Electronic Supplementary Material (ESI) for Polymer Chemistry.

Probing the dendritic architecture through AIE: challenges and successes

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1. Supplemental figures

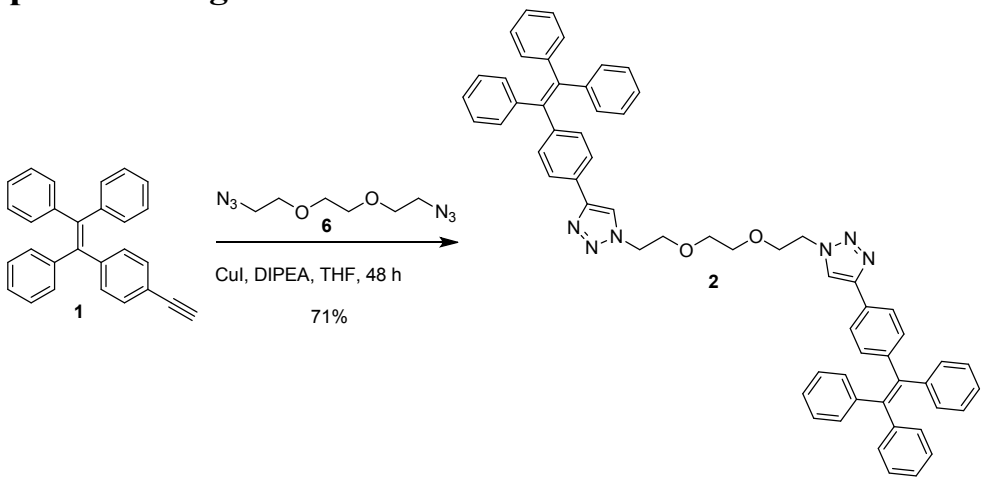


Figure S1 The synthetic route leading to the G0 dendrimer

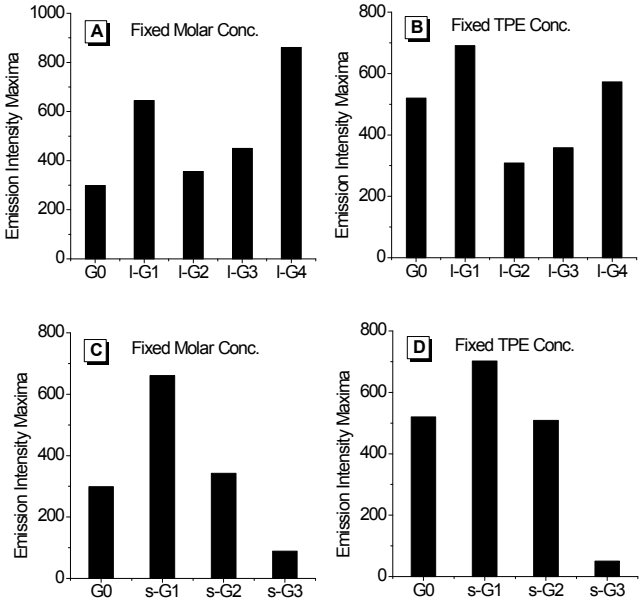


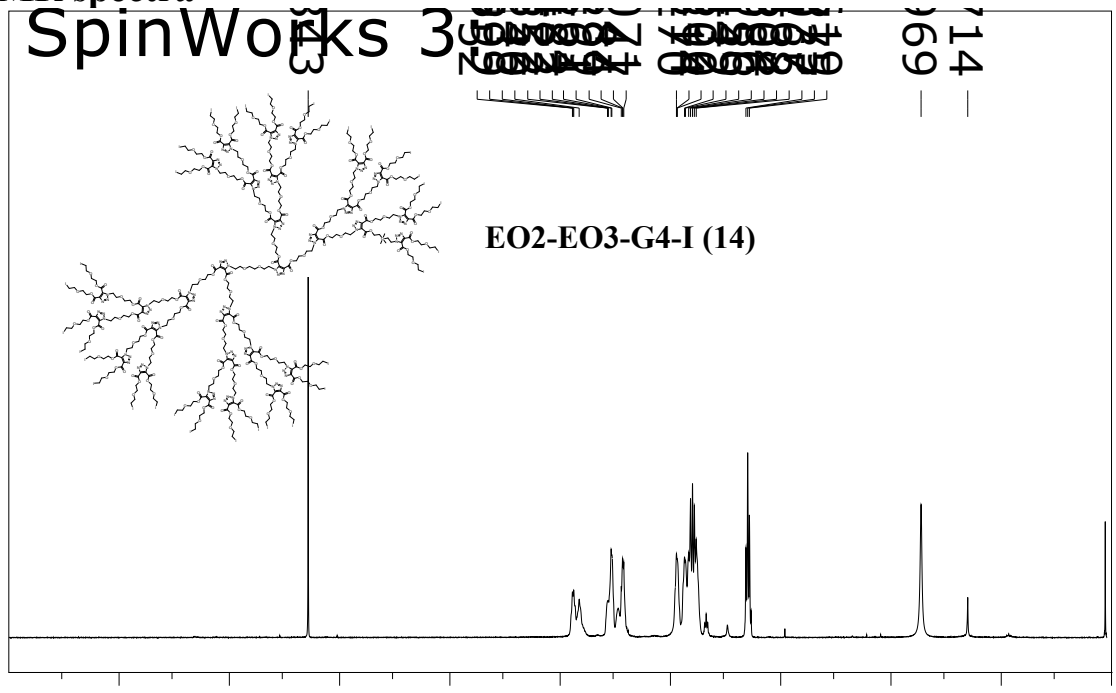
Figure S2. Emission intensity maxima of "long" series at 95 % f_w with a fixed molar concentration of 10^{-5} M (A) and with a fixed concentration of TPE of 10^{-5} M (B). Emission intensity maxima of "short" series at 95 % f_w with a fixed molar concentration of 10^{-5} M (C) and with a fixed concentration of TPE of 10^{-5} M (D) excitation wavelength is 327 nm for all samples.

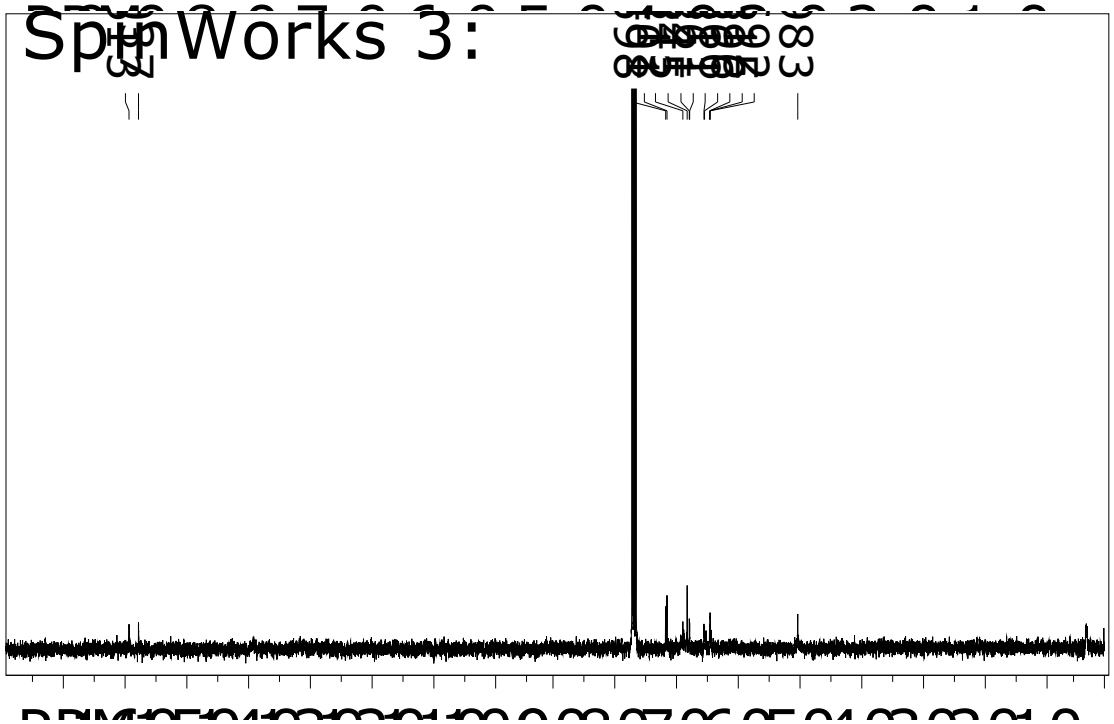
Table 1 **DLS radius of each dendrimer compared with the hard-sphere calculation.**

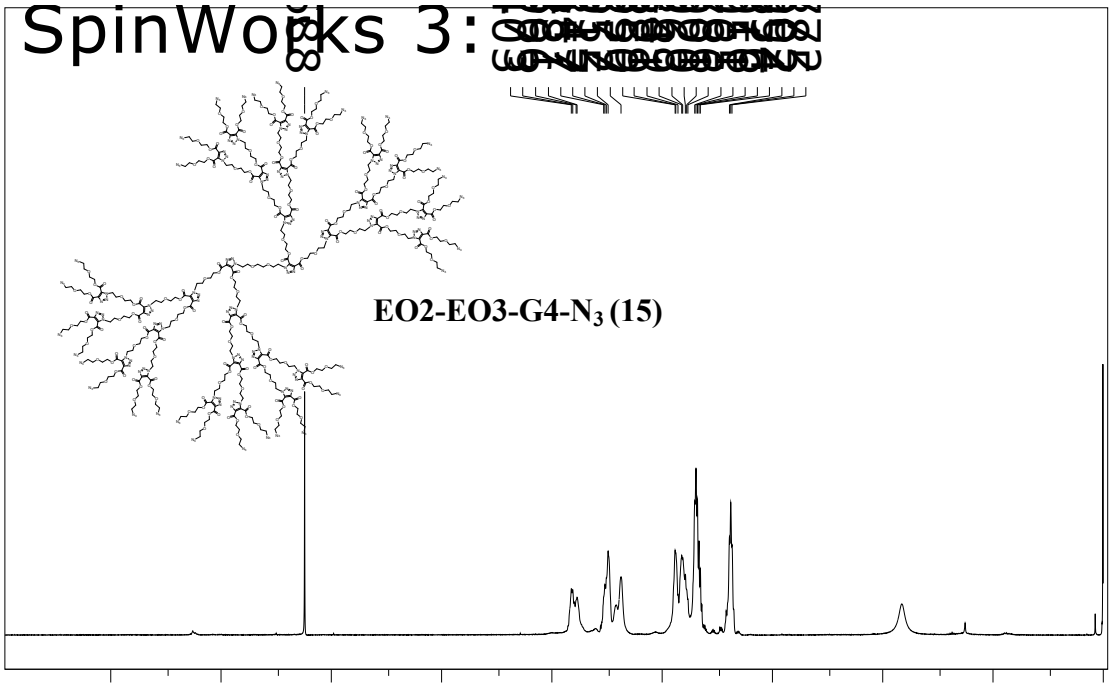
Generation	DLS (nm)	Calc. (nm)
Go (**2**)	N/A	2.52
s-G1 (**3**)	3.05	3.22
s-G2 (**4**)	1.32	3.67
s-G3 (**5**)	2.21	5.11
l-G1 (**20**)	4.13	4.76
l-G2 (**21**)	5.74	6.77
l-G3 (**22**)	8.07	5.95
l-G4 (**23**)	7.24	7.59

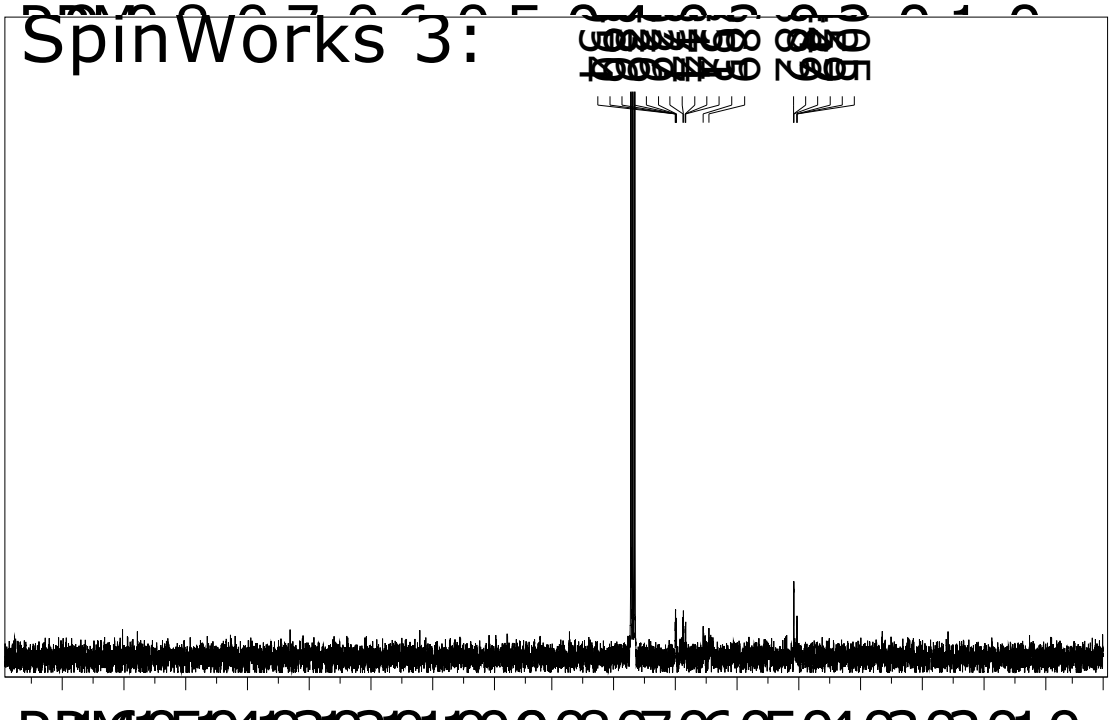
All measurements were conducted in THF, Concentration is 2 x 10^{-5} M. Calculations are the result of a hard-sphere potential energy optimization performed with Hyperchem^{tm} 8.

