Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

T-shaped monopyridazinotetrathiafulvalene-amino acid diad based chiral organogels with aggregation-induced fluorescence emission

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1. Instrumentation

Gelation study

A measured amount of gelator **1** and a measured volume of the solvent were placed in a sealed test tube and heated to obtain a clear solution. And then, the system was left at room temperature. The transition temperatures (T_{gel}) were determined by ball-drop method. An inverted gel was immersed in a water bath initially at or below room temperature, and then was heated (about 2 ^{o}C min^{-1}) slowly up to the point at which the gel fell due to the force of gravity, i.e. the T_{gel}.

NMR experiments

All solution state NMR studies were carried out on Bruker AV-300 Spectrometer (300 MHz for ^{1}H and 75 MHz for ^{13}C) and chemical shifts were referenced relative to tetramethylsilane (δ_H/δ_C=0).

FT-IR spectroscopy

IR spectra were recorded on a Shimadzu FT-IR Prestige-21 instrument with the KBr disk technique.

MALDI-TOF-MS spectrometry

Mass spectra were performed on a Shimadzu Axima CFR^{TM} Plus using a 1,8,9-anthracenetriol (DITH) and β-phenylacrylic acid (CHCA) matrix.

Cyclic voltammetry

Cyclic voltammetry was performed on a CHI660D instrument in benzonitrile (10^{-3} M) with 0.1 M Bu_4NPF_6 as the supporting electrolyte and at a scan rate of 100mVs $^{-1}$. Counter and working electrodes were made of Pt and glass carbon, respectively, and Ag/AgCl was used as the reference electrode. For xerogel measurements, a small amount of the gel was carefully put on the glass carbon electrode, which was left in air for 24 h. This modified glass carbon electrode (as working electrode), together with Pt as the counter electrode and Ag/AgCl as the reference electrode, was put into the benzonitrile solution containing 0.1 M Bu_4NPF_6, and the cyclic voltammograms were recorded at a scanning rate of 100 mV s^{-1}.

UV-Vis spectroscopy

UV-vis spectra were recorded on a Hitachi U-3010 spectrophotometer.

Fluorescence spectroscopy

Fluorescence spectra were recorded on a Shimadzu RF-5301PC fluorescence spectrophotometer.

Circular dichroism (CD) spectroscopy

CD spectra were obtained on Chirascan spectrometer using a 1 mm path-length cell.

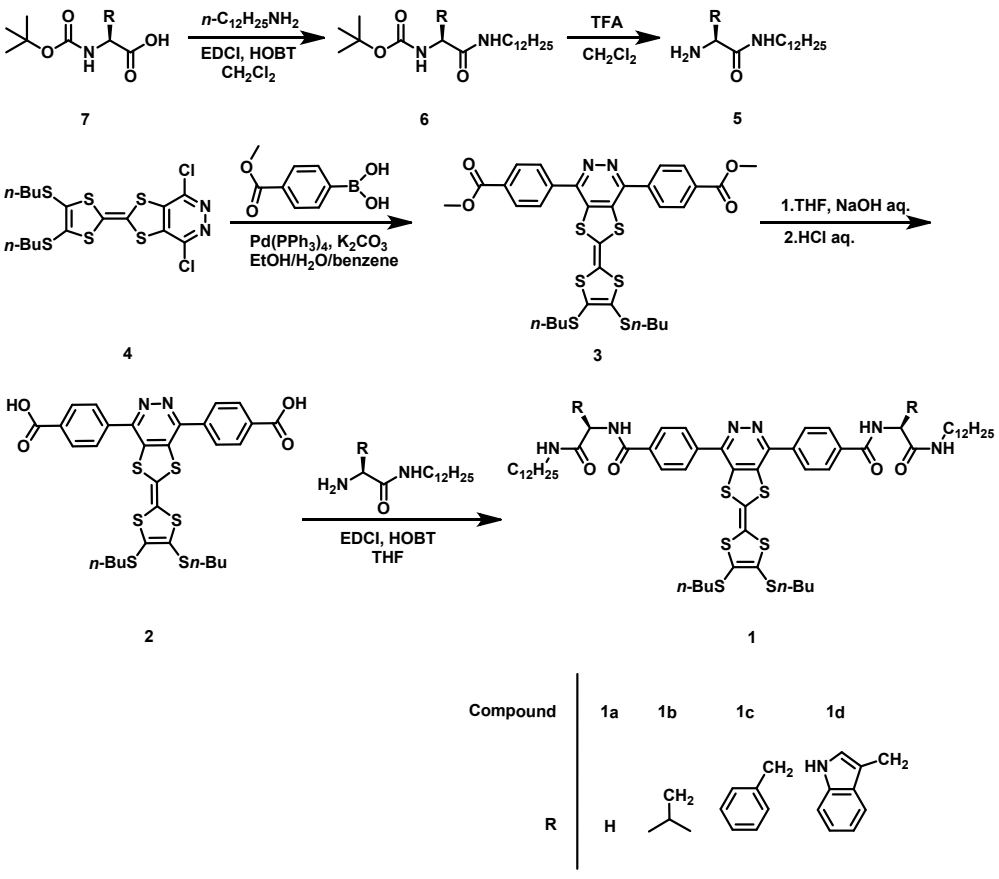
Atomic force microscopy (AFM)

For AFM experiments, 10 μL of sample solution (diluted gels) was drop-casted onto a freshly cleaved mica surface. Each sample was air-dried 48 h in a dust-free environment prior to AFM imaging. The images were obtained by scanning the mica surfaces in air under ambient conditions using Agilent-5500 in tapping mode.

Small-angle X-ray diffracting

Small-angle X-ray scattering (SAXS) measurements were carried out at 298 K on a beamline 1W2A synchrotron radiation X-ray small angle system at Beijing Synchrotron Radiation Facility(λ =1.54Å).

2. Synthesis and characterization of organic compounds



Scheme S1. Synthetic routes of compounds **1a-d**.

All solvents were purified by the standard procedures before use. *p*-(Methoxycarbonyl) phenylboronic acid, $Pd(PPh_3)_4$, 1-(3-(dimethyl-amino)propyl)-3-ethyl-carbodiimide hydrochloride (EDCI) and 1H-benzo[d][1,2,3]triazol-1-ol (HOBT) were purchased from Adamas, and were used as received without further purification. The Boc protection compounds were synthesized according to the traditional methods, and compounds 4, 6a-c were synthesized according to the literature procedure.[1]

Typical procedure for compound 6d

The mixture of **7d** (4.0 g, 0.01314 mol), EDCI (2.7715 g, 0.01446 mol), HOBt (1.9535 g, 0.01446 mol) and *n*-dodecylamine (2.4361 g, 0.01314 mol) was suspended in CH_2Cl_2 (45 mL). The reaction mixture was stirred at room temperature for one day. The solution was successively washed with aqueous HCl (1 M), aqueous NaOH (1 M) and brine. After drying and filtering, the solvent was eliminated and the residue was purified by column chromatography on silica gel using CH_2Cl_2 : ethyl acetate at 20 : 1 to give a white solid (4.4 g, 71%). m.p.: 70-71℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.88 (t, *J* = 6Hz，3H, -*CH*$_2$), 1.287-1.049 (m, 20H, -*CH*$_2$), 1.43 (br, 9H, -*CH*$_3$), 3.344-3.034 (m, 4H, -*CH*$_2$), 4.437- 4.319 (m, 1H, -*CH*), 5.19 (br, 1H, -*NH*), 5.61 (br, 1H, -*NH*), 7.06 (s, 1H, *Py-NH*), 7.165-7.101 (m, 1H, *Ar*)，7.233-7.17 (m, 1H, *Ar*), 7.36 (d, *J* = 9Hz，1H, *Ar*)，7.67 (d, *J* = 9Hz，1H, *Ar*), 8.10 (s, 1H, -*NH*); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 166.39, 151.48, 140.79, 140.50, 131.72, 130.23, 128.10, 127.83, 117.09, 103.82, 52.57, 36.09, 31.71, 21.61, 13.59; MALDI-TOF MS m/z calcd for $C_{28}H_{45}N_3O_3$: 471.35. Found: 471.9 ($[M]^+$, 100)

Cleavage of the N-Boc protecting group and get compounds 5

Trifluoroacetic acid (TFA, 10 mL) was added to a solution of the corresponding N-Boc-protected compound (ca. 2 g) in dichloromethane (15 mL). The solution was stirred at room temperature for 2 h and evaporated. The residue obtained was repeatedly dissolved in dichloromethane and the solvent evaporated to yield the crude trifluoroacetate salt, which was redissolved in dichloromethane (60 mL) and washed with saturated aqueous $NaHCO_3$ (3 x 40 mL) and brine to neutrality. After drying and filtering, evaporation of the solvent afforded the corresponding amine which was used in the next step without further purification.

Typical procedure for compound 3

A mixture of **4** (462.9 mg, 0.9228 mmol), *p*-(methoxycarbonyl)phenyl-boronic acid (664.3 mg, 3.6912 mmol), $Pd(PPh_3)_4$ (511.9 mg, 0.4429 mmol) and K_2CO_3 (918.3 mg, 6.442 mmol) in a mixture of EtOH-H_2O-C_6H_6 at 1 : 1 : 2 (40 mL) was stirred under N_2 at 90 ^{o}C for 12 h. After

cooling, the resulting mixture was dissolved in CH_2Cl_2, washed with water and dried over anhydrous Na_2SO_4. After evaporation of the solvent, the crude product was purified by column chromatography on silica gel using CH_2Cl_2 : ethyl acetate at 30 : 1 to give a yellow solid (429.5 mg, 66.4%). m.p.: 176-177℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.93 (t, 6H, *J* = 9Hz, -*CH*$_3$), 1.485-1.411 (m, 4H, -*CH*$_2$), 1.663-1.575 (m, 4H, -*CH*$_2$), 2.83 (t, *J* = 9Hz，4H, -*CH*$_2$), 4.00 (s, 6H, -*CH*$_3$), 8.01(d, *J* = 9Hz，4H, *Ar*), 8.27 (d, *J* = 9Hz, 4H, *Ar*); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 166.39, 151.48, 140.79, 140.50, 131.72, 130.23, 128.10, 127.83, 117.09, 103.82, 52.57, 36.09, 31.71, 21.61, 13.59; MALDI-TOF MS m/z calcd for $C_{32}H_{32}N_2O_4S_6$: 700.07. Found: 700.08.([M]$^+$, 100).

Typical procedure for compound 2

A mixture of **3** (278.7 mg, 0.3976 mmol) and NaOH (4 M, 20 mL) aqueous solution in THF (30 mL) was stirred at 50 ^{o}C overnight. After cooling and evaporation of the solvent, the pH was adjusted to 2-3. Thereafter, the mixture was filtered and washed with water. The filter cake was dried in vacuum to obtain a brownish yellow solid (215.5 mg, 80.5%). m.p.: 233-234℃. MALDI-TOF MS m/z calcd for $C_{30}H_{28}N_2O_4S_6$: 672.04. Found: 672.0.([M]$^+$, 100).

Typical procedure for compounds 1

The mixture of **2** (0.06 mmol), EDCI (0.13 mmol), HOBT (0.13 mmol) and the corresponding compounds 5 (0.12 mmol) was suspended in THF (10 mL). The reaction mixture was stirred at room temperature for one day. The solvent was eliminated and the residue was taken up in $CHCl_3$. The solution was successively washed with aqueous HCl (1 M), aqueous NaOH (1 M) and brine. After drying and filtering, the solvent was eliminated and the residue was purified by column chromatography on silica gel using CH_2Cl_2 : methanol at 30 : 1 to give a orange-yellow solid.

Compound 1a: Yield 72.5%, m.p.: 189-190℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.955-0.818 (m, 12H, -*CH*$_3$), 1.464-1.241 (m, 40H, -*CH*$_2$), 1.646-1.516 (m,8H, -*CH*$_2$), 1.82 (br, 2H, -*NH*), 2.987-2.662 (m, 4H, -*CH*$_2$), 3.31 (q, *J* = 6 Hz, 4H, -*CH*$_2$), 4.267-4.120 (m, 4H, -*CH*$_2$), 6.81 (br, 1H, -*NH*), 7.79 (br, 1H, -*NH*), 7.97 (d, *J* = 9Hz,4H, *Ar*), 7.87 (d, *J* = 9Hz,4H, *Ar*); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 169.05, 167.37, 151.16, 140.68, 139.43, 135.06, 128.32, 127.93, 127.72, 103.65, 44.13, 39.85, 36.04, 31.93, 31.71, 29.68, 29.66, 29.63, 29.59, 29.49, 29.37, 29.33, 26.97, 22.70, 21.63, 14.14, 13.61; MALDI-TOF MS m/z calcd for $C_{58}H_{84}N_6O_4S_6$: 1120.49. Found:1121.5.([M+H]$^+$, 100).

