Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Amphiphilic Oligoamides as Versatile, Acid-Responsive Gelators

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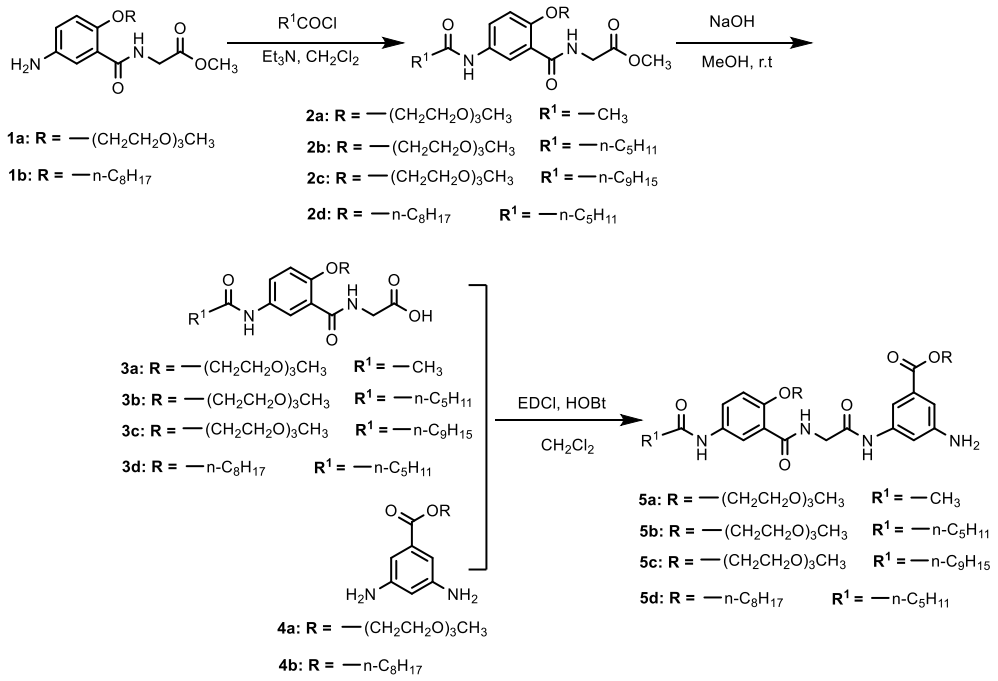
1. Synthesis and Characterization



Scheme S1 Synthetic route to compound **5a-d**

Compounds **1a**, **1b**, **4a** and **4b** were prepared according to the previously reported method.[S1-S7]

General procedure for the synthesis of compounds 2a-2d. A solution of appropriate acid chloride (15.0 mmol) in CH_2Cl_2 (50 mL) was added to a solution of amine **1a** or **1b** (15.0 mmol) and triethylamine (15.0 mmol) in CH_2Cl_2 (100 mL) over a period of 30 minutes at 0 ^oC. After addition, the ice-water bath was removed, and the reaction mixture was allowed to warm to room temperature. After 4 hrs, the solvent was washed with 1 M HCl, saturated aqueous $NaHCO_3$ and NaCl solution in sequence, dried over anhydrous Na_2SO_4 and then concentrated in vacuo. The residue was purified by column chromatography (petroleum ether / acetone = 4 / 1).

Compound 2a. White solid (5.1 g, 82%). IR (KBr, cm^{-1}): 3423, 3354, 3308, 2956, 2894, 2875, 1759, 1687, 1636, 1551, 1499, 1370, 1319, 1251, 1207, 1099. ^1H NMR (400 MHz, $CDCl_3$): δ 8.75 (t, *J* = 5.0 Hz, 1H), 815 (dd, *J* = 9.0, 2.8 Hz, 1H), 7.84 (d, *J* = 2.8 Hz, 1H), 6.93 (d, *J* = 9.0 Hz, 1H), 4.26-4.23 (m, 4H), 3.93 (m, 2H), 3.76 (s, 3H), 3.70 (m, 2H), 3.65-3.62 (m, 4H), 3.51 (m, 2H), 3.35 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.49, 168.95, 165.30, 153.33, 132.72, 125.51, 123.27, 121.20,

113.76, 71.92, 70.69, 70.63, 70.59, 69.21, 68.77, 59.02, 52.24, 41.89, 24.27. ESI-MS: *m/z* calcd for $C_{19}H_{28}N_2O_8$: 412.18; found: 413.34 $[M + H]^+$.

Compound 2b. White solid (6.1 g, 87%). IR (KBr, cm^{-1}): 3378, 3323, 2956, 2931, 2874, 1741, 1682, 1635, 1543, 1498, 1277, 1245, 1215, 1109. ^1H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 8.21 (dd, *J* = 8.9, 2.8 Hz, 1H), 7.80 (s, 1H), 7.54 (s, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 4.28-4.24 (m, 4H), 3.94 (m, 2H), 3.76 (s, 3H), 3.71 (m, 2H), 3.65-3.60 (m, 4H), 3.52 (m, 2H), 3.35 (s, 3H), 2.35 (t, *J* = 7.6 Hz, 2H), 1.71 (m, 2H), 1.36-1.32 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.95, 170.44, 165.22, 153.21, 132.76, 125.40, 123.20, 121.18, 113.69, 71.89, 70.66, 70.60, 70.57, 69.19, 68.76, 58.98, 52.19, 41.85, 37.36, 31.48, 25.36, 22.51, 13.97. ESI-MS: *m/z* calcd for $C_{23}H_{36}N_2O_8$: 468.25; found: 469.43 $[M + H]^+$.

Compound 2c. White solid (6.4 g, 81%). IR (KBr, cm^{-1}): 3449, 3326, 2921, 2870, 2851, 1750, 1692, 1539, 1501, 1361, 1305, 1218, 1125. ^1H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 8.19 (d, *J* = 8.9 Hz, 1H), 7.78 (s, 1H), 7.28 (s, 1H), 6.93 (d, *J* = 8.9 Hz, 1H), 4.27 (m, 4H), 3.94 (m, 2H), 3.78 (s, 3H), 3.73-3.51 (m, 8H), 3.36 (s, 3H), 2.34 (m, 2H), 1.69 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.11, 167.50, 162.31, 150.24, 129.88, 122.46, 120.29, 118.20, 110.72, 68.94, 67.69, 67.64, 67.58, 66.24, 65.80, 56.01, 49.22, 38.91, 34.42, 28.94, 26.55, 26.42, 26.36, 22.74, 19.72, 11.17. ESI-MS: *m/z* calcd for $C_{27}H_{44}N_2O_8$: 524.31; found: 525.52 $[M + H]^+$.

Compound 2d. White solid (4.8 g, 71%). ^1H NMR (400MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.19 (dd, *J* = 9.0, 2.7 Hz, 1H), 7.81 (d, *J* = 2.6 Hz, 1H), 7.28 (s, 1H), 6.96 (d, *J* = 9.0 Hz, 1H), 4.27 (d, *J* = 4.8 Hz, 2H), 4.13 (t, *J* = 6.6 Hz, 2H), 3.79 (s, 3H), 2.35 (t, *J* = 7.5 Hz, 2H), 2.04-1.84 (m, 2H), 1.78-1.69 (m, 2H), 1.50-1.27 (m, 14H), 0.90 (m, 6H).

General procedure for the synthesis of compounds 3a-3d. Compound **2a-2d** (10.0 mmol) was dissolved in MeOH (100 mL), to which the solution of KOH (20.0 mmol, 2 M) was added. The mixture was heated to reflux for 4 hrs. Then, MeOH was removed in vacuo. The aqueous layer was acidified with concentrated HCl until pH = 1, which was extracted with dichloromethane (50 mL × 3). The orginc phase was

dried over anhydrous sodium sulfate, filtered and the solvent was removed under reduced pressure. The residue was purified by column chromatography (CH_2Cl_2 / CH_3OH = 30 / 1).

Compound 3a. White solid (3.8 g, 96%). IR (KBr, cm^{-1}): 3466, 3370, 2931, 2890, 1733, 1647, 1555, 1499, 1252, 1216, 1198, 1102. ^1H NMR(400 MHz, DMSO-*d6*): δ 9.96 (s, 1H), 8.61 (dd, *J* = 8.9, 2.8 Hz, 1H), 8.02 (s, 1H), 7.81 (s, 1H), 7.14 (d, *J* = 9.0 Hz, 1H), 4.24 (m, 2H), 4.01 (m, 2H), 3.82 (m, 2H), 3.60 (m, 2H), 3.53-3.48 (m, 4H), 3.41 (m, 2H), 3.22 (s, 3H), 2.02 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d6*): δ 171.18, 168.06, 164.28, 152.37, 133.13, 123.61, 121.75, 121.50, 114.38, 71.25, 69.86, 69.80, 69.57, 68.82, 68.57, 58.04, 41.44, 23.81. ESI-MS: *m/z* calcd for $C_{18}H_{25}N_2O_8$: 398.17; found: 399.32 $[M + H]^+$.

Compound 3b. White solid (4.4 g, 96%). IR (KBr, cm^{-1}): 3490, 3389, 3305, 2955, 2933, 2870, 2619, 2503, 1727, 1681, 1551, 1498, 1450, 1286. ^1H NMR (400 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.19 (dd, *J* = 8.9, 2.8 Hz, 1H), 7.81 (s, 1H), 7.52 (s, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 4.29 (m, 4H), 3.92 (m, 2H), 3.72-3.61 (m, 8H), 3.37 (s, 3H), 2.36 (t, *J* = 7.6 Hz, 2H), 1.72 (m, 2H), 1.35 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.50, 171.36, 165.62, 153.40, 132.64, 125.60, 123.28, 120.75, 113.63, 71.90, 70.73, 70.65, 70.36, 69.28, 68.84, 58.90, 42.46, 37.38, 31.53, 25.43, 22.52, 14.02. ESI-MS: *m/z* calcd for $C_{22}H_{34}N_2O_8$: 454.23; found: 455.41 $[M + H]^+$.

Compound 3c. White solid (3.2 g, 63%). IR (KBr, cm^{-1}): 3504, 3389, 3309, 2926, 2855, 1730, 1645, 1546, 1497, 1258, 1214, 1105. ^1H NMR(400 MHz, $CDCl_3$) δ 8.85 (s, 1H),8.18 (s, 1H), 8.02 (s, 1H), 7.81 (s, 1H), 7.55 (s, 1H), 4.27 (m, 4H), 3.91 (m, 2H), 3.71-3.61 (m, 8H), 3.41 (s, 3H), 2.36 (t, *J* = 7.0 Hz, 1H), 1.70 (m, 2H), 1.26 (m, 12H), 0.88 (t, *J* = 6.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.29, 170.97, 165.14, 152.93, 132.23, 125.18, 122.89, 120.17, 113.08, 71.43, 70.23, 70.15, 69.92, 68.78, 68.32, 58.42, 41.95, 36.91, 31.50, 29.12, 29.00, 28.94, 25.37, 22.28, 13.74. ESI-MS: *m/z* calcd for $C_{26}H_{42}N_2O_8$: 510.29; found: 511.32 $[M + H]^+$.

Compound 3d. White solid (3.3 g, 75%). ^1H NMR (400MHz, $CDCl_3$) δ 8.78 (t, J = 4.7 Hz, 1H), 8.16 (dd, J = 9.0, 2.7 Hz, 1H), 7.97 (s, 1H), 7.83 (d, J = 2.7 Hz, 1H), 6.92

(d, J = 9.1 Hz, 1H), 4.27 (d, J = 4.8 Hz, 2H), 4.09 (t, J = 6.7 Hz, 2H), 2.36 (t, J = 7.6 Hz, 2H), 1.96 – 1.82 (m, 2H), 1.78 – 1.63 (m, 2H), 1.47 – 1.22 (m, 14H), 0.87 (q, J = 6.9 Hz, 6H).

General procedure for the synthesis of compounds 5a-5d. The appropriate acid **3a-3d** (10.0 mmol), 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide (EDCl, 12.0 mmol) and N-hydroxybenzotriazole (HOBt, 12.0 mmol) were dissolved in dry CH_2Cl_2 (50 mL). After stirring at room temperature for 30 minutes, the solution was added dropwise over a period of 10 minutes to the solution of 3,5-diaminobenzoate (**4a** or **4b**, 10.0 mmol) in CH_2Cl_2 (100 mL). Stirring was continued for 20 hrs. Then, the solvent was extracted with water (50 mL × 3), saturated brine (50 mL × 1). The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography (CH_2Cl_2 / CH_3OH = 15 / 1).

