Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information (ESI)

Position- and region-isomerized derivatives of a V-shaped fluorophore: the unique solution-state dual emission and the unusual force-induced solid-state turn-on emission

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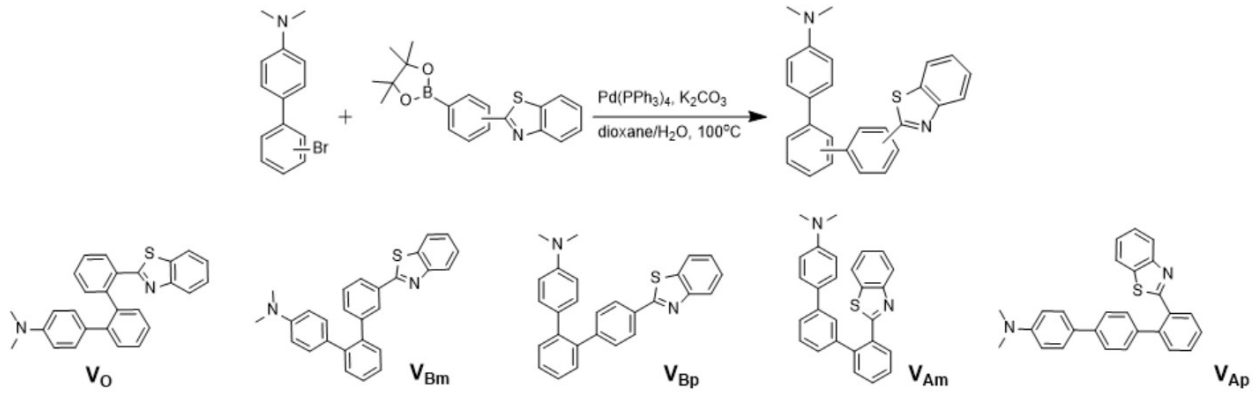
Materials and instruments

All the reagents were analytically pure and some chemicals were further purified by recrystallization or distillation. Melting points were determined by an OptiMelt automated 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 $CDCl_3$ as the solvent. The absorption spectra were measured on a Shimadzu UV 2501(PC)S UV–Vis 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 and the solid-state quantum yields were gained by an integral sphere. The mass spectrum was recorded on a HP 1110 mass spectrometer. 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. The preparation of compound **V** was referred to our previous report (*RSC Adv*., **2017**, *7*, 50720–50728).

Synthetic procedures



At room temperature and N_2 flux, the solution of 2'- or 3'- or 4'-bromo-N,N-dimethyl-[1,1'-biphenyl]-4-amine (12 mmol, 3.3 g) in dioxane / H_2O (4:1, v/v, 10 mL) was injected into the mixture of 2-[2- or 3- or 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]benzo[d]thiazole (10 mmol, 3.37 g), $Pd(PPh_3)_4$ (0.5 mmol, 0.577 g) and K_2CO_3(15 mmol, 2.07g) in dioxane/H_2O (4:1, v/v, 20 mL). The resulted mixture was heated at 100°C for 24 h and then cooled to room temperature. After filtration, the filtrate was diluted with water and extracted by CH_2Cl_2 (3×15 mL). The combined organic layers were dried over anhydrous Na_2SO_4. After the removal of solvent, the residue was purified on a silica gel column chromatography to offer the corresponding product.

2''-(benzo[d]thiazol-2-yl)-N, N-dimethyl-[1,1': 2',1''-terphenyl]-4-amine (**V_O**): 67% yield, white powder; m.p. 150.9-152.3 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ 2.90(s, 6H), 6.44(d, *J*=8.4 Hz, 2H), 6.80(d, *J*=8.8 Hz, 2H), 7.30-7.36(m, 2H), 7.38-7.51(m, 7H), 7.74(d, *J*=8.0 Hz, 1H), 8.79(d, *J*=8.0 Hz, 1H), 8.11-8.13(m, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 40.43, 111.89, 121.21, 123.05, 124.62, 125.68, 126.60, 127.32, 128.58, 129.78, 129.83, 130.02, 130.20, 131.70, 131.92, 133.07, 136.55, 138.16, 141.60, 142.01, 149.02, 152.64, 167.25; EI-MS(70 eV) *m/z* (%) 406(M^+, 100), 392(48), 376(12), 362(10), 286(25), 271(15), 254(5), 228(7), 202(8).

