Electronic Supplementary Information(ESI)

Side chain effect on solid-state emission behaviours and mechanofluorochromic activities of 10*H*-phenothiazinylbenzo[*d*]imidazoles

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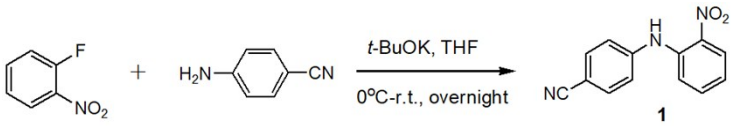
Materials and instruments

All the reagents were analytically pure and some chemicals were further purified by recrystallization or distillation. Melting points were determined by an OptiMelt automatic melting point system. The ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were obtained on a Bruker Avance II DMX 400 spectrometer with DMSO-d_6 or $CDCl_3$ as the solvent. The absorption spectra were measured on a Shimadzu UV 3600 UV-Vis-NIR spectrometer, and the fluorescence spectra were acquired on a Perkin-Elmer LS55 spectrophotometer. The quantum yields were measured with quinine sulfate in 0.1 M sulfuric acid solution (Φ_f=0.55) as the reference. The crystallographic data were determined on a Bruker Gemini Ultra diffractometer with a CCD counter. The powder X-ray diffraction patterns were recorded on DX2700 with Cu-K_α radiation operating at 40 kV and 40 mA by a 0.3°/min scanning rate. Differential scanning calorimetry curves were obtained on a Waters TA Q20 instrument. ML spectrum are recorded on an optical fiber spectrometer with the fiber in 1000 μm diameter and 200-1100 nm acceptable wavelength range.

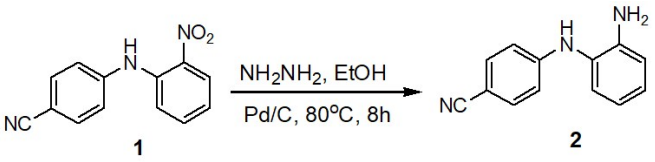
Synthesis of the intermediates and the titled BIMP compounds



1

At 0°C, 4-cyanoaniline (12 mmol, 1.42 g) in anhydrous THF (15 mL) was slowly dropped into the mixture of 2-fluoronitrobenzene (10 mmol, 1.41 g) and *t*-BuOK (12 mmol, 1.34 g) in anhydrous THF (15 mL). The resulted mixture was stirred at 0°C for another 1h and then at room temperature overnight. Water (100 mL) was added and the solution was extracted with ethyl acetate (2×15 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then filtrated. The solvent was removed from the filtrate under reduced pressure and the residue was purified by silica gel column chromatography using petroleum ether/CH_2Cl_2 mixture as the eluent, producing **1** as orange solid.

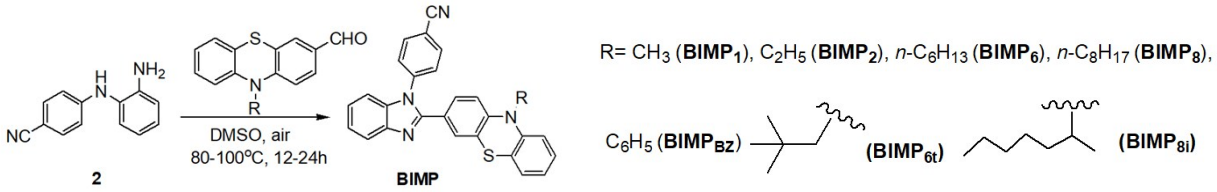
4-(2-nitrophenylamino)benzonitrile (**1**): 77% yield; m.p. 182.3-183.9 °C; ^{1}H NMR(400 MHz, $CDCl_3$) δ(ppm): 6.99(dt, J_1=2.0 Hz, J_2=6.8 Hz, 1H), 7.33(d, J=8.8 Hz, 2H), 7.46-7.54(m, 2H), 7.66(d, J=8.8 Hz, 2H), 8.22(dd, J_1=1.2 Hz, J_2=8.8 Hz, 1H), 9.43(s, 1H); ^{13}C NMR(100 MHz, $CDCl_3$) δ(ppm): 106.86, 117.35, 118.78, 120.23, 121.21, 126.91, 133.86, 135.63, 135.69, 139.50, 143.78.



1 2

At room temperature, hydrazine hydrate (80%wt, 20 mmol) was added into the suspension of **1** (5 mmol) and palladium absorbed on carbon powder (10%wt, 0.25 mmol) in EtOH (15 mL). The resulted mixture was heated at 80°C for 8 h and then cooled to room temperature. After filtration, the filtrate was diluted with water (100 mL) and extracted with EtOAc (2×15 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and the filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography using petroleum ether/EtOAc mixture as the eluent, producing **2** as greyish white solid.

4-(2-aminophenylamino)benzonitrile (**2**): 88% yield; m.p.159.4-161.2°C; ^{1}H NMR(400 MHz, $CDCl_3$) δ(ppm): 3.83(s, br, 2H), 5.72(s, 1H), 6.72(dt, J_1=8.8 Hz, J_2=2.0 Hz, 2H), 6.83(td, J_1=7.6 Hz, J_2=1.2 Hz, 1H), 6.87(d, J=7.6 Hz, 1H), 7.15(d, J=7.6 Hz, 2H), 7.47(dt, J_1=8.8 Hz, J_2=2.0 Hz, 2H); ^{13}C NMR(100 MHz, $CDCl_3$) δ(ppm): 100.61, 113.99, 116.41, 119.19, 120.14, 125.19, 127.03, 127.77, 133.77, 143.00, 149.59.



At room temperature, 10-alkyl-10*H*-phenothiazine-3-carbaldehyde (12 mmol) was added into the solution of **2** (10 mmol) in DMSO (20 mL) and the resulted solution was stirred at 80-100°C in an open vessel for 12-24 h. After cooled to room temperature, the solution was diluted with water (100 mL) and extracted with CH_2Cl_2 (2×15 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and the filtrate was concentrated under reduced pressure. The residue was purified by silica gel column chromatography using petroleum ether/CH_2Cl_2 mixture as the eluent, producing **BIMP** as pale to dark yellow solid or oil. All the products were recrystallized in EtOH/ CH_2Cl_2 mixture to offer the corresponding solids used for all types of measurements.

4-(2-(10-methyl-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile **(BIMP$_1$)**: 87% yield; m.p. 227.9-229.3°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 3.33(s, 3H), 6.64(d, J=8.4 Hz, 1H), 6.79(dd, J_1=1.2 Hz, J_2=8.4 Hz, 1H), 6.94(dt, J_1=1.2 Hz, J_2=7.6 Hz, 1H), 7.07(dd, J_1=1.5 Hz, J_2=8.4 Hz, 1H), 7.10(dd, J_1=1.2 Hz, J_2=7.6 Hz, 1H), 7.16(dt, J_1=1.2 Hz, J_2=7.6 Hz, 1H), 7.20-7.29(m, 2H), 7.35(dt, J_1=1.2 Hz, J_2=6.8 Hz, 1H), 7.41-7.44(m, 3H), 7.80(dt, J_1=1.5 Hz, J_2=8.4 Hz, 2H), 7.86(dt, J_1=1.2 Hz, J_2=7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 35.45, 109.80, 112.29, 113.88, 114.40, 117.89, 120.05, 122.66, 123.09, 123.14, 123.64, 123.76,124.05, 127.27, 127.70, 127.93, 128.06, 128.66, 133.87, 136.27, 141.03, 143.17, 144.79, 147.18, 151.46.

4-(2-(10-ethyl-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile **(BIMP$_2$)**: 81% yield; m.p. 198.7-200.7°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 1.31(t, J=6.8 Hz, 3H), 3.92(q, J=6.8Hz, 2H), 7.00(d, J=8.4 Hz, 2H), 7.06(d, J=7.2 Hz, 1H), 7.16-7.19(m, 2H), 7.22-7.39(m, 5H), 7.73(d, J=8.4 Hz, 2H), 7.81(d, J=7.6 Hz, 1H), 8.13(d, J=8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 12.97, 41.73, 110.68, 111.83, 115.32, 116.21, 118.67, 119.78, 122.47, 123.20, 123.39, 123.55, 123.64, 123.92, 127.58, 127.91, 128.34, 129.11, 134.70, 136.92, 141.07, 143.17, 143.77, 146.00, 151.40.

4-(2-(10-hexyl-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile **(BIMP$_6$)**: 77% yield; m.p. 146.6-148.2 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 0.91(t, *J*=6.8 Hz, 3H), 1.33-1.45(m, 6H), 1.81(hep, *J*=7.2 Hz, 2H), 3.84(t, *J*=7.2 Hz, 2H), 6.74(d, *J*=8.4 Hz, 1H), 6.88(d, *J*=8.0 Hz, 1H), 6.97(t, *J*=7.2 Hz, 1H), 7.11-7.14(m, 2H), 7.19(t, *J*=8.0 Hz, 1H), 7.25-7.33(m, 2H), 7.39(t, *J*=8.0 Hz, 1H), 7.44(d, *J*=2.0 Hz, 1H), 7.48(d, *J*=8.0 Hz, 2H), 7.85(d, *J*=8.0 Hz, 2H), 7.90(d, *J*=8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm): 14.01, 22.59, 26.55, 26.70, 31.42, 47.64, 109.78, 112.27, 114.72, 115.61, 117.92, 120.06, 122.94, 122.98, 123.62, 123.72, 123.98, 125.25, 127.45, 127.52, 128.06, 128.17. 128.42, 133.88, 136.29, 141.06, 143.21, 144.19, 146.76, 151.50.

4-(2-(10-(3,3-dimethylbutyl)-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile (**BIMP$_{6t}$**): 64% yield, m.p. 102.5-104.2 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 6.98(s, 9H), 1.60(dt, J_1=7.6 Hz, J_2=1.2 Hz, 2H), 3.89(dt, J_1=7.6 Hz, J_2=1.2 Hz, 2H), 6.96-7.01(m, 2H), 7.05(d, *J*=8.0 Hz, 1H), 7.15-7.38(m, 7H), 7.70(d, *J*=8.4 Hz, 2H), 7.80(d, *J*=7.6 Hz, 1H), 8.09(d, *J*=8.4 Hz, 2H), 8.35(s, 1H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm): 29.60, 30.33, 43.63, 79.64, 110.66, 111.83, 115.70, 116.56, 118.61, 119.80, 123.42, 123.45, 123.59, 123.75, 123.90, 124.16, 127.73, 128.09, 128.29, 129.07, 129.11, 134.64, 136.92, 141.05, 143.20, 144.31, 146.57, 151.44.

4-(2-(10-phenyl-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile (**BIMP$_{BZ}$**): 68% yield; m.p. 251.2-253.1 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 6.02(d, *J*=8.8 Hz, 1H), 6.13-6.16(m, 1H), 6.73(dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H), 6.83-6.87(m, 2H), 6.99-7.01(m, 1H), 7.22(d, *J*=8.0 Hz, 1H), 7.27-7.31(m, 1H), 7.35-7.40(m, 4H), 7.47(d, *J*=8.8 Hz, 2H), 7.54(t, *J*=8.0Hz, 1H), 7.65(t, *J*=8.0 Hz, 2H), 7.83(d, *J*=8.0 Hz, 2H), 7.88(d, *J*=8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm): 109.73, 112.30, 114.91, 116.10, 117.89, 119.16, 120.04, 120.43, 123.01, 123.05, 123.59, 123.69, 126.70, 127.07, 127.56, 127.87, 128.05, 128.76, 130.94, 131.05, 133.87, 136.34, 140.21, 141.07, 143.20, 143.32, 145.53, 151.29.

4-(2-(10-octyl-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile **(BIMP$_8$)**: 71% yield; m.p.143.7-145.1 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 0.91(t, *J*=7.2 Hz, 3H), 1.28(m, 8H), 1.45(hep, *J*=7.2 Hz, 2H), 1.81(hep, *J*=7.2 Hz, 2H), 3.83(t, *J*=7.2 Hz, 2H), 6.74(d, *J*=8.8 Hz, 1H), 6.87(d, *J*=8.0 Hz, 1H), 6.96(t, *J*=7.6 Hz, 1H),7.13(d, *J*=8.4 Hz, 2H), 7.19(t, *J*=8.4 Hz, 1H), 7.26(d, *J*=8.0 Hz, 1H), 7.33(m, 1H), 7.39(t, *J*=7.2 Hz, 1H), 7.43(d, *J*=2 Hz, 1H), 7.48(d, *J*=8.8 Hz, 2H), 7.84(d, *J*=8.4 Hz, 2H), 7.90(d, *J*=8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm): 14.12, 22.63, 26.73, 26.78, 26.88, 29.18, 29.20, 31.74, 47.64, 109.78, 112.28, 114.70, 115.61, 117.90, 120.04, 122.93, 122.97, 123.61, 123.71, 123.97, 125.22, 127.44, 127.51, 128.06, 128.14, 128.42, 133.57, 136.29, 141.06, 143.20, 144.17, 146.77, 151,50.

4-(2-(10-(2-methylheptyl)-10H-phenothiazin-3-yl)-1H-benzo[d]imidazol-1-yl)benzonitrile **(BIMP$_{8i}$)**: 78% yield; m.p.153.4-154.9^{o}C; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 0.75-0.80(m, 6H), 1.17-1.38(m, 8H), 1.75-1.78(m, 1H), 3.73-3.76(m, 2H), 6.93-6.97(m, 2H), 7.03(d, *J*=8.4 Hz, 1H), 7.11-7.33(m, 6H), 7.39(d, *J*=2 Hz, 1H), 7.65(d, *J*=8.4 Hz, 2H), 7.76(d, *J*=8.0 Hz, 1H), 8.03(d, *J*=8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm): 10.79, 14.24, 22.80, 23.74, 28.28, 30.21, 35.87, 50.72, 110.66, 111.82, 116.22, 117.12, 118.60, 119.81, 123.49, 123.53, 123.81, 123.90, 124.20, 124.95, 127.84, 128.21, 128.26, 128.99, 129.06, 134.60, 136.92, 141.06, 143.22, 144.80, 147.03, 151.52.