Compound 5a. White solid (3.7 g, 54%). IR (KBr, cm^{-1}): 3420, 3375, 3347, 3278, 3246, 3163, 3109, 2928, 2887, 1698, 1636, 1538, 1243, 1220, 1109. ^{1}H NMR (400 MHz，$CDCl_3$): δ 10.00 (s, 1H), 9.96 (s, 1H), 8.70 (t, *J* = 5.3 Hz, 1H), 8.05 (d, *J* = 2.8 Hz, 1H), 7.81 (dd, *J* = 8.9, 2.8 Hz, 1H), 7.35 (s, 1H), 7.17 (s, 1H), 7.15 (s, 1H), 6.92 (s, 1H), 5.44 (s, 2H), 4.33 (m, 2H), 4.27 (m, 2H), 4.15 (m, 2H), 3.87 (m, 2H), 3.72 (m, 2H), 3.61-3.35 (m, 16H), 3.21 (s, 3H), 3.18 (s, 3H), 2.02 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d6*): δ 168.03, 167.33, 166.13, 164.26, 152.42, 149.43, 139.65, 133.08, 130.51, 123.55, 121.77, 121.59, 114.29, 109.78, 108.74, 107.80, 71.24, 71.19, 69.89, 69.86, 69.76, 69.62, 69.50, 68.87, 68.62, 68.44, 63.82, 58.00, 57.97, 43.50, 23.80. ESI-MS: *m/z* calcd for $C_{32}H_{46}N_2O_8$: 678.31; found: 679.60 $[M + H]^+$.

Compound 5b. White solid (4.2 g, 57%). IR (KBr, cm^{-1}): 3456, 3369, 3310, 3278, 3249, 3162, 3110, 2951, 2927, 2871, 1700, 1690, 1636, 1560, 1539, 1497, 1244, 1223, 1107, 1053. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.75 (s, 1H), 9.21 (s, 1H), 8.79 (s, 1H), 8.24 (d, *J* = 6.7 Hz, 1H), 7.84 (s, 3H), 7.78 (s, 1H), 7.39 (s, 1H), 7.02 (s, 1H), 6.85 (d, *J* = 9.0 Hz, 1H), 4.48-4.45 (m, 4H), 4.22 (m, 2H), 4.02 (m, 2H), 3.82-3.47 (m, 18H), 3.34 (s, 3H), 3.29 (s, 3H), 2.42 (t, *J* = 3.5 Hz, 2H), 1.71 (m, 2H), 1.32 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 172.18, 167.01, 166.89,

164.72, 153.40, 147.75, 139.74, 132.52, 130.68, 125.22, 122.66, 120.34, 112.88, 111.06, 110.54, 110.33, 71.89, 71.82, 70.73, 70.58, 70.44, 70.38, 69.22, 69.08, 68.90, 64.55, 58.97, 58.87, 45.32, 37.15, 31.54, 25.24, 22.53, 13.98. ESI-MS: *m/z* calcd for $C_{36}H_{54}N_4O_{12}$: 734.37; found: 735.88 $[M + H]^+$.

Compound 5c. White solid (4.2 g, 53%). IR (KBr, cm^{-1}): 3429, 3364, 3323, 3280, 3251, 3114, 2927, 2857, 1701, 1636, 1539, 1244, 1225, 1112, 1055. ^1H NMR(400MHz, $CDCl_3$) δ 9.59 (s, 1H), 9.18 (s, 1H), 8.44 (s, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.90 (s, 1H), 7.78 (s, 1H), 7.40 (s, 1H), 7.09 (s, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 4.43 (m, 4H), 4.27 (m, 2H), 4.00 (m, 2H), 3.99-3.49 (m, 18H), 3.36 (s, 3H), 3.33 (s, 3H), 2.40 (m, 2H), 1.70(m, 2H), 1.25 (m, 12H), 0.89 (t, *J* = 5.9 Hz, 3H). ^{13}C NMR(100 MHz, $CDCl_3$) δ 171.99, 166.78, 166.60, 164.33, 153.18, 147.70, 139.58, 132.34, 130.42, 124.90, 122.43, 120.08, 110.80, 110.24, 109.96, 71.71, 71.63, 70.53, 70.39, 70.36, 70.15, 69.01, 68.86, 68.66, 64.37, 58.72, 58.62, 45.11, 36.97, 31.71, 29.44, 29.36, 29.29, 29.17, 25.38, 22.47, 13.93. ESI-MS: *m/z* calcd for $C_{40}H_{62}N_4O_{12}$: 790.44; found:791.46 $[M + H]^+$.

Compound 5d. White solid (3.4 g, 50%). ^1H NMR (400MHz, DMSO-*d6*) δ 10.03 (s, 1H), 9.89 (s, 1H), 8.67 (t, *J* = 4.9 Hz, 1H), 8.07 (d, *J* = 2.7 Hz, 1H), 7.81 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.42 (s, 1H), 7.13 (d, *J* = 9.0 Hz, 1H), 7.09 (s, 1H), 6.91 (s, 1H), 5.43 (s, 2H), 4.20-4.12 (m, 6H), 2.27 (t, *J* = 7.4 Hz, 2H), 1.85 (m, 2H), 1.71-1.53 (m, 4H), 1.47- 1.12 (m, 24H), 0.89-0.74 (m, 9H).

Notes and references

[S1] Guo, Z. Q.; Tong, W. L.; Chan, M. C. W. *Chem. Commun.* **2014**, *50*, 1711.

[S2] Raju, M. V. R.; Lin, H. C. *Org. Lett.* **2014**, *16*, 5564.

[S3] Li, M. F.; Yamato, K.; Ferguson, J. S.; Gong, B. *J. Am. Chem. Soc*. **2006**, *128*, 12628.

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[S5] Zeng, H. Q.; Ickes, H.; Flowers, R. A.; Gong., B. *J. Org. Chem*. **2001**, *66*, 3574.

[S7] Zeng, H. Q.; Yang, X. W.; Flowers, R. A.; Gong, B. *J. Am. Chem. Soc.* **2002**, *124*, 2903.

2. Gelation Tests and Additional Gel Images

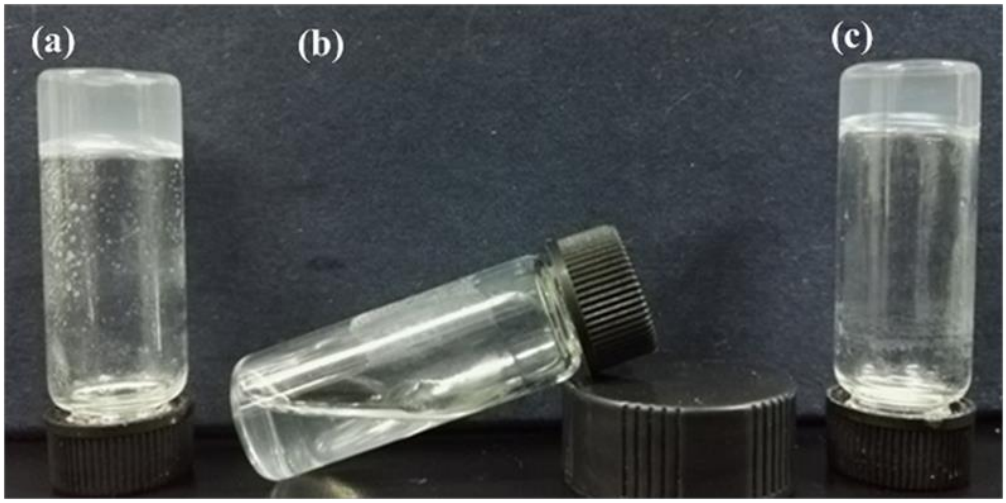


Fig. S1 Images of **G2** at a concentration of 10 mg mL^{-1} under different conditions (a) neutral water; (b) acidulated by HCl (1 M, 5 μL); (c) added 5 μL Et_3N into the acidified solution

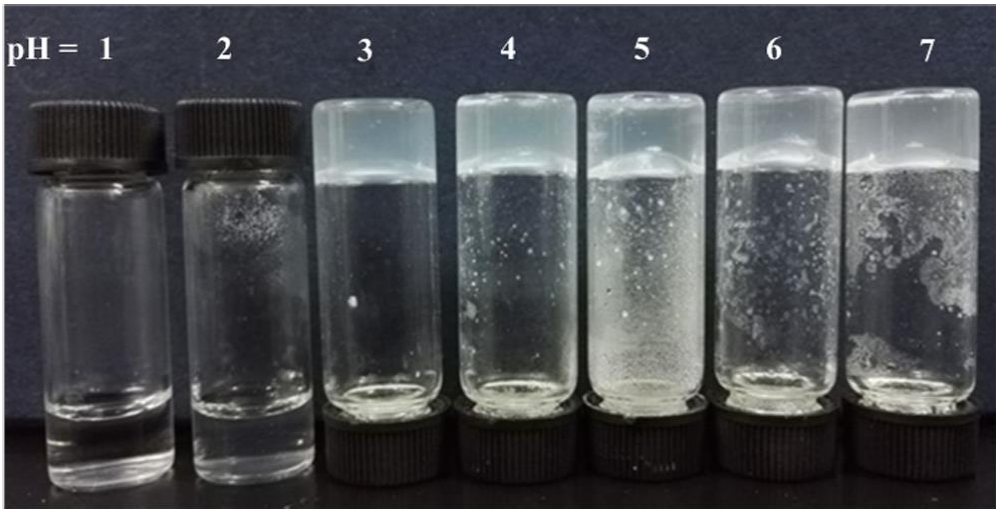


Fig. S2 Images of **G2** at a concentration of 10 mg mL^{-1} in water under different pH (the value of pH is 1 to 7 in turn from left to right)

3. UV-Vis and Fluorescence Spectroscopy

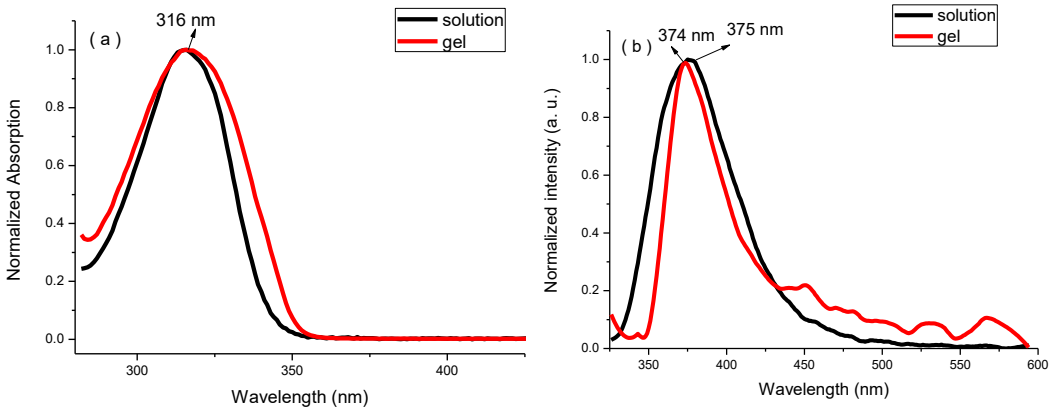


Fig. S3 G2 at a concentration of 0.1 mM and in the gel state (15 mg mL^{-1}) in benzene at room temperature (a) Absorption spectra (1 mm path length) (b) Fluorescence emission spectra (λex = 307 nm).

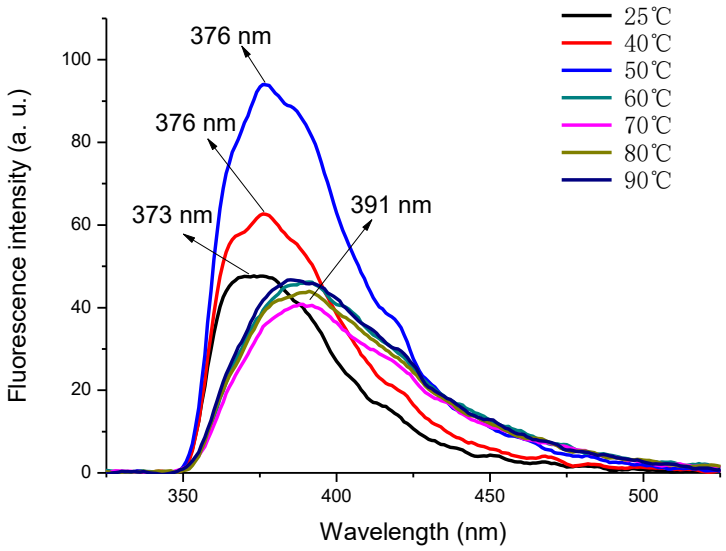


Fig. S4 The fluorescence emission spectra change of **G2** in H_2O (10 mg mL^{-1}) at different temperature (λex = 307 nm).

