Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A sensitive colorimetric and fluorescent sensor based on imidazolium-functionalized squaraines for the detection of GTP and alkaline phosphatase in aqueous solution

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I. General Remarks

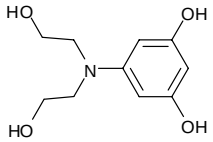
NMR spectra were obtained on a Bruker AV II-400 MHz or a Varian Inova 400 spectrometer. The ^{1}H NMR (400 MHz) chemical shifts were measured relative to $CDCl_3$, D_2O or DMSO-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm; D_2O: δ = 4.79 ppm; DMSO-d_6: δ = 2.50 ppm). The ^{13}C NMR (100 MHz) chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm; DMSO-d_6: δ = 39.52 ppm). High-resolution mass spectra (HRMS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected. Absorption spectra were detected on a HITACHI U-2910 absorption spectrophotometer. Fluorescence spectra were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer. TEM studies were carried out on a HITACHI H-600IV, operating at 75 kV. Dynamic light scattering (DLS) experiments were recorded on a Brookhaven BI-200SM Laser Light Scattering Goniometer. Fluorescence images was examined under a fluorescence microscopy (OLYMPUS IX71) irradiated by green light source (540-580 nm).

Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. Tetrahydrofuran was dried by heating at reflux over sodium/benzophenone and freshly distilled prior to use. *n*-Butanol was dried by heating at reflux over sodium and distilled prior to use. Benzene was treated firstly by shaking with concentrated H_2SO_4 until free from thiophene, and then with water, dilute NaOH and water again. This mixture was then dried with sodium and distilled prior to use. All syntheses and manipulations were carried out under dry N_2 atmosphere. The semisquaraine **7** was synthesized according to the reference.[1]

Water was distilled for twice in the optical spectroscopic studies. The sodium salts of ATP and GTP were purchased from J&K Scientific Ltd. (Beijing, China). The sodium salts of other nucleotides were purchased from Biotogether Co., Ltd. (Nanjing, China). Stock solutions (6 mM) of nucleotides (the sodium salts of ATP, GTP, ADP, GDP, AMP, GMP, UMP, CMP) and anions (CH_3CO_2Na, Na_2SO_4, NaF, NaCl, NaBr, NaI, $NaNO_3$, $NaHCO_3$, $NaH_2PO_4{\cdot}2H_2O$, $Na_4P_2O_7$) in HEPES buffer (10 mM, pH = 7.2) were stored at

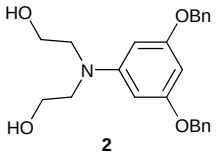
-20 ^{o}C and used within a few days. Stock solutions of host (10 μM) were prepared in HEPES buffer (10 mM, pH = 7.2). Each time a 3 mL of host solution was filled in a quartz cell of 1 cm of optical path length and the stock solution of anion was dropped into a quartz cell using a microsyringe. The volume of aions stock solution added was less than 100 μL to remain the concentration of host constant. For all measurements, The emission slits of fluorescence spectra were set at 5.0 nm if not specified.

II. Synthesis and characterization of ImSQ4, ImSQ8 and ImSQ12



1

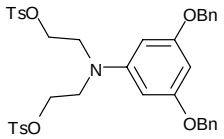
1 was synthesized according to the procedure described in the previous literature.[2] A mixture of phloroglucinol dihydrate (8.0 g, 49 mmol) and diethanolamine (4.6 g, 44 mmol) were dissolved in a mixture of toluene (50 mL) and *n*-butanol (50 mL). The mixture was refluxed with azeotropic distillation of water for 3 h, during this time period reaction solution turned to red. After being cooled, the solvent was removed under reduced pressure. The crude residue was purified by silica column chromatography (EtOAc/petroleum = 1/30~1/5, v/v) to afford the product **1** as a pink solid (5.8 g, 62% yield).



2

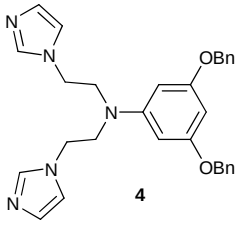
To a suspension of K_2CO_3 (14.5 g, 105 mmol) in DMF (100 mL) was added **1** (5.6 g, 26.3 mmol) and benzyl chloride (12.1 mL, 105 mmol). The resulting mixture was then reflux for 4 h. Water (60 mL) was added and the mixture was extracted with EtOAc (3 × 60 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by column chromatography on silica gel (CH_2Cl_2/EtOAc = 2/1, v/v) to afford the desired product **2** as an off-white solid (5.6 g, 54% yield). M.p.: 90-91 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ

= 3.42 (s, 2H), 3.50 (t, J = 4.8 Hz, 4H), 3.77 (t, J = 4.8 Hz, 4H), 5.01 (s, 4H), 5.95 (s, 2H), 6.10 (s, 1H), 7.30-7.42 (m, 10H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.7, 61.0, 70.2, 90.8, 93.6, 127.7, 128.1, 128.7, 137.2, 149.8, 161.0 ppm. HRMS (ESI^+): calcd for $C_{24}H_{28}NO_4$ $[M+H]^+$ 394.2018, found 394.2010.



3

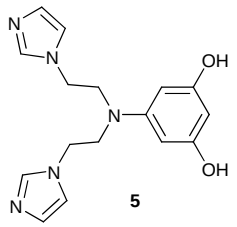
Tosyl chloride (4.6 g, 24.1 mmol) in dicloromethane (20 mL) was added dropwise to a solution of **2** (3.8 g, 9.7 mmol) and triethylamine (4.1 mL, 29.5 mmol) in dicloromethane (20 mL). The solution was then stirred at room temperature overnight. After the triethylamine hydrochloride salt had been removed by filtration, the filtrate was evaporated to dryness. The crude material was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1, v/v) to afford **3** as colorless oil (5.4 g, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.38 (s, 6H), 3.49 (t, J = 6.0 Hz, 4H), 4.05 (t, J = 6.0 Hz, 4H), 4.97 (s, 4H), 5.71 (s, 2H), 6.05 (s, 1H), 7.24 (d, J = 8.4 Hz, 4H), 7.31-7.42 (m, 10H), 7.69 (d, J = 8.0 Hz, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.8, 50.6, 66.8, 70.2, 91.5, 92.8, 127.7, 128.0, 128.2, 128.8, 130.0, 132.8, 137.1, 145.1, 147.8, 161.1 ppm. HRMS (ESI^+): calcd for $C_{38}H_{40}NO_8S_2$ $[M+H]^+$ 702.2195, found 702.2171.



4

Sodium hydride (60% in mineral oil, 0.88 g, 21.9 mmol) was added to a solution of imidazole (1.35 g, 19.9 mmol) in THF (20 mL). After the solution had been stirred for 30 min at 40 °C, the THF (15 mL) solution of **3** (5.95 g, 8.5 mmol) was added dropwise over 30 min. The resulting mixture was then stirred vigorously for 12 h at 75 °C. Subsequently, the reaction was quenched by water and extracted with CH_2Cl_2 (3×15 mL). The combined organic layers was concentrated in vacuo and purified by flash column

chromatography on silica gel (CH_2Cl_2/CH_3OH = 16/1, v/v) to give **4** as a light yellow powder (3.5 g, 83% yield). M.p.: 126-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.13 (t, J = 5.2 Hz, 4H), 3.83 (t, J = 5.2 Hz, 4H), 5.04 (s, 4H), 5.86 (s, 2H), 6.18 (s, 1H), 6.74 (s, 2H), 7.04 (s, 2H), 7.26 (m, 2H), 7.31-7.41 (m, 10H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 43.5, 51.4, 69.1, 91.1, 92.1, 119.6, 127.7, 127.8, 128.4, 128.5, 137.4, 137.5, 148.4, 160.5 ppm. HRMS (ESI^+): calcd for $C_{30}H_{32}N_5O_2$ $[M+H]^+$ 494.2556, found 494.2558.

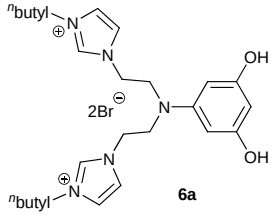


5

A mixture of 5% Pd/C (0.24 g) and **4** (2.5 g, 5.0 mmol) in MeOH (15 mL) was hydrogenated at 1.5 MPa in an autoclave and stirred at room temperature overnight. Subsequently, the reaction mixture was filtered and washed with MeOH. The solid residues containing product and catalyst were heated with DMF at 120 °C, filtered immediately. The filtrate was removed in vacuo to obtain **5** as an off-white solid (1.5 g, 96% yield), which was carried forward to further reactions without further purifications.

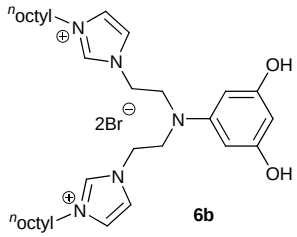
General procedure for the synthesis of 6a–c

n-Bromoalkane (1 mL) was added to a solution of **5** (0.31 g, 1.0 mmol) in DMF (6 mL). The solution was then stirred vigorously for 24 h at 75 °C. Subsequently, the reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (CH_2Cl_2/CH_3OH = 10/1, v/v) to afford the desired product as an off-white solid. Further purification was taken by recrystalization from isopropanol and hexane.



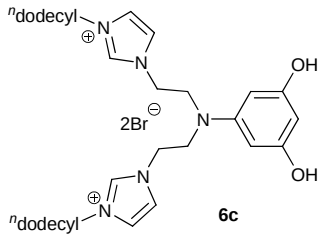
6a

6a: 0.46 g, 78%. M.p.: 200-201 °C. ^{1}H NMR (400 MHz, D_2O): δ = 0.85 (t, J = 7.2 Hz, 6H), 1.07-1.18 (m, 4H), 1.50-1.57 (m, 4H), 3.80 (t, J = 4.8 Hz, 4H), 3.98 (t, J = 7.2 Hz, 4H), 4.40 (t, J = 4.8 Hz, 4H), 5.48 (s, 2H), 5.66 (s, 1H), 7.37 (t, J = 1.6 Hz, 2H), 7.52 (t, J = 1.6 Hz, 2H), 8.54 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.3, 18.7, 31.3, 46.1, 48.5, 48.9, 91.1, 92.9, 122.2, 122.9, 136.5, 148.3, 159.2 ppm. HRMS (ESI$^+$): calcd for $C_{24}H_{37}N_5O_2Br$ $[M\text{-}Br]^+$ 506.2131, found 506.2131.



6b

6b: 0.50 g, 71%. M.p.: 188-189 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 0.86 (t, J = 6.4 Hz, 6H), 1.24 (s, 20H), 1.70 (t, J = 6.8 Hz, 4H), 3.61 (s, 4H), 4.10 (t, J = 6.8 Hz, 4H), 4.30 (s, 4H), 5.55 (s, 2H), 5.65 (s, 1H), 7.78 (s, 2H), 7.81 (s, 2H), 8.92 (s, 2H), 9.21 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.2, 22.3, 25.7, 28.5, 28.7, 29.6, 31.4, 46.2, 49.0, 49.3, 91.3, 93.0, 122.4, 123.1, 136.7, 148.4, 159.4 ppm. HRMS (ESI$^+$): calcd for $C_{32}H_{52}N_5O_2$ $[M\text{-}2Br\text{-}H]^+$ 538.4121, found 538.4119.

