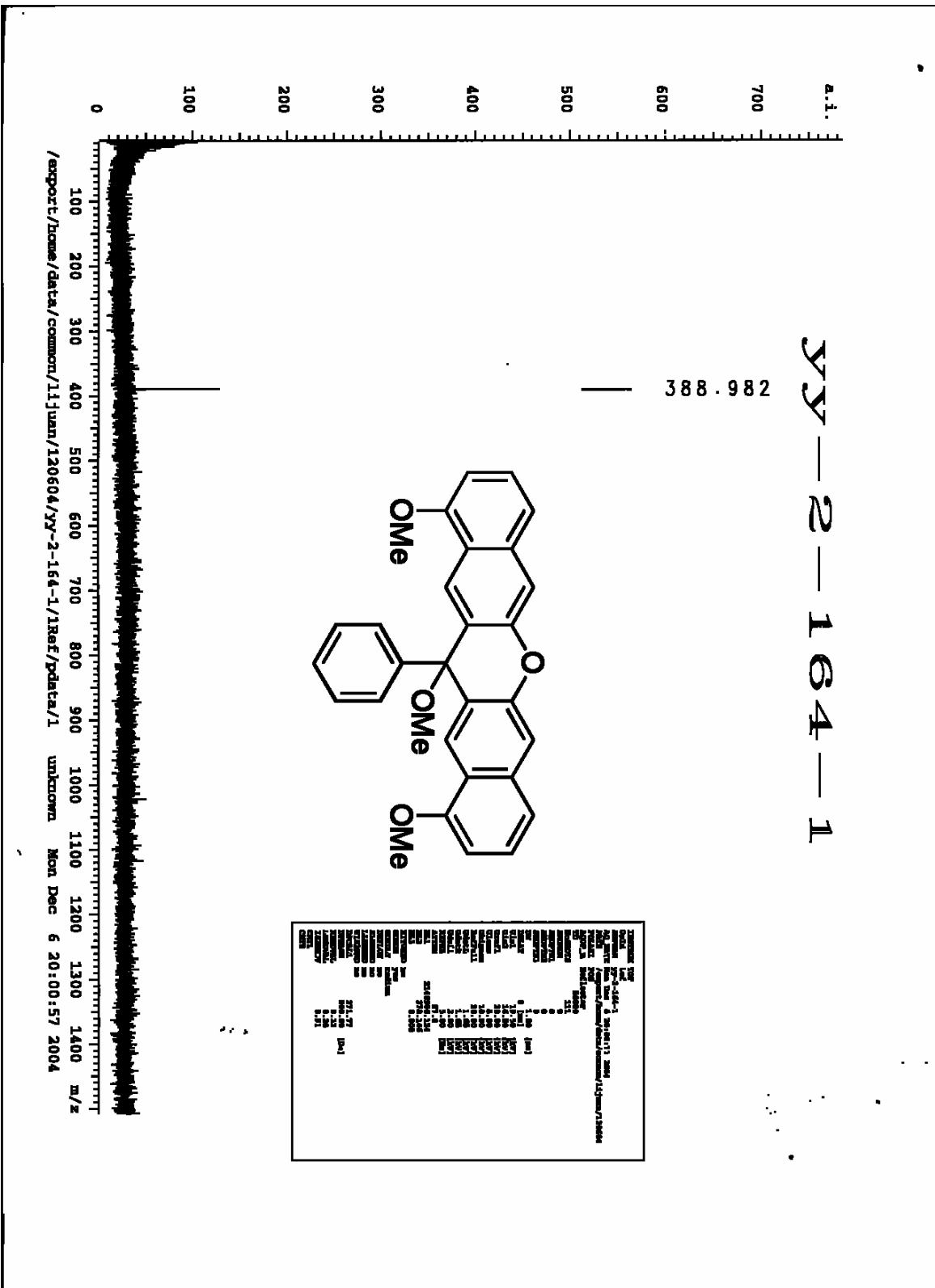
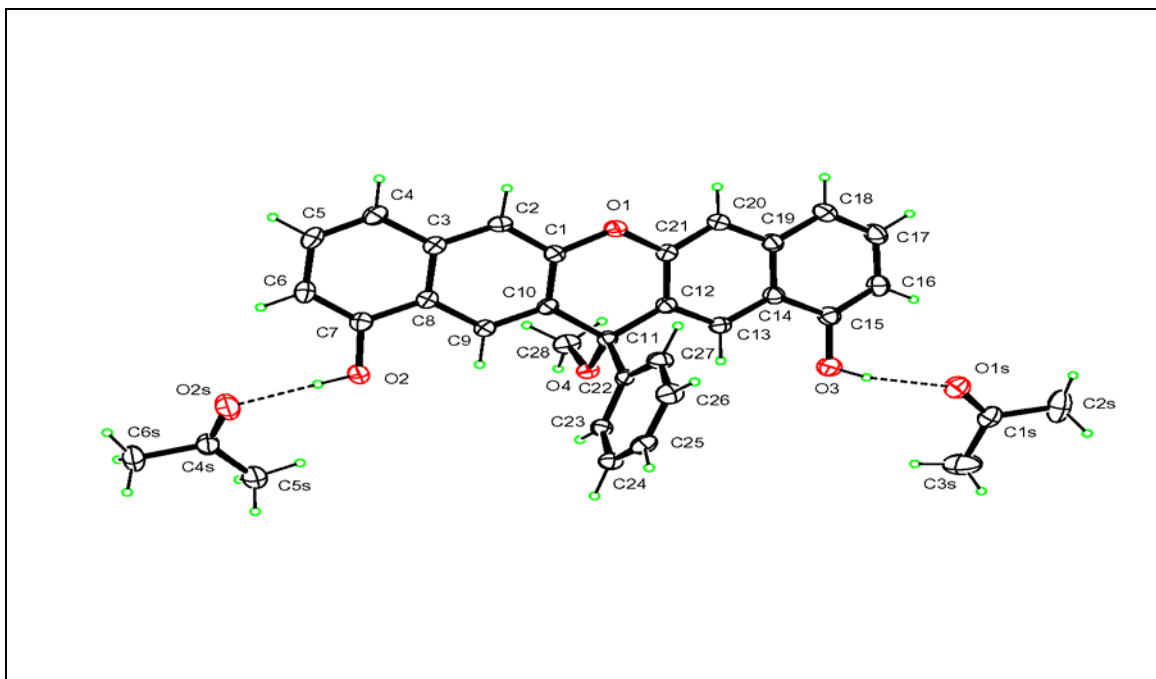


Figure S27. MALDI TOF of 10.



**Figure S28.** Ortep drawing of **10** with two acetone solvates.

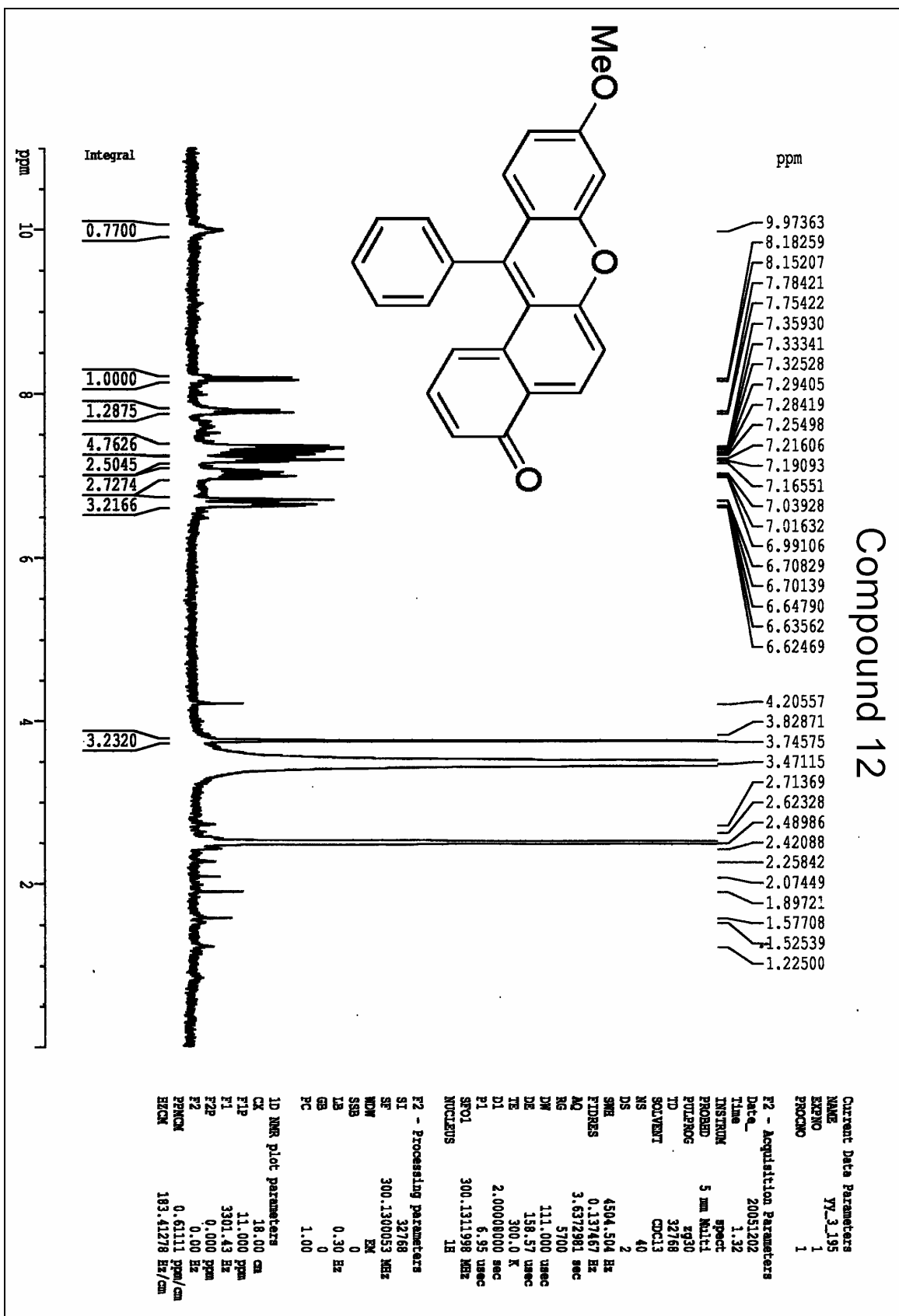


Figure S29. <sup>1</sup>H NMR of 12.

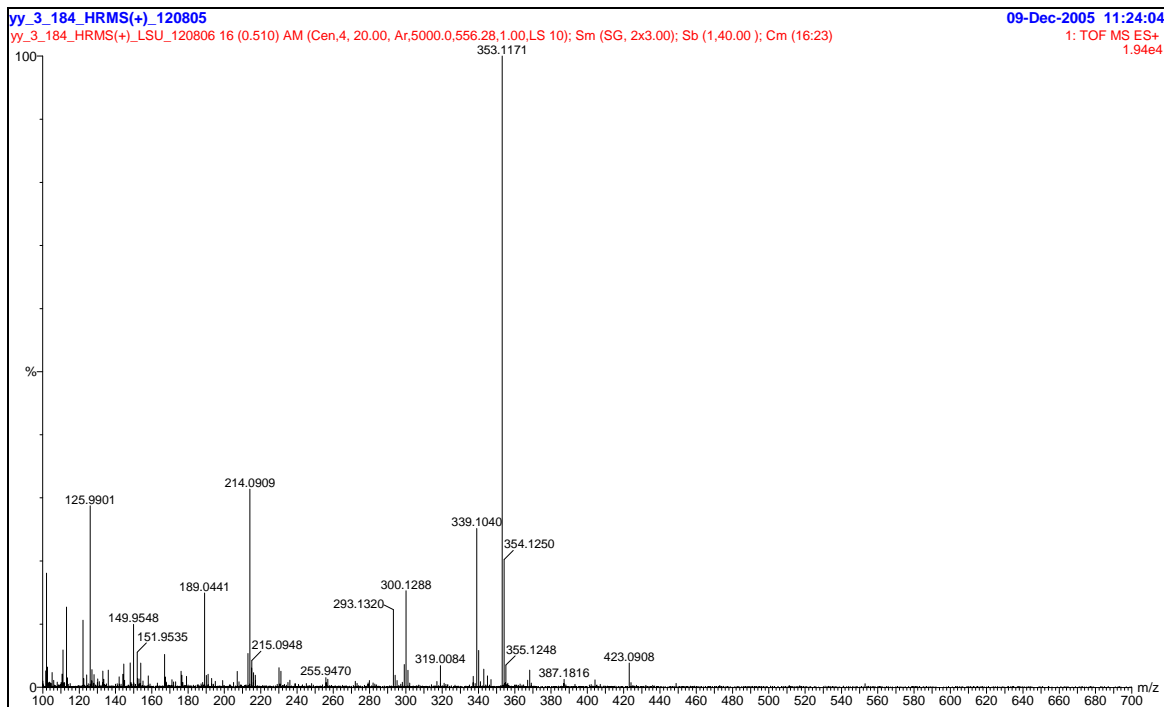


Figure S30. HRMS of 12.

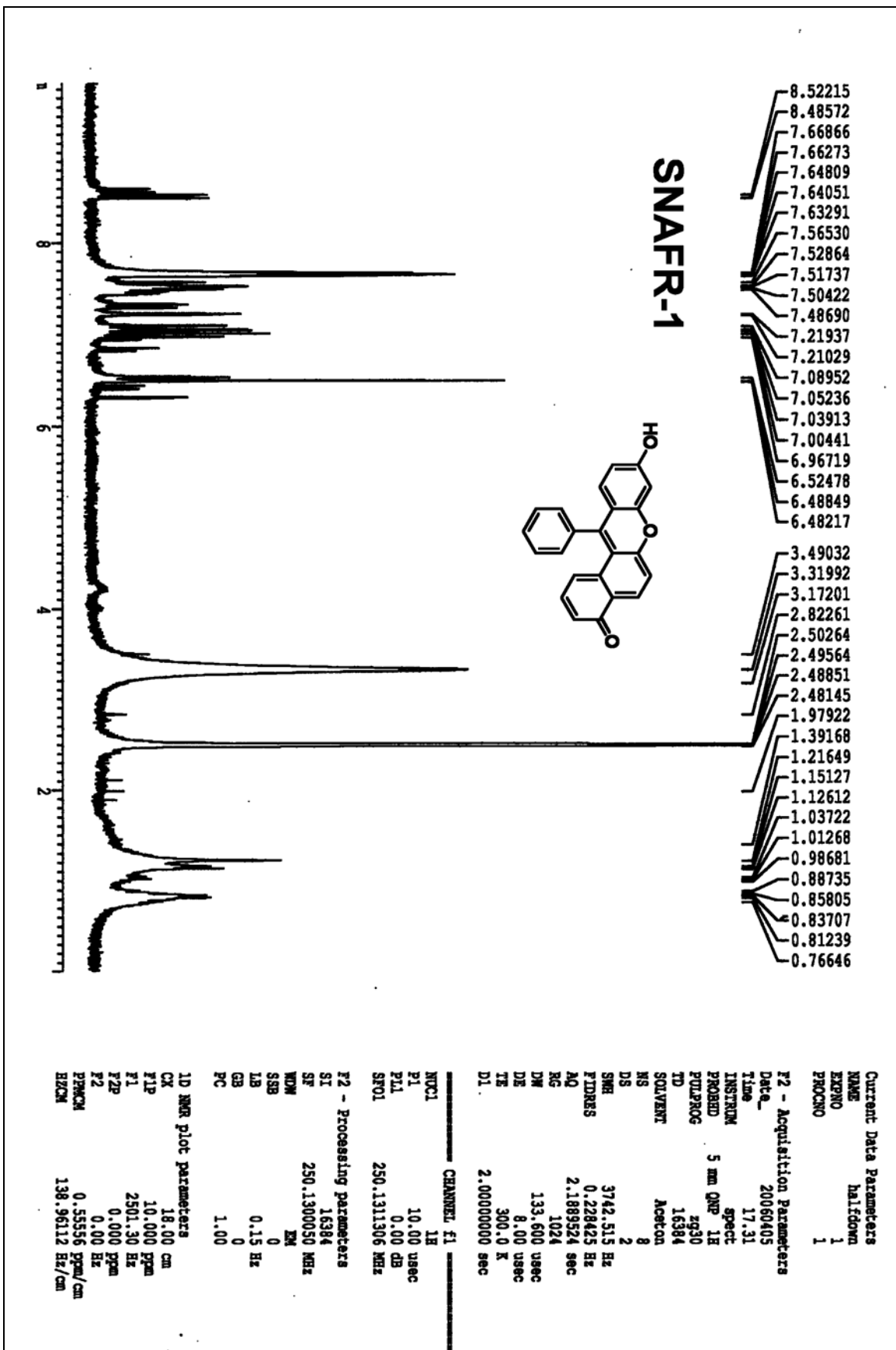
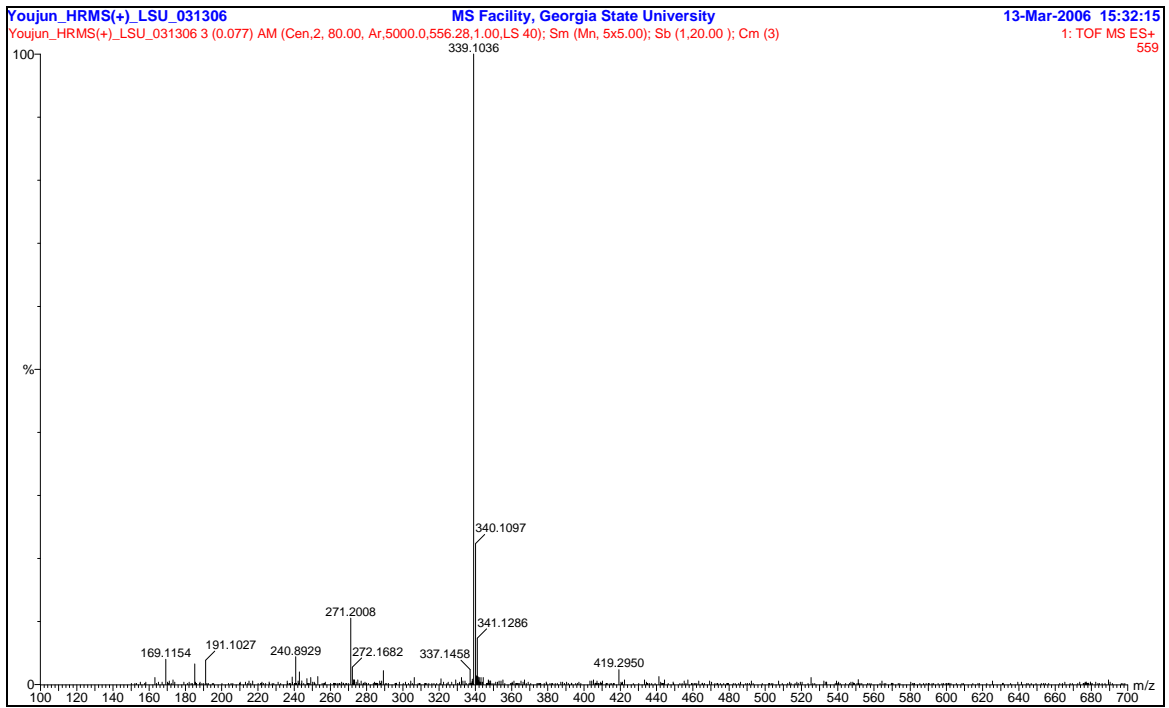


Figure S31. <sup>1</sup>H NMR of SNAFR-1.



**Figure S32. HRMS of SNAFR-1.**



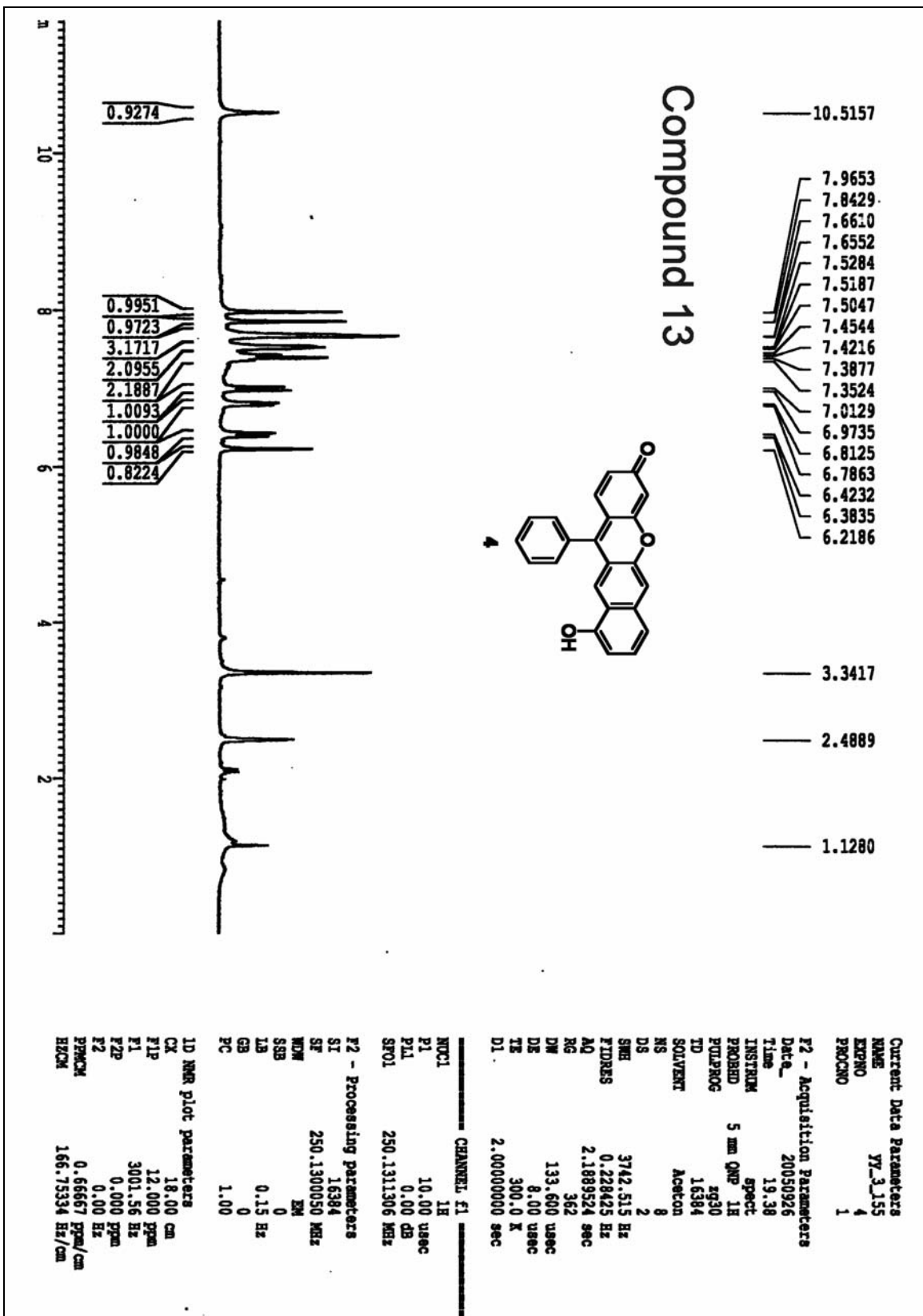


Figure S33. <sup>1</sup>H NMR of 13.