Compound 1b: Yield 68.2%, m.p.: 231-232℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.999-0.814 (m, 12H, -*CH*$_3$), 1.177-1.009 (m, 12H, -*CH*$_3$), 1.496-1.246 (m, 38H, -*CH*$_2$), 1.688-1.529 (m, 8H, -*CH*$_2$), 1.987-1.700 (m, 8H, -*CH*$_2$), 2.81(t, *J* = 9Hz，4H, -*CH*$_2$), 3.22-3.070 (m, 2H, -*CH*$_2$), 3.501-3.356

(m, 2H, -CH_2), 5.058-4.889 (m, 2H, -*CH*),7.3 (br, 1H, -*NH*), 7.45 (br, 2H, -*NH*), 7.70 (d, *J* = 9Hz,4H, *Ar*), 7.82(d, *J* = 9Hz, 4H, *Ar*), 7.97 (br, 1H, -*NH*); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 172.11, 167.22, 150.90, 135.67, 128.25, 128.20, 128.05, 127.96, 127.56, 52.25, 41.04, 39.79, 39.72, 35.98, 31.94, 31.76, 31.72, 29.69, 29.51, 29.41, 27.11, 25.09, 22.85, 22.71, 21.68, 14.14, 13.63; MALDI-TOF MS m/z calcd for$C_{66}H_{100}N_6O_4S_6$: 1232.61. Found: 1233.9.([M+H]$^+$, 100).

Compound 1c: Yield 67.3%, m.p.: 226-227℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.96-0.827 (m, 12H, -CH_3), 1.459-1.243 (m, 44H, -CH_2), 1.651-1.557 (m, 4H, -CH_2), 1.77 (br, 1H, -*NH*), 2.906-2.710 (m, 4H, -CH_2), 3.363-3.021 (m, 8H, -CH_2), 5.236-5.100 (m, 2H, -*CH*), 7.00 (br, 2H, -*NH*), 7.4-7.287 (m, 10H, *Ar*), 7.71 (d, *J* = 9Hz, 4H, *Ar*), 7.79 (d, *J* = 9Hz, 4H, *Ar*), 7.88（br, 1H, -*NH*); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 175.47, 170.87, 166.92, 137.06, 135.52, 129.52, 128.60, 128.53, 128.44, 128.28, 128.25, 128.19, 128.03, 127.94, 127.67, 126.88, 55.32, 39.72, 38.85, 38.77, 36.02, 32.00, 31.95, 31.77, 31.72, 29.73, 29.70, 29.63, 29.47, 29.40, 29.34, 27.06, 26.98, 22.72, 21.66, 14.15, 13.64; MALDI-TOF MS m/z calcd for $C_{72}H_{96}N_6O_4S_6$: 1300.58. Found: 1301.6.([M+H]$^+$, 100).

Compound 1d: Yield 61.4%, m.p.: 224-225℃. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.915-0.742 (m, 12H, -CH_3), 1.4-1.175 (m, 44H, -CH_2), 1.537-1.433 (m, 4H, -CH_2), 3.272-3.023 (m, 8H, -CH_2), 4.792-4.673 (m, 2H, -*CH*), 7.102-6.952(m, 4H, *Ar*), 7.24 (s, 2H,*Py-NH*), 7.315 (d, *J* = 9Hz，2H, *Ar*), 7.695 (d, *J* = 9Hz，2H, *Ar*), 7.89 (d, *J* = 9Hz，4H, *Ar*), 8.05 (d, *J* = 6Hz，4H, *Ar*),8.73 (d, *J* = 9Hz, 2H, -*NH*), 10.80 (br, 1H, -*NH*); ^{13}C NMR (75 MHz, DMSO) δ: 171.78, 165.88, 151.88, 140.27, 138.94, 136.53, 136.28, 128.73, 128.08, 127.74, 127.46, 124.07, 121.31, 118.98, 118.63, 111.77, 110.99, 54.92, 35.61, 34.84, 31.77, 31.67, 30.87, 29.59, 29.52, 29.48, 29.23, 26.74, 22.57, 21.27, 14.41, 13.85; MALDI-TOF MS m/z calcd for $C_{76}H_{98}N_8O_4S_6$: 1378.60. Found: 1377.3 ([M-H]$^+$, 100).

Reference:

1. (a) N. Zheng, H. Li, G. Sun, K. Zhong, B. Yin, *Org. Biomol. Chem.* **2013**, *11*, 5100-5108; (b) S. Debnath, A. Shome, S. Dutta, P. K. Das, *Chem. Eur. J.* **2008**, *14*, 6870-6881; (c) Y, Dai, X, Zhao, X, Su, G, Li, A. Zhang, *Macromol. Rapid. Commun.* **2014**, *35*, 1326-1331; (d) S. Basak, N. Nandi, A. Baral, A. Banerjee, *Chem. Commun.* **2015**, *51*, 780-783.

3. Additional data

Table S1 Gelation properties of **1a-d** in various solvents.

Solvents	**1a**	**1b**	**1c**	**1d**
CH_2Cl_2	P	S	TG(1.7)	IS
$CHCl_3$	S	S	S	IS
THF	S	S	TG(3.8)	IS
1,4-dioxane	OG[a] (6.0[b])	P	OG(2.0)	OG(6.0)
CCl_4	TG (4.2)	S	TG (5.0)	sS
Ethyl acetate	IS	IS	IS	IS
Benzene	TG(10.0)	S	TG(10)	sS
Toluene	TG(6.0)	S	TG (5)	sS
Xylene	TG(5.0)	S	TG(3.7)	sS
Phemethylol	S	S	S	S
n-Hexane	IS	IS	PG	IS
Cyclohexane	IS	IS	PG	IS
PE	IS	IS	IS	IS
Acetone	IS	IS	IS	IS
Acetonitrile	IS	IS	IS	IS
Aether	IS	IS	IS	IS
Methanol	IS	IS	IS	IS
Ethanol	IS	IS	IS	IS
DMF	SG(5.0)	SG(5.0)	SG(5.0)	S
DMSO	OG(1.6)	S	OG(1.8)	TG(5.0)
Glacial acetic acid	OG (4.0)	OG(4.0)	OG (4.0)	OG(4.0)

[a]OG = Opaque gel; TG = Transparent gel; P = Precipitation; S = Soluble; IS = Insoluble; SG = Sonication gel

[b]CGC = the critical gelation concentrations (mg/mL) at room temperature.

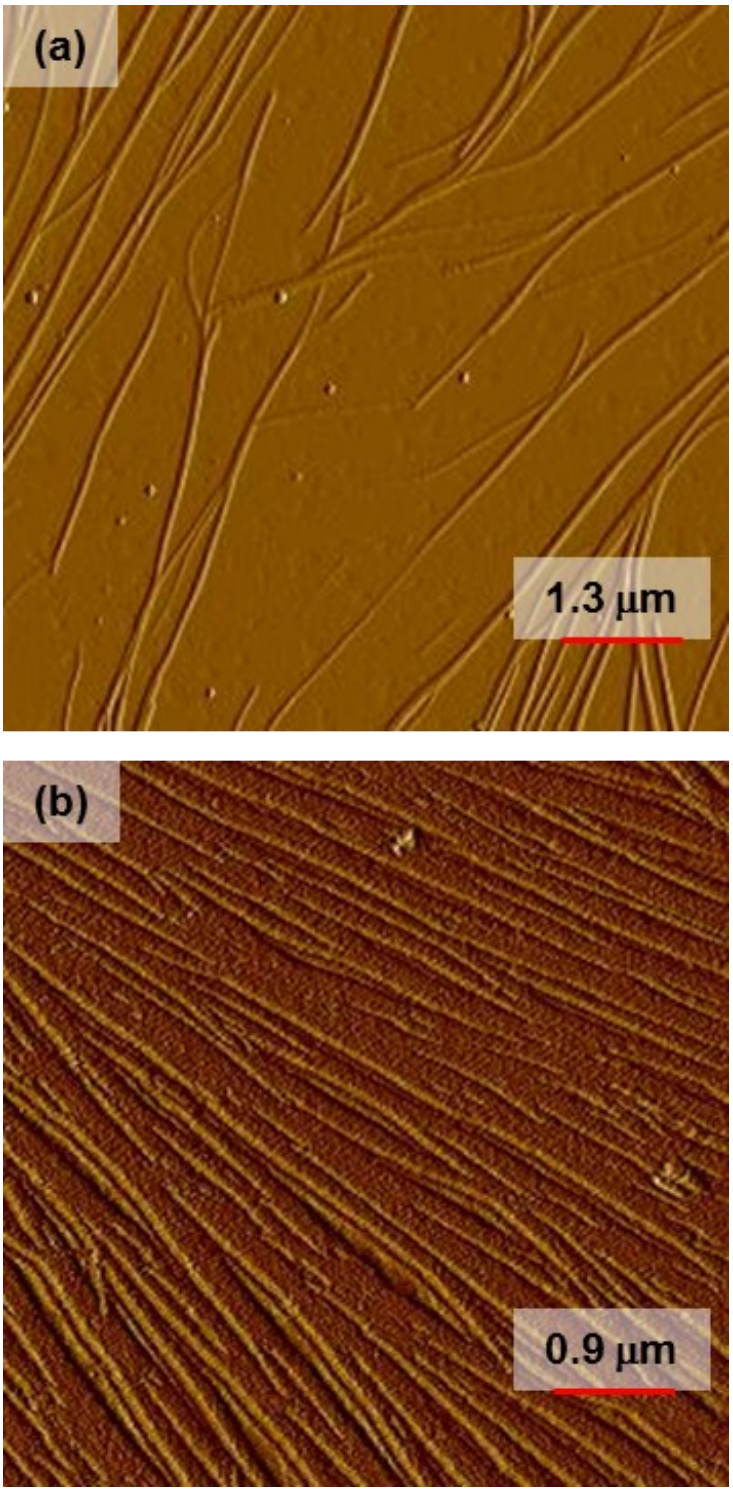


Figure S1. AFM images of organogels of **1c** and **1d** in DMSO (a, b).

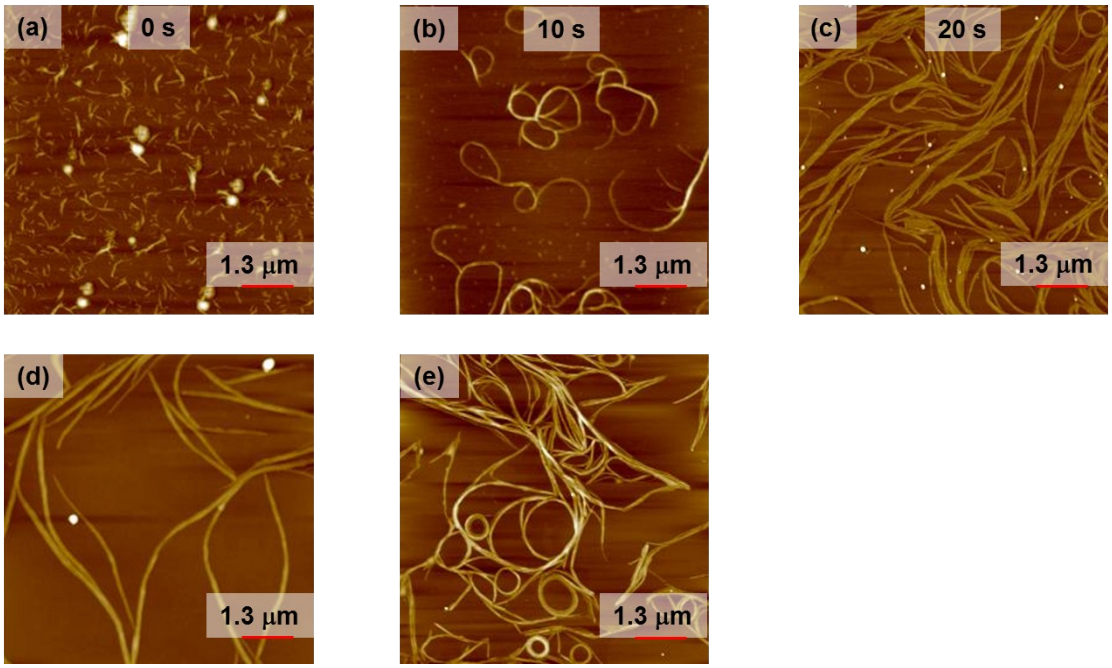


Figure S2. AFM observations of the conversion process of the gelator **1b** in DMF by sonication for different times (a-c), and AFM images of sonication organogels of **1a** and **1c** in DMF.