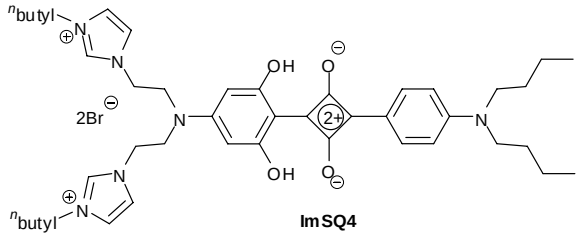


6c

6c: 0.65 g, 80%. M.p.: 180-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.87 (t, J = 7.2 Hz, 6H), 1.25-1.33 (m, 36H), 1.91 (s, 4H), 3.78 (s, 4H), 4.19 (t, J = 7.2 Hz, 4H), 4.44 (s, 4H), 5.65 (s, 1H), 6.23 (s, 2H), 7.19 (s, 2H), 8.21 (s, 2H), 8.28 (s, 2H), 10.02 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.9, 22.1, 25.5, 28.4, 28.7, 28.8, 28.98, 29.02, 29.4, 31.3, 46.1, 48.8, 49.2, 91.2, 93.0, 122.2, 122.9, 136.4, 148.2, 159.2 ppm. HRMS (ESI$^+$): calcd for $C_{40}H_{69}N_5O_2Br$ $[M\text{-}Br]^+$ 730.4635, found 730.4634.

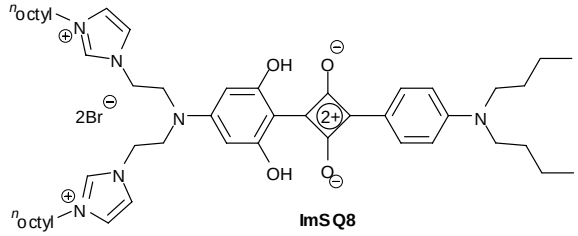
General procedure for the synthesis of ImSQ4, ImSQ8 and ImSQ12

3-(4-(dibutylamino)phenyl)-4-hydroxycyclobut-3-ene-1,2-dione **7** (150 mg, 0.50 mmol) was reacted with the imidazolium salt **6** (0.60 mmol) in a mixture of distilled *n*-butanol (3 mL) and benzene (3 mL) at reflux for 10 h. The solvent was removed in vacuo after the reaction mixture was cooled down to room temperature. The residue was washed with ether and filtrated. Further purification was taken by recrystalization from isopropanol and hexane, the desired product was gained as a green solid.



ImSQ4

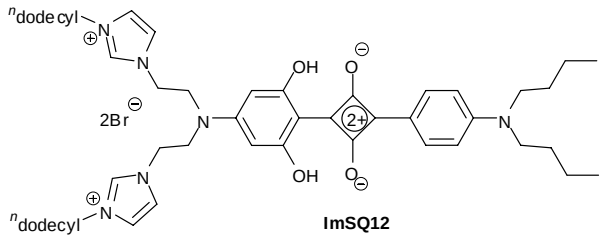
ImSQ4: 147 mg, 34%. M.p.: 195-198 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.91 (t, J = 7.2 Hz, 6H), 0.97 (t, J = 7.2 Hz, 6H), 1.31-1.38 (m, 8H), 1.59-1.62 (m, 4H), 1.84-1.86 (m, 4H), 3.36 (s, 4H), 4.24 (s, 8H), 4.73 (s, 4H), 5.81 (s, 2H), 6.66 (d, J = 8.8 Hz, 2H), 7.35 (s, 2H), 7.97 (d, J = 8.8 Hz, 2H), 8.06 (s, 2H), 10.11 (s, 2H), 12.44 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.6, 14.0, 19.6, 20.3, 29.6, 31.9, 46.8, 49.8, 50.1, 51.3, 93.3, 106.2, 112.6, 117.5, 122.1, 123.9, 132.6, 137.1, 152.9, 159.4, 164.8, 166.8, 178.0, 182.2 ppm. HRMS (ESI$^+$): calcd for $C_{42}H_{58}N_6O_4Br$ $[M\text{-}Br]^+$ 789.3703, found 789.3696.



ImSQ8

ImSQ8: 149 mg, 30%. M.p.: 218-220 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 0.69 (t, J = 6.4 Hz, 6H), 0.91 (t, J = 6.4 Hz, 6H), 1.04-1.10 (m, 20H), 1.31-1.34 (m, 4H), 1.50-1.52 (m, 8H), 3.49 (s, 4H), 4.00-4.04 (m, 8H), 4.48 (s, 4H), 5.47 (s, 2H), 6.96 (d, J = 8.4 Hz, 2H), 7.78 (s, 2H), 7.87-7.92 (m, 4H), 9.19 (s, 2H), 12.32 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.77, 13.84, 19.5, 22.1, 25.7, 28.7, 29.2, 30.2, 31.4, 46.5, 47.8, 48.9, 50.3, 92.1, 105.0, 113.3, 116.5, 122.5, 123.3, 131.6, 136.5, 153.0, 159.8, 163.5, 164.9, 175.2, 181.8 ppm. HRMS (ESI$^+$): calcd for $C_{50}H_{74}N_6O_4Br$ $[M\text{-}Br]^+$ 901.4955,

found 901.4952.



ImSQ12

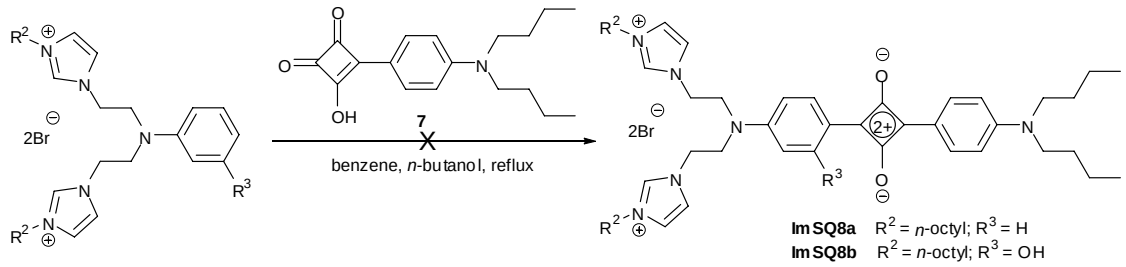
ImSQ12: 160 mg, 29%. M.p.: 211-214 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.86 (t, J = 7.2 Hz, 6H), 0.97 (t, J = 7.2 Hz, 6H), 1.20-1.28 (m, 36H), 1.38 (q, J = 7.2 Hz, 4H), 1.61 (s, 4H), 1.85 (s, 4H), 3.35 (s, 4H), 4.23 (s, 4H), 4.29 (s, 4H), 4.78 (s, 4H), 5.82 (s, 2H), 6.65 (d, J = 8.4 Hz, 2H), 7.29 (s, 2H), 7.97 (d, J = 8.4 Hz, 2H), 8.12 (s, 2H), 10.20 (s, 2H), 12.48 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.0, 14.2, 20.3, 22.8, 26.5, 29.2, 29.4, 29.59, 29.64, 29.7, 30.4, 32.0, 46.9, 49.9, 50.4, 51.3, 93.3, 106.4, 112.6, 117.6, 121.9, 124.0, 132.6, 137.2, 152.9, 159.4, 164.8, 166.9, 178.2, 182.2 ppm. HRMS (ESI$^+$): calcd for $C_{58}H_{90}N_6O_4Br$ $[M\text{-}Br]^+$ 1013.6207, found 1013.6207.

III. References

1. K. Liang, K.-Y. Law and D. G. Whitten, *J. Phys. Chem. B*, 1997, **101**, 540.

2. K. J. Wallace, M. Gray, Z. Zhong, V. M. Lynch and E. V. Anslyn, *Dalton Trans.*, 2005, 2436.

IV. The failed synthetic route to imidazolium-functionalized squaraines



Scheme S1 The failed synthetic route to imidazolium-functionalized squaraines.

The bisimidazolium-containing aniline derivatives with one or no *meta*-hydroxyl group on the benzene ring could not deliver the desired squaraines.

V. Photophysical properties of ImSQ4, ImSQ8 and ImSQ12

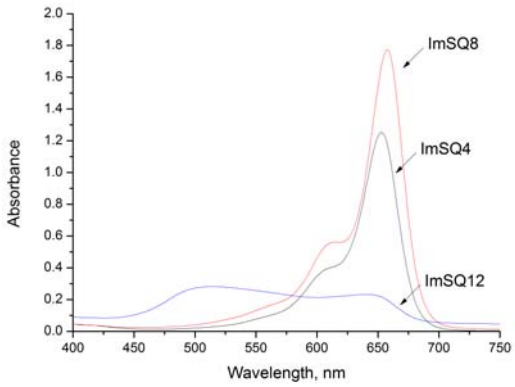


Fig. S1 Absorption spectra of **ImSQ4, ImSQ8** and **ImSQ12** (10 μM) in HEPES buffer (10 mM, pH = 7.2).

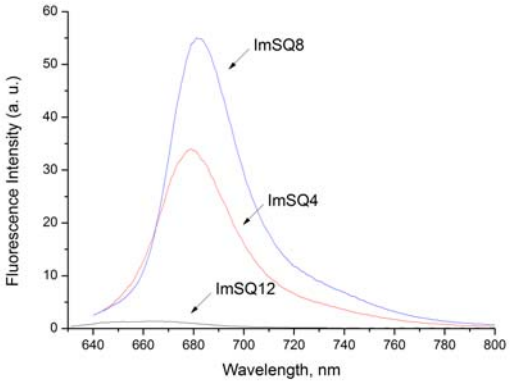


Fig. S2 Fluorescent emission spectra of **ImSQ4, ImSQ8** and **ImSQ12** (10 μM) in HEPES buffer (10 mM, pH = 7.2).

