Supporting Information

Cu-catalysed oxidative C–H/C–H coupling polymerisation of benzodiimidazoles: an efficient approach to regioregular polybenzodiimidazoles for blue-emitting materials

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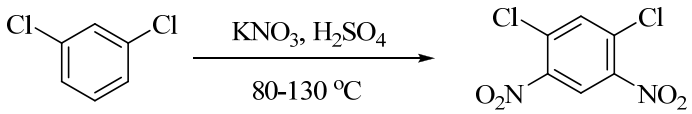
I. General remarks

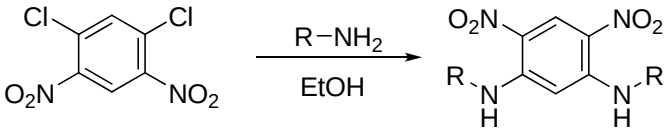
Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. $Cu(OAc)_2$ was washed with acetic anhydride using a Soxhlet extractor for 5 days prior to use. Benzodiimidazole derivatives were synthesized according to the literature procedures.[1] NMR spectra were obtained on a Bruker AMX-400. The ^1H NMR (400 MHz) chemical shifts were reported relative to $CDCl_3$ as the internal reference ($CDCl_3$: δ = 7.26 ppm); The ^{13}C NMR (100 MHz) chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ = 77.16 ppm). High-resolution mass spectra (HR-MS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected. Gel permeation chromatography (GPC) measurements were performed on a LC-20AD system using $CHCl_3$ as eluent and polystyrene as standards at a column temperature of 40 ºC. Thermogravimetric analysis (TGA) was carried out using NETZSCH TG 209F1 Iris at a heating rate of 10 ºC/min under N_2 atmosphere. Absorption spectra were recorded on HITACHI U-2910 spectrophotometer. Fluorescence spectra and absolute quantum yields were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer with a calibrated integrating sphere system. To reduce the fluctuation in the excitation intensity, the lamp was kept on for 1 hour prior to the experiment.

II. Synthesis of the benzodiimidazole derivatives

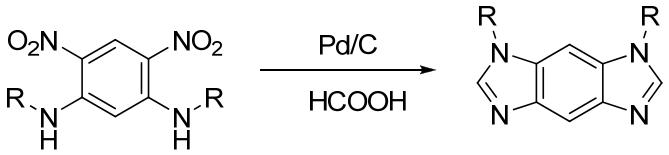


To a well-stirred mixture of 7.31 g (50 mmol) of *m*-dichlorobenzene with 25 g (247.5 mmol) of potassium nitrate was added 80 mL of concentrated sulfuric acid in one portion. The temperature of the reaction mixture rose during a few minutes to 80 ºC and kept the temperature for 30 minutes. And then rose the temperature to 130 ºC for 4 h. After the reaction mixture was cooled to room temperature, it was poured into

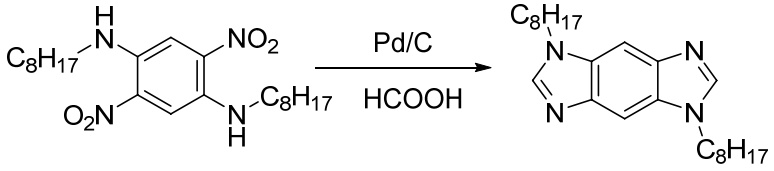
crushed ice. A yellow precipitated was collected and washed by water (3×100 mL). The resulting solid was recrystallized with ethyl alcohol, affording 1,5-dichloro-3,4-dinitrobenzene as a yellow solid (10.82 g, 91.1% yield).



After 1,5-dichloro-3,4-dinitrobenzene (1.00 g, 4.22 mmol) was dissolved in EtOH (75 mL), amine (16.9 mmol) was added in a single portion. The mixture was then placed in an oil bath at 80 ºC and stirred for 48 h. The mixture was poured into H_2O (200 mL) which caused solids to precipitate. The solids (N^1,N^3-dialkyl-4,6-dinitrobenzene-1,3-diamine) were collected via vacuum filtration, rinsed with H_2O, and dried under vacuum.



N^1,N^3-Dialkyl-4,6-dinitrobenzene-1,3-diamine (2.44 mmol) was suspended in HCO_2H (88%, 100 mL). To the suspension was added HCO_2Na (1.99 g, 29.2 mmol) and Pd/C (103 mg, 3 wt %, 0.05 mmol Pd). The mixture was heated in an oil bath at 140 ºC for 48 h. Upon completion, the cooled reaction mixture was filtered through celite and the filtrate volume was reduced to ca. 20 mL under vacuum. The solution was then added slowly into a vigorously stirred saturated solution of aqueous Na_2CO_3 (150 mL). Precipitated solids were collected via vacuum filtration, rinsed with H_2O. Purification via silica gel column chromatography (petroleum ether/acetone = 1/1, v/v) afforded the desired product.



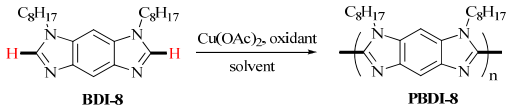
N^1,N^4-Dioctyl-3,6-dinitrobenzene-1,4-diamine[2] (2.23 g, 5.29 mmol) was suspended

in HCO_2H (88%, 80 mL). To the suspension was added HCO_2Na (8.0 g, 118 mmol) and Pd/C (1.8 g, 5 wt %). The mixture was heated in an oil bath at 140 ºC for 40 h. Upon completion, the cooled reaction mixture was filtered through celite and the filtrate volume was reduced to ca. 20 mL under vacuum. The solution was then added slowly into a vigorously stirred saturated solution of aqueous Na_2CO_3 (150 mL). Precipitated solids were collected via vacuum filtration, rinsed with H_2O. Purification via silica gel column chromatography (petroleum ether/acetone = 1/1, v/v) afforded the desired product (800 mg, 39.5%).

III. Optimization of the oxidative C–H/C–H coupling polymerization

1,7-Dioctyl-1*H*,7*H*-benzo[1,2-*d*:4,5-*d*]diimidazole (**BDI-8**, 0.25 mmol), $Cu(OAc)_2$ (9 mg, 20 mol%) and oxidant were dissolved in solvent (1 mL). The reaction container was purged with O_2 for 30 min to remove air and then heated at 140 ºC for 24 h. The mixture was cooled to room temperature, and the polymer was precipitated by slowly adding the mixture of CH_3OH and H_2O. The resulting solid was filtered and subjected to Soxhlet extraction in methanol, acetone and hexane for the removal of low molecular weight materials and impurities. The remaining polymer was extracted with chloroform, precipitated again from methanol, filtered, washed with methanol and dried under vacuum.

Table S1 Optimization of the Cu-catalysed oxidative C–H/C–H coupling polymerisation[a]



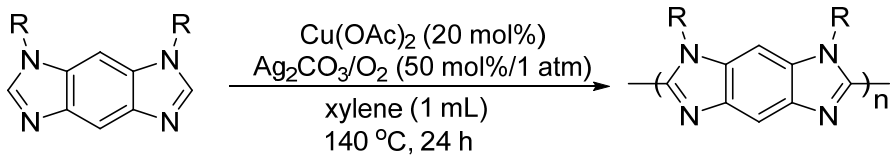
BDI-8 PBDI-8

Entry	Oxidant[b]	Solvent	Yield[c]	*M*n[d]	PDI[d]
1	Ag_2CO_3 (1.5)/O_2	xylene	63%	8100	1.78
2	Ag_2CO_3 (1.0)/O_2	xylene	70%	3300	3.08
3	Ag_2CO_3/O_2	xylene	66%	32000	1.52
4	Ag_2CO_3 (0.2)/O_2	xylene	67%	8200	3.55
5[e]	–	xylene	70%	2700	2.63
6[e]	–	DMF	64%	2200	2.21
7[f]	Ag_2CO_3/O_2	xylene	71%	6700	2.32
8	Ag_2CO_3/O_2	dioxane	67%	5800	2.47
9	Ag_2CO_3/O_2	dioxane/DMF	67%	4700	3.27
10	Ag_2CO_3/O_2	toluene	74%	5300	3.46

11	Ag_2CO_3/O_2	toluene/$CHCl_3$	63%	4200	1.93
12[g]	Ag_2CO_3/O_2	xylene	68%	31500	2.16

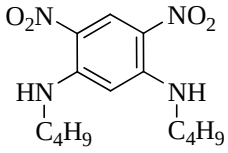
[a] Reaction conditions: **BDI-8** (0.25 mmol), $Cu(OAc)_2$ (20 mol%), Ag_2CO_3 (0.5 equiv), and solvent (1.0 mL) under O_2 (1 atm) at 140 ºC for 24 h; [b] The number in parentheses is the equivalent of Ag_2CO_3; [c] The products were obtained by reprecipitation from $CHCl_3$/MeOH after Soxhlet extraction; [d] Estimated by gel permeation chromatography (GPC) on polystyrene standards; [e] $Cu(OAc)_2$ (1.0 equiv); [f] $Cu(OAc)_2 \cdot H_2O$; [g] 48 h.

IV. General procedure for the oxidative C–H/C–H coupling polymerization of benzodiimidazoles



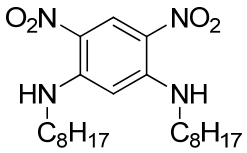
The benzodiimidazole derivative (0.25 mmol), $Cu(OAc)_2$ (9 mg, 20 mol%) and Ag_2CO_3 (34.5 mg, 50 mol%) were dissolved in xylene (1 mL). The reaction container was purged with O_2 for 30 min to remove air and then heated at 140 ºC for 24 h. The mixture was cooled to room temperature, and the polymer was precipitated by slowly adding the mixture of CH_3OH and H_2O. The resulting solid was filtered and subjected to Soxhlet extraction in methanol, acetone and hexane for the removal of low molecular weight materials and impurities. The remaining polymer was extracted with chloroform, precipitated again from methanol, filtered, washed with methanol and dried under vacuum.

V. Characterization data of products



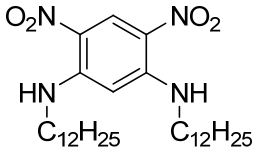
***N*[1],*N*[3]-Dibutyl-4,6-dinitrobenzene-1,3-diamine**

A yellow powder, m.p.100-102 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.01 (t, J = 7.4 Hz, 6H), 1.46-1.55 (m, 4H), 1.72-1.79 (m, 4H), 3.25-3.30 (m, 4H), 5.64 (s, 1H), 8.31 (s, 2H), 9.22 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.9, 20.4, 30.6, 43.2, 90.2, 124.2, 129.7, 148.8 ppm. HRMS (ESI^+): calculated for $C_{14}H_{22}O_4N_4Na$ $[M+Na]^+$ 333.1539, found 333.1536.



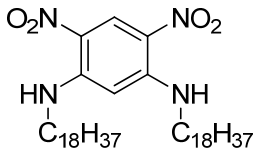
4,6-Dinitro-*N*^{1},*N*^{3}-dioctylbenzene-1,3-diamine

A yellow powder, m.p. 76-78 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.89 (t, J = 6.8 Hz, 6H), 1.29-1.49 (m, 20H), 1.72-1.80 (m, 4H), 3.24-3.29 (m, 4H), 5.63 (s, 1H) , 8.31 (s, 2H), 9.22 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.2, 28.6, 29.3, 29.4, 31.9, 43.5, 90.2, 124.2, 129.7, 148.8 ppm. HRMS (ESI^+): calculated for $C_{22}H_{38}O_4N_4$ Na $[M+Na]^+$ 445.2791, found 445.2788.



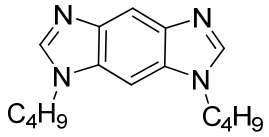
***N*^{1},*N*^{3}-Didodecyl-4,6-dinitrobenzene-1,3-diamine**

A yellow powder, m.p. 84-86 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, J = 6.8 Hz, 6H), 1.26-1.36 (m, 32H), 1.42-1.49 (m, 4H), 1.73-1.80 (m, 4H), 3.24-3.29(m, 4H), 5.63 (s, 1H) , 8.32 (s, 2H), 9.23 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.3, 22.8, 27.2, 28.6, 29.4, 29.5, 29.6, 29.7, 29.77, 29.79, 32.1, 43.5, 90.2, 124.2, 129.8, 148.8 ppm. HRMS (ESI^+): calculated for $C_{30}H_{54}O_4N_4$ Na $[M+Na]^+$ 557.4043, found 557.4045.



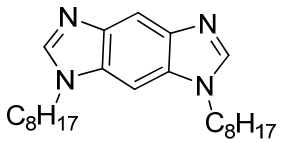
4,6-Dinitro-*N*^{1},*N*^{3}-dioctadecylbenzene-1,3-diamine

A yellow powder, m.p. 82-84 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, J = 6.8 Hz, 6H), 1.25-1.36 (m, 56H), 1.42-1.47 (m, 4H), 1.72-1.80 (m, 4H), 3.24-3.29 (m, 4H), 5.63 (s, 1H), 8.32 (s, 2H), 9.23 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.3, 22.8, 27.2, 28.6, 29.4, 29.5, 29.65, 29.73, 29.80, 29.81, 29.83, 29.9, 32.1, 43.5, 90.2, 124.2, 129.8, 148.8 ppm. HRMS (ESI$^+$): calculated for $C_{42}H_{78}O_4N_4Na$ $[M+Na]^+$ 725.5921, found 725.5919.



1,7-Dibutyl-1*H*,7*H*-benzo[1,2-*d*:4,5-*d*]diimidazole (BDI-4)

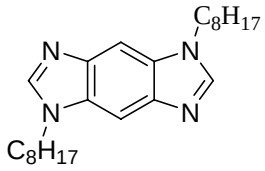
A white powder, m.p. 76-78 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.93-0.97 (m, 6H), 1.33-1.40 (m, 4H), 1.85-1.90 (m, 4H), 4.16-4.20 (m, 4H), 7.19 (s, 1H), 7.89 (s, 2H), 8.16 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.7, 20.2, 31.5, 45.0, 88.3, 110.3, 132.1, 141.1, 143.7 ppm. HRMS (ESI$^+$): calculated for $C_{16}H_{23}N_4$ $[M+H]^+$ 271.1923, found 271.1920.



1,7-Dioctyl-1*H*,7*H*-benzo[1,2-*d*:4,5-*d*]diimidazole (BDI-8)

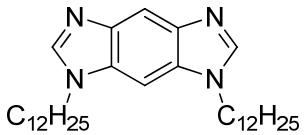
A white powder, m.p. 72-74 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.84 (t, J = 6.6 Hz, 6H), 1.22-1.32 (m, 20H), 1.86-1.91 (m, 4H), 4.17 (t, J = 7.0 Hz, 4H), 7.18 (s, 1H), 7.89 (s, 2H), 8.17 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.1, 22.7, 27.0,

29.2, 29.5, 31.8, 45.3, 88.3, 110.3, 132.0, 141.1, 143.7 ppm. HRMS (ESI^+): calculated for $C_{24}H_{39}N_4$ $[M+H]^+$ 383.3175, found 383.3173.