2. NMR spectra






SpinWorks 3:
EO2-EO3-G4-N3 (15)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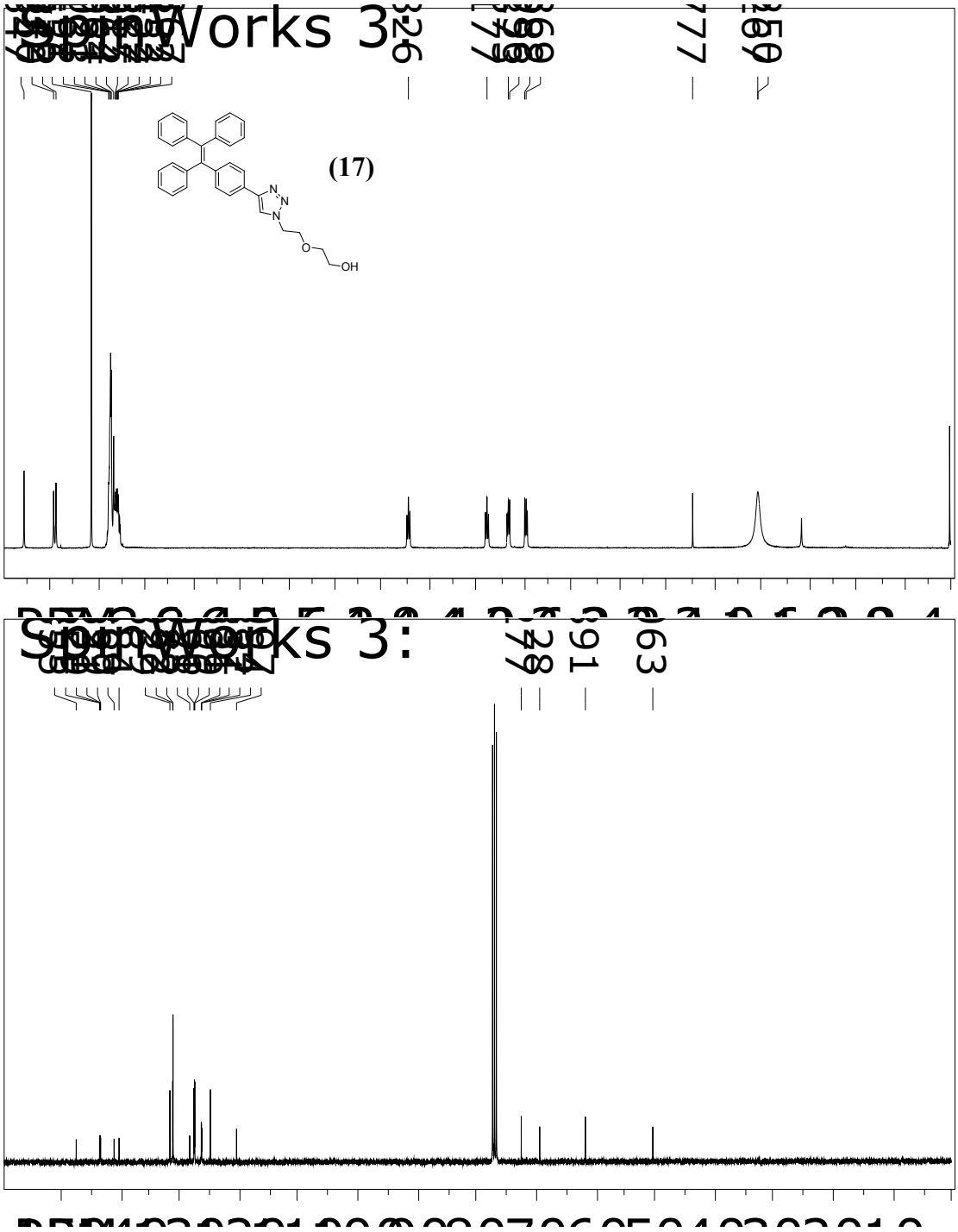
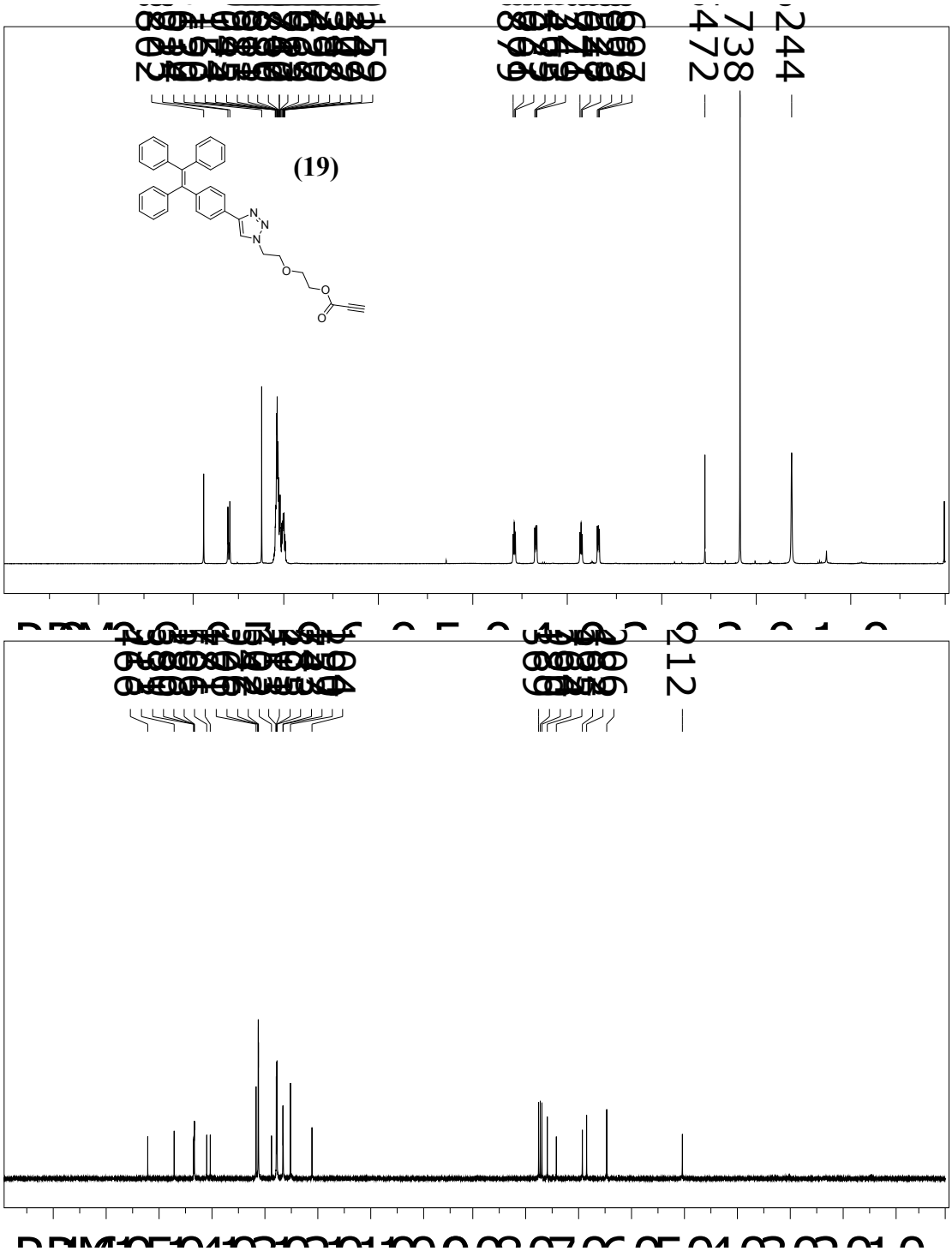
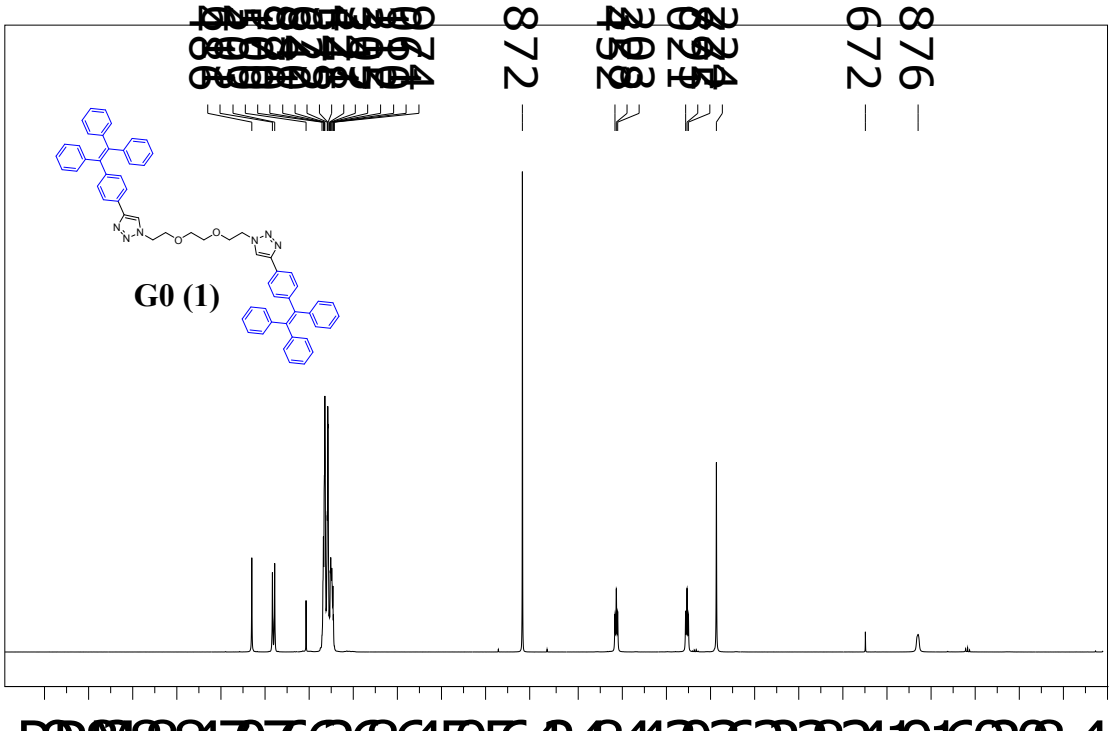
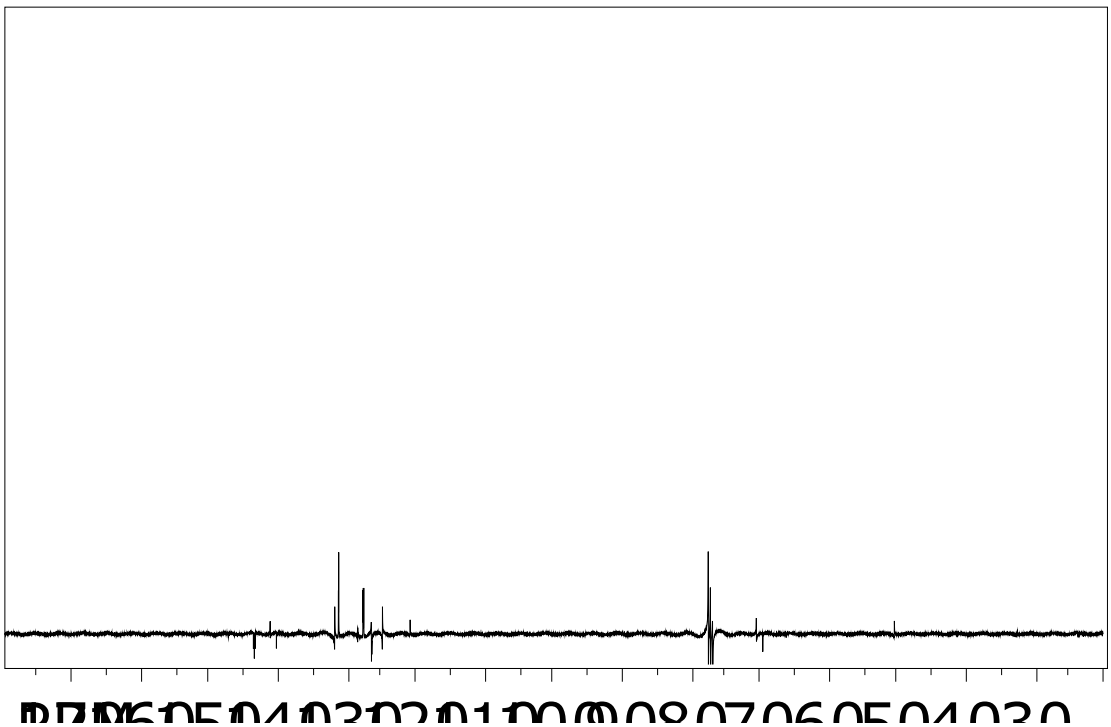
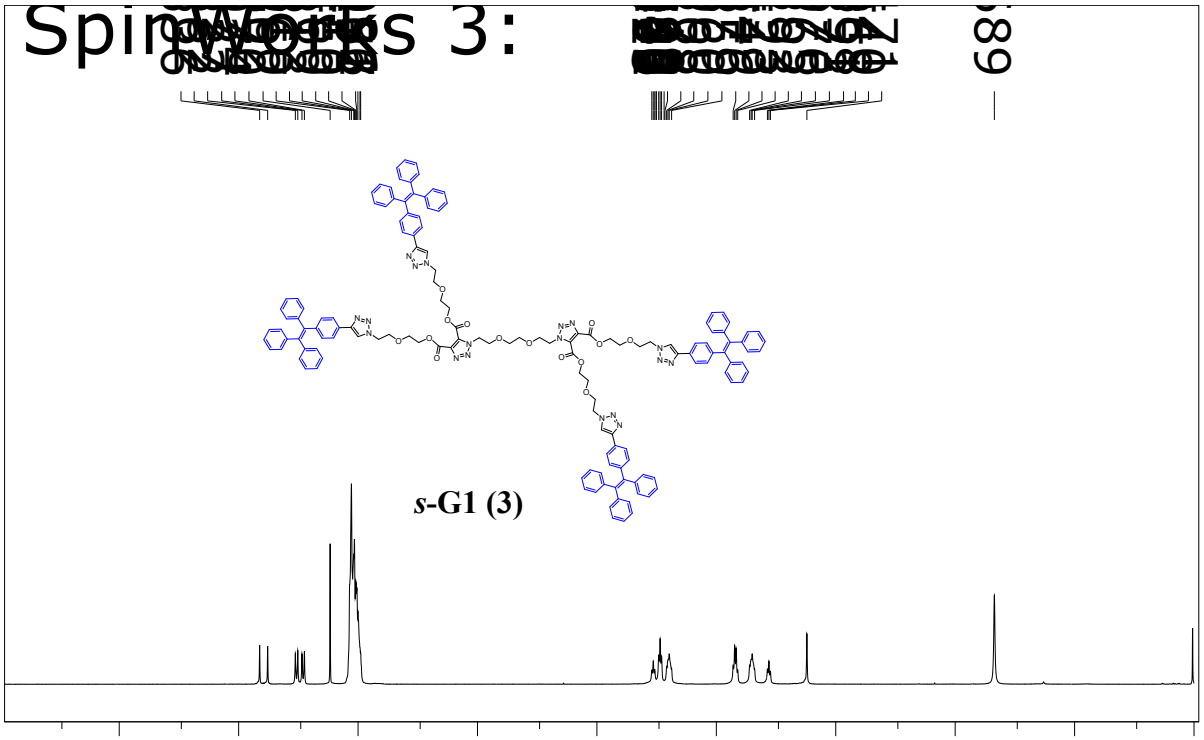
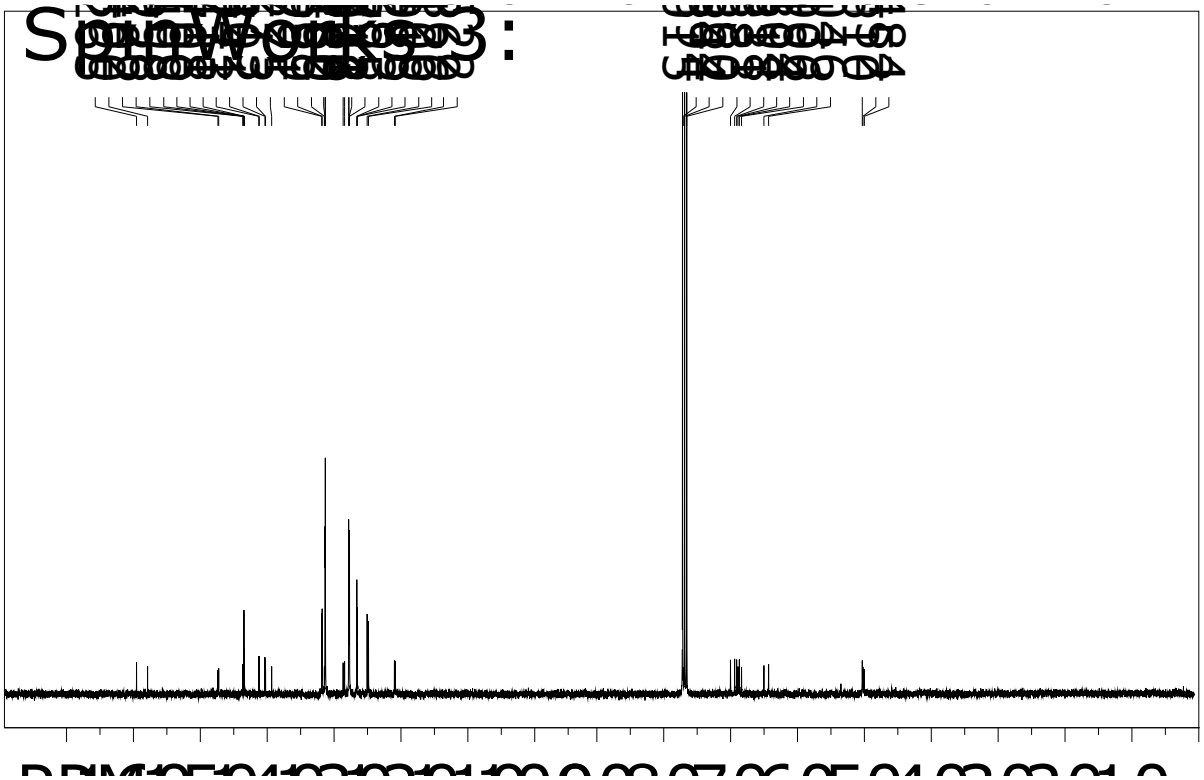