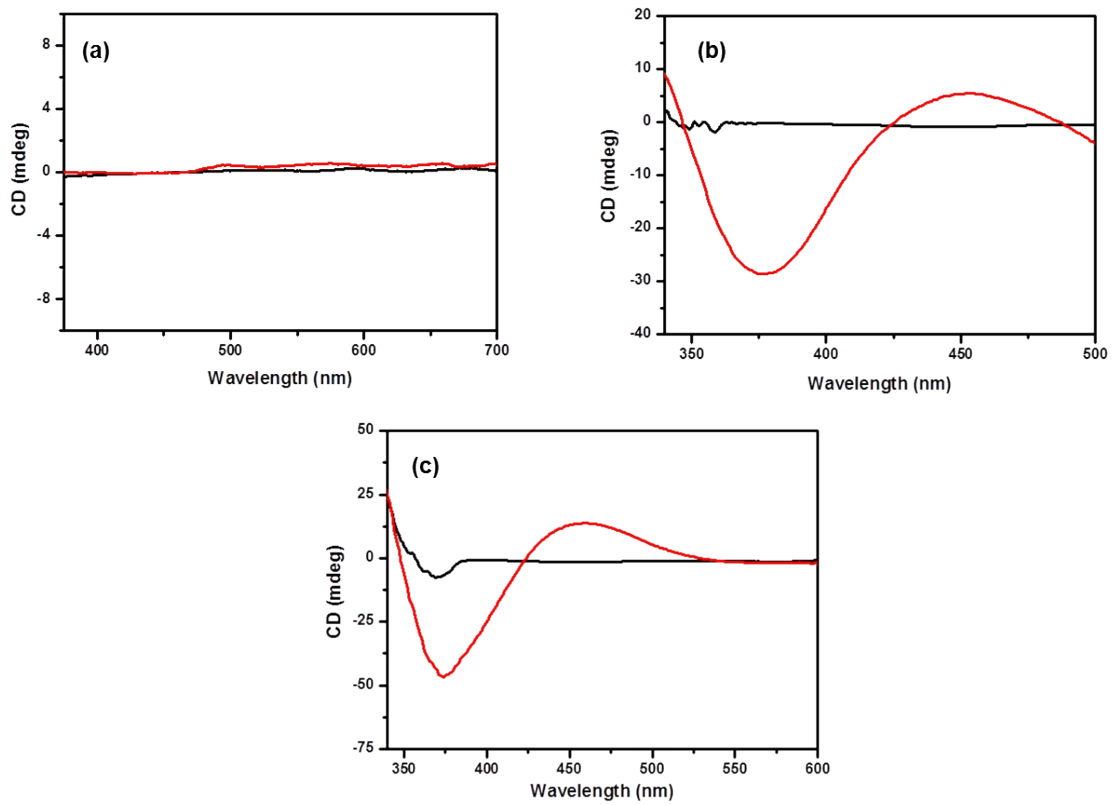


Figure S3. CD spectra of **1a** (a), **1c** (b) and **1d** (c) in $CHCl_3$ solution and 1,4-dioxane gels. Solutions are black lines and gels are red lines.

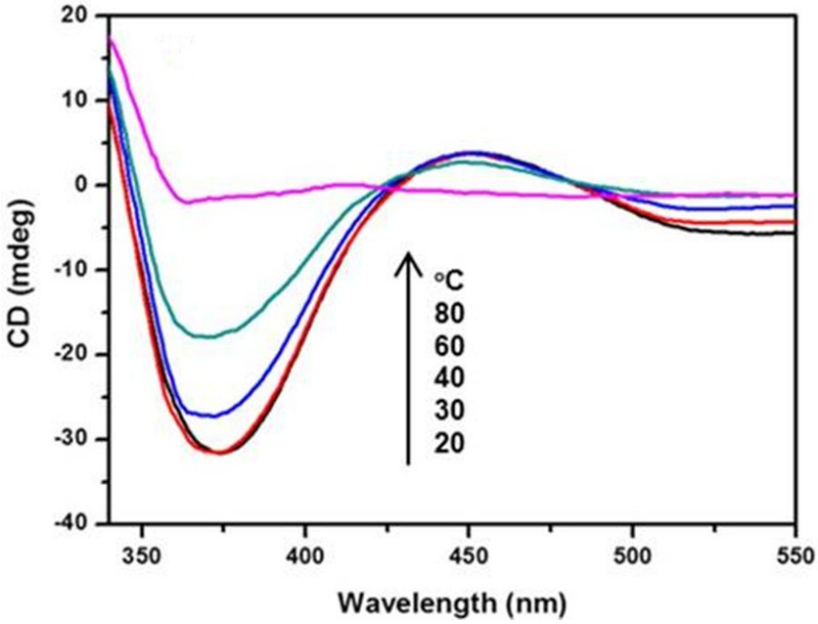


Figure S4. Temperature-dependence of the CD spectra of the organogel of **1c** in 1,4-dioxane. The concentration is 10 mg/mL.

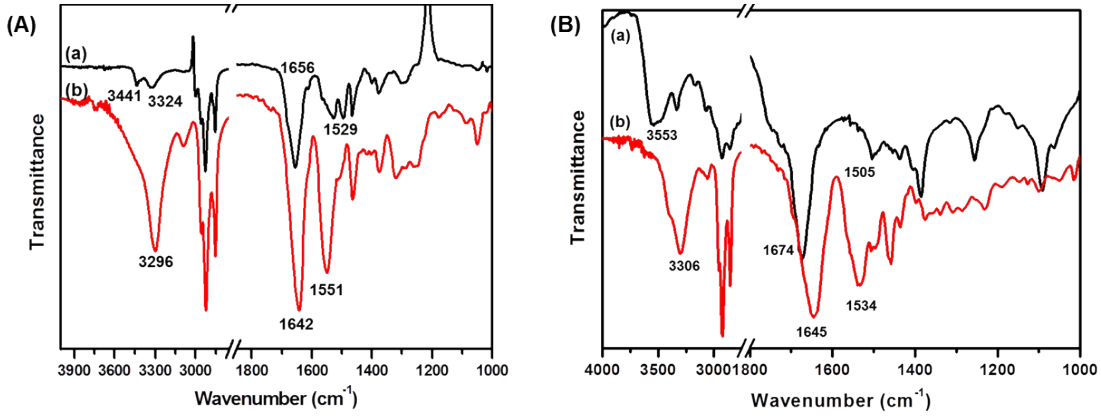


Figure S5. FTIR spectra of (A) **1a** and (B) **1d** in $CHCl_3$ solution (a), xerogel from 1,4-dioxane (b).

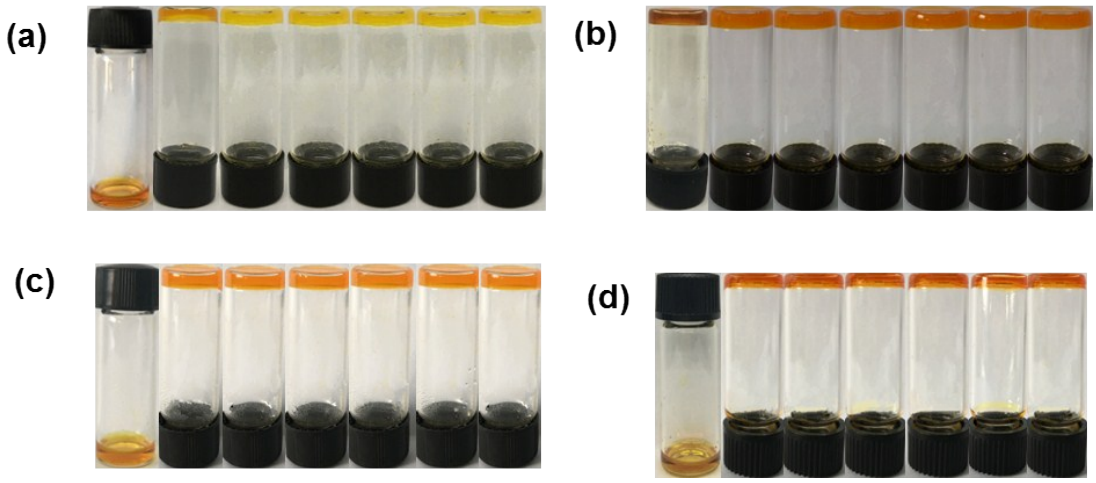


Figure S6. Photographs of the **1c** and **1d** organogels in 1,4-dioxane (a, c) and DMSO (b, d) upon the addition of 5.0 equiv. of each anion. From left to right is addition of F^-, Cl^-, Br^-, I^-, AcO^-, HSO_4^- and $H_2PO_4^-$.

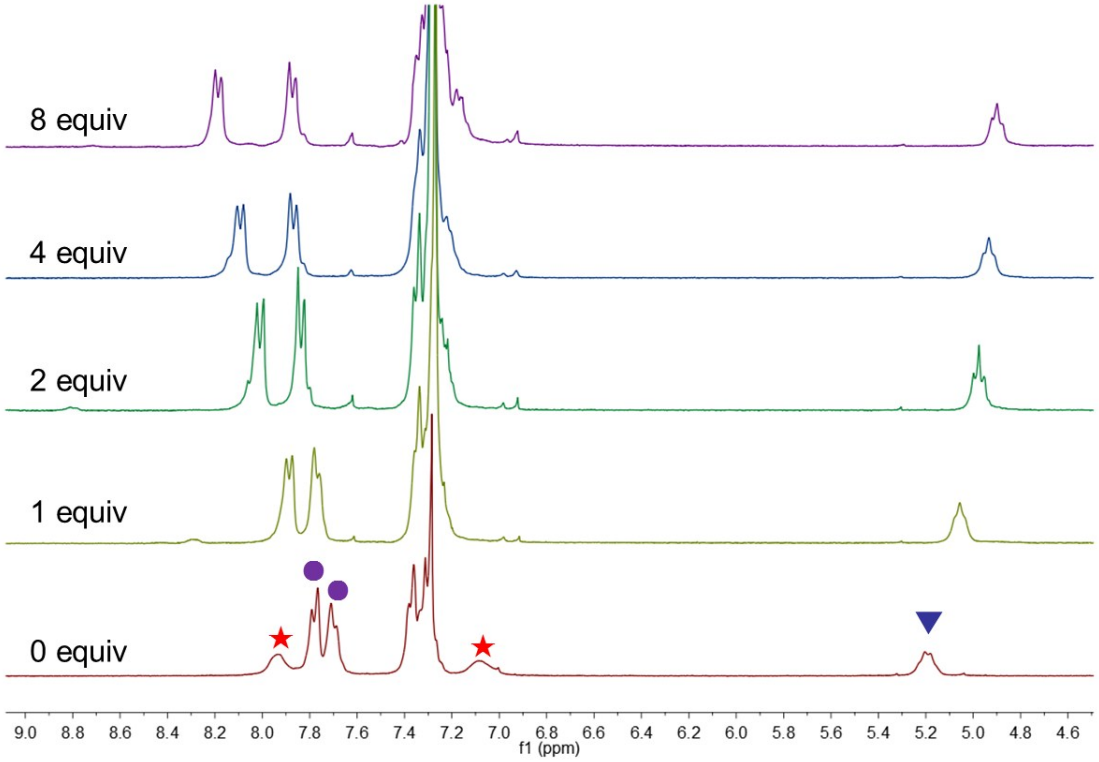


Figure S7. Partial ^1H NMR spectra of **1c** in $CDCl_3$ (5 mg/mL) upon the addition of F^-. ★: the amide N-H; ▼: the C-H on the Phe residues; ●: the aromatic proton on T-shaped skeleton.

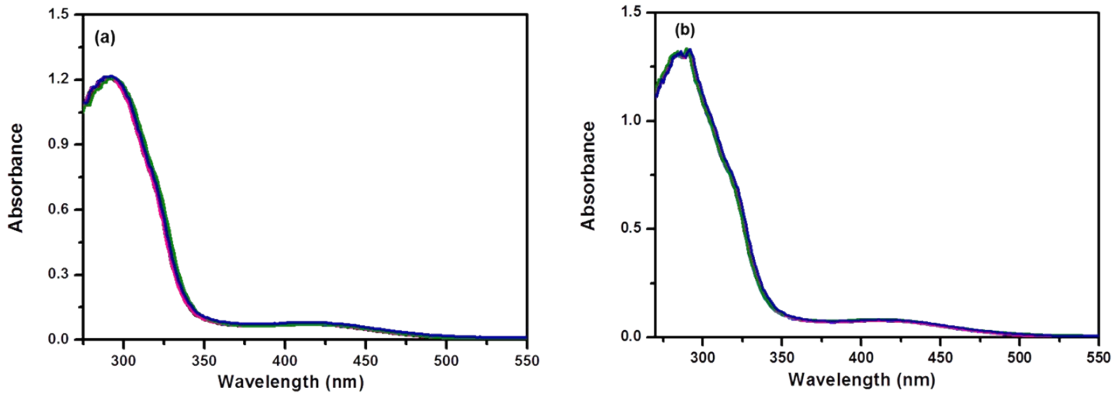


Figure S8. UV-Vis spectra of (a) **1c** in 1,4-dioxane (3×10^{-5} M) and (b) **1d** in DMSO (3×10^{-5} M) with increasing addition of F^- (0-20 equiv).