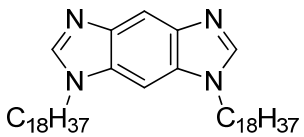
1,5-Dioctyl-1,5-dihydrobenzo[1,2-*d*:4,5-*d*]diimidazole (BDI-8′)

A white powder, m.p. 106-108 ºC, ^1H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, J = 6.8 Hz, 6H), 1.22-1.30 (m, 20H), 1.87-1.92 (m, 4H), 4.19 (t, J = 7.0 Hz, 4H), 7.72 (s, 2H), 7.93 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.1, 22.7, 26.9, 29.2, 29.5, 31.8, 45.4, 99.1, 131.6, 141.6, 144.2 ppm. HRMS (ESI^+): calculated for $C_{24}H_{39}N_4$ $[M+H]^+$ 383.3175, found 383.3173.



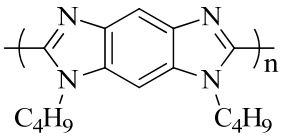
1,7-Didodecyl-1*H*,7*H*-benzo[1,2-*d*:4,5-*d*]diimidazole (BDI-12)

A white powder, m.p. 70-72 ºC, ^1H NMR (400 MHz, $CDCl_3$): δ = 0.87 (t, J = 6.6 Hz, 6H), 1.24-1.35 (m, 36H), 1.87-1.96 (m, 4H), 4.20 (t, J = 7.0 Hz, 4H), 7.20 (s, 1H), 7.92 (s, 2H), 8.19 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.3, 29.5, 29.57, 29.61, 29.68, 29.73, 29.74, 32.0, 45.4, 88.3, 110.5, 132.1, 141.2, 143.8 ppm. HRMS (ESI^+): calculated for $C_{32}H_{55}N_4$ $[M+H]^+$ 495.4427, found 495.4426.



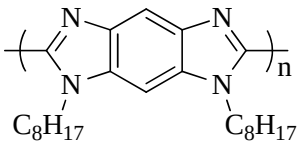
1,7-Dioctadecyl-1*H*,7*H*-benzo[1,2-*d*:4,5-*d*]diimidazole (BDI-18)

A white powder, m.p. 68-70 ºC, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.87 (t, J = 6.8 Hz, 6H), 1.24-1.34 (m, 60H), 1.90-1.94 (m, 4H), 4.20 (t, J = 7.0 Hz, 4H), 7.21 (s, 1H), 7.93 (s, 2H), 8.18 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.3, 29.5, 29.57, 29.61, 29.7, 29.76, 29.79, 29.83, 32.1, 45.4, 88.4, 110.3, 132.1, 141.1, 143.7 ppm. HRMS (ESI^+): calculated for $C_{44}H_{79}N_4$ $[M+H]^+$ 663.6305, found 663.6308.



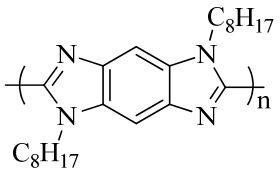
PBDI-4

According to the general procedure, **PBDI-4** was obtained as a brown solid (42 mg, 63% yield). Mn = 22500, PDI = 2.09. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.94-0.99 (m, 6H), 1.43 (s, 4H), 1.97 (s, 4H), 5.11 (s, 4H), 7.43 (s, 1H), 8.30 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.9, 20.3, 31.9, 45.3, 89.4, 110.2, 134.8, 140.7, 144.0.



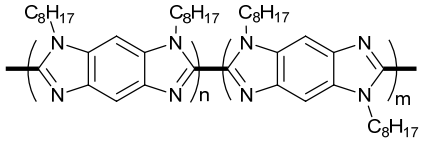
PBDI-8

According to the general procedure, **PBDI-8** was obtained as a brown solid (63 mg, 66% yield). Mn= 32000, PDI = 1.52. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.83 (s, 6H), 1.23 (s, 20H), 1.98 (s, 4H), 5.09 (s, 4H), 7.43 (s, 1H), 8.32 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.3, 29.77, 29.84, 31.9, 45.6, 89.3, 110.4, 134.8, 140.8, 144.0. The structure of **PBDI-8** was further confirmed by ^{1}H-^{1}H NOESY spectrum and HMQC (^{13}C-^{1}H COSY) spectrum.



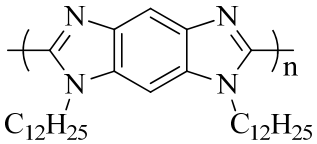
PBDI-8′

According to the general procedure, **PBDI-8′** was obtained as a brown solid (67 mg, 71% yield). Mn= 5800, PDI = 1.33. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.85 (s, 6H), 1.24-1.28 (m, 20H), 2.01 (s, 4H), 5.08 (s, 4H), 7.95 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.7, 27.0, 29.3, 29.8, 31.9, 45.6, 99.7, 134.0, 141.5, 144.4.



COPBDI-8

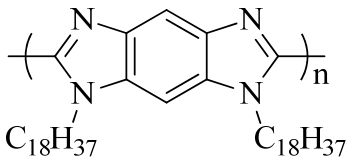
According to the general procedure, **COPBDI-8** was obtained as a brown solid (57 mg, 61% yield). Mn= 4100, PDI = 1.50. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.82 (s, 11H), 1.24 (m, 36H), 1.98 (m, 7.7H), 5.08 (s, 4H), 7.43 (s, 1H), 7.93 (s, 1.8H), 8.34 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.3, 29.8, 31.8, 45.5, 134.8, 140.8, 141.6, 144.5.



PBDI-12

According to the general procedure, **PBDI-12** was obtained as a brown solid (78 mg, 63% yield). Mn= 37200, PDI = 1.68. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.84-0.88 (m, 6H), 1.22-1.25 (m, 36H), 1.98 (s, 4H), 5.09 (s, 4H), 7.43 (s, 1H), 8.33 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.46, 29.51, 29.79, 29.83, 32.1,

45.7, 89.3, 110.4, 134.8, 140.8, 144.0.



PBDI-18

According to the general procedure, **PBDI-18** was obtained as a brown solid (140 mg, 85% yield). Mn = 44500, PDI = 1.32. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.86 (s, 6H), 1.25 (s, 60H), 1.99 (s, 4H), 5.10 (s, 4H), 7.43 (s, 1H), 8.33 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.8, 27.1, 29.46, 29.51, 29.79, 29.84, 32.1, 45.6, 89.3, 110.3, 134.9, 140.8, 144.0.

VI. References

1. A. J. Boydston, P. D. Vu, O. L. Dykhno, V. Chang, A. R. Wyatt, A. S. Stockett, E. T. Ritschdorff, J. B. Shear and C. W. Bielawski, *J. Am. Chem. Soc.*, 2008, **130**, 3143.
2. Z.-L. Zhou, S.-T. Lam, L. Zhao, US20130237725.

VII. Absorption spectra of the polymers

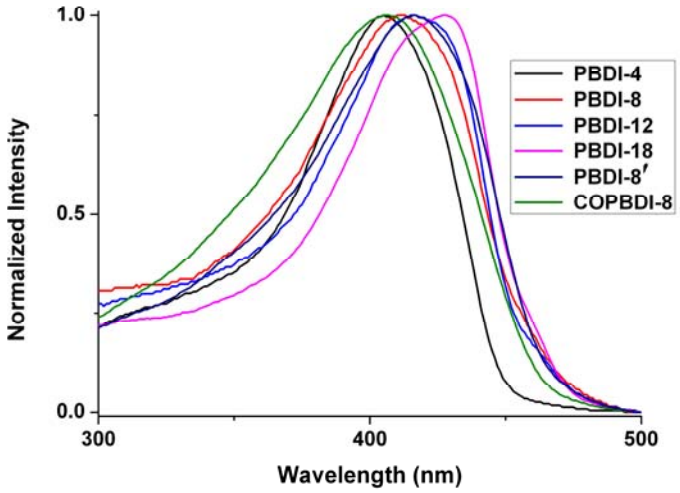


Fig. S1. Absorption spectra of **PBDI-4**, **PBDI-8**, **PBDI-12**, **PBDI-18, PBDI-8′** and **COPBDI-8** in $CHCl_3$.

VIII. Emission spectra of the polymers in PS film

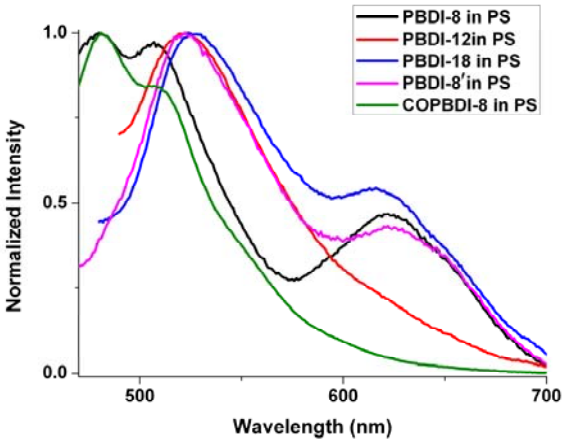


Fig. S2. Emission spectra of **PBDI-8**, **PBDI-12**, **PBDI-18, PBDI-8′** and **COPBDI-8** in PS (c = 1 wt%) film.

IX. TGA curves of the polymers

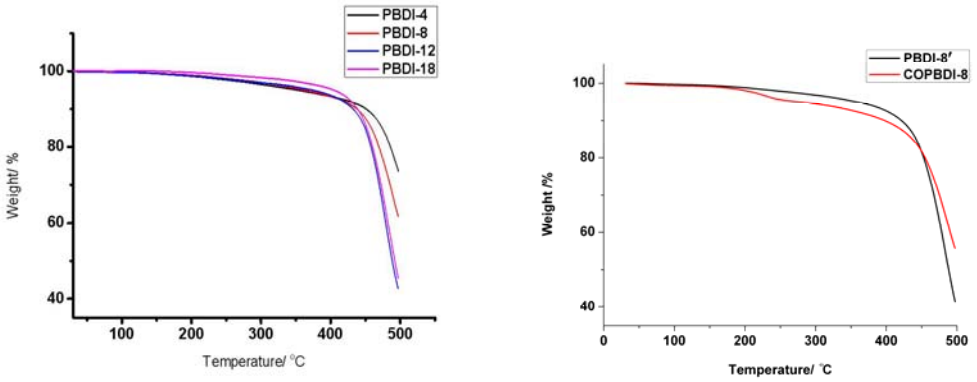


Fig. S3. TGA curves of **PBDI-4**, **PBDI-8**, **PBDI-12** and **PBDI-18** (left); TGA curves of **PBDI-8′** and **COPBDI-8** (right).