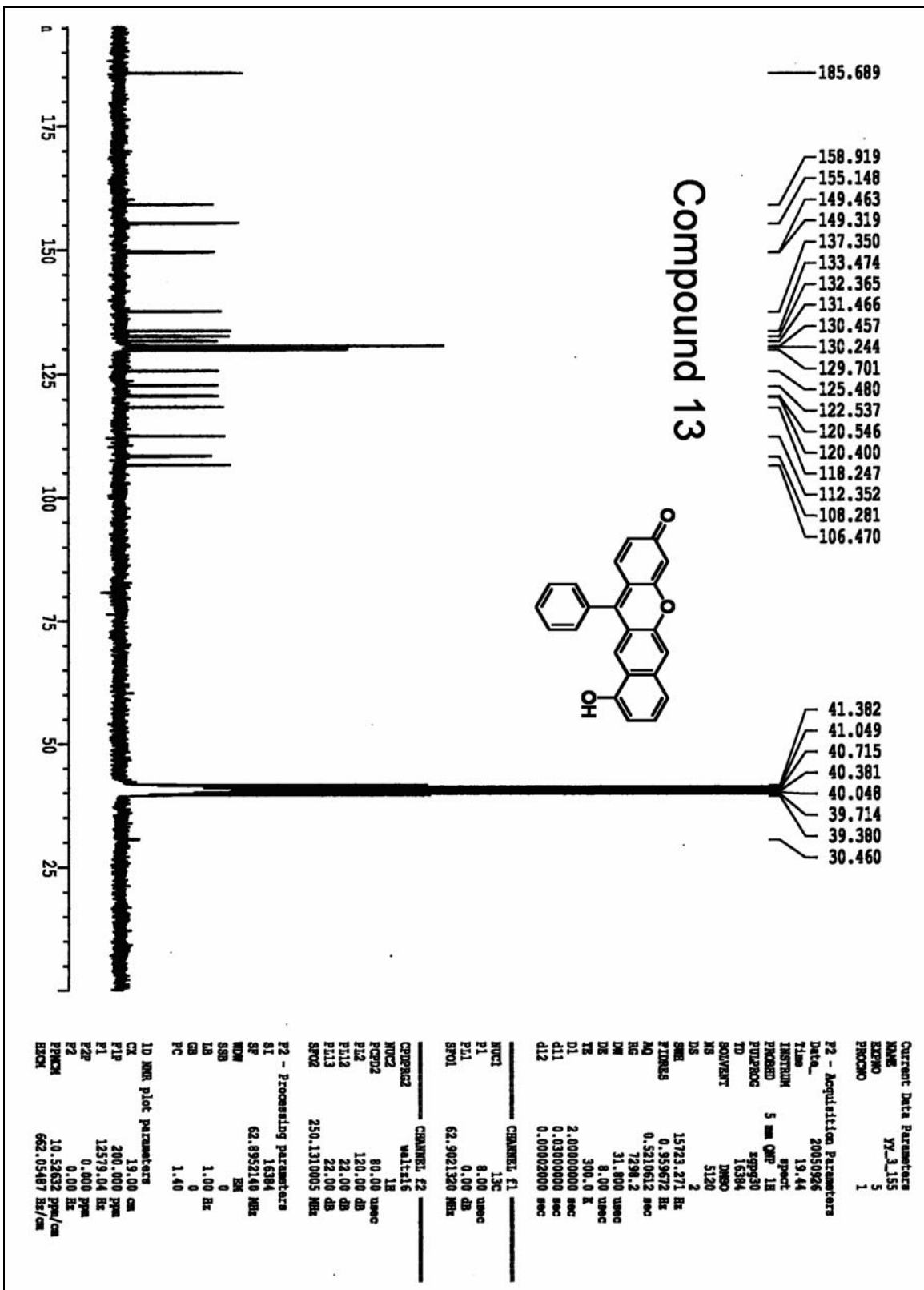


Figure S34. <sup>13</sup>C NMR of 13.

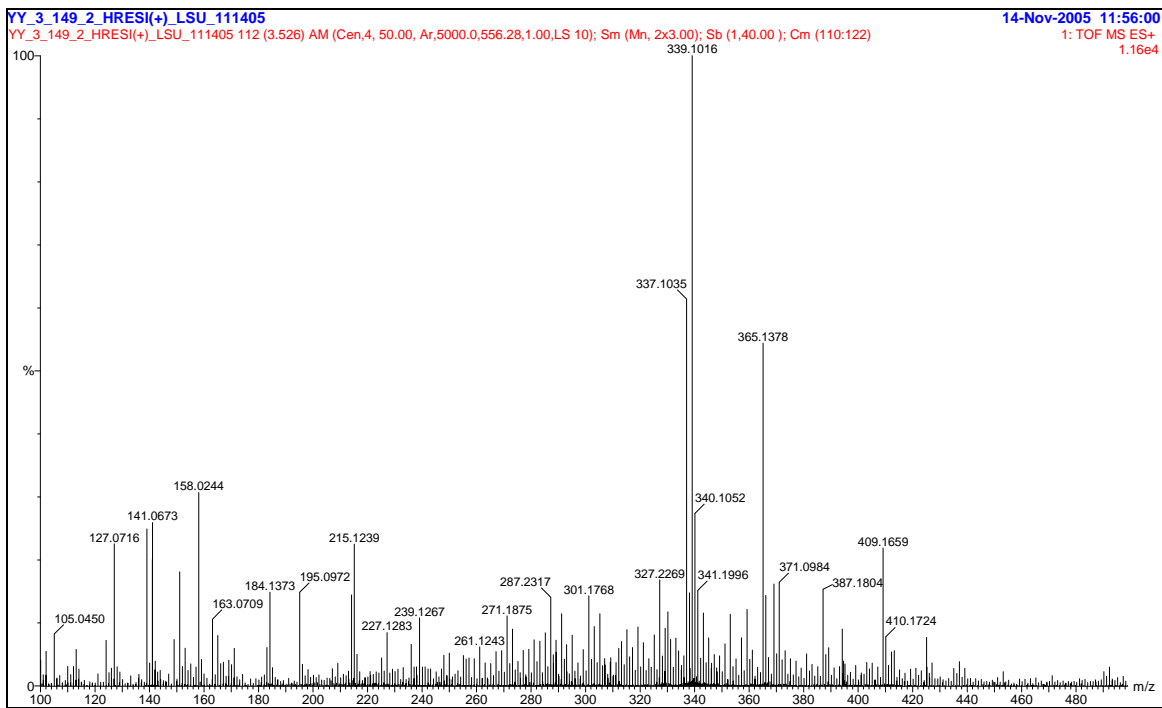


Figure S35. HRMS of 13.

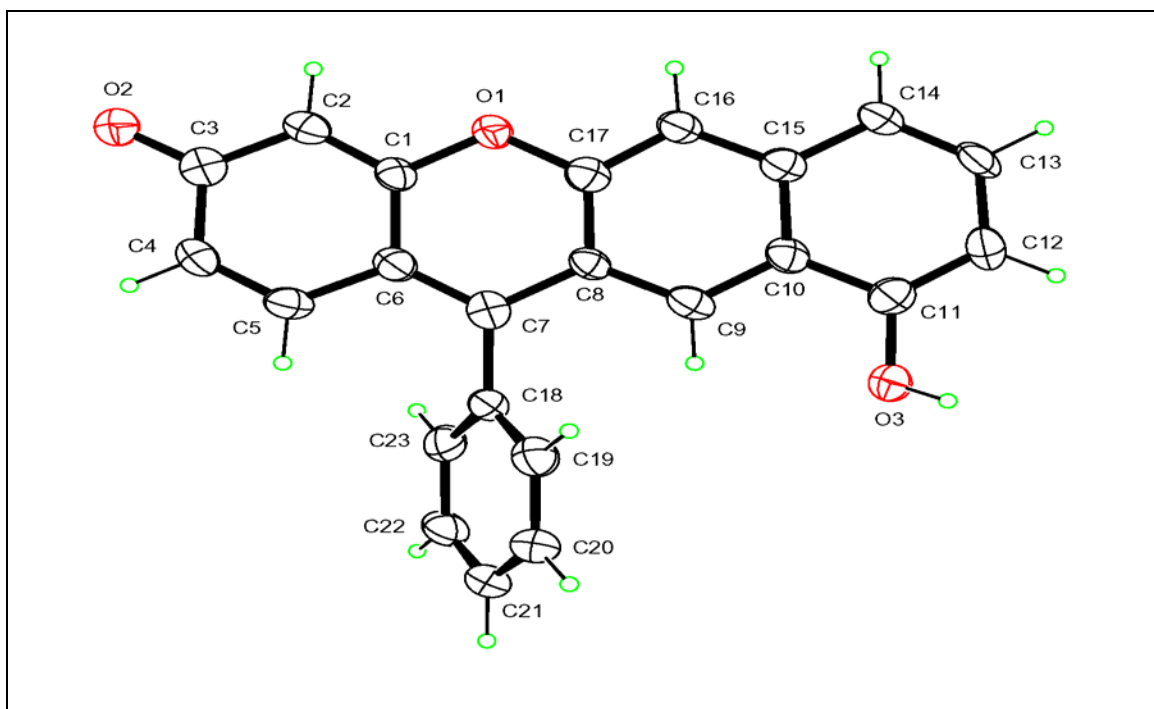


Figure S36. Ortep drawing of 13.

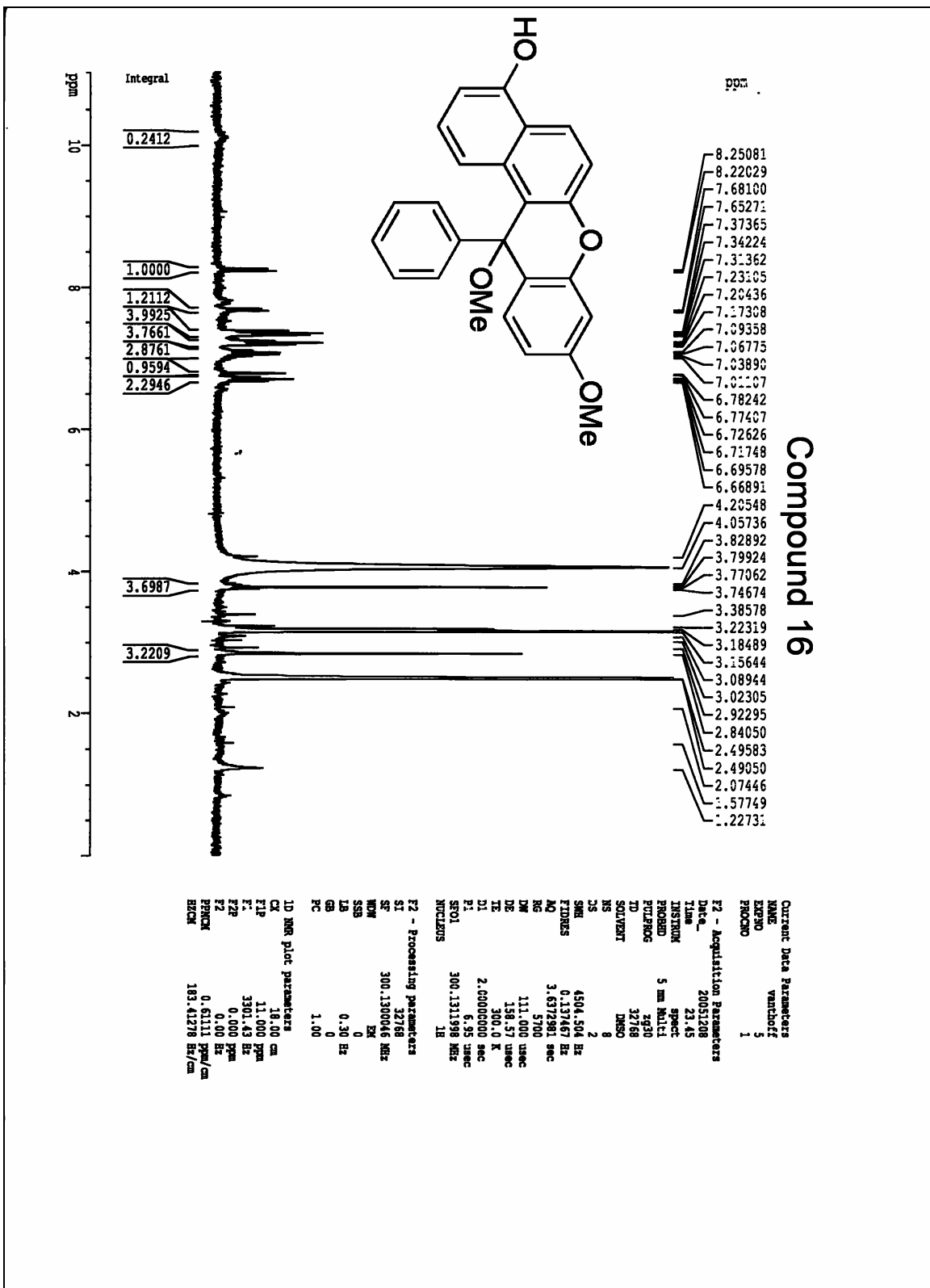
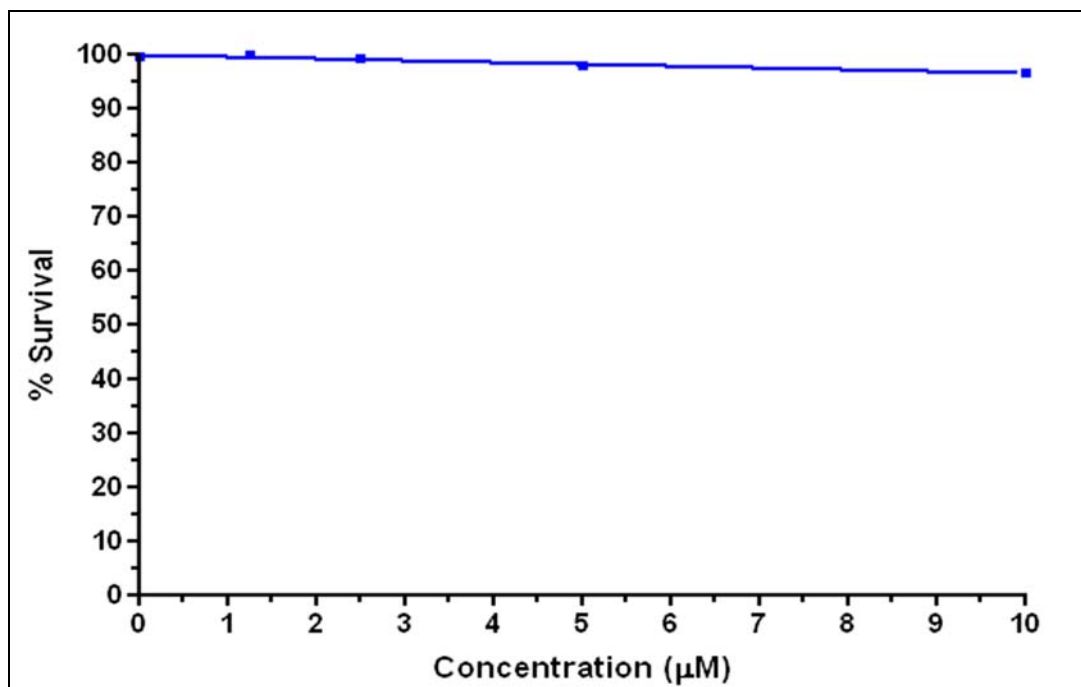
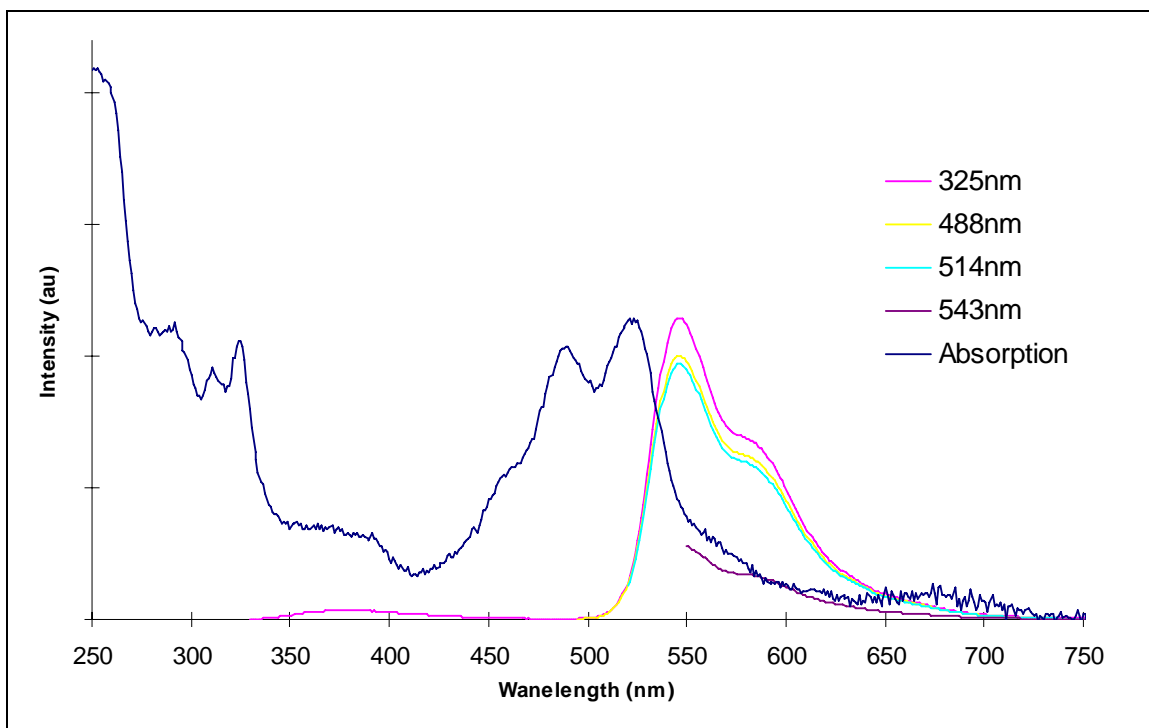


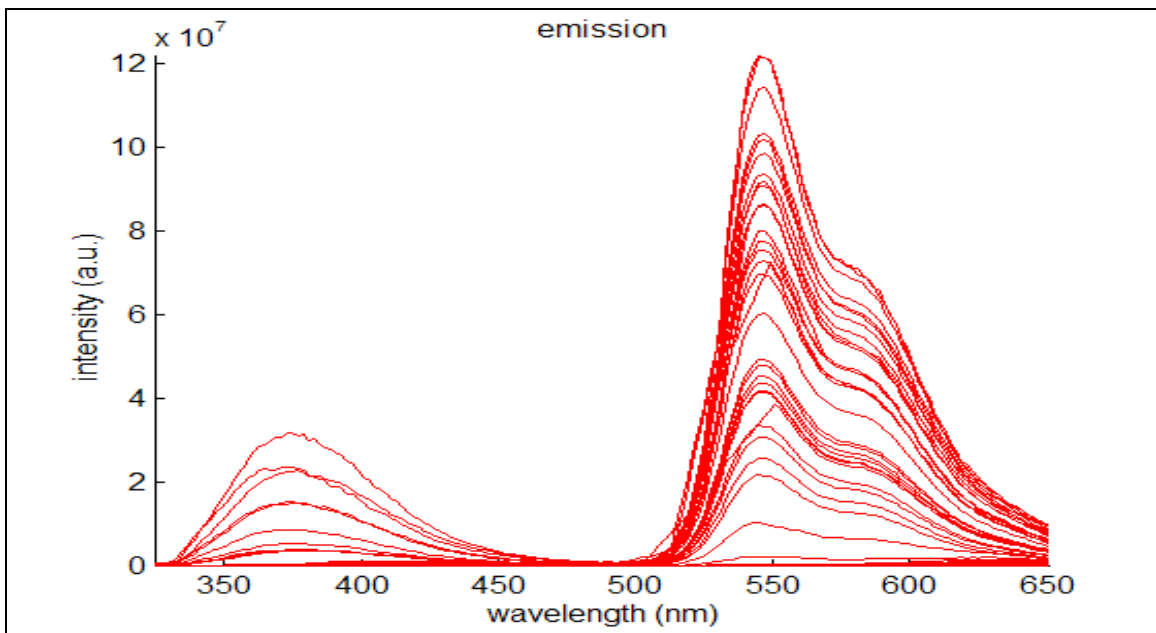
Figure S37. <sup>1</sup>H NMR of 16.



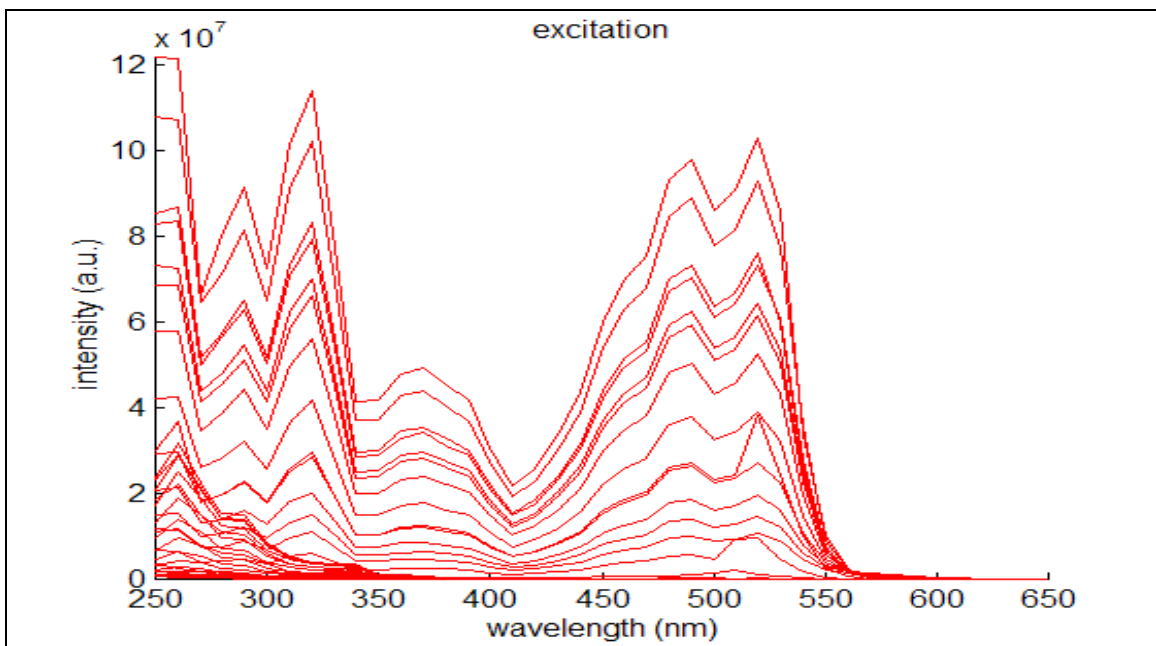
**Figure S38.** Cytotoxicity Study of SNAFR-1. Cells were loaded overnight at the concentrations indicated. Negative control (100% kill) was achieved by adding Saponin to 0.1% and 0 uM was used as 100% Viable for standardization purposes. Triplicates of each concentration were run. Error bars are not visible at the scale of the graph. Viability was measured using the CellTiter Blue Cell Viability Kit from Promega.



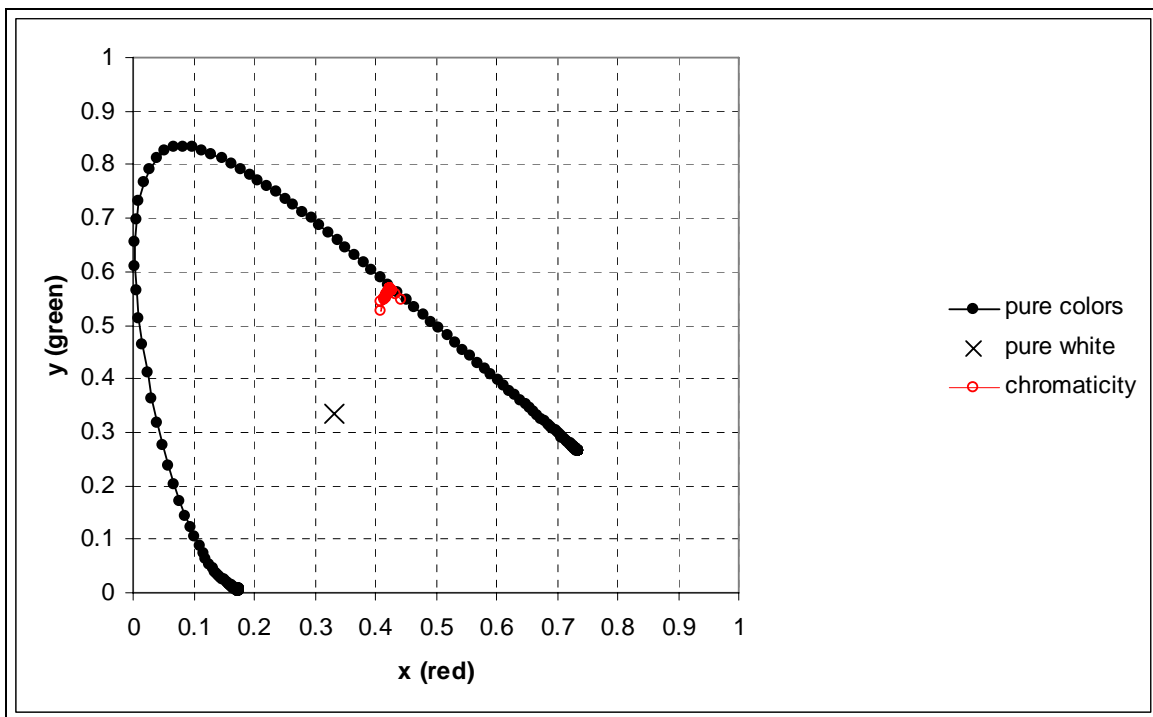
**Figure S39.** Absorption spectrum of 30 µM SNAFR-1 in MeOH and emission spectra excited at wavelengths corresponding to common laser lines. UV-Vis absorption spectrum normalized to emission spectra.