(17)
N
N
N
O
OH

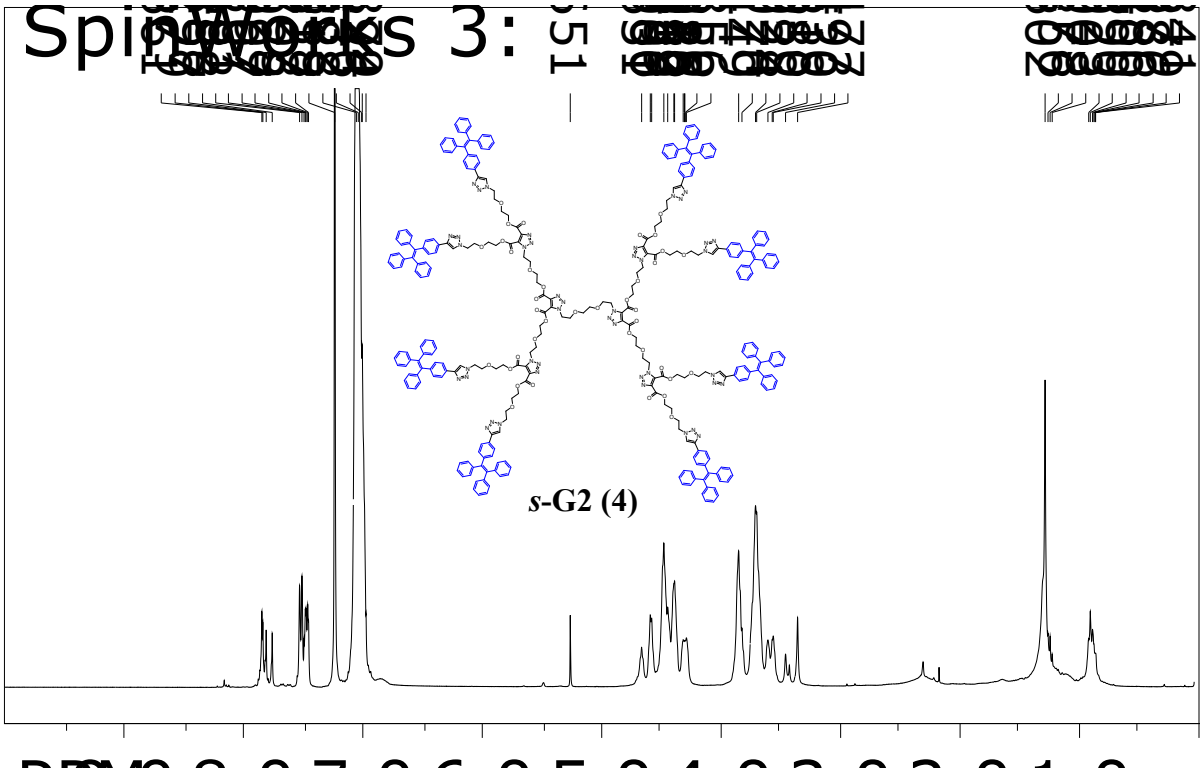

(19)


8.72
6.72
8.76
G0 (1)




s-G1 (3)

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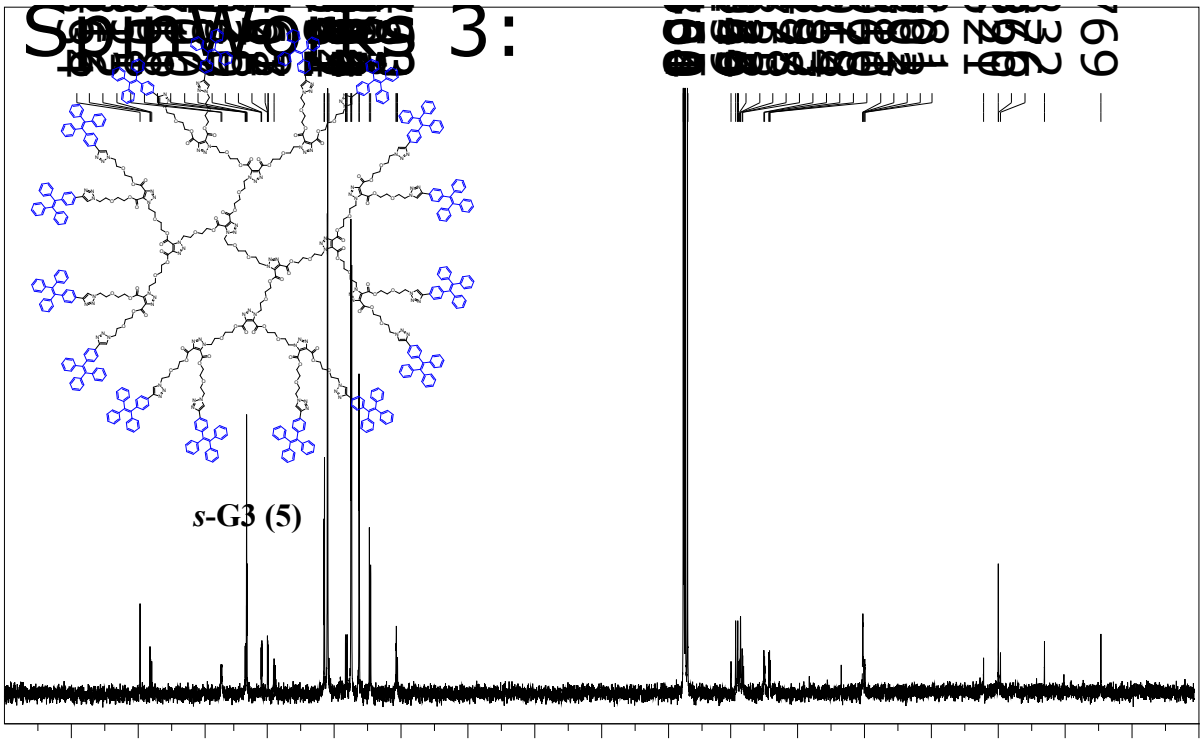
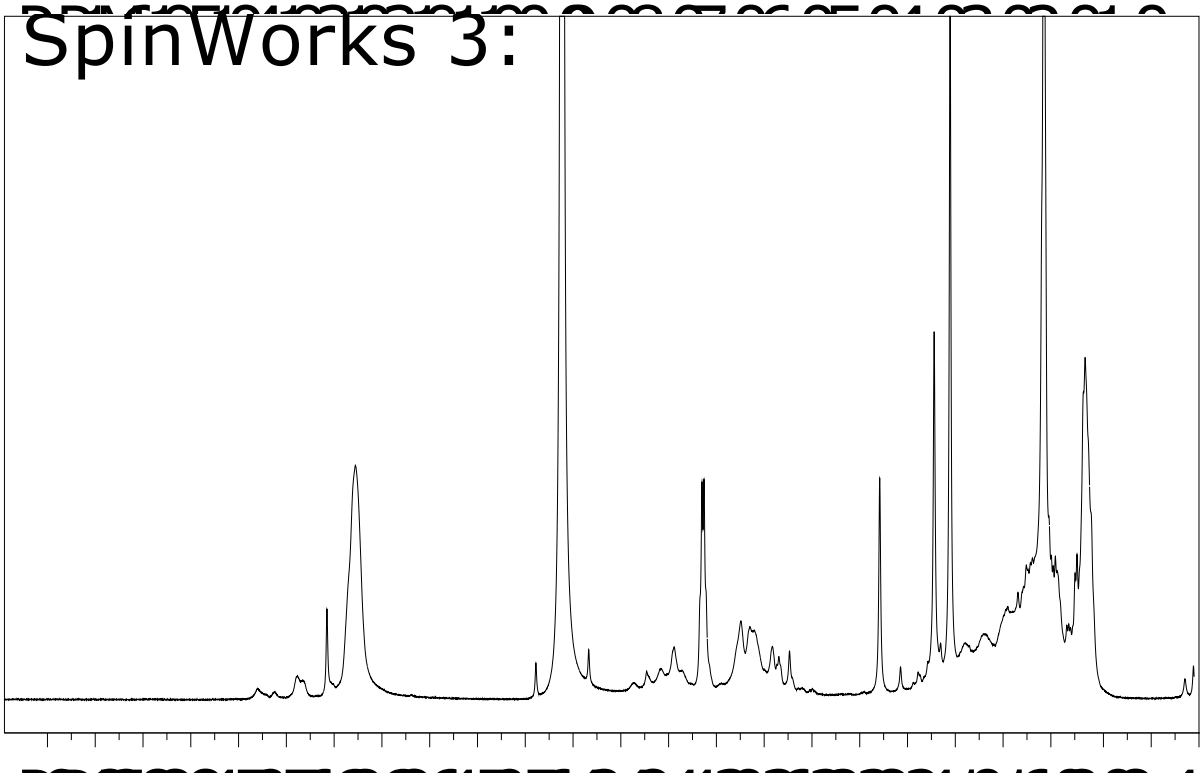