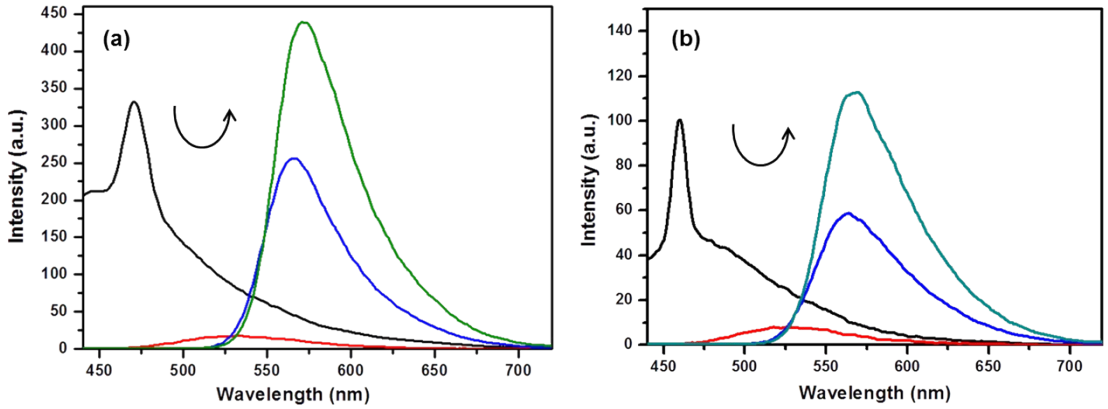


Figure S9. Fluorescence spectra of **1a** (a) and **1d** (b) in 1,4-dioxane at different concentrations. 1×10^{-5} M (black line), 1×10^{-3} M (red line), 5×10^{-3} M (CGC, blue line), 8×10^{-3} M (green line).

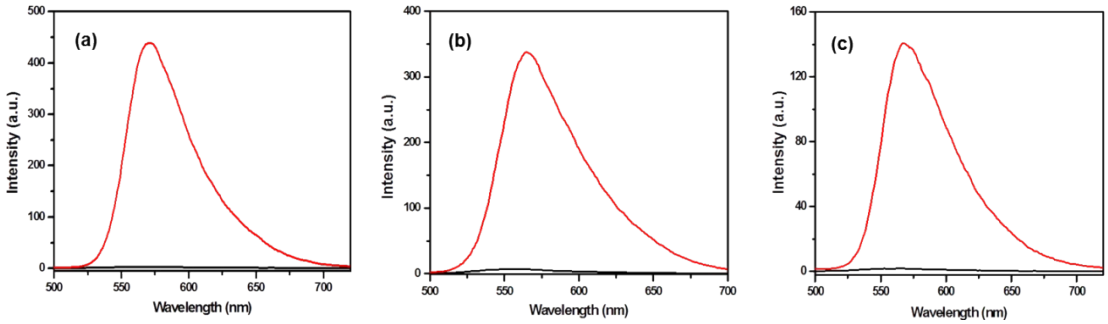


Figure S10. Fluorescence spectra of **1a** (a), **1c** (b) and **1d** (c) in the gel phase (red) and hot solution (black) in 1,4-dioxane (10 mg/mL).

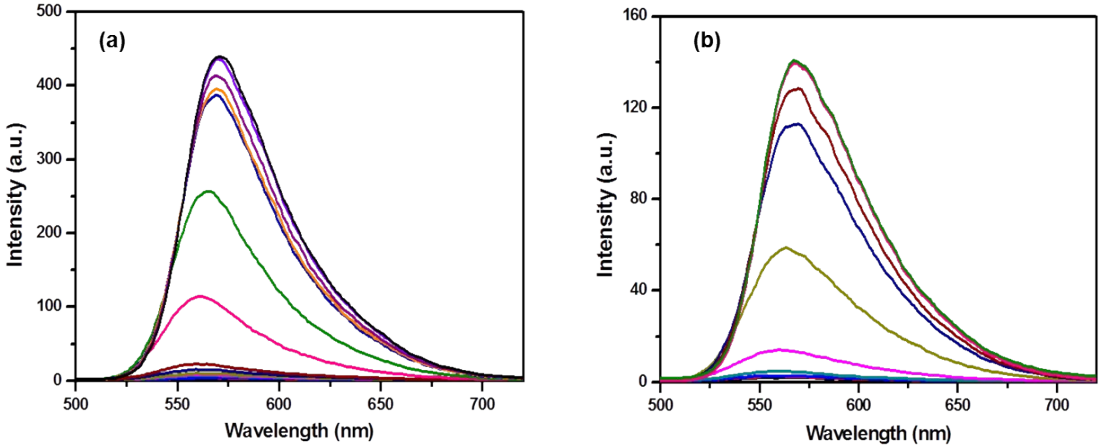


Figure S11. Time-dependent fluorescence changes of gelator **1a** (a) and **1d** (d) in 1,4-dioxane (10 mg/mL).

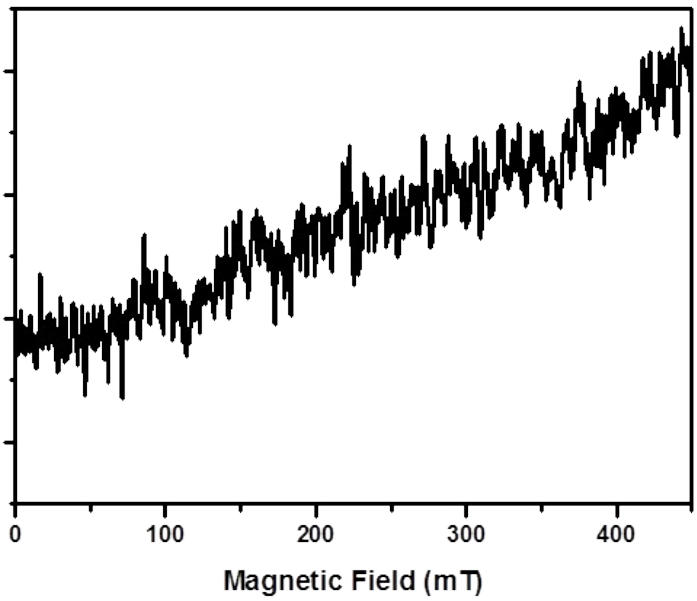


Figure S12. EPR spectrum of the binary gel of **1c** with 0.5 equiv C_{60}.

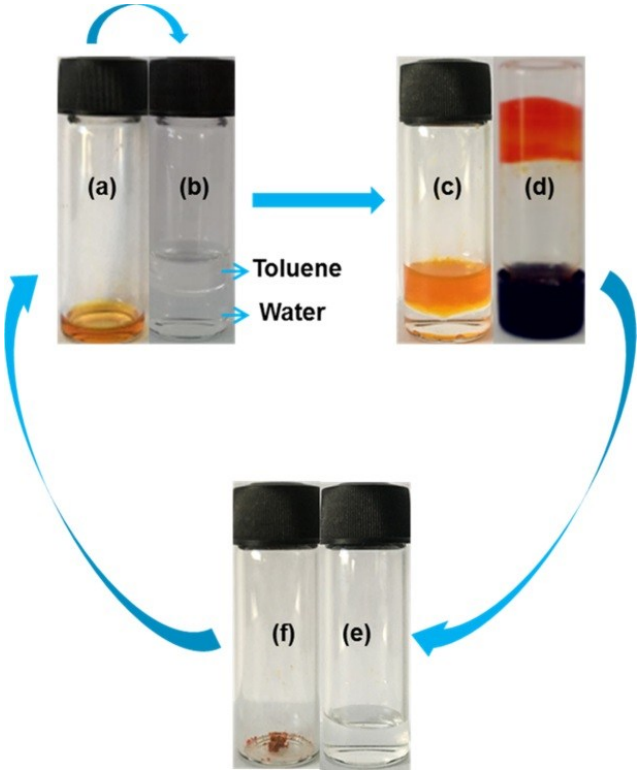


Figure S13. Room-temperature phase-selective gelation and recovery of gelator 1c: (a) 100 μL $CHCl_3$ solution of **1c** (14 mg), (b) 400μL of water and 300μL of the toluene mixture, (c) the mixture of (a) and (b) induces the phase-selective gelation at room temperature, (d) the inclined tube after the selective gelation, (e) the separated water and (f) recovered xerogel of **1c**.