3''-(benzo[d]thiazol-2-yl)-N, N-dimethyl-[1,1': 2',1''-terphenyl]-4-amine (**V_{Bm}**): 74% yield, white powder; m.p. 160.4-161.7°C; ^{1}H NMR (400MHz, $CDCl_3$) δ 3.02(s, 6H), 6.79(d, *J*=8.0 Hz, 2H), 7.24(d, *J*=7.6 Hz, 1H), 7.35(t, *J*=8.0 Hz, 1H), 7.40(t, *J*=8.0 Hz, 1H), 7.47(m, 3H), 7.51-7.62(m, 5H), 7.74(d, *J*=8.0 Hz, 1H), 8.11(d, *J*=8.4 Hz, 1H), 8.18(dd, J_1= 7.6 Hz, J_2=2 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 40.64, 112.82, 121.38, 123.20, 124.87, 125.65, 125.87, 127.68, 127.73, 127.87, 128.69, 130.03, 130.35, 130.89, 132.75, 136.76, 140.53, 141.10, 141.97, 149.94, 152.78, 167.84; EI-MS(70 eV) *m/z* (%) 406(M^+, 100), 391(45), 376(10), 362(15), 273(17), 254(7), 227(15), 202(5).

4''-(benzo[d]thiazol-2-yl)-N,N-dimethyl-[1,1':2',1''-terphenyl]-4-amine (**V_{Bp}**): 81% yield, pale yellow powder; m.p. 183.4-185.2°C; ^{1}H NMR (400MHz, $CDCl_3$) δ 3.06(s, 6H), 6.86(d, *J*=8.4 Hz, 2H), 7.33-7.40(m, 3H), 7.48(dd, J_1=1.2 Hz, J_2=8.0 Hz,1H), 7.53(dt, J_1=2 Hz, J_2=8.0 Hz, 2H), 7.56(t, *J*=2Hz, 1H), 7.58-7.62(m, 4H), 7.76(d, *J*=8.0 Hz, 1H), 8.11(d, *J*=8.0 Hz, 1H), 8.13(dd, J_1=2Hz, J_2=8.0 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 40.64, 112.87, 121.41, 123.23, 124.86, 125.85, 125.96,127.59, 127.62, 130.07, 130.35, 130.50, 130.93, 132.73, 136.78, 137.78, 140.41, 141.67, 150.08, 152.86, 168.01; EI-MS(70 eV) *m/z* (%) 406 (M^+, 100), 391(52), 376(13), 362(17), 253(8), 203(5).

2''-(benzo[d]thiazol-2-yl)-N,N-dimethyl-[1,1':3',1''-terphenyl]-4-amine (**V_{Am}**): 61% yield, white powder; m.p. 127.6-129.2°C; ^{1}H NMR (400MHz, $CDCl_3$) δ 2.95(s, 6H), 6.66(dd, J_1=1.2 Hz, J_2=7.2 Hz, 2H), 7.13(dd, J_1=2Hz, J_2=7.2 Hz, 2H), 7.28-7.31(m, 1H), 7.37(m, 1H), 7.41-7.57(m, 6H), 7.93(dd, J_1=1.2 Hz, J_2=8.0 Hz, 1H), 8.02-8.06(m, 2H), 8.12(dd, J_1=1.2 Hz, J_2=8.0 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 40.53, 112.23, 121.60, 123.22, 125.12, 125.39, 126.27, 126.79, 127.95, 128.51, 129.06, 130.59, 130.69, 132.77, 133.42, 135.15, 139.25, 140.81, 143.07, 149.32, 154.18, 168.33; EI-MS(70 eV) *m/z* (%) 406 (M^+, 100), 389(35), 262(10), 254(7), 202(17).

2''-(benzo[d]thiazol-2-yl)-N,N-dimethyl-[1,1':4',1''-terphenyl]-4-amine (**V_{Ap}**): 78% yield, yellowish green powder; m.p. 183.1-184.6°C; ^{1}H NMR (400MHz, $CDCl_3$) δ 2.91(s, 6H), 6.59(d, *J*=7.6 Hz, 2H), 7.03(d, *J*=8.4 Hz, 2H), 7.31(d, *J*=8.0 Hz, 2H), 7.35-7.49(m, 6H), 7.88(d, *J*=8.0 Hz, 1H), 7.96(d, *J*=8.0 Hz, 2H), 8.04(d, *J*=8.4 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 40.38, 112.04, 121.61, 123.10, 125.09, 126.30,

126.74, 127.18, 128.00, 130.46, 130.52, 130.62, 130.67, 131.45, 135.03, 139.22, 140.77, 145.18, 149.22, 154.18, 168.12; EI-MS(70 eV) *m/z* (%) 406(M^+, 100), 389(33), 316(7), 286(8), 254(5), 202(13).