VI. Related experiments of the host-guest recognition

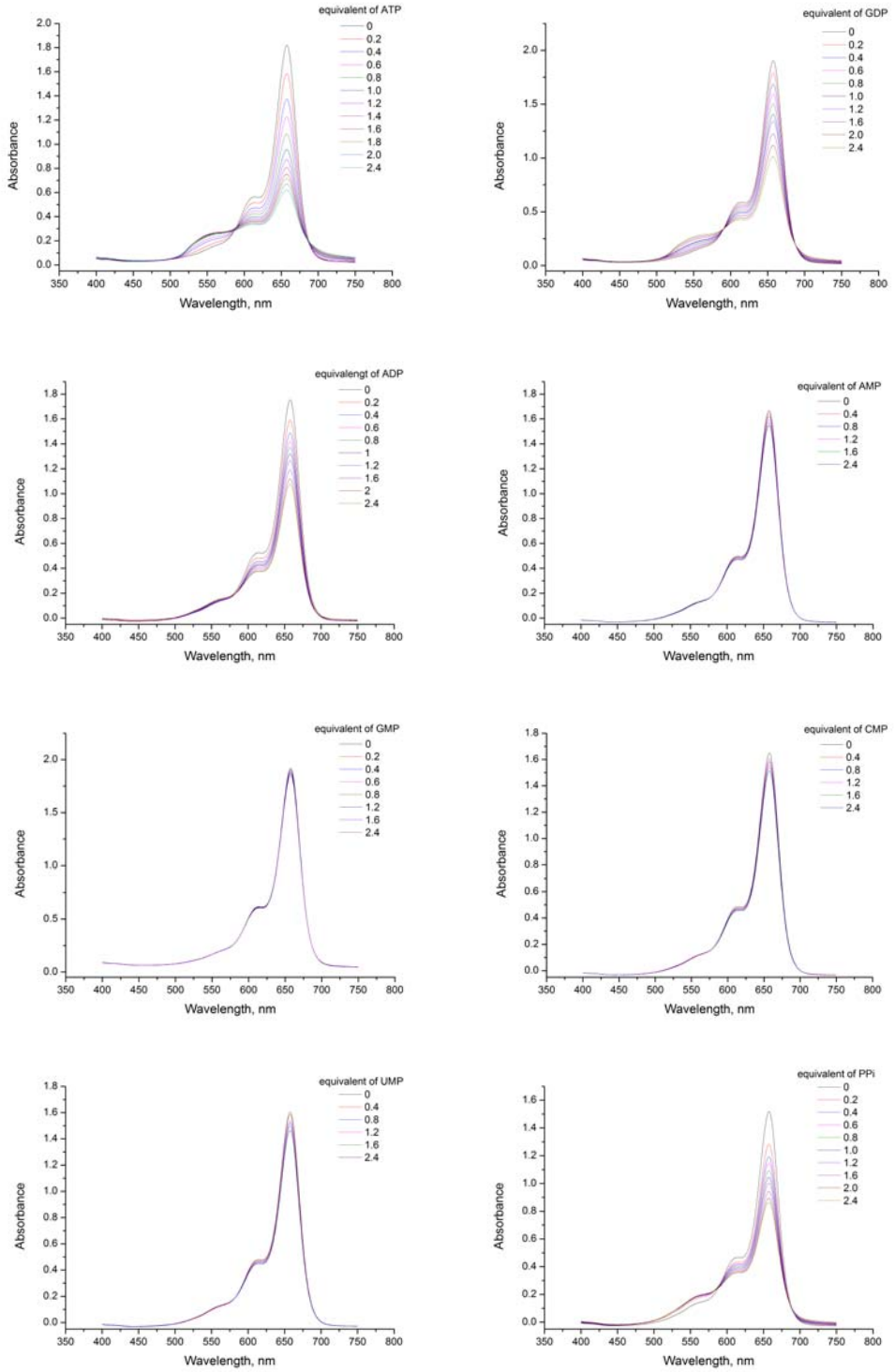


Fig. S3-1 Absorption spectra of **ImSQ8** (10 μM) upon addition of different anions in HEPES buffer (10 mM, pH = 7.2).

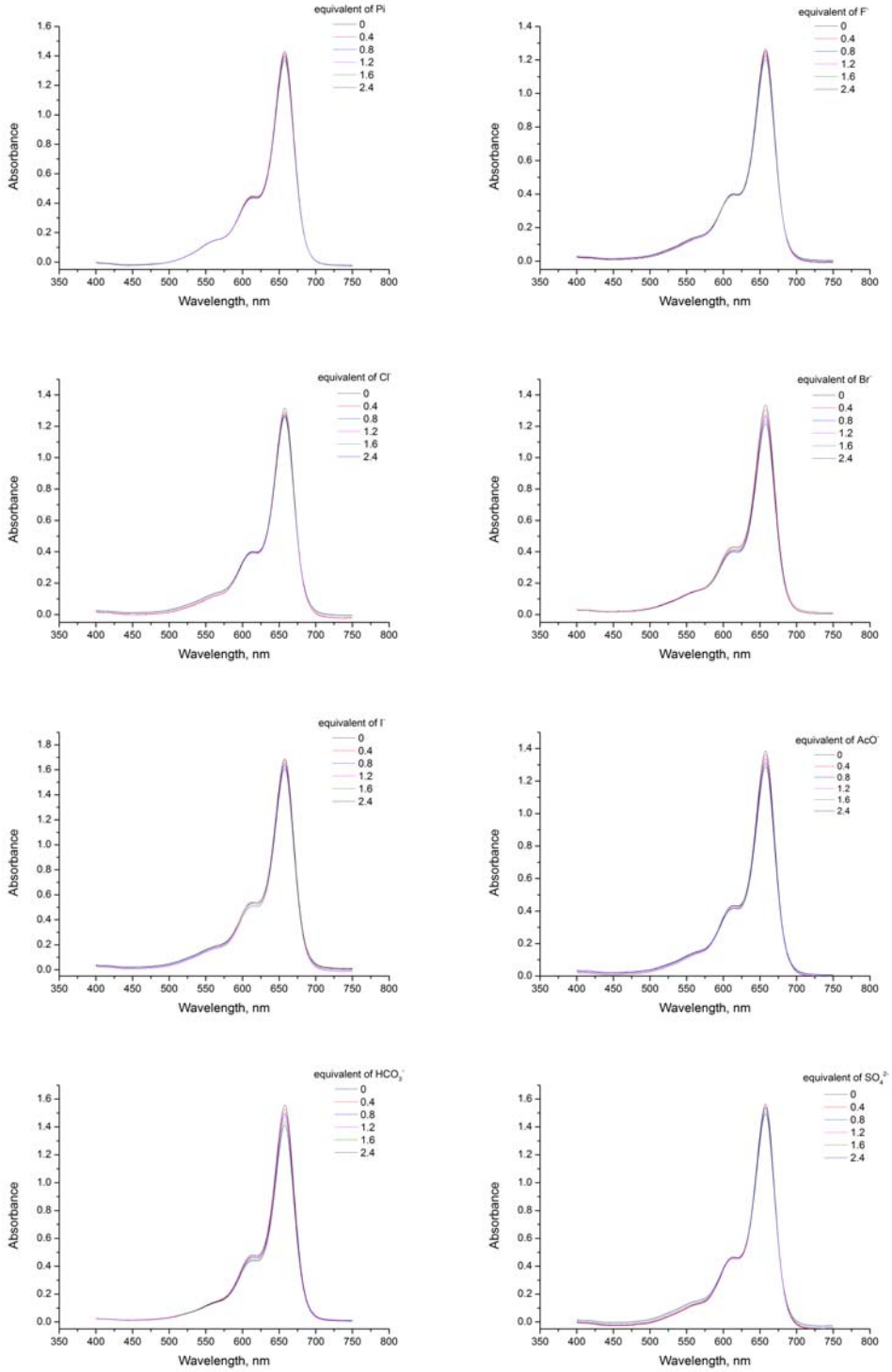


Fig. S3-2 Absorption spectra of **ImSQ8** (10 μM) upon addition of different anions in HEPES buffer (10 mM, pH = 7.2).

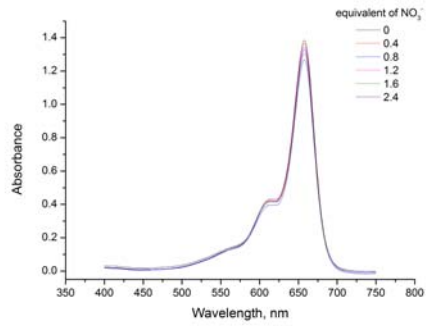


Fig. S3-3 Absorption spectra of **ImSQ8** (10 μM) upon addition of different anions in HEPES buffer (10 mM, pH = 7.2).

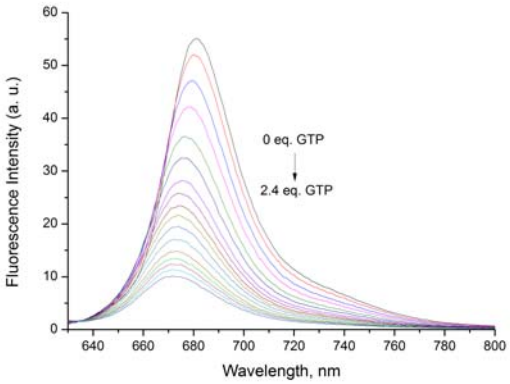


Fig. S4 Fluorescent emission spectra of **ImSQ8** (10 μM) upon addition of GTP in HEPES buffer (10 mM, pH = 7.2). λ_{ex} = 613 nm.

VII. Calculation of the detection limit

The typical limit of detection (LOD) is obtained by using the equation followed:

$$\mathrm{LOD} = \frac{3 \times \mathrm{SD}}{\mathrm{S}}$$

Where SD is the standard deviation of the background (**ImSQ8** in HEPES buffer (10 mM, pH = 7.2)) and S is the sensitivity. S can be obtained from the slope of the linear fit.

VIII. Fluorescence image of live cells

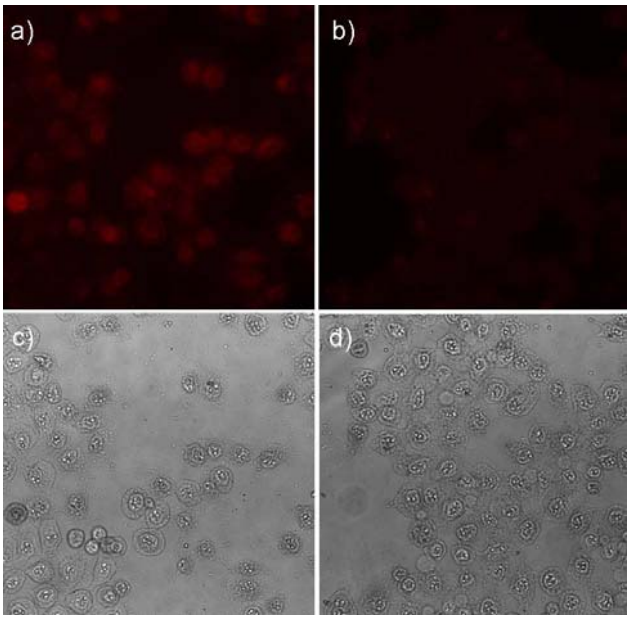


Fig. S5 Fluorescence microscopy images of Bel-7402 cells treated with **ImSQ8** (20 μM) in physiological saline containing 1% DMSO: (a) before and (b) after adding GTP (30 equiv). (c)/(d) were the brightfield images corresponding to (a)/(b), respectively.