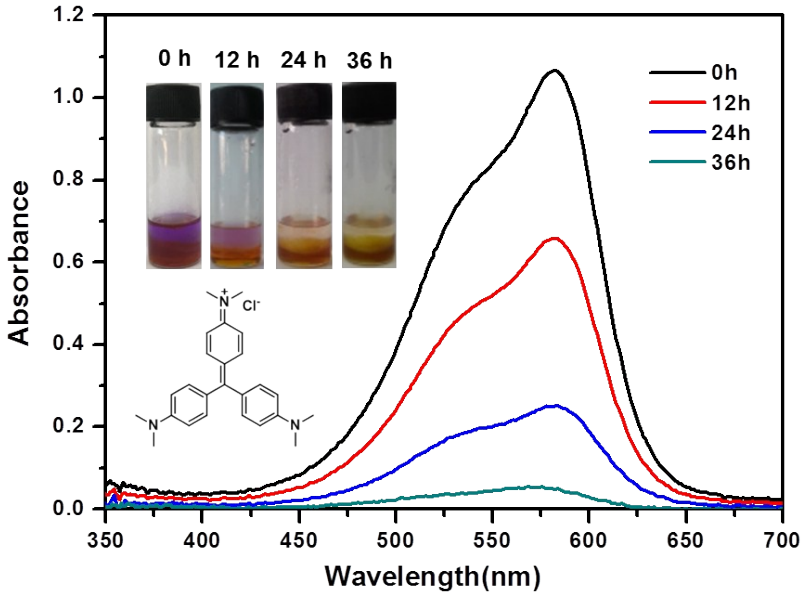
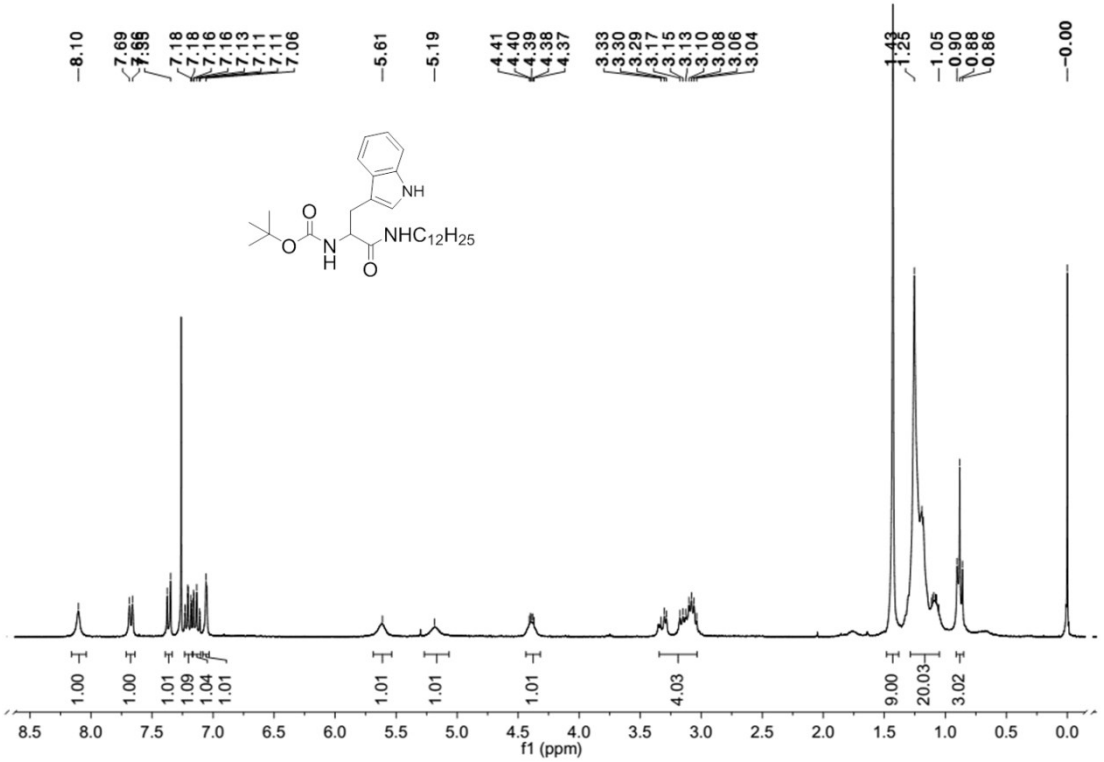
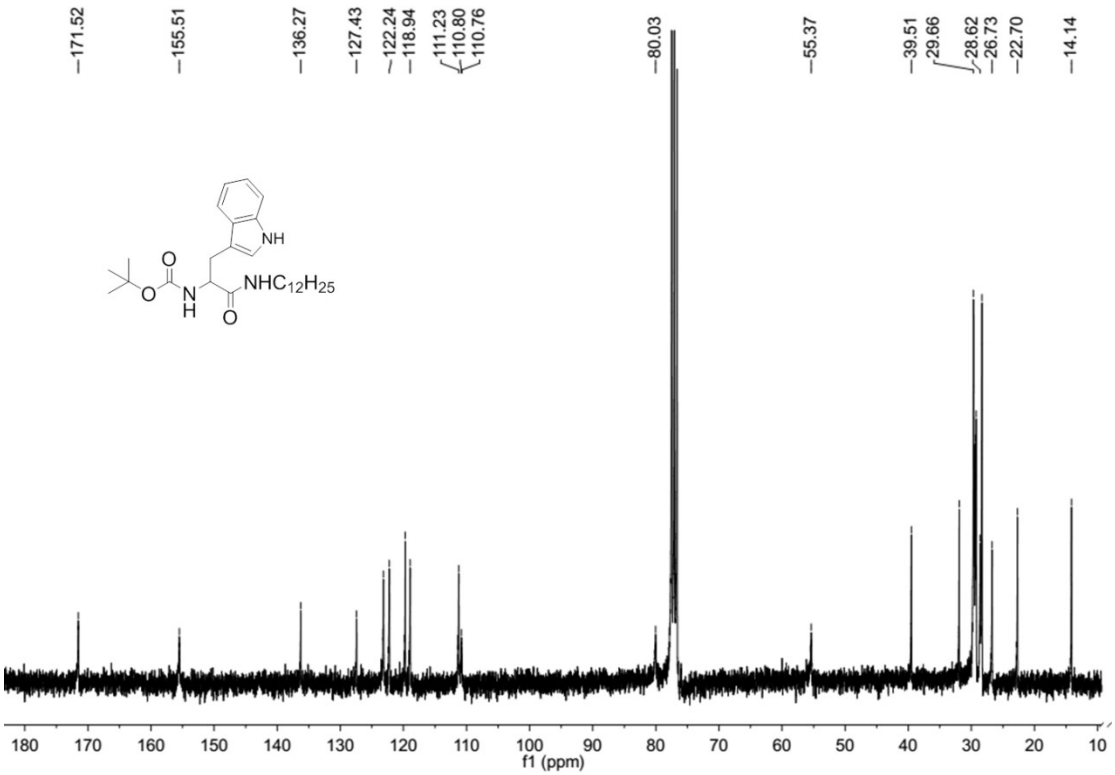
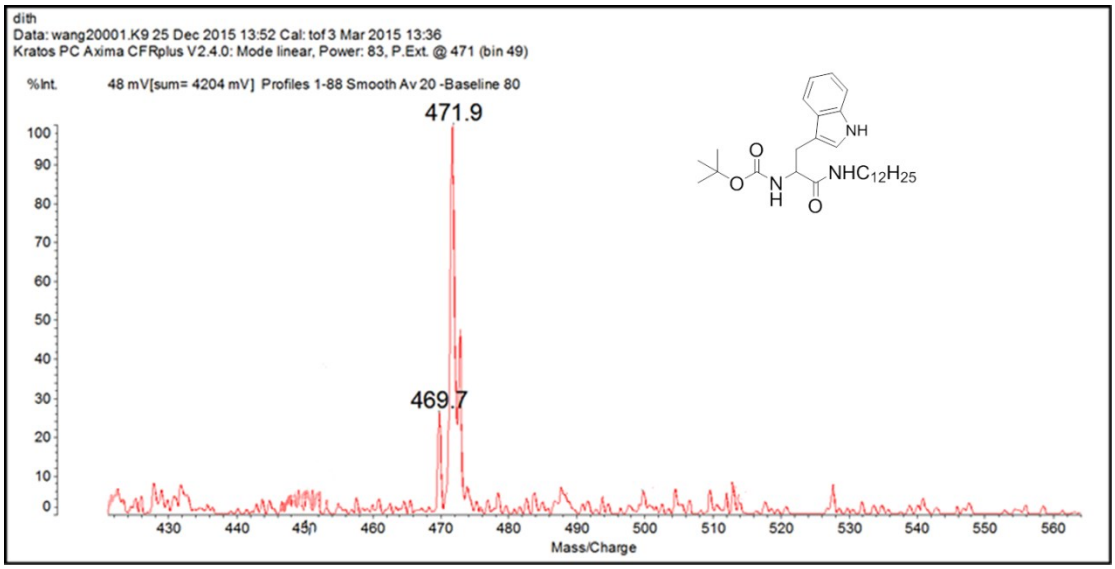


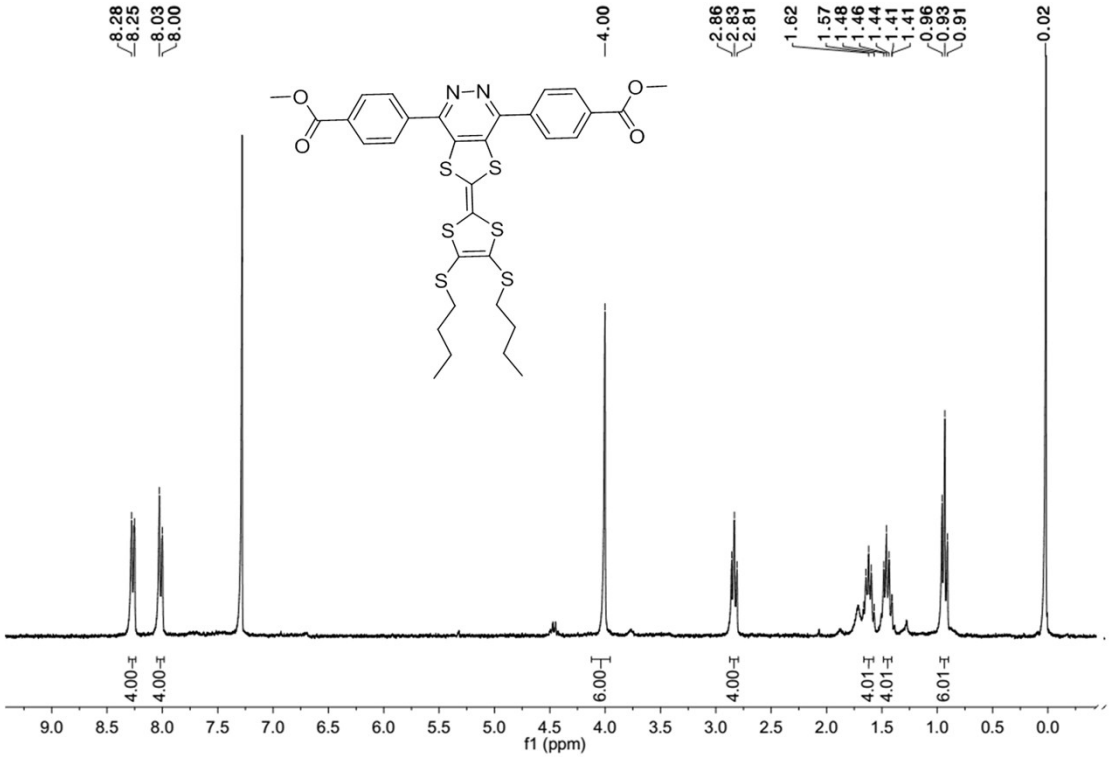
Figure S14. Absorption spectra of aqueous solutions crystal violet after adsorption by organogel **1c** in 1,4-dioxane for different times; 1.0 mL of crystal violet solution (2×10^{-4} M) was added on the top of 0.4 mL gel and the samples were tested at room temperature.

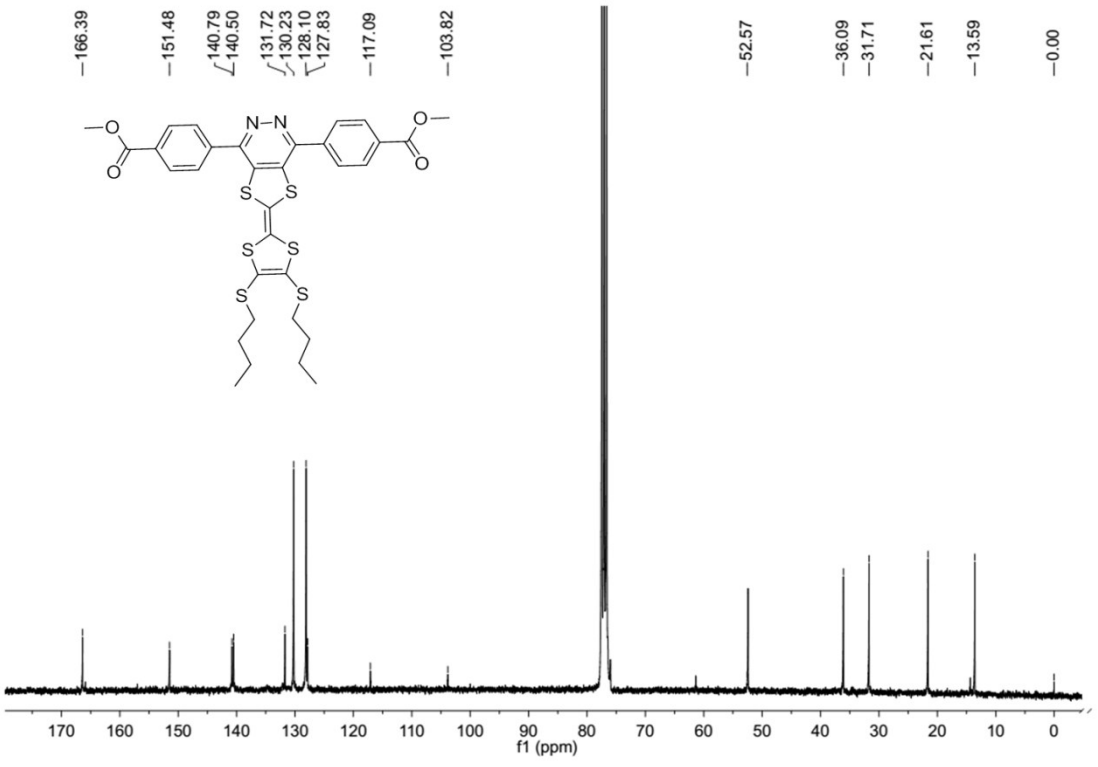
3. ^{1}H, ^{13}C NMR and MALDI-TOF-MS Spectra