s-G3 (5)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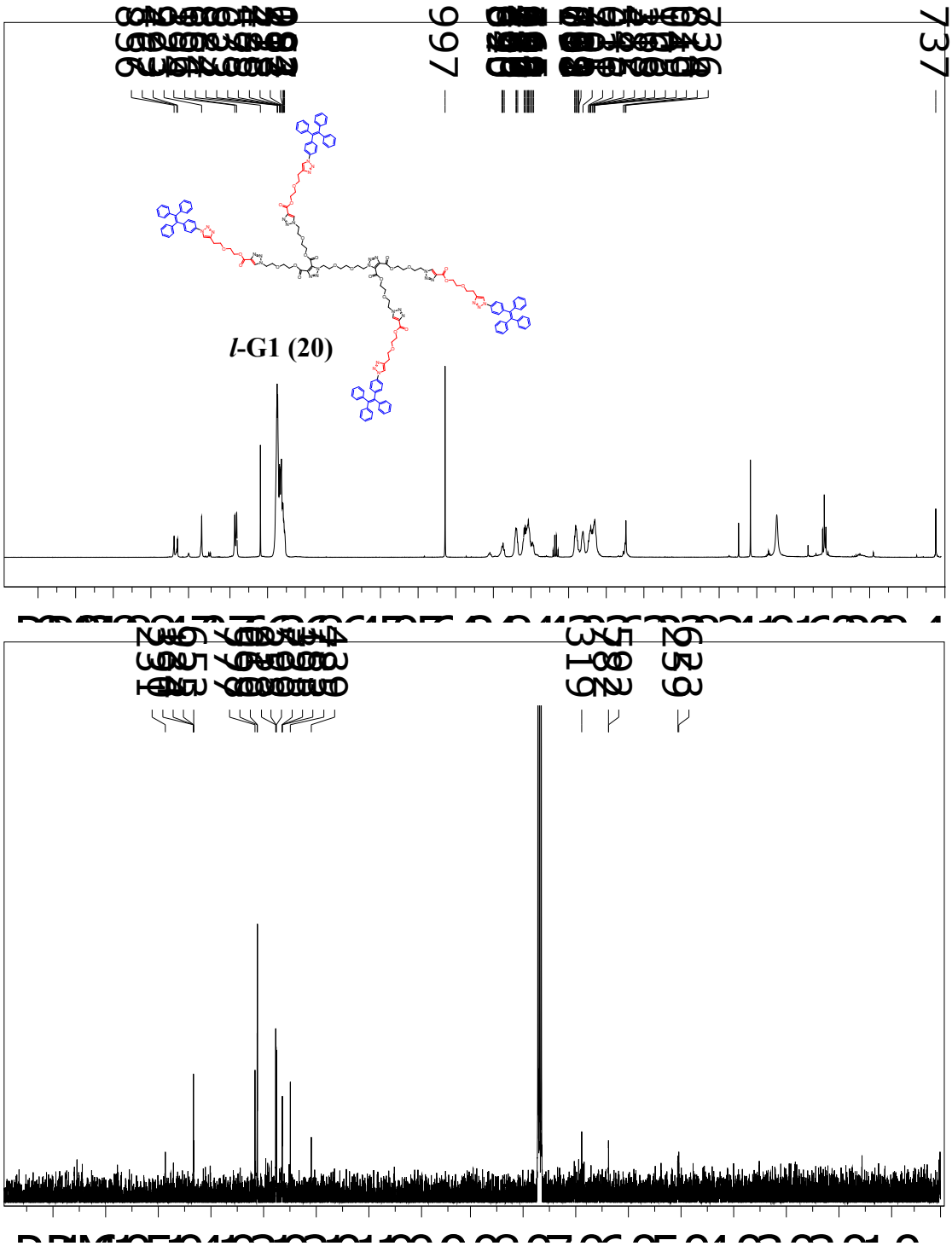
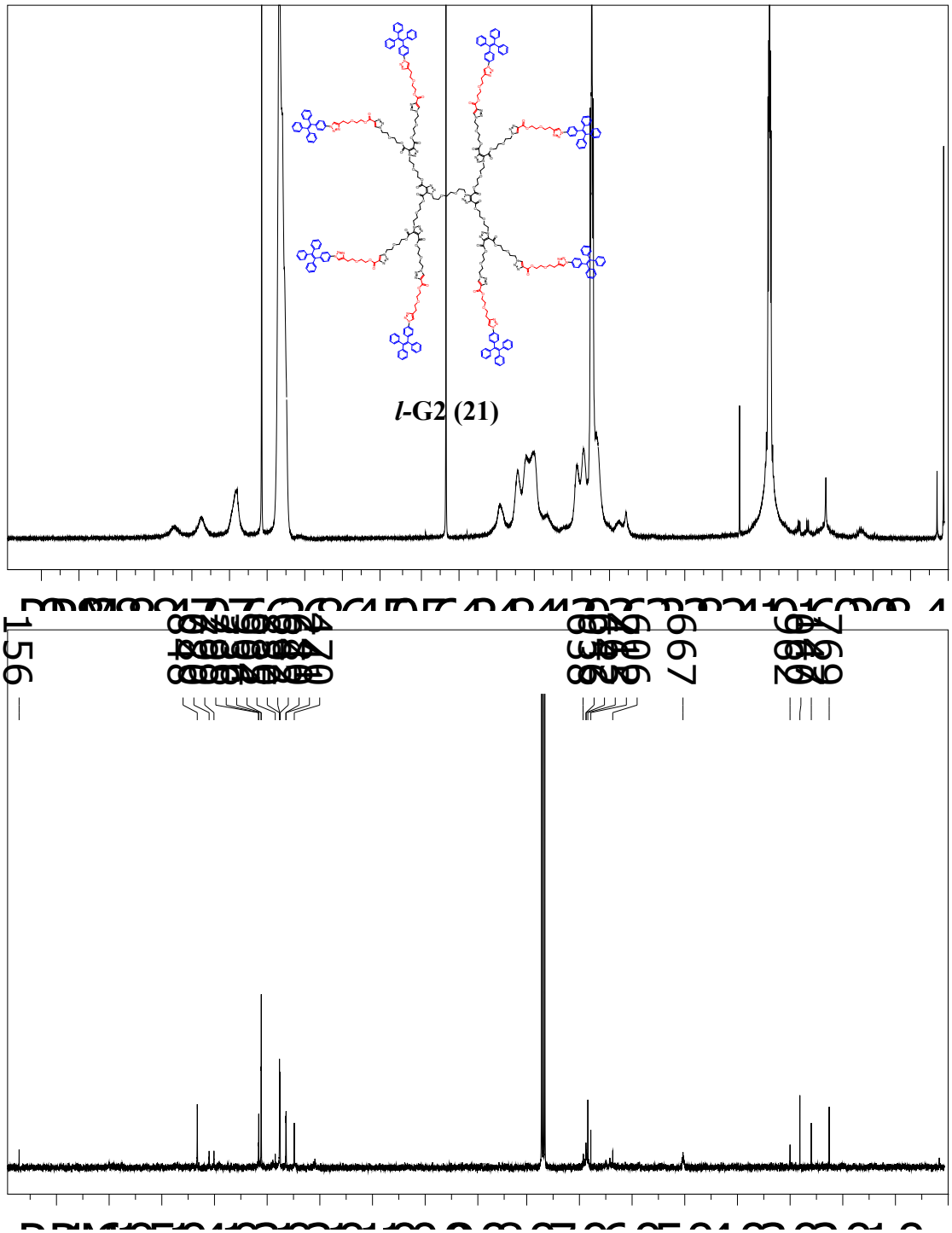
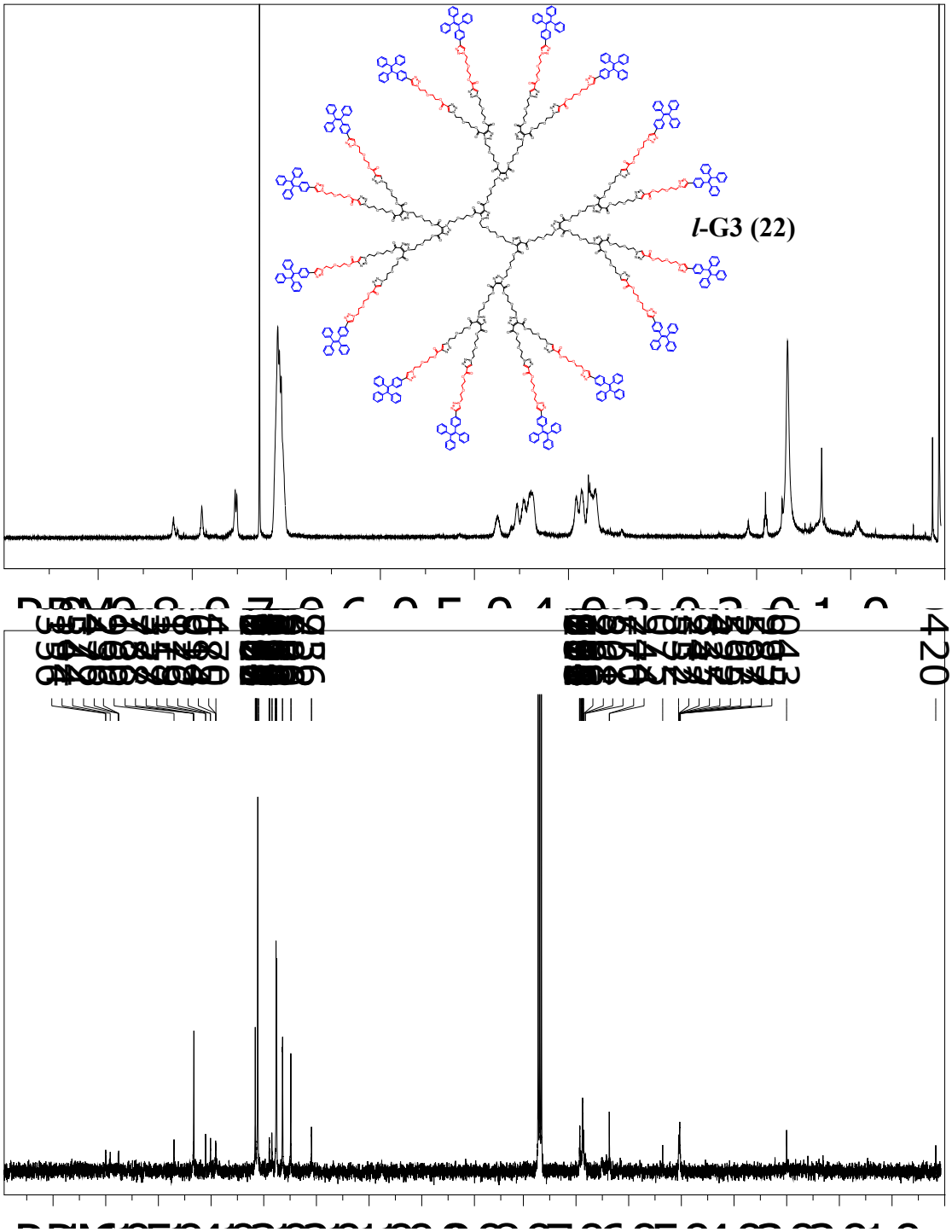

l-G1 (20)


l-G2 (21)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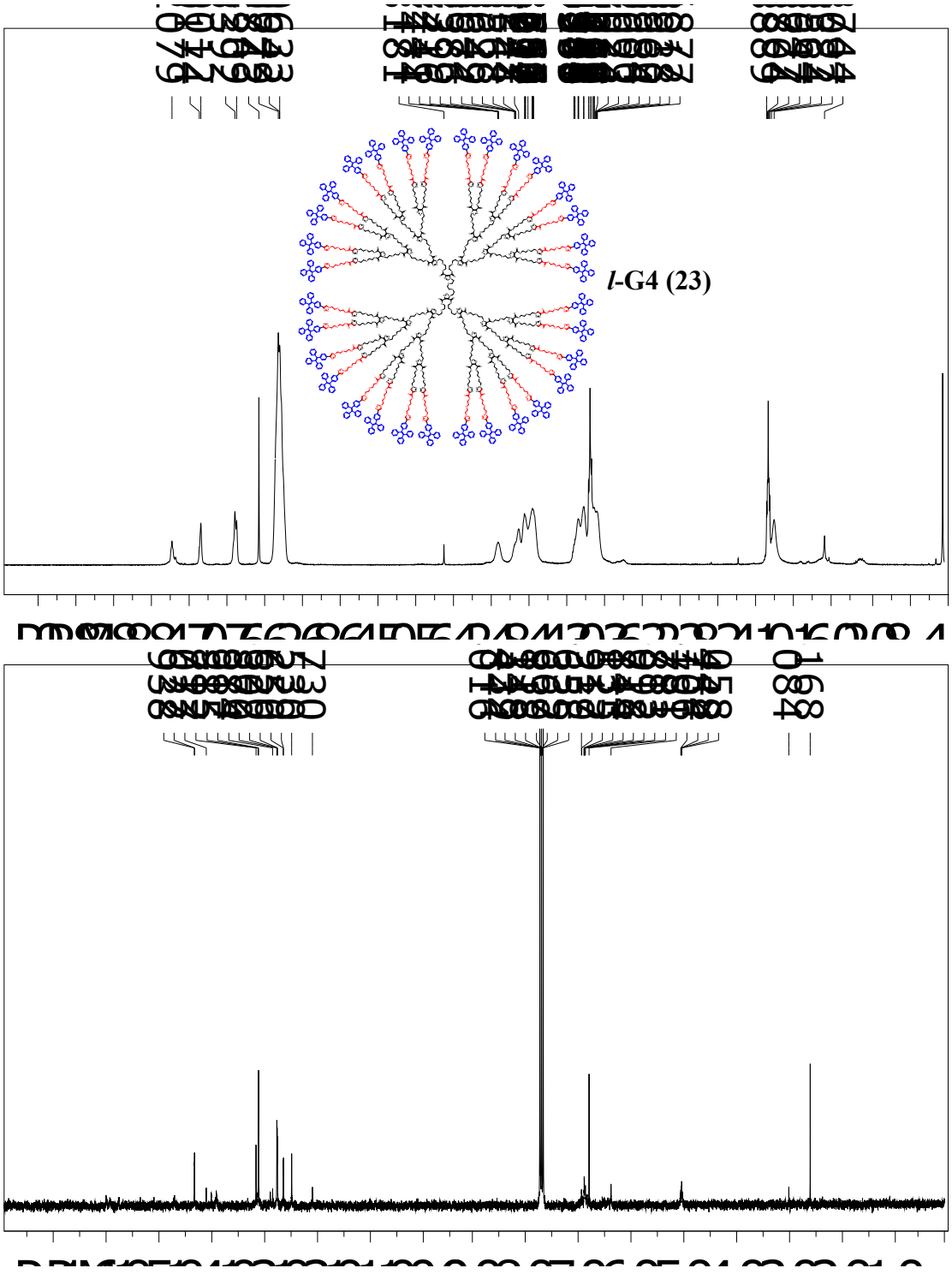

l-G4 (23)

3. Infrared spectra

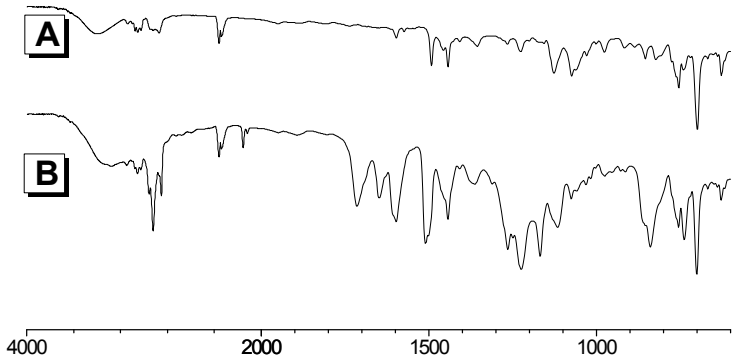


Figure S3. Infrared spectra from compound **17** (A) and compound (**19**) (B)