IX. DLS measurements of aggregates in HEPES buffer

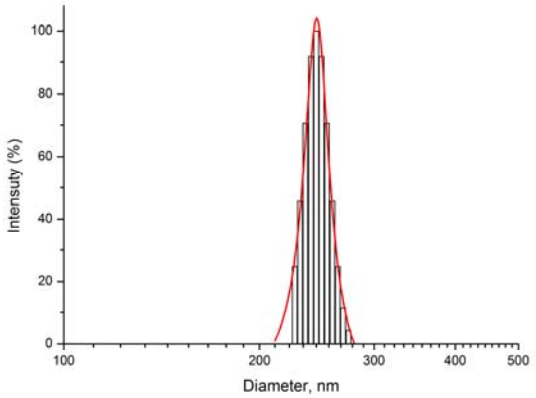
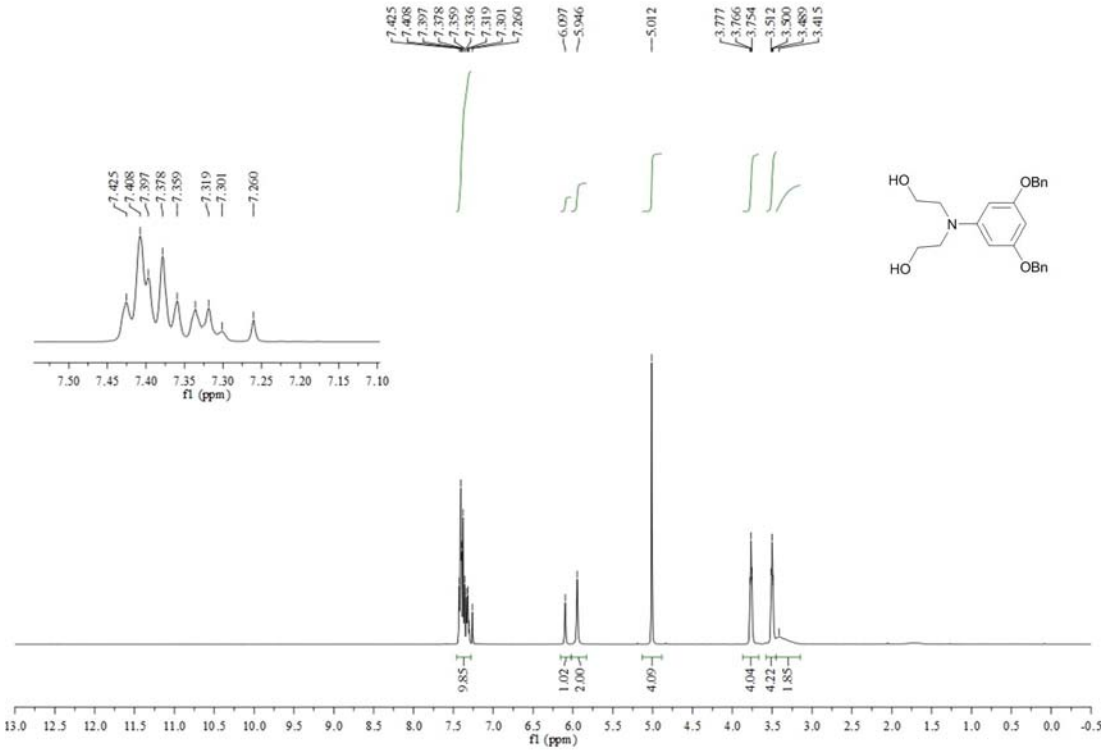
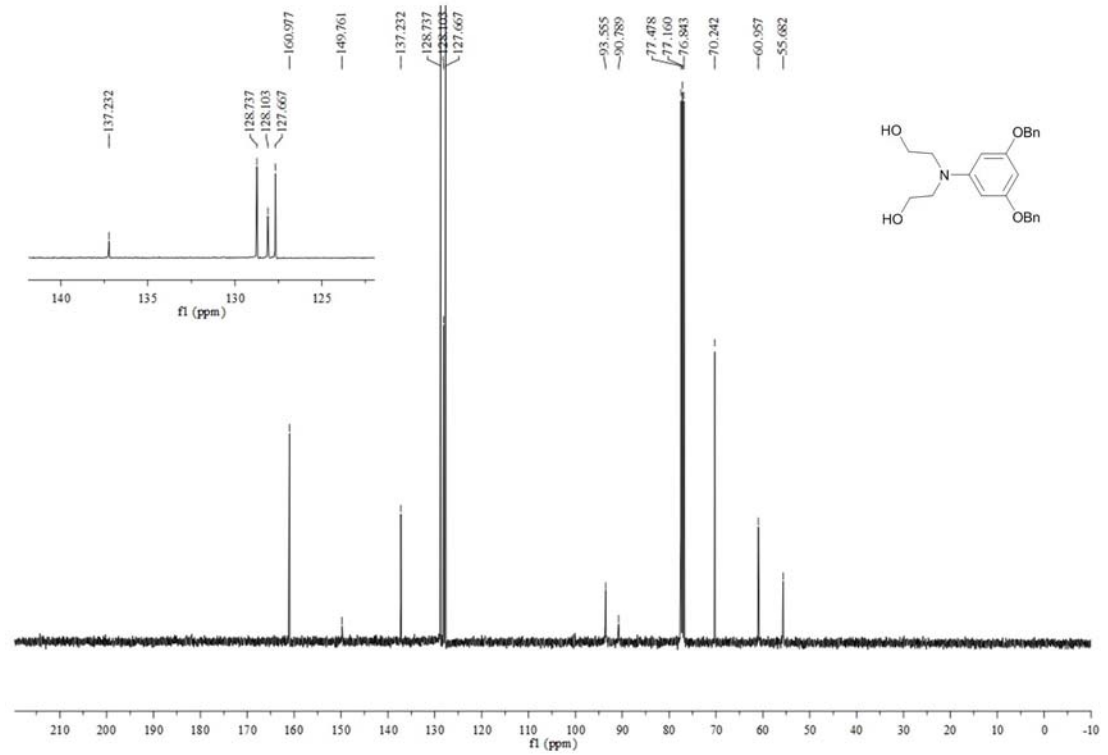
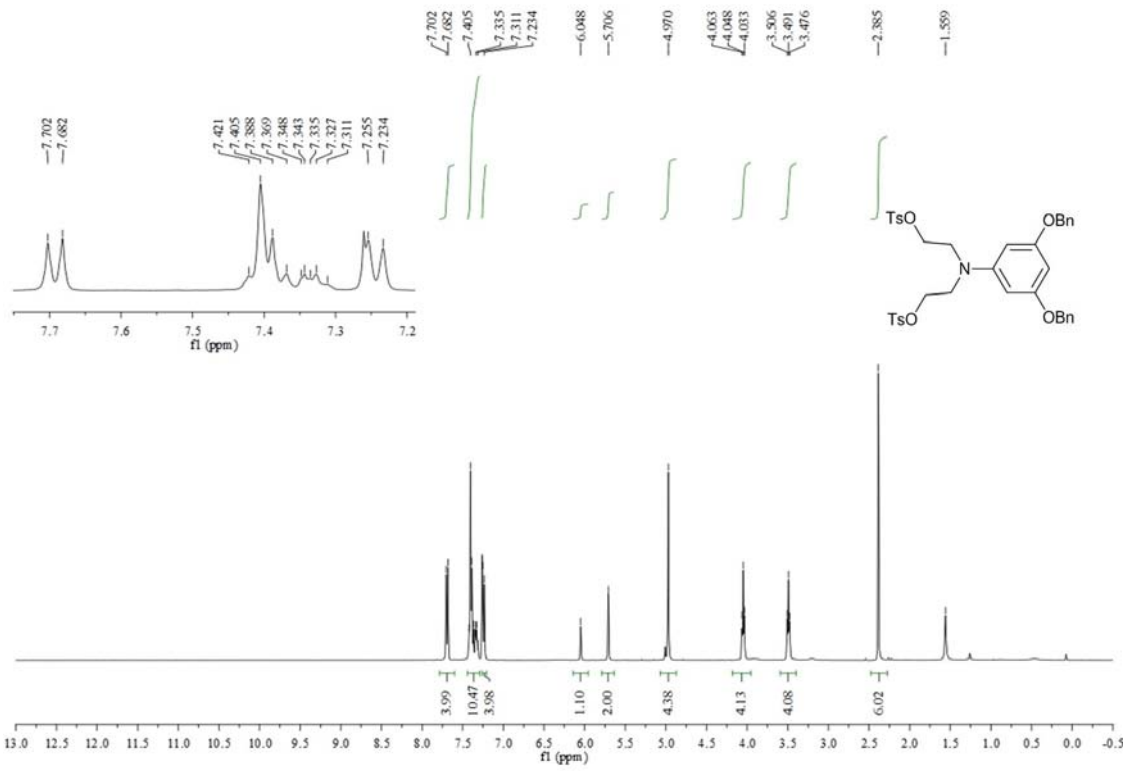


Fig. S6 CONTIN plot from DLS measurements at 90^{o} on **ImSQ8** (40 μM) in HEPES buffer (10 mM, pH = 7.2) in the presence of GTP (2.0 equiv.).