Table S1 Crystallographic data for **$BIMP_1$**, **$BIMP_2$** and **$BIMP_6$**

	$BIMP_1$ (CCDC 1919632)	**$BIMP_2$ (1919633)**	**$BIMP_6$ (CCDC1919634)**
	a = 7.9212(3) Å	*a* = 8.5519(7) Å	*a* = 8.6242(2) Å
	b = 9.5348(3) Å	*b* = 10.6954(8) Å	*b* = 13.3809(3) Å
	c = 14.0962(5) Å	*c* = 12.9906(11) Å	*c* = 11.9133(3) Å
	α =88.056(1) °	*α* = 87.540(7) °	*α* = 90 °
	β =89.137(1) °	*β* = 74.165(7) °	*β* = 108.743(1) °
	γ =84.091(1) °	*γ* = 76.420(7) °	*γ* = 90 °
Temperature	170 K	293 K	170 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Volume	1058.31(6)	1110.87(16)	1301.88(5)
Space group	P_{-1}	P_{-1}	P_{21}
Hall group	$-P_1$	$-P_1$	P_{2yb}
Density	1.351 g/cm^3	1.329 g/cm^3	1.277 g/cm^3
Z	2	2	2
Mu	0.176 / mm	0.170 / mm	0.153 / mm
F_{000}	448.0	464.0	528.0
h, k, l (max)	13, 16, 23	10, 12, 15	12, 19, 17
N_{ref}	10807	4069	7405
T_{min}, T_{max}	0.937, 0.981	0.920, 0.934	0.695, 0.746
Data completeness	0.987	0.998	1.79/0.93
θ (max)	37.076	25.348	30.521
$R_{reflections}$	0.0466 (8253)	0.0481 (2894)	0.0317 (6879)
$wR^2_{reflections}$	0.1342 (10671)	0.1262 (4059)	0.0821 (7405)
S	1.025	1.025	1.037
N_{par}	290	290	335
Flack parameter	----	----	0.033 (0.015)

Table S2 Crystallographic data for **$BIMP_{6t}$**, **$BIMP_8$** and **$BIMP_{BZ}$**

	$BIMP_{6t}$·$CHCl_3$ (CCDC1919636)	**$BIMP_8$ (CCDC1919635)**	**$BIMP_{BZ}$ (CCDC1919637)**
	a = 13.5139(3)Å	*a* = 11.5485(12) Å	*a* = 9.8655(4) Å
	b = 15.4850(4) Å	*b* = 8.0467(7) Å	*b* = 10.2689(4) Å
	c = 15.7111(3) Å	*c* = 31.393(4) Å	*c* = 12.5214(5) Å
	α = 90 °	*α* = 90 °	*α* = 87.488(1) °
	β = 110.006(1) °	*β* = 93.842(4) °	*β* = 70.801(1) °
	γ = 90 °	*γ* = 90 °	*γ* = 83.510(1) °
Temperature	170 K	273 K	170 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Volume	3089.35(12)	2910.8(5)	1190.26(8)
Space group	$P_{21/n}$	$P_{21/n}$	P_{-1}
Hall group	$-P_{2yn}$	$-P_{2yn}$	$-P_1$
Density	1.333 g/cm^3	1.206 g/cm^3	1.374 g/cm^3
Z	4	4	2
Mu	0.349 / mm	0.140 / mm	0.166 / mm
F_{000}	1288.0	1120.0	512.0
h, k, l (max)	16, 19, 19	16, 11, 44	12, 12, 15
N_{ref}	6274	8464	4837
T_{min}, T_{max}	0.689, 0.745	0.709, 0.746	0.689, 0.745
Data completeness	0.992	0.992	0.989
ϑ (max)	26.386	30.056	26.392
$R_{reflections}$	0.0441(5333)	0.1046(4654)	0.0344(4418)
$wR^2_{reflections}$	0.1151(6274)	0.3696(8464)	0.0916(4837)
S	1.038	1.278	1.044
N_{par}	401	382	334

Table S3 Crystallographic data for **$BIMP_{8i}$**

	$BIMP_{8i}$ (CCDC1919652)
	a = 7.7139(3)Å
	b = 11.3447(4) Å
	c = 16.7455(7) Å
	α = 100.235(1) ^{o}
	β = 91.830(1) ^{o}
	γ = 94.809(1) ^{o}
Temperature	170 K
Wavelength	0.71073 Å
Volume	1435.39(10)
Space group	P_{-1}
Hall group	$-P_1$
Density	1.223 g/cm^3
Z	2
Mu	0.142/ mm
F_{000}	560.0
h, k, l (max)	9, 14, 21
N_{ref}	6306
T_{min}, T_{max}	0.674, 0.746
Data completeness	0.992
θ *(max)*	27.148
$R_{reflections}$	0.0965(5374)
$wR^2_{reflections}$	0.2721(6306)
S	1.063
N_{par}	373

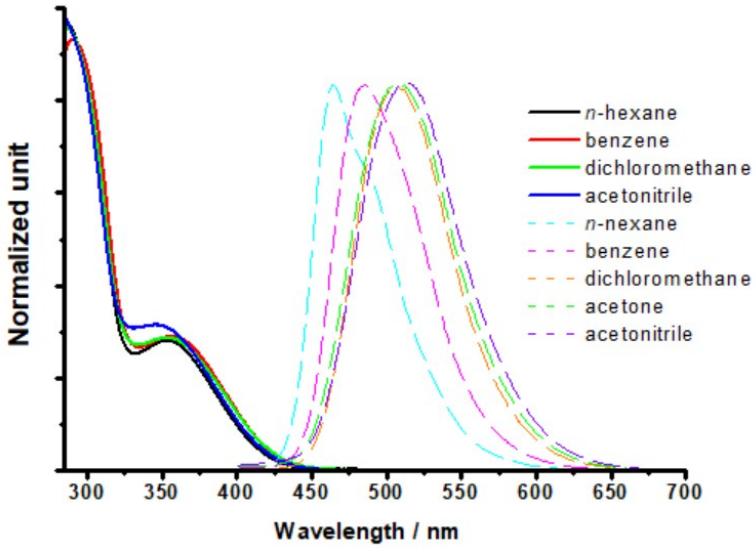


Fig. S1 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_1$** in different solvents

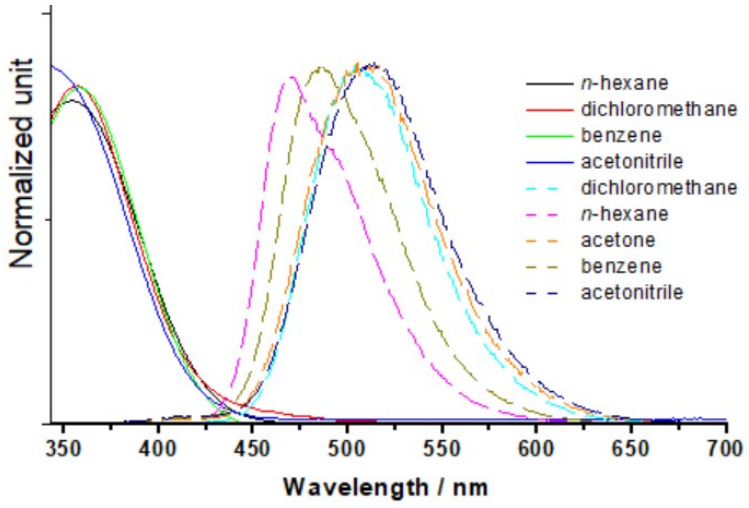


Fig. S2 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_6$** in different solvents

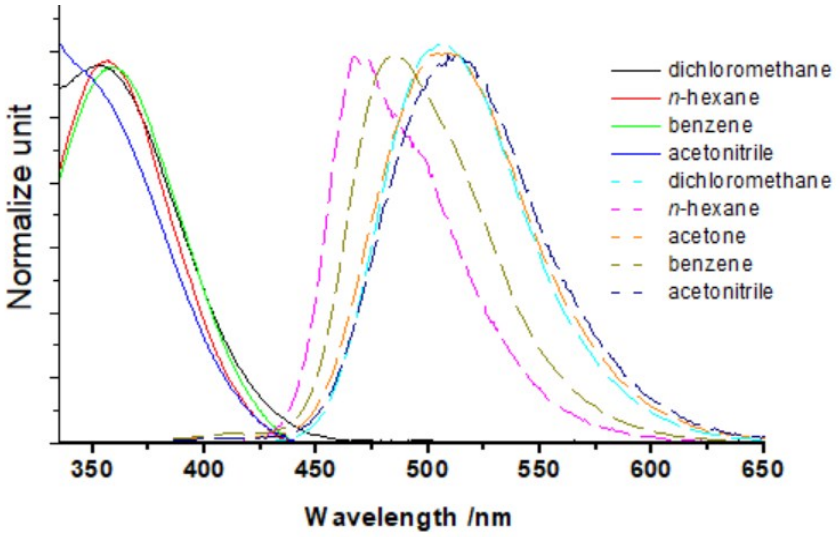


Fig. S3 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_{6t}$** in different solvents

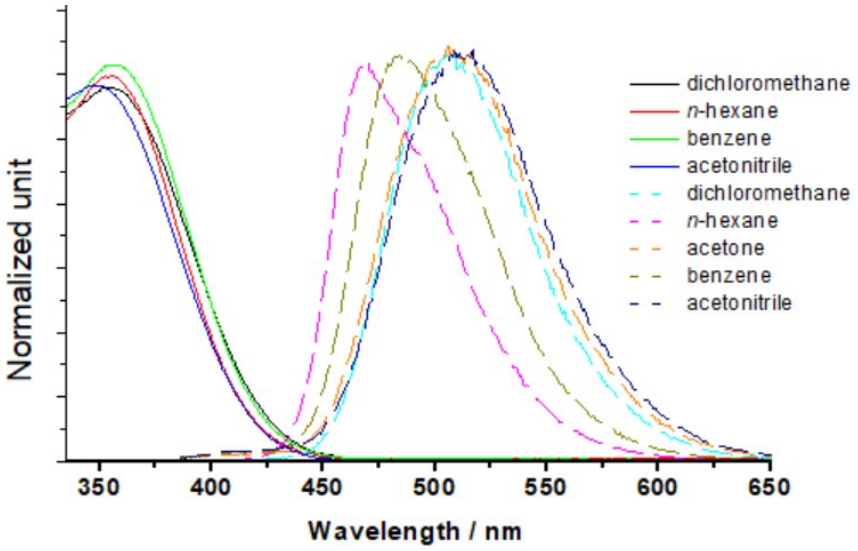


Fig. S4 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_{8}$** in different solvents

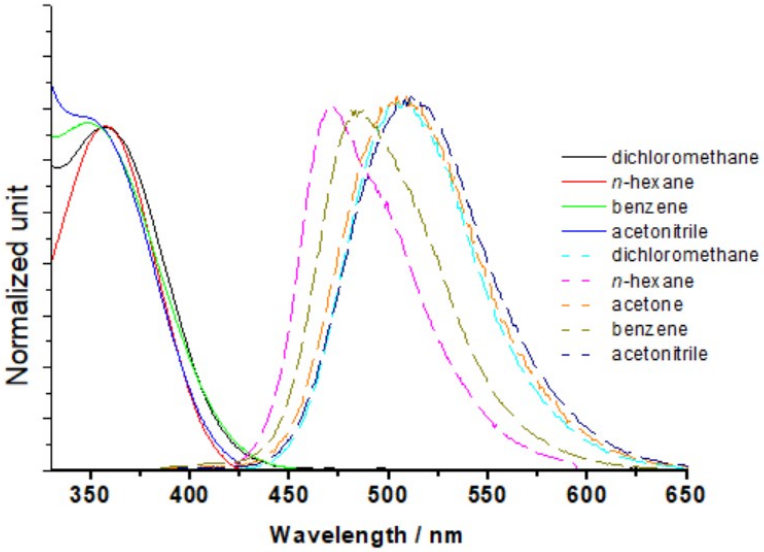


Fig. S5 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_{8i}$** in different solvents

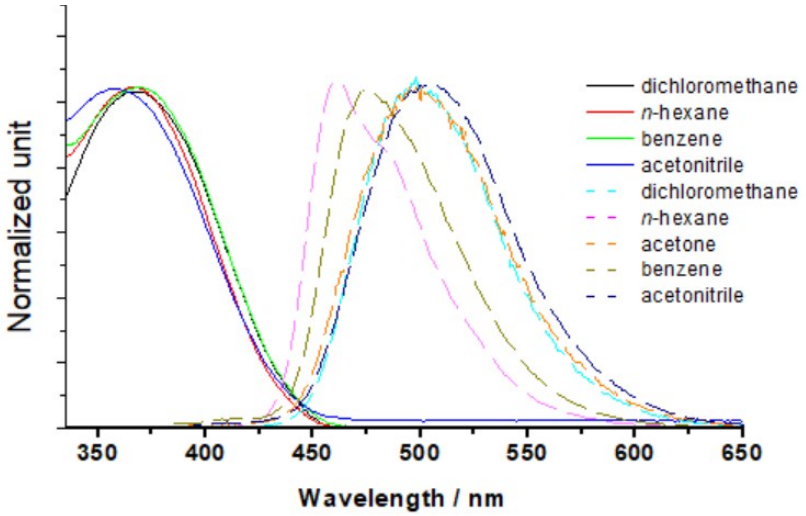


Fig. S6 Absorption (solid lines) and emission spectra (dash lines) of **BIMP$_{BZ}$** in different solvents

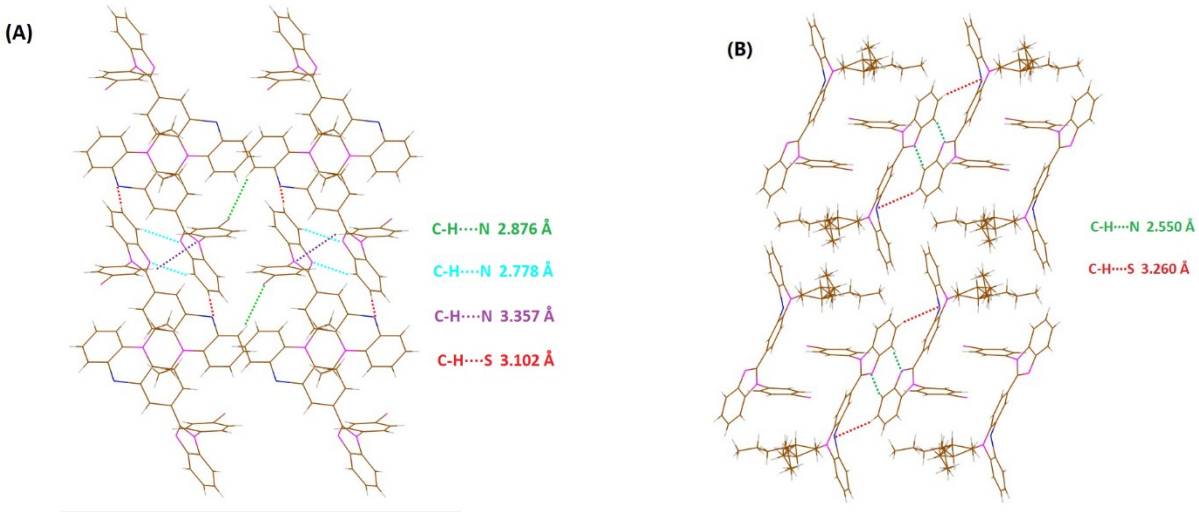


Fig. S7 Molecular packings of **BIMP$_2$** (A) and **BIMP$_{8i}$** (B)

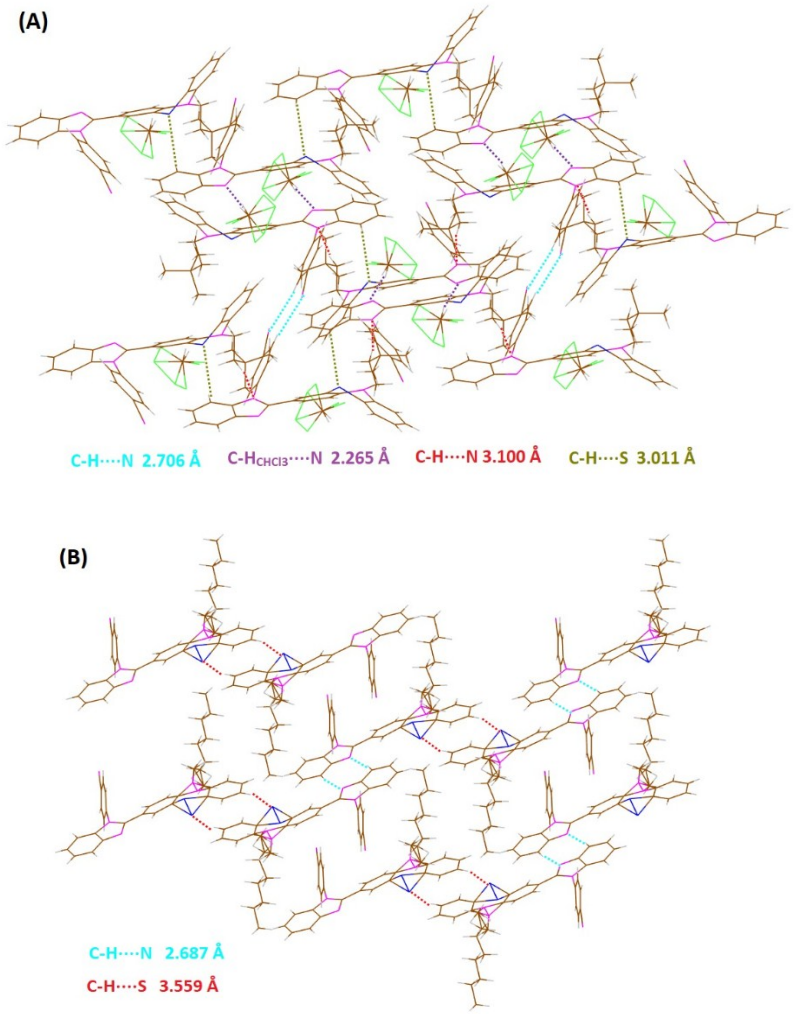


Fig. S8 Molecular packings of **BIMP$_{6t}$** (A) and **BIMP$_8$** (B)