4. 1D and 2D NMR Spectroscopy

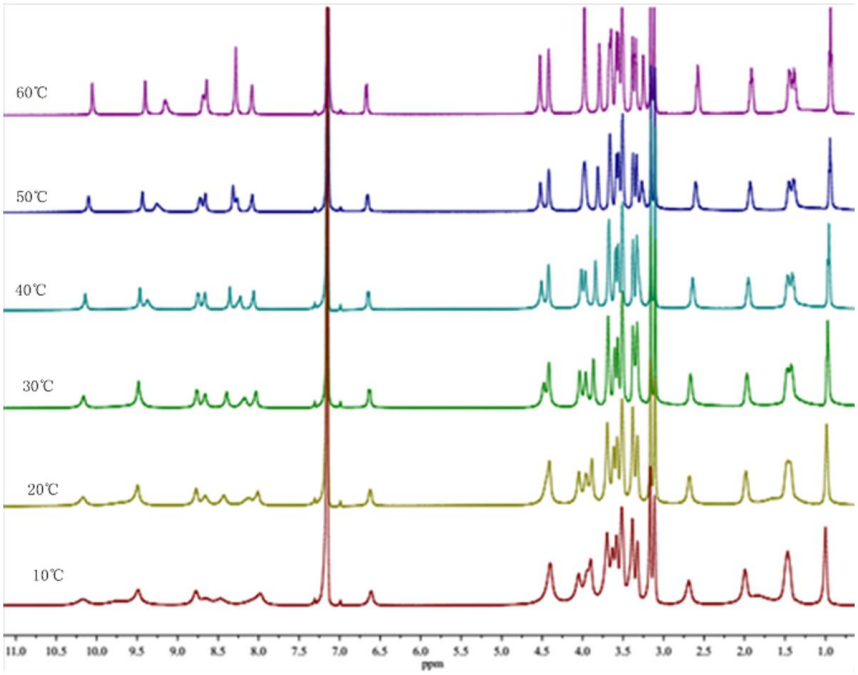


Fig. S5 Variable temperature ^{1}H NMR spectra of compound **G2** (20 mM, C_6D_6)

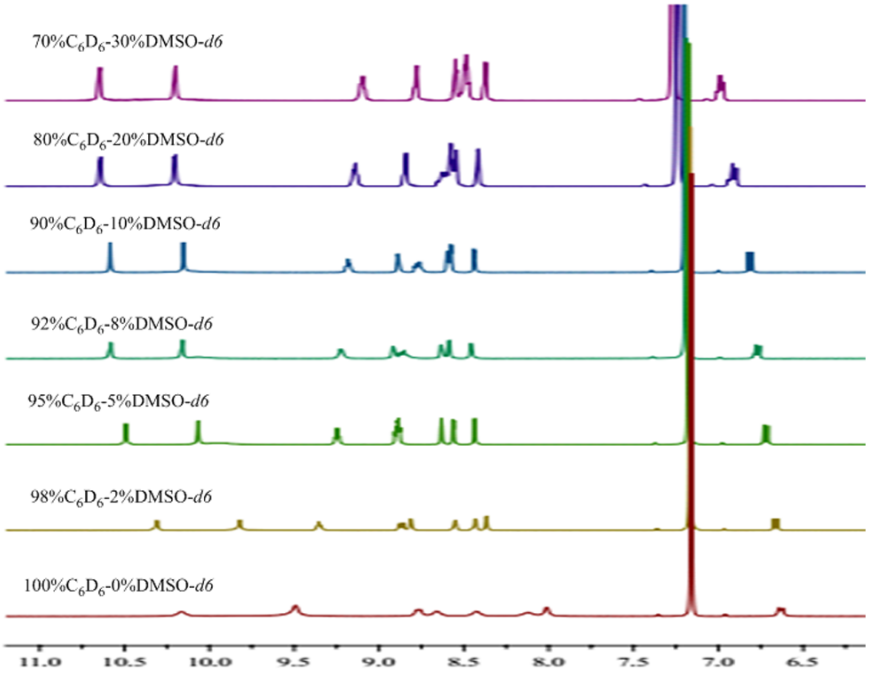


Fig. S6 Solvent-dependent ^{1}H NMR spectra of compound **G2** (20 mM, 25℃, C_6D_6-DMSO-d_6)

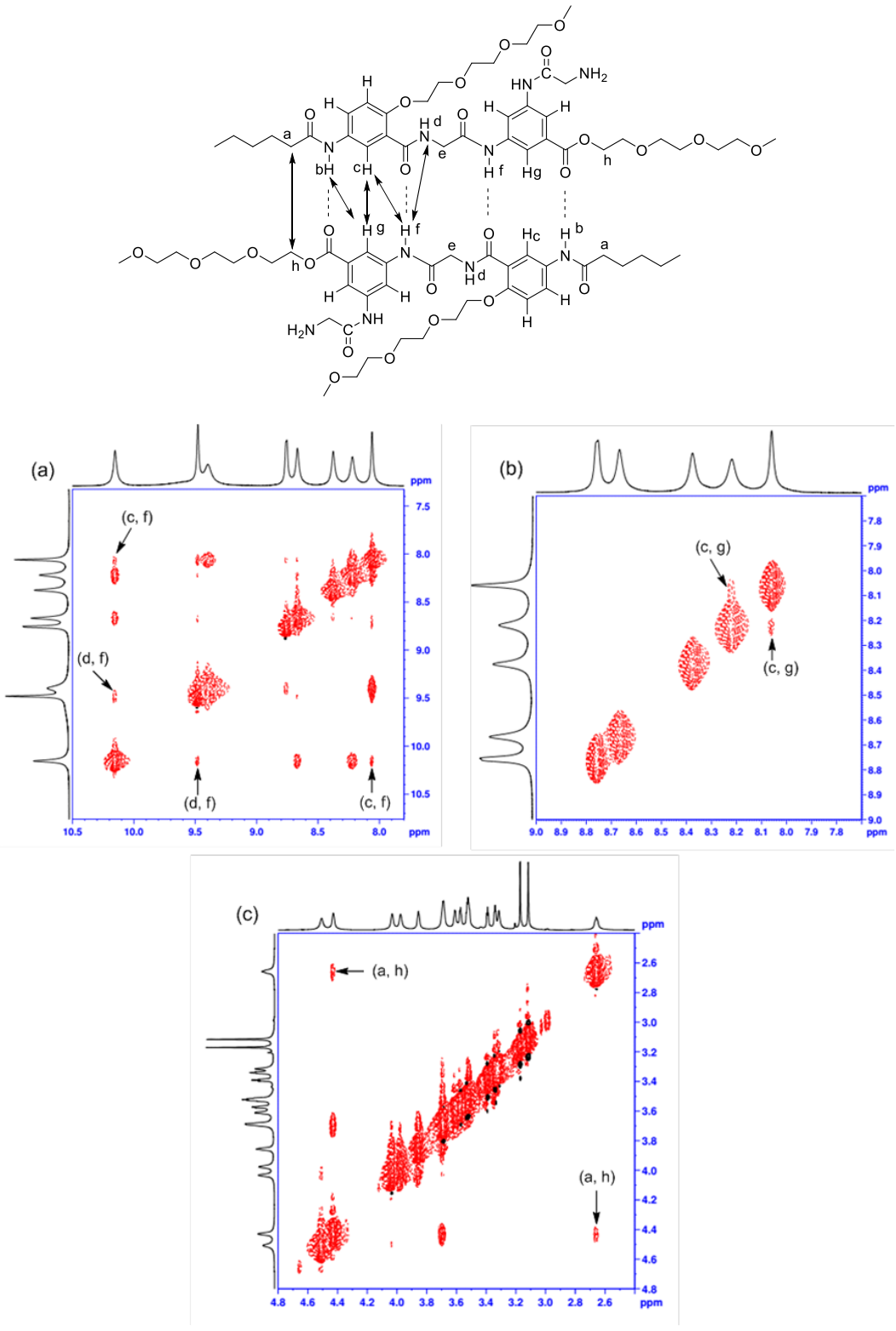


Fig. S7 Partial Spectra of NEOSY (**G2**, 20 mM in C_6D_6)

5. Loading and releasing experiments

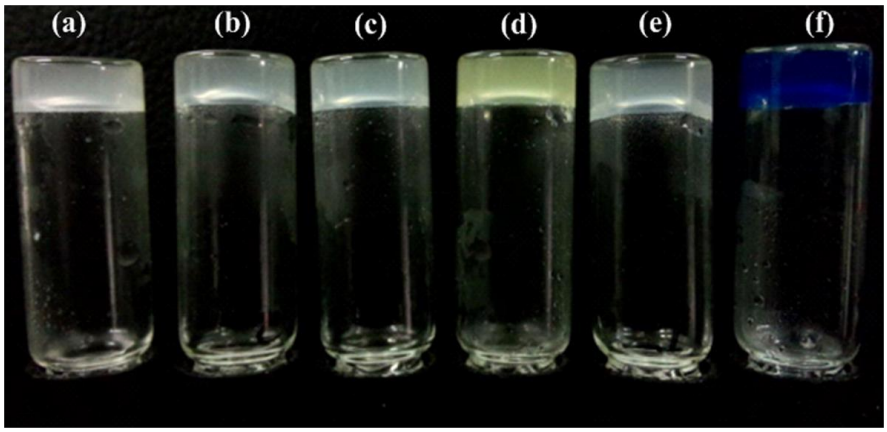


Fig. S8 The pictures of the hydrogels with different compounds, (a) **G2** + zinc acetate, (b) **G2** + streptomycin sulphate, (c) **G2** + chloramphenicol, (d) **G2** + tetracycline, (e) **G2** + benzyl penicillin, (f) **G2** + methylene blue. The hydrogel are formed in the condition of **G2** (5.0 mg) in the aqueous solutions of different drugs (1.0 mM, 500 μL), respectively.

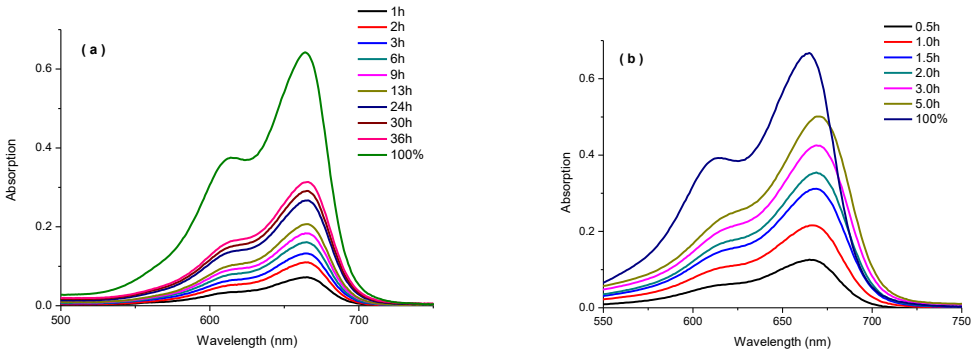


Fig. S9 Absorption spectra of **MB** releasing from the hydrogel **G2** in different conditions, (a) pure water , (b) water containing 1‰ glacial acetic acid