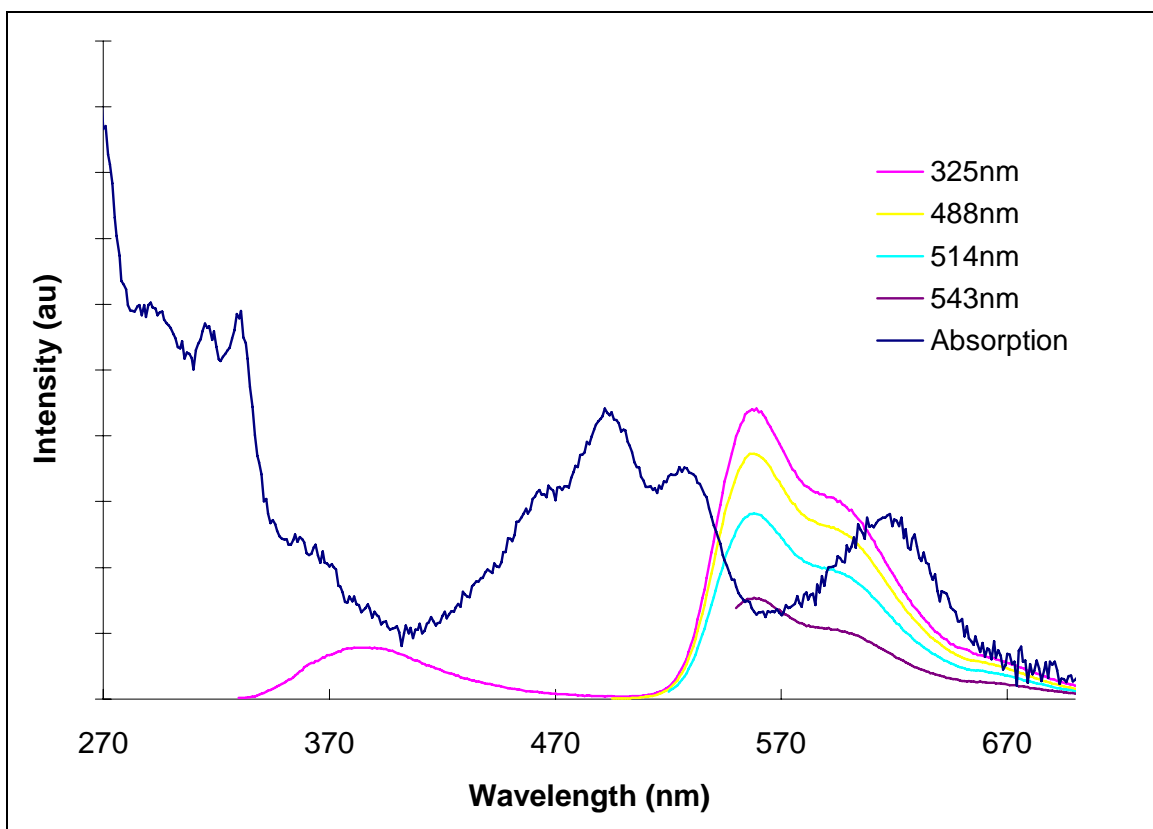
**Figure S40.** Emission of 30  $\mu\text{M}$  SNAFR-1 as a function of excitation in MeOH.



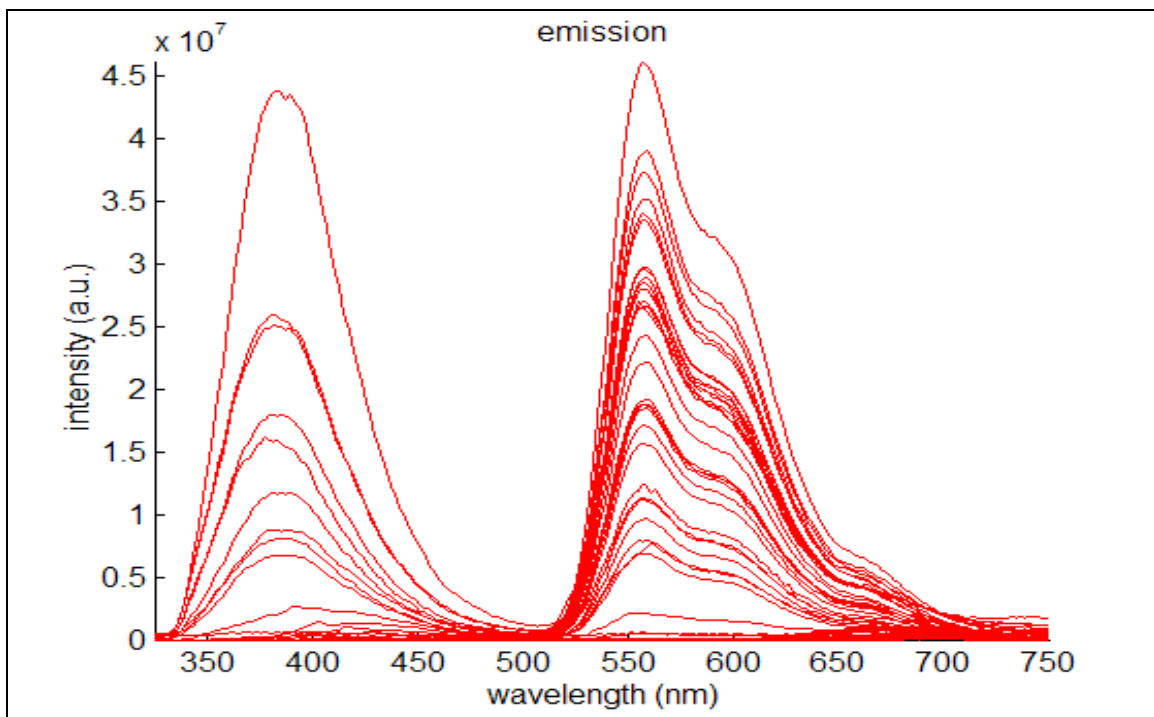
**Figure S41.** Excitations of 30  $\mu\text{M}$  SNAFR-1 as a function of emission in MeOH.



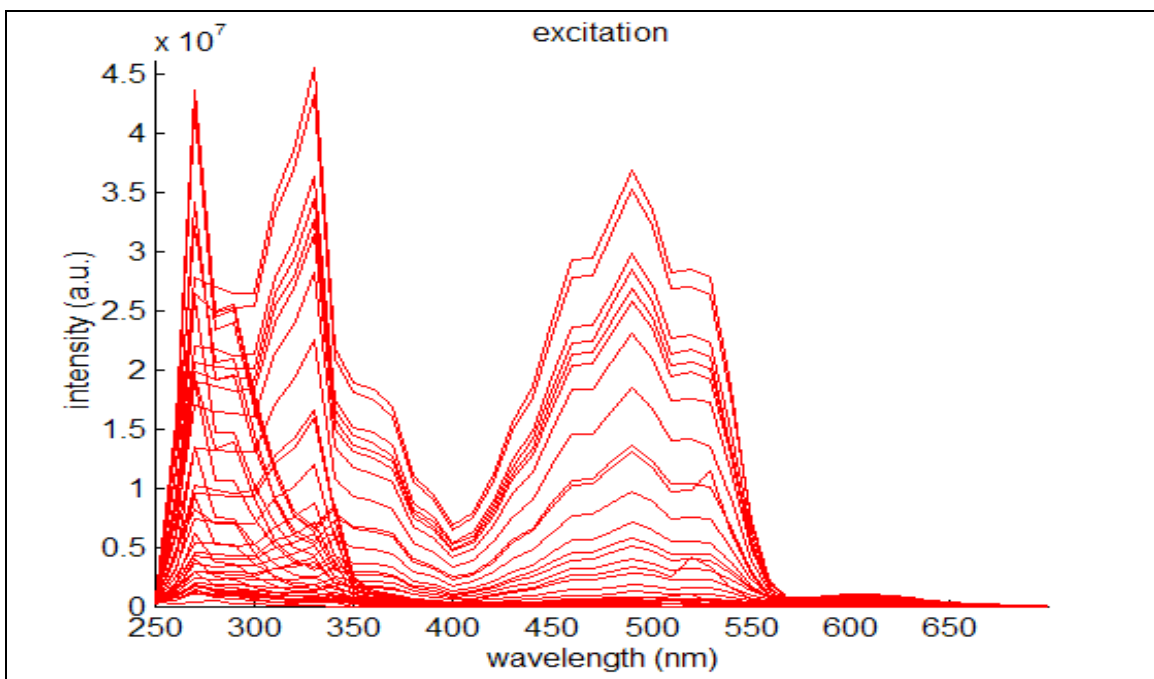
**Figure S42.** Chromaticity diagram of 30  $\mu\text{M}$  SNAFR-1 in MeOH with excitation wavelength between 260 nm and 550 nm plotted in a 1931 CIE diagram.



**Figure S43.** Absorption spectrum of 30  $\mu\text{M}$  SNAFR-1 in DMSO and emission spectra excited at wavelengths corresponding to common laser lines. UV-Vis absorption spectrum normalized to emission spectra.

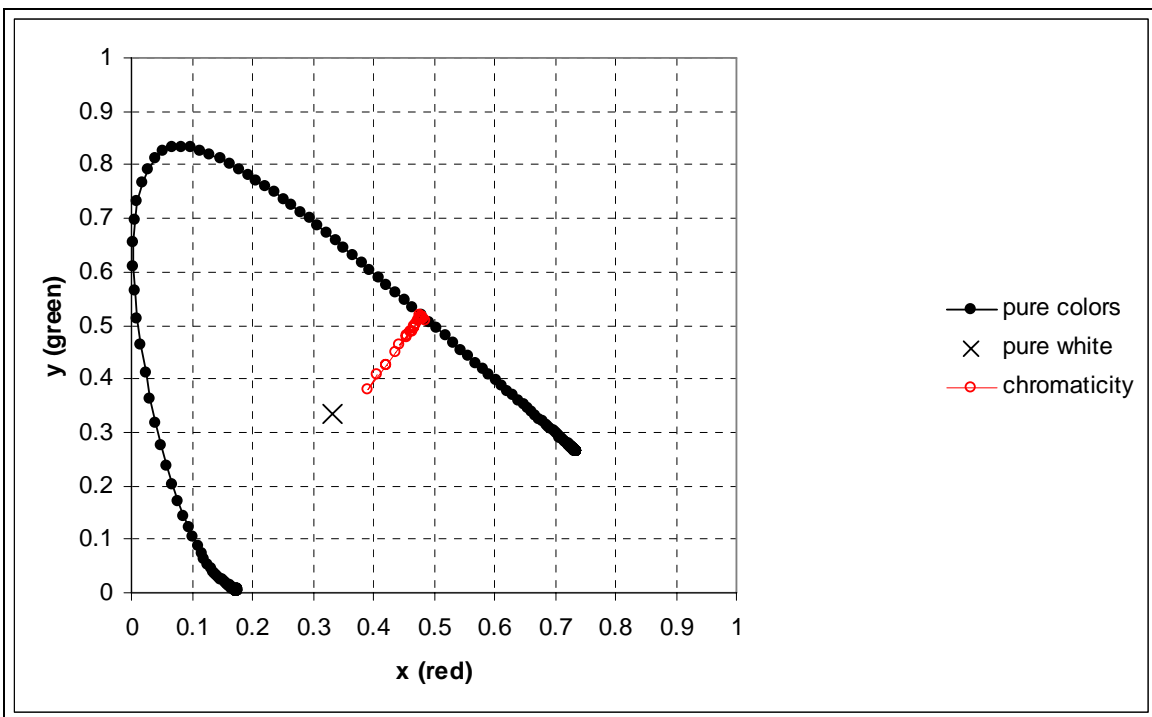


**Figure S44.** Emission of 30  $\mu\text{M}$  SNAFR-1 as a function of excitation in DMSO.

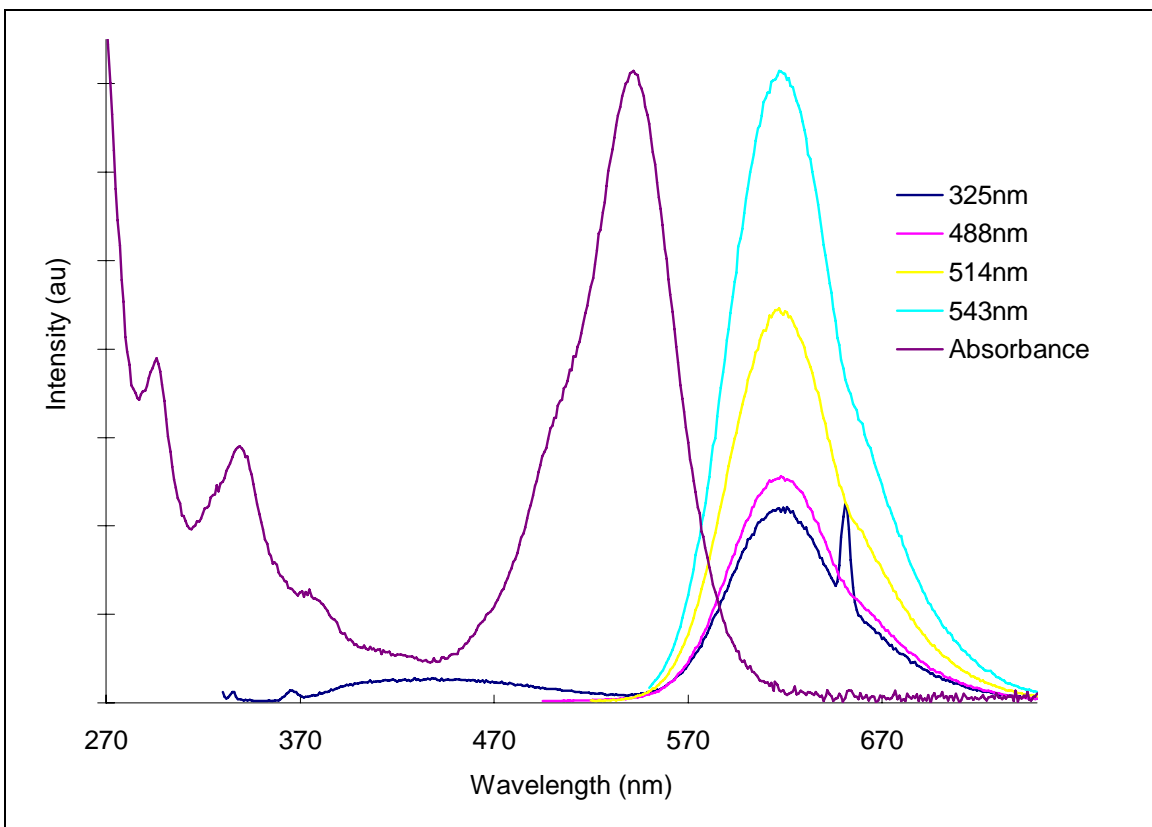


**Figure S45.** Excitation of 30  $\mu\text{M}$  SNAFR-1 as a function of emission in DMSO.

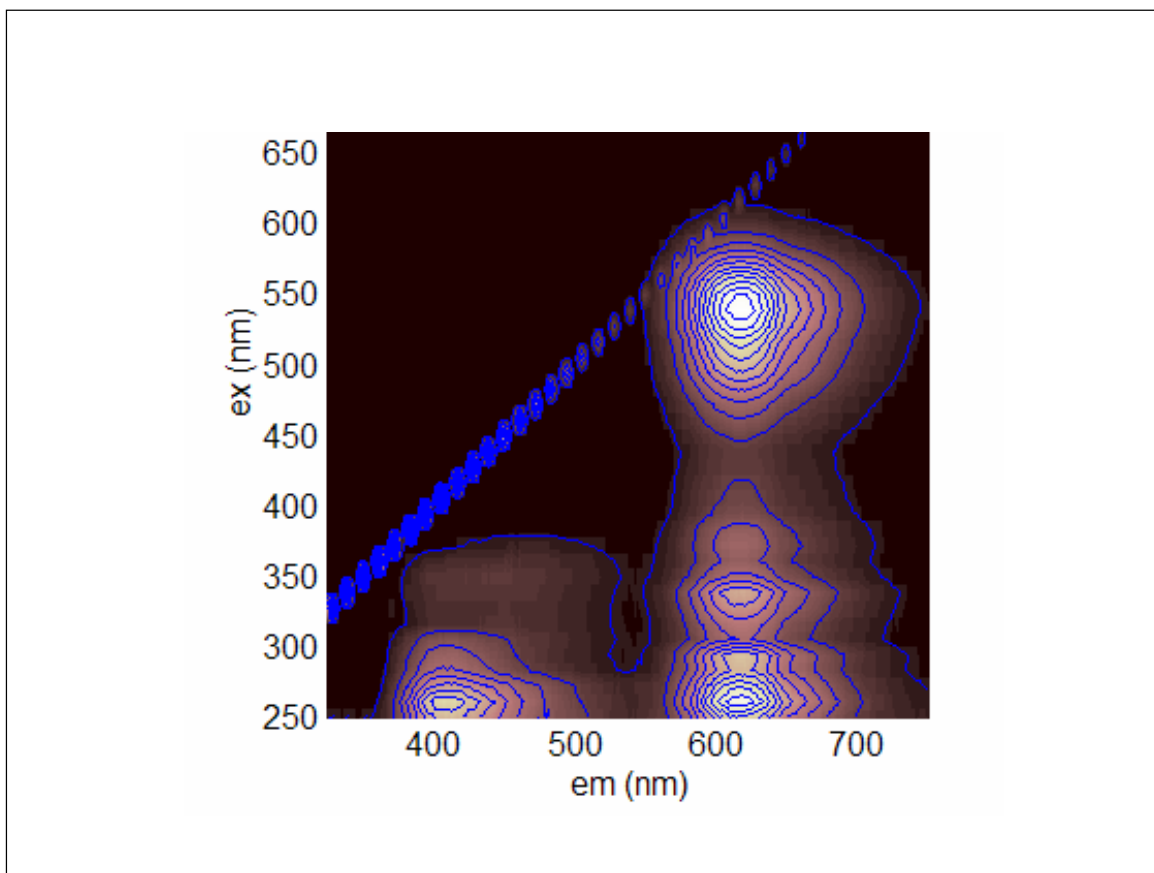




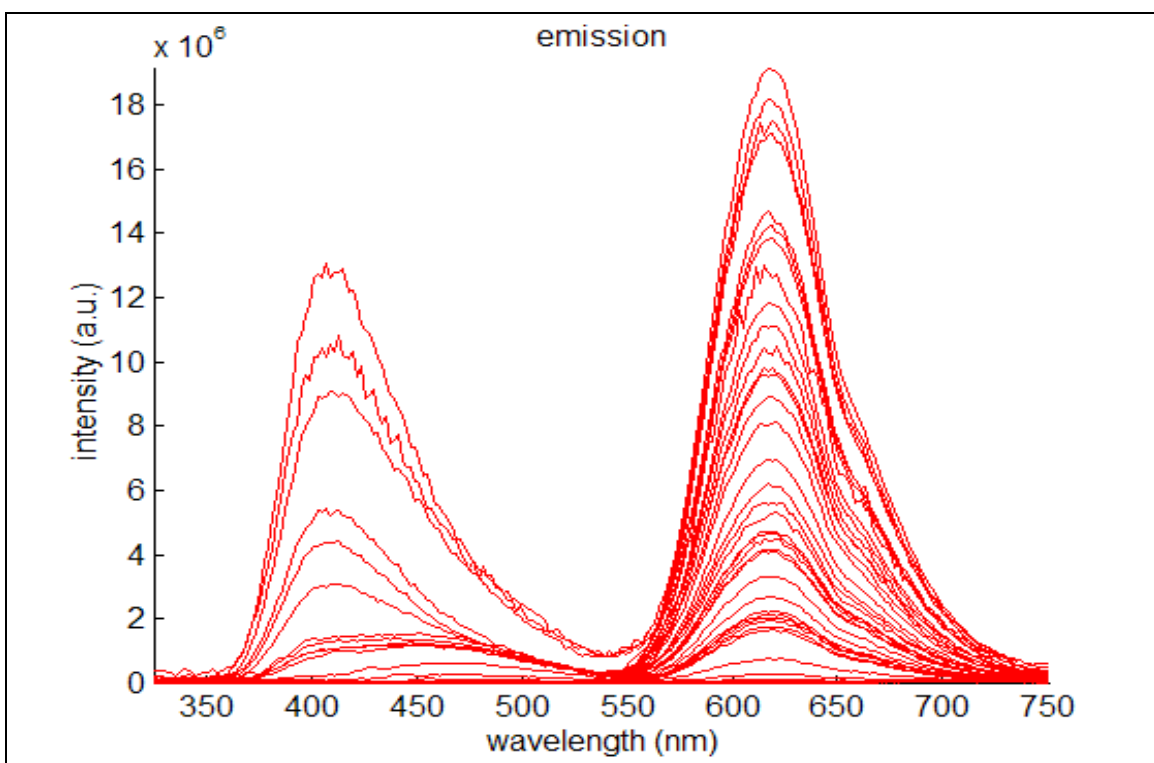
**Figure S46.** Chromaticity diagram of 30  $\mu\text{M}$  **SNAFR-1** in DMSO with excitation wavelength between 260 nm and 550 nm plotted in a 1931 CIE diagram.



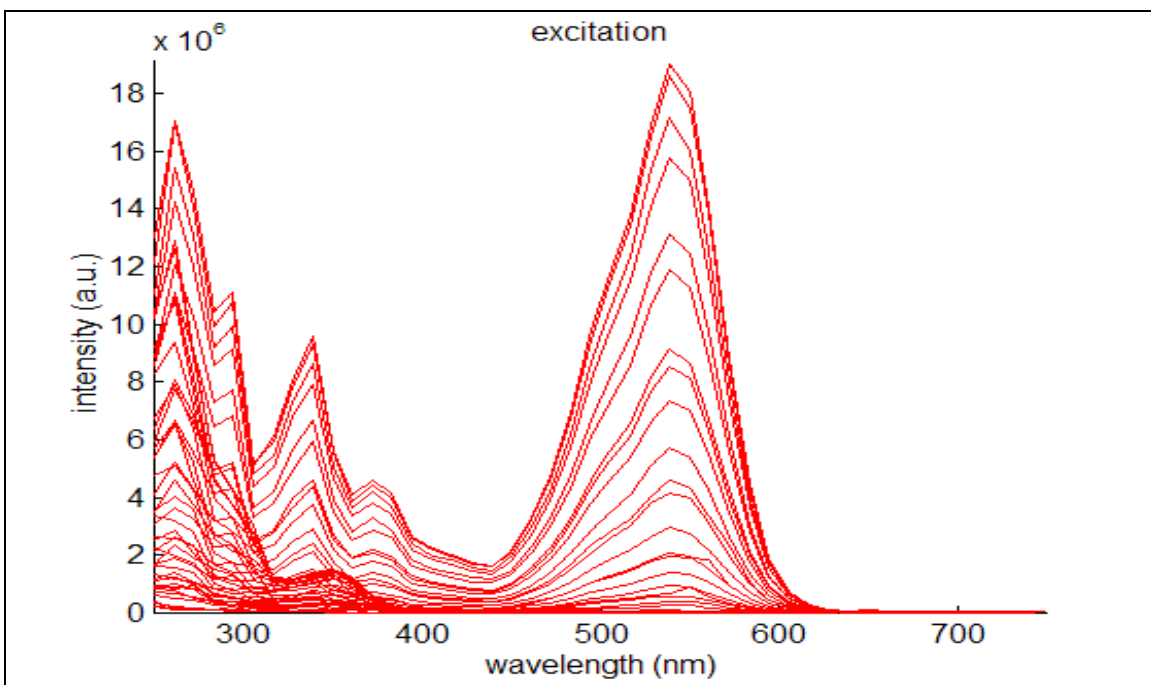
**Figure S47.** Absorption spectrum of 30  $\mu\text{M}$  **SNAFR-1** in 0.1M NaOH and emission spectra excited at wavelengths corresponding to common laser lines. UV-Vis absorption spectrum normalized to emission spectra.