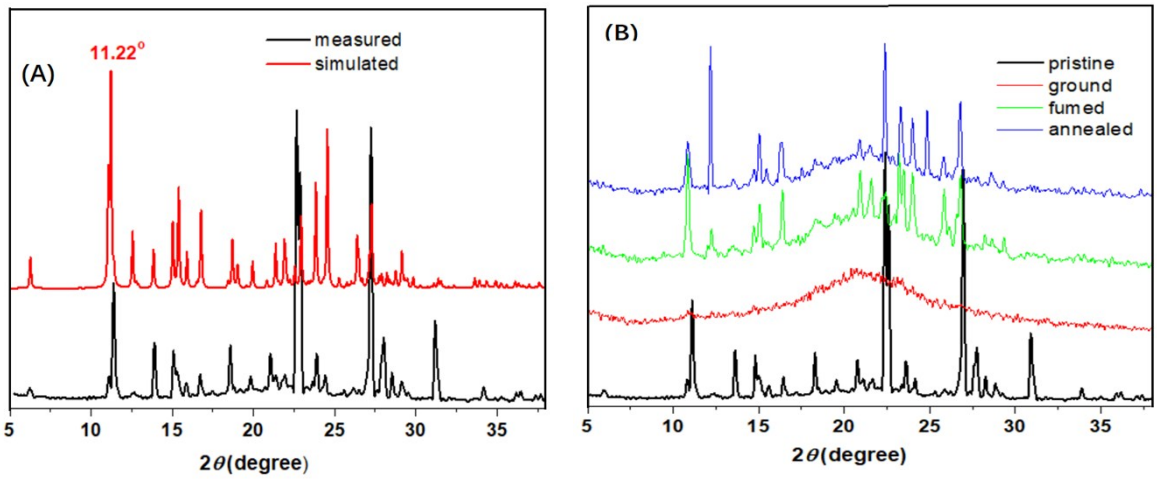


Fig. S9 PXRD patterns of **BIMP$_1$** under measured and simulated conditions (A) and other conditions (B)

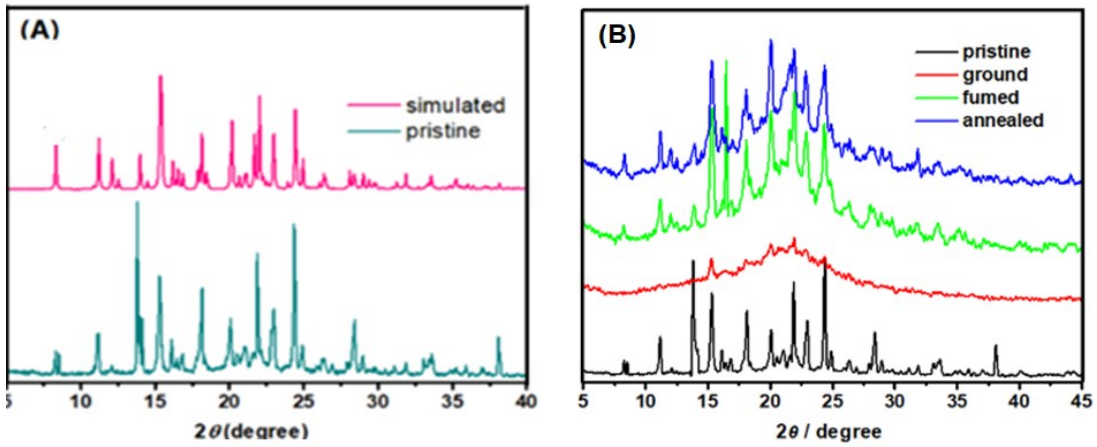


Fig. S10 PXRD patterns of **BIMP$_2$** under measured and simulated conditions (A) and other conditions (B)

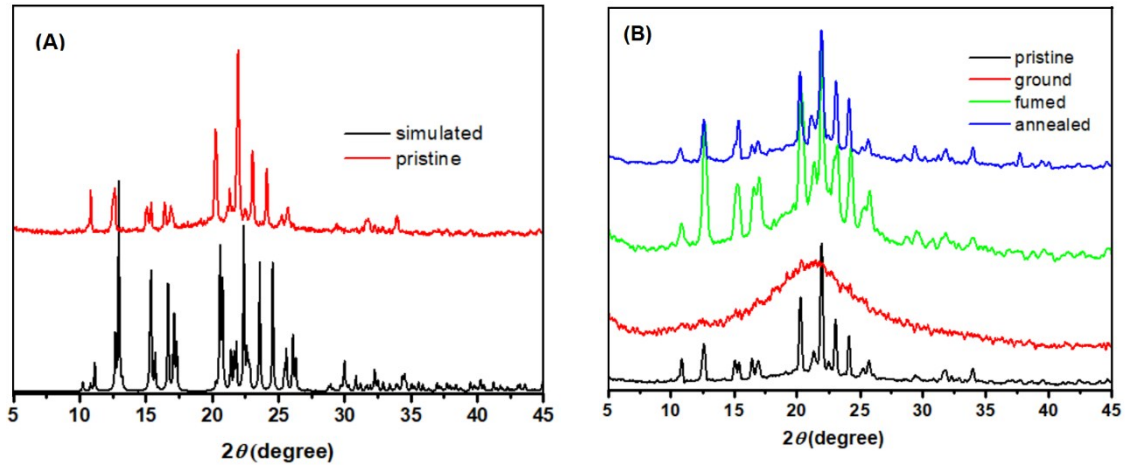


Fig. S11 PXRD patterns of **BIMP$_6$** under measured and simulated conditions (A) and other conditions (B)

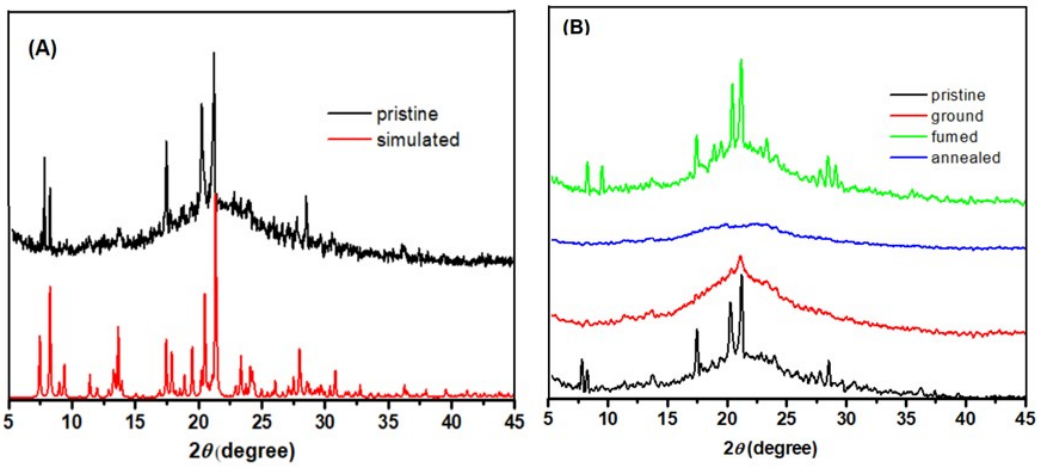


Fig. S12 PXRD patterns of **BIMP$_{6t}$** under measured and simulated conditions (A) and other conditions (B)

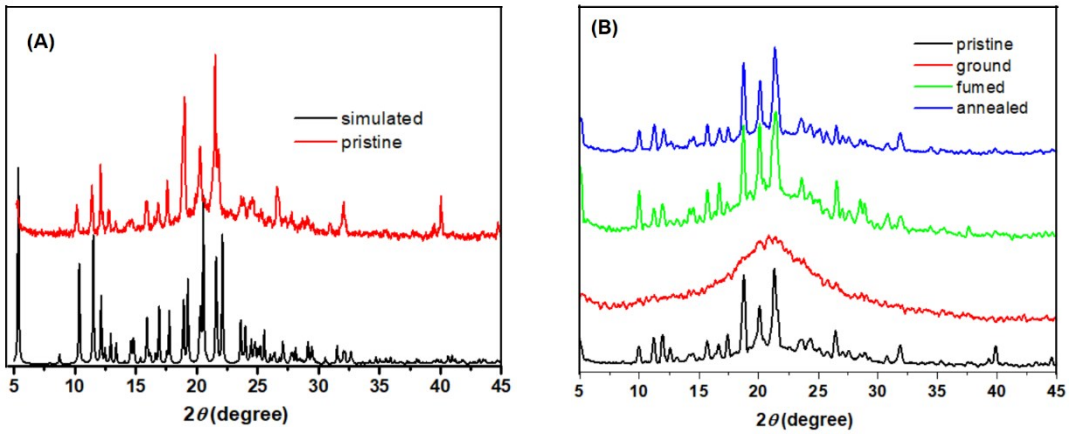


Fig. S13 PXRD patterns of **BIMP$_{8i}$** under measured and simulated conditions (A) and other conditions (B)

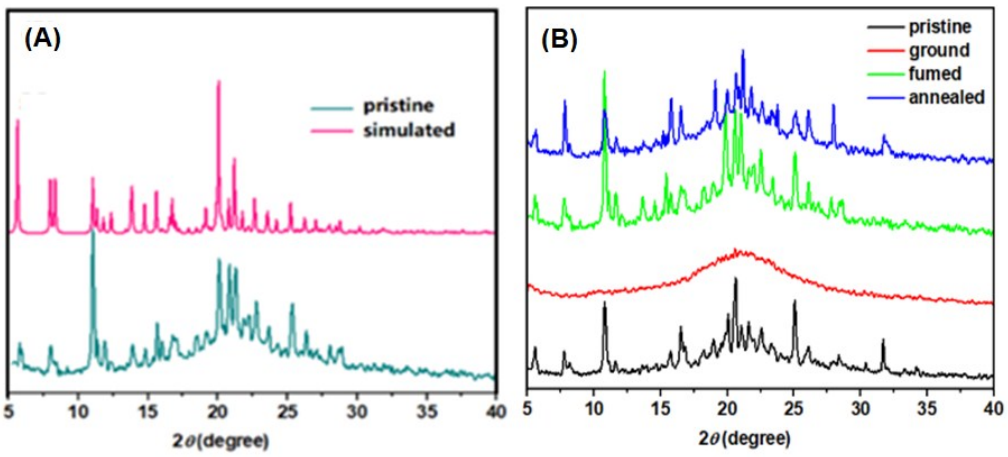


Fig. S14 PXRD patterns of **BIMP$_{8}$** under measured and simulated conditions (A) and other conditions (B)

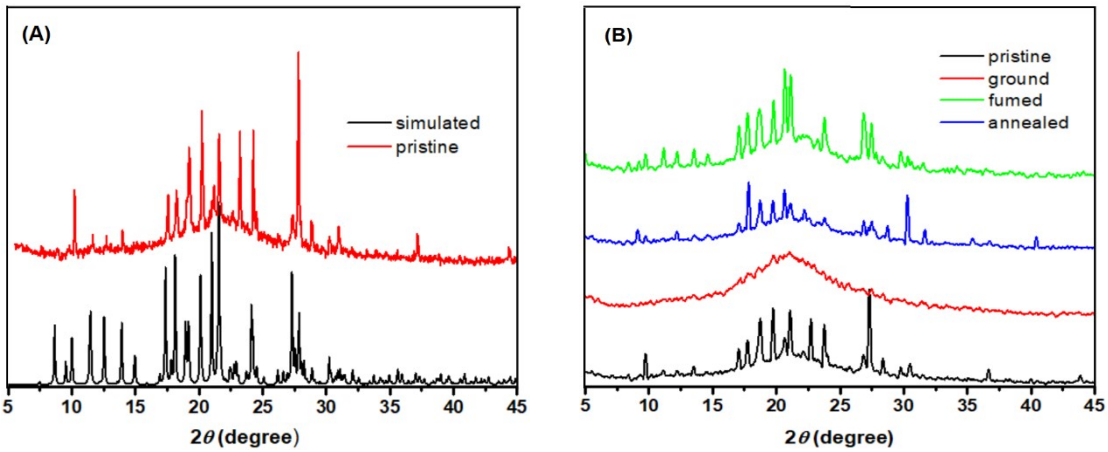


Fig. S15 PXRD patterns of **BIMP$_{BZ}$** under measured and simulated conditions (A) and other conditions (B)

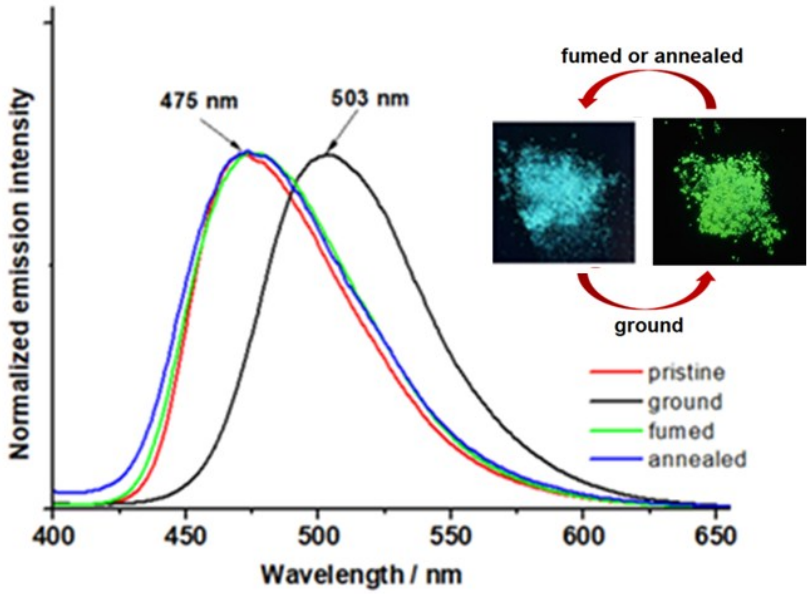


Fig. S16 Solid-state emission spectra of **BIMP$_1$** under different conditions (inserted: photos taken under 365 nm UV irradiation)

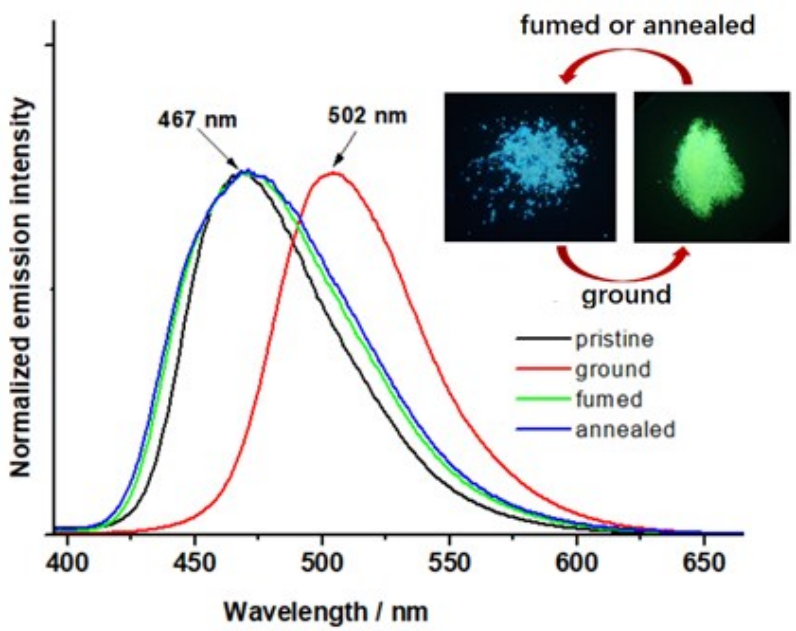


Fig. S17 Solid-state emission spectra of **$BIMP_6$** under different conditions (inserted: photos taken under 365 nm UV irradiation)