X-ray structure analysis

Single crystals of the title compounds grown in MeCN/EtOH were selected for the X-ray analysis. The diffraction data were collected on a Bruker CCD area-detector diffractometer equipped with a graphite-monochromated Mo-K_α radiation (λ=0.71073 Å). The unit cell parameters were determined from a least-squares refinement of the setting angles. The structure was solved by direct methods and refined on F^2 by the full-matrix least-squares methods with SHELXS-97. The refinement was carried out by full-matrix least squares method on the positional and anisotropic temperature parameters of the non-hydrogen atoms using SHELXL-97. All H atoms were placed in the idealized positions and constrained to ride on their parent atoms.Crystallographic data for compound **V** (CCDC 1551667)**, $\mathbf{V_O}$** (CCDC 1834425), **$\mathbf{V_{Bm}}$** (CCDC 1834423), **$\mathbf{V_{Bp}}$** (CCDC 1834424) and **$\mathbf{V_{Am}}$** (CCDC 1844322) were deposited at CCDC center and can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/ data_request/ cif.

Table S1 Crystallographic data for **$\mathbf{V_O}$** and **V**

$\mathbf{V_O}$	**V**
a = 7.398(1) Å	a = 6.1982(5) Å
b = 14.3691(15) Å	b = 24.956(2) Å
c = 20.4895(16) Å	c =10.8550(9) Å
α = 90° *β* = 91.329 (8)° *γ* = 90°	*α* = 90 ° *β* = 97.234(8) ° *γ* =90 °
Temperature 293 K	170 K
Volume 2177.5(4)	1665.7(2)
Space group P 2_1/n	P 2_1/c
Hall group - P 2_{yn}	-P 2_{ybc}
Density 1.240 g/cm^3	1.318 g/cm^3
Z 4	4
Mu 0.164 / nm	0.198 / nm
F_{000} 856.0	696.0
h, k, l (max) 8, 17, 24	7, 30, 13
N_{ref} 3970	3045
T_{min}, T_{max} 0.641, 1.000	0.766, 1.000
$R_{reflections}$ 0.0641 (2040)	0.0592 (2445)
$wR^2_{reflections}$ 0.1843 (3970)	0.1526(3045)
S 1.005	1.079
N_{par} 273	219

Table S2 Crystallographic data for $\mathbf{V_{Bm}}$ and $\mathbf{V_{Bp}}$

	$\mathbf{V_{Bm}}$	$\mathbf{V_{Bp}}$
	a = 10.7946(7) Å	a = 12.2955(11) Å
	b = 7.7940(6) Å	b = 13.9512(11) Å
	c = 25.0193(18) Å	c = 12.4705(14) Å
	α = 90° β = 96.088(6) ° γ = 90°	α = 90 ° β = 102.145(9) ° γ =90 °
Temperature	180 K	180 K
Volume	2093.1(3)	2091.3 (3)
Space group	P 2_1/c	P 2_1
Hall group	- P 2_{ybc}	-P 2_{yb}
Density	1.290 g/cm^3	1.291 g/cm^3
Z	4	4
Mu	0.171 / nm	0.171 / nm
F_{000}	856.0	856.0
h, k, l (max)	13, 9, 30	14, 16, 15
N_{ref}	3809	5954
T_{min}, T_{max}	0.936, 1.000	0.878, 1.000
$R_{reflections}$	0.0425 (2919)	0.0555 (4526)
$wR^2_{reflections}$	0.1056 (3809)	0.1520 (5954)
S	1.016	1.045
N_{par}	273	558

Table S3 Crystallographic data for $\mathbf{V_{Am}}$

	$\mathbf{V_{Am}}$
	a = 41.697(4) Å
	b = 11.1157(11) Å
	c = 9.2068(8) Å
α = 90°	β = 93.753(6) ° γ = 90°
Temperature	293 K
Volume	4258.1(7)
Space group	P 2_1/c
Hall group	- P 2_{ybc}
Density	1.268 g/cm^3
Z	8
Mu	0.168 / nm
F_{000}	1712.0
h, k, l (max)	50, 13, 11
N_{ref}	7791
T_{min}, T_{max}	0.939, 0.978
$R_{reflections}$	0.0649 (4103)
$wR^2_{reflections}$	0.1622 (7765)
S	1.020
N_{par}	545