6. IR, HRMS, ^{1}H NMR and ^{13}C NMR Spectra of G1-G6

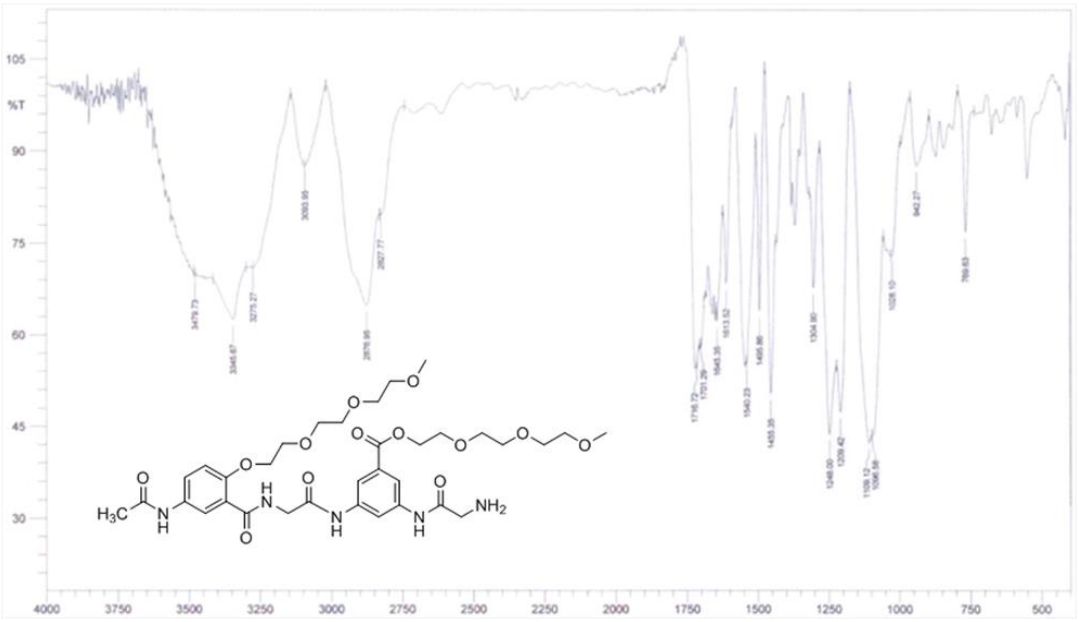


Fig. S10 IR Spectra of Compound **G1**

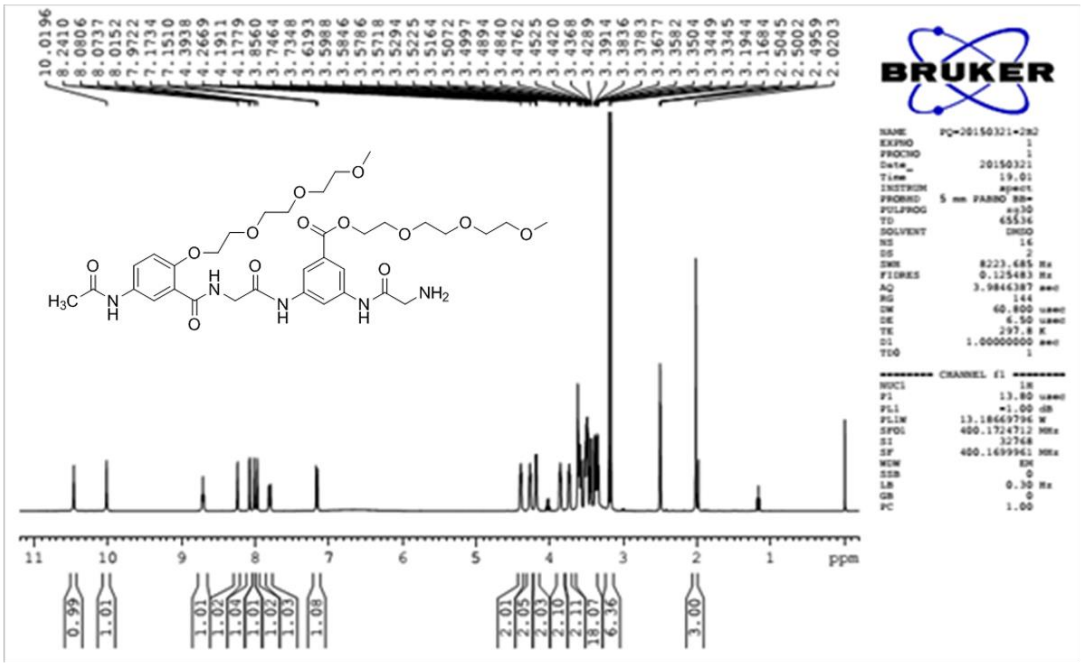


Fig. S11 ^{1}H NMR Spectra of Compound **G1** (4 mM, DMSO-d_6)

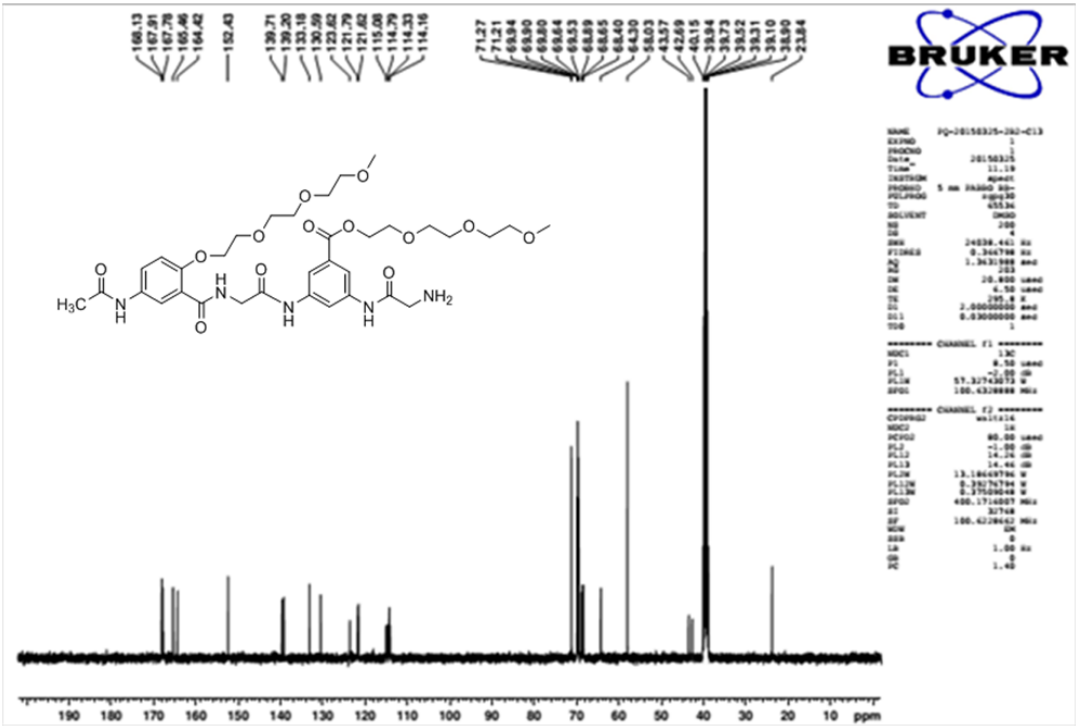
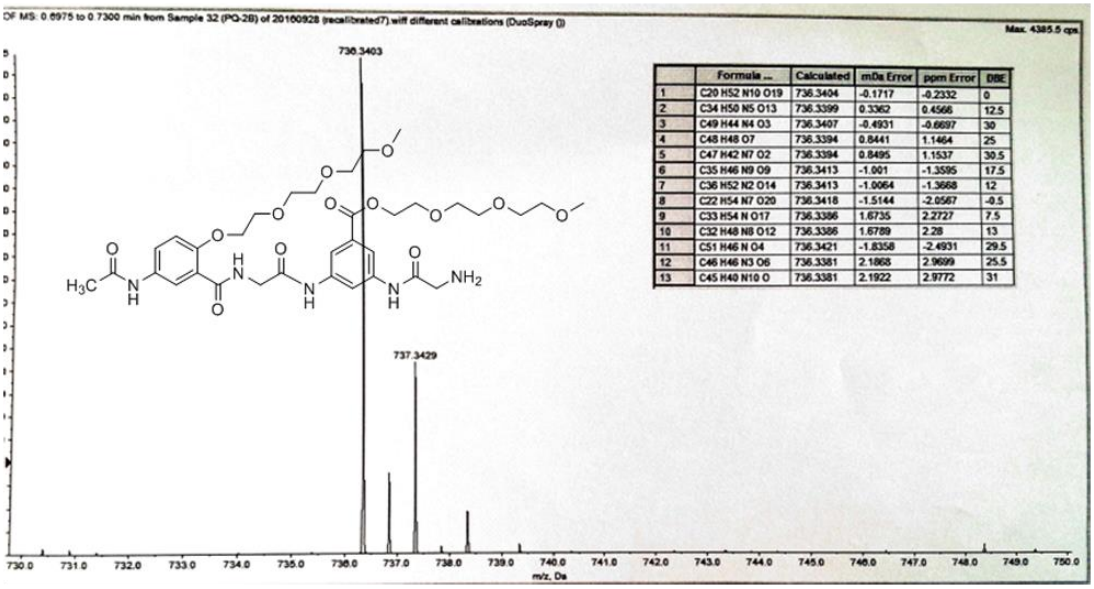


Fig. S12 ^{13}C NMR Spectra of Compound **G1** (20 mM, DMSO-d_6)



	Formula ...	Calculated	mDa Error	ppm Error	DBE
1	C20 H52 N10 O19	736.3404	-0.1717	-0.2332	0
2	C34 H50 N5 O13	736.3399	0.3362	0.4566	12.5
3	C49 H44 N4 O3	736.3407	-0.4931	-0.6697	30
4	C48 H48 O7	736.3394	0.8441	1.1464	25
5	C47 H42 N7 O2	736.3394	0.8495	1.1537	30.5
6	C35 H46 N9 O9	736.3413	-1.001	-1.3595	17.5
7	C36 H52 N2 O14	736.3413	-1.0064	-1.3668	12
8	C22 H54 N7 O20	736.3418	-1.5144	-2.0567	-0.5
9	C33 H54 N O17	736.3386	1.6735	2.2727	7.5
10	C32 H48 N8 O12	736.3386	1.6789	2.28	13
11	C51 H46 N O4	736.3421	-1.8358	-2.4931	29.5
12	C46 H46 N3 O6	736.3381	2.1868	2.9699	25.5
13	C45 H40 N10 O	736.3381	2.1922	2.9772	31