X. ^{1}H-^{1}H NOESY and HMQC (^{13}C-^{1}H COSY) spectra of PBDI-8

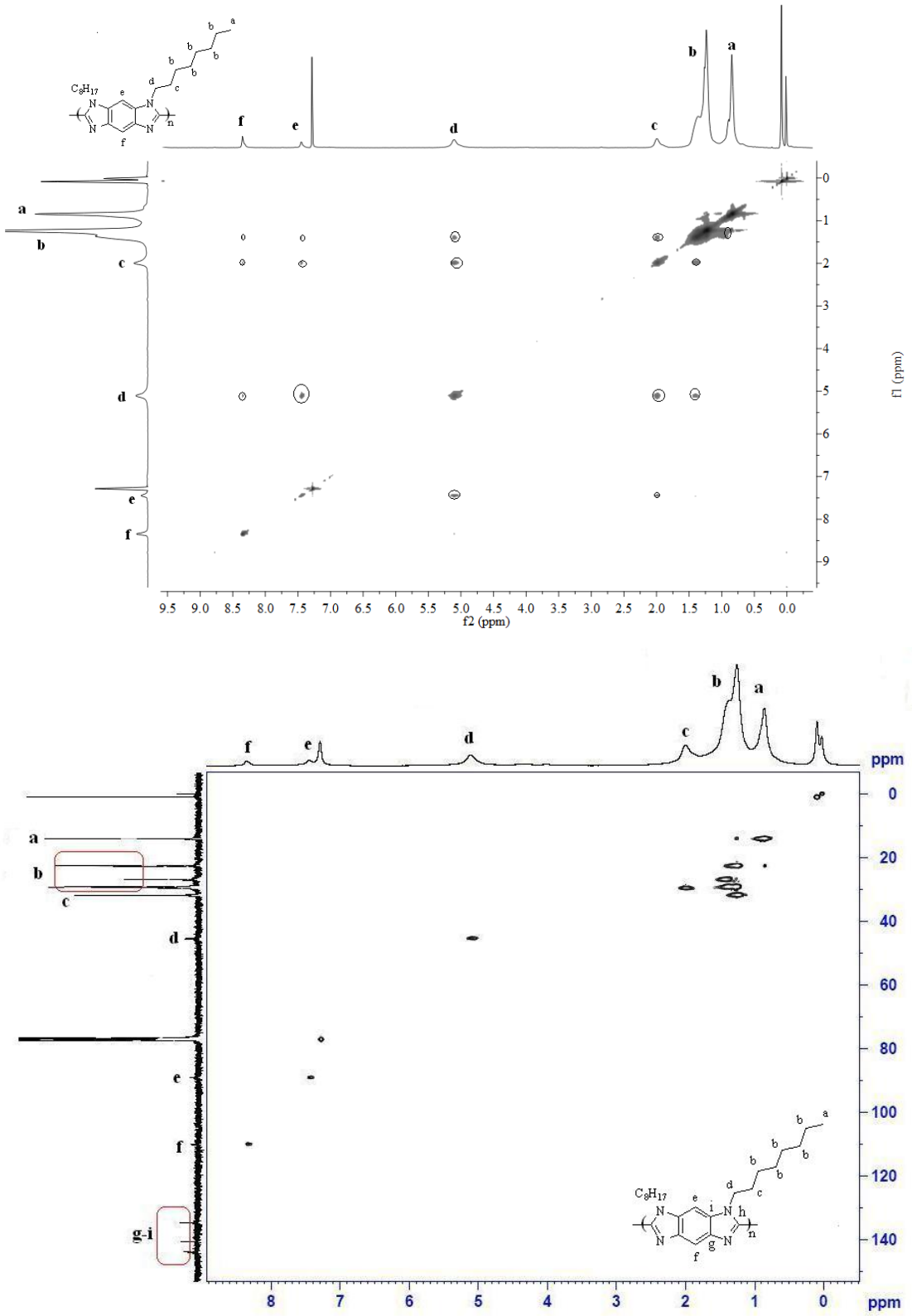
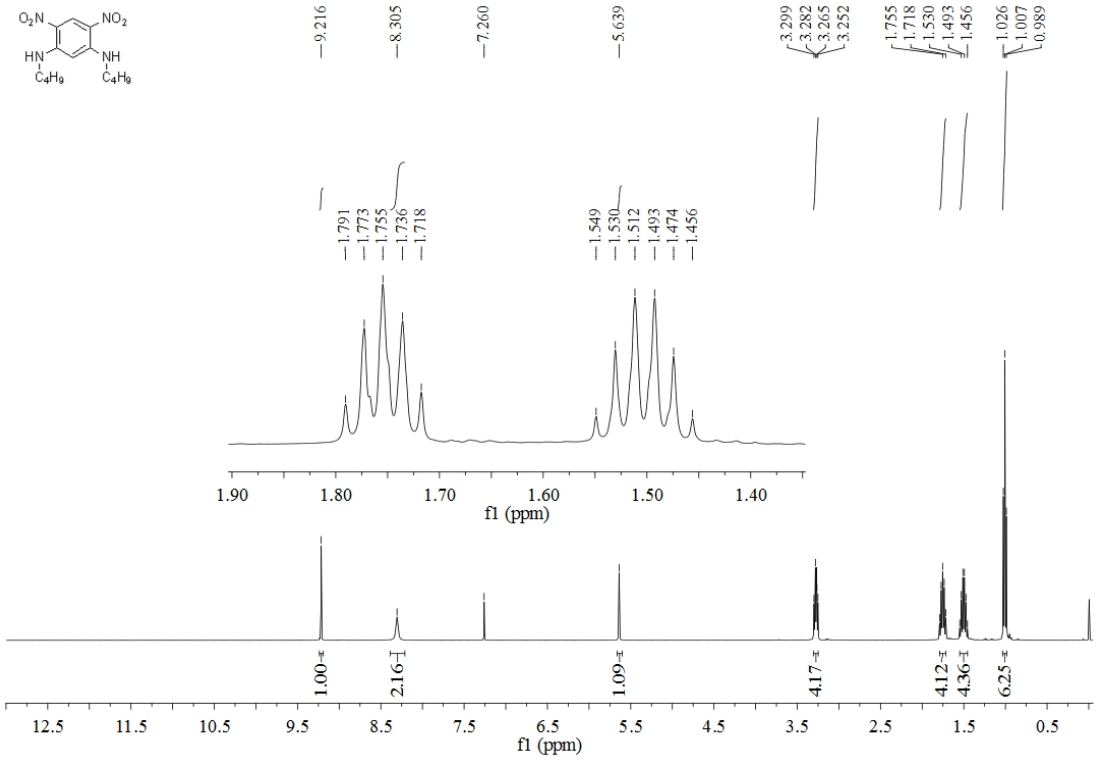
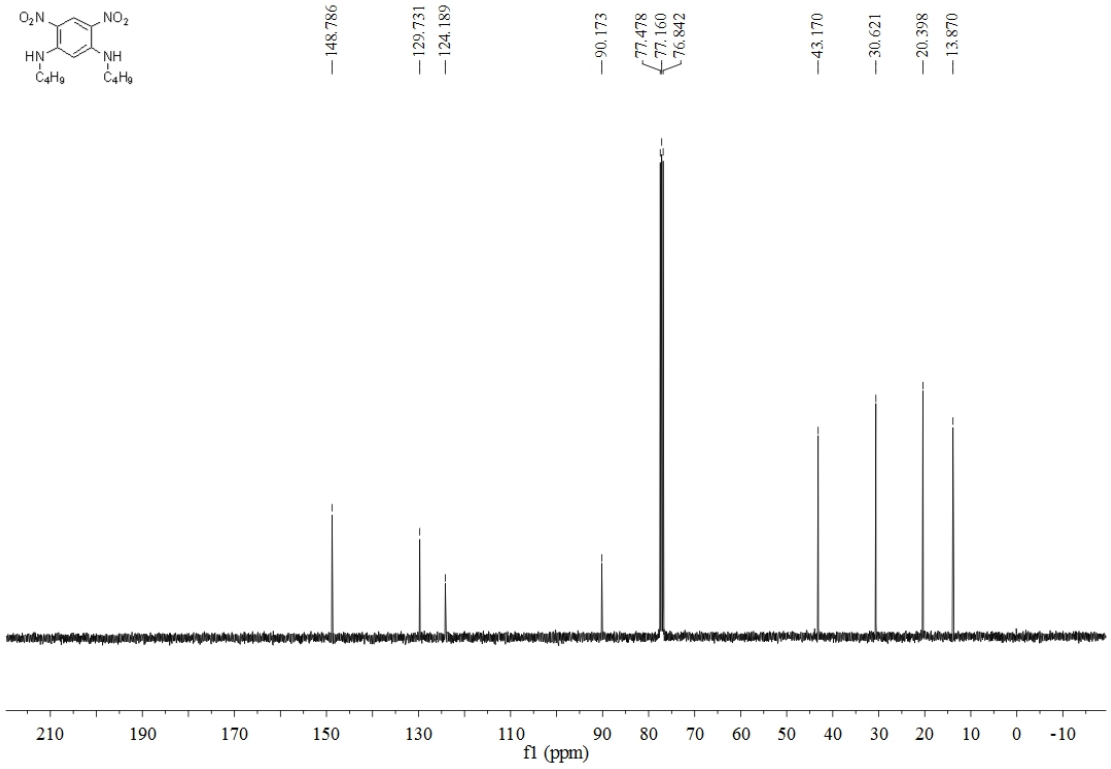
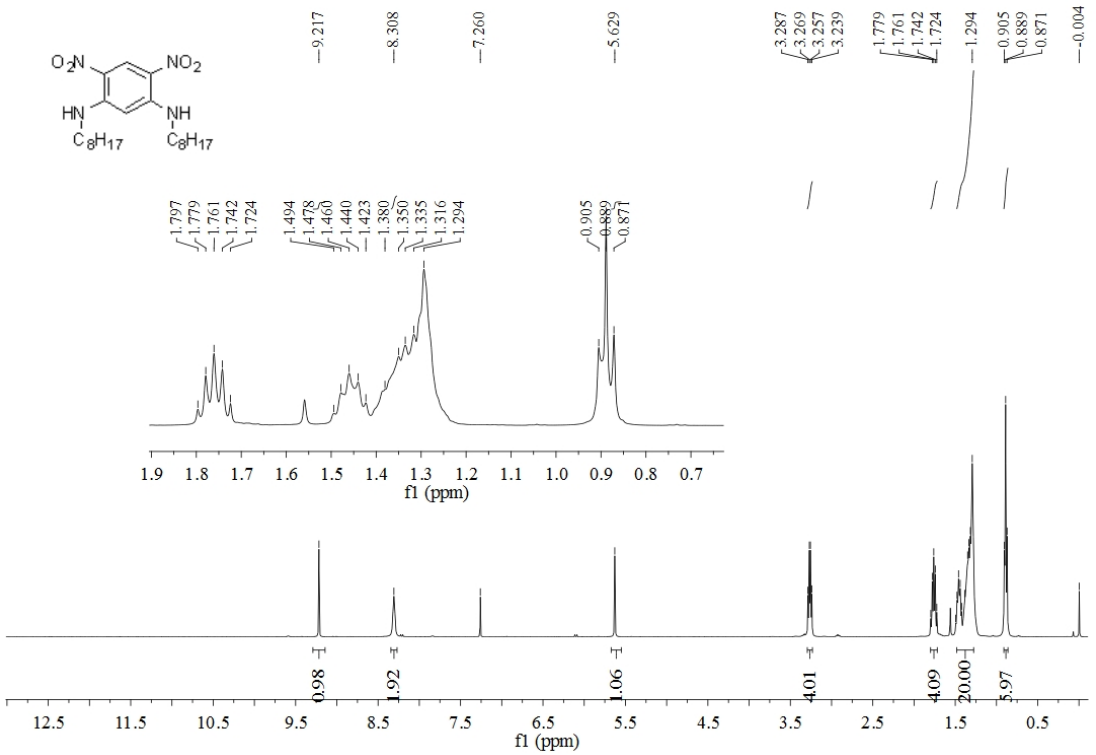