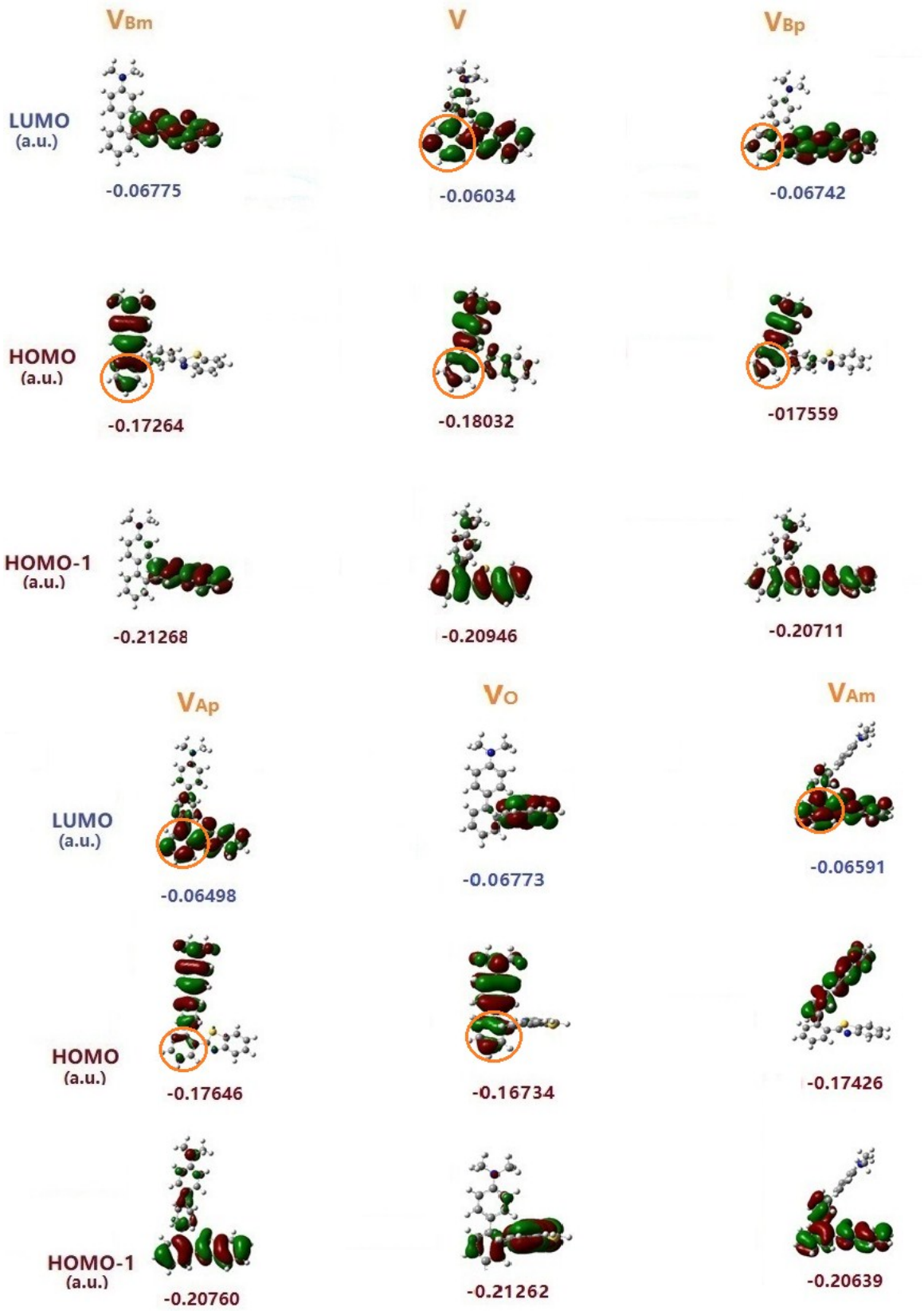


Fig. S1 Electronic distributions on frontier molecular orbits calculated by TD-DFT at B3LYP/6-31G (d, p) level (solid-line cycles: delocalization with electrons)