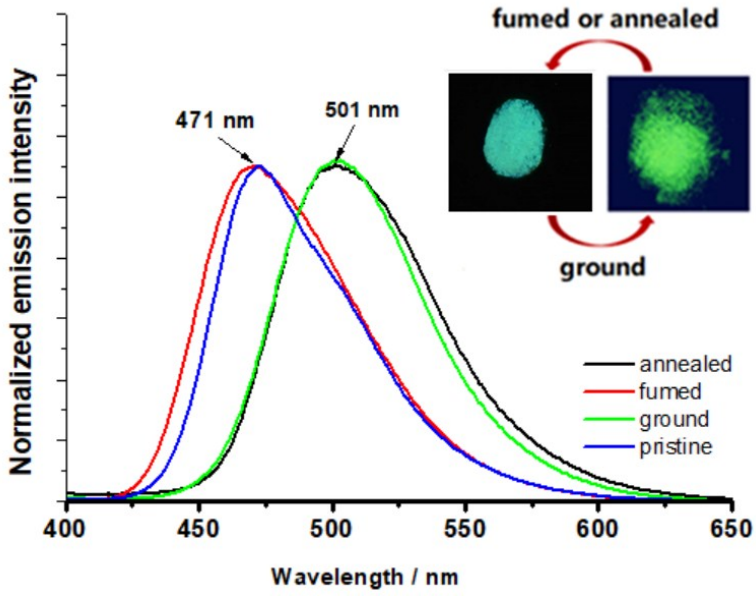


Fig. S18 Solid-state emission spectra of **$BIMP_{6t}$** under different conditions (inserted: photos taken under 365 nm UV irradiation)

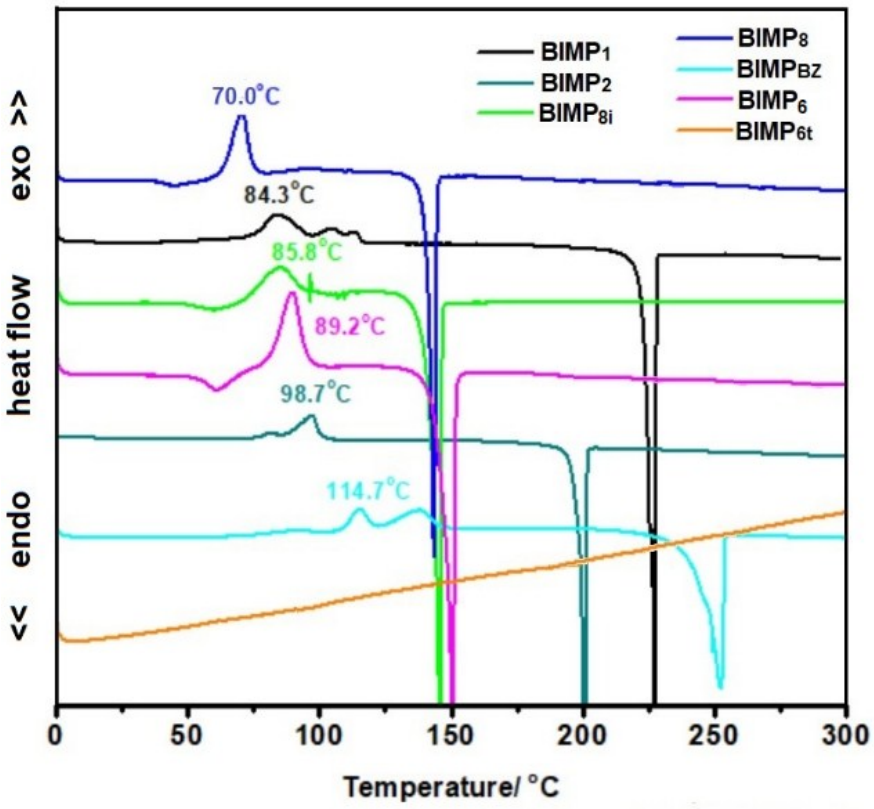
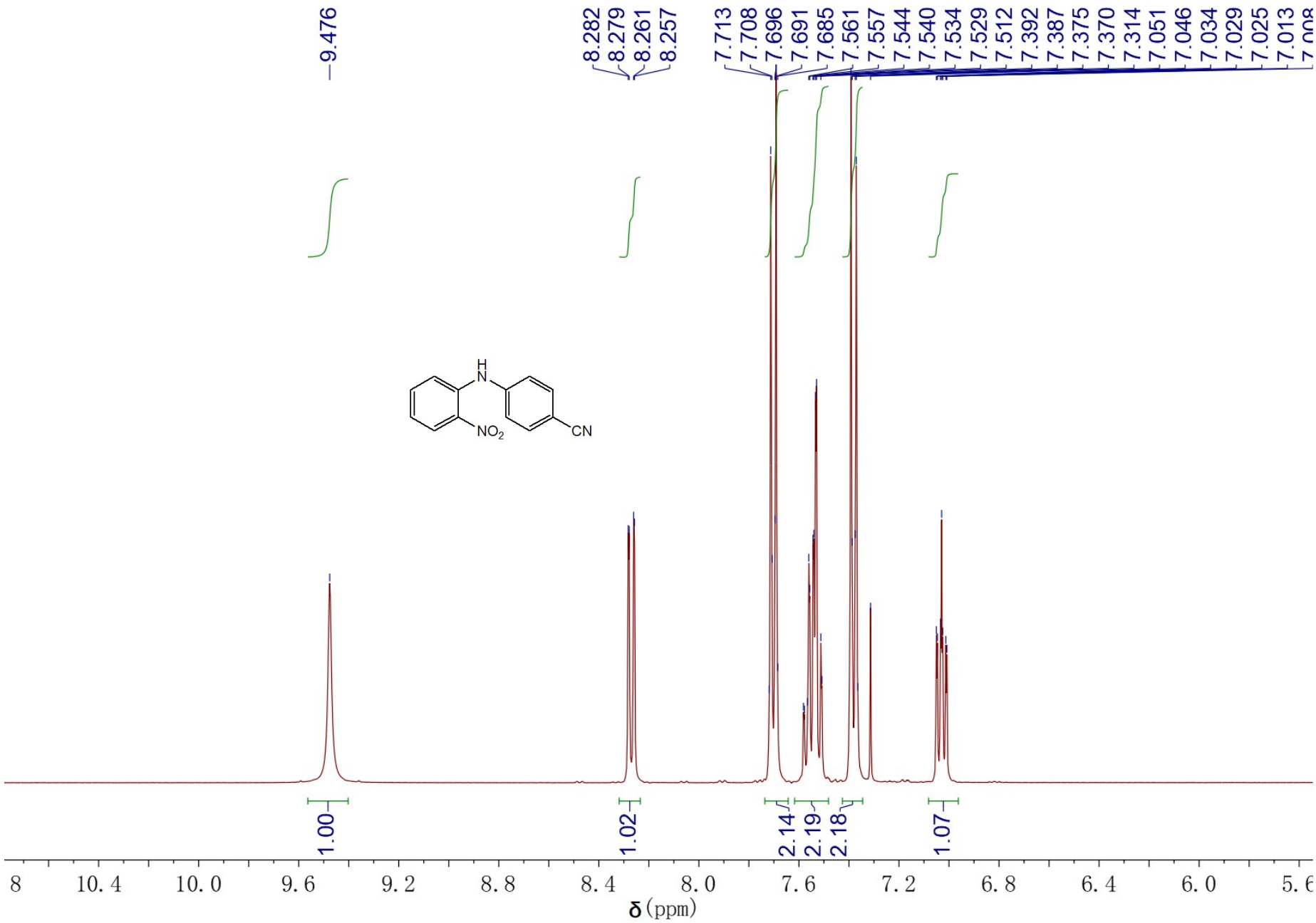


Fig. S19 DSC curves of the ground **BIMP** samples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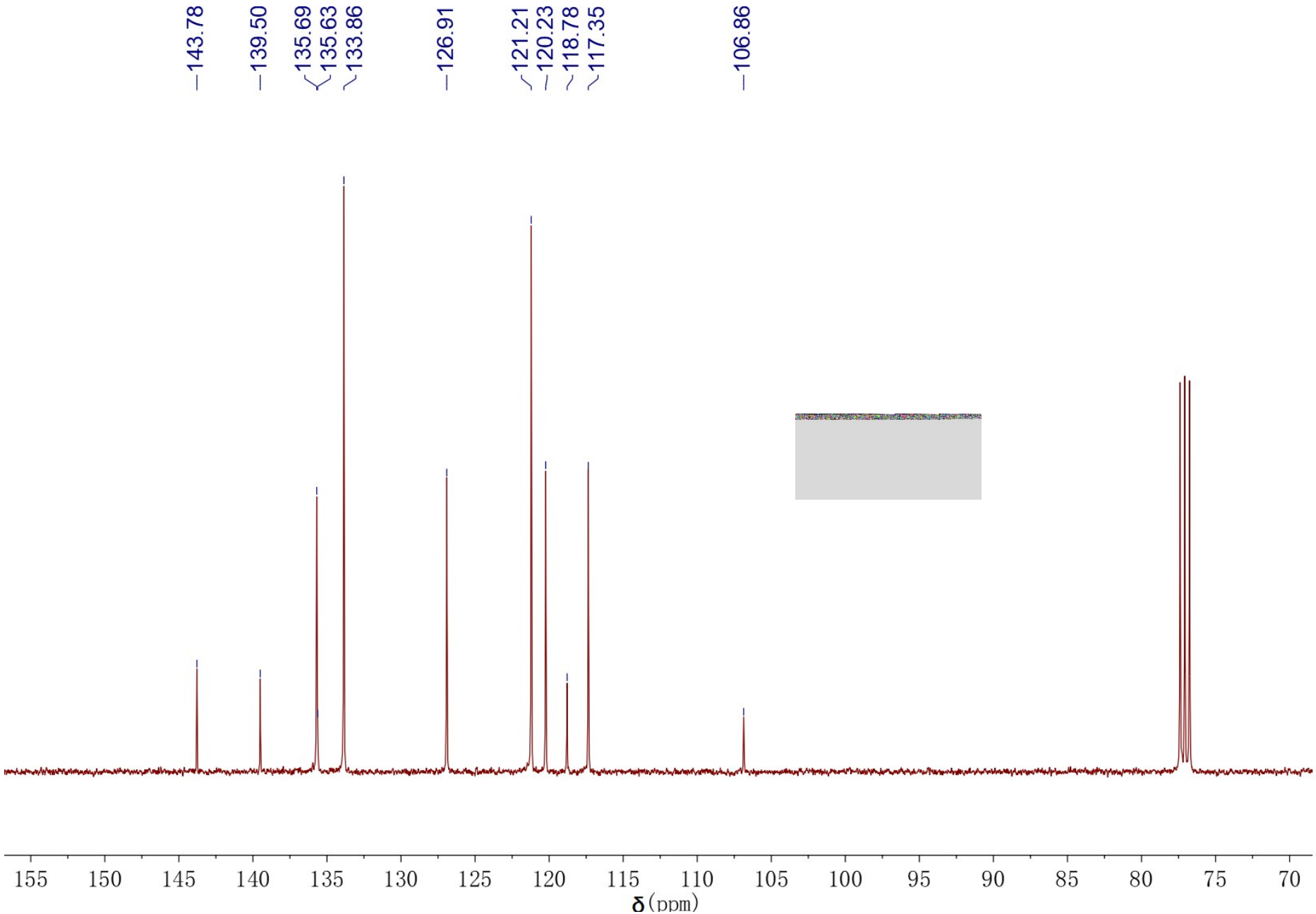
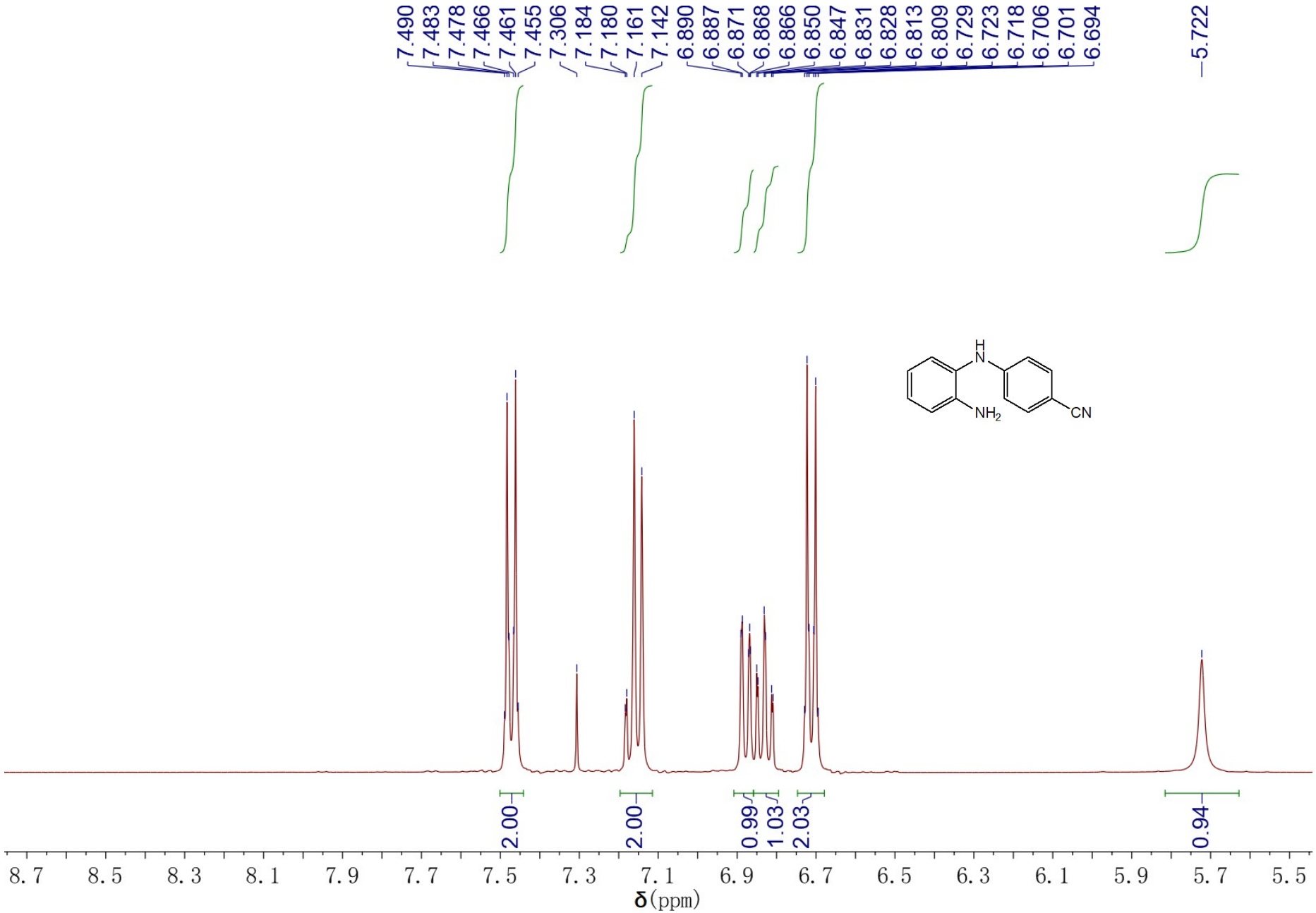
8.279
8.261
8.257
7.713
7.708
7.696
7.691
7.685
7.561
7.557
7.544
7.540
7.534
7.529
7.512
7.392
7.387
7.375
7.370
7.314
7.051
7.046
7.034
7.029
7.025
7.013
H
N
NO2
CN
1.00
1.02
2.14
2.19
2.18
1.07
8
10.4
10.0
9.6
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
δ(ppm)