Fig. S13 HRMS Spectra of Compound **G1**

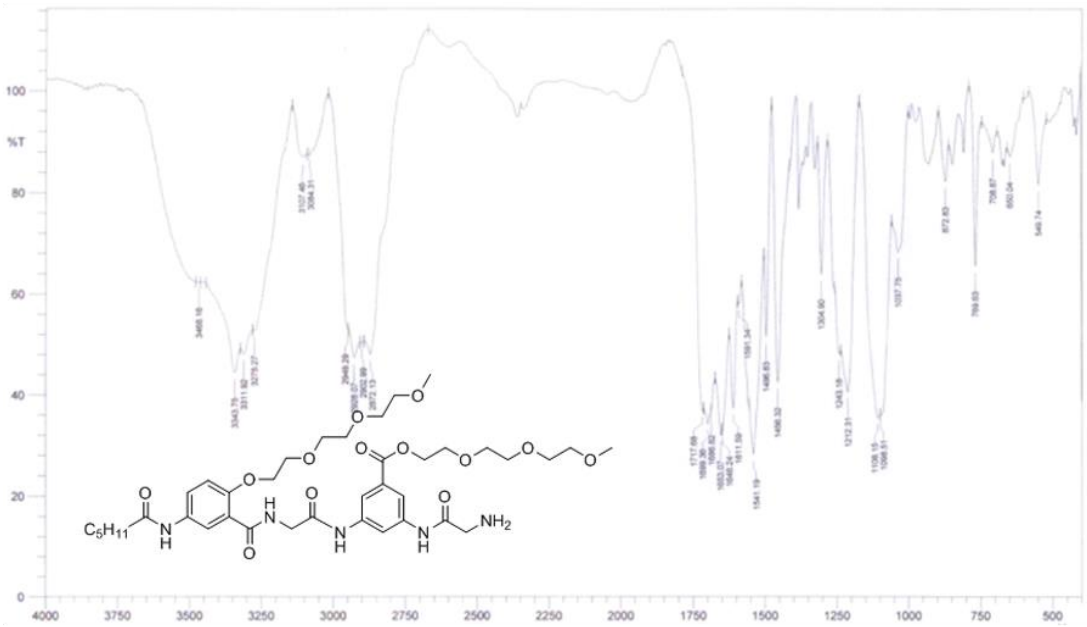


Fig. S14 IR Spectra of Compound **G2**

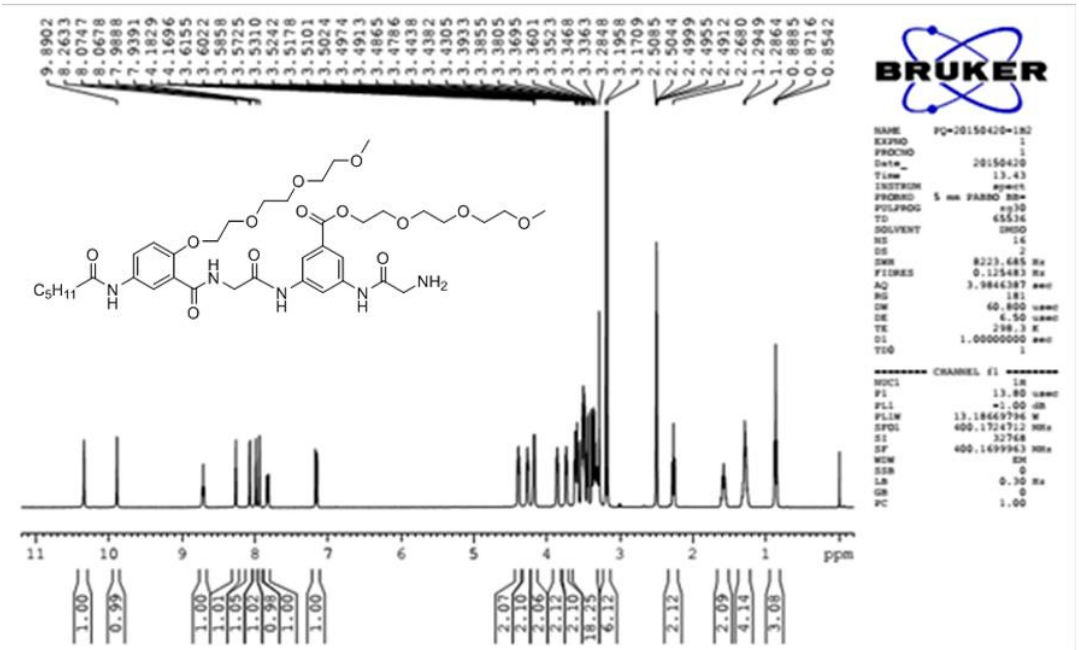


Fig. S15 ^{1}H NMR Spectra of Compound **G2** (4 mM, DMSO-d_6)

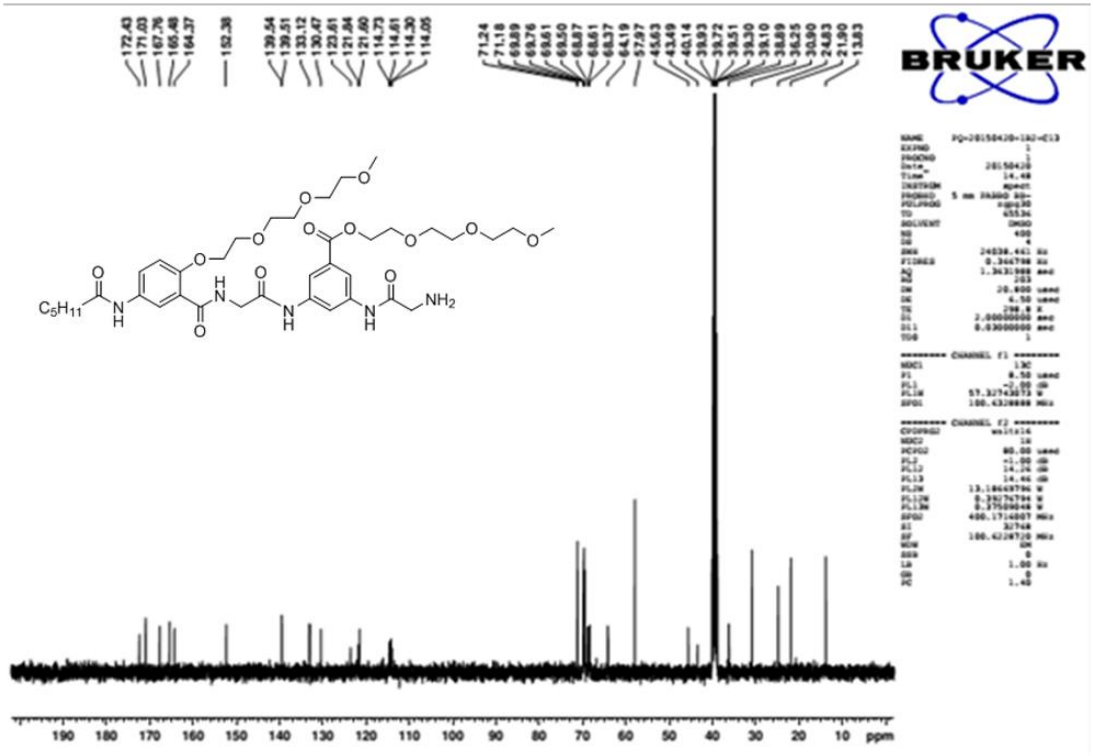
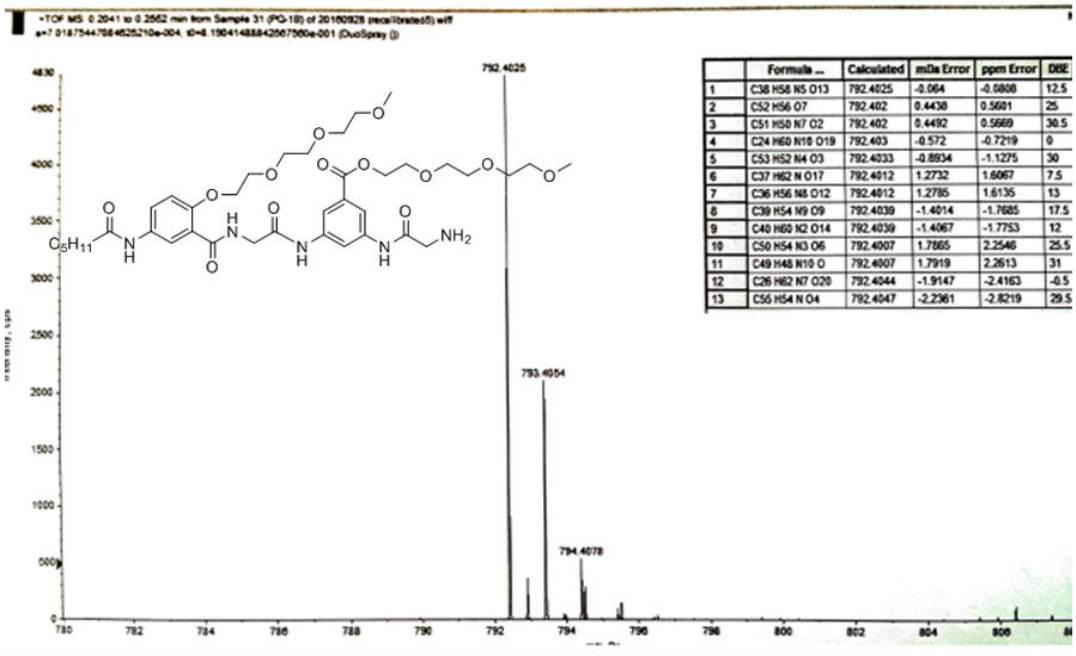


Fig. S16 ^{13}C NMR Spectra of Compound **G2** (20 mM, DMSO-d_6)



	Formula ...	Calculated	mDa Error	ppm Error	DBE
1	C38 H58 N5 O13	792.4025	-0.064	-0.0808	12.5
2	C52 H56 O7	792.402	0.4438	0.5601	25
3	C51 H50 N7 O2	792.402	0.4492	0.5669	30.5
4	C24 H60 N10 O19	792.403	-0.572	-0.7219	0
5	C53 H52 N4 O3	792.4033	-0.8934	-1.1275	30
6	C37 H62 N O17	792.4012	1.2732	1.6067	7.5
7	C36 H56 N8 O12	792.4012	1.2785	1.6135	13
8	C39 H54 N9 O9	792.4039	-1.4014	-1.7685	17.5
9	C40 H60 N2 O14	792.4039	-1.4067	-1.7753	12
10	C50 H54 N3 O6	792.4007	1.7665	2.2546	25.5
11	C49 H48 N10 O	792.4007	1.7919	2.2613	31
12	C26 H62 N7 O20	792.4044	-1.9147	-2.4163	-0.5
13	C55 H54 N O4	792.4047	-2.2361	-2.8219	29.5

Fig. S17 HRMS Spectra of Compound **G2**

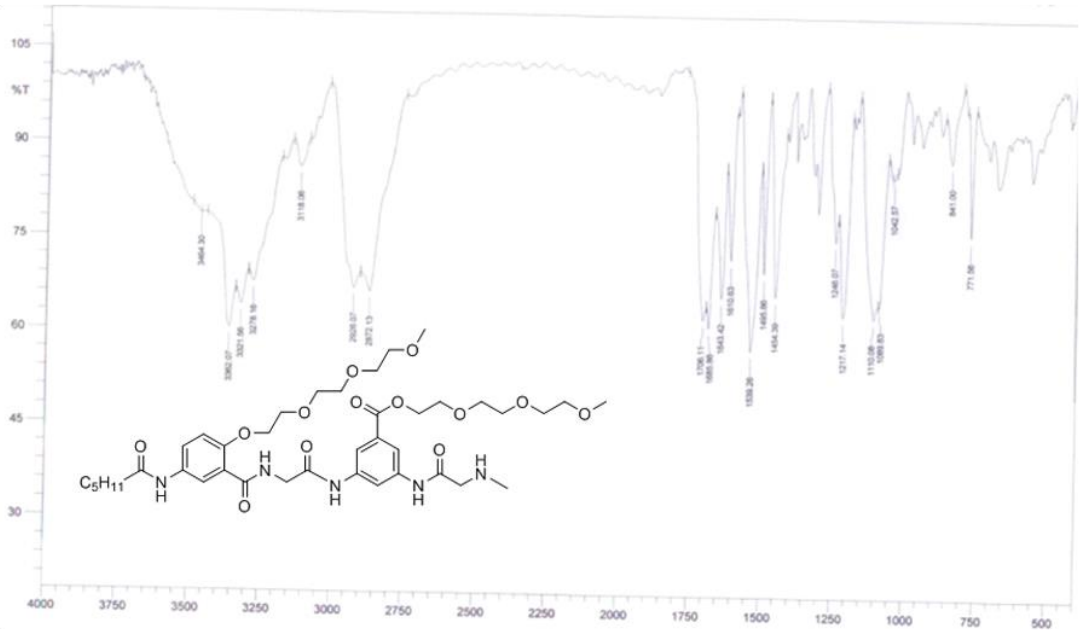


Fig. S18 IR Spectra of Compound **G3**

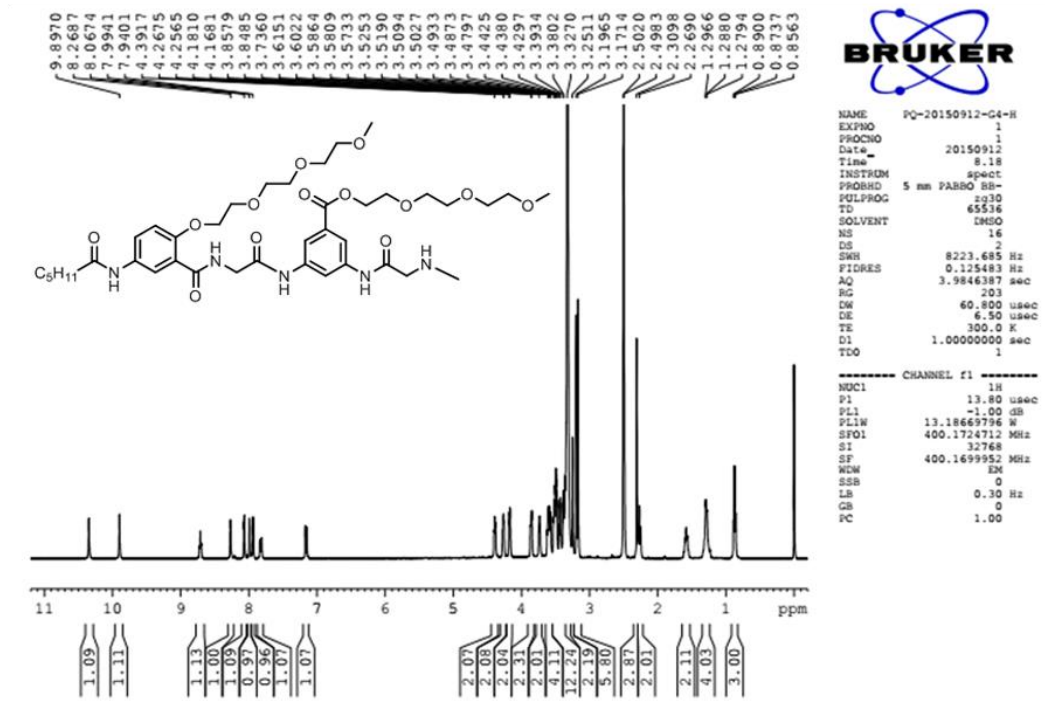


Fig. S19 ^{1}H NMR Spectra of Compound **G3** (4 mM, DMSO-d_6)