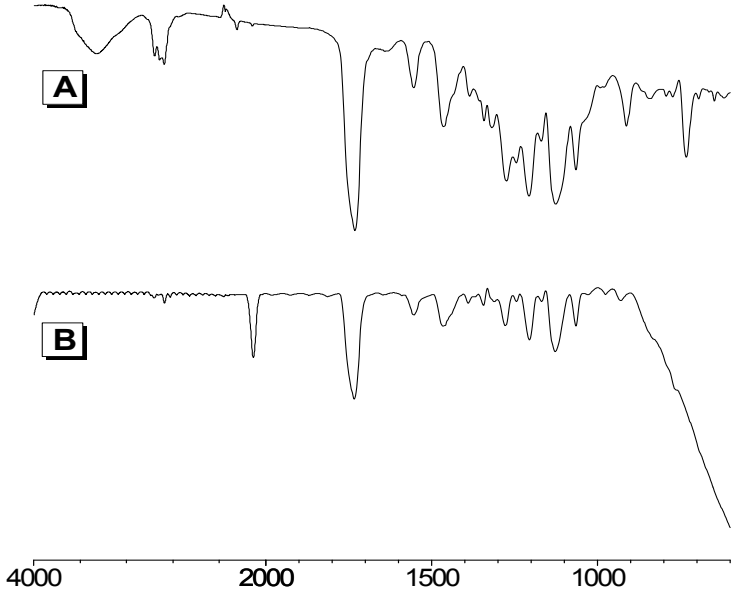


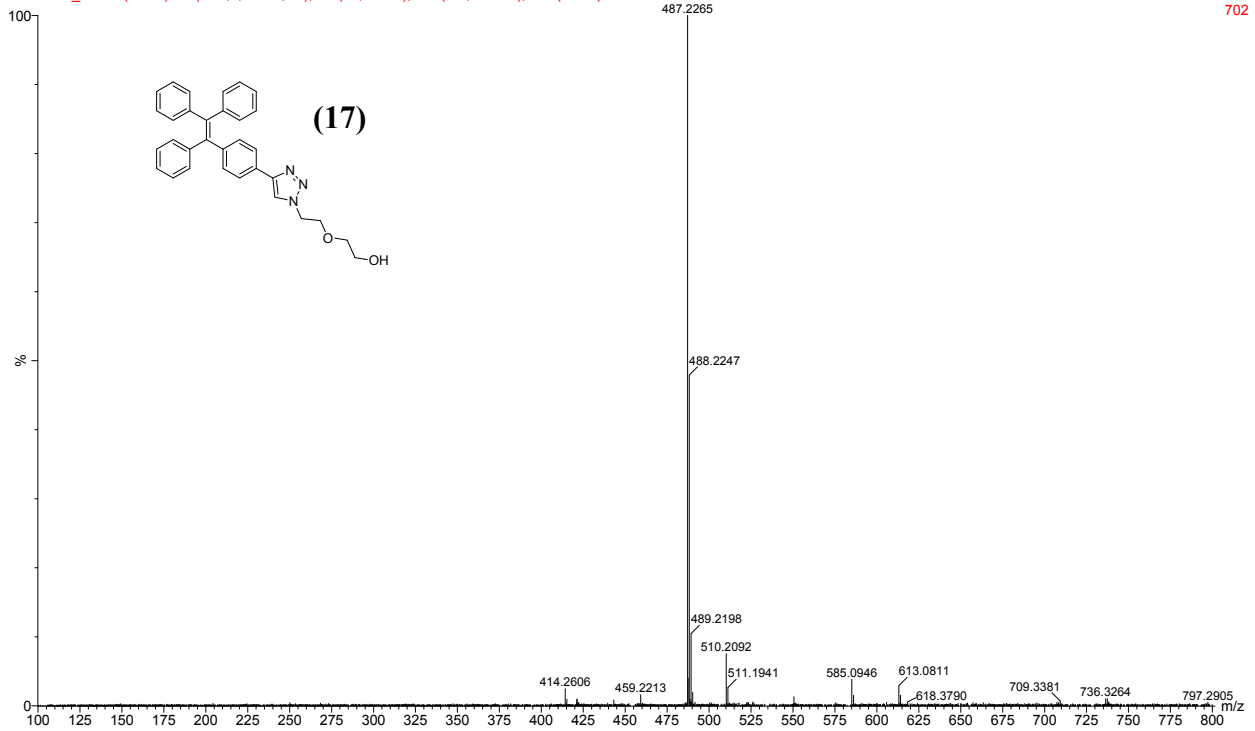
Figure S4. Infrared spectra from EO3-EO2-G4-I (**14**) (A) and EO3-EO2-G4-N_3 (**15**) (B)

4. Mass spectra

arm-HK-97-111, MW=487; DCTB

tan130419_17 22 (0.732) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (22:27)

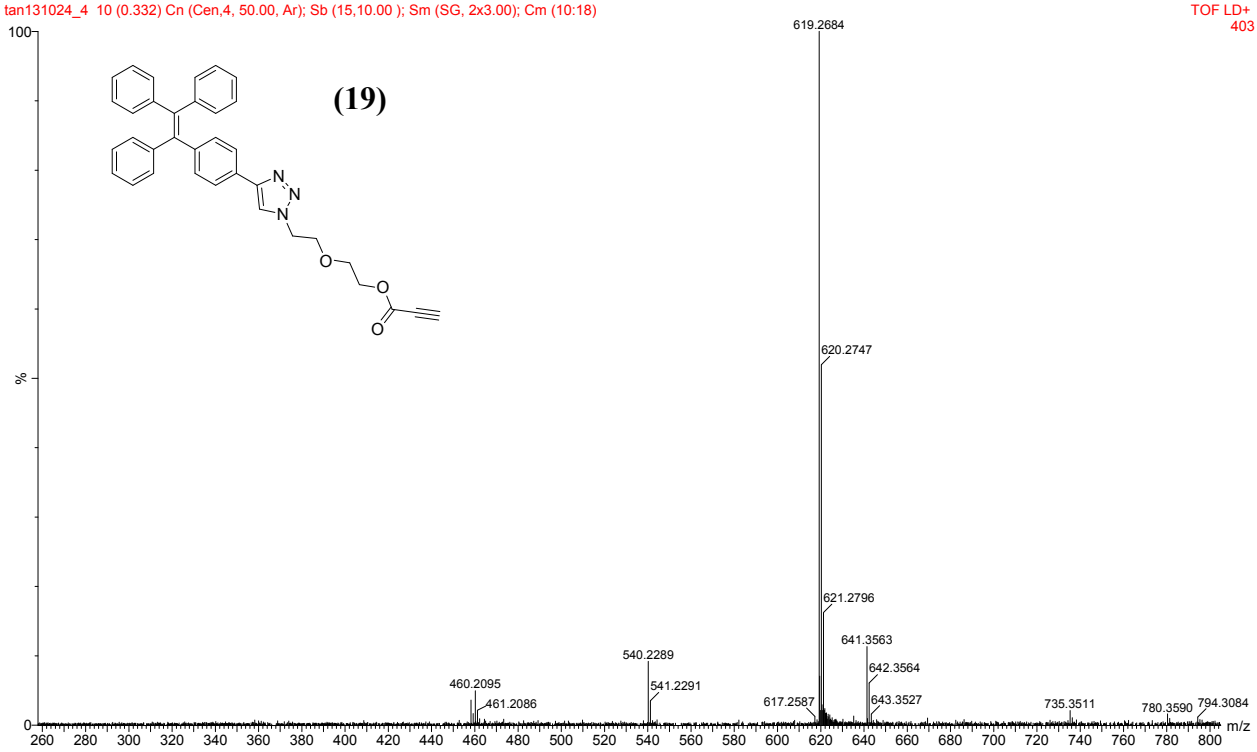
TOF LD+
702

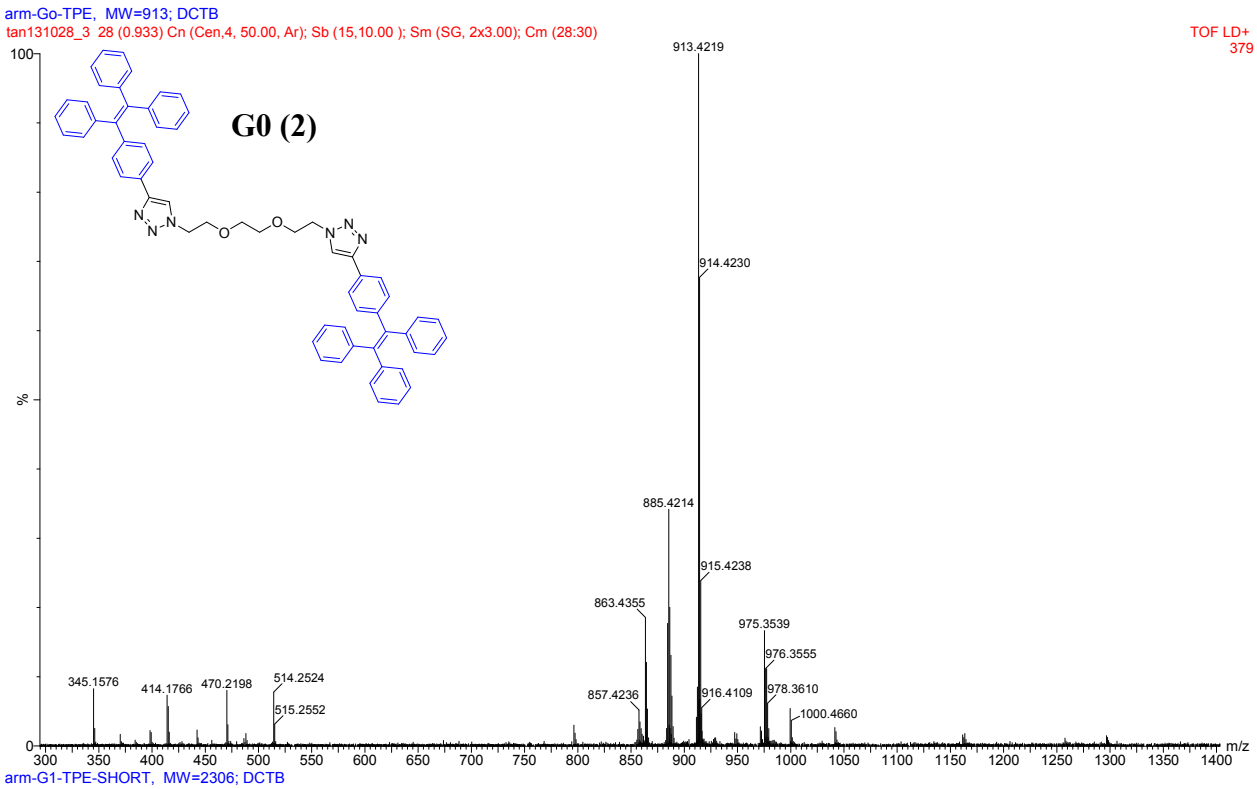


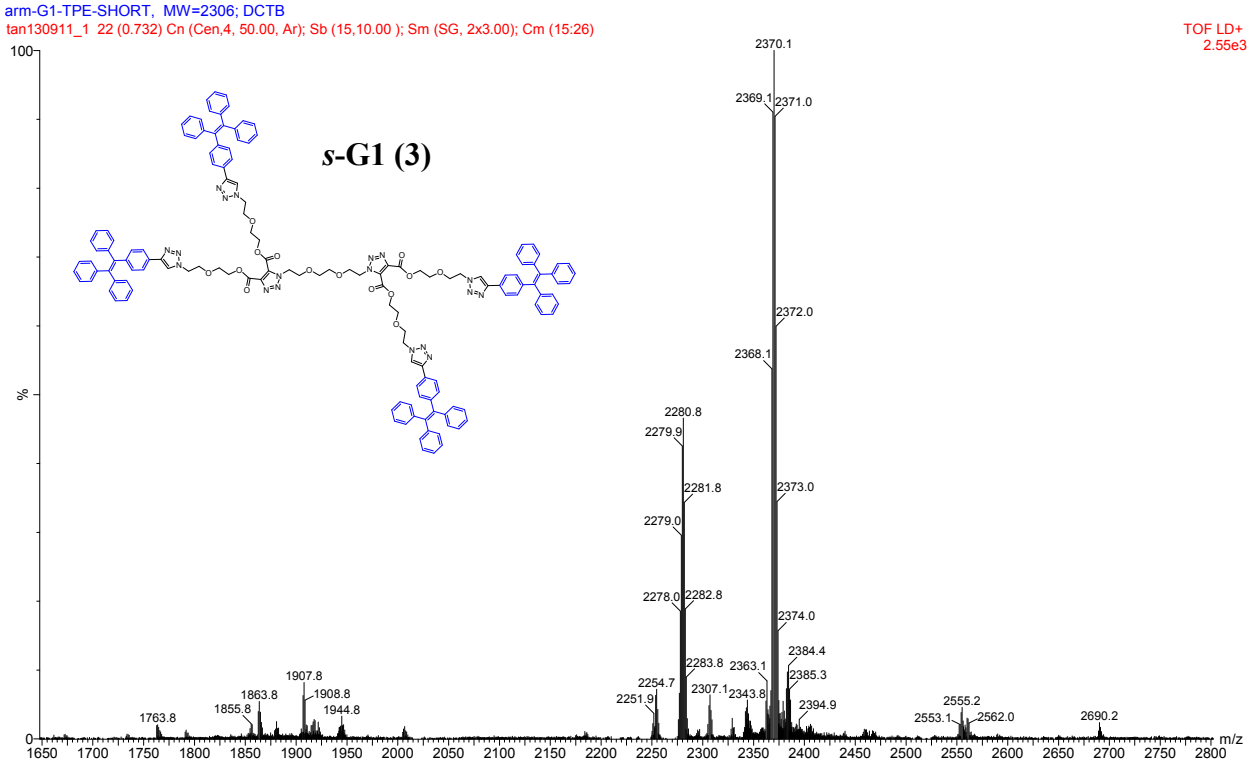
arm-TPE-PEG-ESTER, MW=539; DCTB

tan131024_4 10 (0.332) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (10:18)