X. Copies of ^{1}H and ^{13}C NMR spectra






7.702
7.682
7.405
7.335
7.311
7.234
6.048
5.706
4.970
4.063
4.048
4.033
3.506
3.491
3.476
2.385
1.559
7.421
7.405
7.388
7.369
7.348
7.343
7.335
7.327
7.311
7.255
7.234
TsO
OBn
N
TsO
OBn
f1 (ppm)
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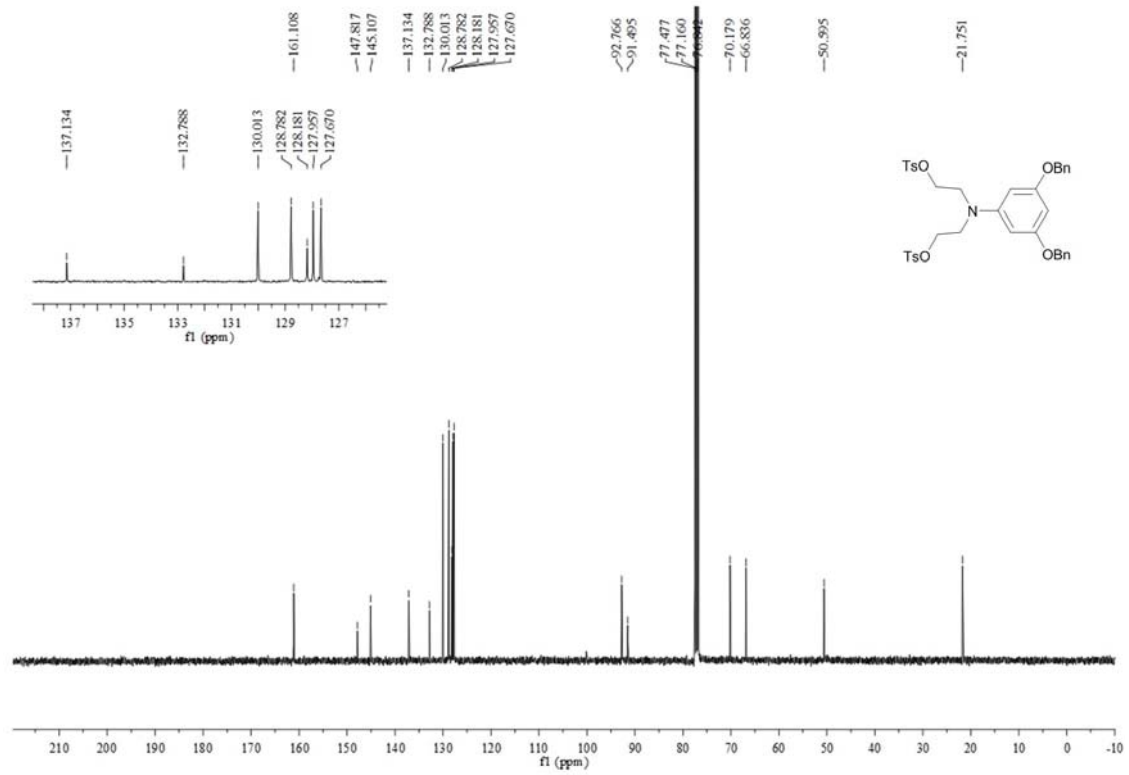
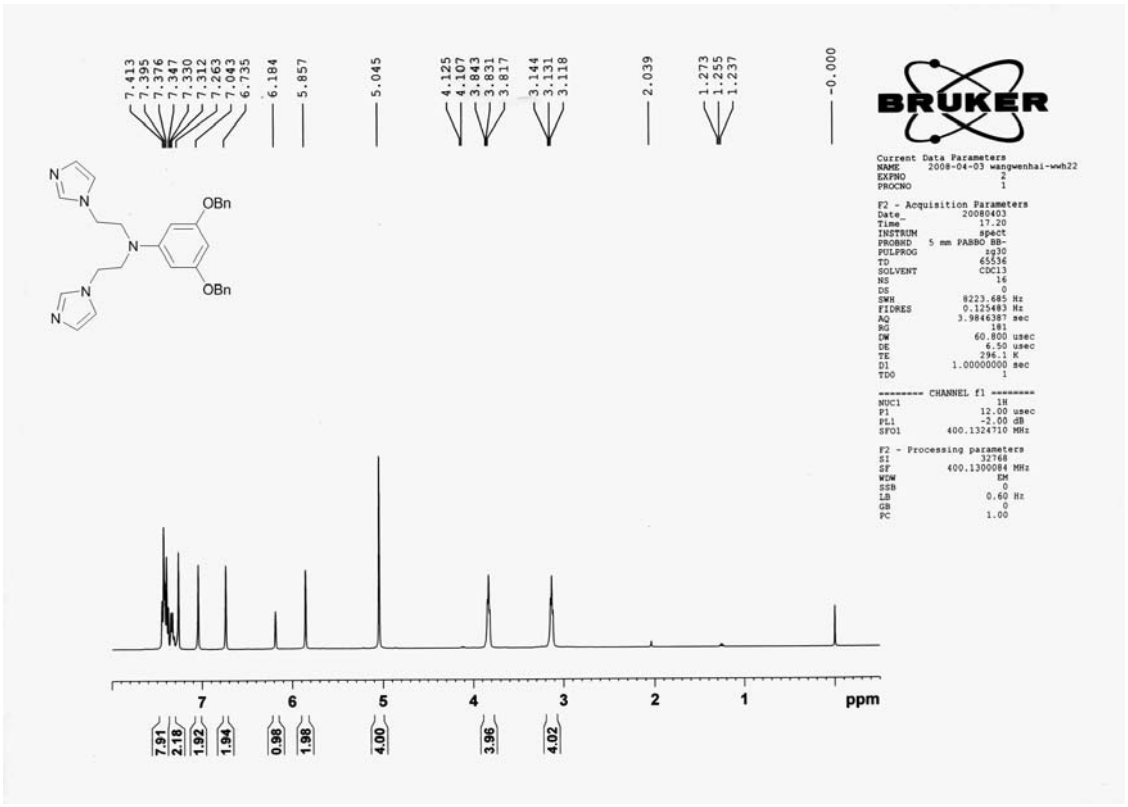
10.47
3.98
1.10
2.00
4.38
4.13
4.08
6.02
f1 (ppm)


161.108
147.817
145.107
137.134
132.788
130.013
128.782
128.181
127.957
127.670
92.766
91.495
77.427
77.160
76.894
70.179
66.836
50.595
21.751
137.134
132.788
130.013
128.782
128.181
127.957
127.670
TsO
OBn
N
TsO
OBn
f1 (ppm)
f1 (ppm)