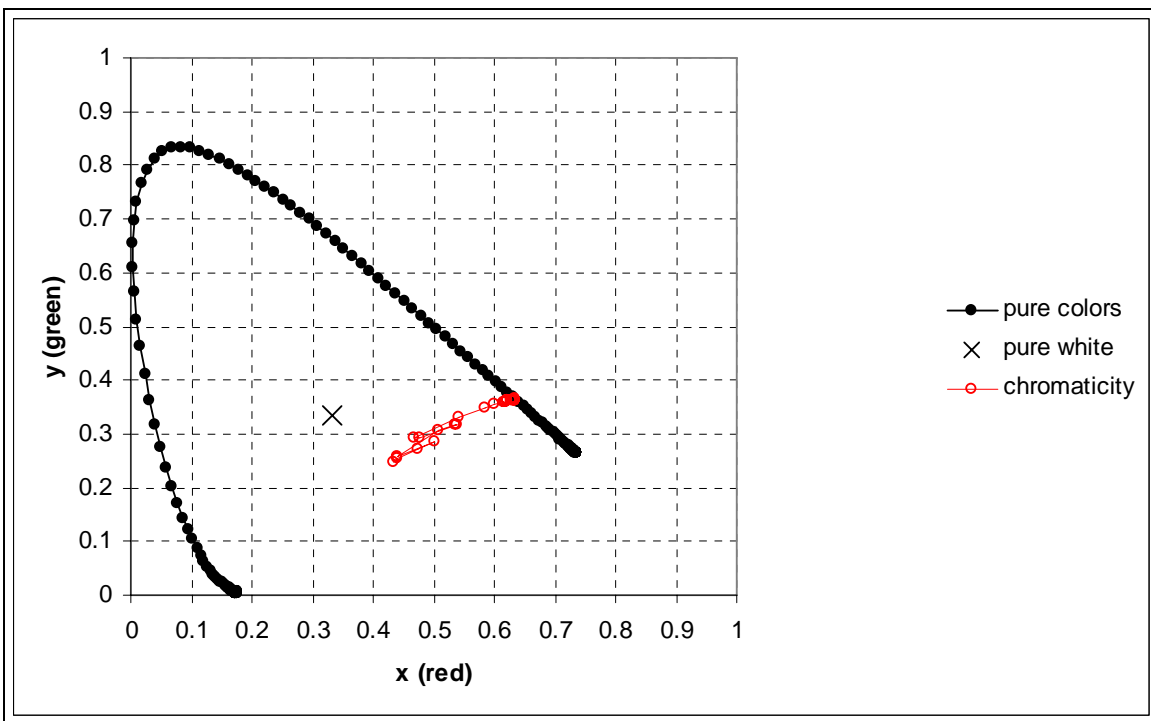
**Figure S48.** EEM of 30  $\mu\text{M}$  SNAFR-1 in 0.1 M NaOH.



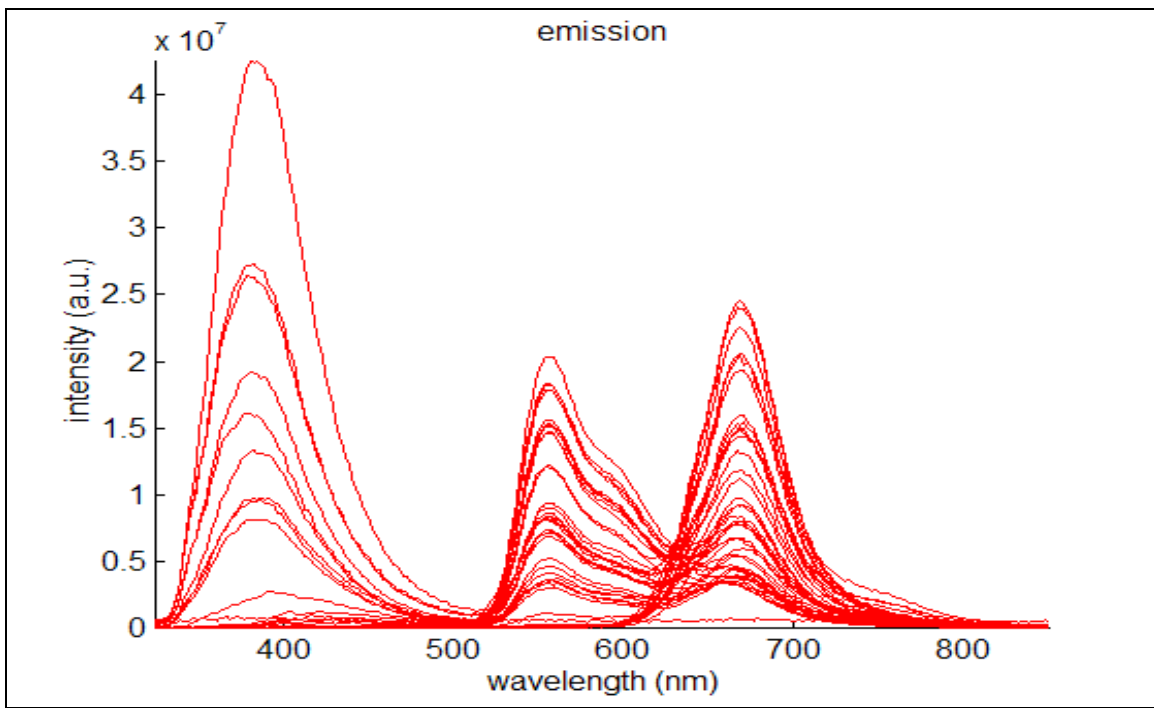
**Figure S49.** Emission of 30  $\mu\text{M}$  SNAFR-1 as a function of excitation in 0.1 M NaOH.



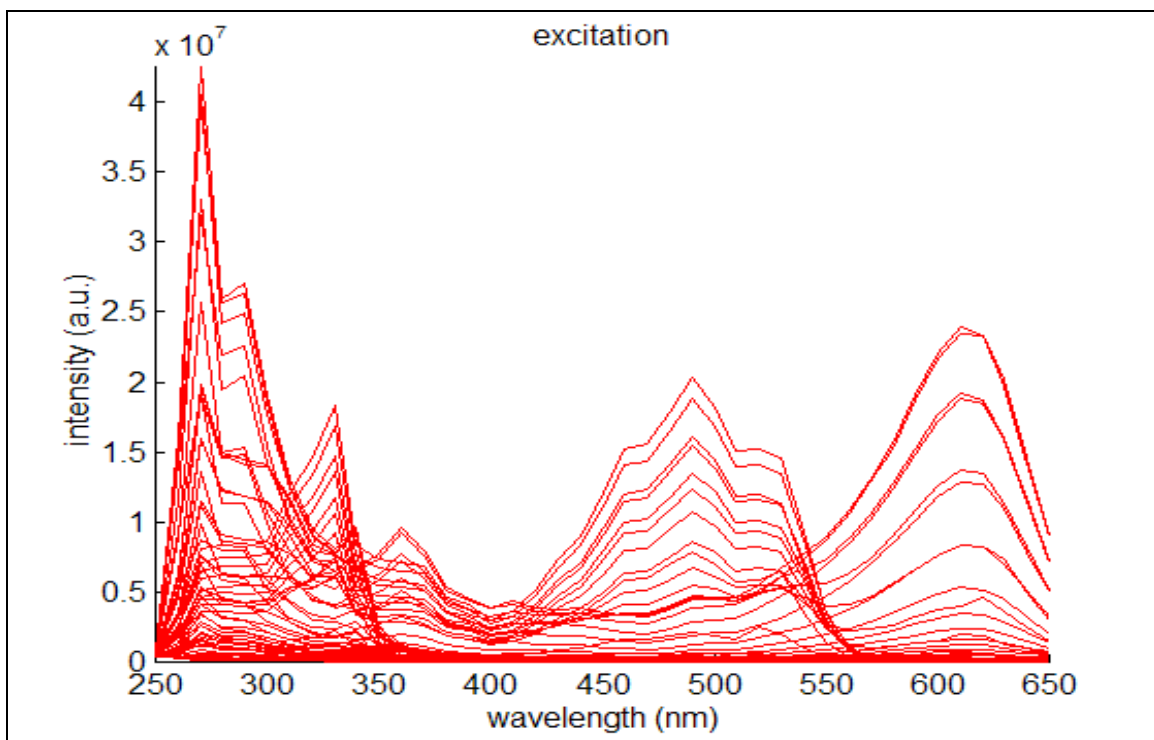
**Figure S50.** Excitation of 30  $\mu\text{M}$  SNAFR-1 as a function of emission in 0.1 M NaOH.



**Figure S51.** Chromaticity diagram of 30  $\mu\text{M}$  SNAFR-1 in 0.1 M NaOH with excitation wavelength between 260 nm and 600 nm plotted in a 1931 CIE diagram.



**Figure S52.** Emission of 30  $\mu\text{M}$  SNAFR-1 as a function of excitation in DMSO with 0.25% phosphate buffer pH 7.



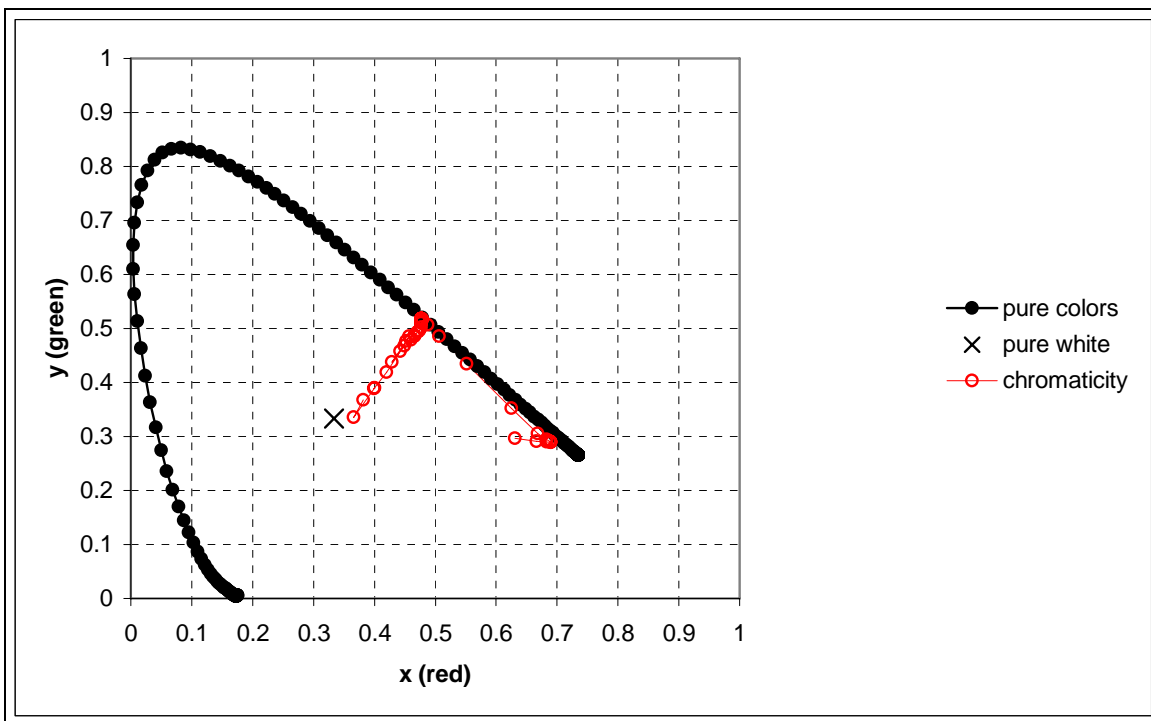
**Figure S53.** Excitation of 30  $\mu\text{M}$  SNAFR-1 as a function of Emission in DMSO with 0.25% phosphate buffer pH 7.

**Table S1.** Apparent  $pK_a$  values calculated for **SNFR-1** in DMSO with 0.25% phosphate buffer (50mM).

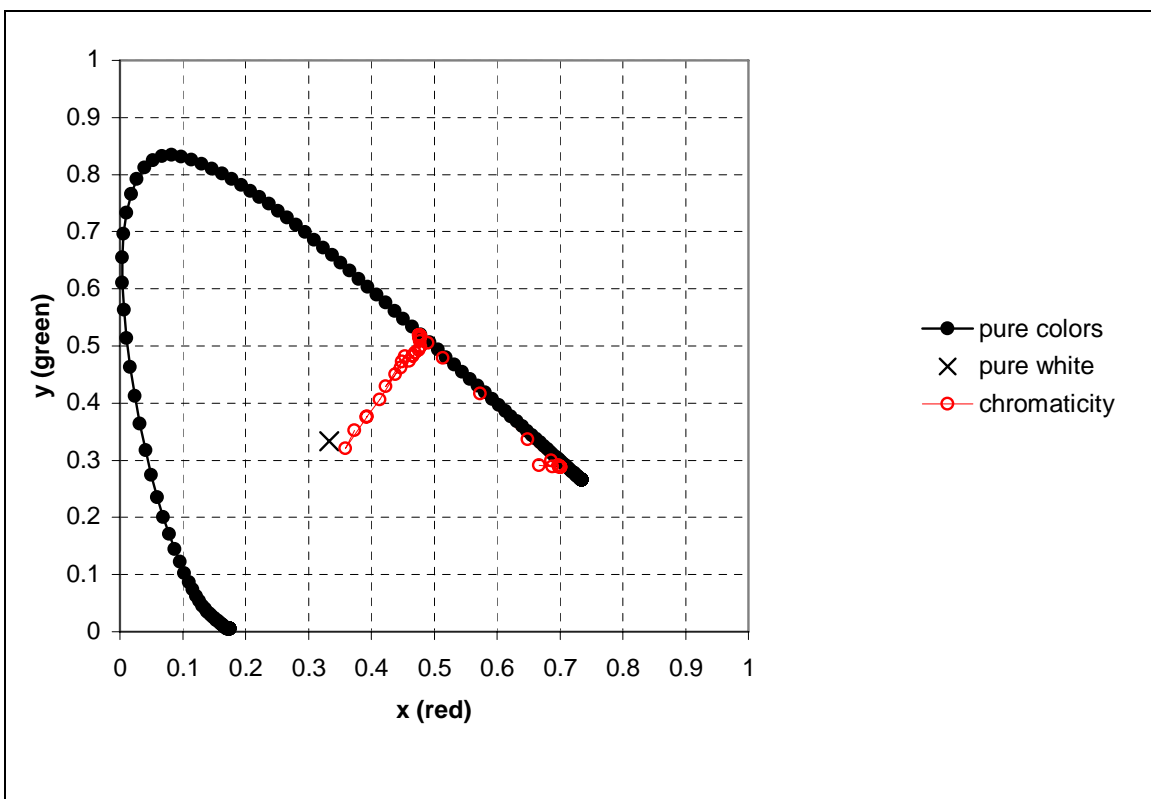
Method	$\lambda_{ex}$	$\lambda_1/\lambda_2$	$R_{max}$	$R_{min}$	$pK_a$
Em	325	670/656	1.22	0.91	5.93
Em	325	592/656	2.87	0.53	5.92
Em	325	559/656	4.31	0.96	5.97
Em	514	678/660	1.01	0.75	5.93
Em	514	592/660	2.89	0.53	5.92
Em	514	559/660	4.27	0.94	5.97
Em	543	674/637	2.75	1.13	5.99
Em	543	592/637	1.60	0.24	5.91
Em	543	558/637	2.33	0.43	5.96
Abs		614/538	3.95	1.14	5.94
Abs		520/538	1.14	0.69	5.96
Abs		493/538	1.48	0.56	5.93
Abs		467/538	1.05	0.40	5.96
Abs		520/427	2.39	1.53	6.09
Abs		493/427	3.09	1.25	5.99
Abs		466/427	2.19	0.89	6.02
Abs		411/427	1.13	0.70	5.96
Abs		362/427	2.11	1.60	6.03
Abs		362/345	1.14	0.84	6.10
Abs		330/345	2.23	1.34	5.96
Abs		330/311	1.10	0.64	5.99
Abs		296/311	1.37	1.13	6.05

**Table S2.** Chromaticity coordinates of 30  $\mu\text{M}$  SNAFR-1 in DMSO with 0.25% phosphate buffer (50 mM) as a function of excitation wavelength and added buffer pH.

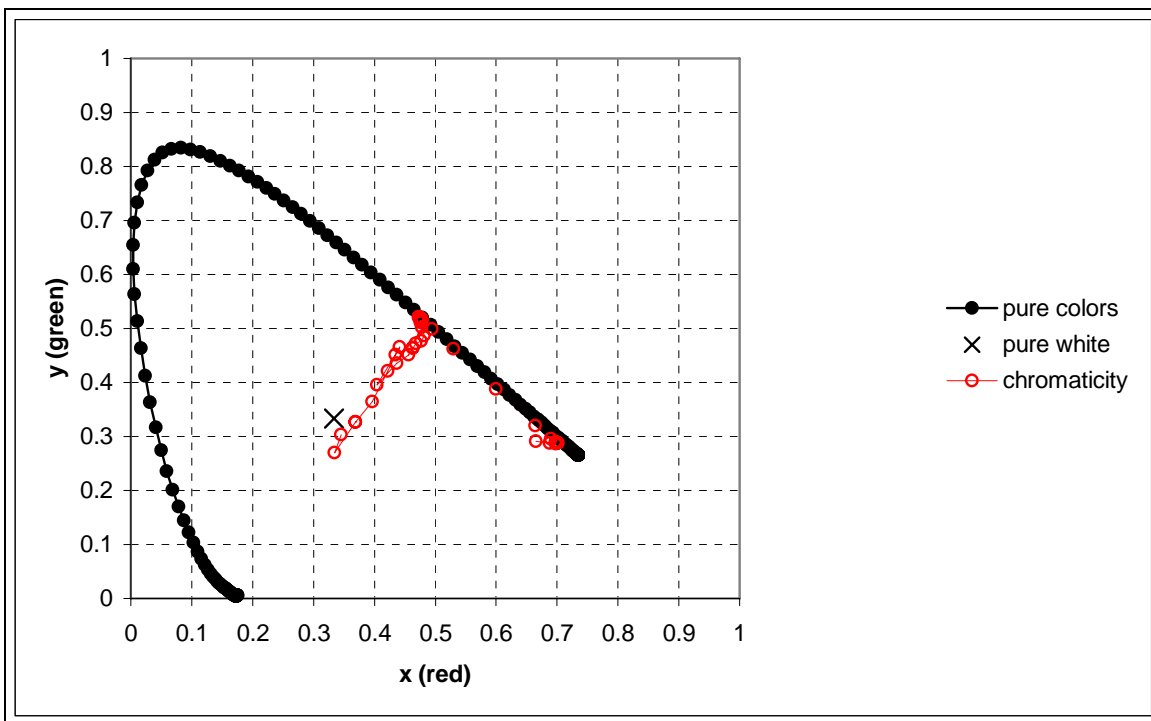
$\lambda_{\text{ex}}$	pH 4		pH 5		pH 6		pH 7		pH 8	
	x	y	x	y	x	y	x	y	x	y
270	0.37	0.34	0.36	0.32	0.33	0.27	0.36	0.30	0.30	0.18
280	0.40	0.39	0.39	0.38	0.37	0.33	0.36	0.30	0.33	0.23
290	0.40	0.39	0.39	0.38	0.37	0.33	0.39	0.34	0.33	0.22
300	0.42	0.42	0.41	0.41	0.40	0.36	0.41	0.40	0.36	0.25
310	0.44	0.46	0.44	0.45	0.42	0.42	0.43	0.44	0.38	0.31
320	0.45	0.48	0.45	0.47	0.43	0.45	0.43	0.46	0.39	0.36
330	0.46	0.49	0.45	0.48	0.44	0.47	0.40	0.38	0.39	0.38
340	0.43	0.44	0.42	0.43	0.40	0.40	0.44	0.43	0.35	0.28
350	0.45	0.47	0.45	0.46	0.44	0.44	0.46	0.44	0.42	0.33
360	0.46	0.48	0.46	0.47	0.46	0.45	0.46	0.46	0.46	0.36
370	0.47	0.49	0.47	0.48	0.46	0.46	0.46	0.46	0.47	0.38
380	0.47	0.49	0.47	0.48	0.46	0.46	0.47	0.47	0.47	0.37
390	0.47	0.49	0.47	0.49	0.47	0.47	0.48	0.47	0.47	0.39
400	0.47	0.50	0.48	0.49	0.48	0.48	0.48	0.48	0.49	0.39
410	0.48	0.50	0.48	0.50	0.48	0.49	0.48	0.50	0.50	0.41
420	0.48	0.51	0.48	0.51	0.48	0.50	0.47	0.51	0.49	0.44
430	0.48	0.51	0.48	0.51	0.48	0.51	0.47	0.52	0.48	0.47
440	0.48	0.52	0.48	0.52	0.48	0.52	0.47	0.52	0.48	0.49
450	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52	0.47	0.51
460	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52	0.46	0.53
470	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52	0.46	0.53
480	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52	0.46	0.53
490	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52	0.47	0.53
500	0.48	0.52	0.48	0.52	0.48	0.52	0.47	0.52	0.47	0.52
510	0.48	0.52	0.48	0.52	0.48	0.52	0.47	0.52	0.48	0.51
520	0.48	0.52	0.48	0.52	0.48	0.52	0.48	0.52	0.49	0.50
530	0.48	0.52	0.48	0.52	0.48	0.52	0.49	0.50	0.50	0.49
540	0.49	0.51	0.49	0.51	0.49	0.50	0.53	0.46	0.55	0.44
550	0.51	0.49	0.51	0.48	0.53	0.46	0.60	0.38	0.62	0.36
560	0.55	0.43	0.57	0.42	0.60	0.39	0.67	0.32	0.68	0.31
570	0.62	0.35	0.65	0.34	0.66	0.32	0.69	0.29	0.70	0.29
580	0.67	0.31	0.69	0.30	0.69	0.30	0.70	0.29	0.70	0.29
590	0.68	0.29	0.70	0.29	0.70	0.29	0.70	0.29	0.70	0.29
600	0.69	0.29	0.70	0.29	0.70	0.29	0.70	0.29	0.71	0.29
610	0.69	0.29	0.70	0.29	0.70	0.29	0.70	0.29	0.71	0.29
620	0.69	0.29	0.70	0.29	0.70	0.29	0.70	0.29	0.71	0.29
630	0.68	0.29	0.70	0.29	0.70	0.29	0.69	0.29	0.70	0.29
640	0.67	0.29	0.69	0.29	0.69	0.29	0.66	0.29	0.70	0.29
650	0.63	0.30	0.67	0.29	0.67	0.29	0.66	0.29	0.68	0.29



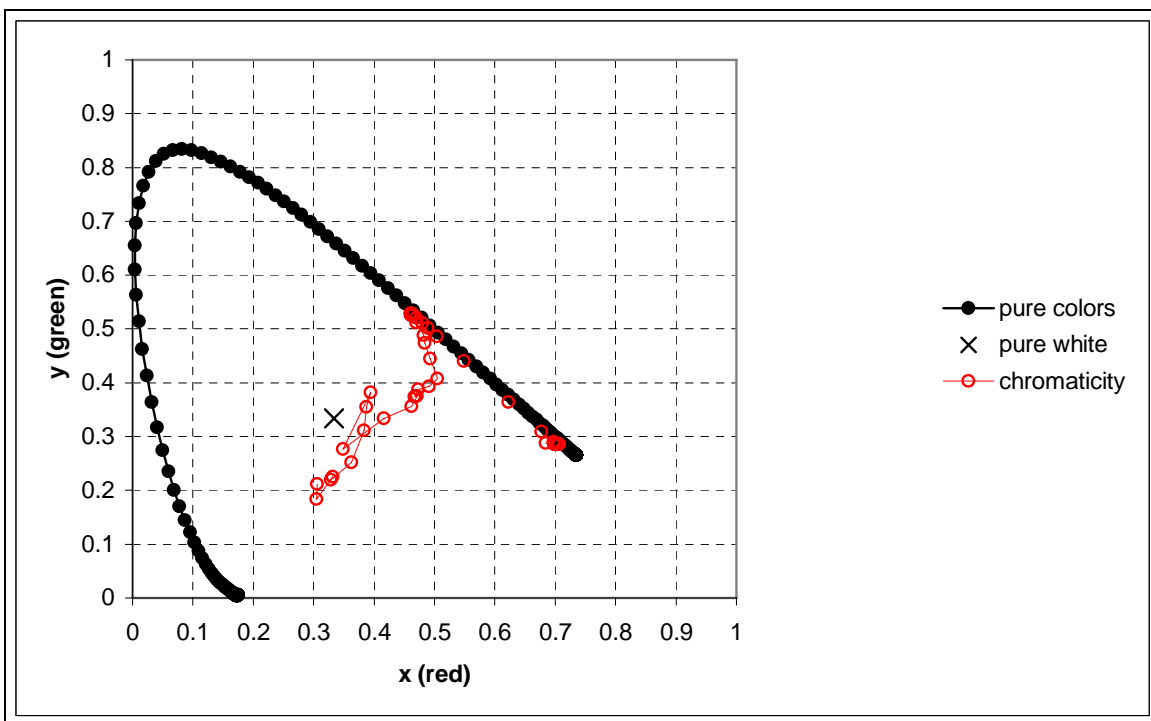
**Figure S54.** Chromaticity coordinates for emissions collected with excitation wavelength between 270 nm and 650 nm plotted in a 1931 CIE diagram for 30  $\mu\text{M}$  **SNAFR-1** in DMSO with 0.25% phosphate buffer (50 mM, pH 4).