Fig. S4. ^{1}H-^{1}H NOESY and HMQC (^{13}C-^{1}H COSY) spectra of **PBDI-8.**

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



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7.260
5.629
3.287
3.269
3.257
3.239
1.779
1.761
1.742
1.724
1.294
0.905
0.889
0.871
-0.004
1.797
1.779
1.761
1.742
1.724
1.494
1.478
1.460
1.440
1.423
1.380
1.350
1.335
1.316
1.294
0.905
0.889
0.871
1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7
f1 (ppm)
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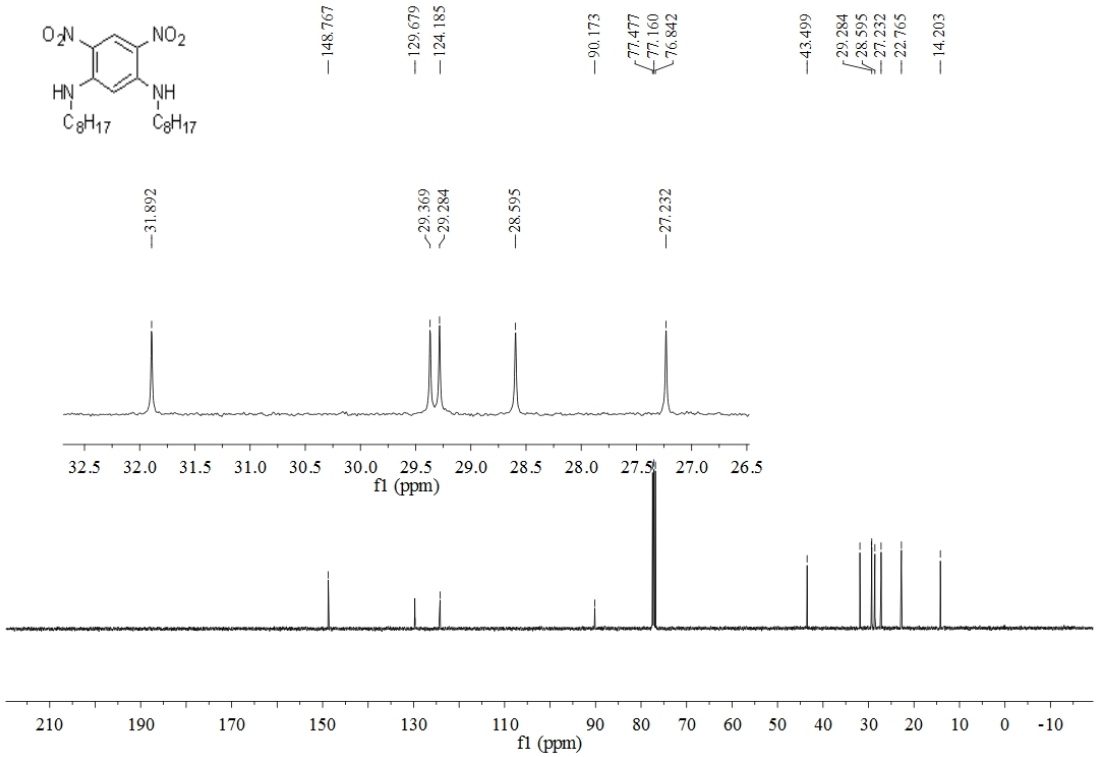
1.92
1.06
4.01
4.09
20.00
5.97
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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124.185
90.173
77.477
77.160
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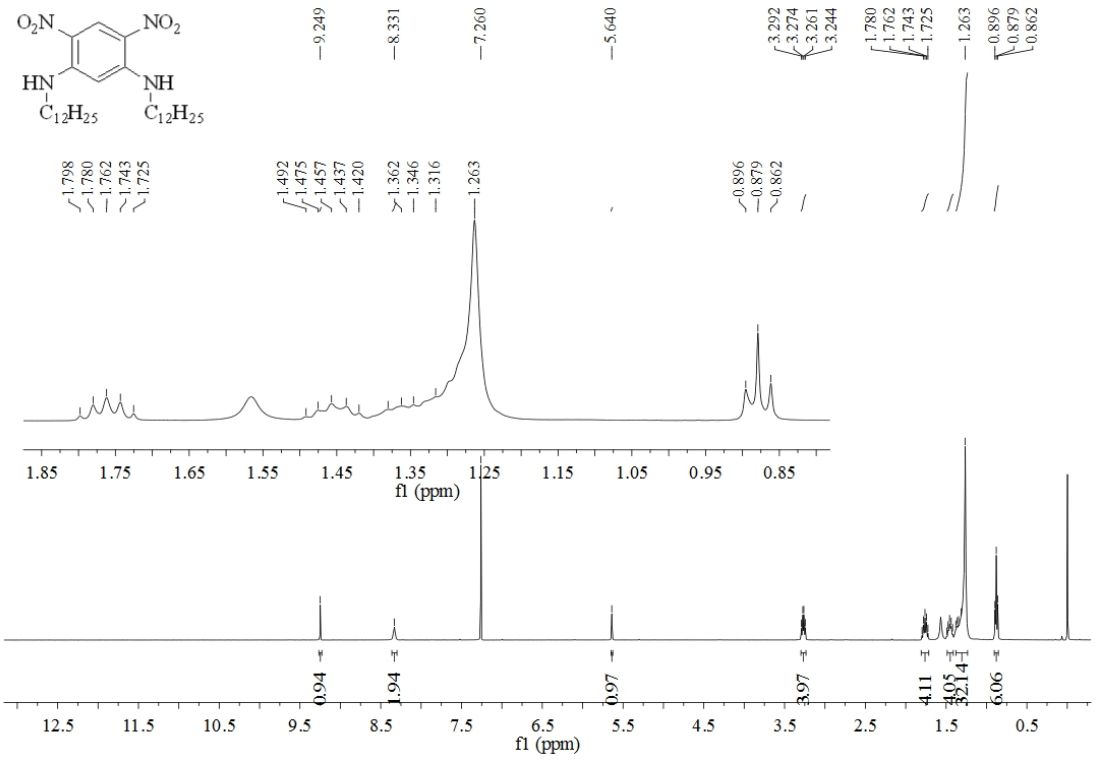
29.284
28.595
27.232
22.765
14.203
31.892
29.369
29.284
28.595
27.232
32.5 32.0 31.5 31.0 30.5 30.0 29.5 29.0 28.5 28.0 27.5 27.0 26.5
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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3.244
1.780
1.762
1.743
1.725
1.263
0.896
0.879
0.862
1.798
1.780
1.762
1.743
1.725
1.492
1.475
1.457
1.437
1.420
1.362
1.346
1.316
1.85 1.75 1.65 1.55 1.45 1.35 1.25 1.15 1.05 0.95 0.85
f1 (ppm)
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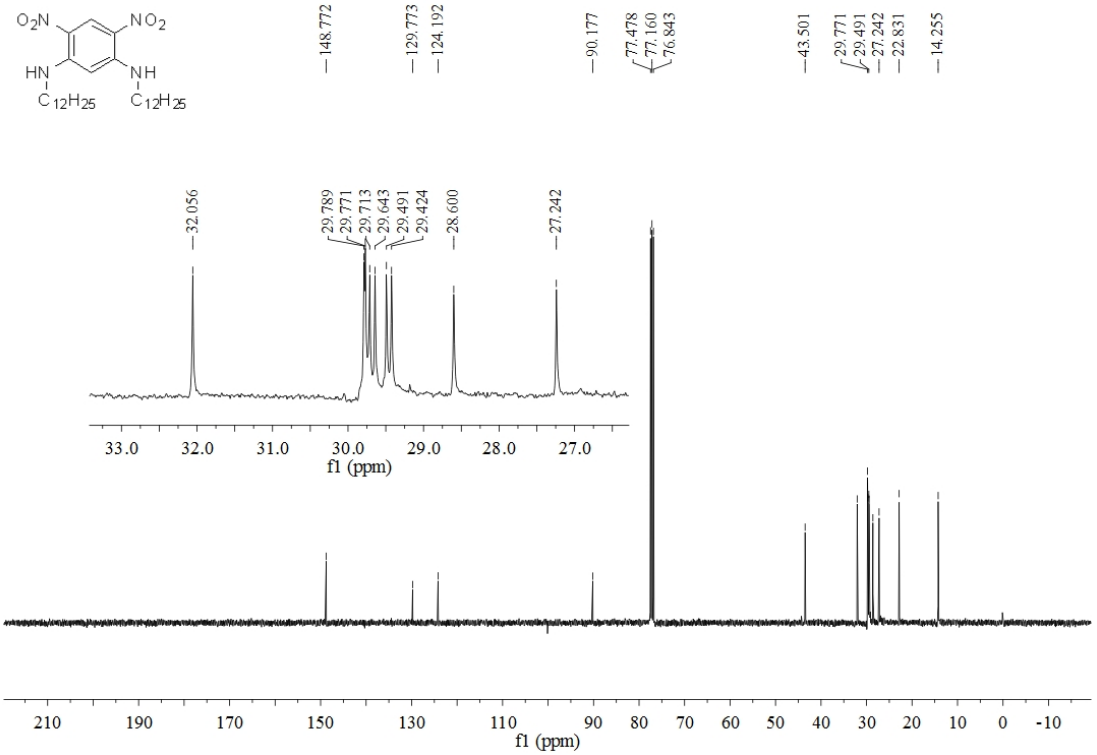
1.94
0.97
3.97
4.11
2.05
32.14
6.06
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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NH
C12H25
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76.843
43.501
29.771
29.491
27.242
22.831
14.255
32.056
29.789
29.771
29.713
29.643
29.491
29.424
28.600
27.242
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f1 (ppm)
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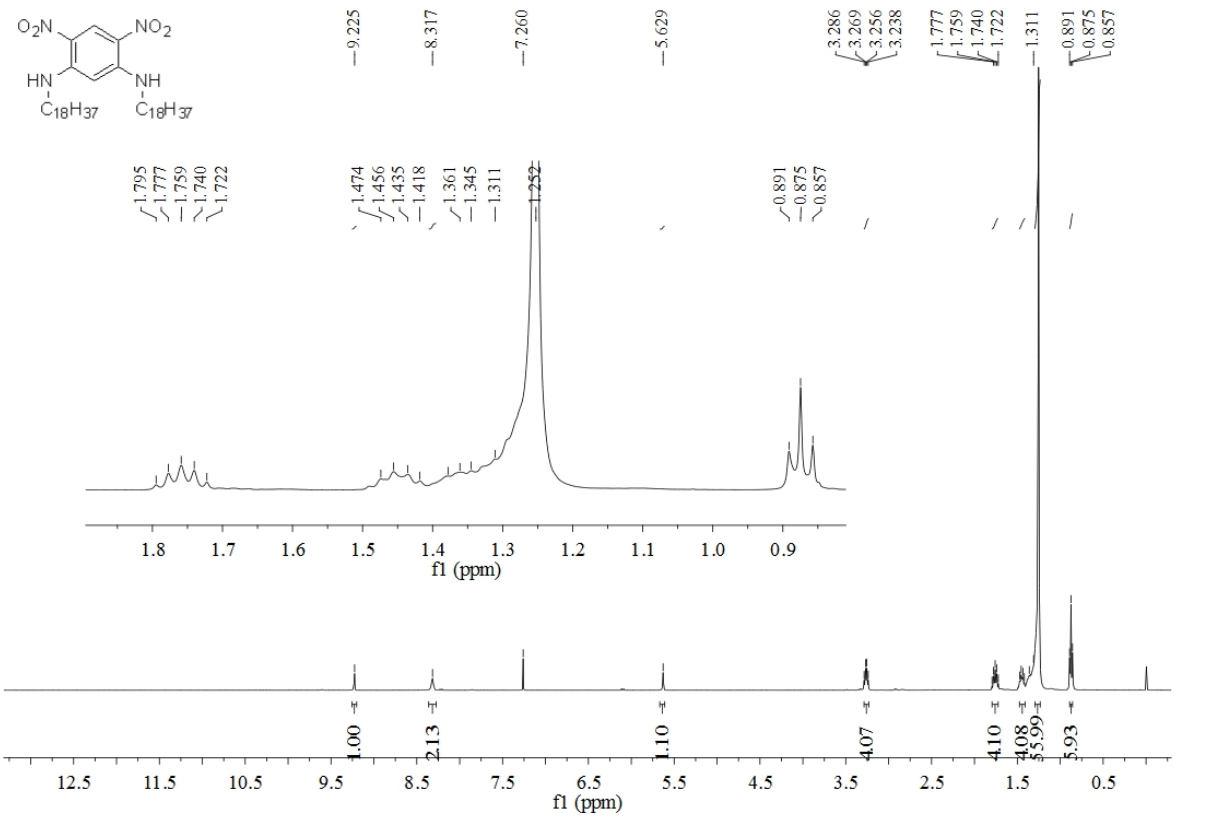
f1 (ppm)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3.238
1.777
1.759
1.740
1.722
1.311
0.891
0.875
0.857
1.795
1.777
1.759
1.740
1.722
1.474
1.456
1.435
1.418
1.361
1.345
1.311
1.252
0.891
0.875
0.857
1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9
f1 (ppm)
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2.13
1.10
4.07
4.10
4.08
5.99
5.93
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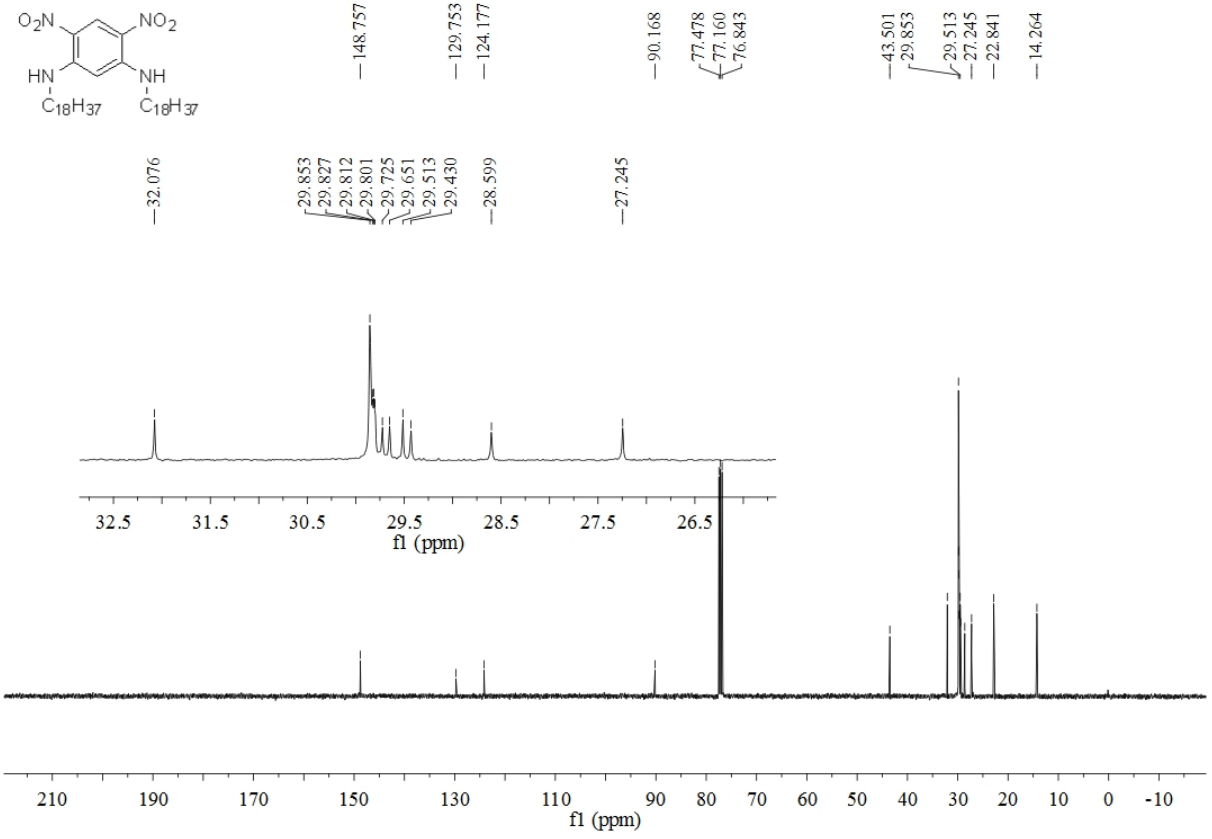
f1 (ppm)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NO2
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NH
C18H37
C18H37
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77.160
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43.501
29.853
29.513
27.245
22.841
14.264
32.076
29.853
29.827
29.812
29.801
29.725
29.651
29.513
29.430
28.599
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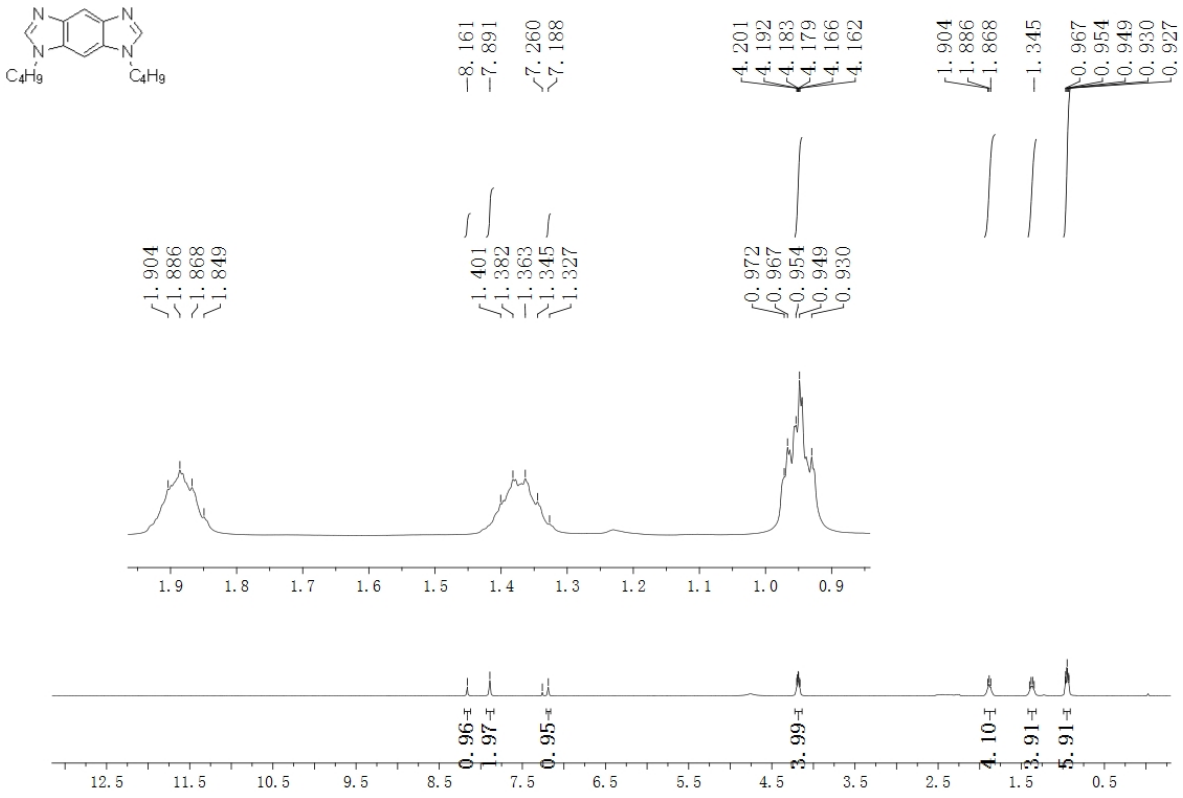
32.5 31.5 30.5 29.5 28.5 27.5 26.5
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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1.904
1.886
1.868
1.345
0.967
0.954
0.949
0.930
0.927
1.904
1.886
1.868
1.849
1.401
1.382
1.363
1.345
1.327
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0.949
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0.95
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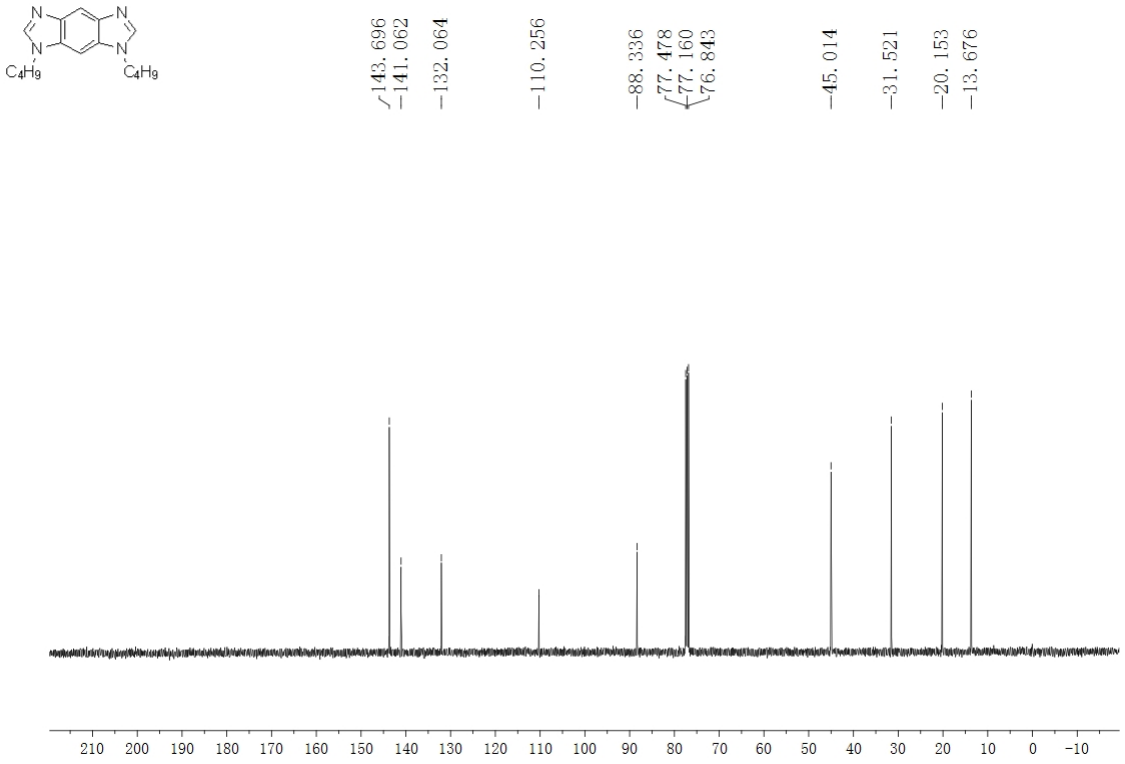
3.91
5.91