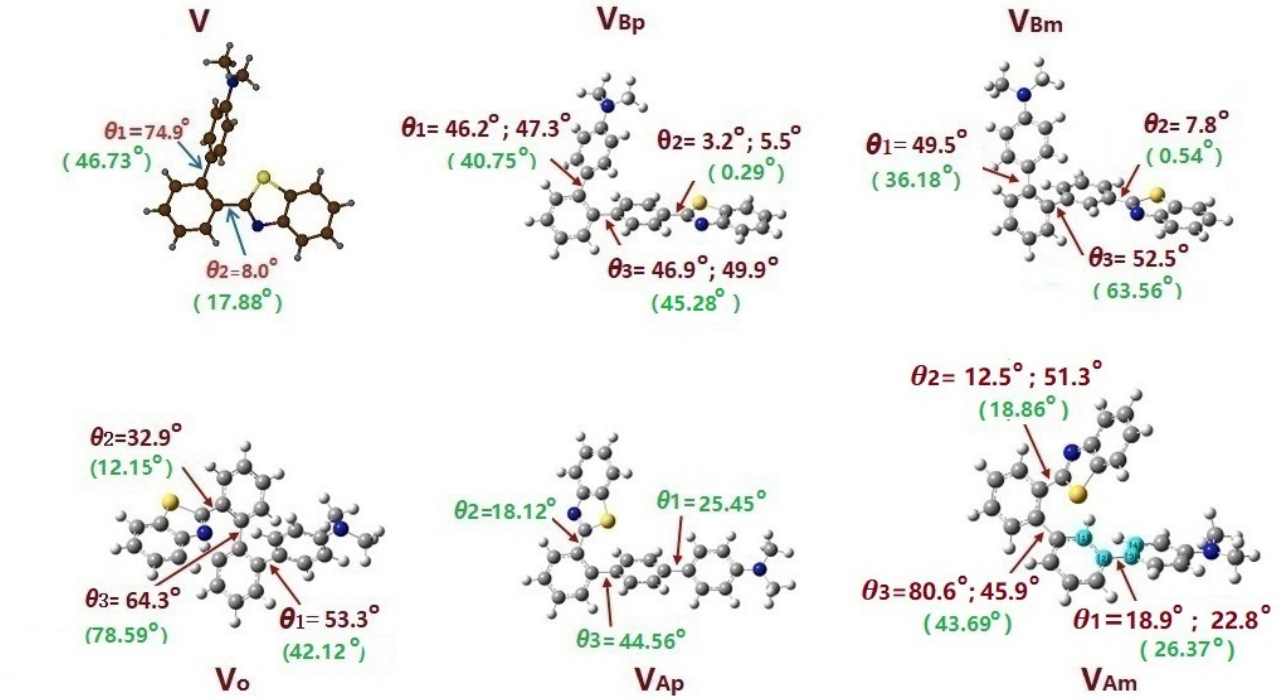


Fig. S2 Excited-state geometries of V-shaped fluorophores in crystalline phase (red) and in gas phase (green) calculated by TD-DFT at B3LYP/6-31G (d, p) level