**Figure S55.** Chromaticity coordinates for emissions collected with excitation wavelength between 270 nm and 650 nm plotted in a 1931 CIE diagram for 30  $\mu\text{M}$  **SNAFR-1** in DMSO with 0.25% phosphate buffer (50 mM, pH 5).



**Figure S56.** Chromaticity coordinates for emission spectra collected with excitation wavelength between 270 nm and 650 nm plotted in a 1931 CIE diagram for a solution of 30  $\mu\text{M}$  **SNAFR-1** in DMSO with 0.25% phosphate buffer (50 mM, pH 6).



**Figure S57.** Chromaticity coordinates for emission spectra collected with excitation wavelength between 270 nm and 650 nm plotted in a 1931 CIE diagram for a solution of 30  $\mu\text{M}$  **SNAFR-1** in DMSO with 0.25% phosphate buffer (50 mM, pH 8).



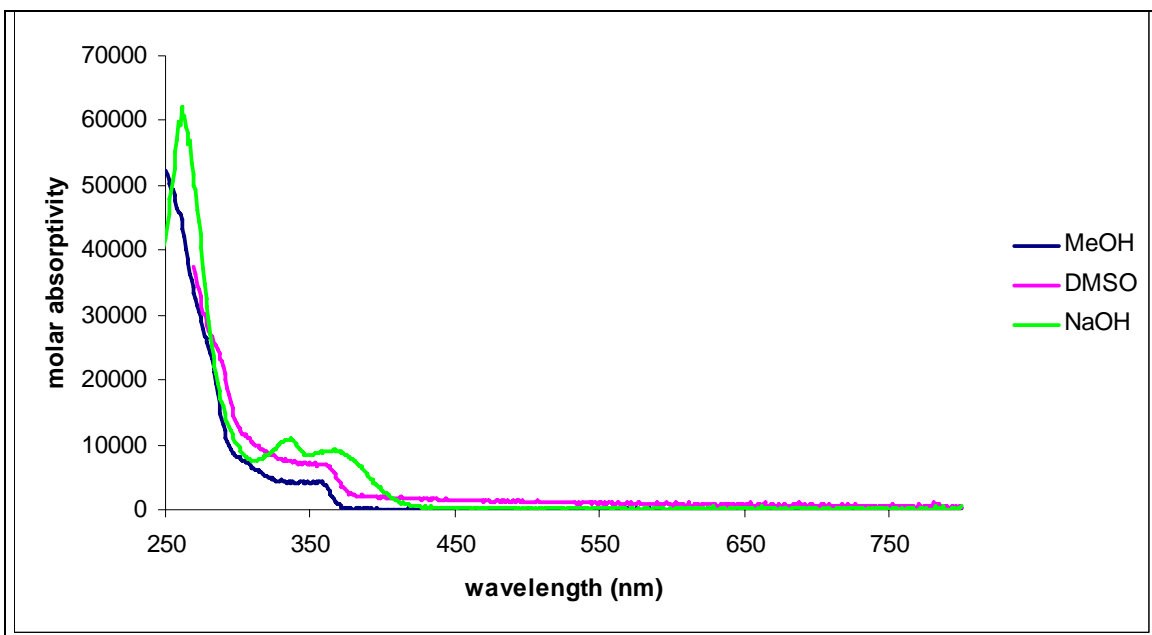


Figure S58. Absorption spectra of **10** in MeOH, DMSO and 0.1 M NaOH.

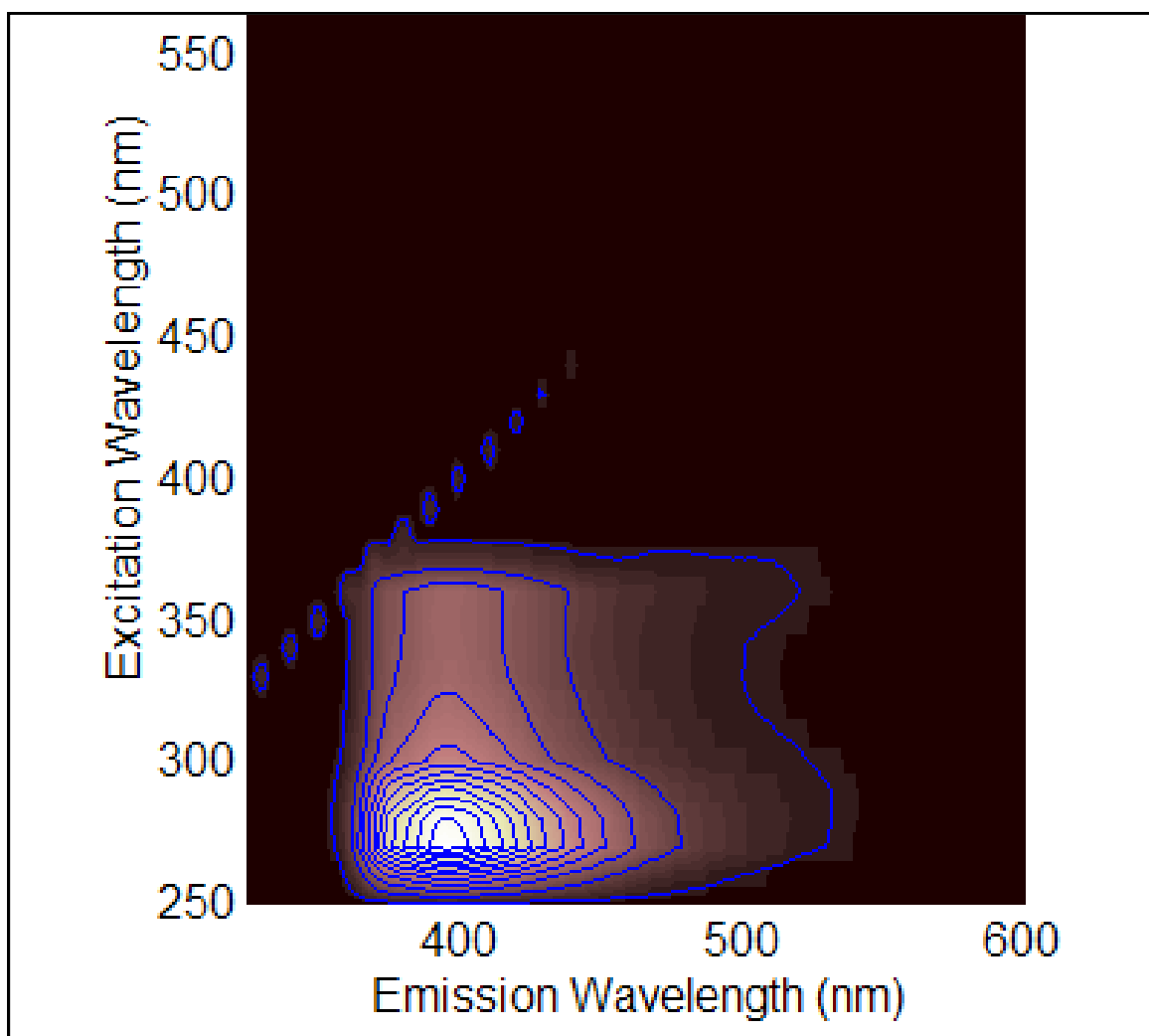
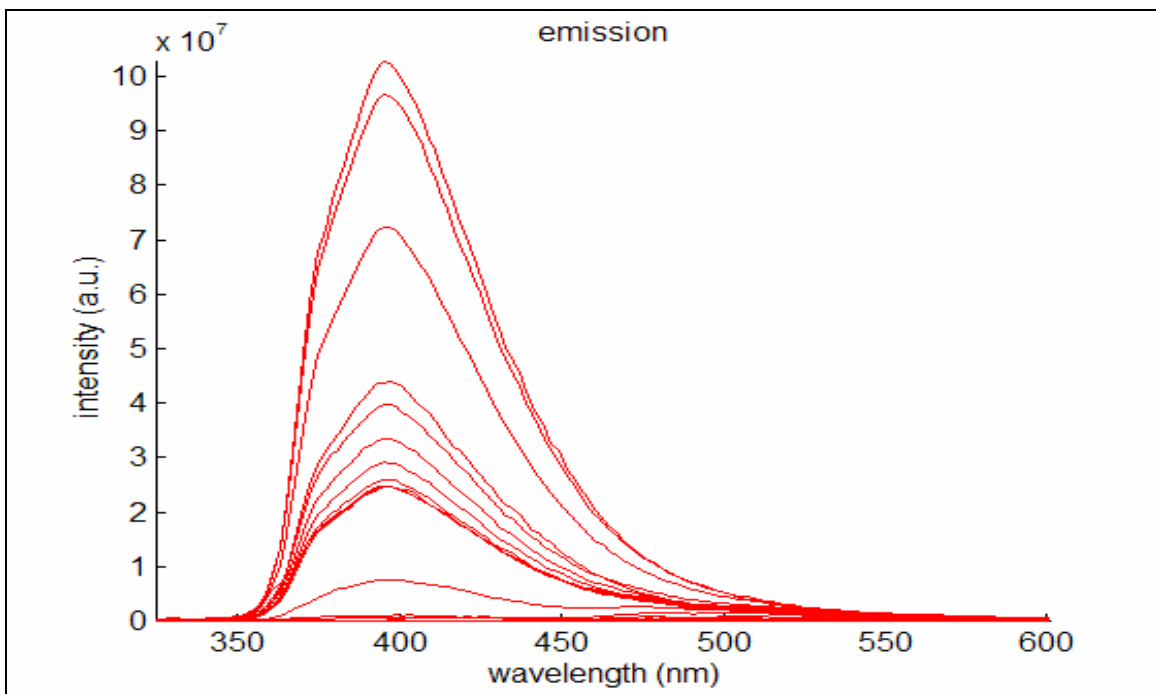
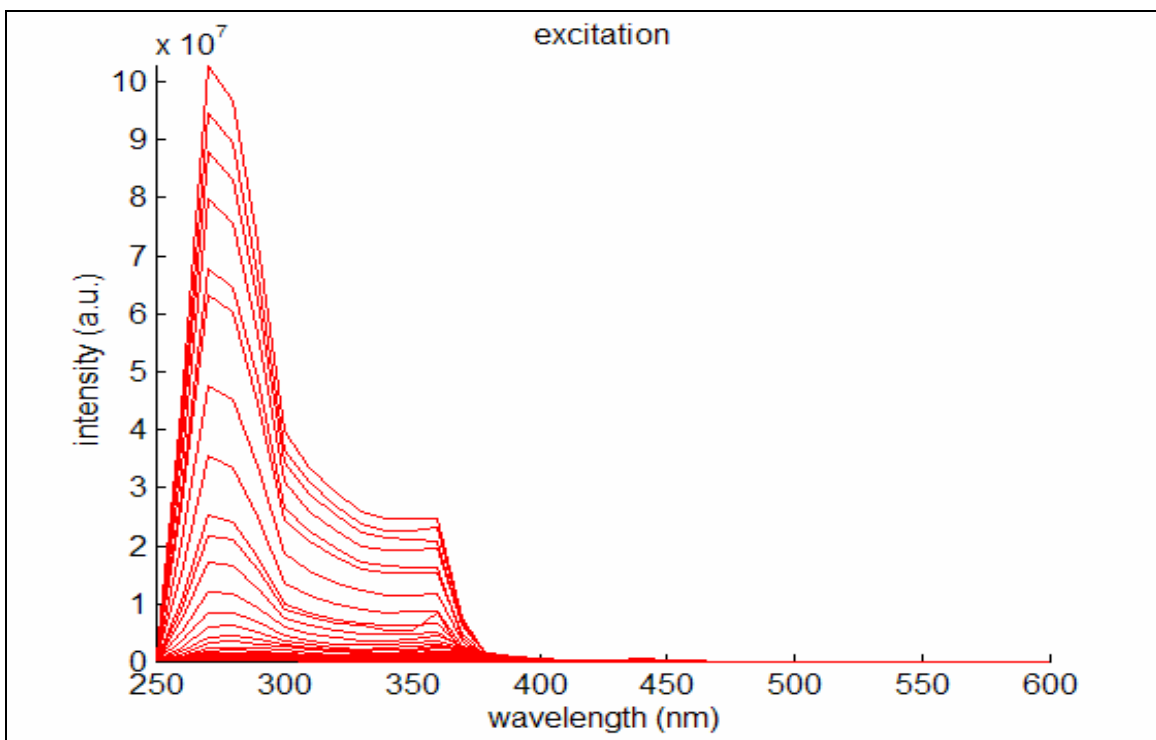


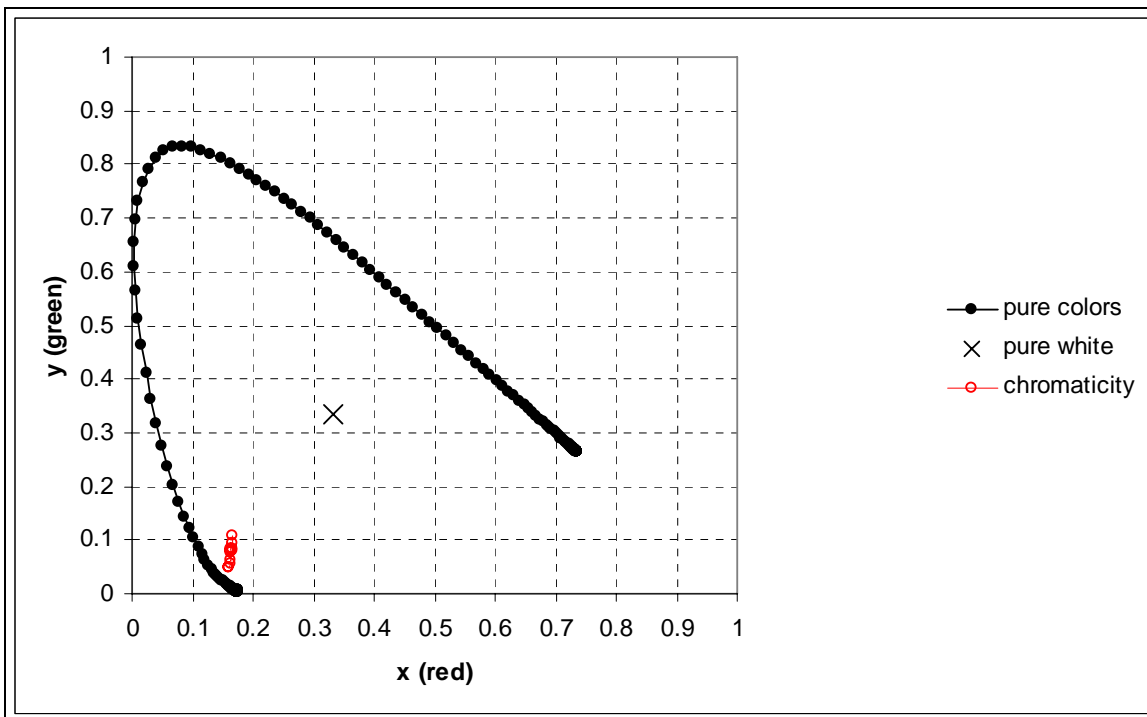
Figure S59. EEM of 10 μM **10** in DMSO.



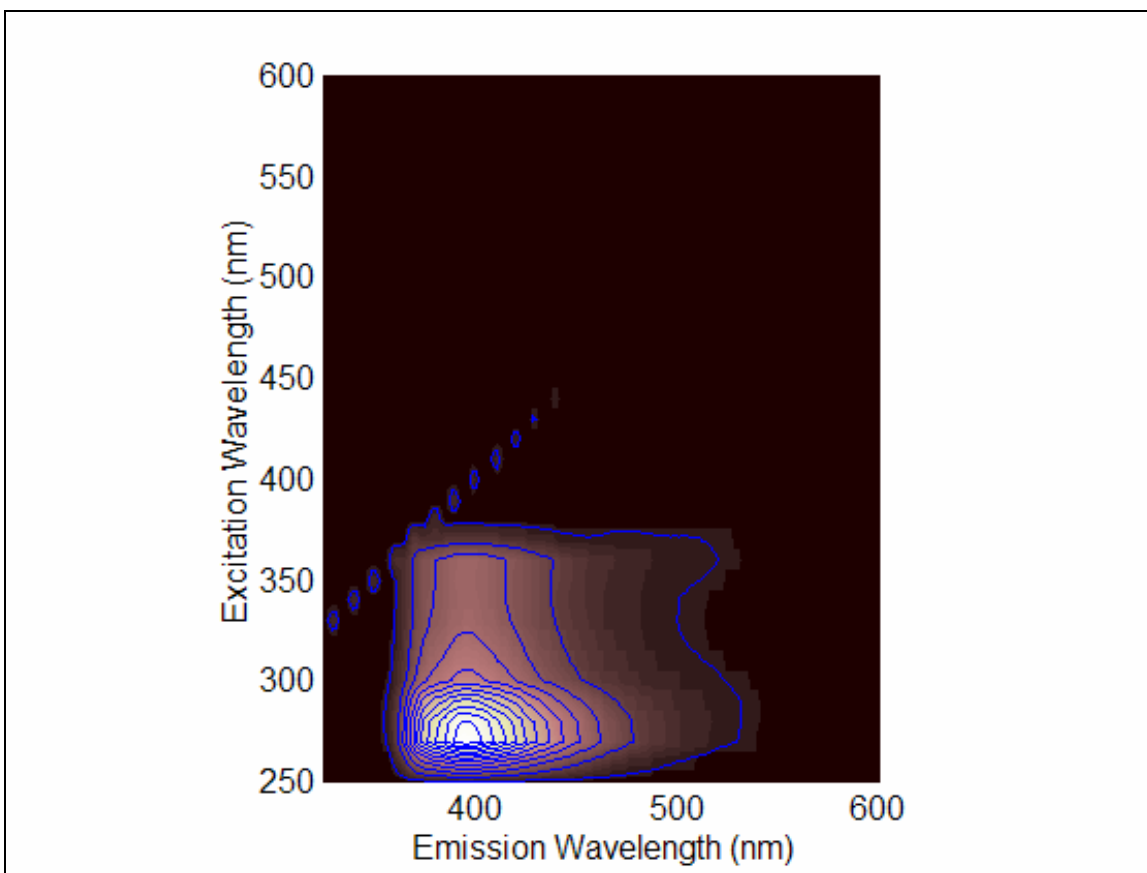
**Figure S60.** Emission of 10  $\mu\text{M}$  **10** as a function of excitation in DMSO.



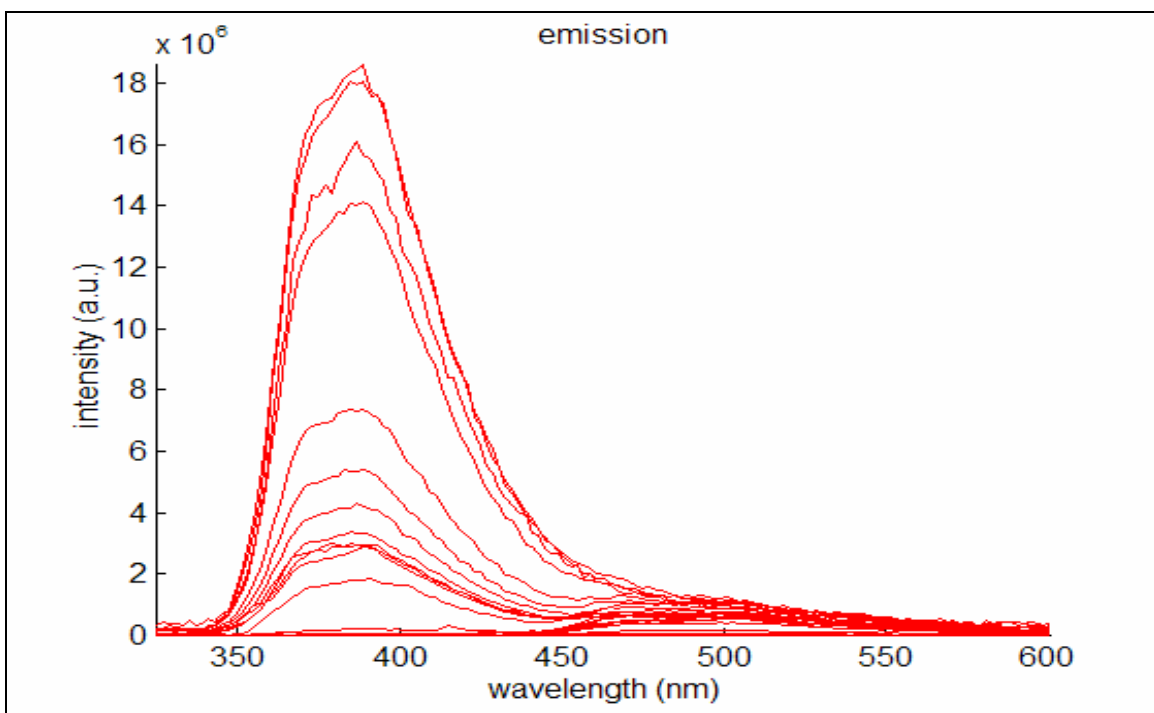
**Figure S61.** Excitation of 10  $\mu\text{M}$  **10** as a function of emission in DMSO.