7.413
7.395
7.376
7.347
7.330
7.312
7.263
7.043
6.735
6.184
5.857
5.045
4.125
4.107
3.843
3.831
3.817
3.144
3.131
3.118
2.039
1.273
1.255
1.237
-0.000
BRUKER
OBn
OBn
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PROCNO 1
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Time_ 17.20
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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
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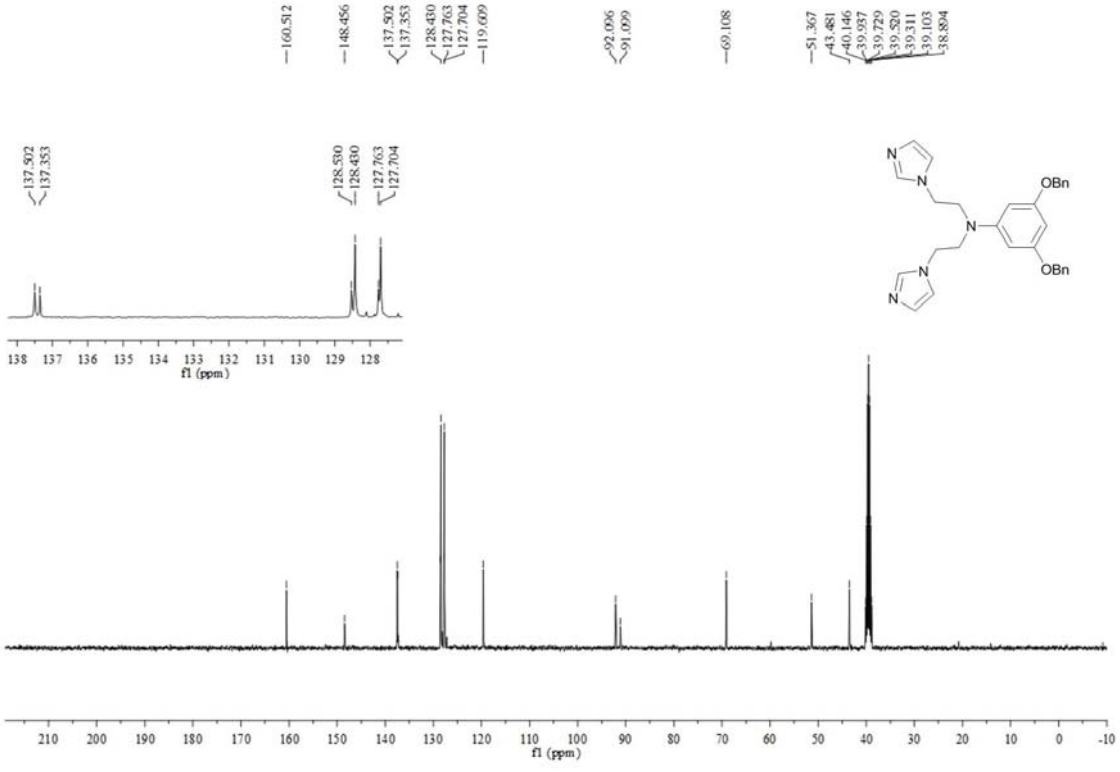
7.91
2.18
1.92
1.94
0.98
1.98
4.00
3.96
4.02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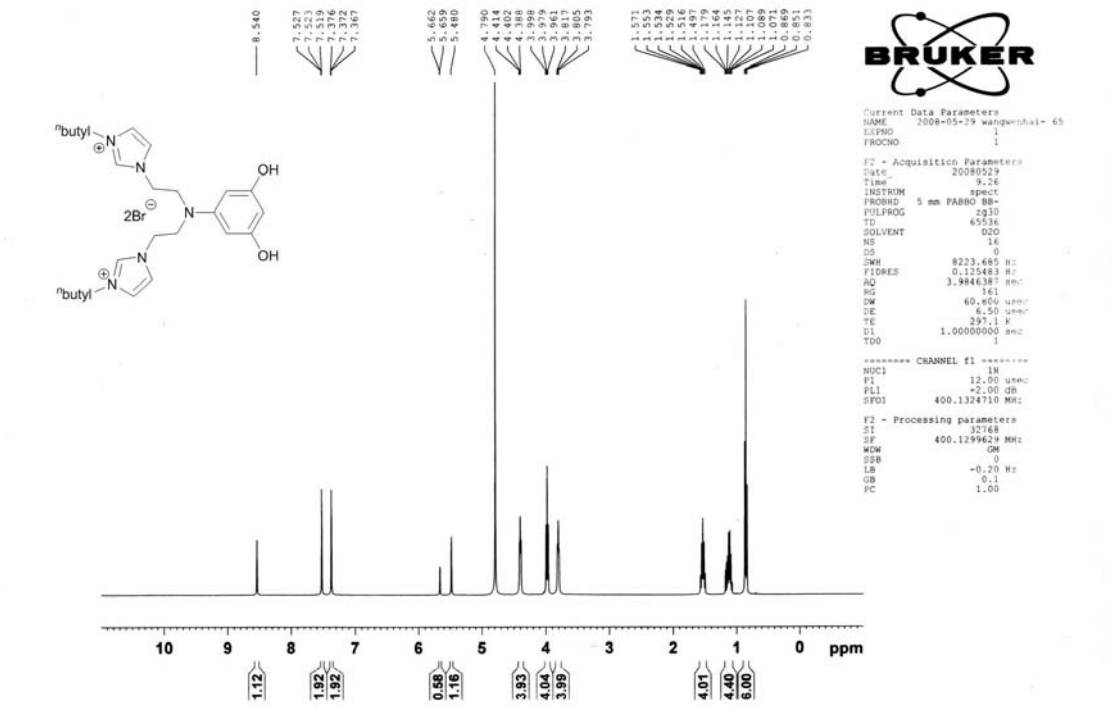
148.456
137.502
137.353
128.430
127.763
127.704
119.609
92.096
91.099
69.108
51.367
43.481
40.146
39.937
39.729
39.520
39.311
39.103
38.894
OBn
OBn
138 137 136 135 134 133 132 131 130 129 128
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.527
7.523
7.519
7.376
7.372
7.367
5.662
5.659
5.480
4.790
4.414
4.402
4.388
4.086
3.979
3.961
3.817
3.805
3.793
1.571
1.553
1.534
1.529
1.516
1.497
1.179
1.164
1.155
1.137
1.107
1.089
1.071
0.869
0.851
0.833
BRUKER
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PROCNO 1
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Time 9.26
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT D2O
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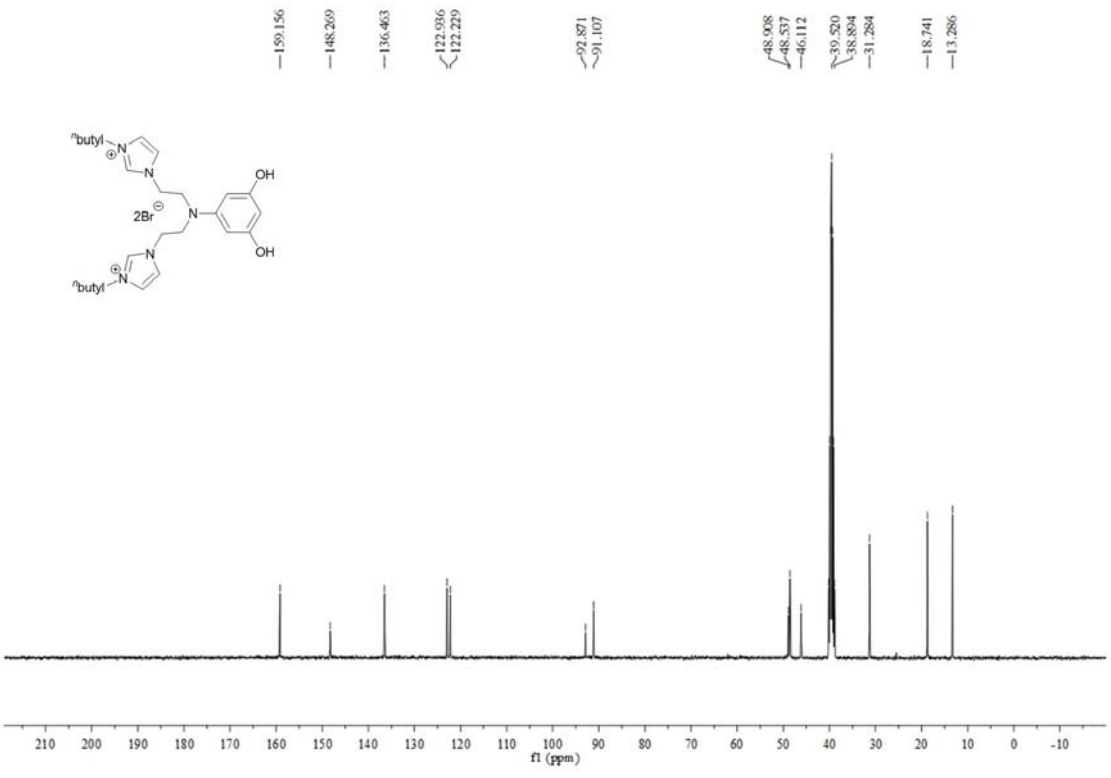
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299629 MHz
WDW GM
SSB 0
LB -0.20 Hz
GB 0.1
PC 1.00
nbutyl
2Br
OH
OH
10 9 8 7 6 5 4 3 2 1 0 ppm
1.12
1.92
1.92
0.58
1.16
3.93
4.04
3.99
4.01
4.40
6.00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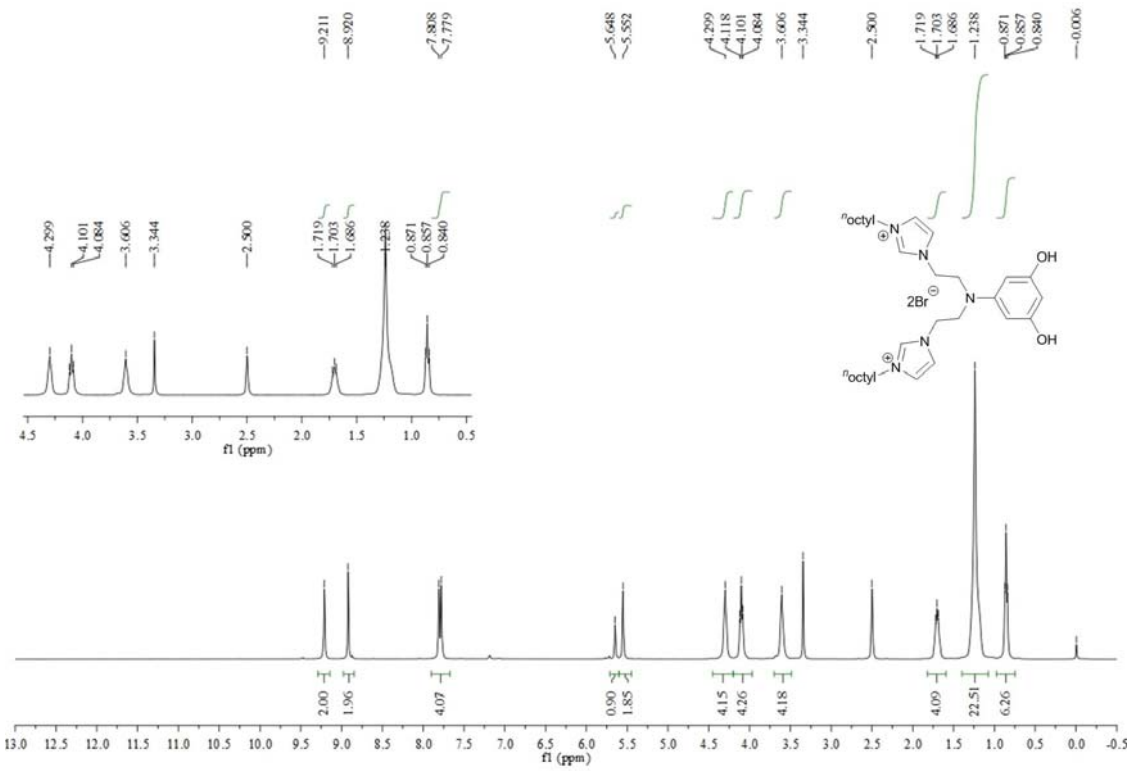
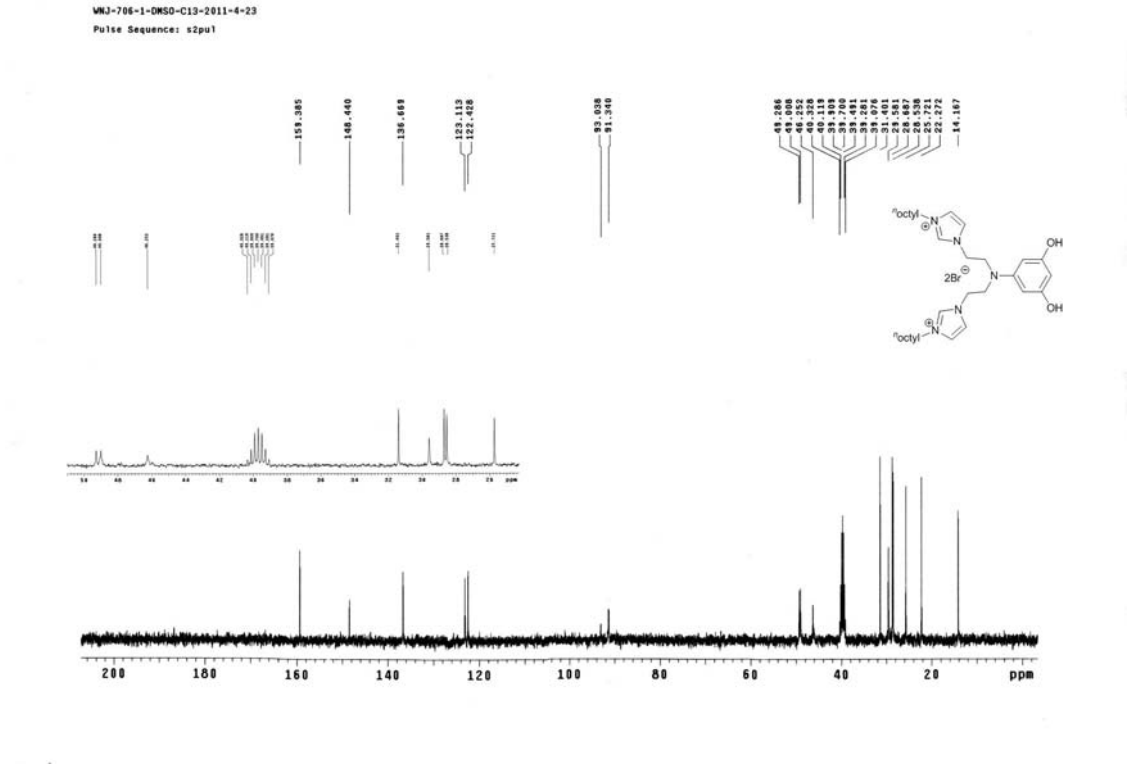
148.269
136.463
122.936
122.229
92.871
91.107
48.908
48.537
46.112
39.520
38.804
31.284
18.741
13.286
nbutyl
2Br
OH
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.211
8.920
7.808
7.779
5.648
5.552
4.299
4.118
4.101
4.084
3.606
3.344
2.500
1.719
1.703
1.686
1.238
0.871
0.857
0.840
0.006
2.00
1.96
4.07
0.90
1.85
4.15
4.26
4.18
4.09
22.51
6.26
f1 (ppm)
nOctyl
2Br
OH
OH