C4H9
C4H9
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132.064
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77.478
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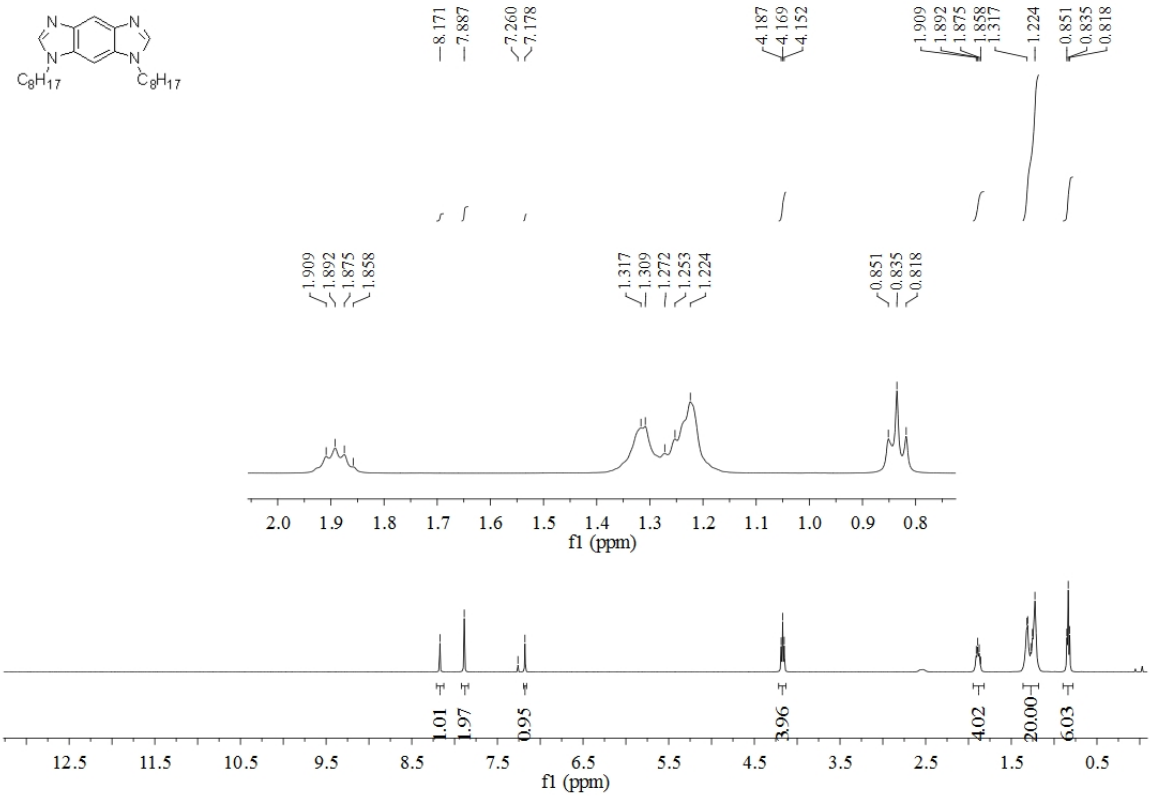
76.843
45.014
31.521
20.153
13.676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4.152
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1.892
1.875
1.858
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1.224
0.851
0.835
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f1 (ppm)
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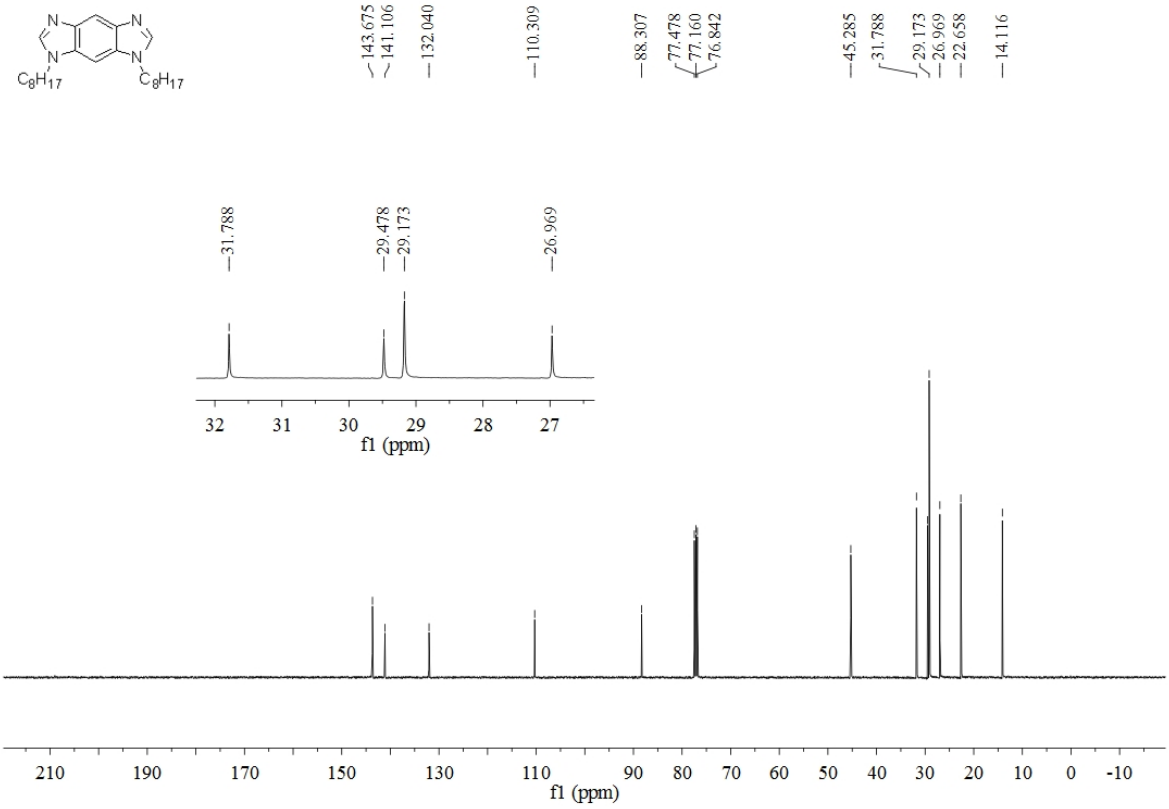
0.95
3.96
4.02
20.00
6.03
f1 (ppm)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76.842
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22.658
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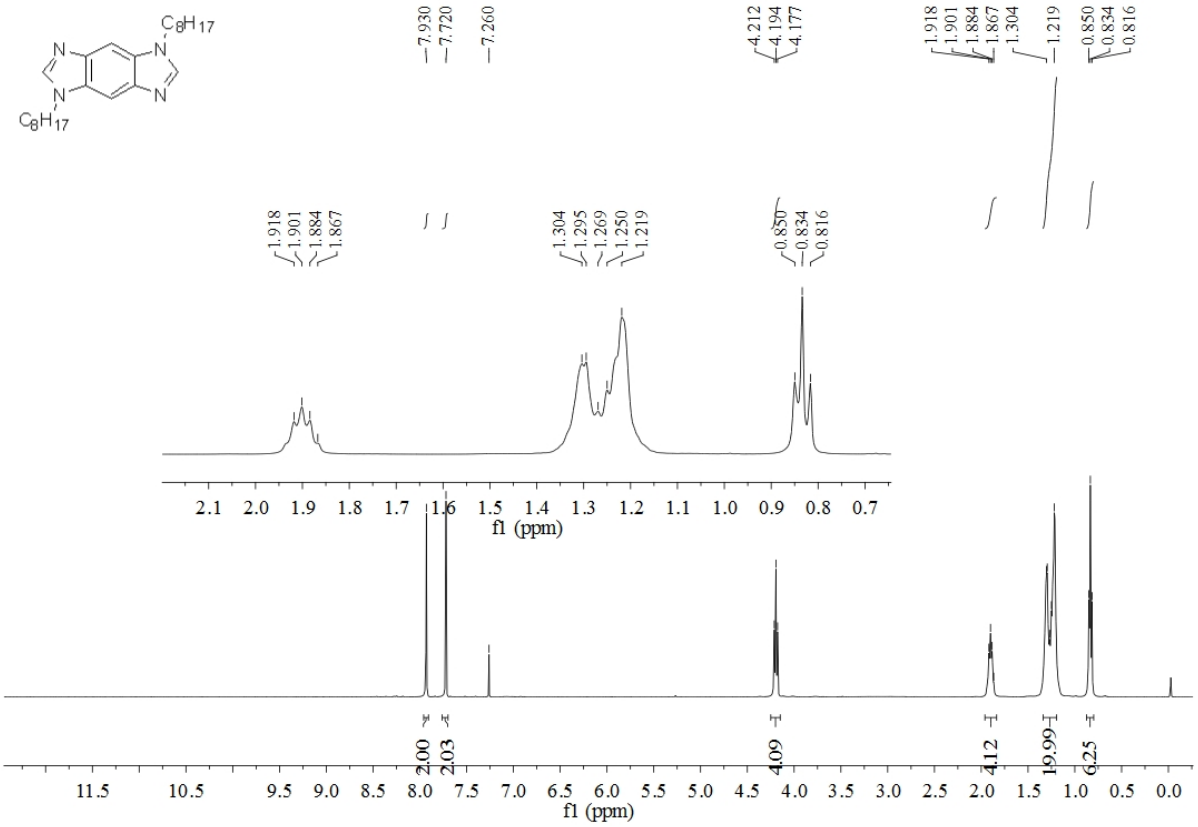
29.173
26.969
f1 (ppm)
f1 (ppm)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7.260
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4.177
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1.901
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1.867
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1.219
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0.834
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fl (ppm)
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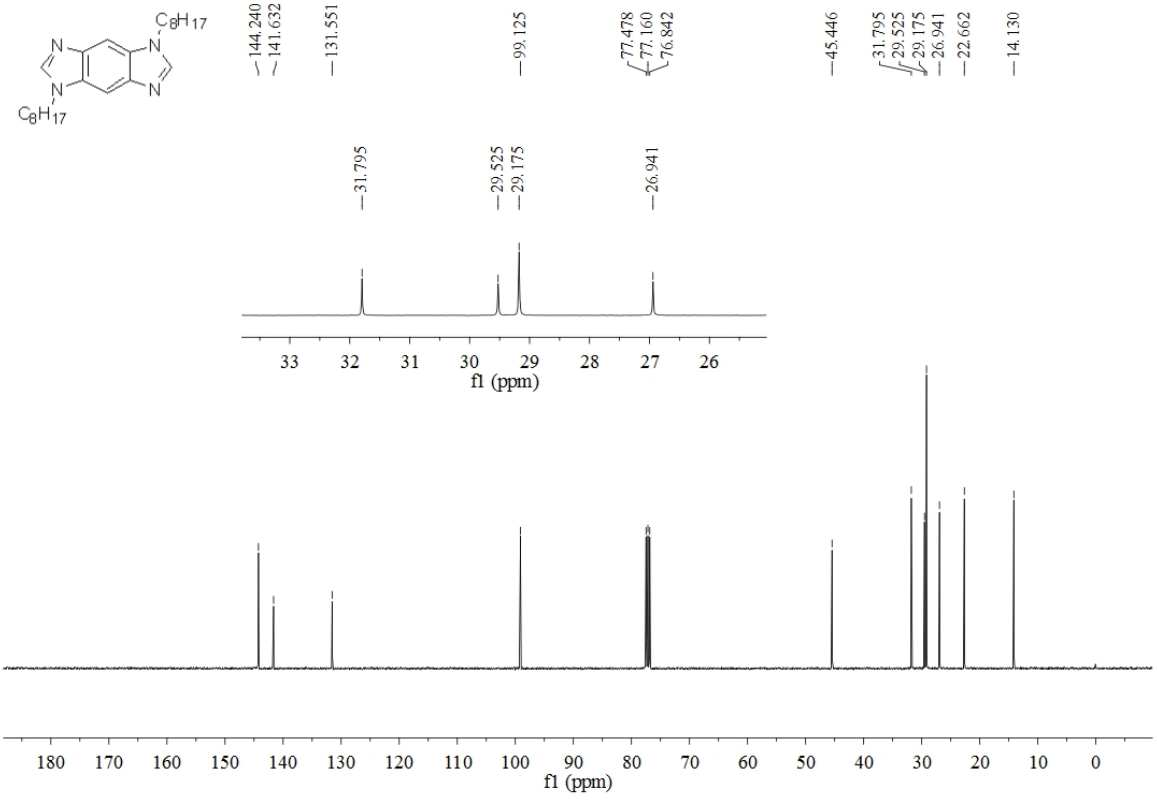
4.12
19.99
6.25