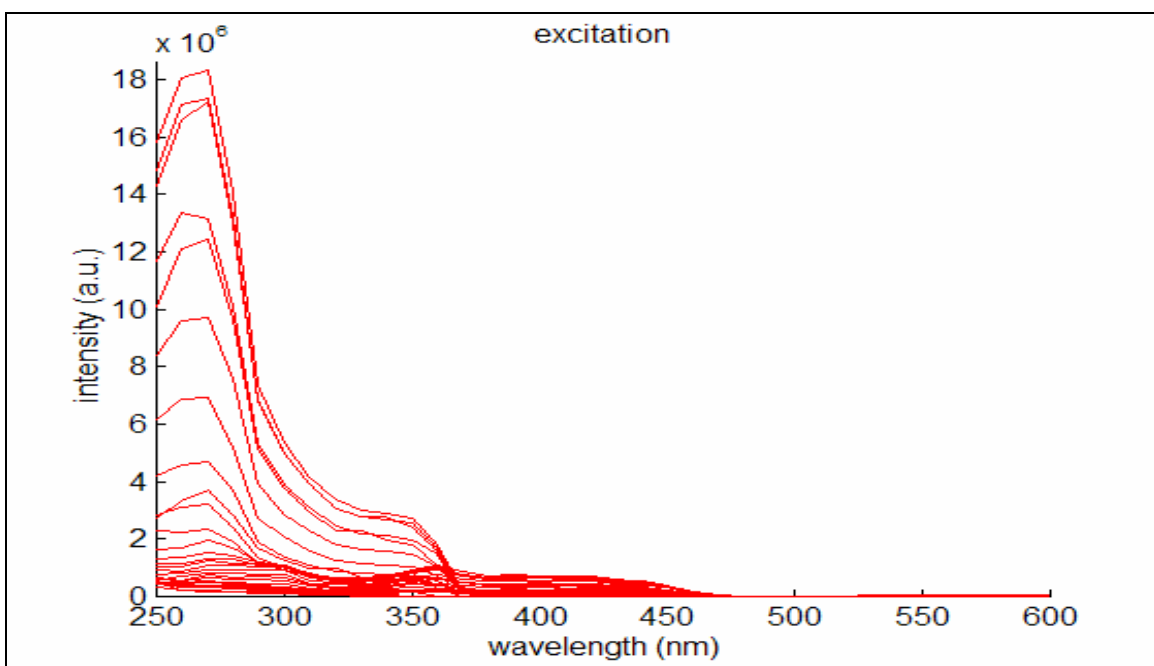
**Figure S62.** Chromaticity diagram of 10  $\mu\text{M}$  **10** in DMSO between 270 nm and 370 nm plotted in a 1931 CIE diagram.



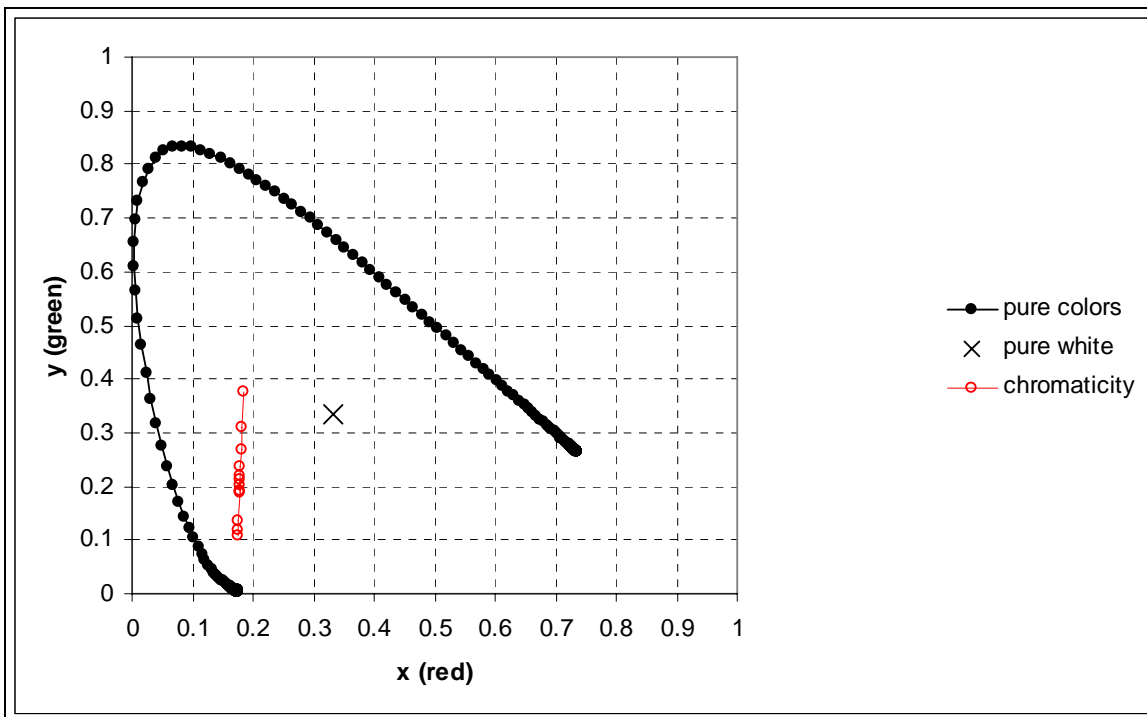
**Figure S63.** EEM of 10  $\mu\text{M}$  **10** in MeOH.



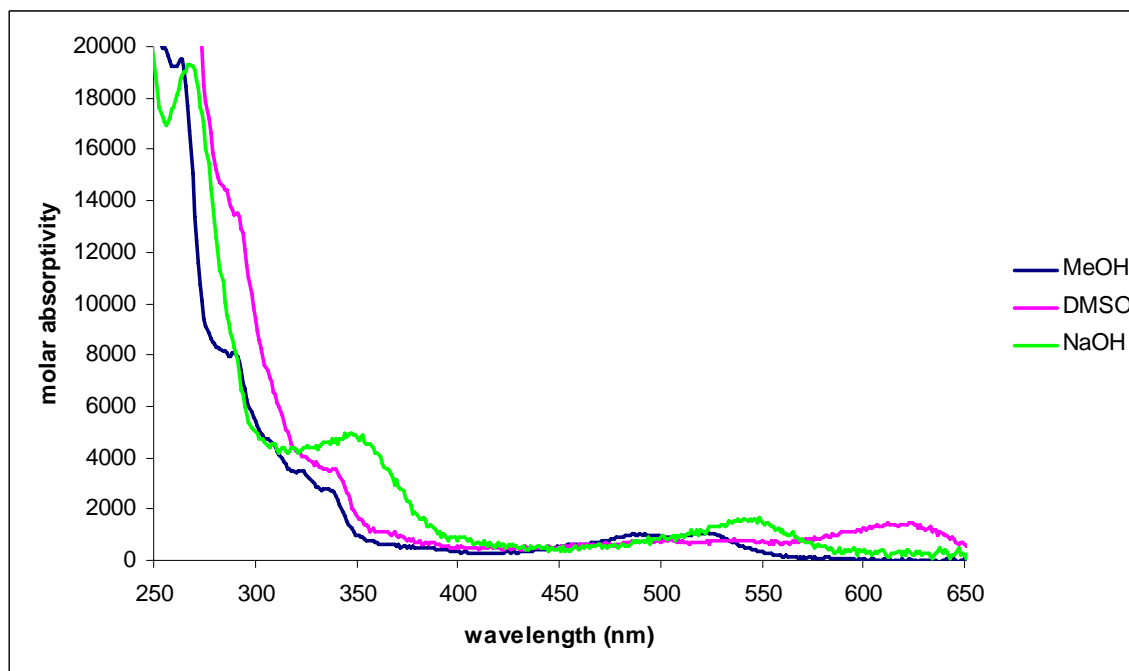
**Figure S64.** Emission of 10  $\mu\text{M}$  **10** as a function of excitation in MeOH.



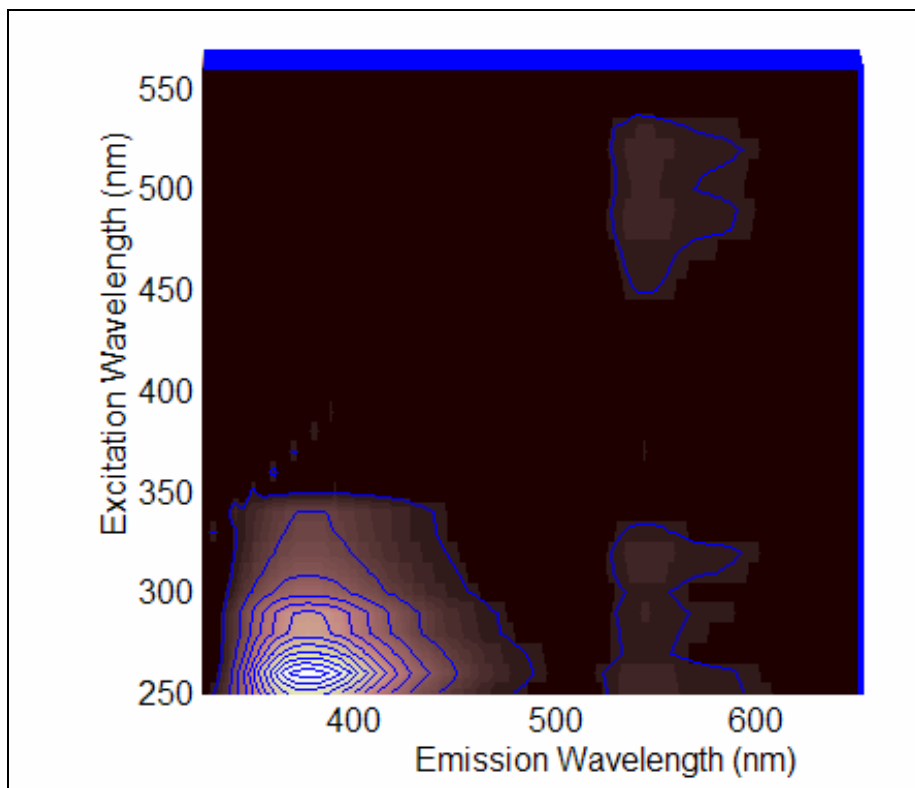
**Figure S65.** Excitation of 10  $\mu\text{M}$  **10** as a function of emission in MeOH.



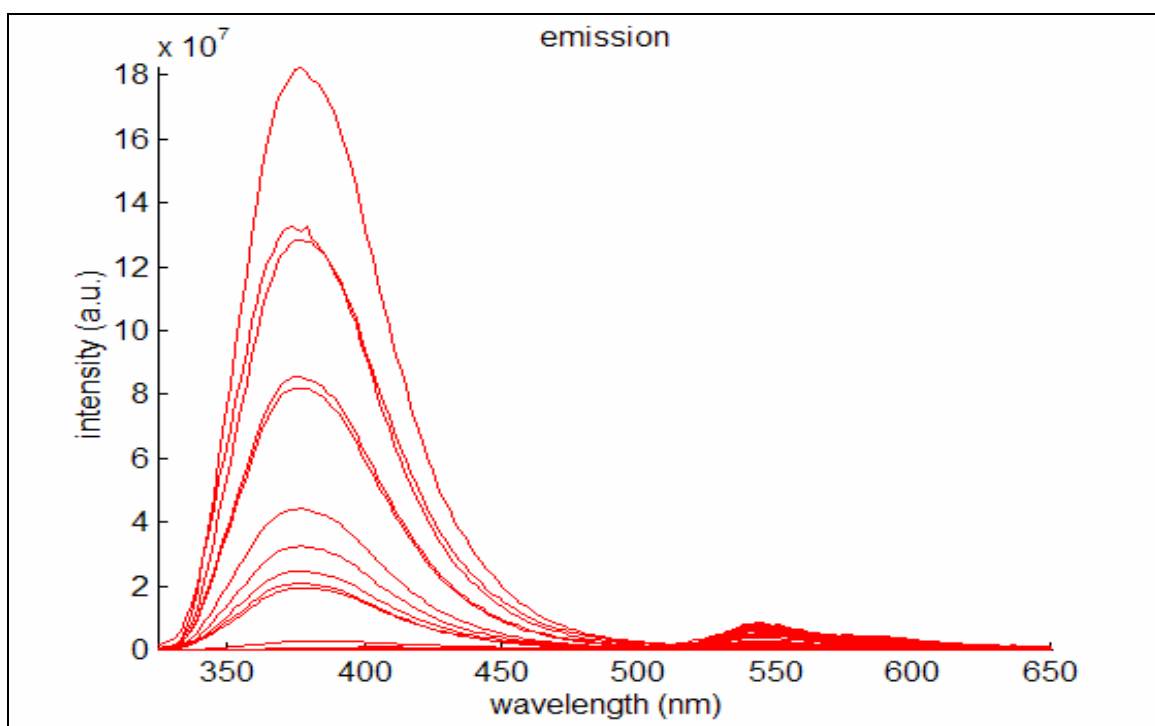
**Figure S66.** Chromaticity diagram of 10  $\mu$ M **10** in MeOH between 270 nm and 370 nm plotted in a 1931 CIE diagram.



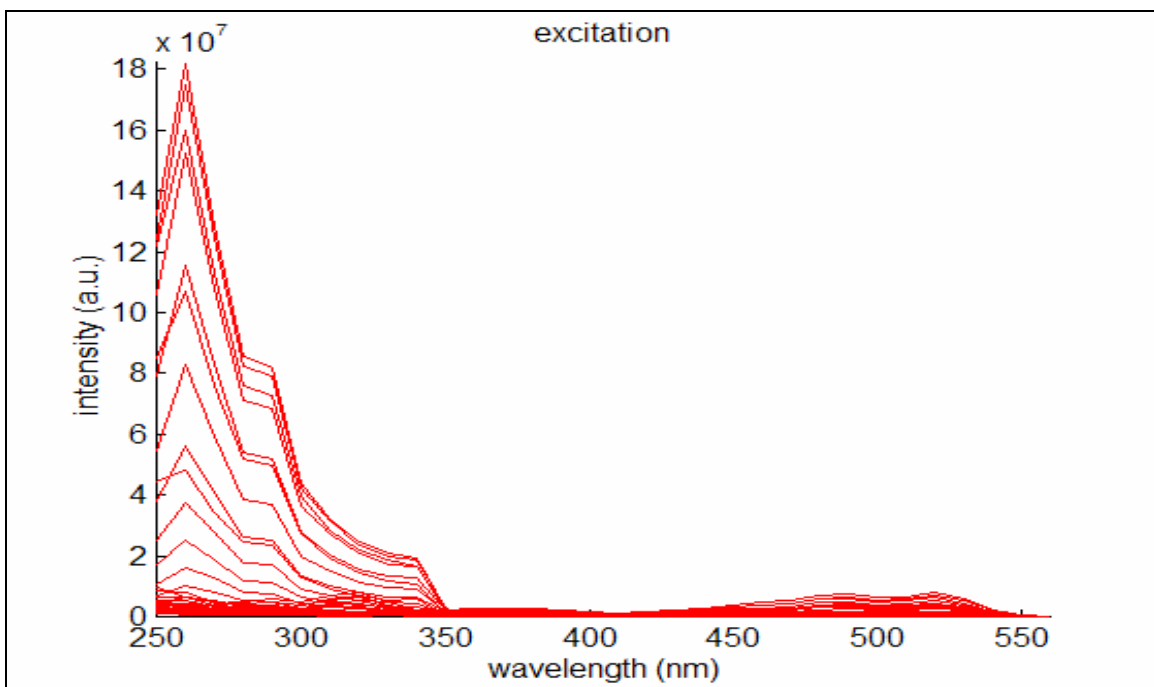
**Figure S67.** Absorption spectra of **12** in MeOH, DMSO and 0.1 M NaOH.



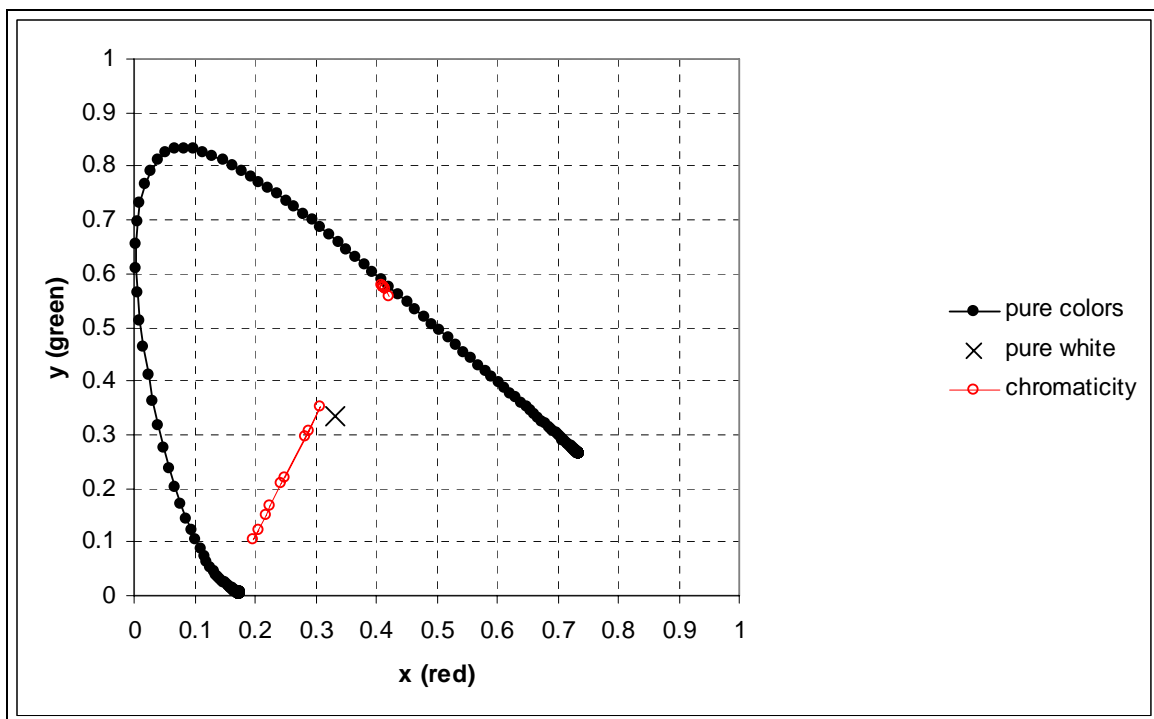
**Figure S68.** EEM of 10 μM **12** in MeOH.



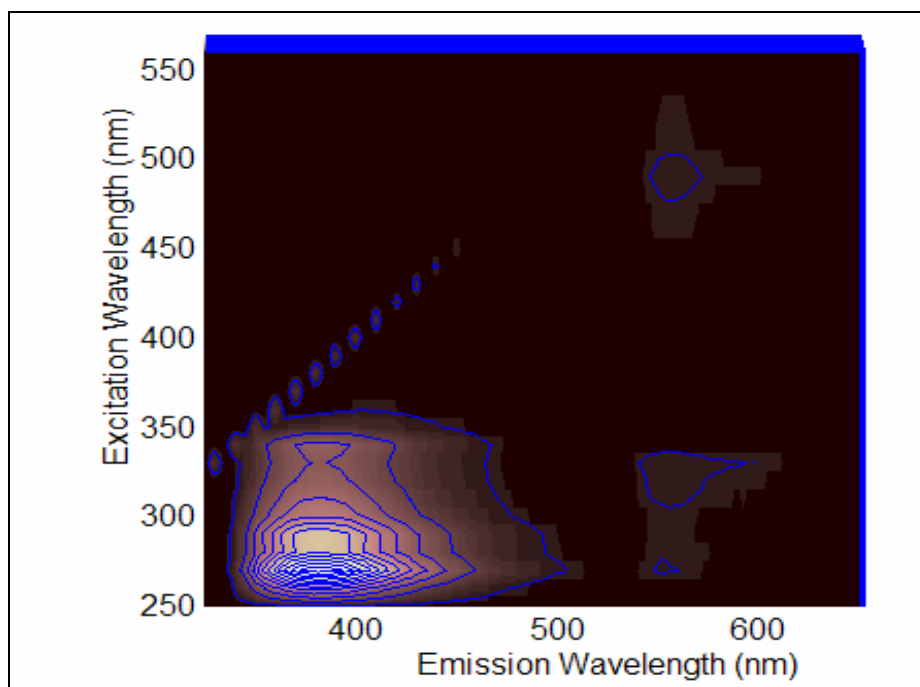
**Figure S69.** Emission of 10 μM **12** as a function of excitation in MeOH.



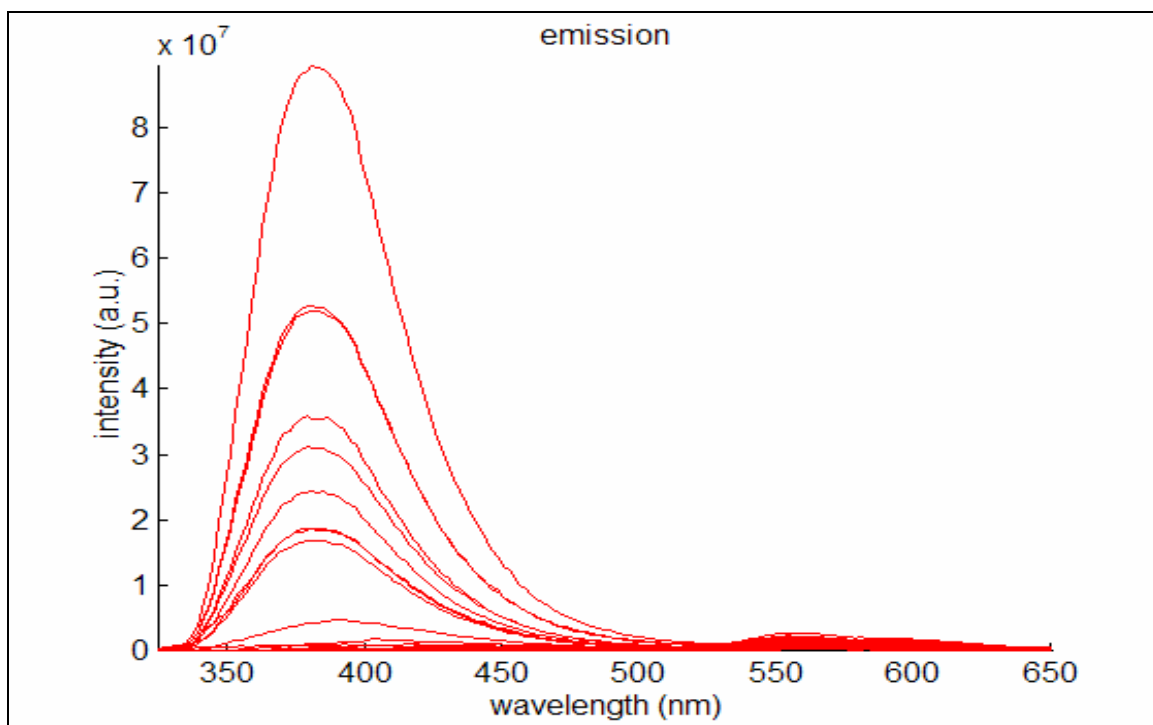
**Figure S70.** Excitation of 10  $\mu\text{M}$  **12** as a function of emission in MeOH.



**Figure S71.** Chromaticity diagram of 10  $\mu\text{M}$  **12** in MeOH from 260 nm to 340 nm and from 440 nm to 540 nm plotted in a 1931 CIE diagram.



**Figure S72.** EEM of 10  $\mu\text{M}$  **12** in DMSO.



**Figure S73.** Emission of 10  $\mu\text{M}$  **12** as a function of excitation in DMSO.



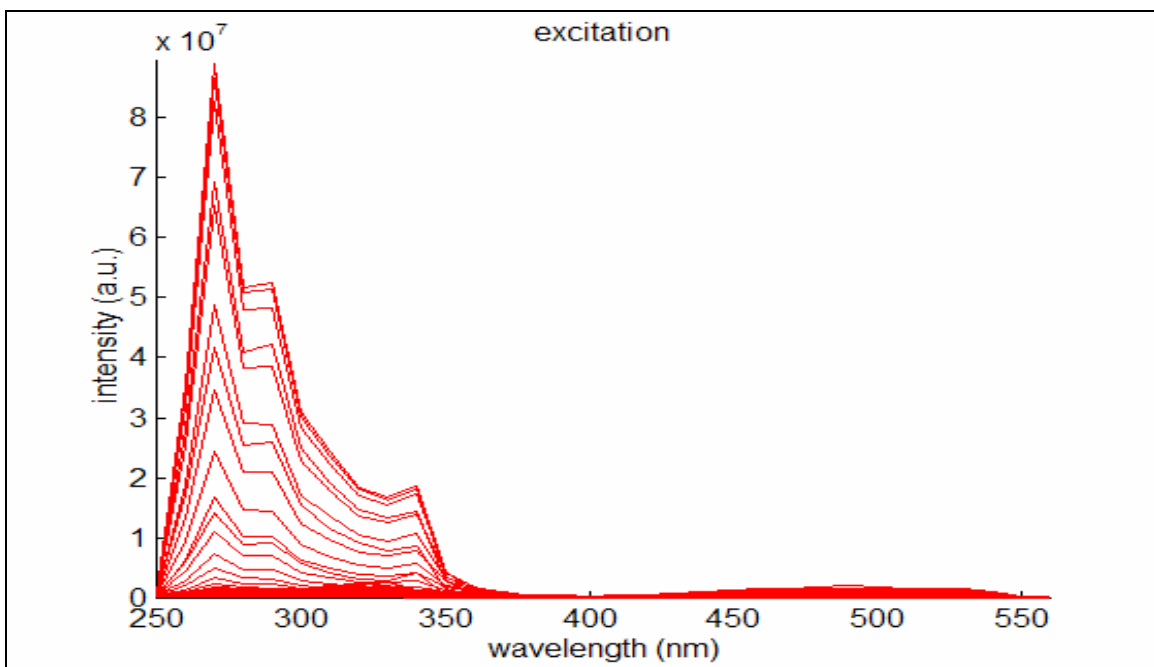


Figure S74. Excitation of 10  $\mu\text{M}$  **12** as a function of emission in DMSO.