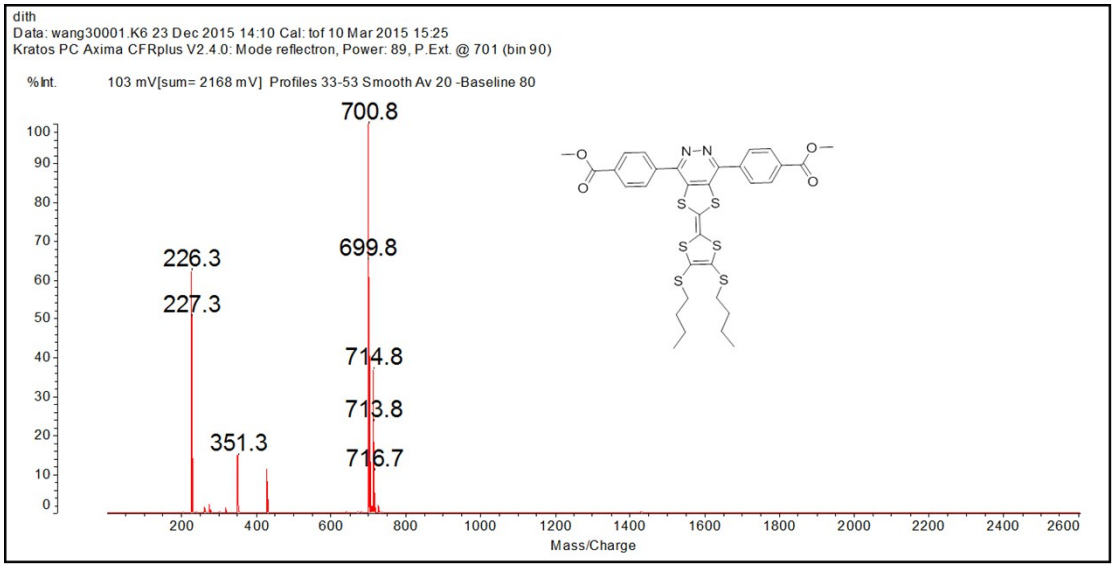


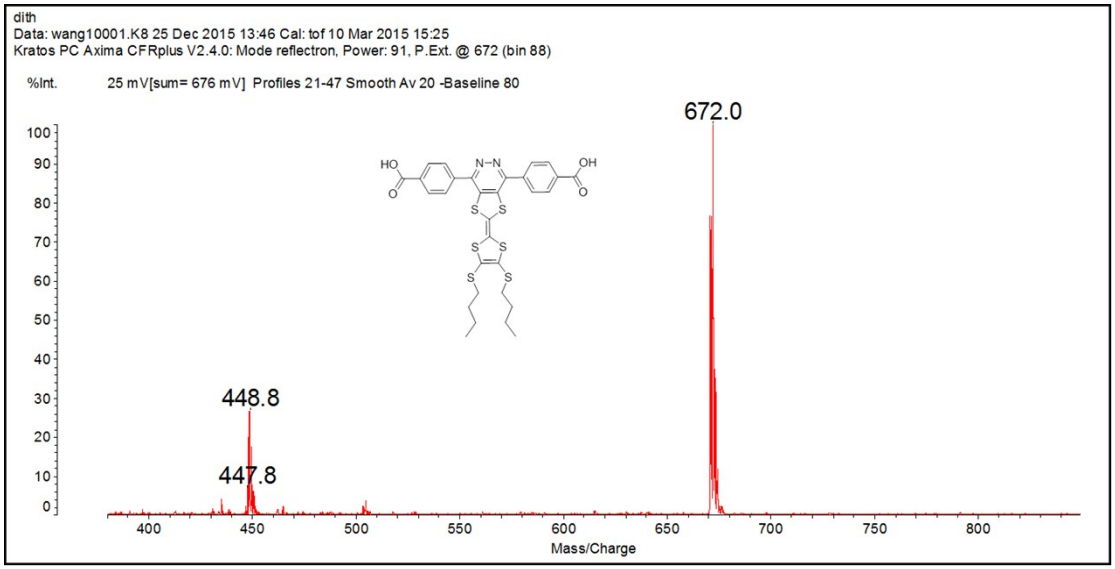

171.52
155.51
136.27
127.43
122.24
118.94
111.23
110.80
110.76
80.03
55.37
39.51
29.66
28.62
26.73
22.70
14.14
NH
O
O
N
H
O
NHC12H25
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

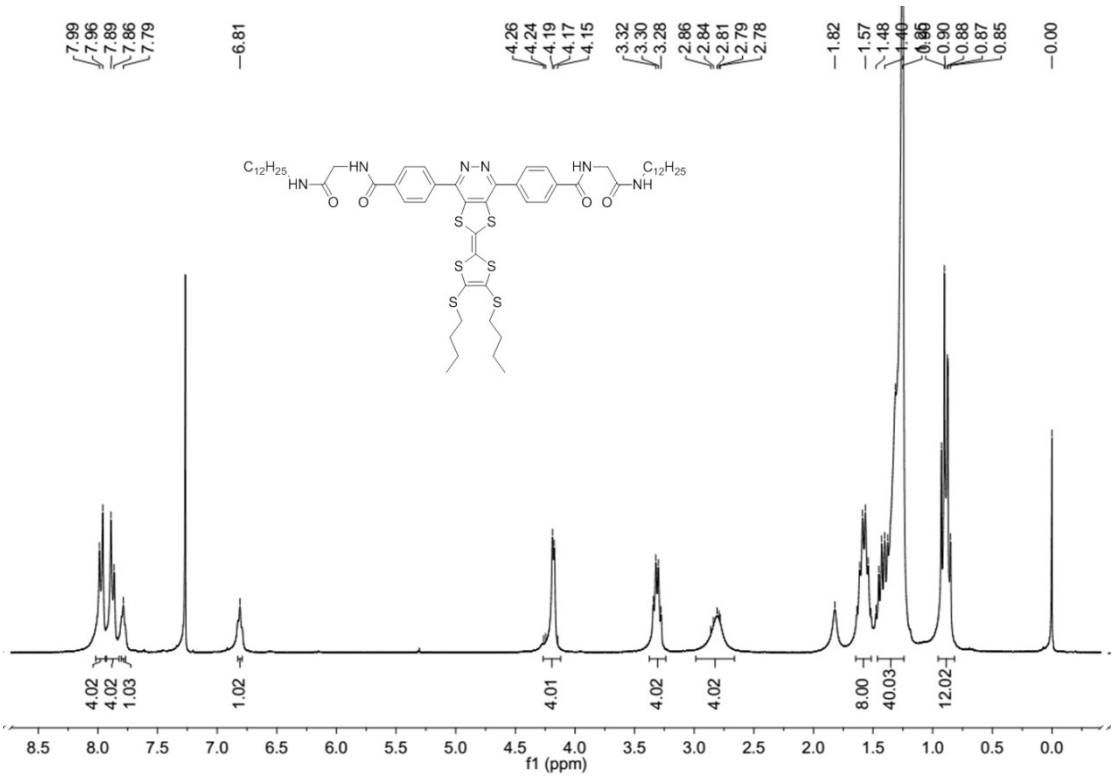

dith
Data: wang20001.K9 25 Dec 2015 13:52 Cal: tof 3 Mar 2015 13:36
Kratos PC Axima CFRplus V2.4.0: Mode linear, Power: 83, P.Ext. @ 471 (bin 49)
%Int.
48 mV[sum= 4204 mV] Profiles 1-88 Smooth Av 20 -Baseline 80
471.9
469.7
NH
O
O
N
H
O
NHC12H25
100 90 80 70 60 50 40 30 20 10 0
430 440 450 460 470 480 490 500 510 520 530 540 550 560
Mass/Charge

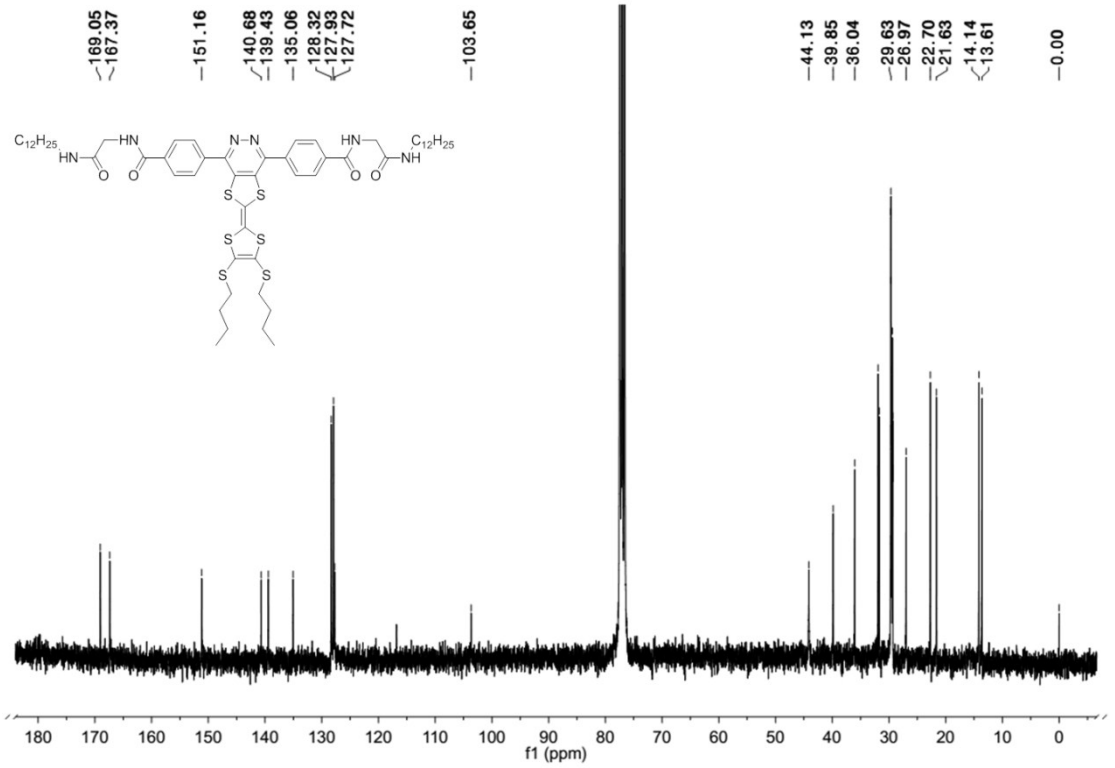

8.28
8.25
8.03
8.00
4.00
2.86
2.83
2.81
1.62
1.57
1.48
1.46
1.44
1.41
1.41
0.96
0.93
0.91
0.02
N–N
O
O
O
O
S
S
S
S
S
S
4.00
4.00
6.00
4.00
4.01
4.01
6.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

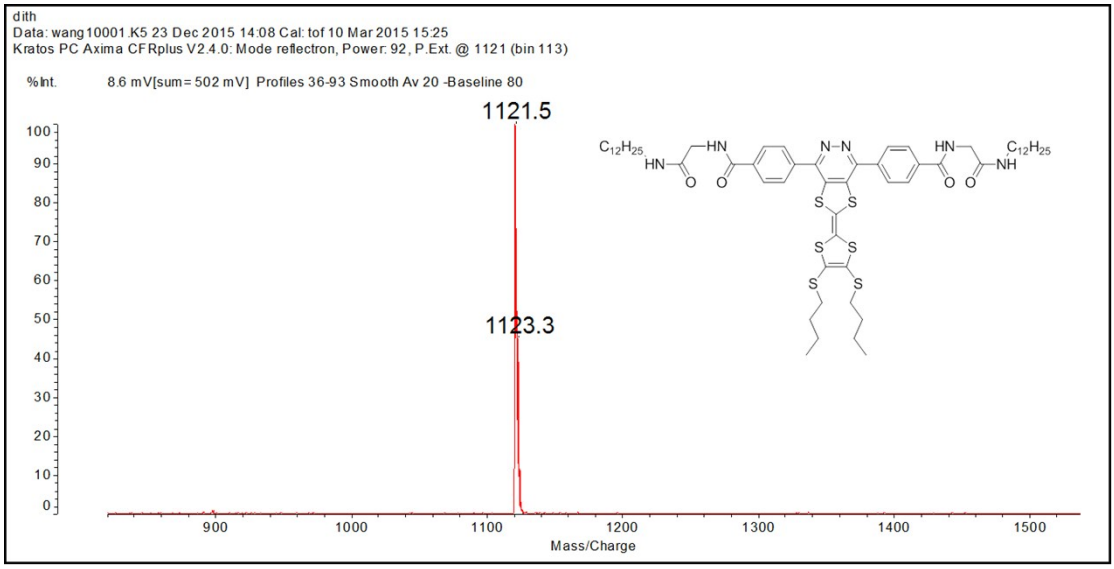

166.39
151.48
140.79
140.50
131.72
130.23
128.10
127.83
117.09
103.82
52.57
36.09
31.71
21.61
13.59
0.00
N–N
O
O
O
O
S
S
S
S
S
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