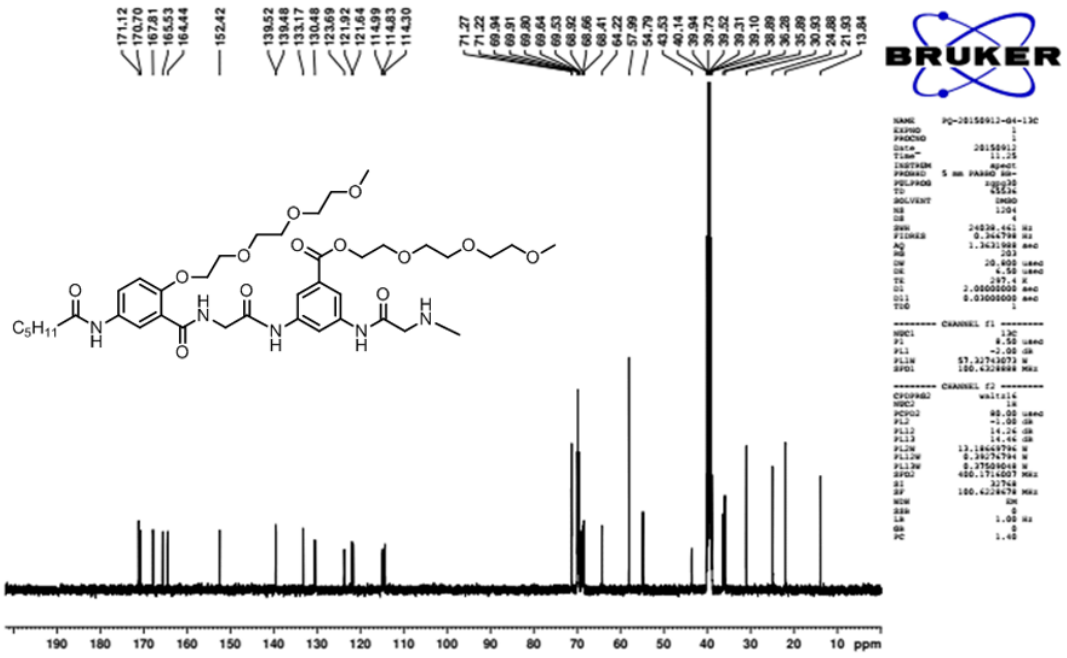
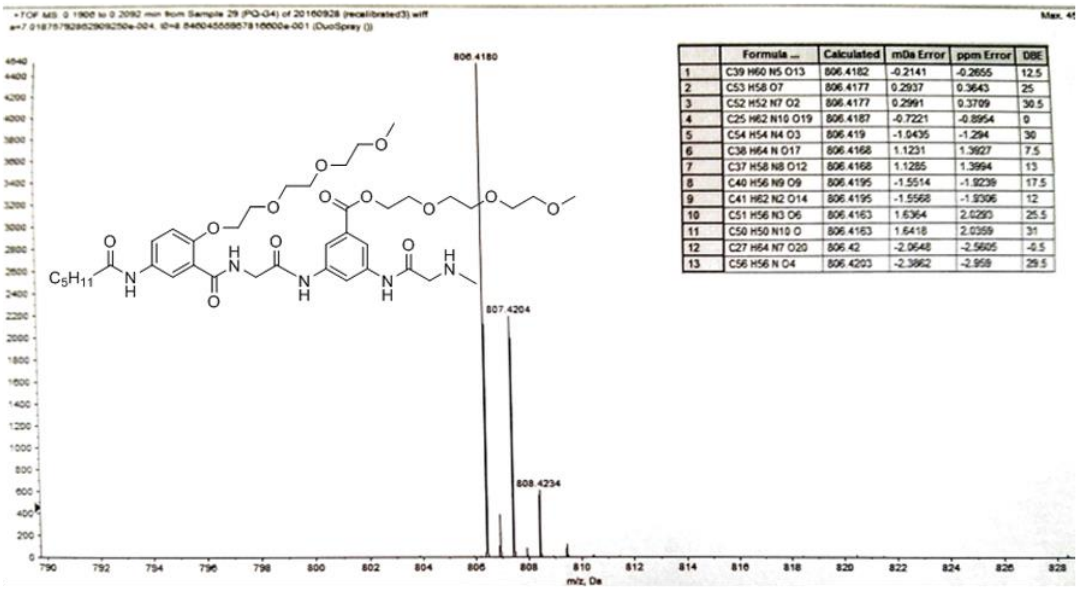


Fig. S20 ^{13}C NMR Spectra of Compound **G3** (20 mM, DMSO-d_6)



	Formula ...	Calculated	mDa Error	ppm Error	DBE
1	C39 H60 N5 O13	806.4182	-0.2141	-0.2655	12.5
2	C53 H58 O7	806.4177	0.2937	0.3643	25
3	C52 H52 N7 O2	806.4177	0.2991	0.3709	36.5
4	C25 H62 N10 O19	806.4187	-0.7221	-0.8954	0
5	C54 H54 N4 O3	806.419	-1.0435	-1.294	38
6	C38 H64 N O17	806.4168	1.1231	1.3927	7.5
7	C37 H58 N8 O12	806.4168	1.1285	1.3994	13
8	C40 H56 N9 O9	806.4195	-1.5514	-1.9239	17.5
9	C41 H62 N2 O14	806.4195	-1.5568	-1.9306	12
10	C51 H56 N3 O6	806.4163	1.6364	2.0293	25.5
11	C50 H50 N10 O	806.4163	1.6418	2.0359	31
12	C27 H64 N7 O20	806.42	-2.9648	-2.5605	-5.5
13	C56 H56 N O4	806.4293	-2.3862	-2.958	29.5

Fig. S21 HRMS Spectra of Compound **G3**

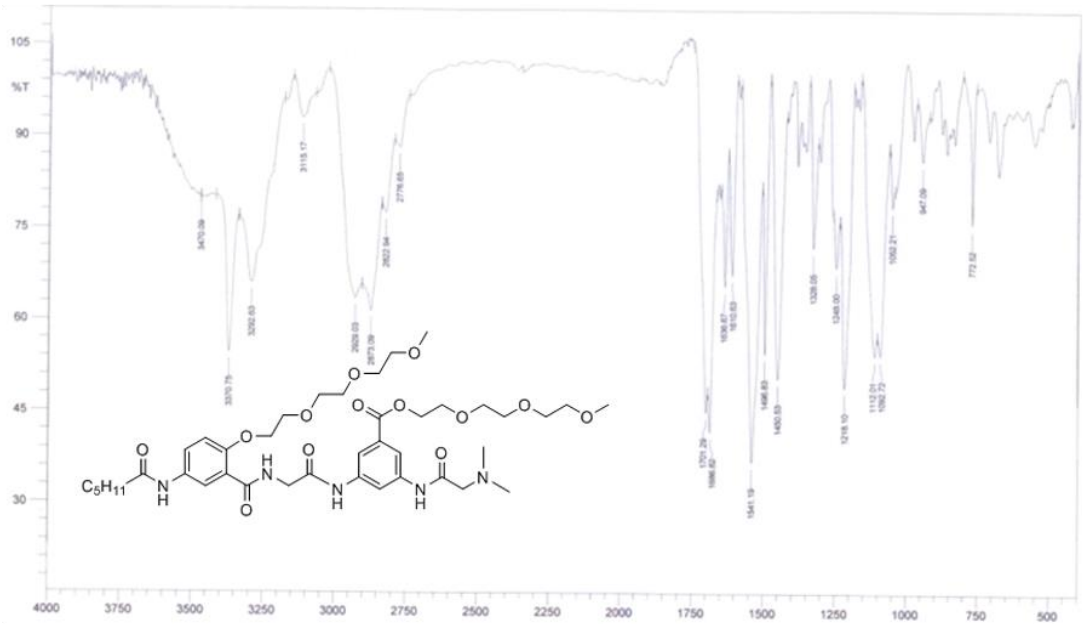


Fig. S22 IR Spectra of Compound **G4**

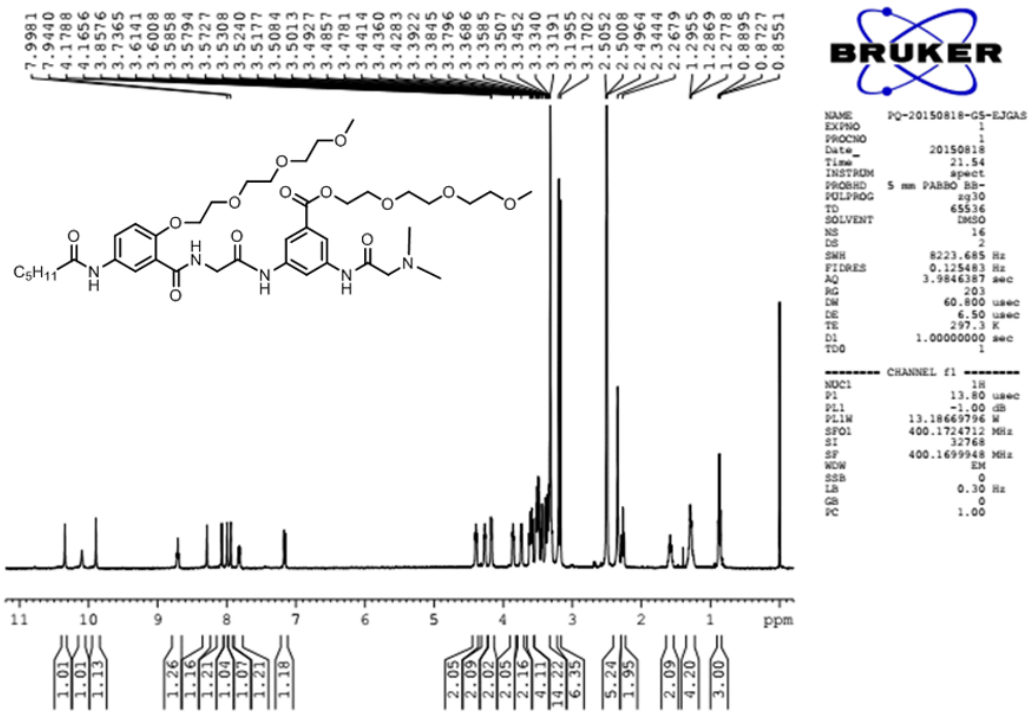


Fig. S23 ^{1}H NMR Spectra of Compound **G4** (4 mM, DMSO-d_6)