143.78
139.50
135.69
135.63
133.86
126.91
121.21
120.23
118.78
117.35
106.86
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
δ(ppm)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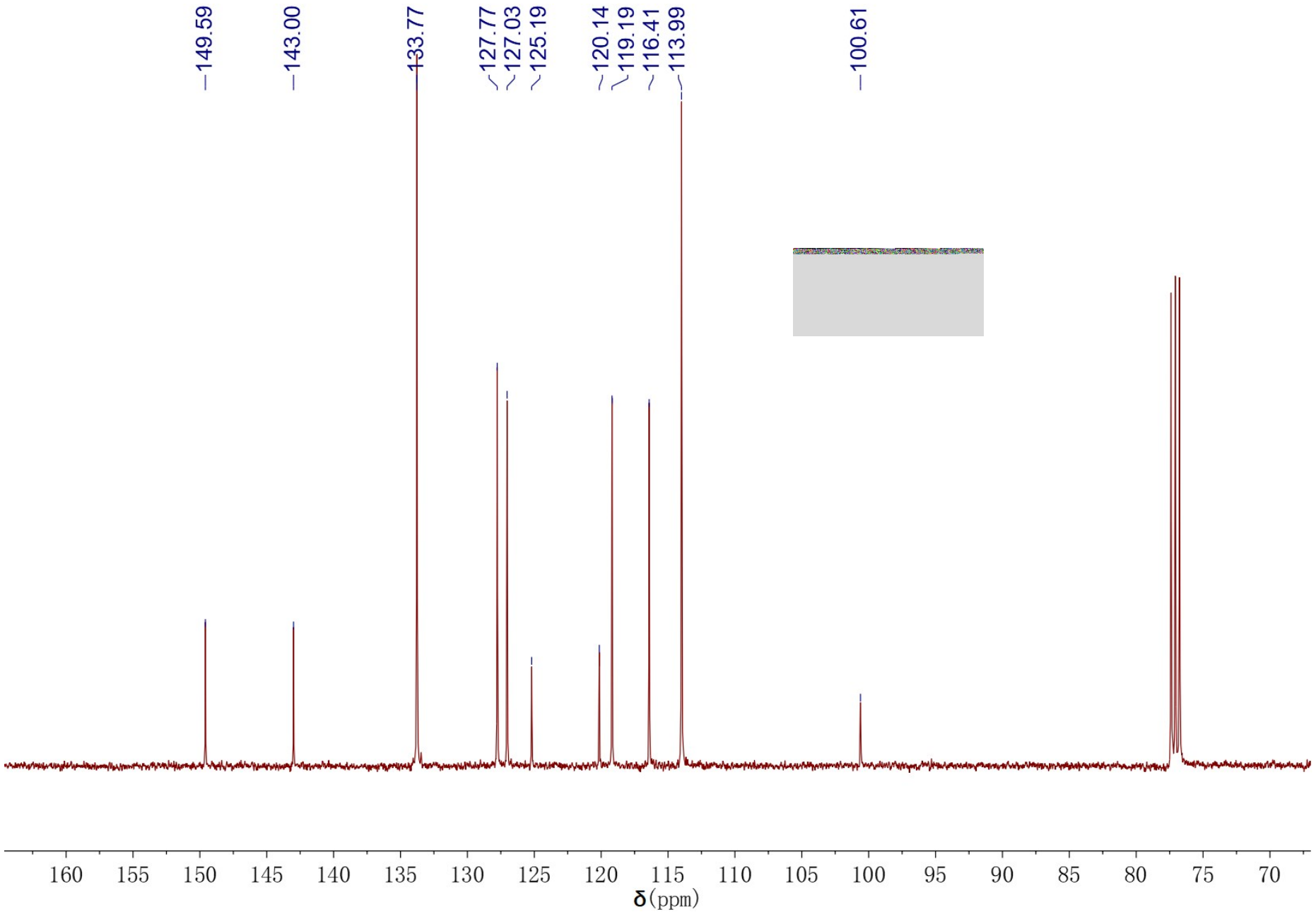
7.483
7.478
7.466
7.461
7.455
7.306
7.184
7.180
7.161
7.142
6.890
6.887
6.871
6.868
6.866
6.850
6.847
6.831
6.828
6.813
6.809
6.729
6.723
6.718
6.706
6.701
6.694
5.722
H
N
NH2
CN
2.00
2.00
0.99
1.03
2.03
0.94
8.7
8.5
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
6.5
6.3
6.1
5.9
5.7
5.5
δ(ppm)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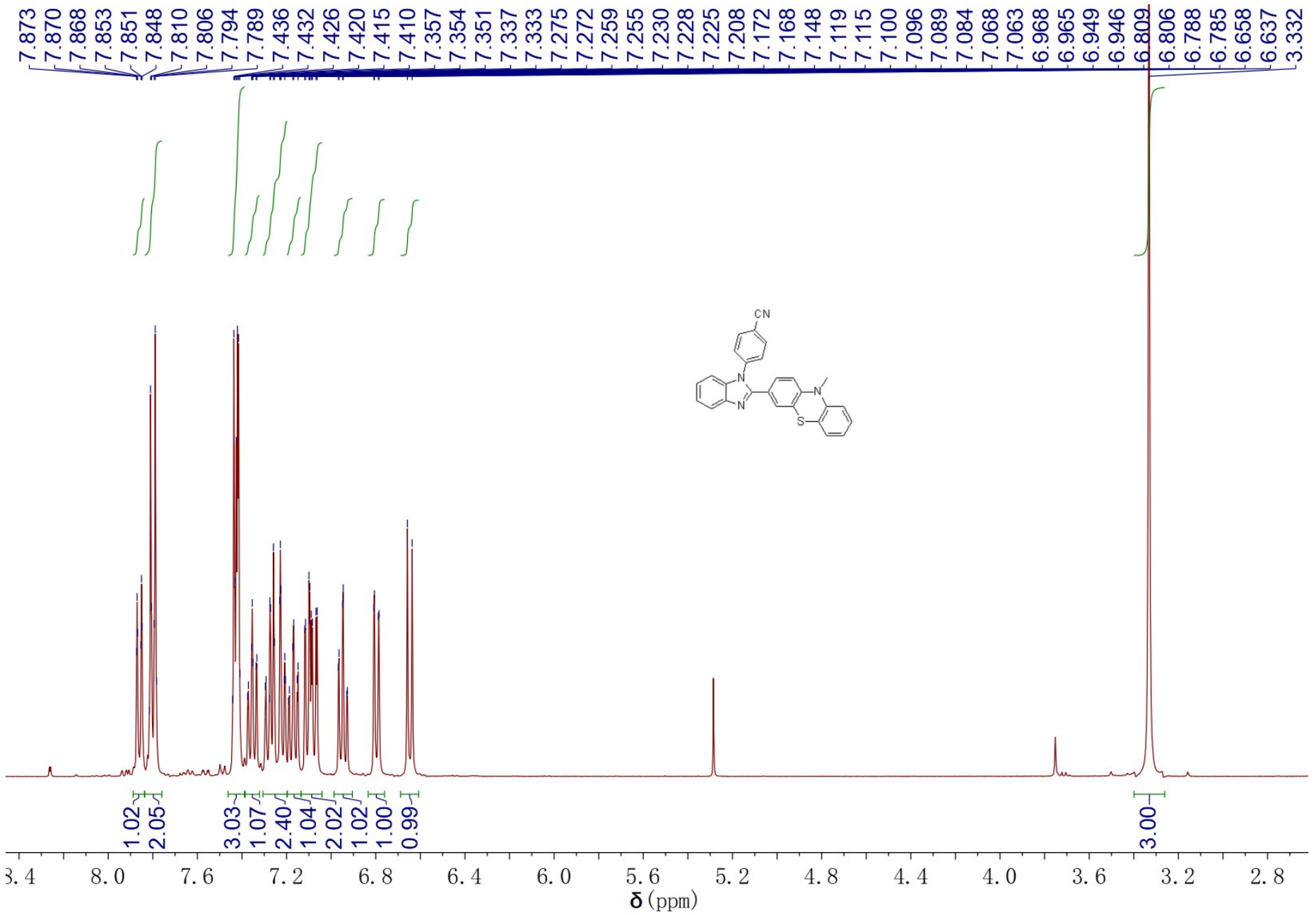
143.00
133.77
127.77
127.03
125.19
120.14
119.19
116.41
113.99
100.61
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
δ(ppm)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7.868
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7.851
7.848
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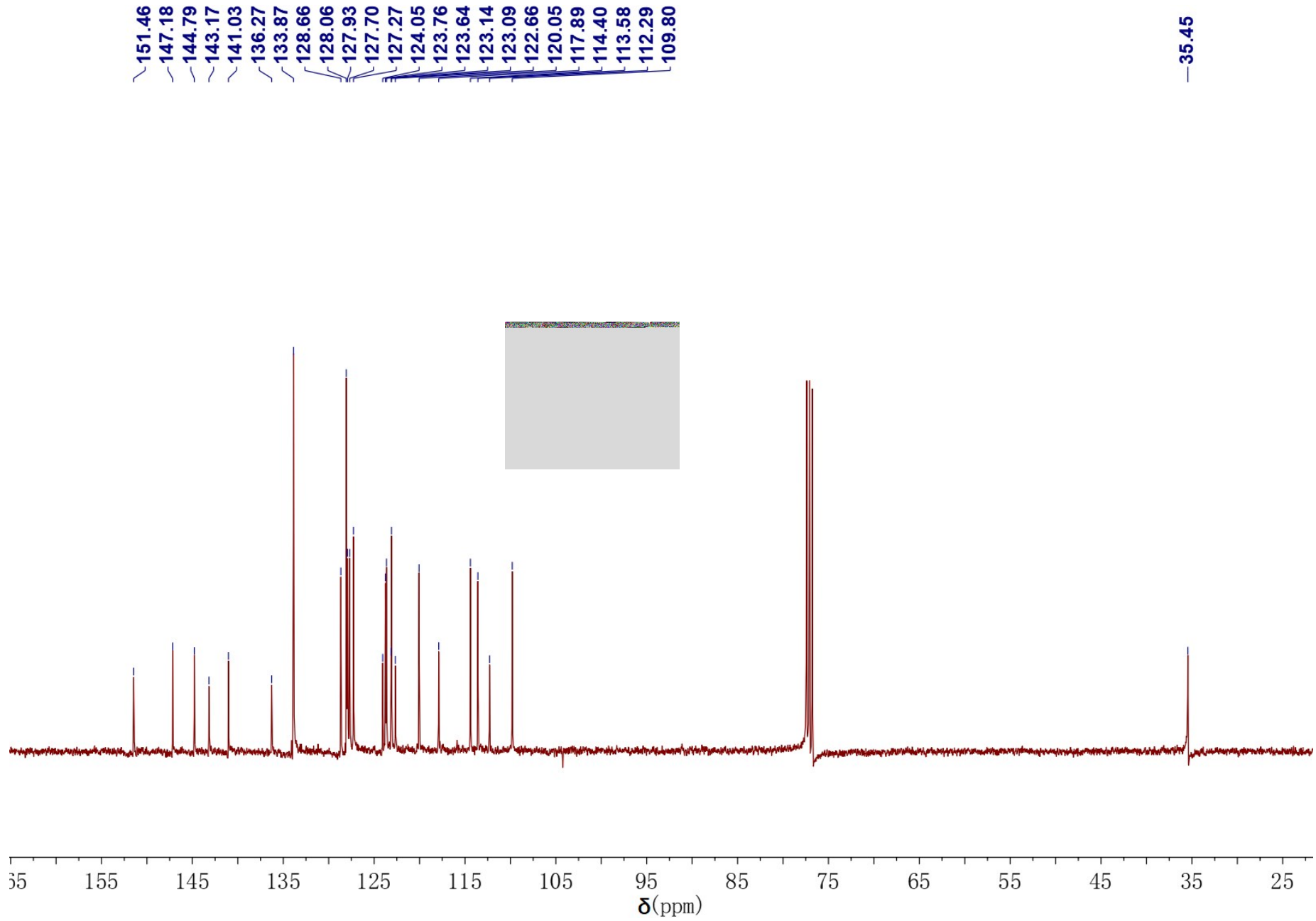
7.806
7.794
7.789
7.436
7.432
7.426
7.420
7.415
7.410
7.357
7.354
7.351
7.337
7.333
7.275
7.272
7.259
7.255
7.230
7.228
7.225
7.208
7.172
7.168
7.148
7.119
7.115
7.100
7.096
7.089
7.084
7.068
7.063
6.968
6.965
6.949
6.946
6.809
6.806
6.788
6.785
6.658
6.637
3.332
CN
N
N
N
S
1.02
2.05
3.03
1.07
2.40
1.04
2.02
1.02
1.00
0.99
3.00
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
δ (ppm)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136.27
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128.66
128.06
127.93
127.70
127.27
124.05
123.76
123.64
123.14
123.09
122.66
120.05
117.89
114.40
113.58
112.29
109.80
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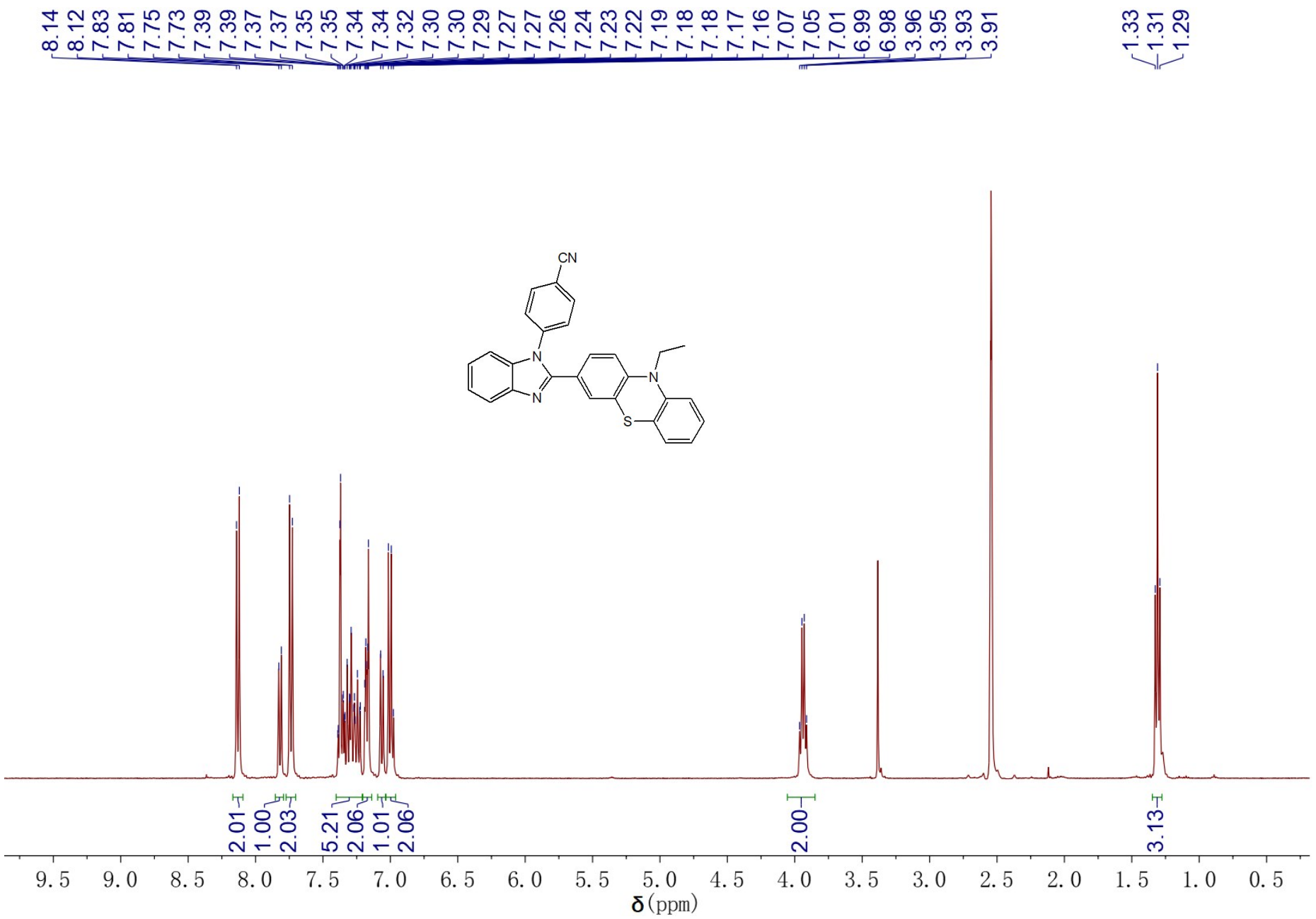
155
145
135
125
115
105
95
85
75
65
55
45
35
25
δ(ppm)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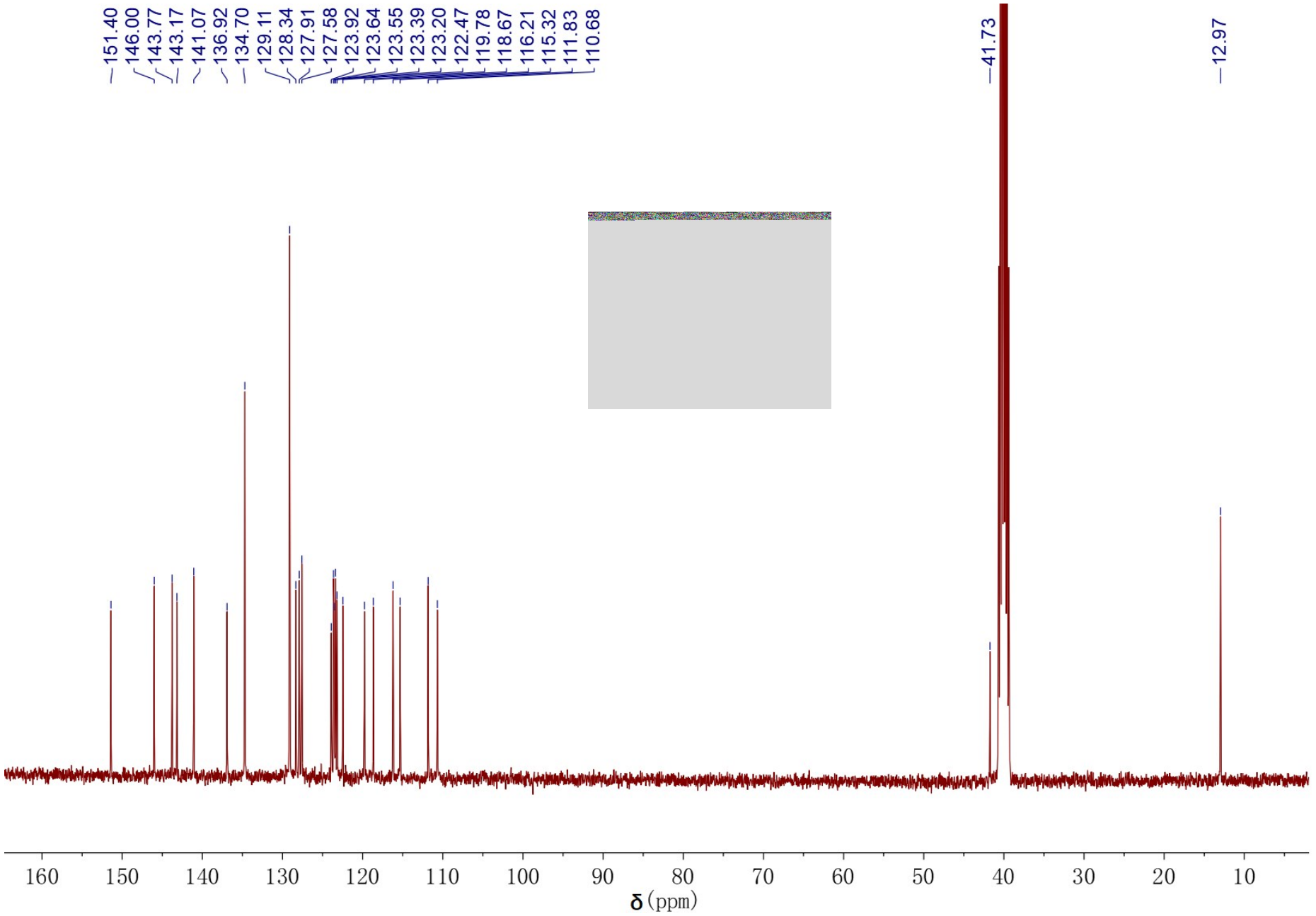
7.73
7.39
7.39