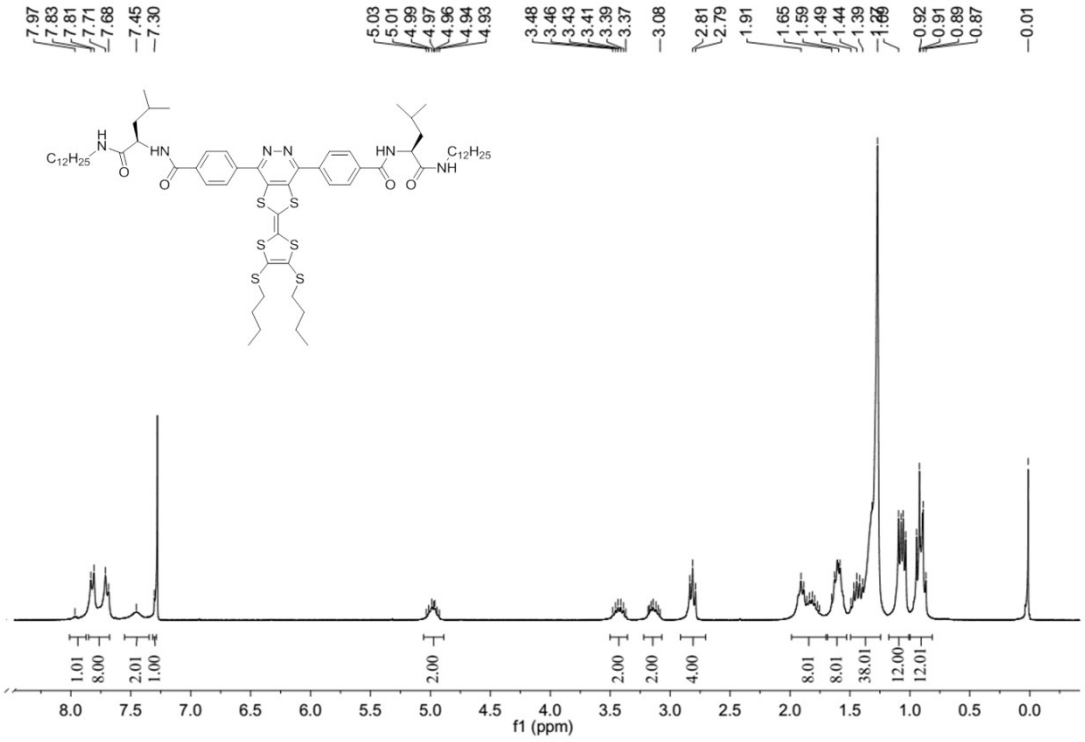

dith
Data: wang30001.K6 23 Dec 2015 14:10 Cal: tof 10 Mar 2015 15:25
Kratos PC Axima CFRplus V2.4.0: Mode reflectron, Power: 89, P.Ext. @ 701 (bin 90)
%Int.
103 mV[sum= 2168 mV] Profiles 33-53 Smooth Av 20 -Baseline 80
700.8
699.8
226.3
227.3
714.8
713.8
351.3
716.7
Mass/Charge

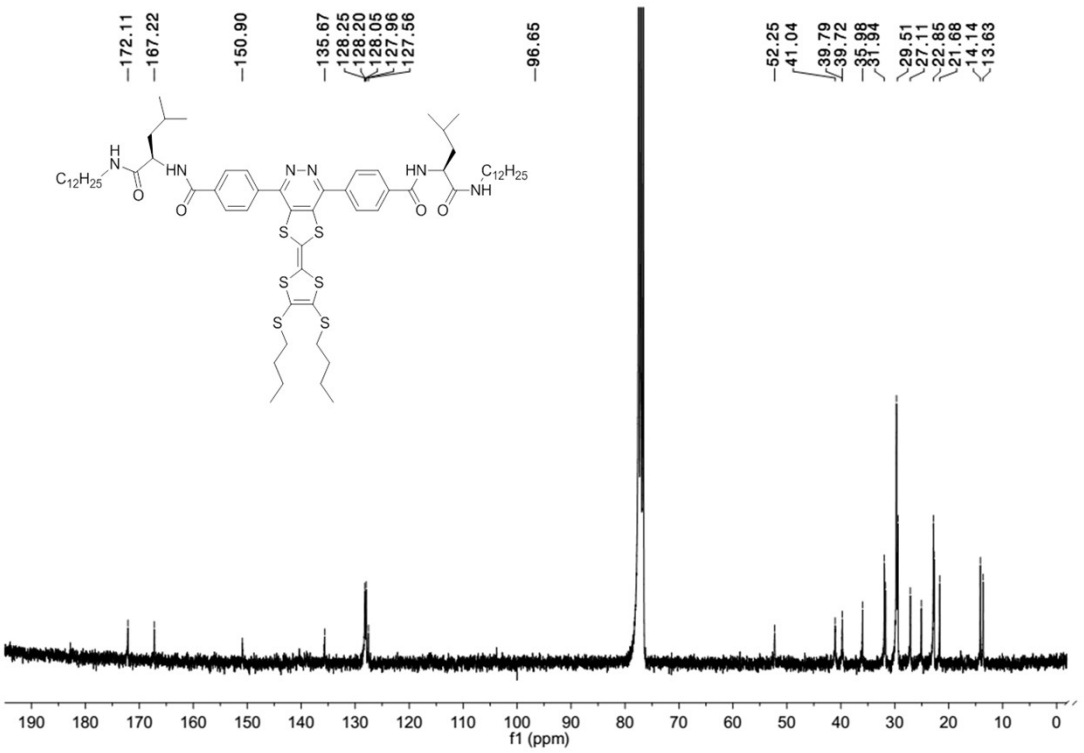

dith
Data: wang10001.K8 25 Dec 2015 13:46 Cal: tof 10 Mar 2015 15:25
Kratos PC Axima CFRplus V2.4.0: Mode reflectron, Power: 91, P.Ext. @ 672 (bin 88)
%Int.
25 mV[sum= 676 mV] Profiles 21-47 Smooth Av 20 -Baseline 80
672.0
448.8
447.8
Mass/Charge

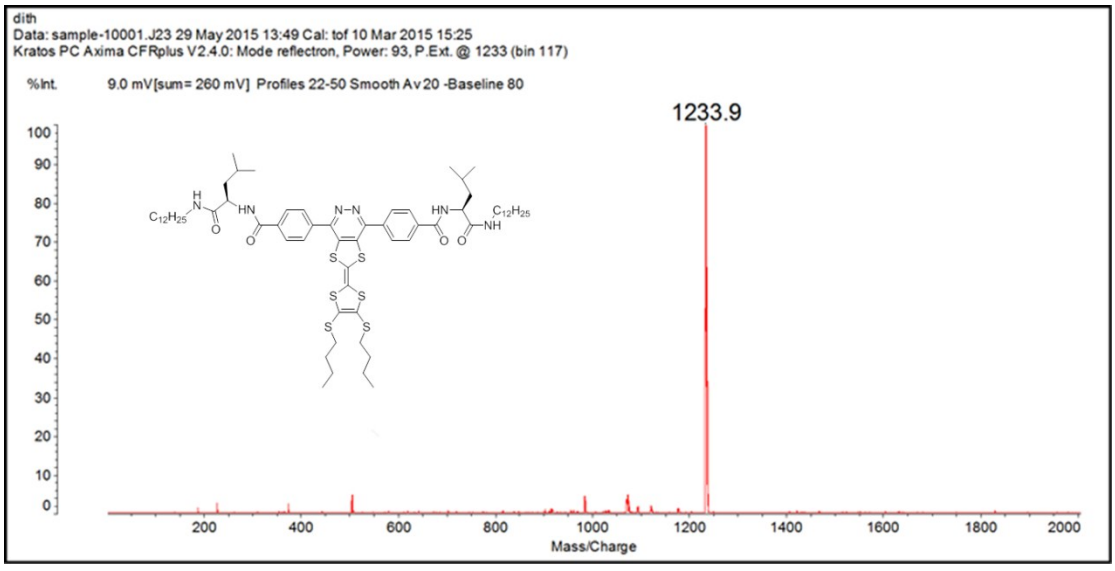

7.99
7.96
7.89
7.86
7.79
6.81
4.26
4.24
4.19
4.17
4.15
3.32
3.30
3.28
2.86
2.84
2.81
2.79
2.78
1.82
1.57
1.48
1.40
0.90
0.88
0.87
0.85
0.00
4.02
4.02
1.03
1.02
4.01
4.02
4.02
8.00
40.03
12.02
f1 (ppm)

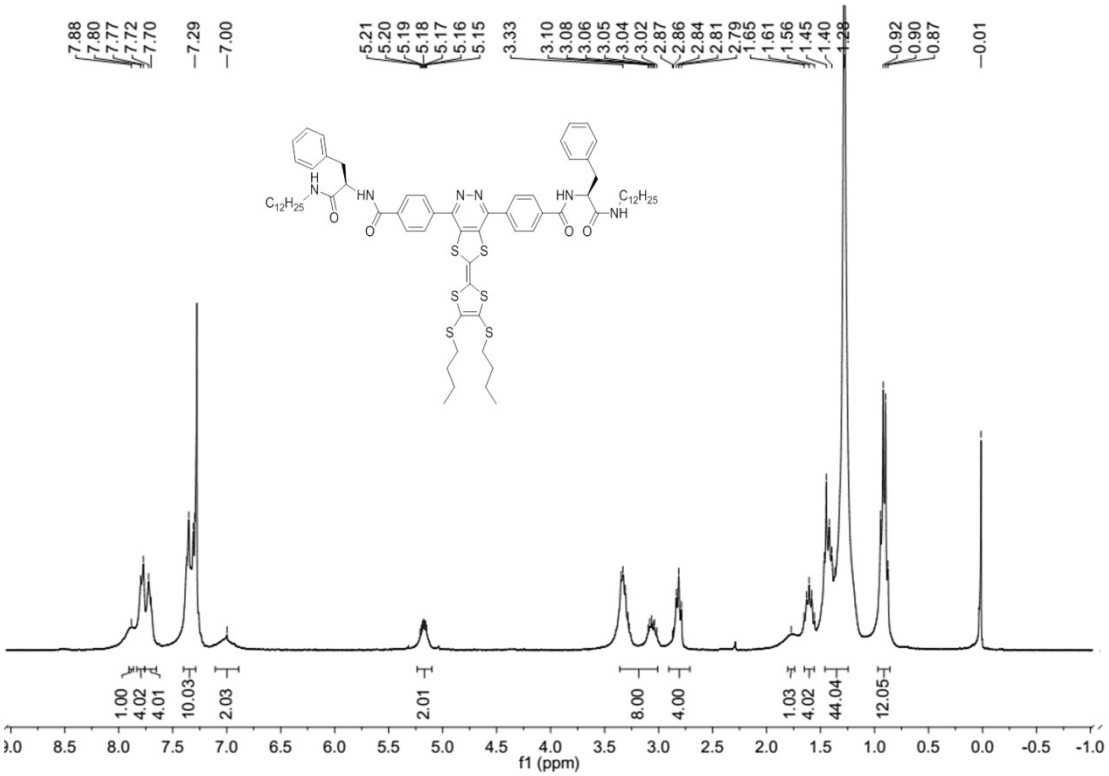

169.05
167.37
151.16
140.68
139.43
135.06
128.32
127.93
127.72
103.65
44.13
39.85
36.04
29.63
26.97
22.70
21.63
14.14
13.61
0.00
f1 (ppm)

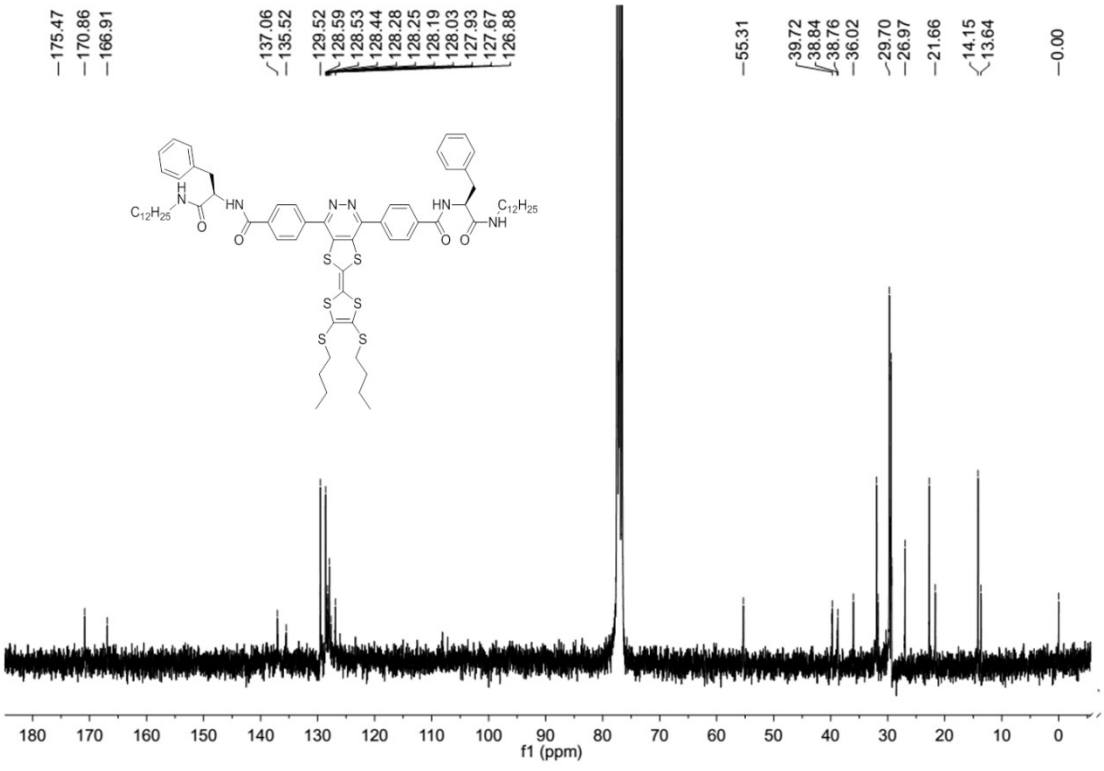

dith
Data: wang10001.K5 23 Dec 2015 14:08 Cal: tof 10 Mar 2015 15:25
Kratos PC Axima CFRplus V2.4.0: Mode reflectron, Power: 92, P.Ext. @ 1121 (bin 113)
%Int.
8.6 mV[sum=502 mV] Profiles 36-93 Smooth Av 20 -Baseline 80
1121.5
1123.3
Mass/Charge