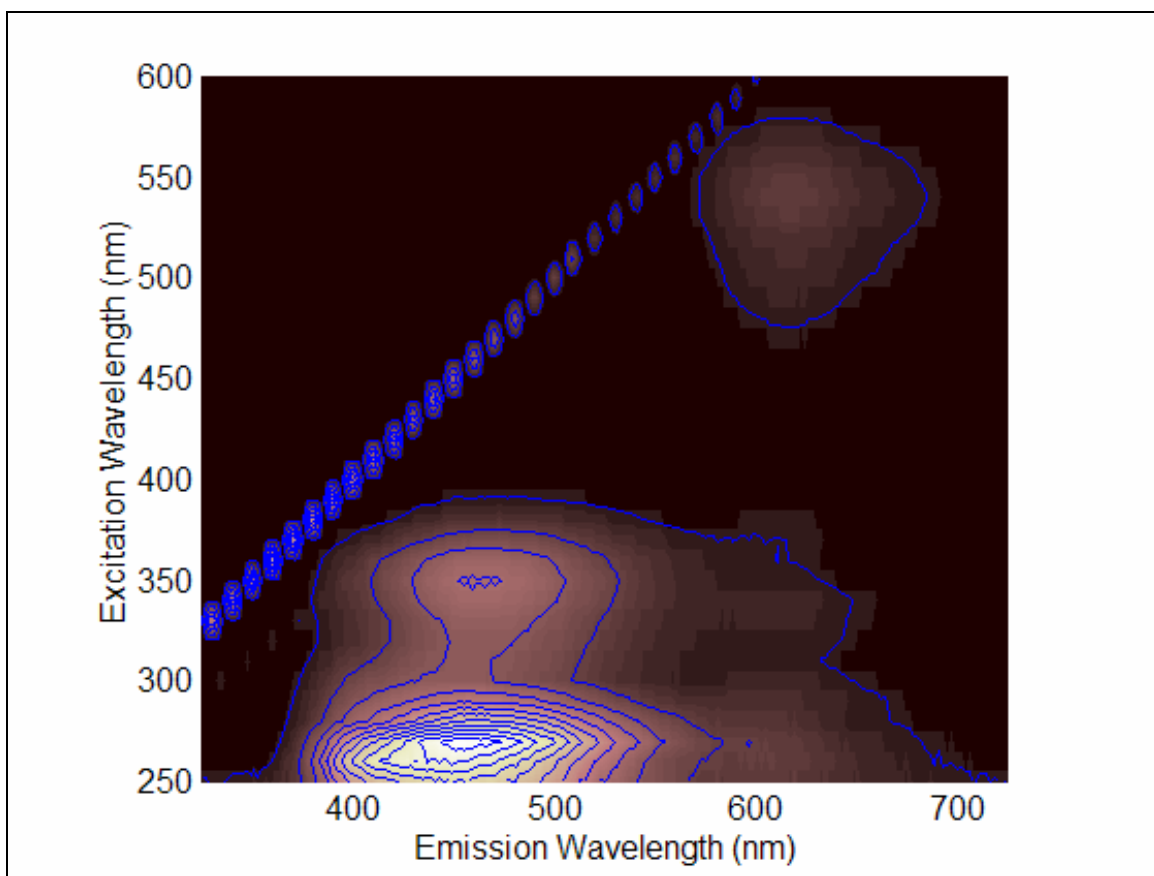
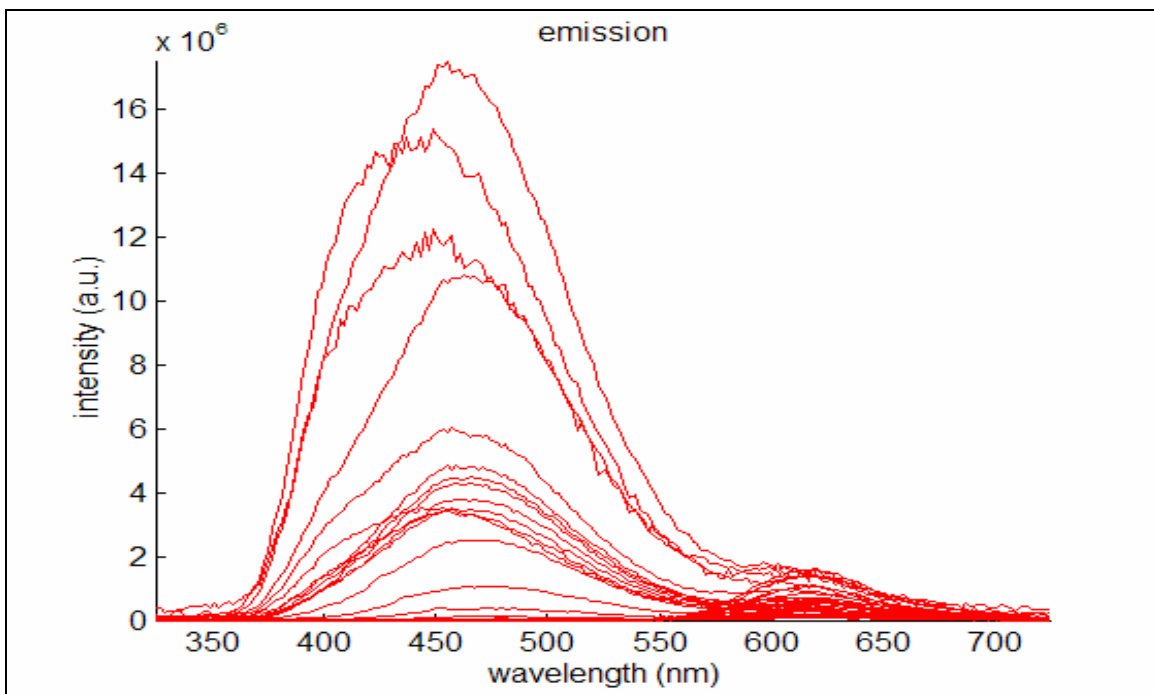
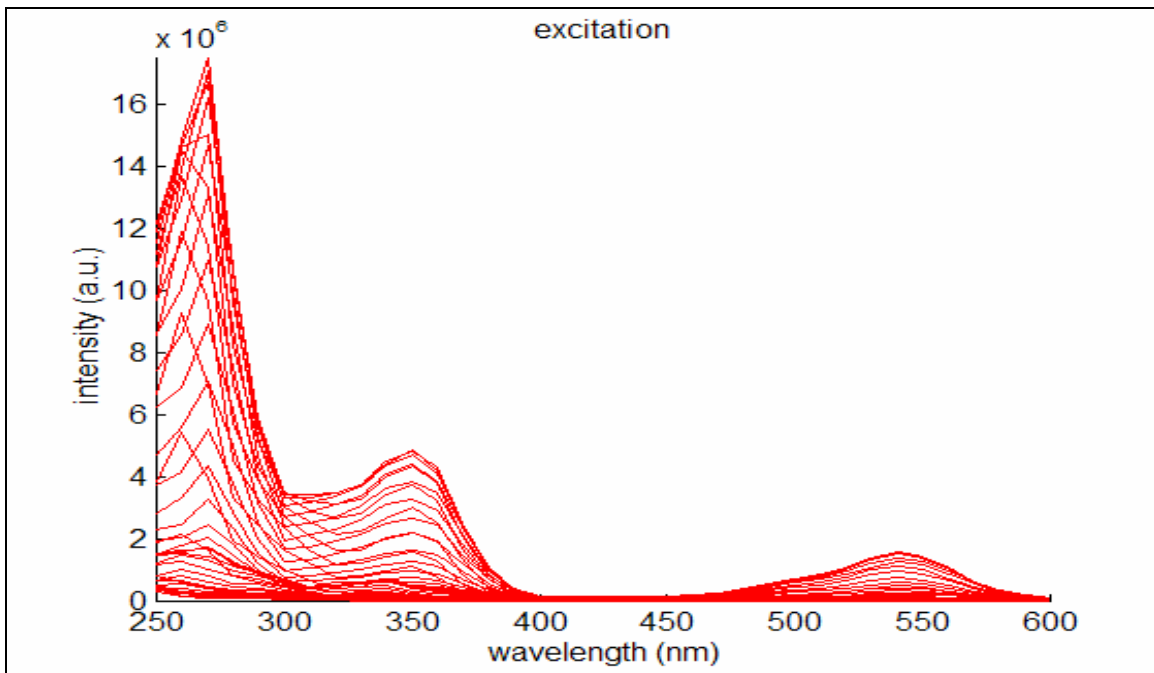


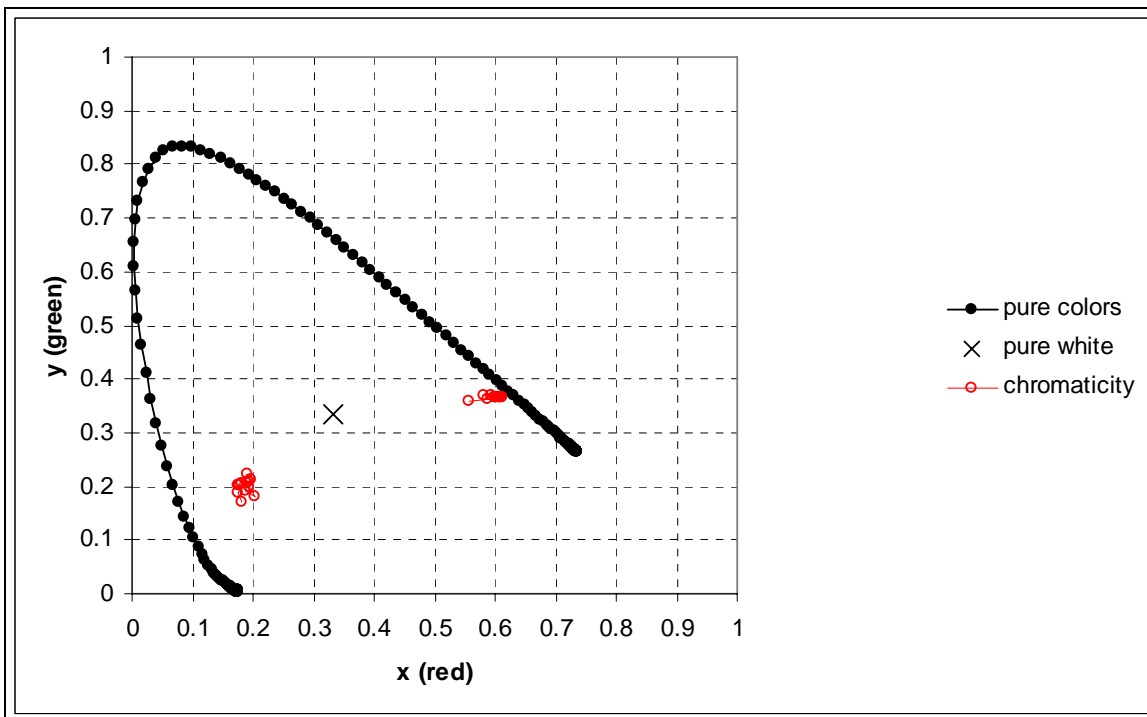
Figure S75. EEM of 10  $\mu\text{M}$  **12** in 0.1 M NaOH.



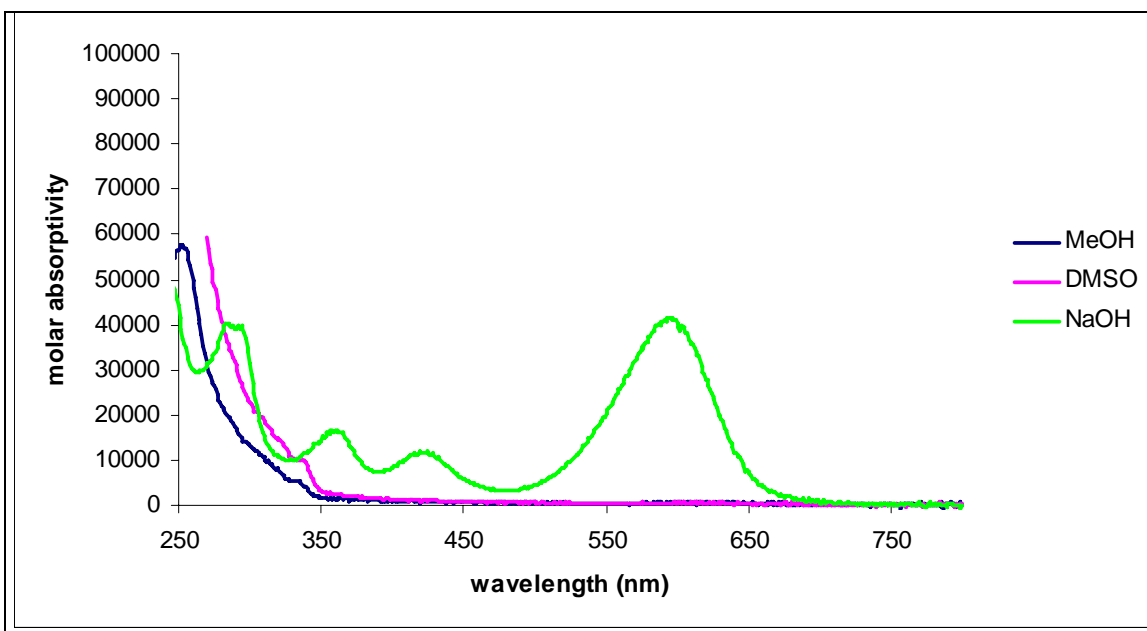
**Figure S76.** Emission of 10  $\mu\text{M}$  **12** as a function of excitation in 0.1 M NaOH.



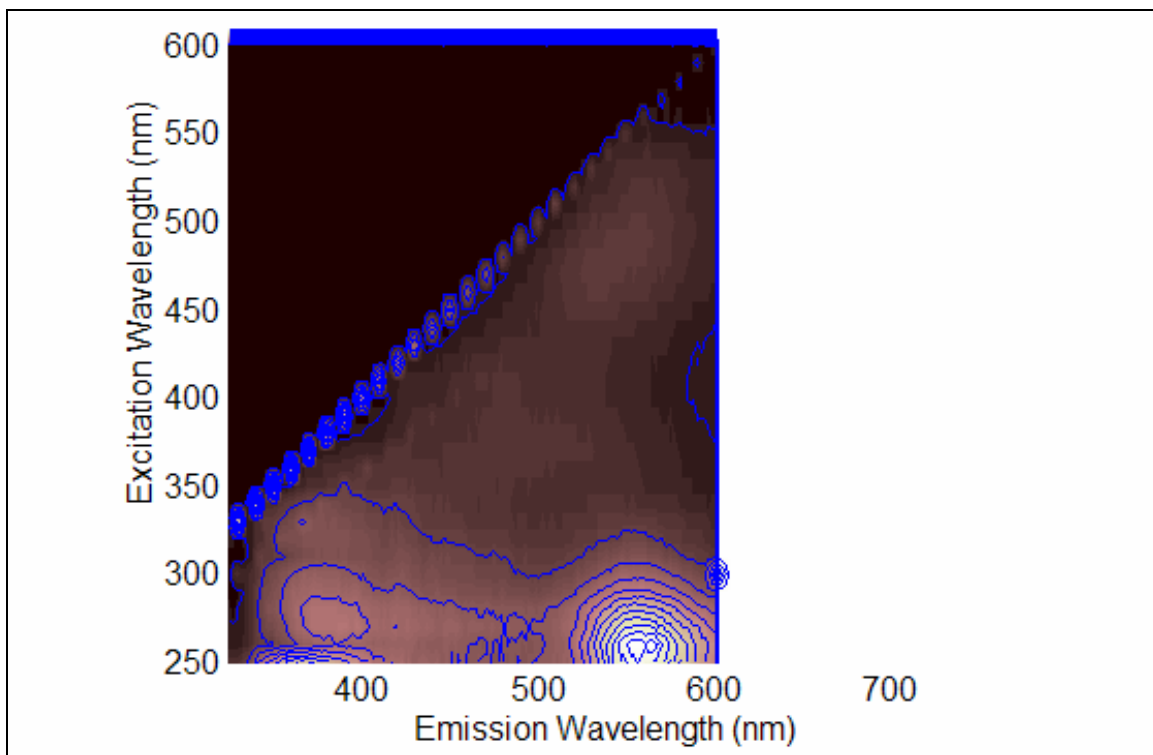
**Figure S77.** Excitation of 10  $\mu\text{M}$  **12** as a function of emission in 0.1 M NaOH.



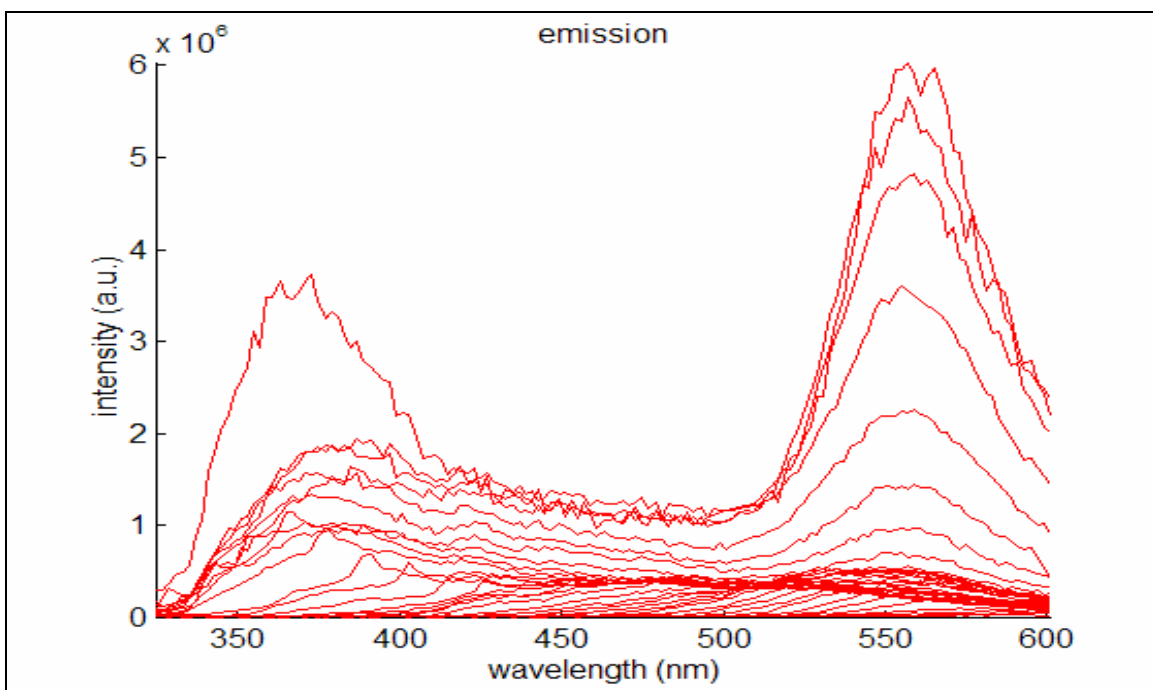
**Figure S78.** Chromaticity diagram of 10  $\mu$ M **12** in 0.1 M NaOH from 260 nm to 370 nm and from 480 nm to 580 nm plotted in a 1931 CIE diagram.



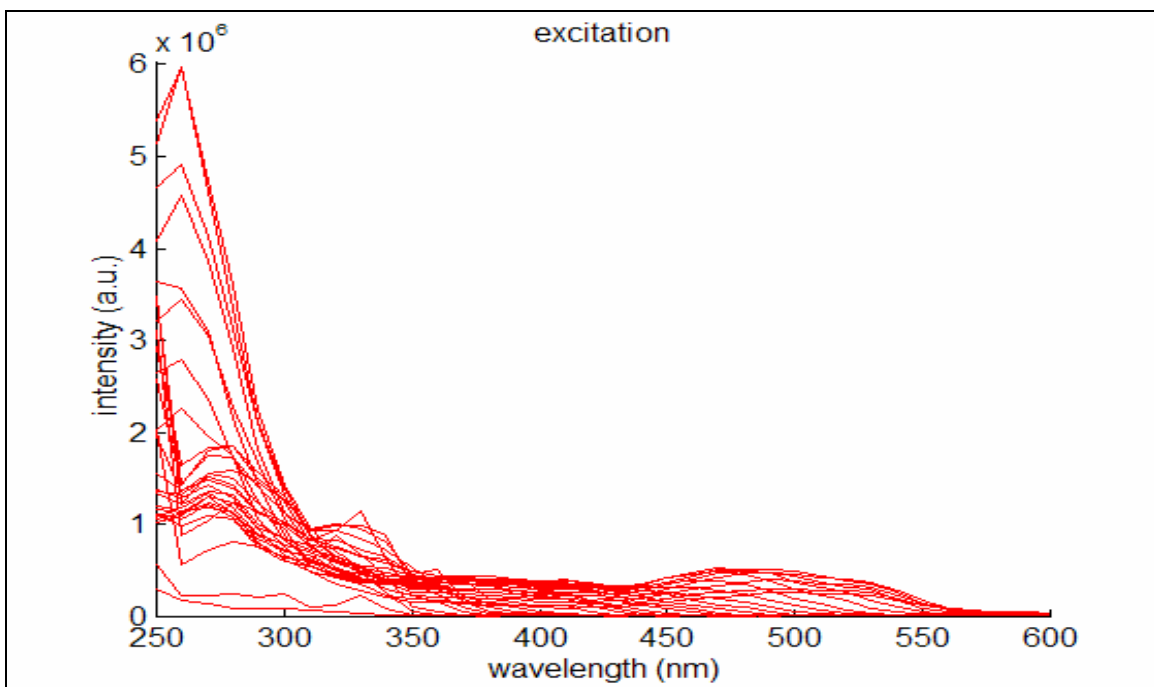
**Figure S79.** Absorption spectra of **14** in MeOH, DMSO and 0.1 M NaOH.