WNJ-706-1-DMSO-C13-2011-4-23
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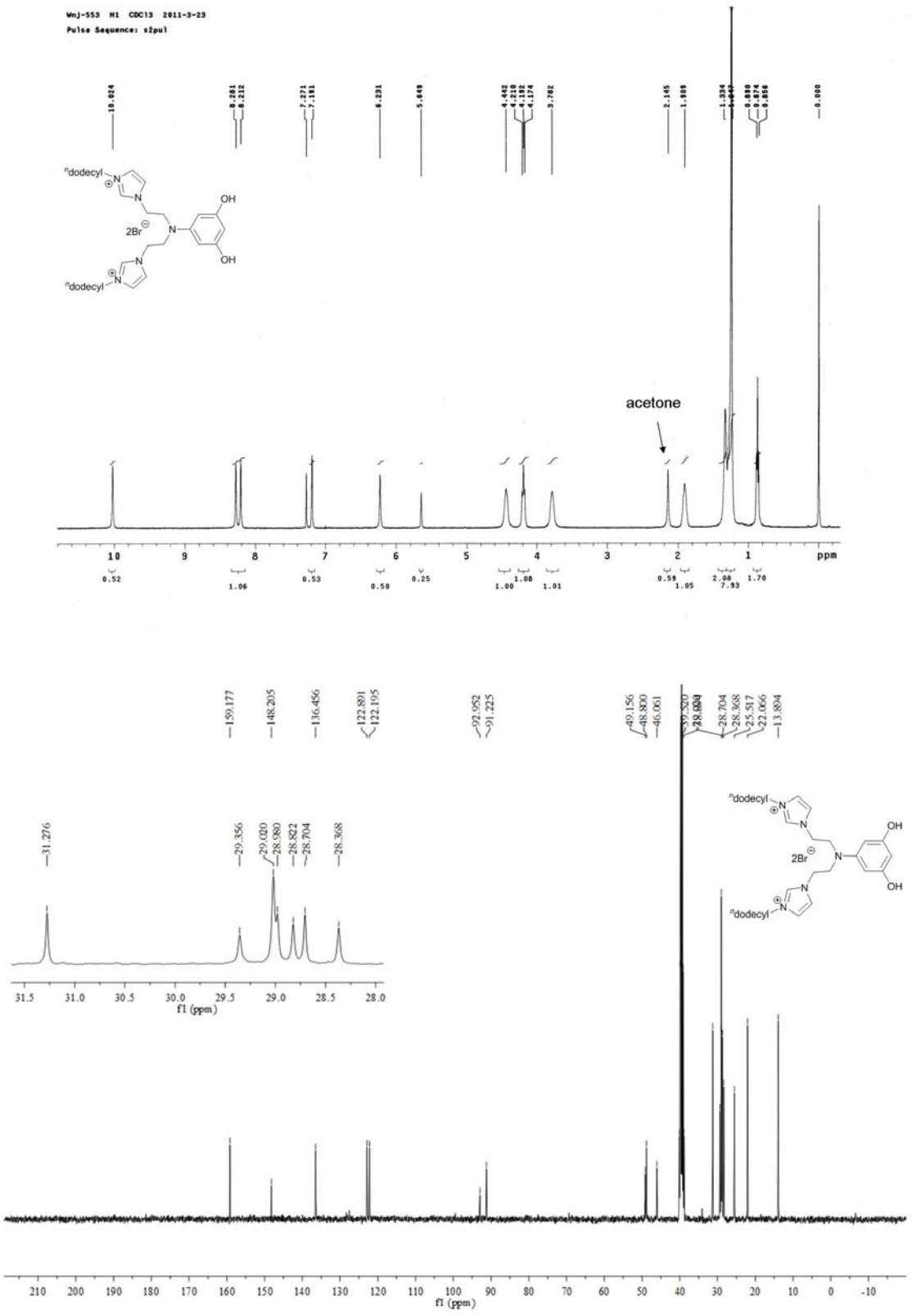
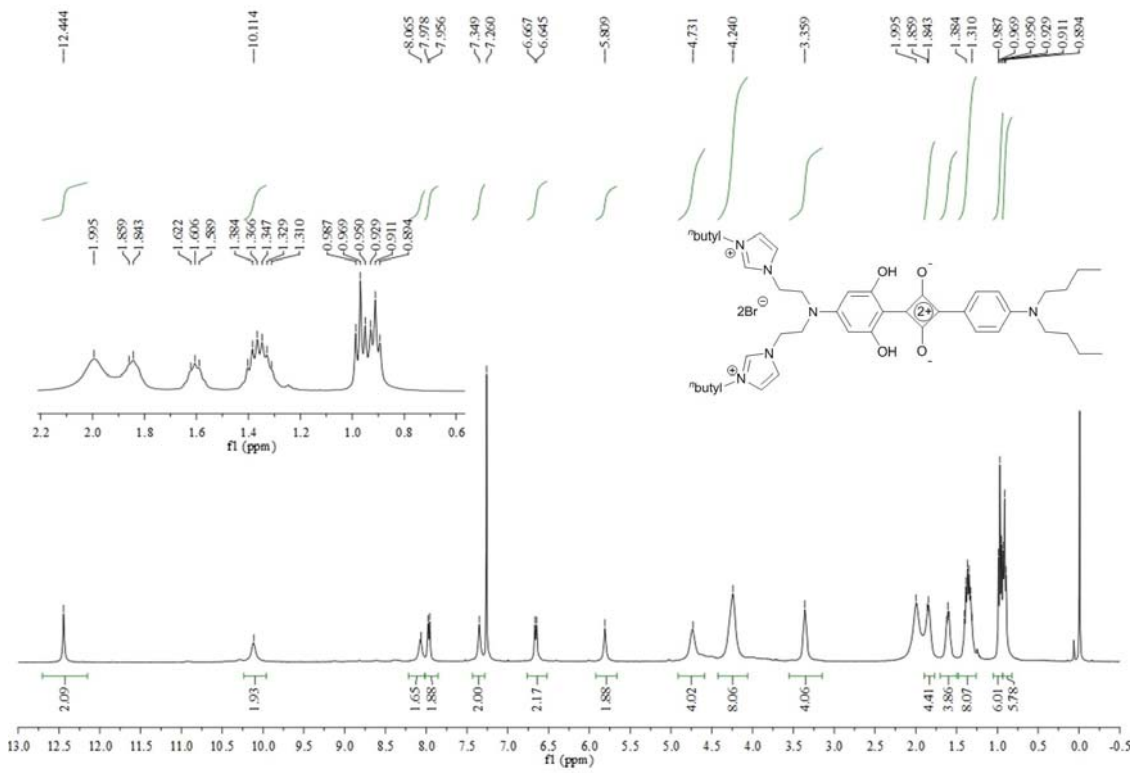
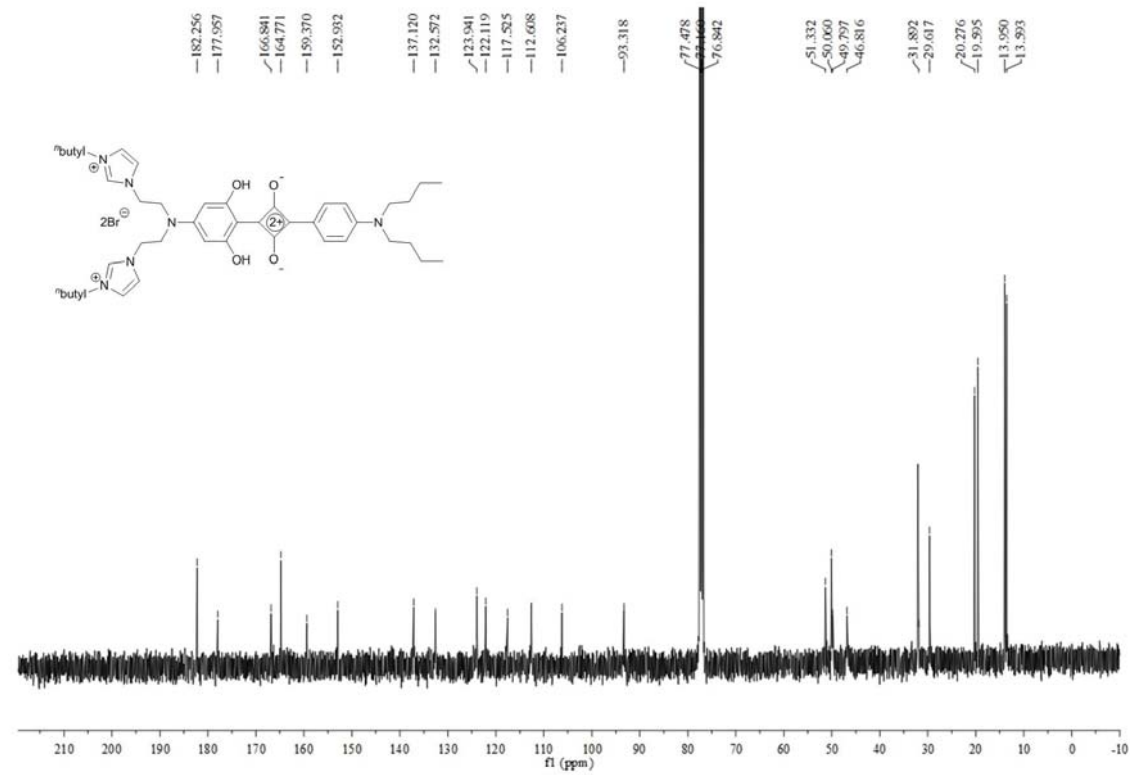
136.669
123.113
122.428
93.038
91.340
14.167
nOctyl
2Br
OH
OH
ppm


Wnj-553 H1 CDCl3 2011-3-23
Pulse Sequence: s2pul
acetone
ppm
f1 (ppm)