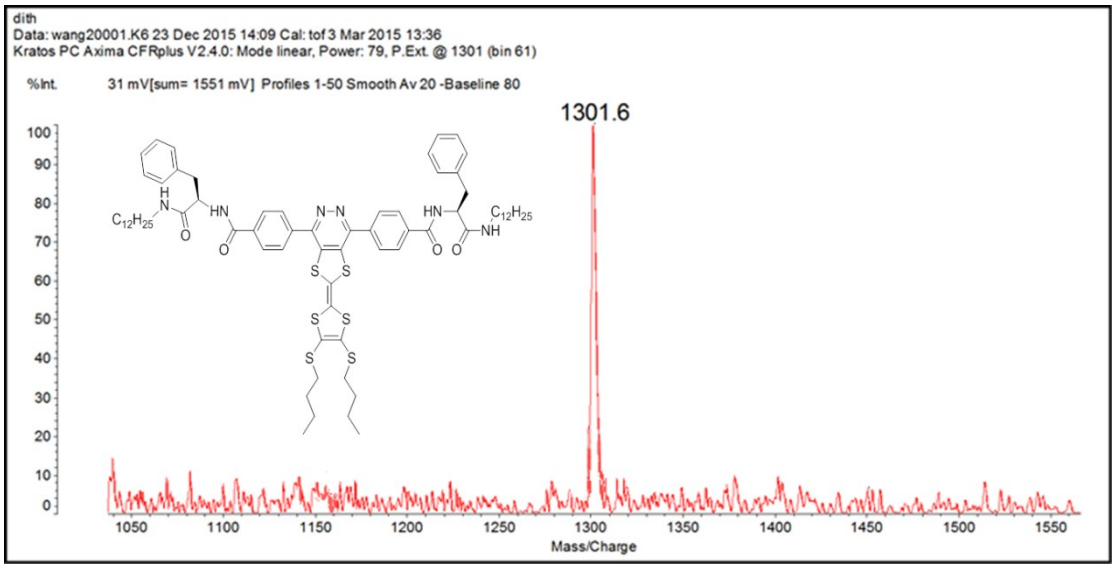

f1 (ppm)

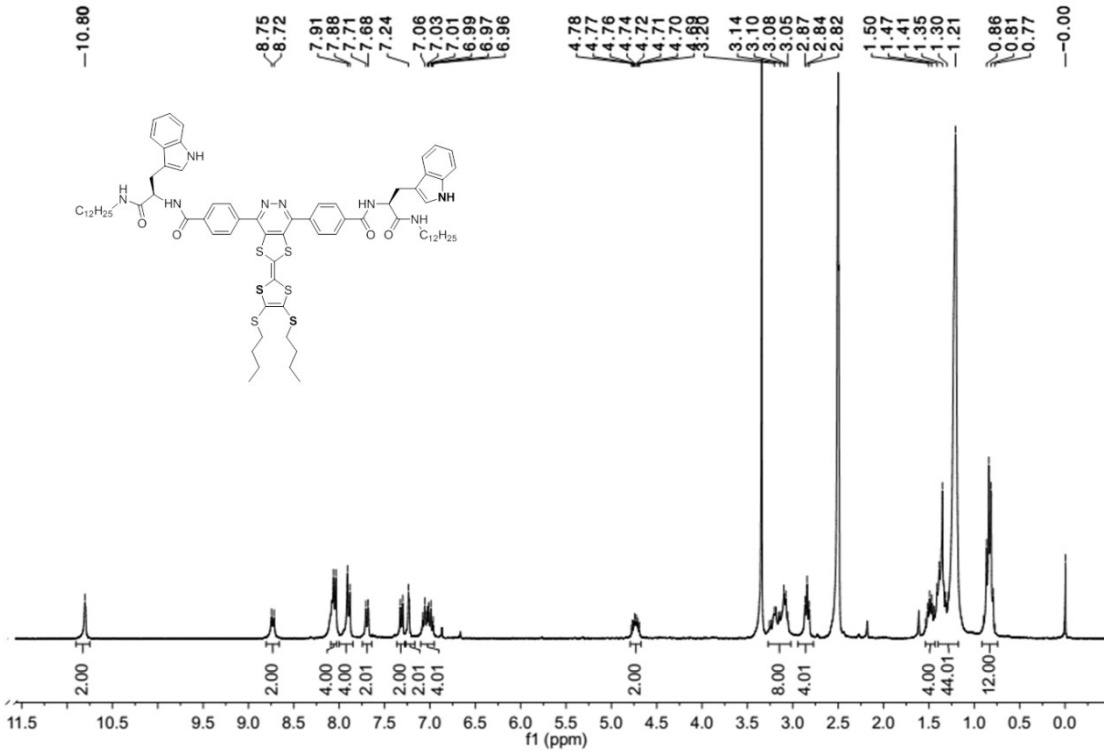

172.11
167.22
150.90
135.67
128.25
128.20
128.05
127.96
127.56
96.65
52.25
41.04
39.79
39.72
35.98
31.94
29.51
27.11
22.85
21.68
14.14
13.63
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

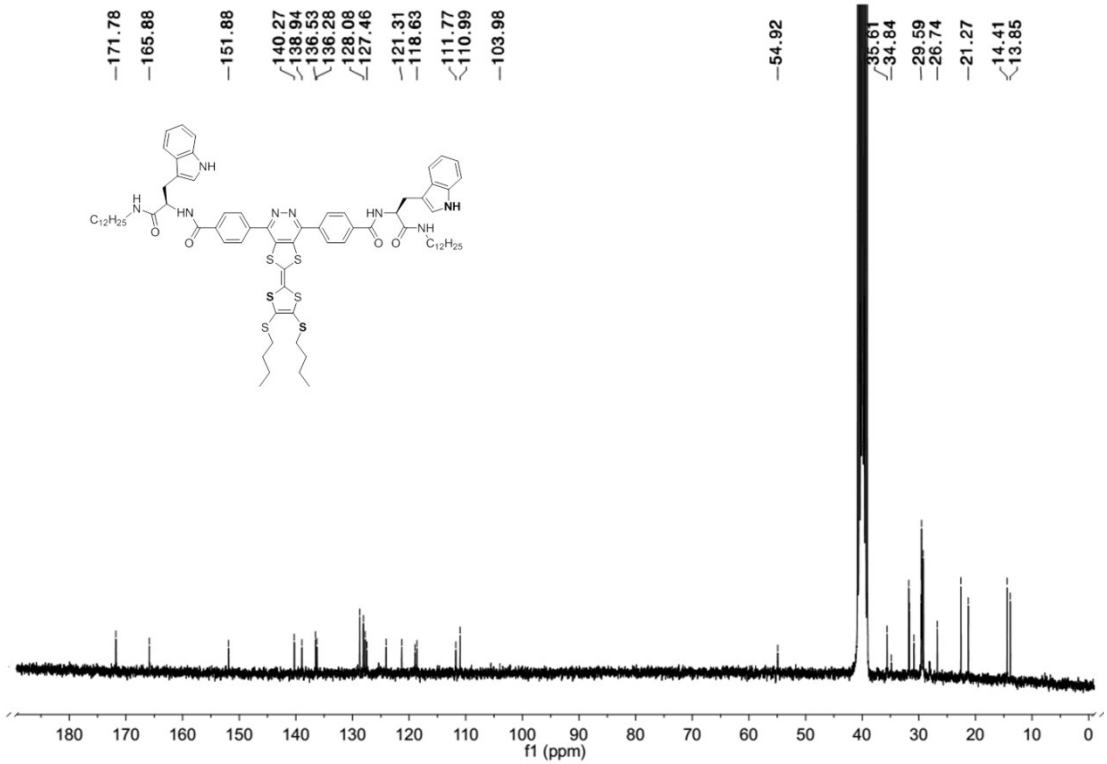

dith
Data: sample-10001.J23 29 May 2015 13:49 Cal: tof 10 Mar 2015 15:25
Kratos PC Axima CFRplus V2.4.0: Mode reflectron, Power: 93, P.Ext. @ 1233 (bin 117)
%Int.
9.0 mV[sum= 260 mV] Profiles 22-50 Smooth Av 20 -Baseline 80
1233.9
100 90 80 70 60 50 40 30 20 10 0
200 400 600 800 1000 1200 1400 1600 1800 2000
Mass/Charge

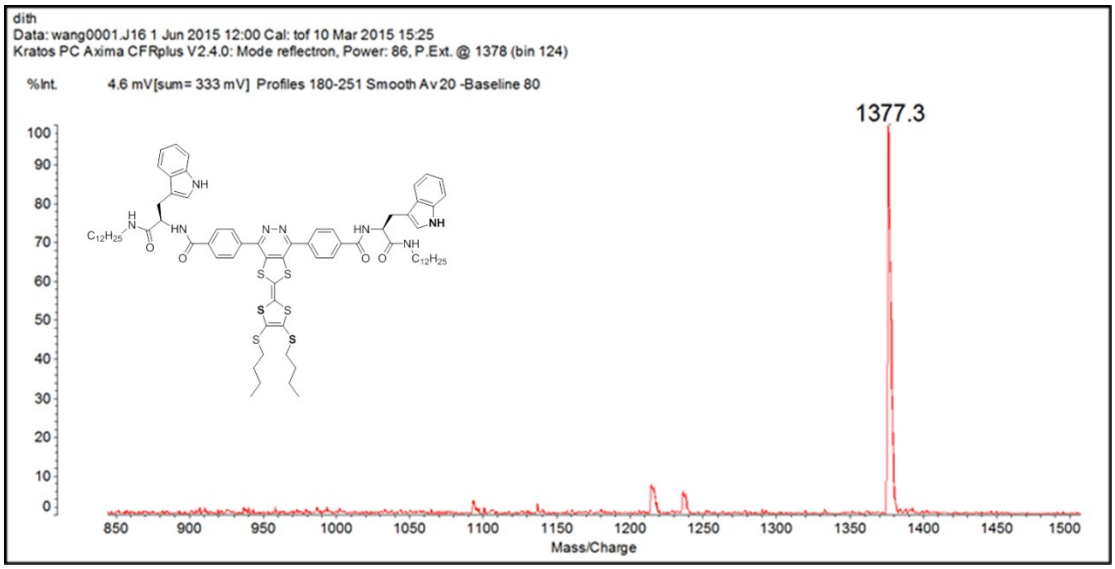

7.88
7.80
7.77
7.72
7.70
7.29
7.00
5.21
5.20
5.19
5.18
5.17
5.16
5.15
3.33
3.10
3.08
3.06
3.05
3.04
3.02
2.87
2.86
2.84
2.81
2.79
1.65
1.61
1.56
1.45
1.40
1.28
0.92
0.90
0.87
0.01
1.00
4.02
4.01
10.03
2.03
2.01
8.00
4.00
1.03
4.02
44.04
12.05
f1 (ppm)


175.47
170.86
166.91
137.06
135.52
129.52
128.59
128.53
128.44
128.28
128.25
128.19
128.03
127.93
127.67
126.88
55.31
39.72
38.84
38.76
36.02
29.70
26.97
21.66
14.15
13.64
0.00
f1 (ppm)


dith
Data: wang20001.K6 23 Dec 2015 14:09 Cal: tof 3 Mar 2015 13:36
Kratos PC Axima CFRplus V2.4.0: Mode linear, Power: 79, P.Ext. @ 1301 (bin 61)
%Int.
31 mV[sum= 1551 mV] Profiles 1-50 Smooth Av 20 -Baseline 80
1301.6
Mass/Charge


f1 (ppm)


171.78
165.88
151.88
140.27
138.94
136.53
136.28
128.08
127.46
121.31
118.63
111.77
110.99
103.98
54.92
35.61
34.84
29.59
26.74
21.27
14.41
13.85
f1 (ppm)


dith
Data: wang0001.J16 1 Jun 2015 12:00 Cal: tof 10 Mar 2015 15:25
Kratos PC Axima CFRplus V2.4.0: Mode reflectron, Power: 86, P.Ext. @ 1378 (bin 124)
%Int.
4.6 mV[sum= 333 mV] Profiles 180-251 Smooth Av 20 -Baseline 80
1377.3
Mass/Charge