C8H17
C8H17
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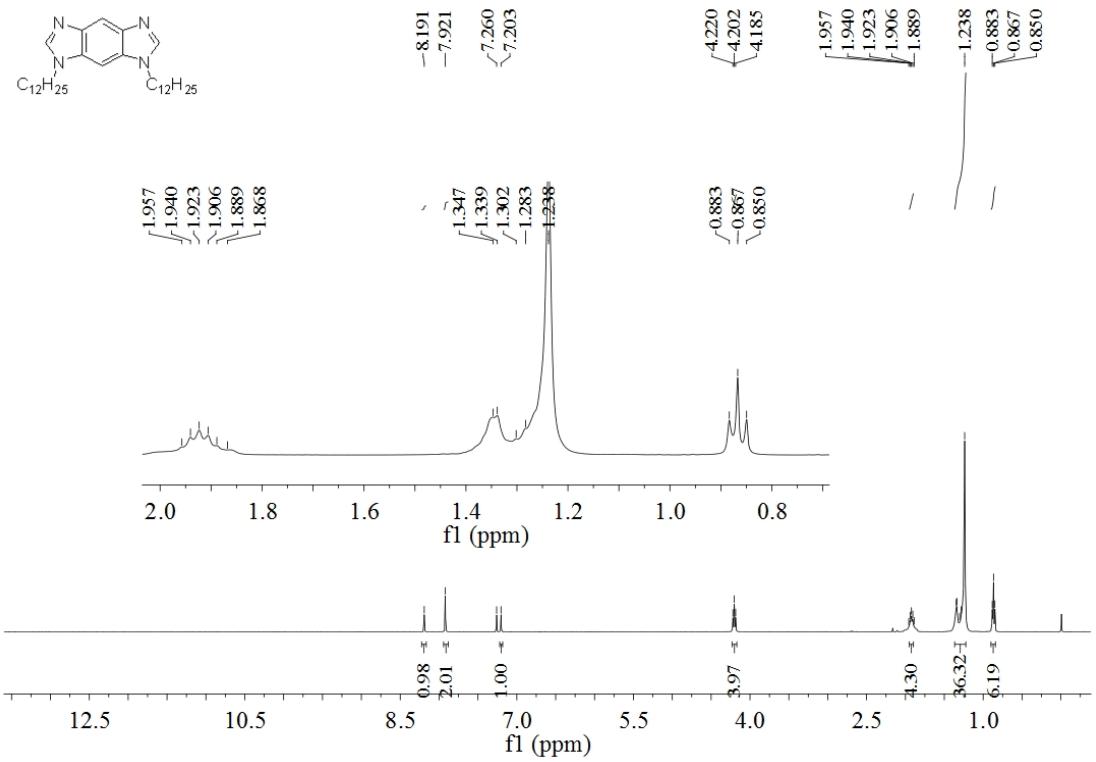
14.130
fl (ppm)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1.238
0.883
0.867
0.850
1.957
1.940
1.923
1.906
1.889
1.868
1.347
1.339
1.302
1.283
1.238
0.883
0.867
0.850
2.0
1.8
1.6
1.4
1.2
1.0
0.8
f1 (ppm)
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1.00
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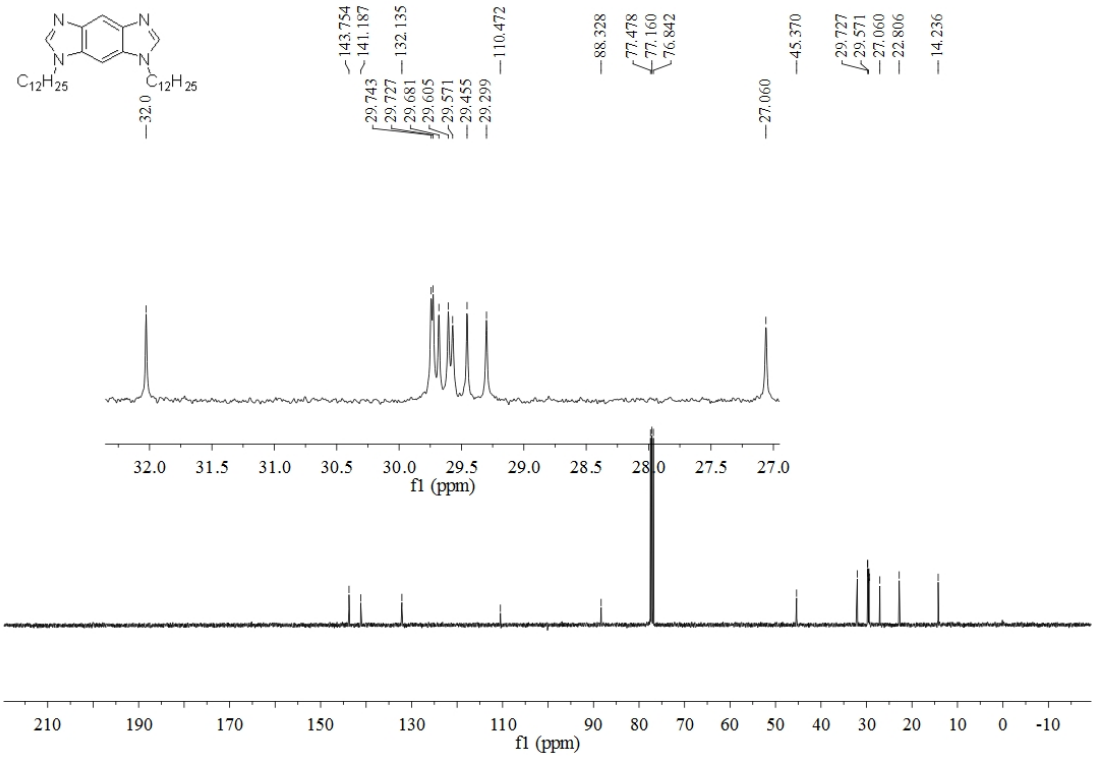
1.0
f1 (ppm)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29.299
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77.160
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27.060
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28.0
27.5
27.0
f1 (ppm)
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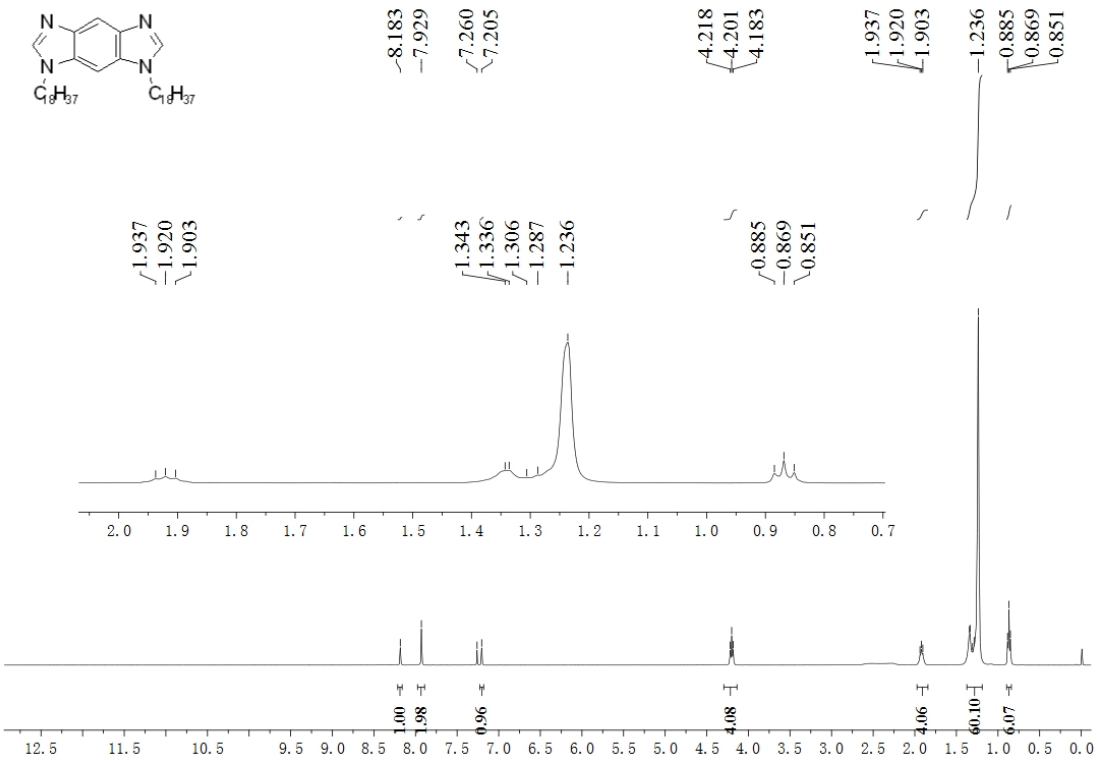
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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1.937
1.920
1.903
1.236
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0.869
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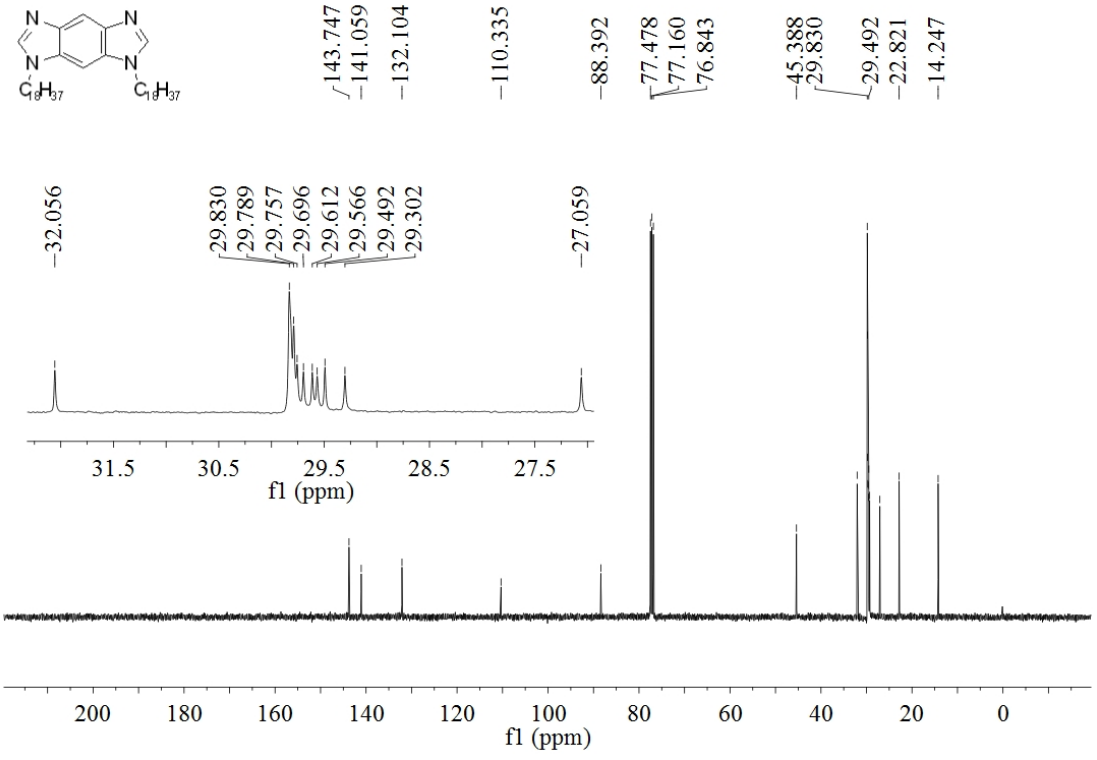
4.08
4.06
60.10
6.07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14.247
32.056
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29.566