12.444
10.114
8.065
7.978
7.956
7.349
7.260
6.667
6.645
5.809
4.731
4.240
3.359
1.995
1.859
1.843
1.622
1.606
1.589
1.384
1.366
1.347
1.329
1.310
0.987
0.969
0.950
0.929
0.911
0.894
nbutyl
2Br
OH
OH
2+
f1 (ppm)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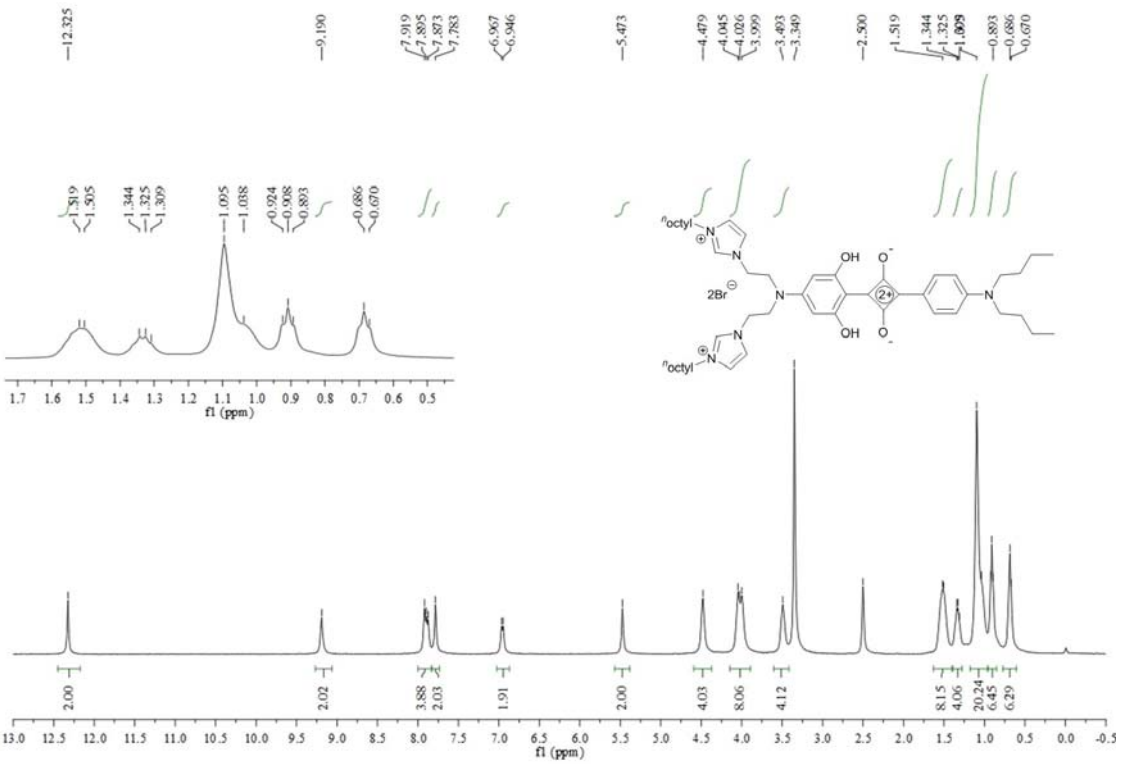
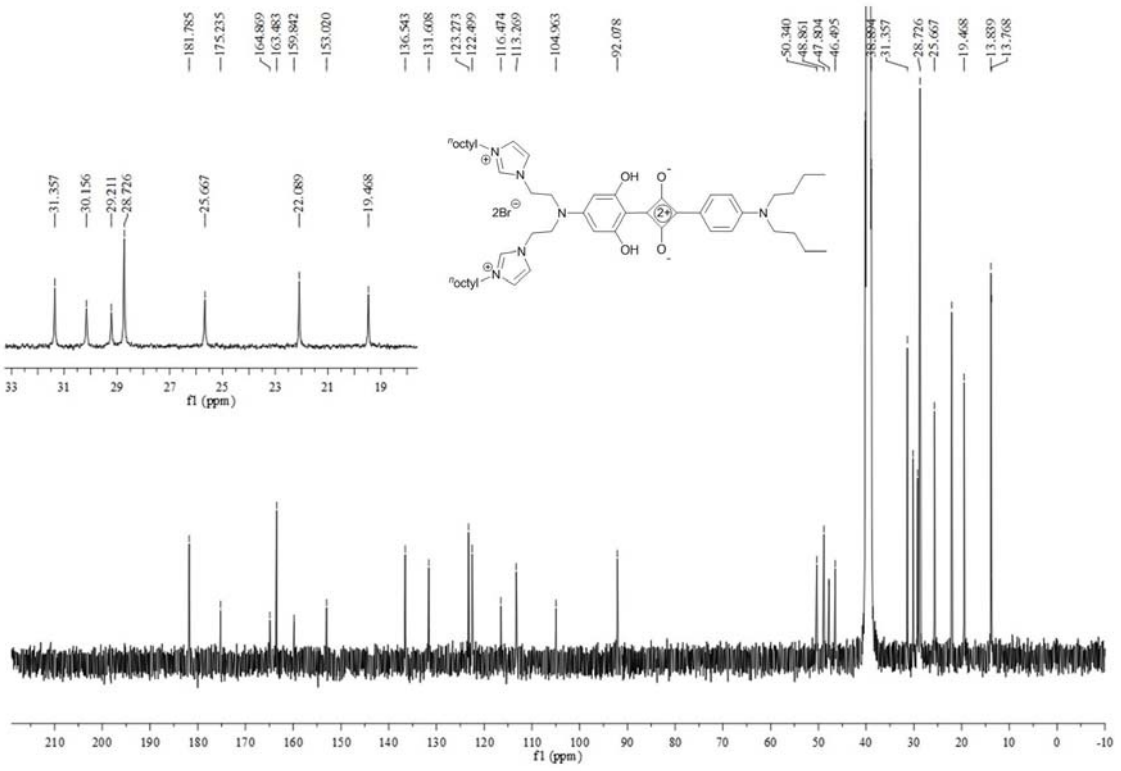
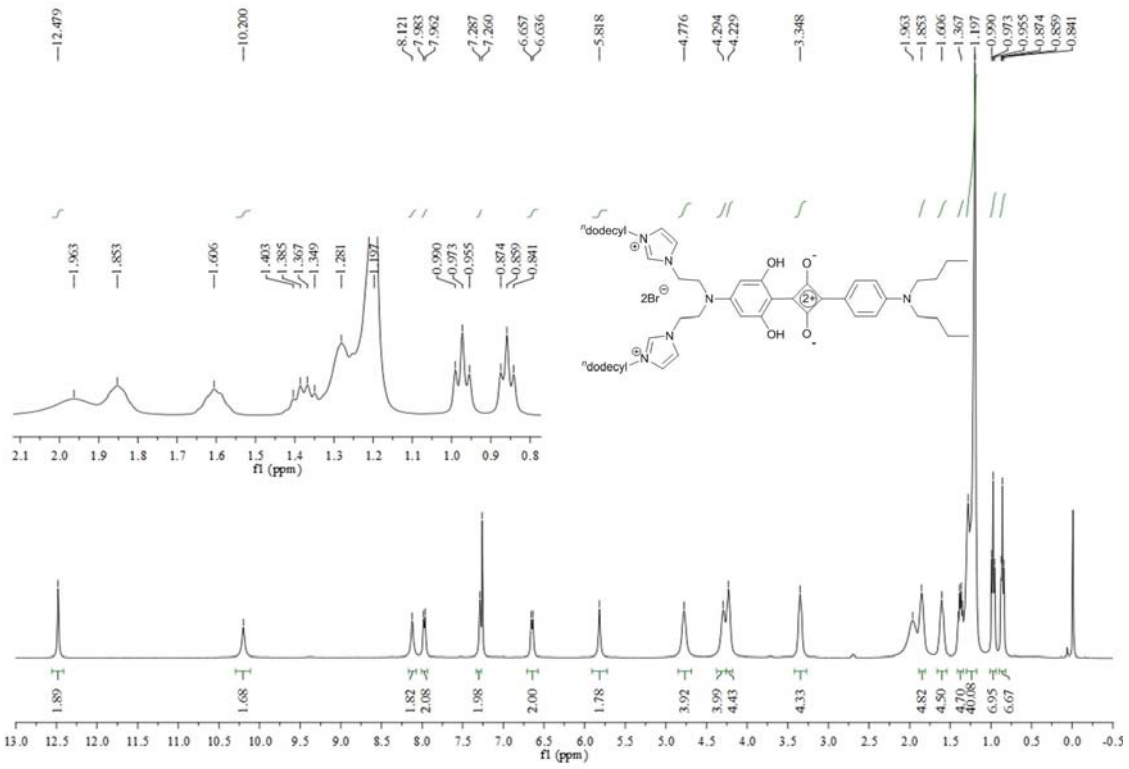
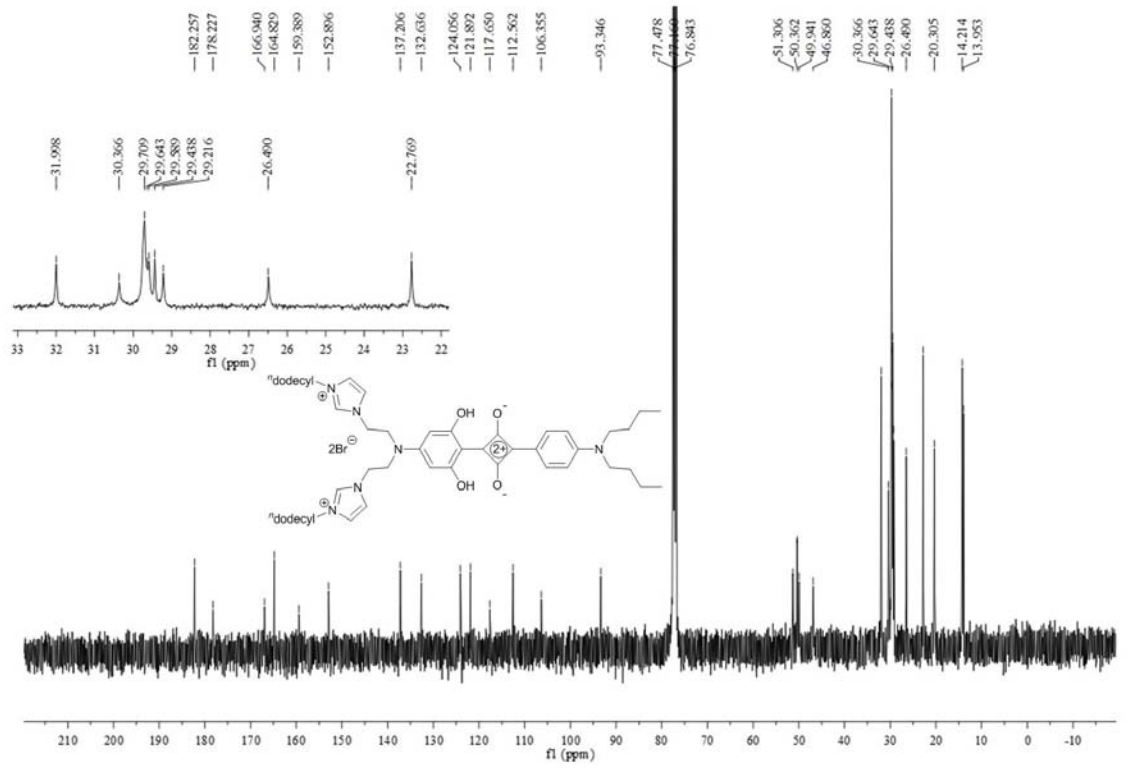
177.957
166.841
164.771
159.370
152.932
137.120
132.572
123.941
122.119
117.525
112.608
106.237
93.318
77.478
76.842
51.332
50.060
49.797
46.816
31.892
29.617
20.276
19.595
13.950
13.933
nbutyl
2Br
OH
OH
2+
f1 (ppm)


12.325
9.190
7.919
7.895
7.873
7.783
6.967
6.946
5.473
4.479
4.045
4.026
3.999
3.493
3.349
2.500
1.519
1.344
1.325
1.309
1.095
1.088
0.924
0.908
0.893
0.686
0.670
nOctyl
2Br
OH
O
2+
N
f1 (ppm)


181.785
175.235
164.869
163.483
159.842
153.020
136.543
131.608
123.273
122.499
116.474
113.269
104.963
92.078
50.340
48.861
47.804
46.495
38.884
31.357
28.726
25.667
19.468
13.839
13.768
31.357
30.156
29.211
28.726
25.667
22.089
19.468
nOctyl
2Br
OH
O
2+
N
f1 (ppm)


12.479
10.200
8.121
7.583
7.562
7.287
7.260
6.657
6.636
5.818
4.776
4.294
4.229
3.348
1.963
1.853
1.606
1.403
1.385
1.367
1.349
1.281
1.197
0.990
0.973
0.955
0.874
0.859
0.841
1.89
1.68
1.82
2.08
1.98
2.00
1.78
3.92
3.99
4.43
4.33
4.82
4.50
4.70
40.08
6.95
6.67
f1 (ppm)
ndodecyl
2Br
OH
O
2+
N


182.257
178.227
166.940
164.829
159.389
152.896
137.206
132.636
124.056
121.892
117.650
112.562
106.355
93.346
77.478
76.843
51.306
50.362
49.941
46.860
30.366
29.643
29.438
26.490
20.305
14.214
13.953
31.998
30.366
29.709
29.643
29.589
29.438
29.216
26.490
22.769
f1 (ppm)
ndodecyl
2Br
OH
O
2+
N