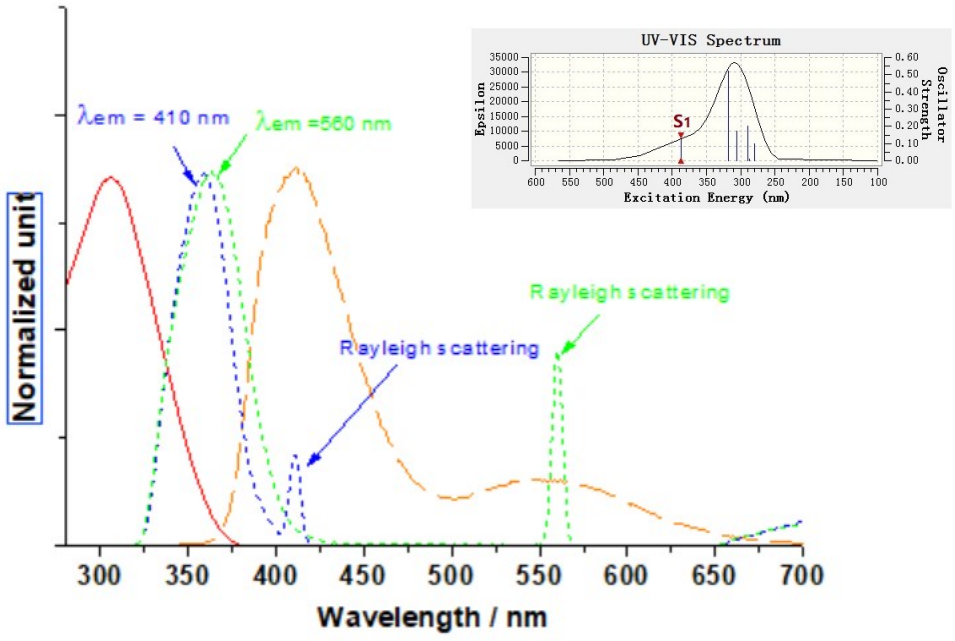


Fig. S3 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=330 nm) spectra of $\mathbf{V_{Ap}}$ in acetone (50 μM) [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

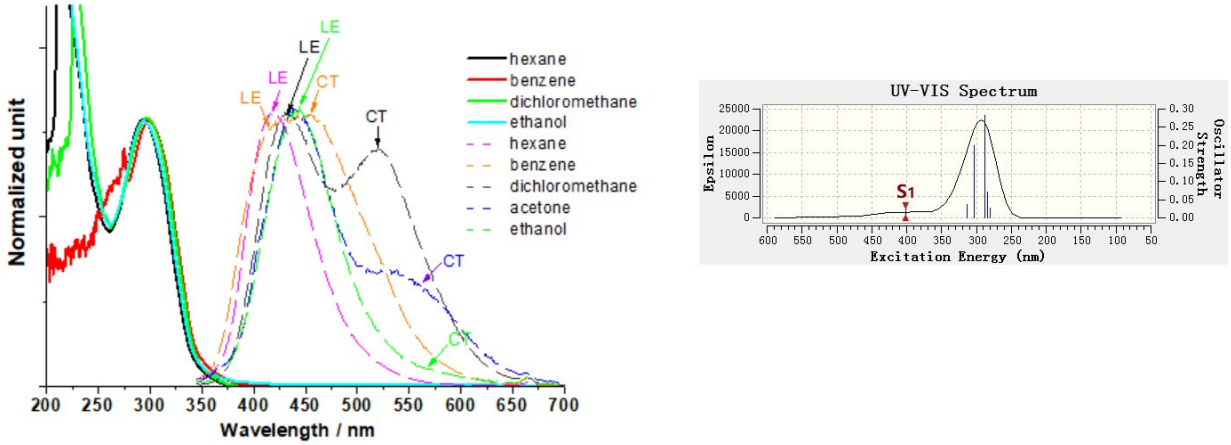


Fig. S4 Absorption (solid lines) and emission spectra (dash lines, λ_{ex}=330 nm, slit width / nm : ex 5; em 5) of compound $\mathbf{V_O}$ (500 μM) in different solvents [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

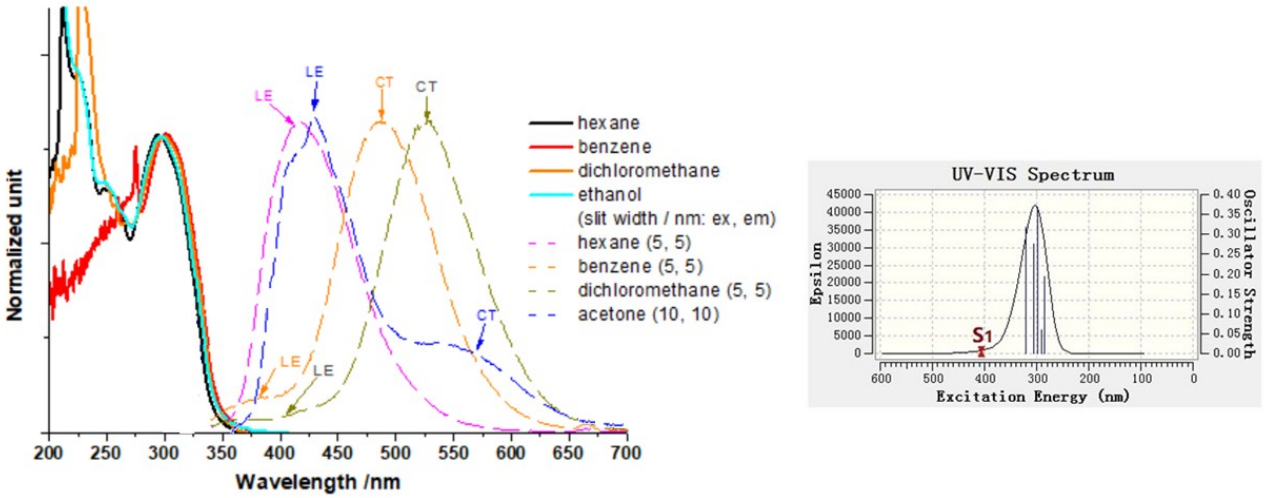


Fig. S5 Absorption (solid lines) and emission spectra (dash lines, λ_{ex}=330 nm) of compound $\mathbf{V_{Bm}}$ (500 μM) in different solvents [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