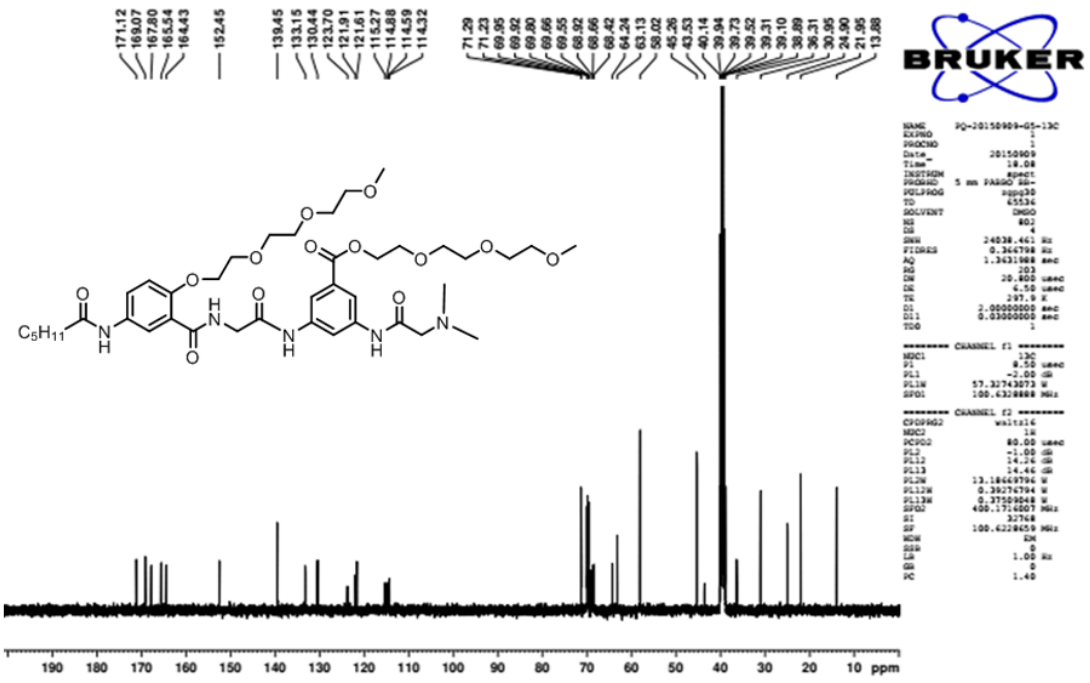


Fig. S24 ^{13}C NMR Spectra of Compound **G4** (20 mM, DMSO-d_6)

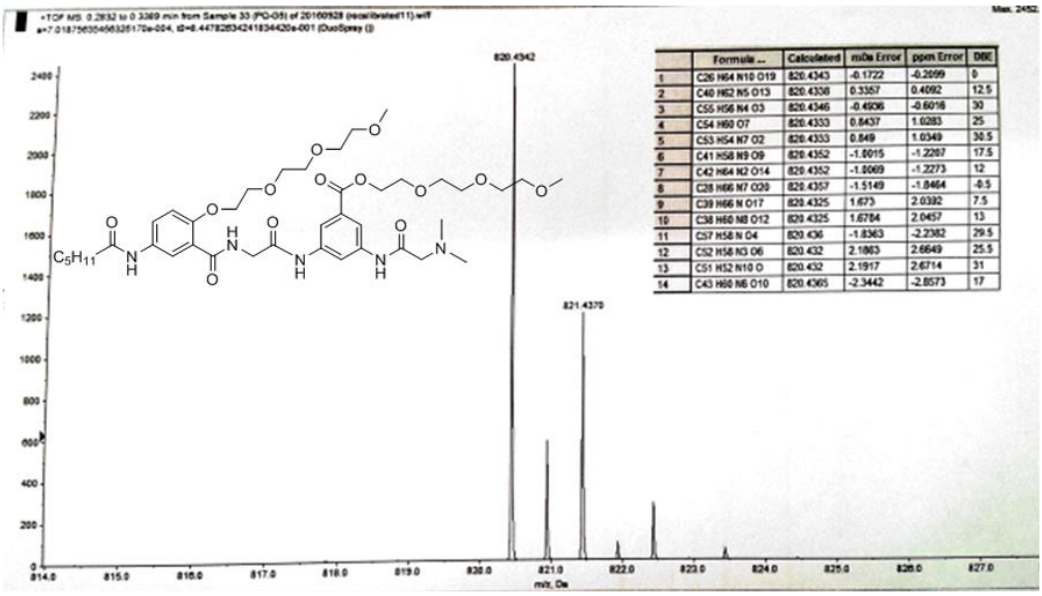


Fig. S25 HRMS Spectra of Compound **G4**

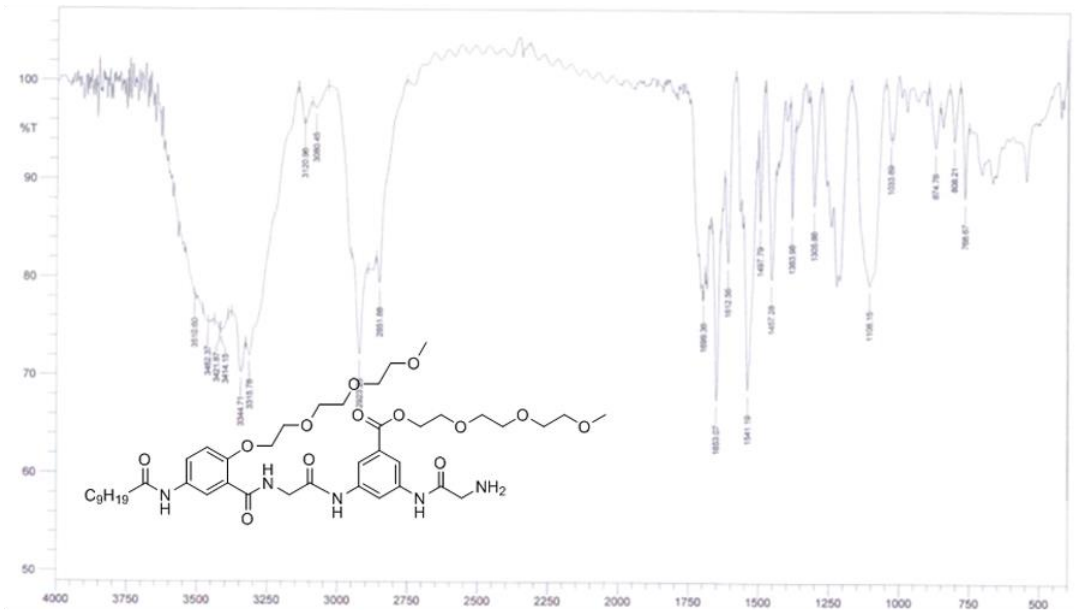


Fig. S26 IR Spectra of Compound **G5**

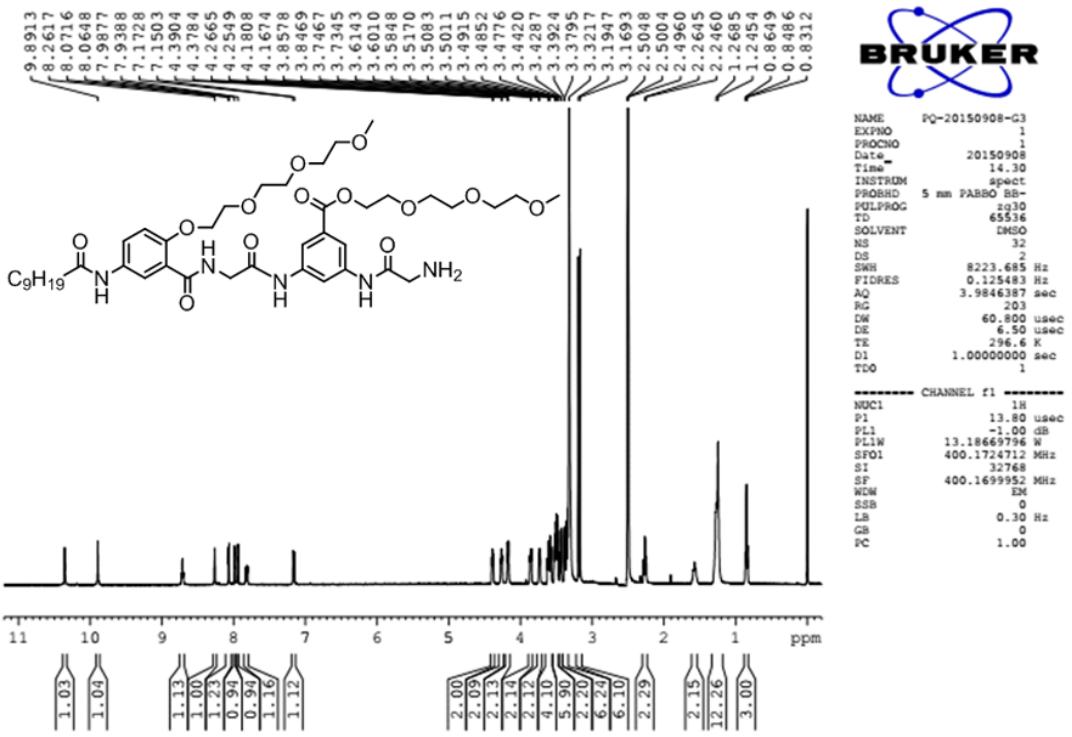


Fig. S27 ^{1}H NMR Spectra of Compound **G5** (4 mM, DMSO-d_6)

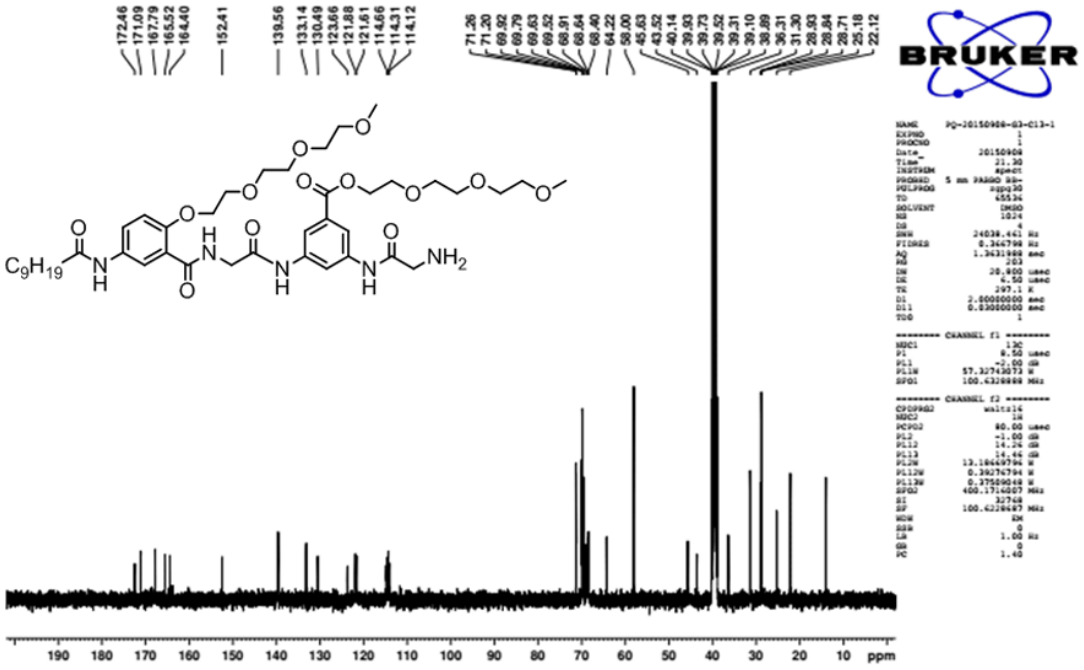
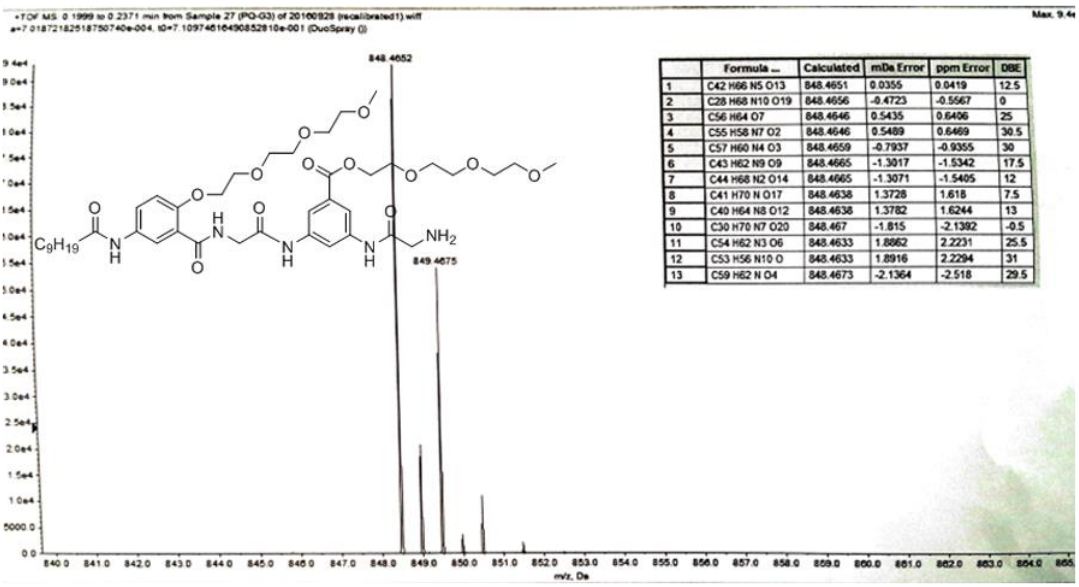