TOF LD+
403




arm-Go-TPE, MW=913; DCTB
tan131028_3 28 (0.933) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (28:30)
TOF LD+
379
G0 (2)
913.4219
914.4230
885.4214
915.4238
863.4355
975.3539
976.3555
978.3610
916.4109
857.4236
1000.4660
345.1576
414.1766
470.2198
514.2524
515.2552
%
m/z


arm-G1-TPE-SHORT, MW=2306; DCTB
tan130911_1 22 (0.732) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (15:26)
TOF LD+
2.55e3
s-G1 (3)
2370.1
2369.1
2371.0
2372.0
2368.1
2280.8
2279.9
2281.8
2373.0
2279.0
2278.0
2282.8
2374.0
2384.4
2283.8
2363.1
2254.7
2385.3
2307.1
2343.8
2251.9
2394.9
1907.8
1863.8
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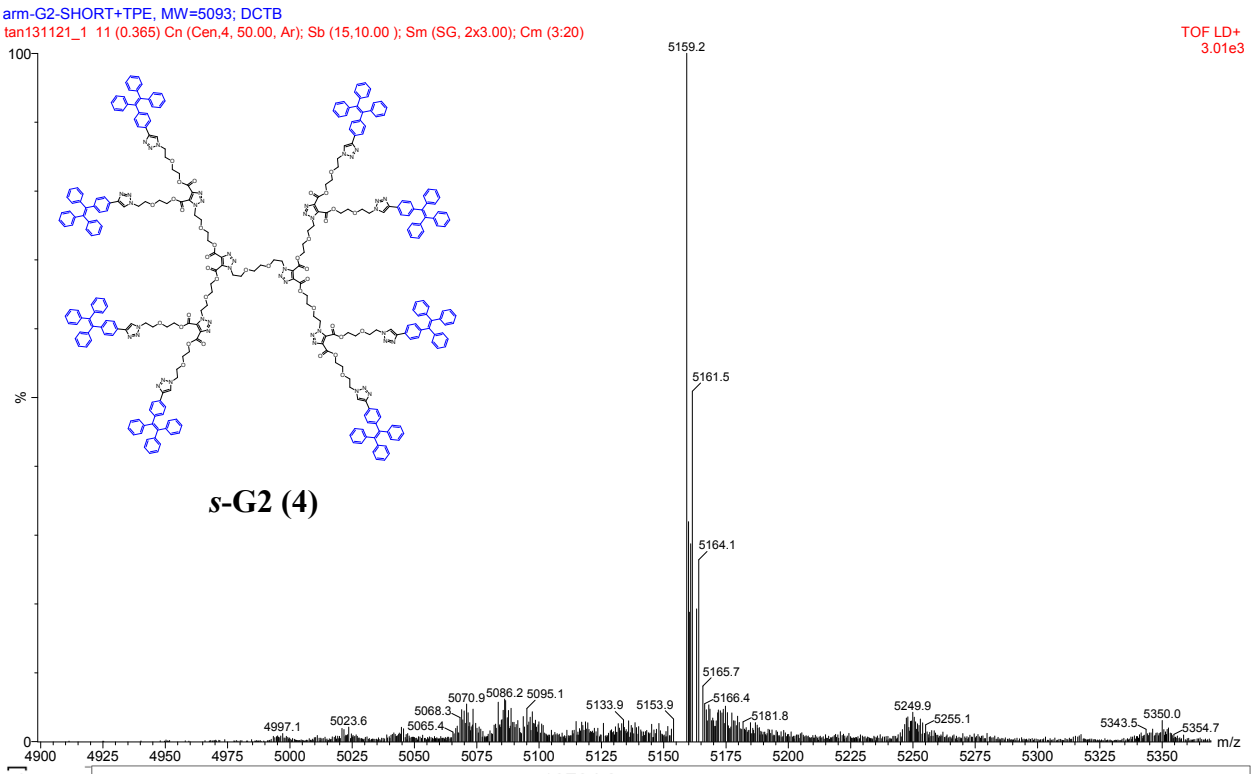
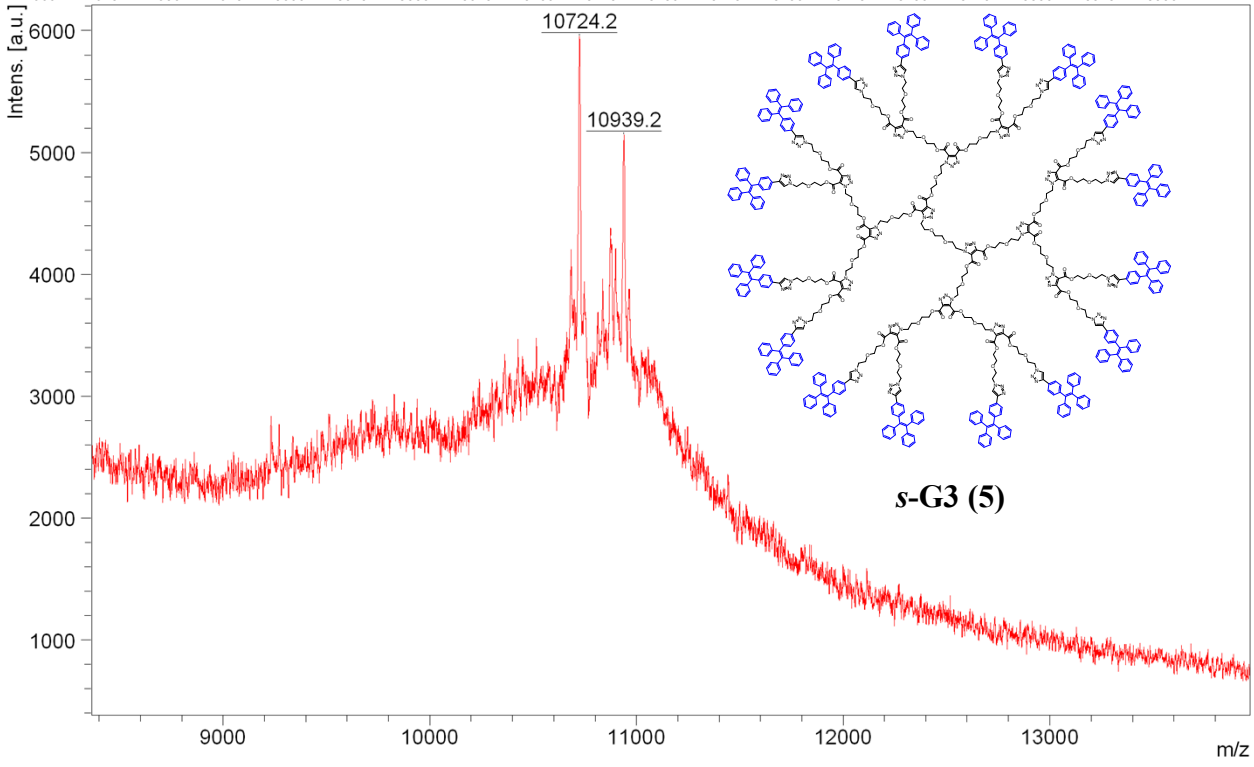
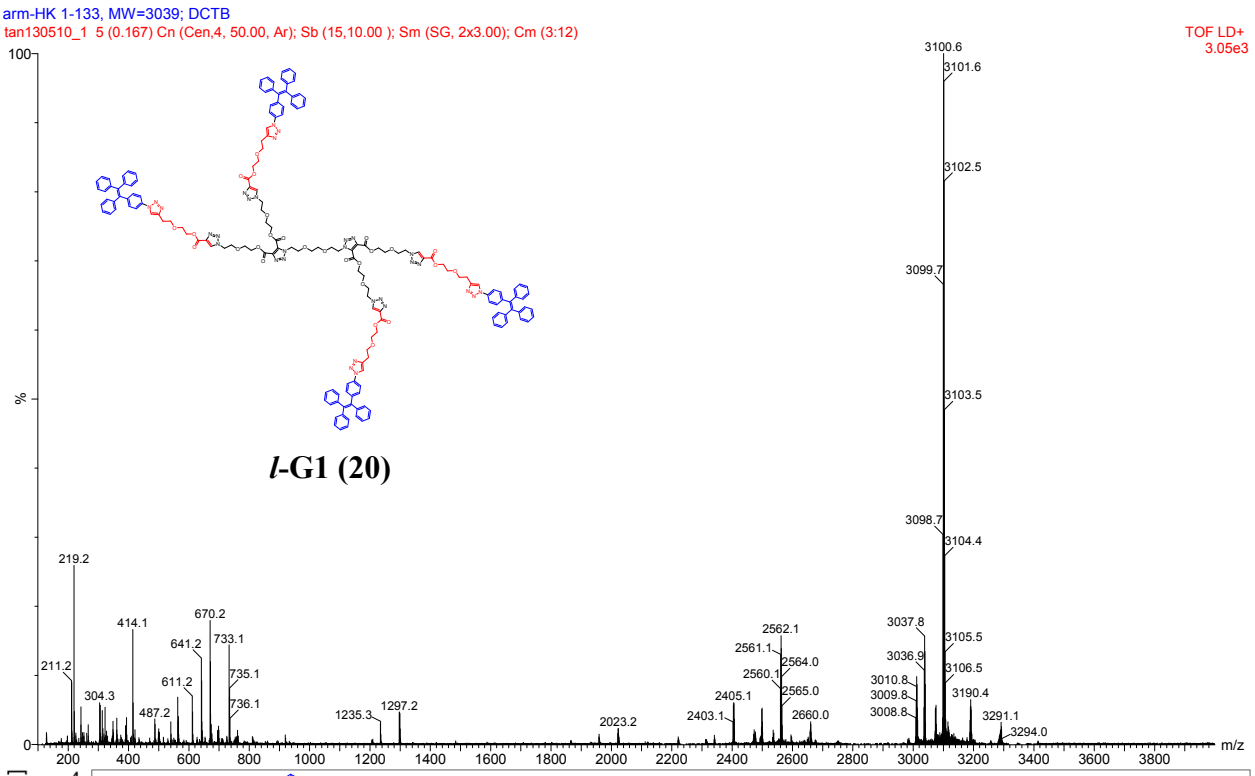
2553.1
2562.0
2690.2
%
m/z

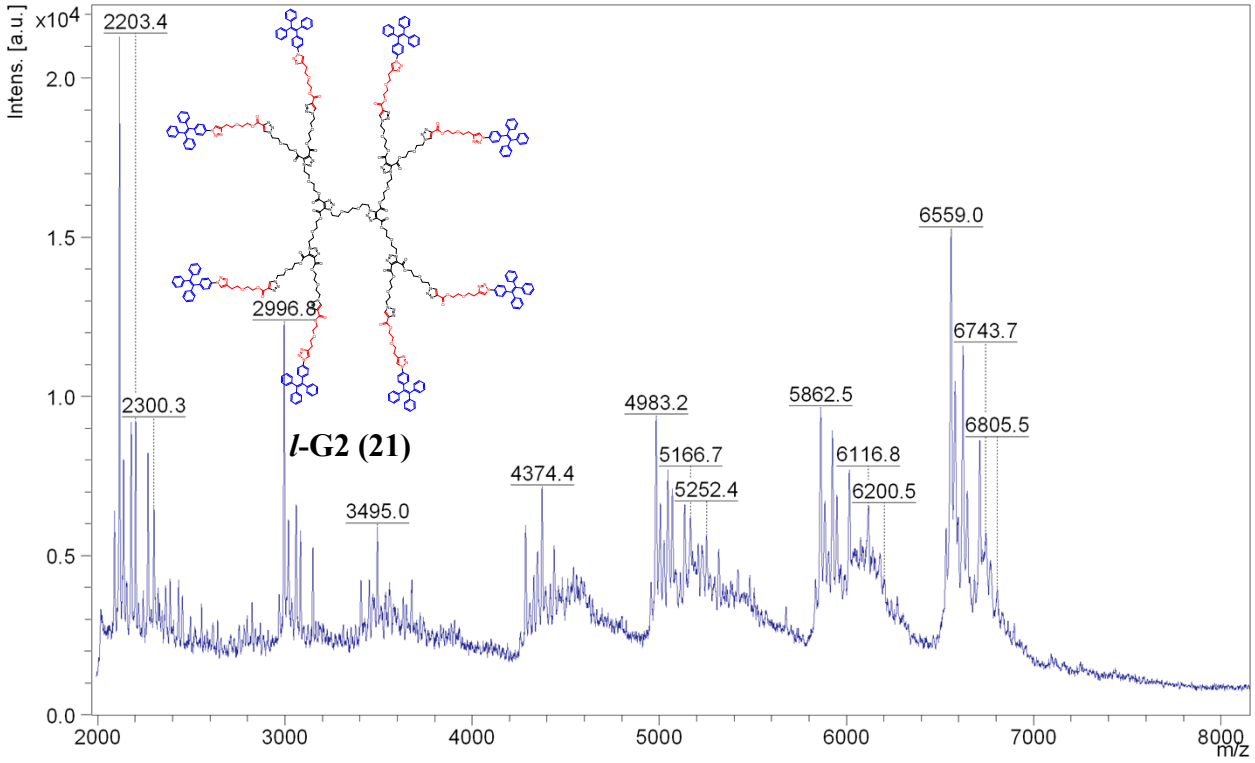

arm-G2-SHORT+TPE, MW=5093; DCTB
tan131121_1 11 (0.365) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (3:20)
TOF LD+
3.01e3
100
%
0
5159.2
5161.5
5164.1
5165.7
5166.4
5181.8
5133.9
5153.9
5086.2
5095.1
5070.9
5068.3
5065.4
5023.6
4997.1
5249.9
5255.1
5343.5
5350.0
5354.7
4900
4925
4950
4975
5000
5025
5050
5075
5100
5125
5150
5175
5200
5225
5250
5275
5300
5325
5350
m/z