29.492
29.302
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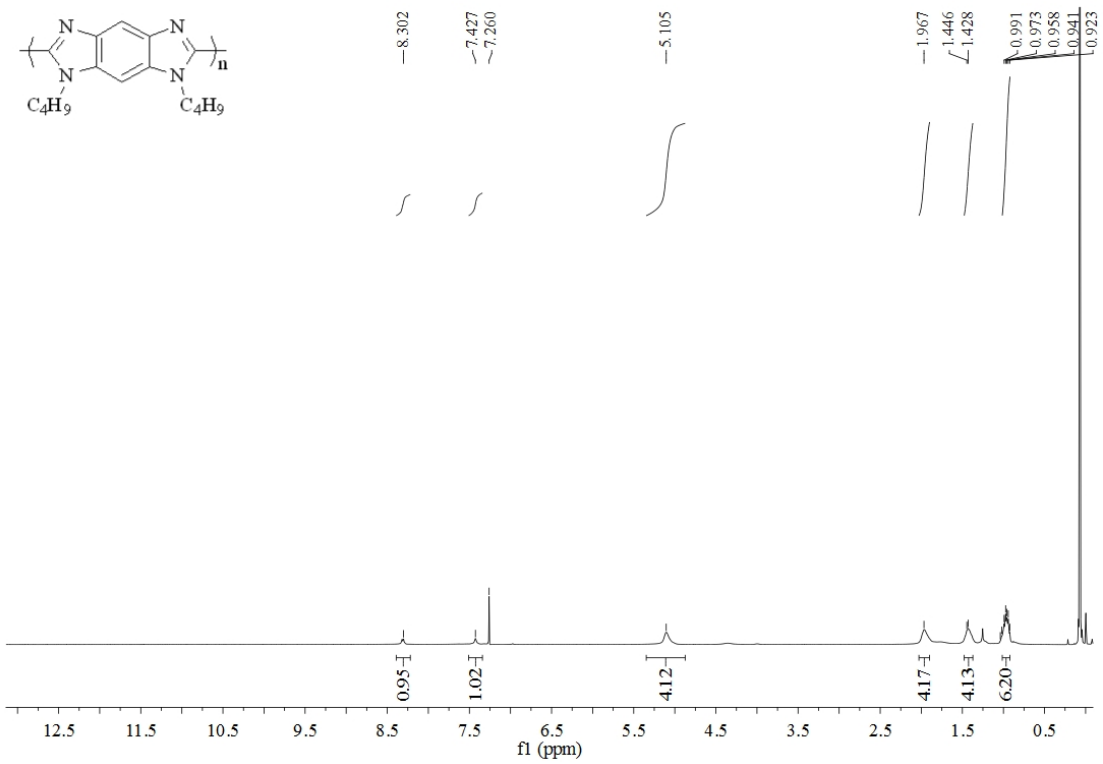
f1 (ppm)
f1 (ppm)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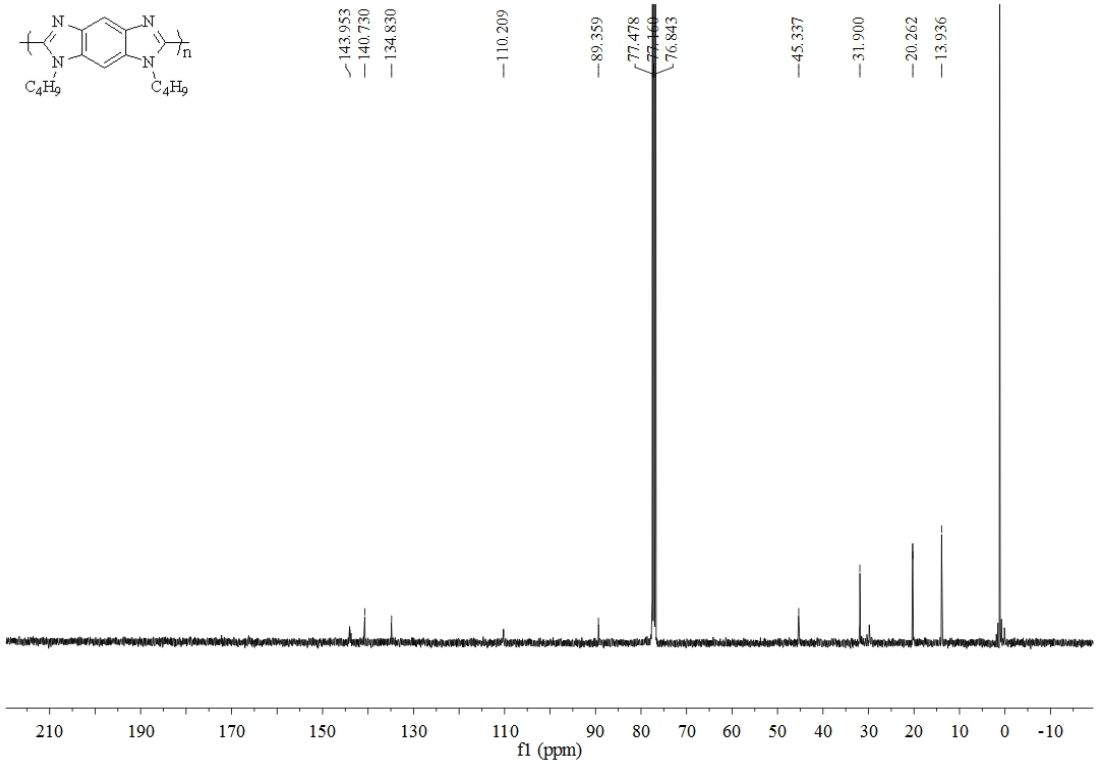
0.958
0.941
0.923
0.95
1.02
4.12
4.17
4.13
6.20
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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20.262
13.936
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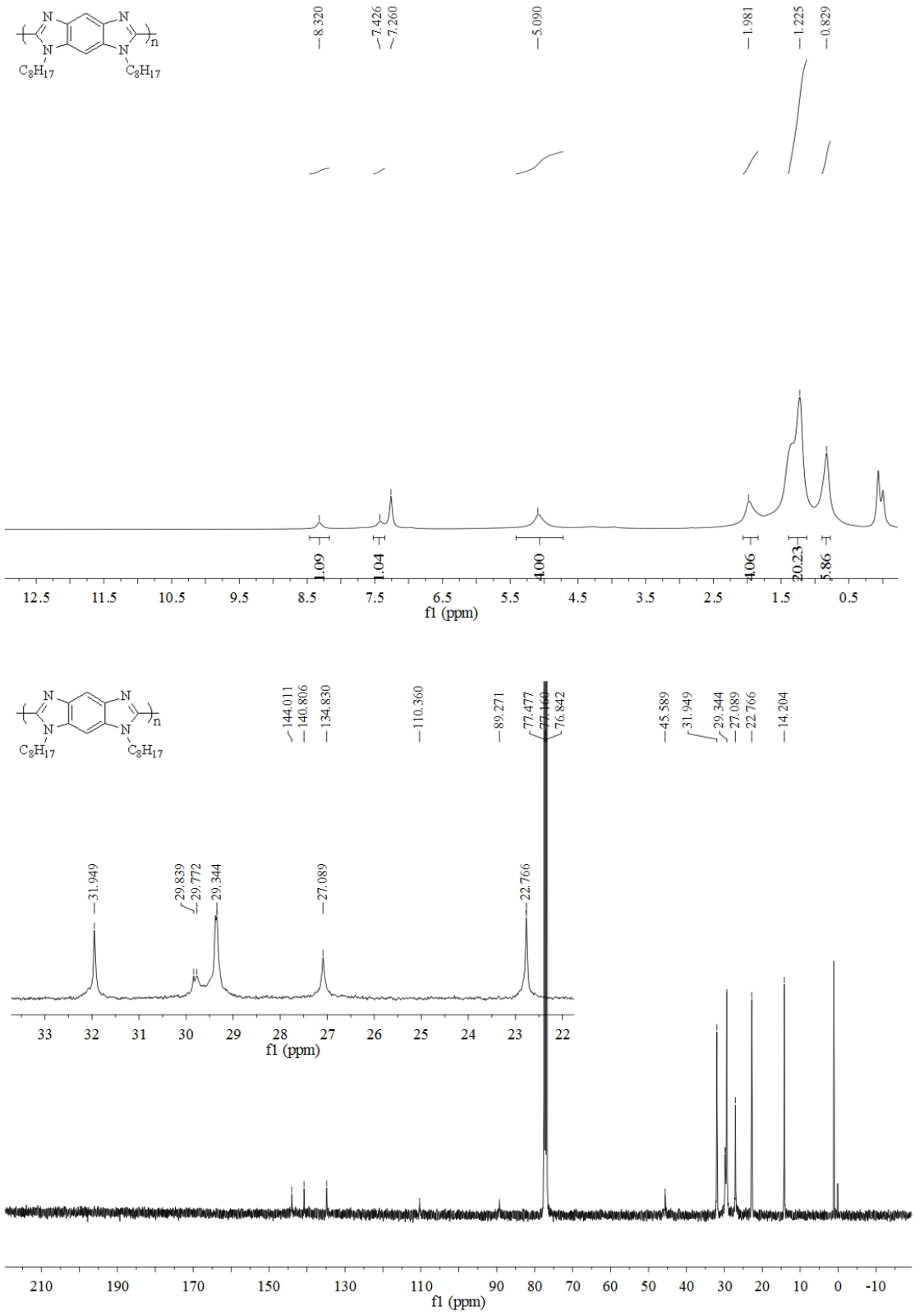
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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4.06
20.23
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f1 (ppm)
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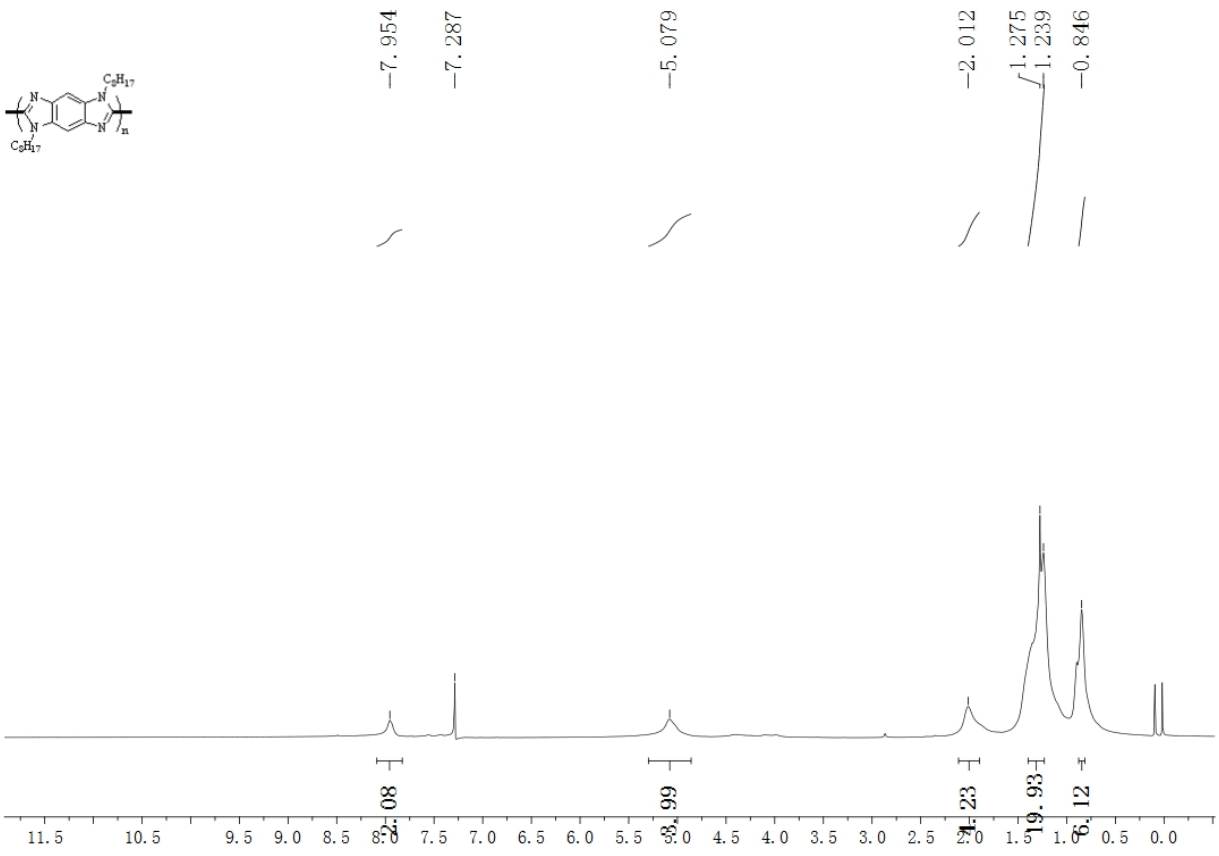
140.806
134.830
110.360
89.271
77.477
77.160
76.842
45.589
31.949
29.344
27.089
22.766
14.204
31.949
29.839
29.772
29.344
27.089
22.766
f1 (ppm)
f1 (ppm)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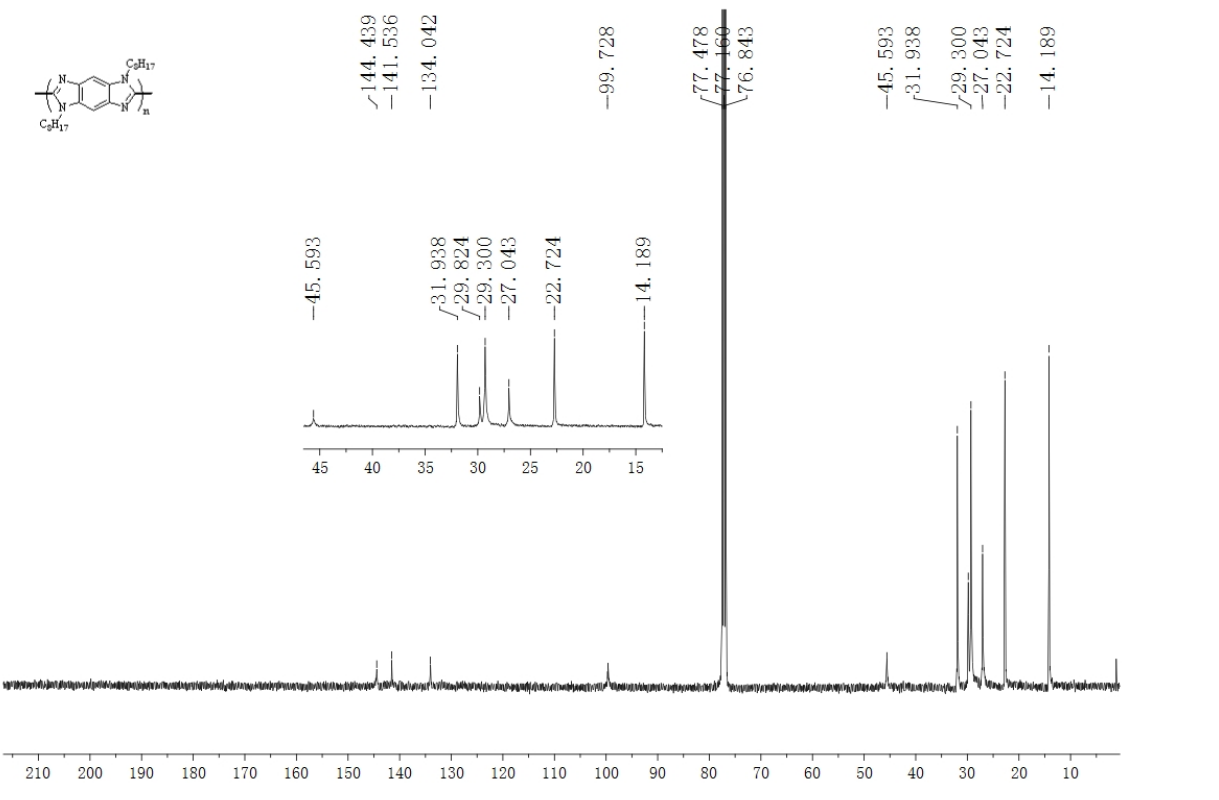
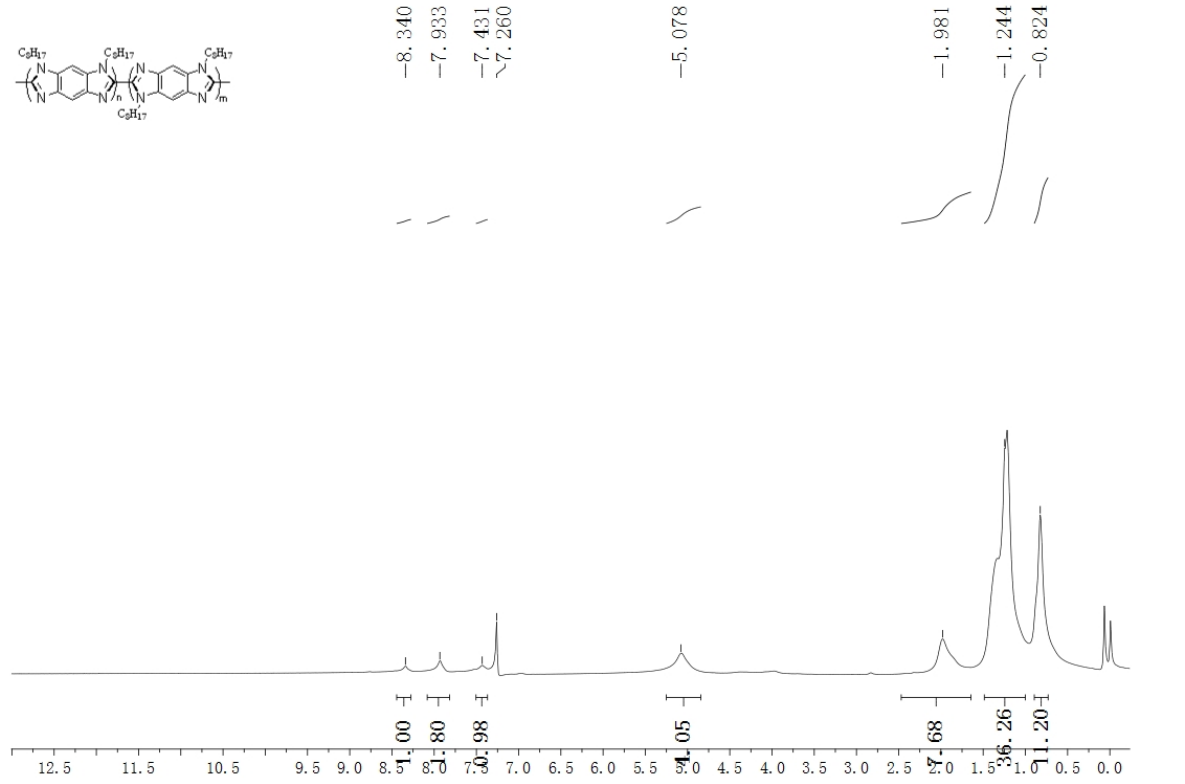
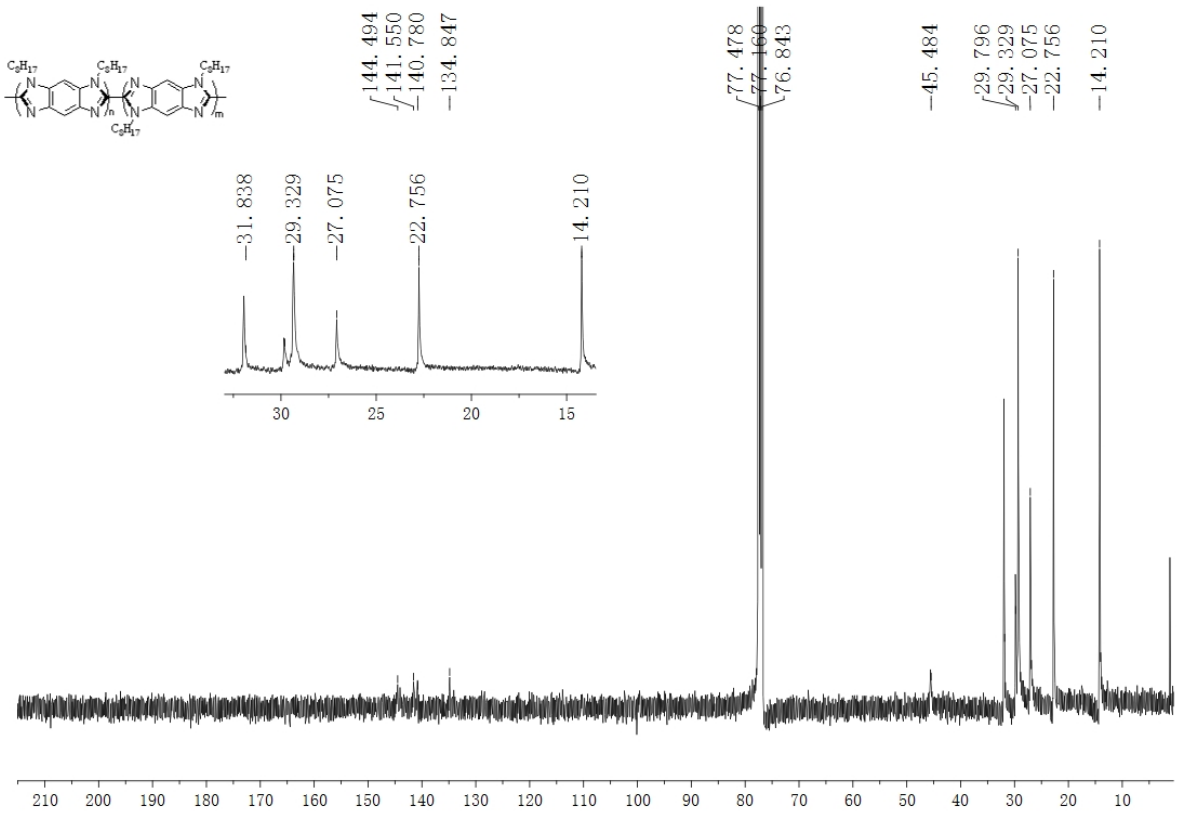
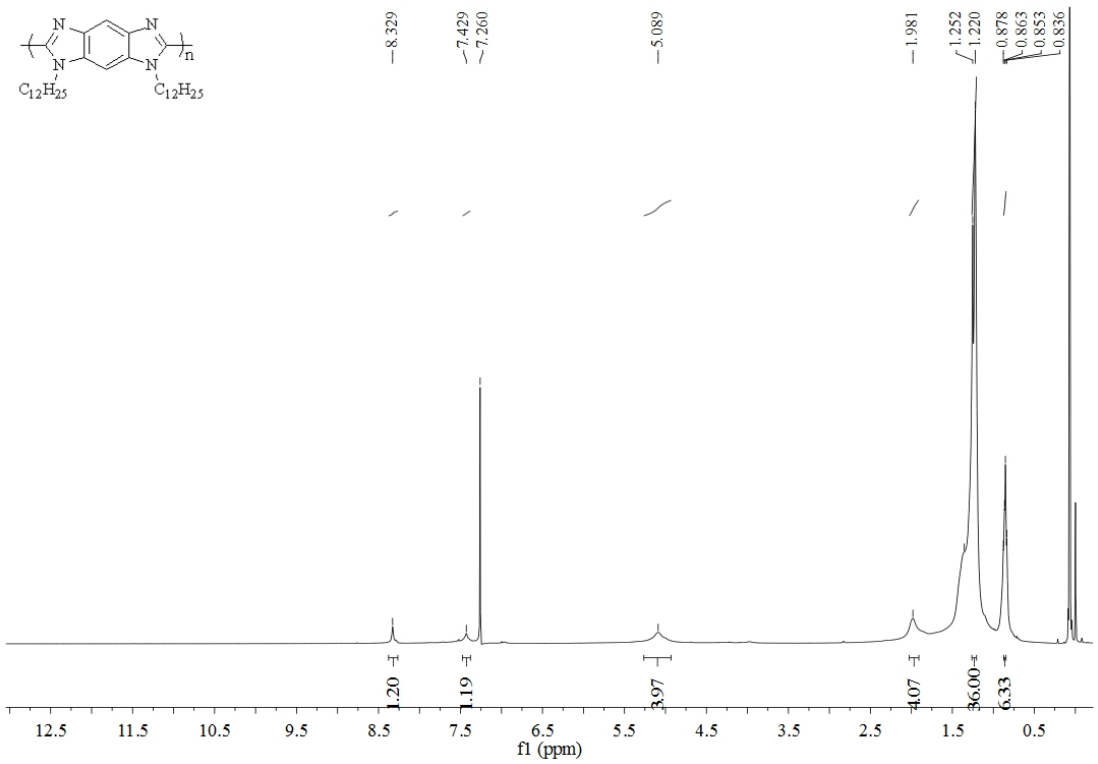
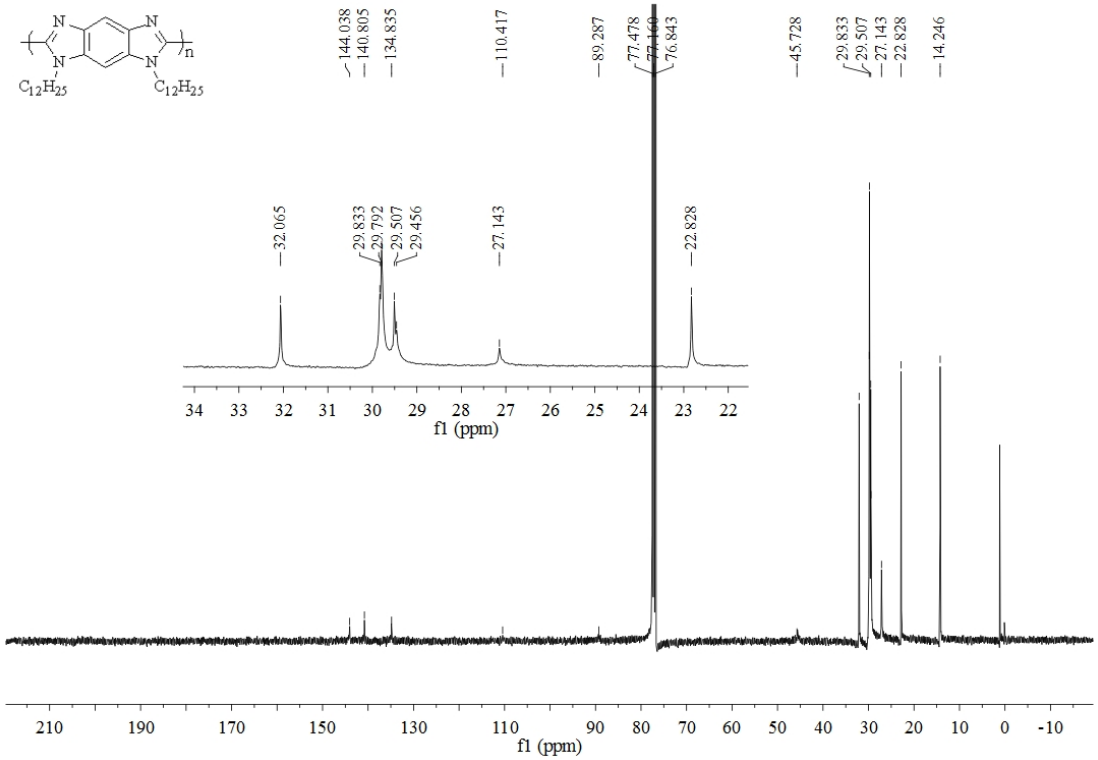
7.287
5.079
2.012
1.275
1.239
0.846
2.08
3.99
4.23
19.93
6.12