7.37
7.37
7.35
7.35
7.34
7.34
7.32
7.30
7.30
7.29
7.27
7.27
7.26
7.24
7.23
7.22
7.19
7.18
7.18
7.17
7.16
7.07
7.05
7.01
6.99
6.98
3.96
3.95
3.93
3.91
1.33
1.31
1.29
CN
N
N
N
S
2.01
1.00
2.03
5.21
2.06
1.01
2.06
2.00
3.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ(ppm)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129.11
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127.58
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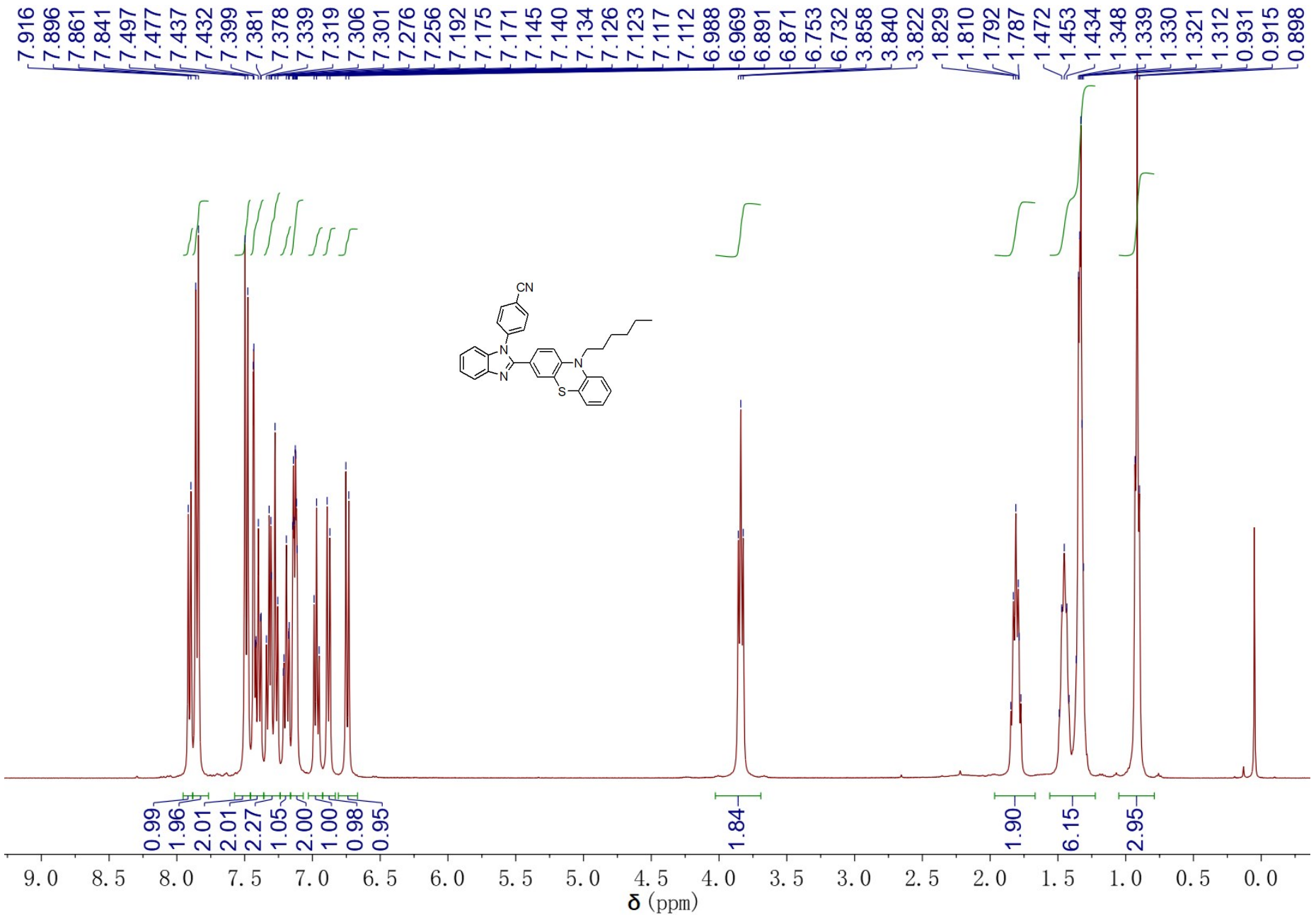
123.64
123.55
123.39
123.20
122.47
119.78
118.67
116.21
115.32
111.83
110.68
41.73
12.97
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ (ppm)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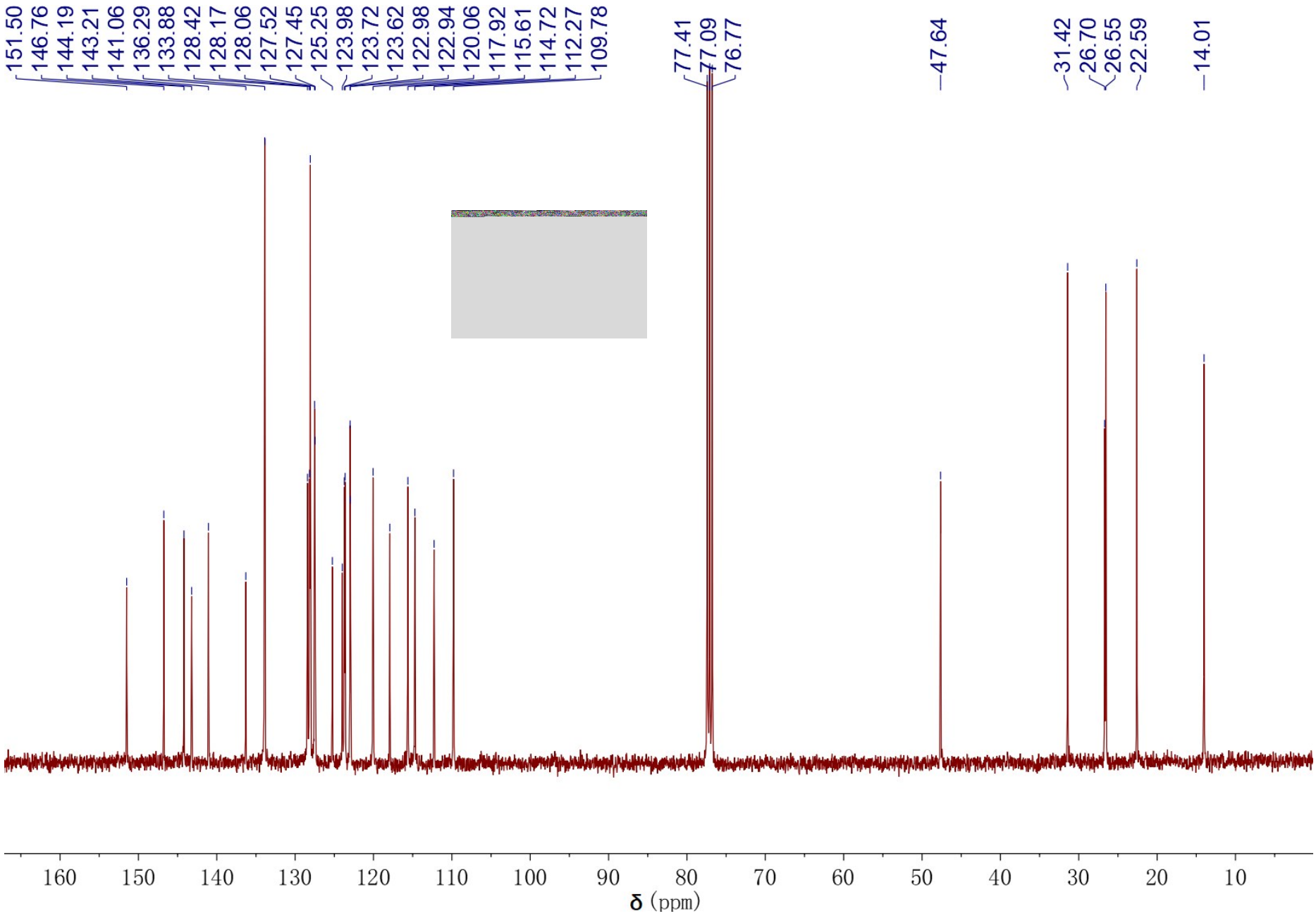
7.306
7.301
7.276
7.256
7.192
7.175
7.171
7.145
7.140
7.134
7.126
7.123
7.117
7.112
6.988
6.969
6.891
6.871
6.753
6.732
3.858
3.840
3.822
1.829
1.810
1.792
1.787
1.472
1.453
1.434
1.348
1.339
1.330
1.321
1.312
0.931
0.915
0.898
CN
N
N
N
S
0.99
1.96
2.01
2.01
2.27
1.05
2.00
1.00
0.98
0.95
1.84
1.90
6.15
2.95
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
δ (ppm)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127.45
125.25
123.98
123.72
123.62
122.98
122.94
120.06
117.92
115.61
114.72
112.27
109.78
77.41
77.09
76.77
47.64
31.42
26.70
26.55
22.59
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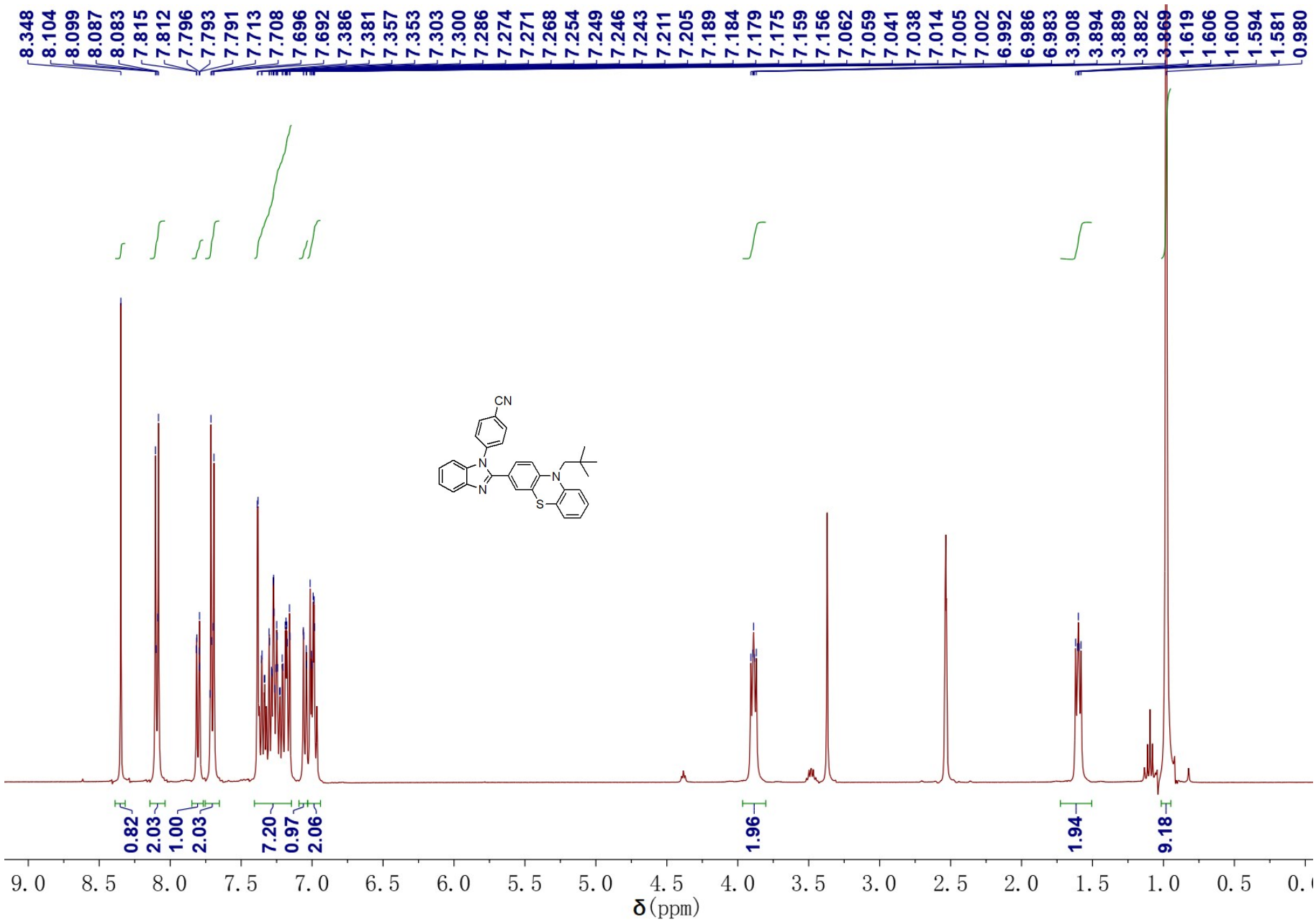
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ (ppm)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7.796
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7.791
7.713
7.708
7.696
7.692
7.386
7.381
7.357
7.353
7.303
7.300
7.286
7.274
7.271
7.268
7.254
7.249
7.246
7.243
7.211
7.205
7.189
7.184
7.179
7.175
7.159
7.156
7.062
7.059
7.041
7.038
7.014
7.005
7.002
6.992
6.986
6.983
3.908
3.894
3.889
3.882
3.869
1.619
1.606
1.600
1.594
1.581
0.980