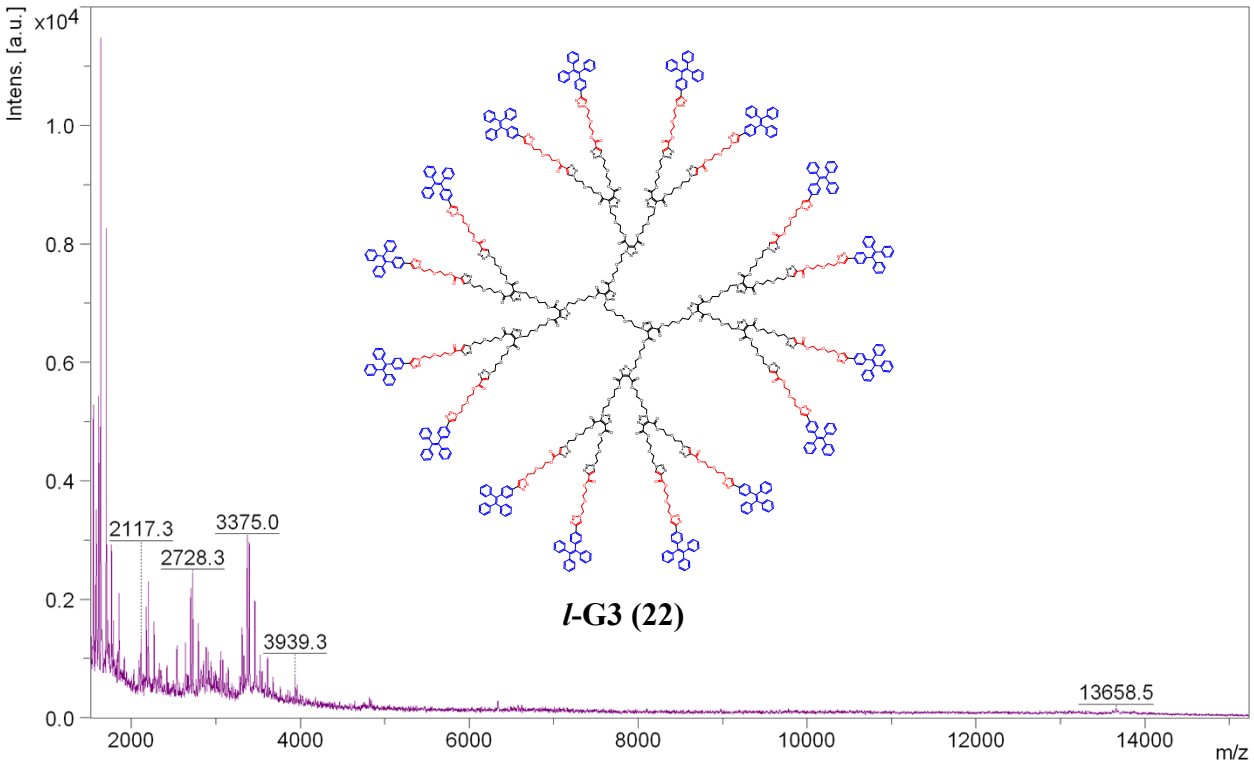
s-G2 (4)


Intens. [a.u.]
6000
5000
4000
3000
2000
1000
10724.2
10939.2
9000
10000
11000
12000
13000
m/z

s-G3 (5)


arm-HK 1-133, MW=3039; DCTB
tan130510_1 5 (0.167) Cn (Cen,4, 50.00, Ar); Sb (15,10.00); Sm (SG, 2x3.00); Cm (3:12)
TOF LD+
3.05e3
l-G1 (20)
%
m/z


l-G2 (21)
Intens. [a.u.]
x10^4
m/z


Intens. [a.u.]
x10^4
1.0
0.8
0.6
0.4
0.2
0.0
2117.3
2728.3
3375.0
3939.3
13658.5
2000
4000
6000
8000
10000
12000
14000
m/z

***l*-G3 (22)**

5. PL spectra

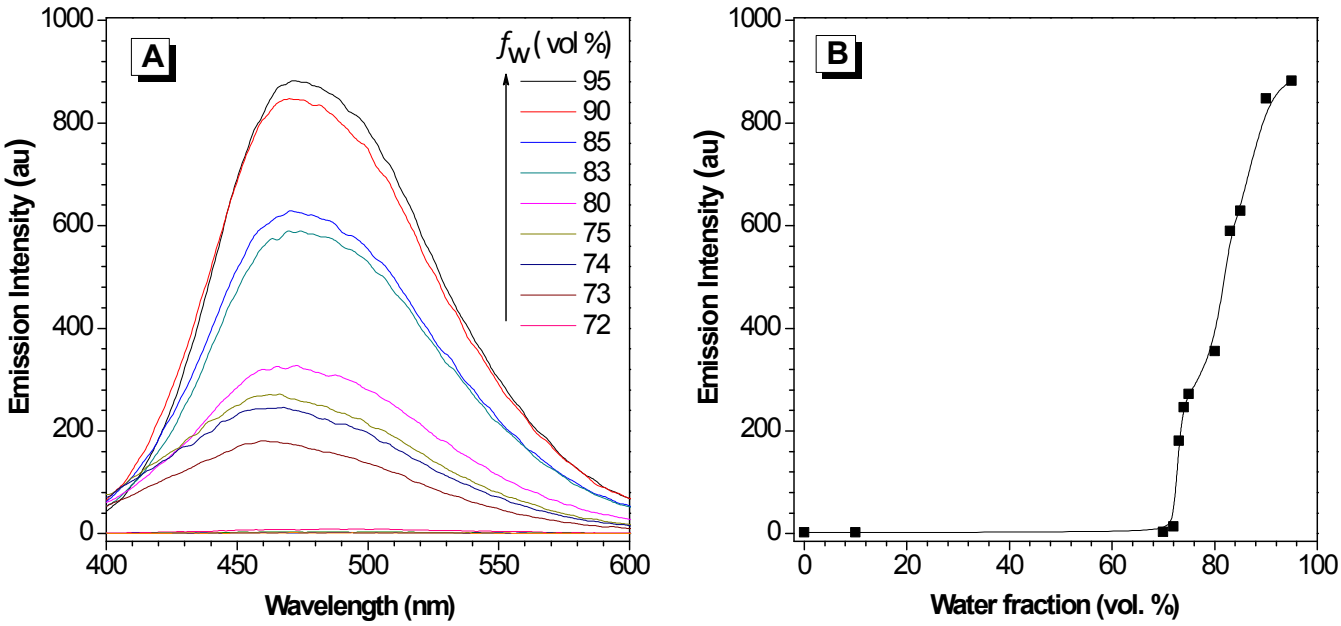


Figure. S4 (A) Emission spectra of G0 (**2**) in THF–water mixtures. (B) Plot of the intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

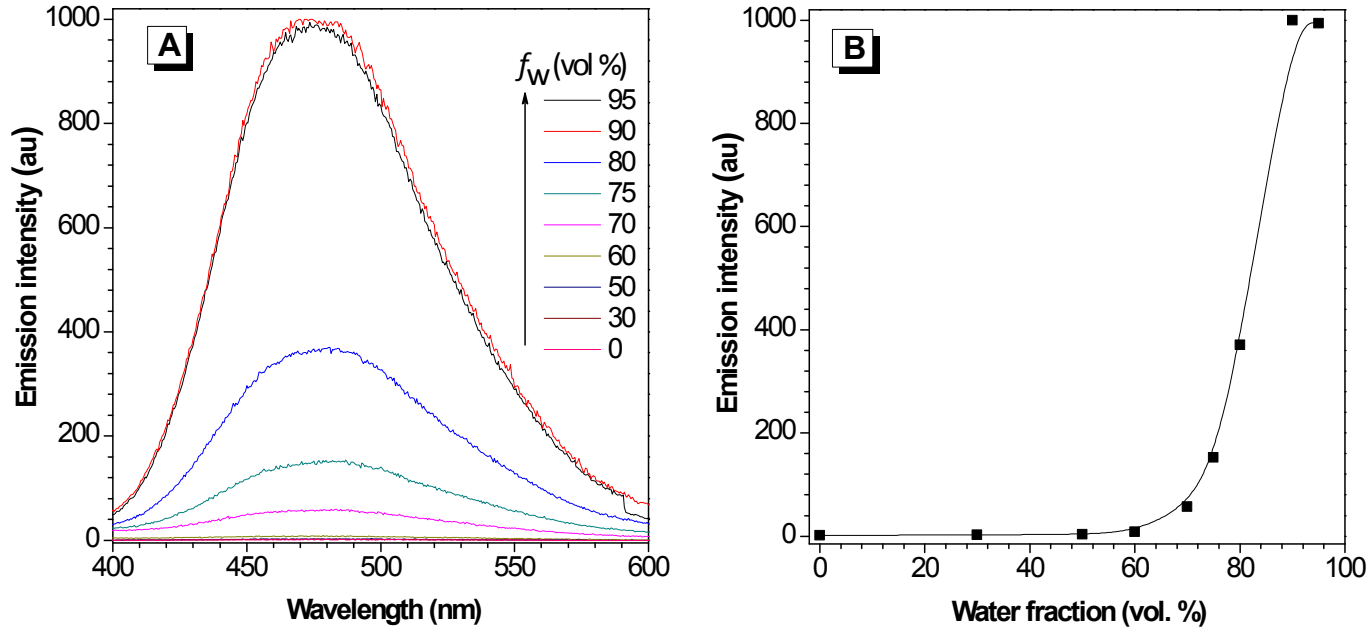


Figure. S5 (A) Emission spectra of *s*-G1 (**3**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

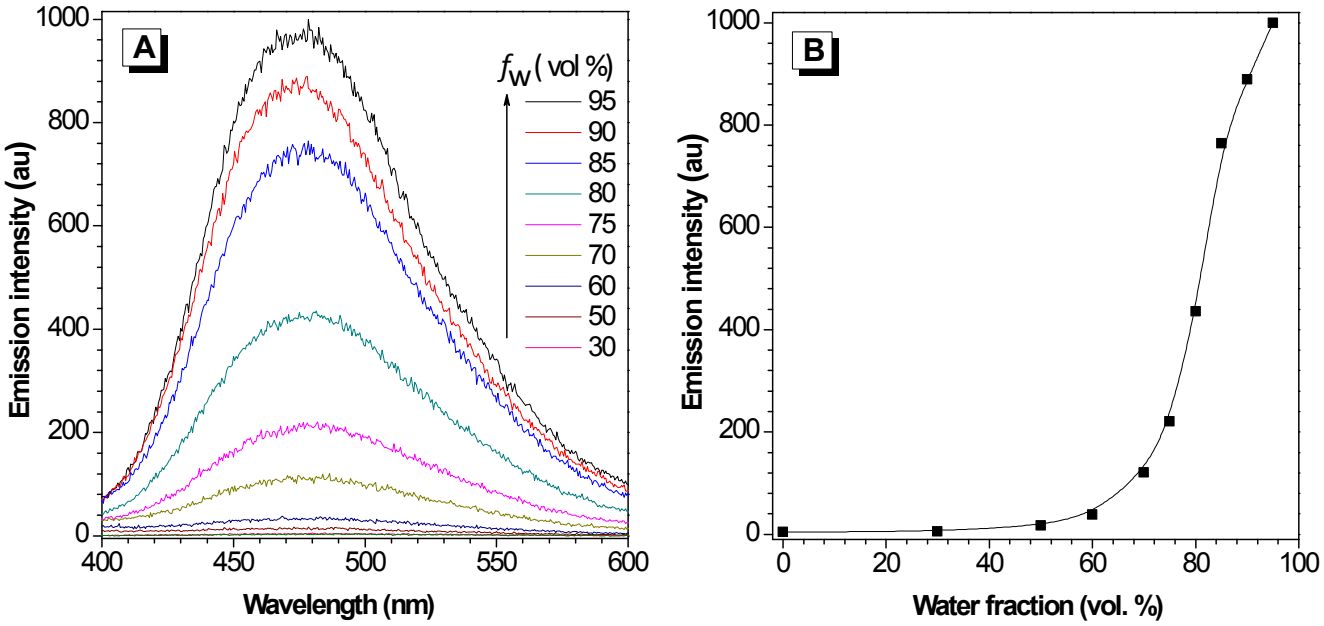


Figure. S6 (A) Emission spectra of *s*-G2 (**4**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

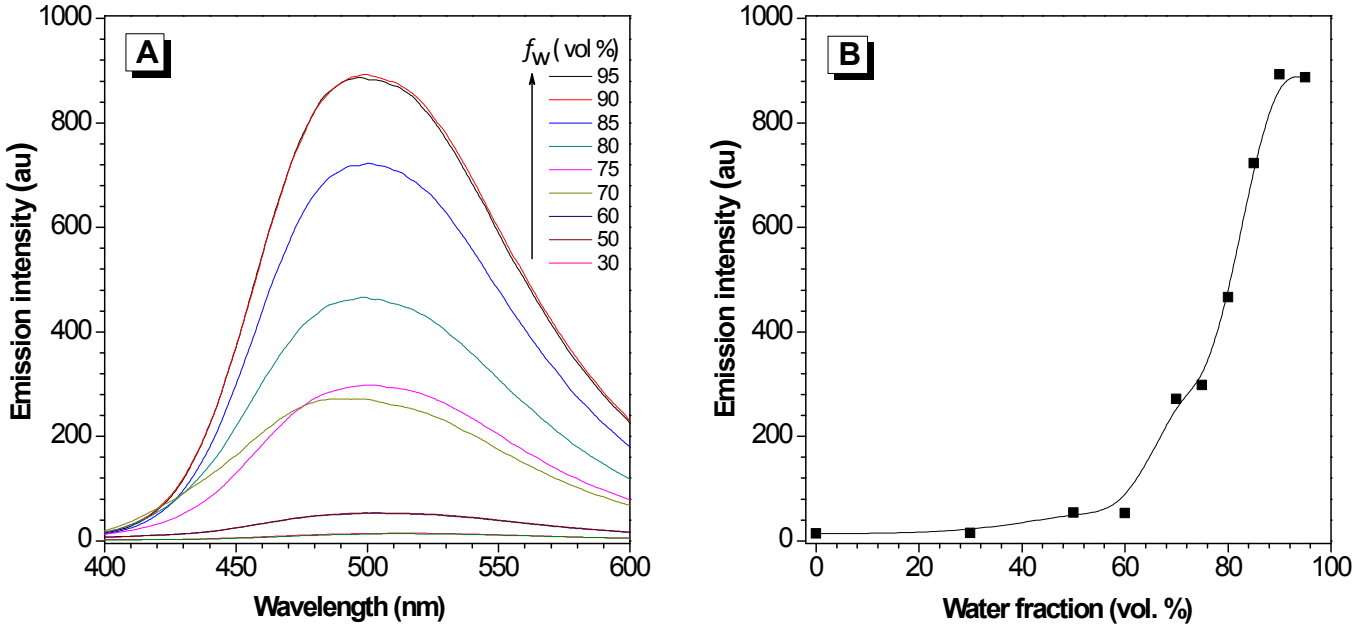


Figure. S7 (A) Emission spectra of *s*-G3 (**5**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