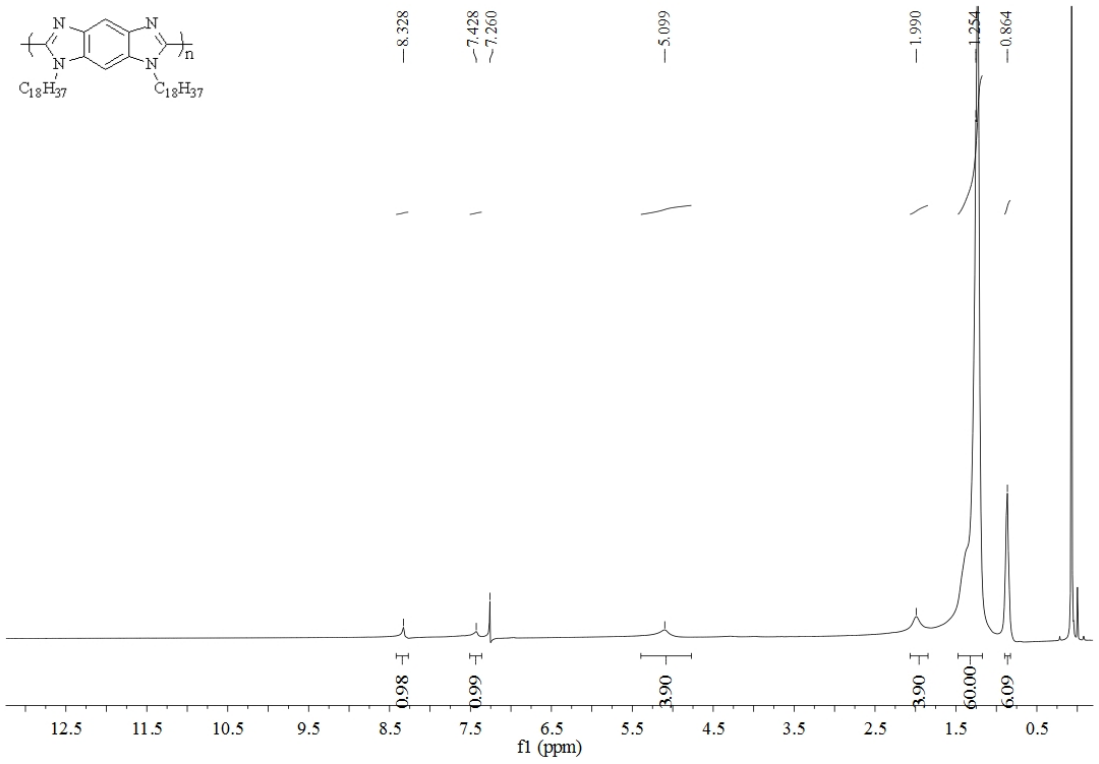

144.439
141.536
134.042
99.728
77.478
77.160
76.843
45.593
31.938
29.300
27.043
22.724
14.189


8.340
7.933
7.431
7.260
5.078
1.981
1.244
0.824
1.00
1.80
0.98
4.05
7.68
36.26
11.20


144.494
141.550
140.780
134.847
77.478
77.160
76.843
45.484
29.796
29.329
27.075
22.756
14.210
31.838
29.329
27.075
22.756
14.210


8.329
7.429
7.260
5.089
1.981
1.252
1.220
0.878
0.863
0.853
0.836
1.20
1.19
3.97
4.07
36.00
6.33
f1 (ppm)


144.038
140.805
134.835
110.417
89.287
77.478
77.160
76.843
45.728
29.833
29.507
27.143
22.828
14.246
32.065
29.833
29.792
29.507
29.456
27.143
22.828
f1 (ppm)


8.328
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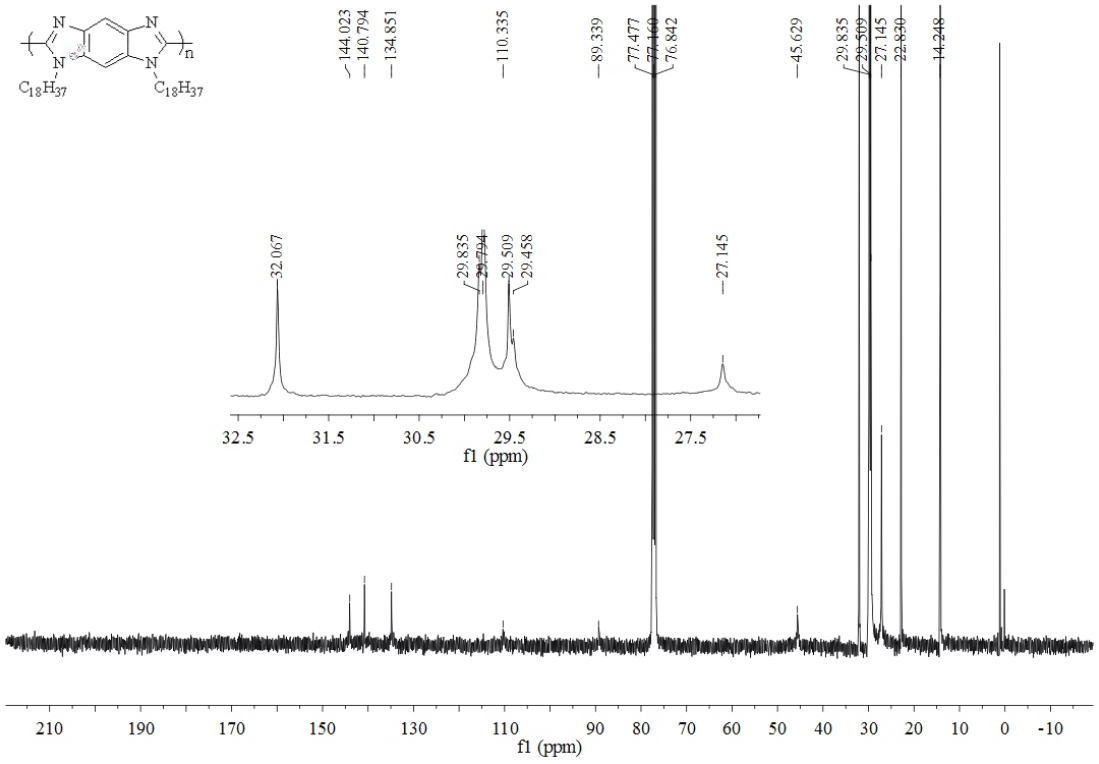
7.260
5.099
1.990
1.254
0.864
0.98
0.99
3.90
3.90
60.00
6.09
f1 (ppm)


144.023
140.794
134.851
110.335
89.339
77.477
77.160
76.842
45.629
29.835
29.509
27.145
22.830
14.248
32.067
29.835
29.794
29.509
29.458
27.145
f1 (ppm)
f1 (ppm)