Fig. S28 ^{13}C NMR Spectra of Compound **G5** (20 mM, DMSO-d_6)



	Formula ...	Calculated	mDa Error	ppm Error	DBE
1	C42 H66 N5 O13	848.4651	0.0355	0.0419	12.5
2	C28 H68 N10 O19	848.4656	-0.4723	-0.5567	0
3	C56 H64 O7	848.4646	0.5435	0.6406	25
4	C55 H58 N7 O2	848.4646	0.5489	0.6469	30.5
5	C57 H60 N4 O3	848.4659	-0.7937	-0.9355	30
6	C43 H62 N9 O9	848.4665	-1.3017	-1.5342	17.5
7	C44 H68 N2 O14	848.4665	-1.3071	-1.5405	12
8	C41 H70 N O17	848.4638	1.3728	1.618	7.5
9	C40 H64 N8 O12	848.4638	1.3782	1.6244	13
10	C30 H70 N7 O20	848.467	-1.815	-2.1392	-0.5
11	C54 H62 N3 O6	848.4633	1.8862	2.2231	25.5
12	C53 H56 N10 O	848.4633	1.8916	2.2294	31
13	C59 H62 N O4	848.4673	-2.1364	-2.518	29.5

Fig. S29 HRMS Spectra of Compound **G5**

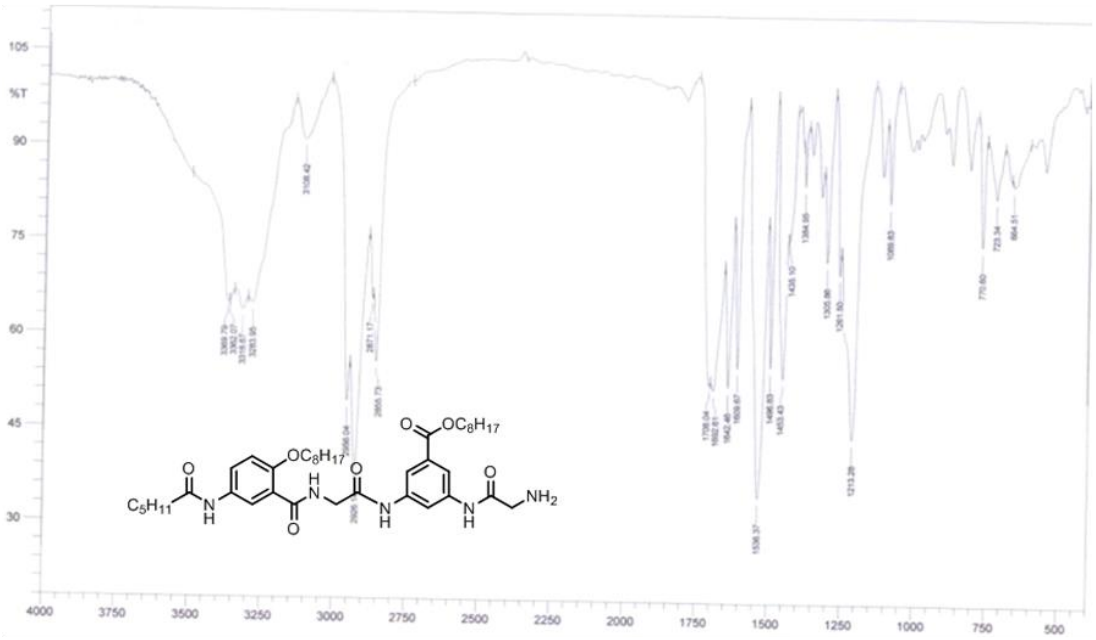


Fig. S30 IR Spectra of Compound **G6**

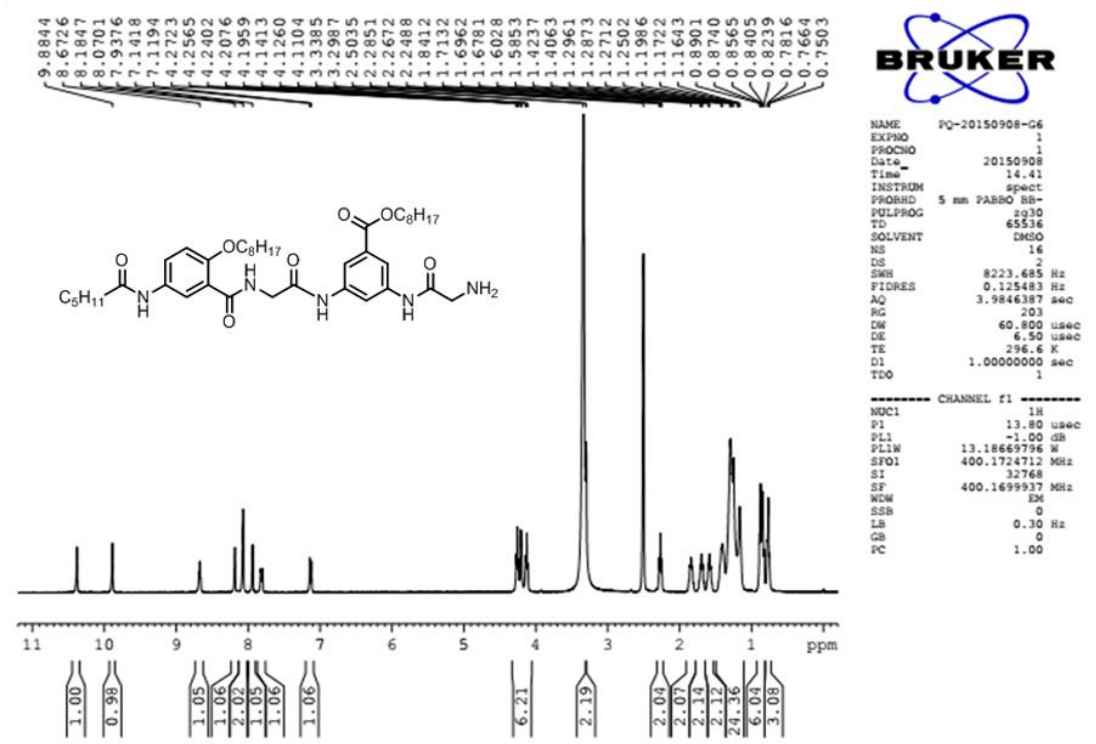


Fig. S31 ^{1}H NMR Spectra of Compound **G6** (4 mM, DMSO-d_6)

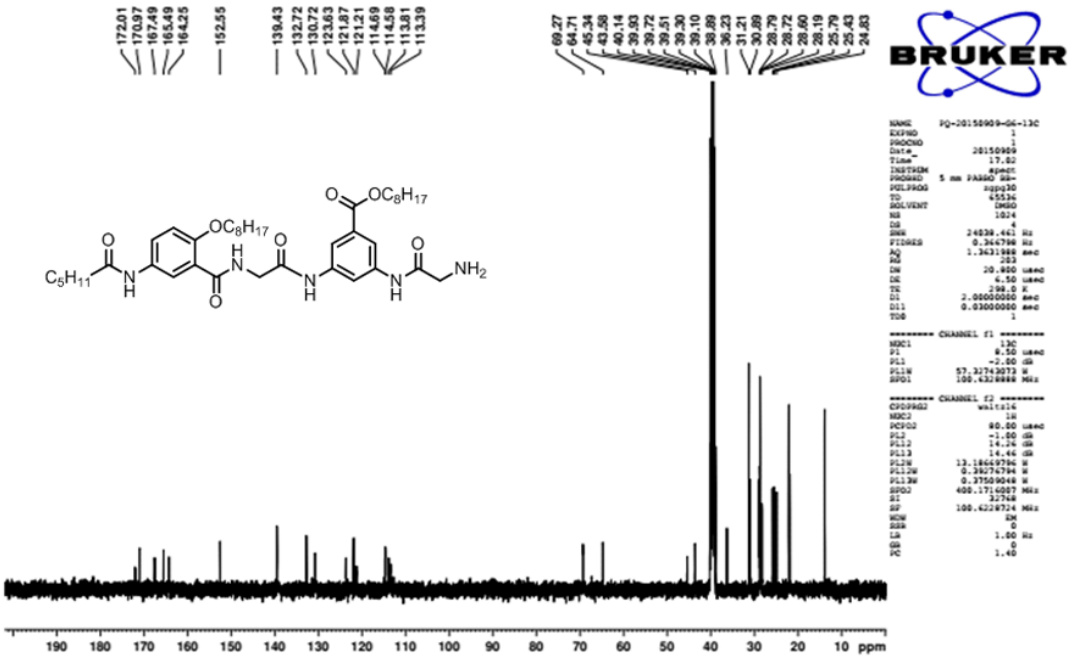
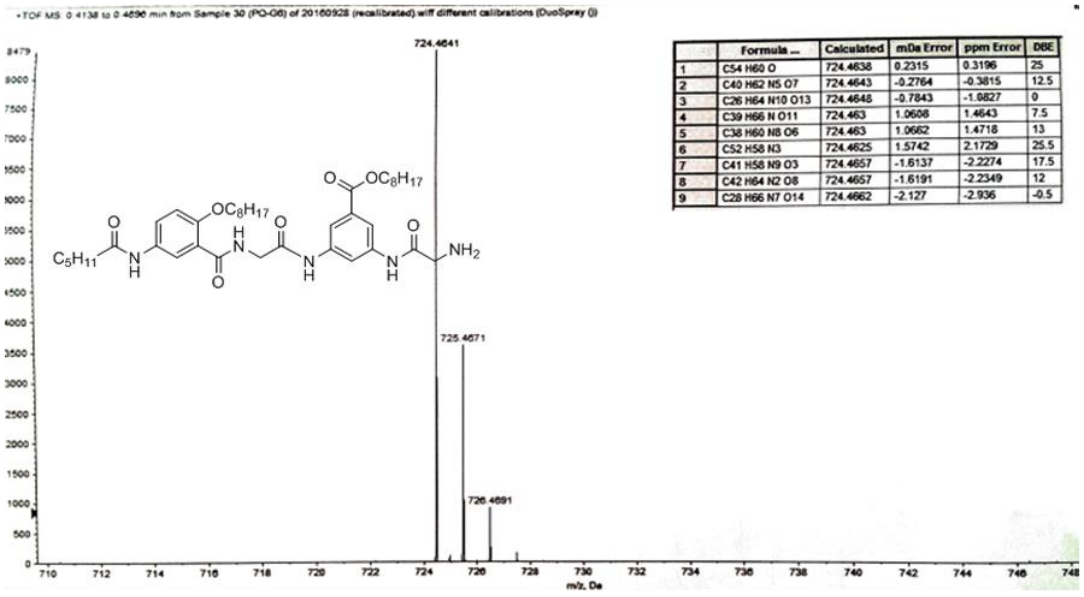


Fig. S32 ^{13}C NMR Spectra of Compound **G6** (20 mM, DMSO-d_6)



	Formula ...	Calculated	mDa Error	ppm Error	DBE
1	C54 H60 O	724.4638	0.2315	0.3196	25
2	C40 H62 N5 O7	724.4643	-0.2764	-0.3815	12.5
3	C26 H64 N10 O13	724.4648	-0.7843	-1.0827	0
4	C39 H66 N O11	724.463	1.0608	1.4643	7.5
5	C38 H60 N8 O6	724.463	1.0662	1.4718	13
6	C52 H58 N3	724.4625	1.5742	2.1729	25.5
7	C41 H58 N9 O3	724.4657	-1.6137	-2.2274	17.5
8	C42 H64 N2 O8	724.4657	-1.6191	-2.2349	12
9	C28 H66 N7 O14	724.4662	-2.127	-2.936	-0.5

Fig. S33 HRMS Spectra of Compound **G6**