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N
N
S
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2.03
1.00
2.03
7.20
0.97
2.06
1.96
1.94
9.18
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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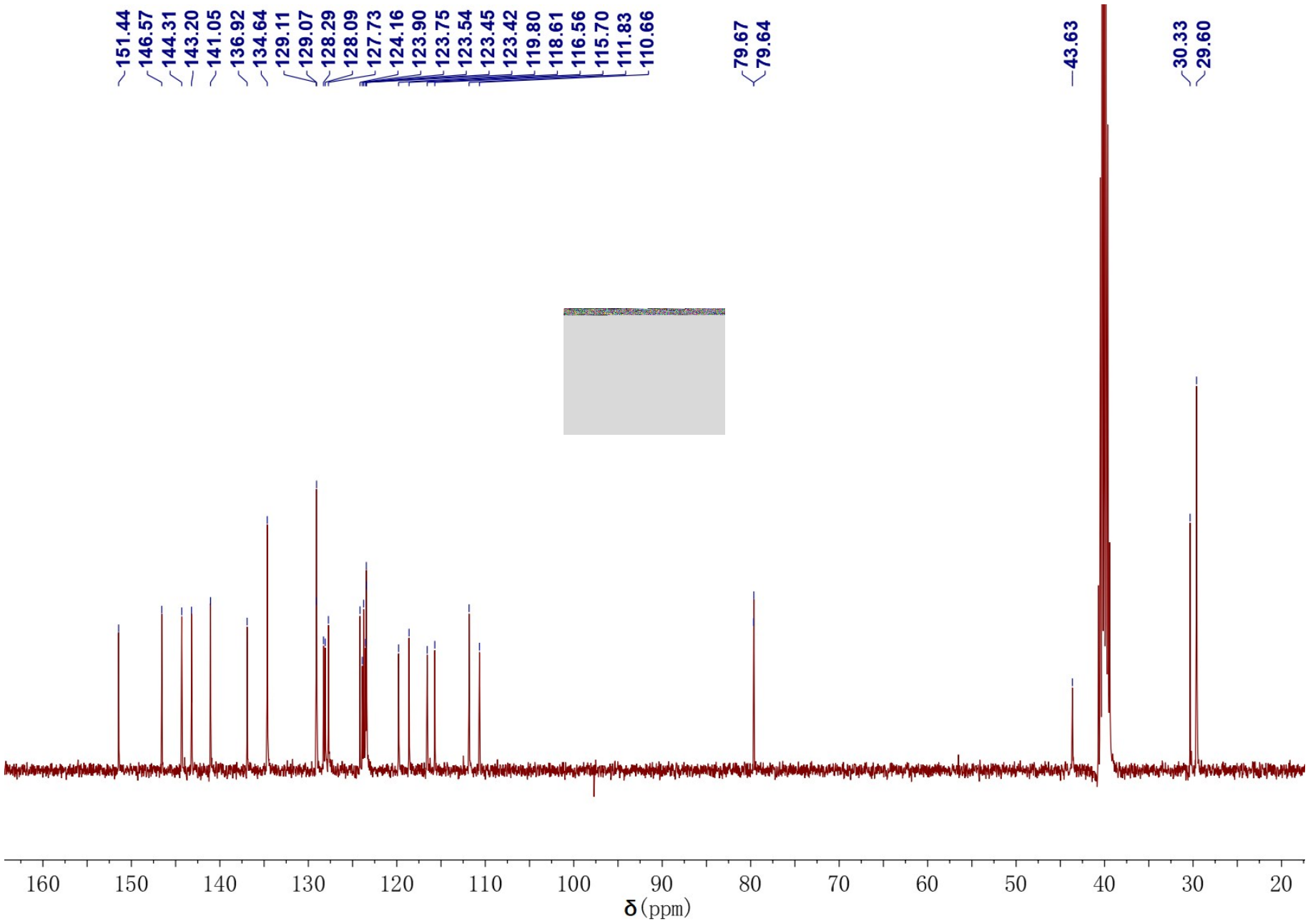
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ(ppm)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123.45
123.42
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116.56
115.70
111.83
110.66
79.67
79.64
43.63
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150
140
130
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110
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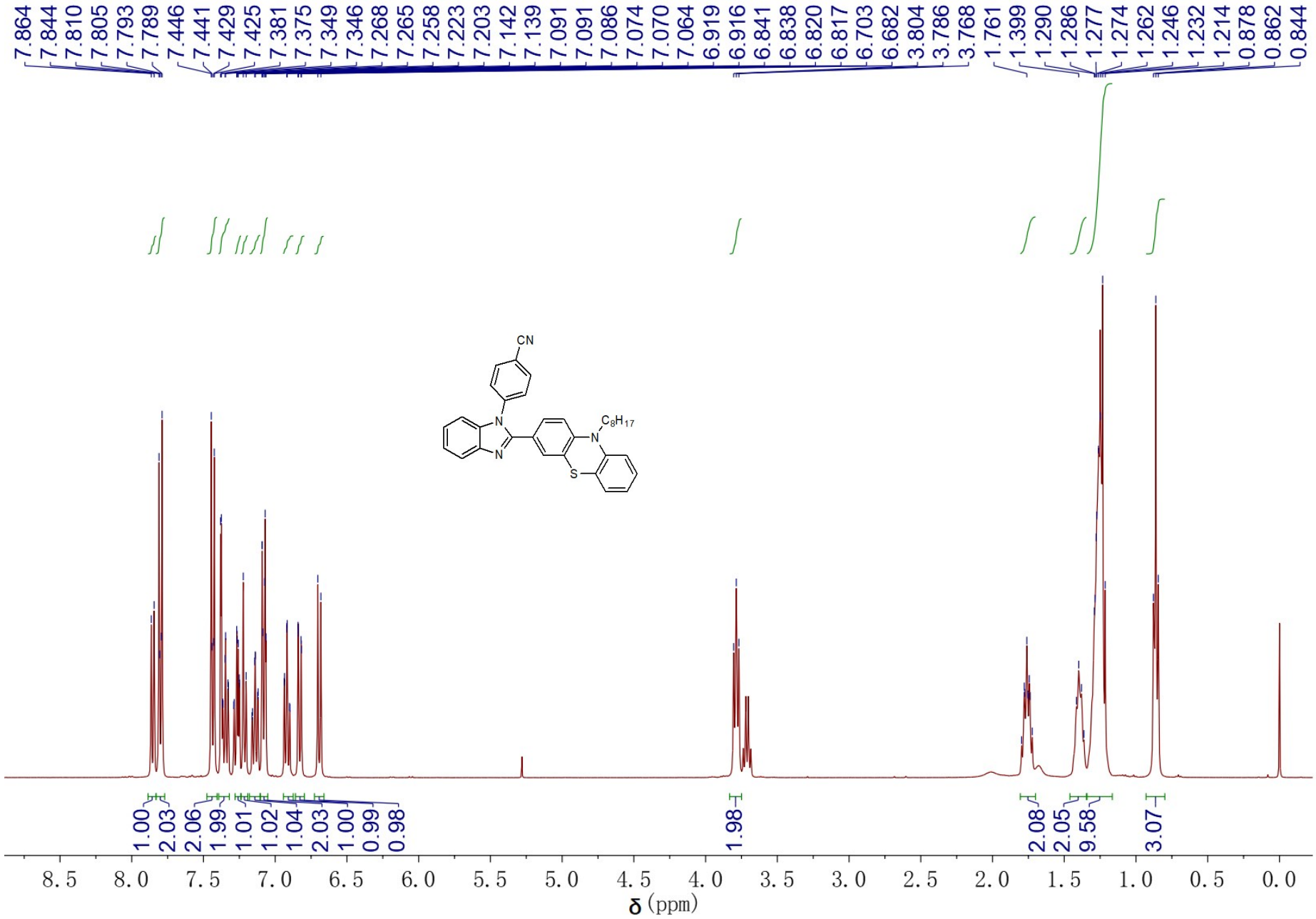
90
80
70
60
50
40
30
20
δ(ppm)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7.268
7.265
7.258
7.223
7.203
7.142
7.139
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7.091
7.086
7.074
7.070
7.064
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6.916
6.841
6.838
6.820
6.817
6.703
6.682
3.804
3.786
3.768
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1.399
1.290
1.286
1.277
1.274
1.262
1.246
1.232
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0.862
0.844
CN
N
N
C8H17
N
S
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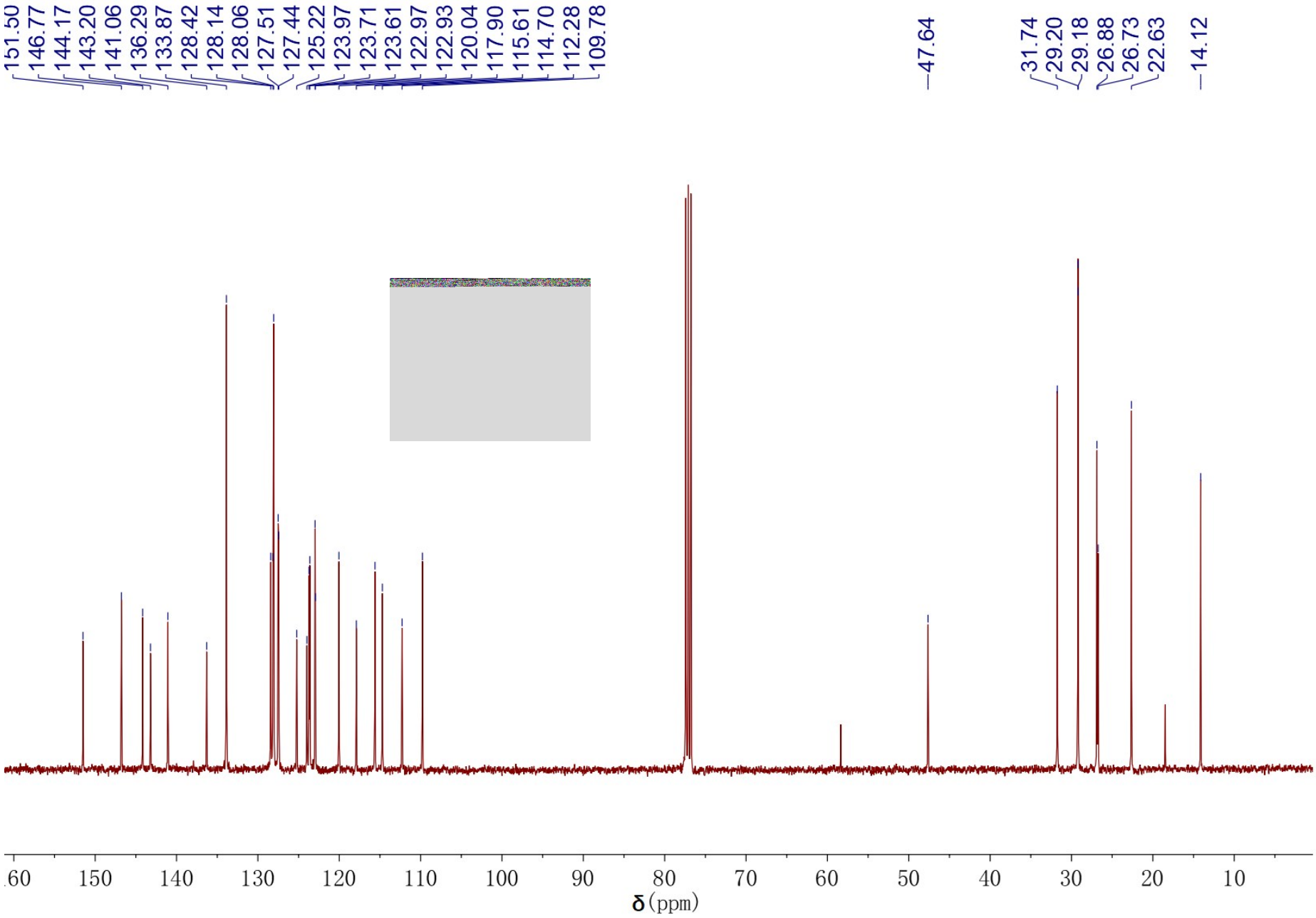
2.03
2.06
1.99
1.01
1.02
1.04
2.03
1.00
0.99
0.98
1.98
2.08
2.05
9.58
3.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)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123.71
123.61
122.97
122.93
120.04
117.90
115.61
114.70
112.28
109.78
47.64
31.74
29.20
29.18
26.88
26.73
22.63
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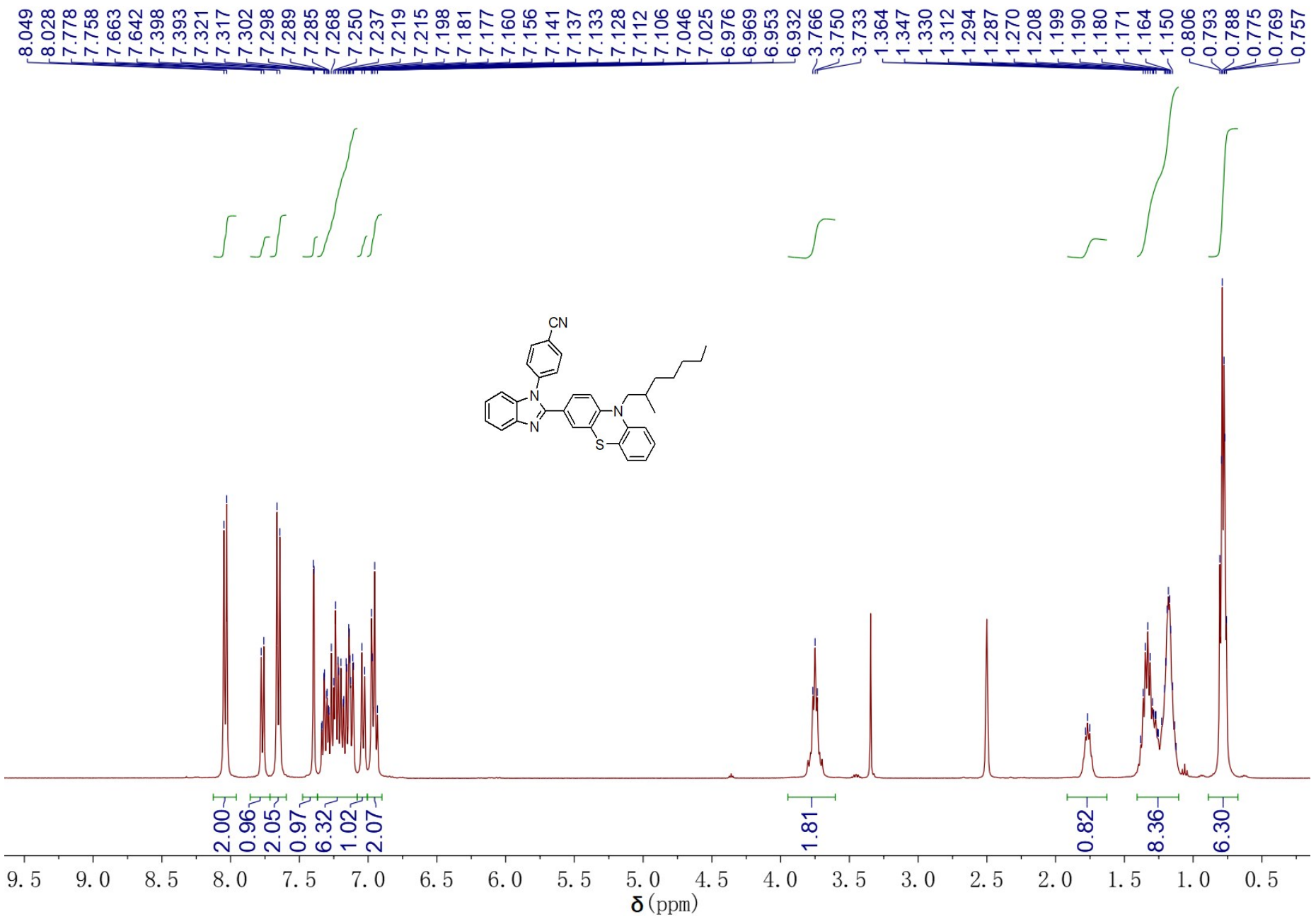
130
120
110
100
90
80
70
60
50
40
30
20
10
δ(ppm)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7.289
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7.250