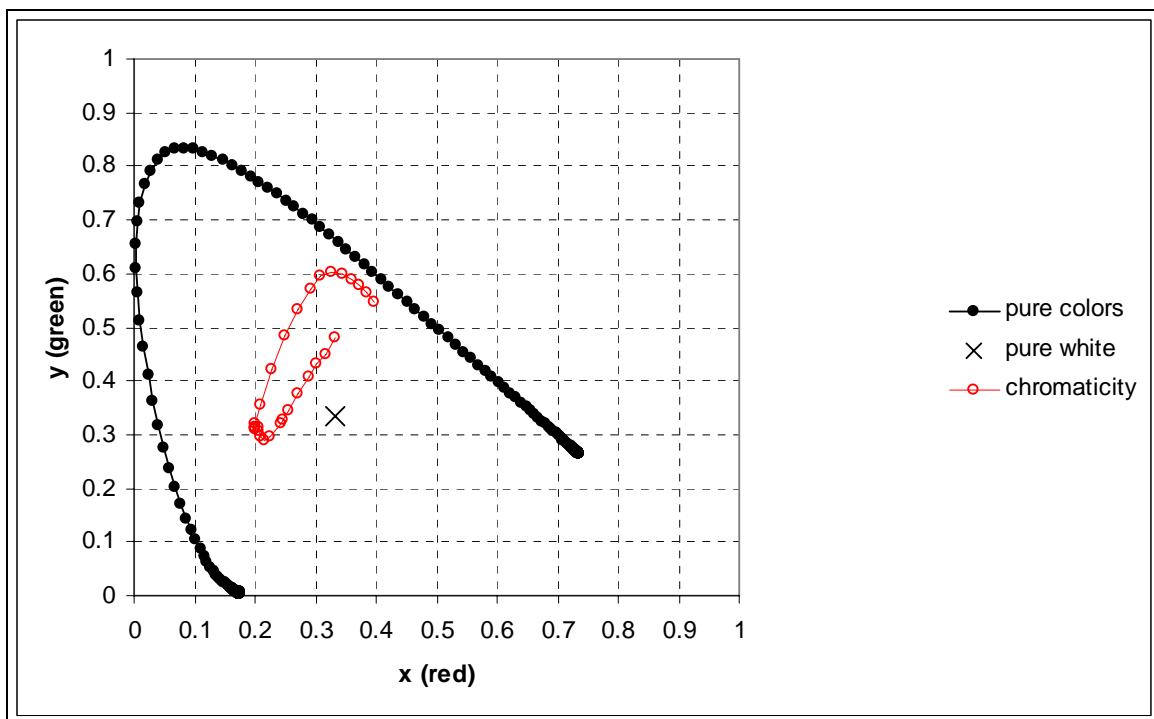
**Figure S80.** EEM of 10  $\mu\text{M}$  **14** in MeOH.



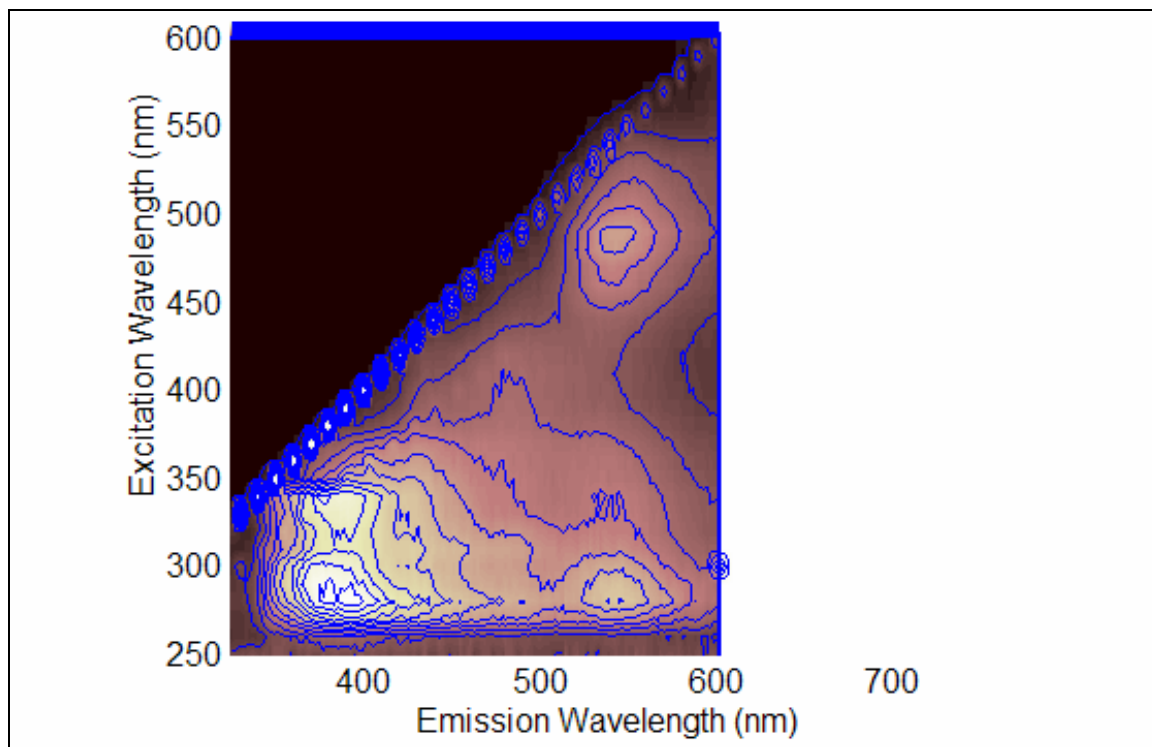
**Figure S81.** Emission of 10  $\mu\text{M}$  **14** as a function of excitation in MeOH.



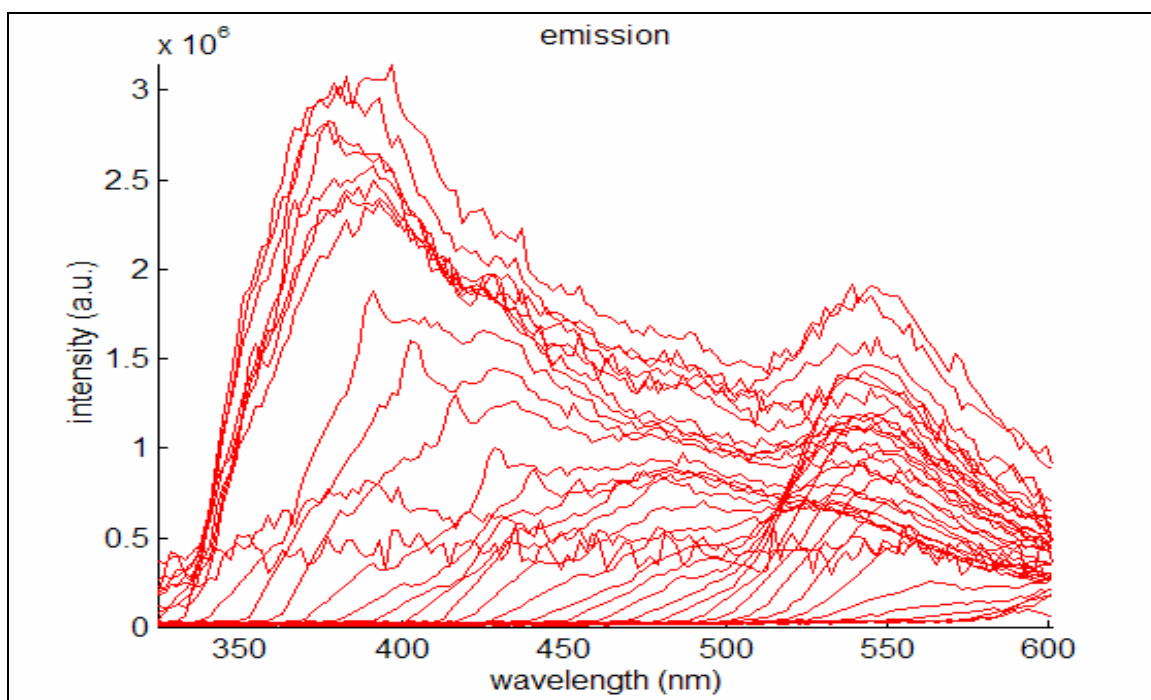
**Figure S82.** Excitation of 10  $\mu\text{M}$  **14** as a function of emission in MeOH.



**Figure S83.** Chromaticity diagram of 10  $\mu\text{M}$  **14** in MeOH between 260 nm and 540 nm plotted in a 1931 CIE diagram.



**Figure S84.** EEM of 10 μM **14** in DMSO.



**Figure S85.** Emission of 10 μM **14** as a function of excitation in DMSO.

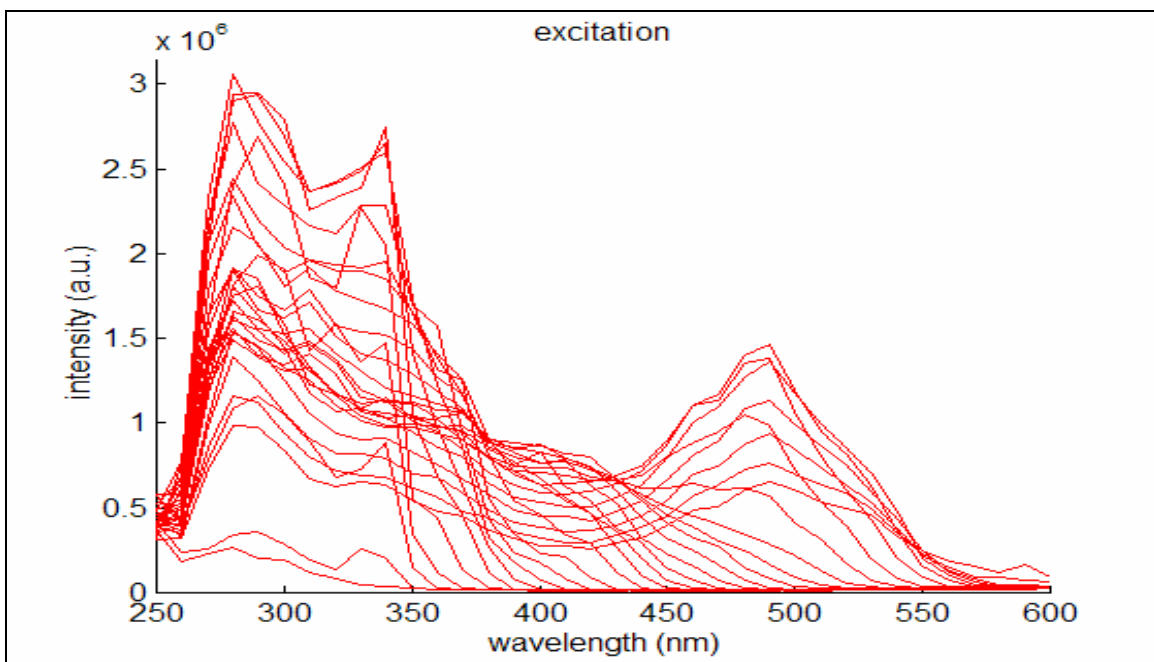


Figure S86. Excitation of 10  $\mu\text{M}$  **14** as a function of emission in DMSO.

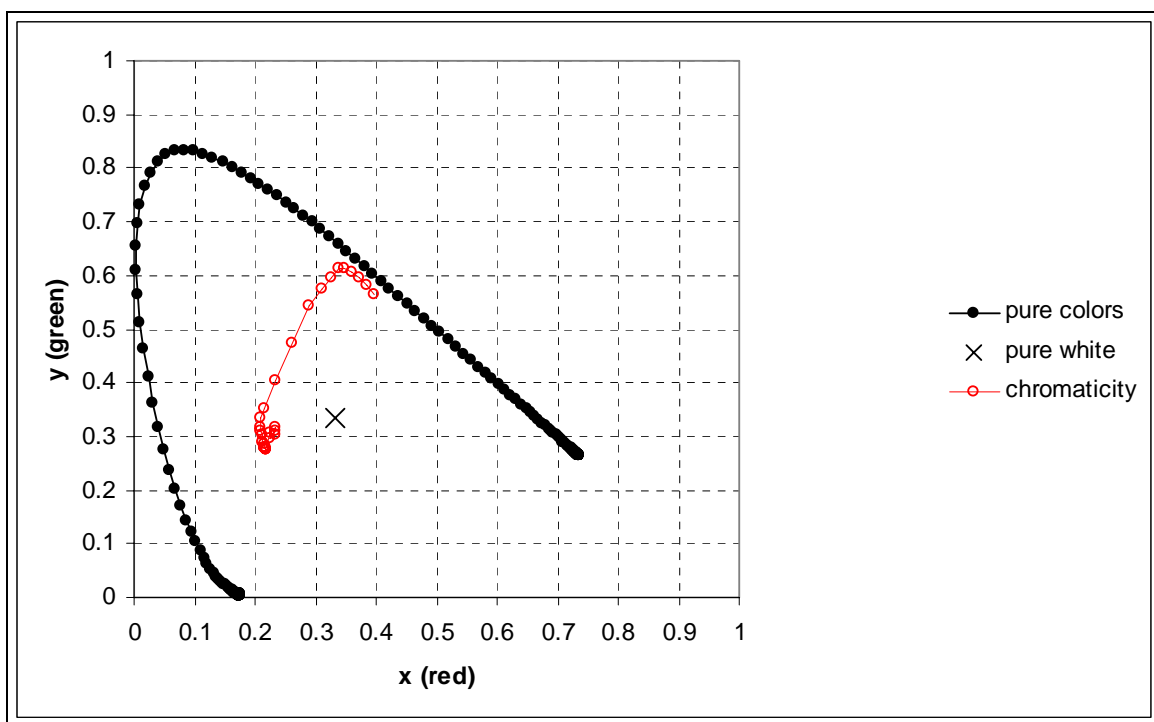
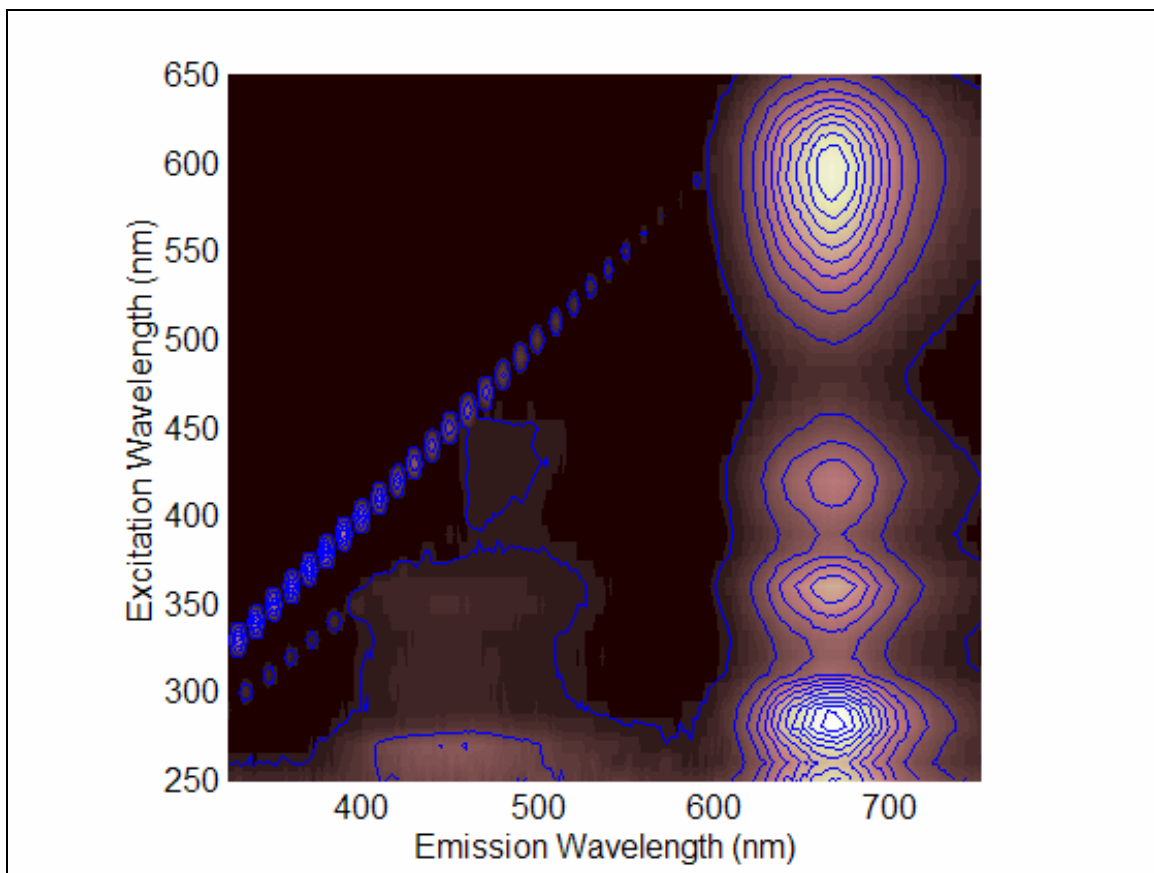
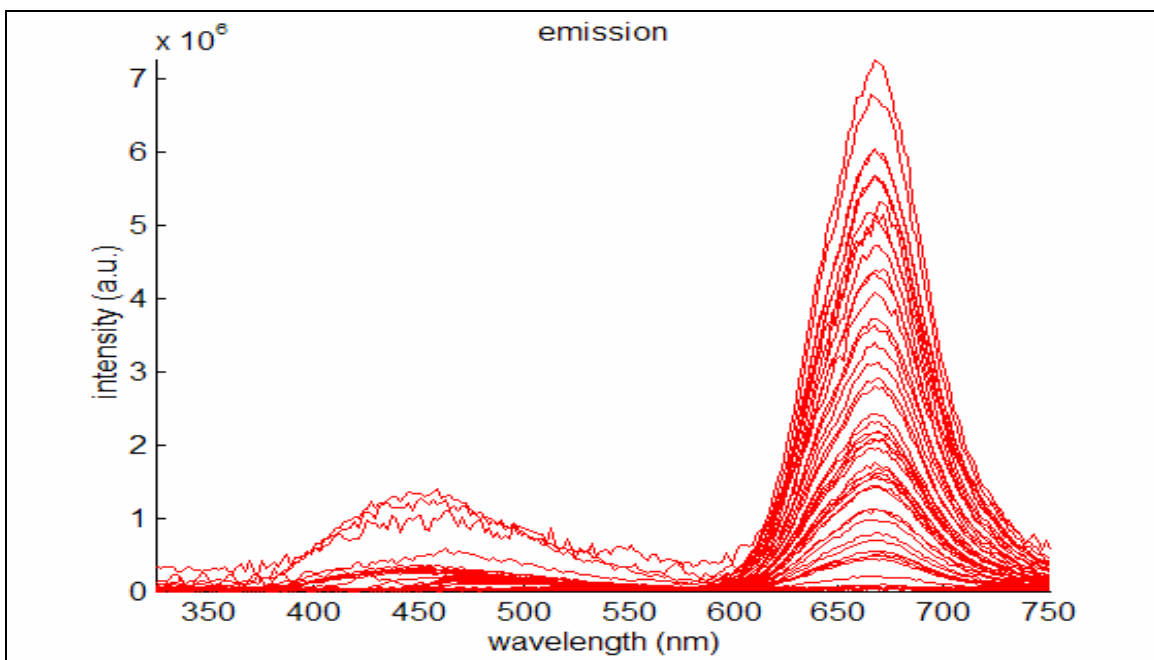


Figure S87. Chromaticity diagram of 10  $\mu\text{M}$  **14** in DMSO between 260 nm and 540 nm plotted in a 1931 CIE diagram.

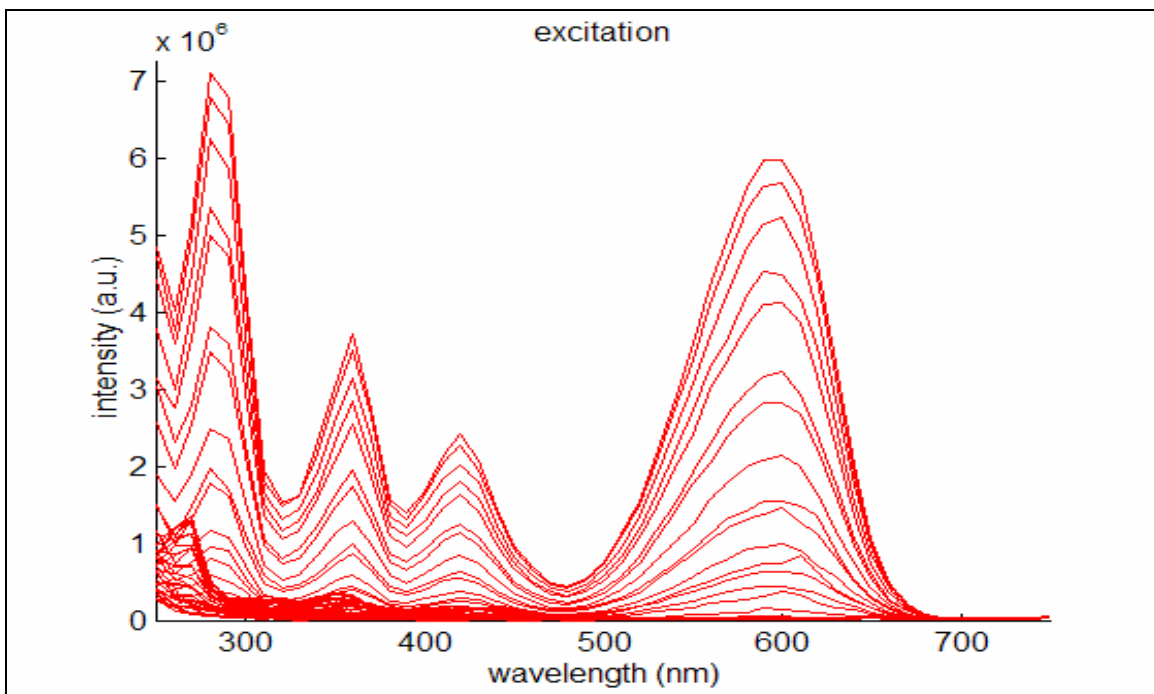


**Figure S88.** EEM of 10  $\mu\text{M}$  **14** in 0.1 M NaOH.

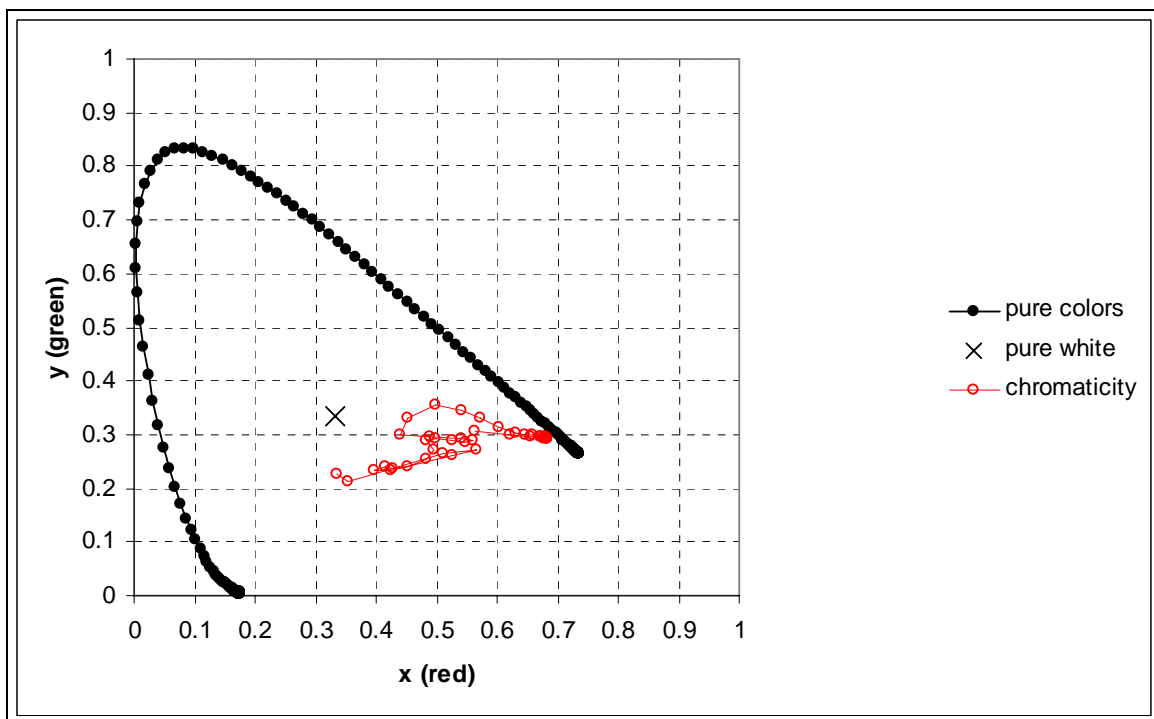


**Figure S89.** Emission of 10  $\mu\text{M}$  **14** as a function of excitation in 0.1 M NaOH.





**Figure S90.** Excitation of 10  $\mu\text{M}$  **14** as a function of emission in 0.1 M NaOH.



**Figure S91.** Chromaticity diagram of 10  $\mu\text{M}$  **14** in 0.1 M NaOH between 260 nm and 650 nm plotted in a 1931 CIE diagram.