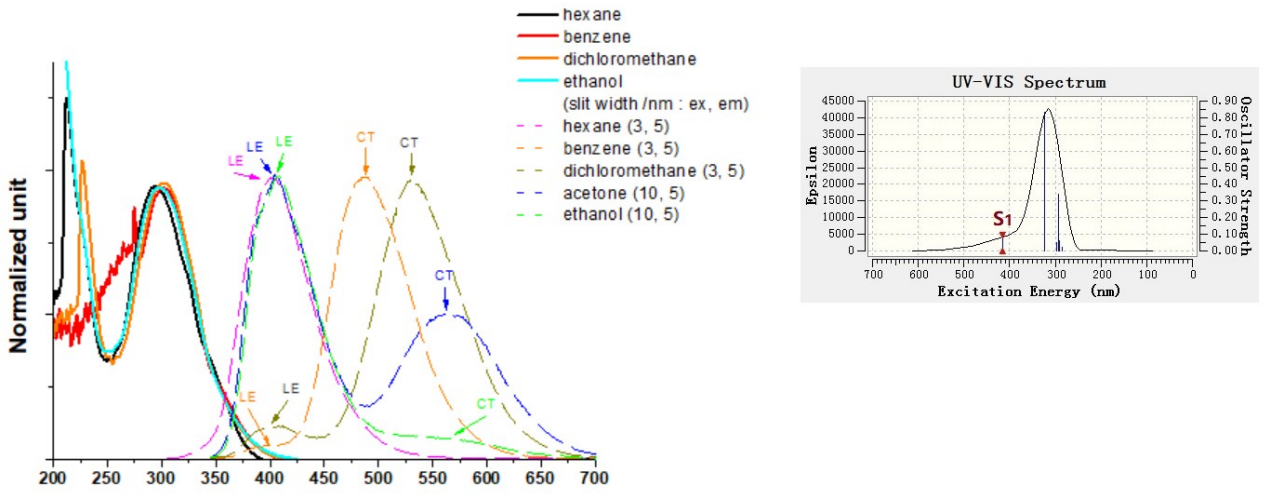


Fig. S6 Absorption (solid lines) and emission spectra (dash lines, λ_{ex}=330 nm) of compound $\mathbf{V_{Bp}}$ (50 μM) in different solvents [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

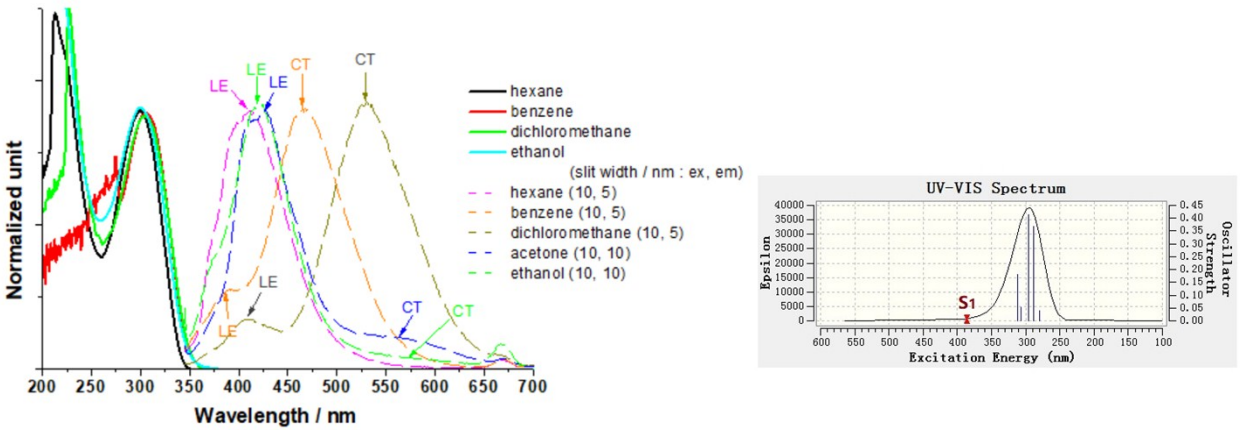


Fig. S7 Absorption (solid lines) and emission spectra (dash lines, λ_{ex}=330 nm) of compound $\mathbf{V_{Am}}$ (500 μM) in different solvents [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