7.237
7.219
7.215
7.198
7.181
7.177
7.160
7.156
7.141
7.137
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7.106
7.046
7.025
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6.969
6.953
6.932
3.766
3.750
3.733
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1.347
1.330
1.312
1.294
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1.190
1.180
1.171
1.164
1.150
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0.775
0.769
0.757
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N
N
S
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0.96
2.05
0.97
6.32
1.02
2.07
1.81
0.82
8.36
6.30
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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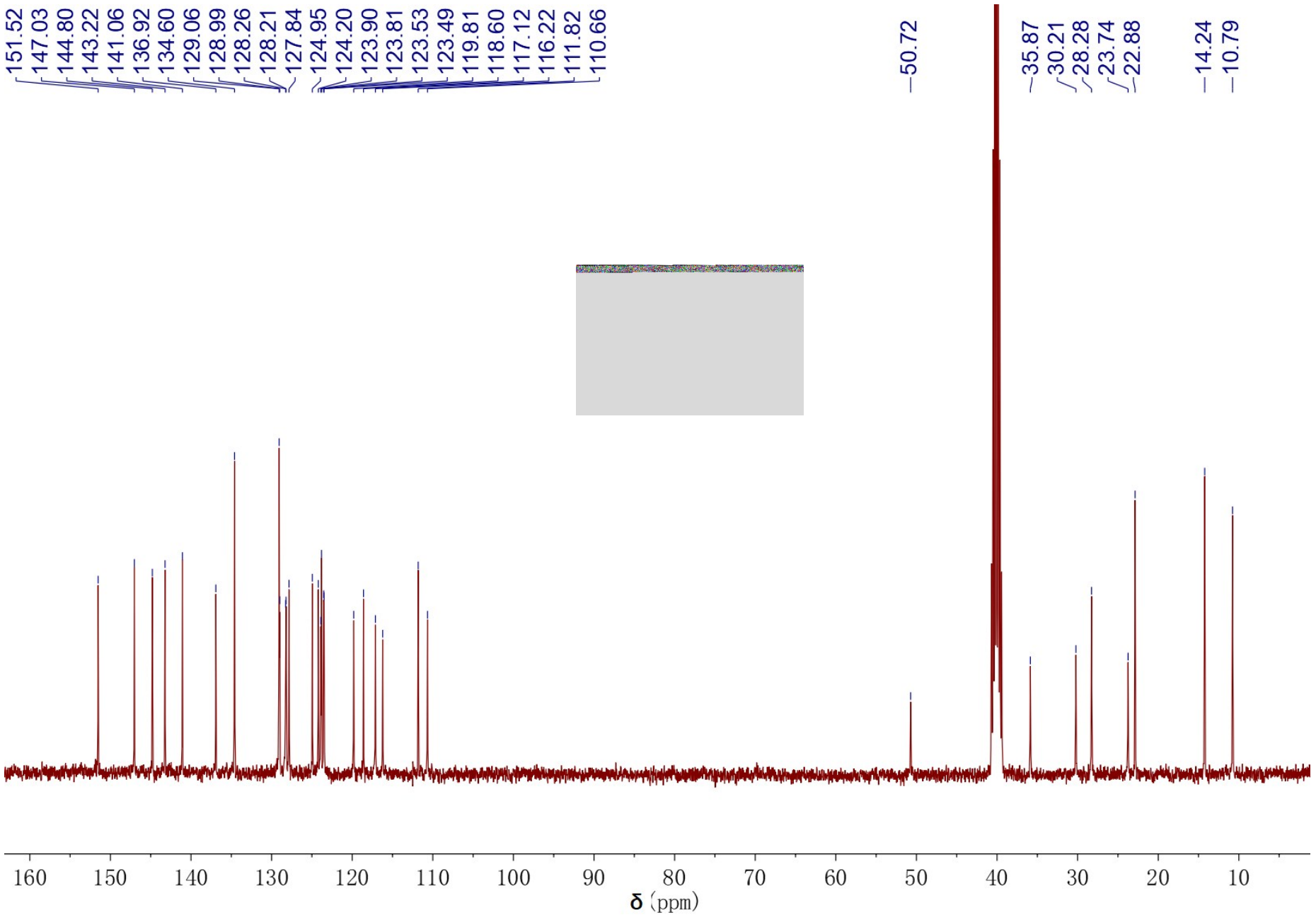
3.0
2.5
2.0
1.5
1.0
0.5
δ(ppm)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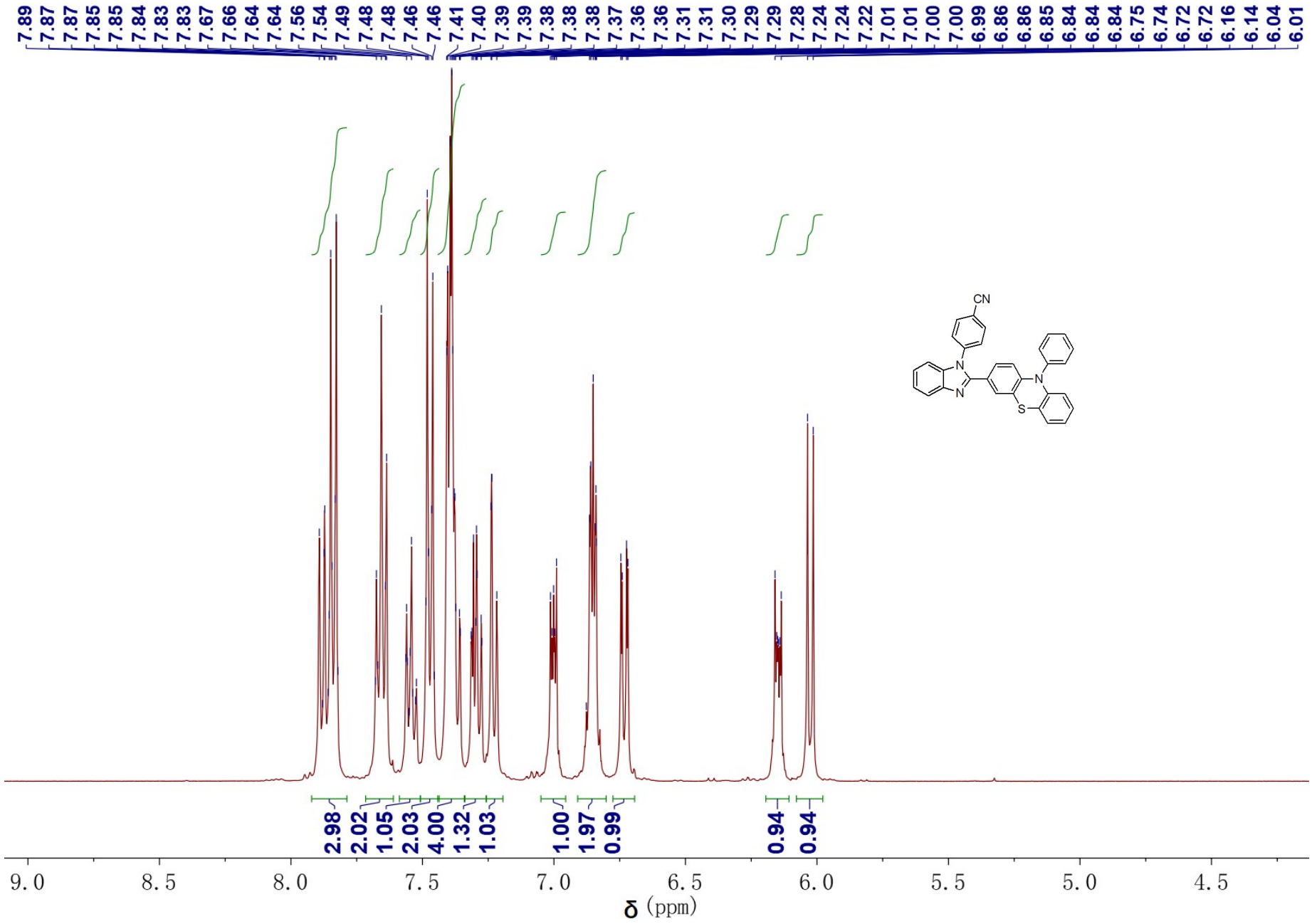
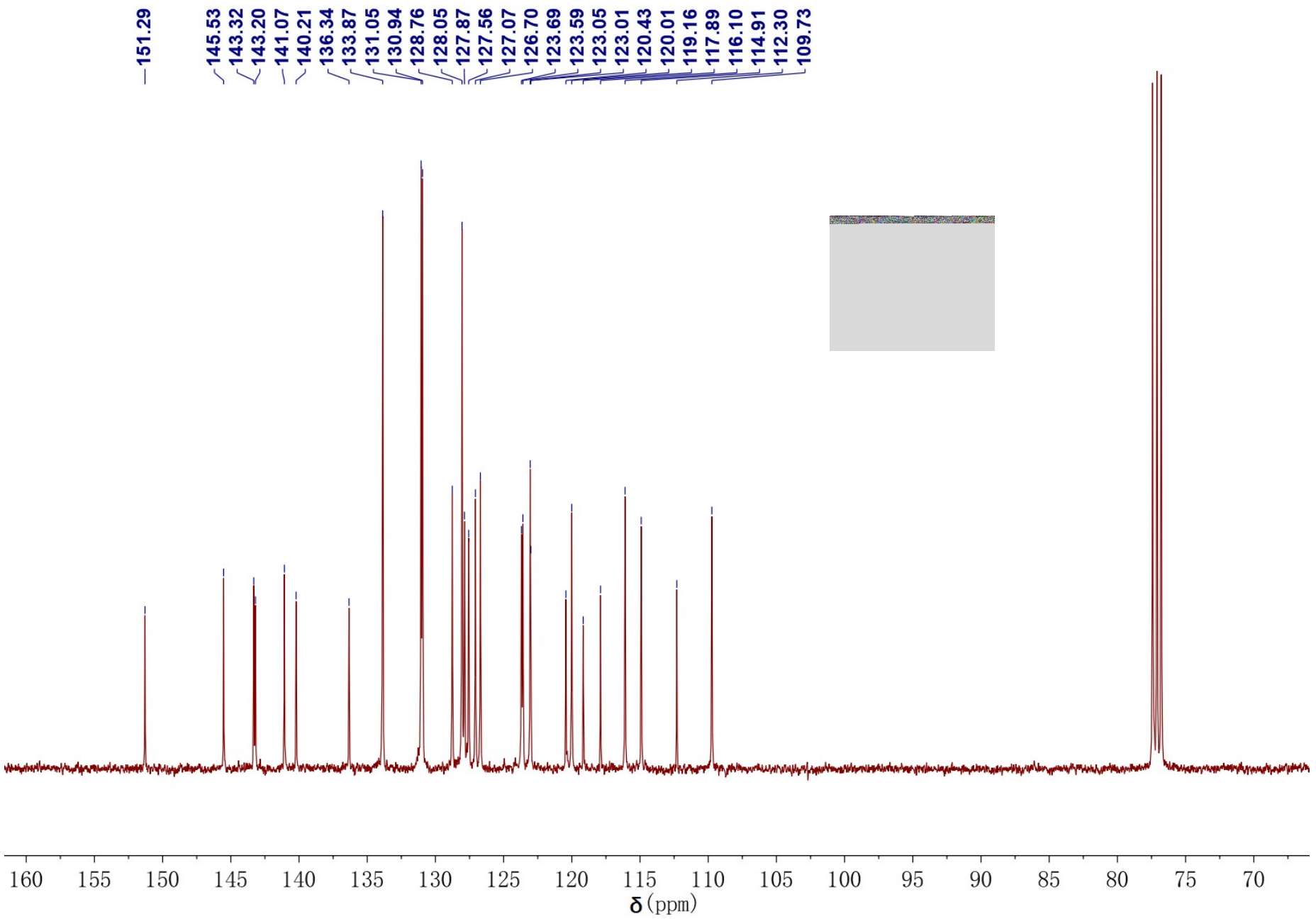
123.53
123.49
119.81
118.60
117.12
116.22
111.82
110.66
50.72
35.87
30.21
28.28
23.74
22.88
14.24
10.79
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
δ (ppm)


7.89 7.87 7.87 7.85 7.85 7.84 7.83 7.83 7.67 7.66 7.64 7.64 7.56 7.54 7.49 7.48 7.48 7.46 7.46 7.41 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.36 7.36 7.31 7.31 7.30 7.29 7.29 7.28 7.24 7.24 7.22 7.01 7.01 7.00 7.00 6.99 6.86 6.86 6.85 6.84 6.84 6.84 6.75 6.74 6.72 6.72 6.16 6.14 6.04 6.01
CN
N
N
N
S
2.98 2.02 1.05 2.03 4.00 1.32 1.03 1.00 1.97 0.99 0.94 0.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5
δ (ppm)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145.53
143.32
143.20
141.07
140.21
136.34
133.87
131.05
130.94
128.76
128.05
127.87
127.56
127.07
126.70
123.69
123.59
123.05
123.01
120.43
120.01
119.16
117.89
116.10
114.91
112.30
109.73
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
δ(ppm)