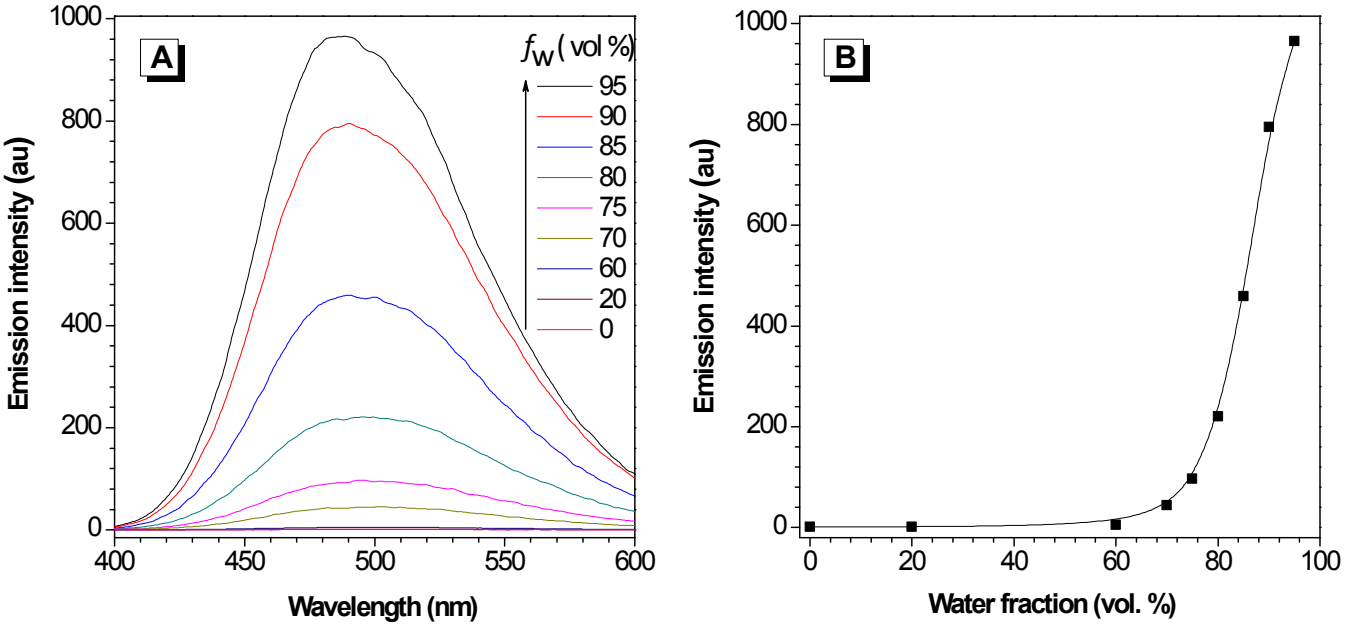


Figure. S8 (A) Emission spectra of *l*-G1 (**20**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

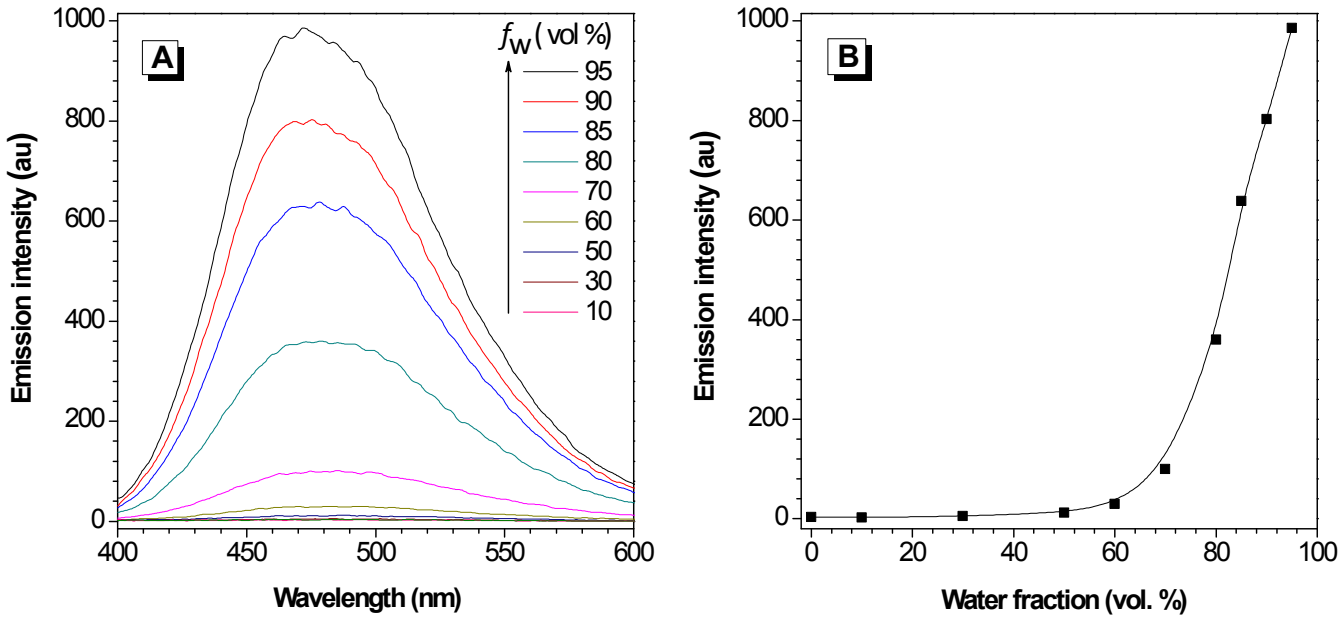


Figure. S9 (A) Emission spectra of *l*-G2 (**21**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

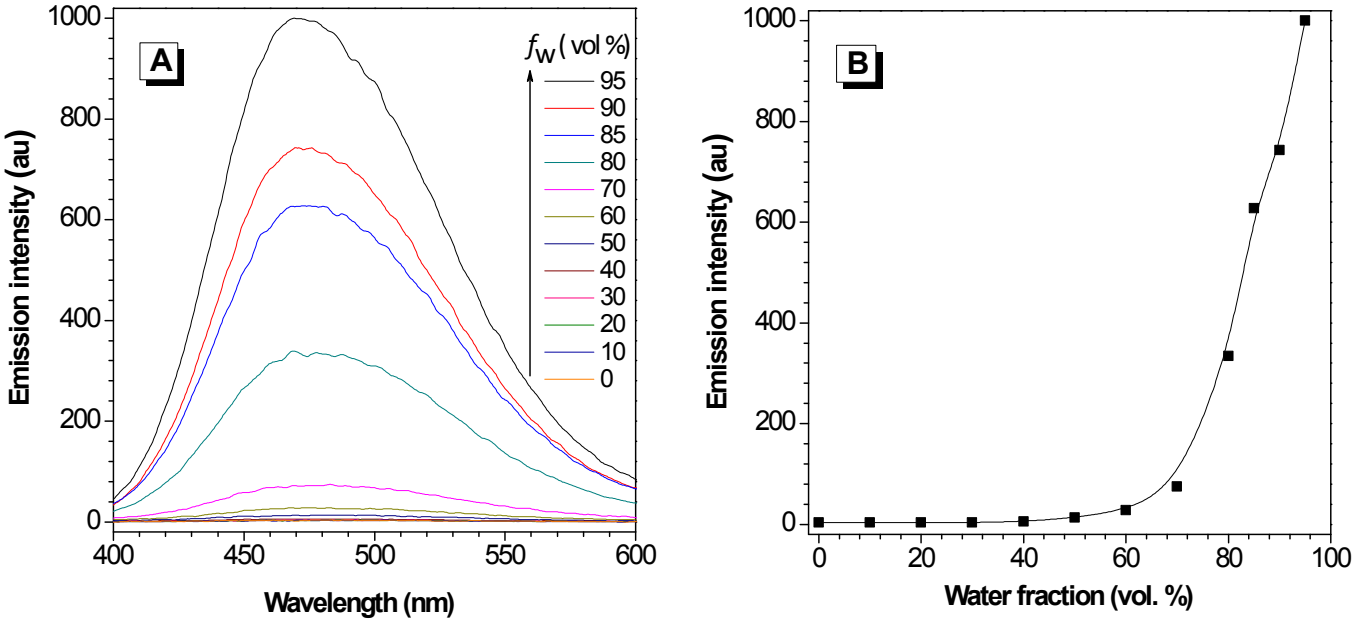


Figure. S10 (A) Emission spectra of *l*-G3 (**22**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

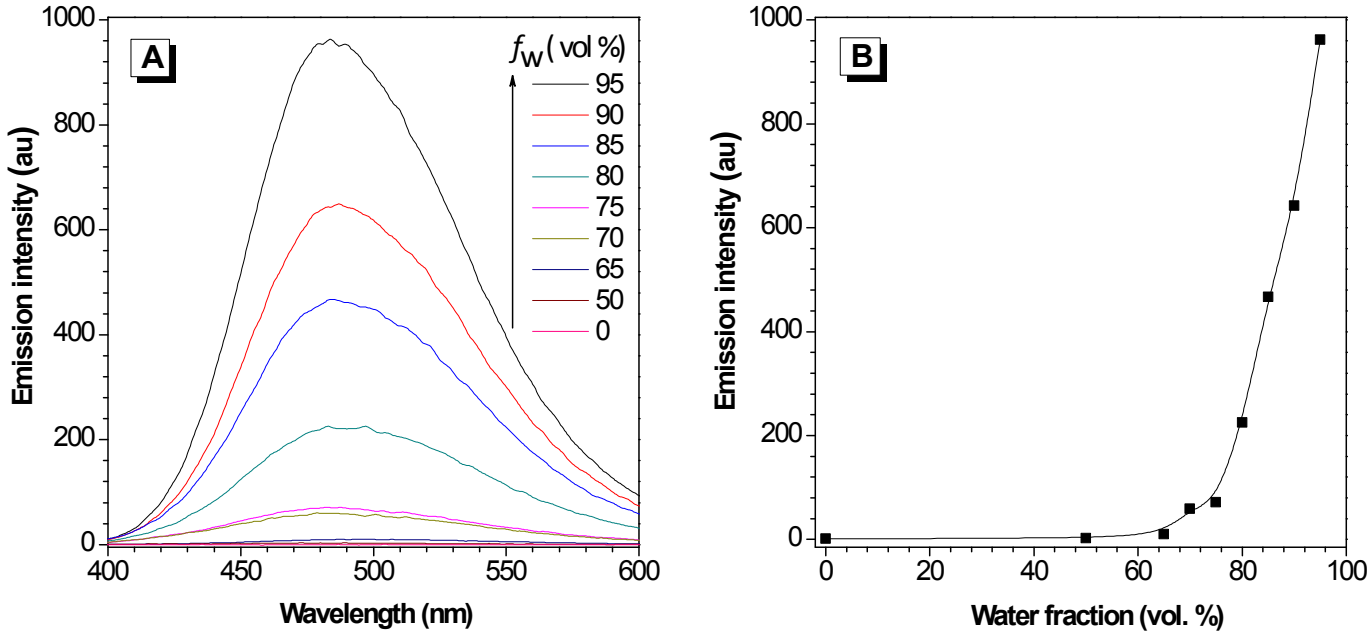


Figure. S11 (A) Emission spectra of *l*-G4 (**23**) in THF–water mixtures. (B) Plot of intensity values versus the compositions of the aqueous mixtures. Solution concentration: 10^{-5} M; excitation wavelength: 327 nm.

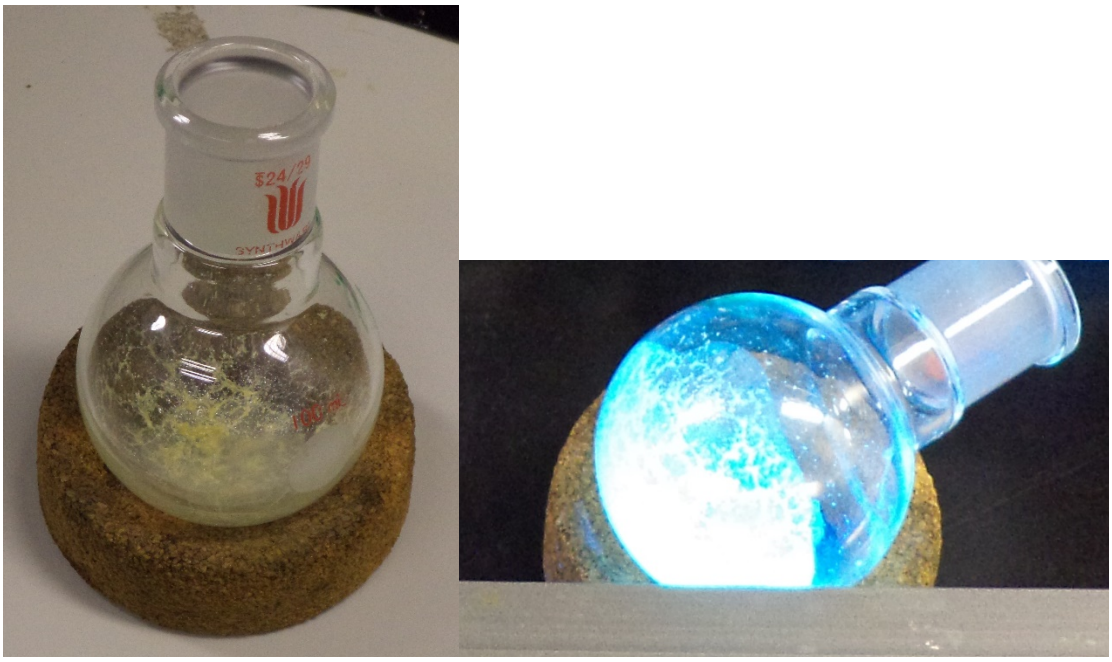


Figure S12. (A) G4-*l* (**23**) dried in a flask. It is a yellow flaky solid. (B) The very same flask exposed to UV light.