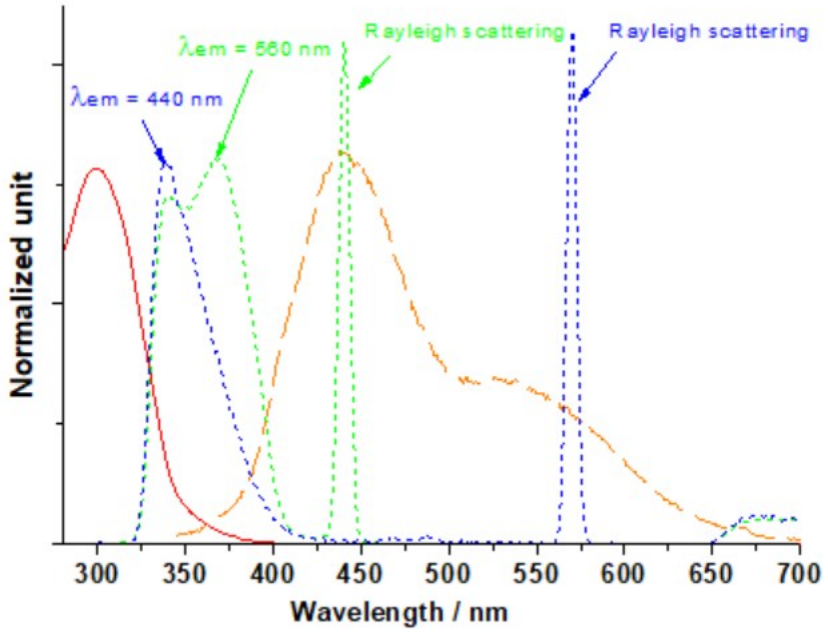


Fig. S8 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=330 nm) spectra of $\mathbf{V_O}$ in acetone (500 μM)

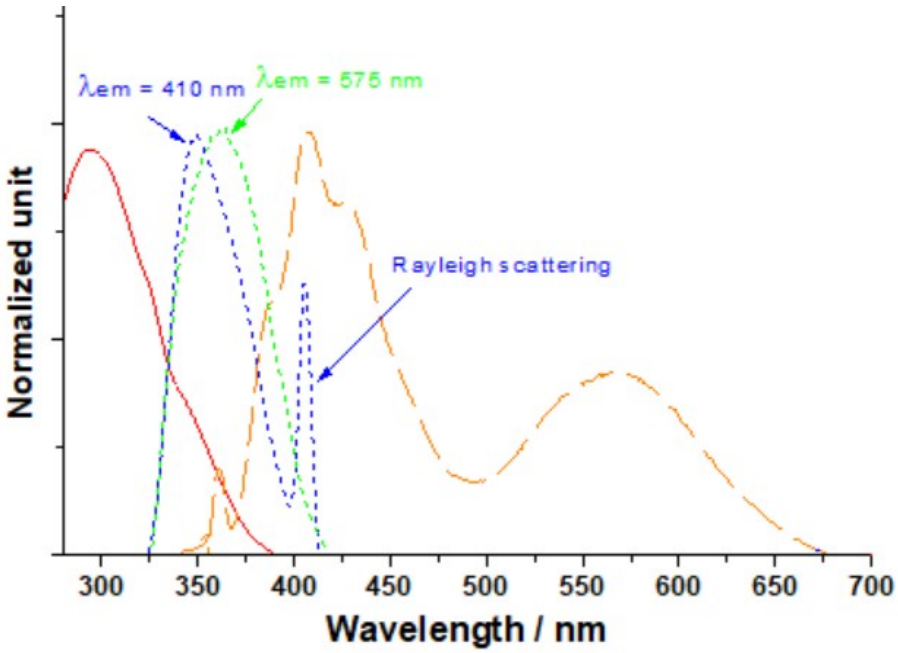


Fig. S9 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=330 nm) spectra of $\mathbf{V_{Bp}}$ in acetone (50 μM)

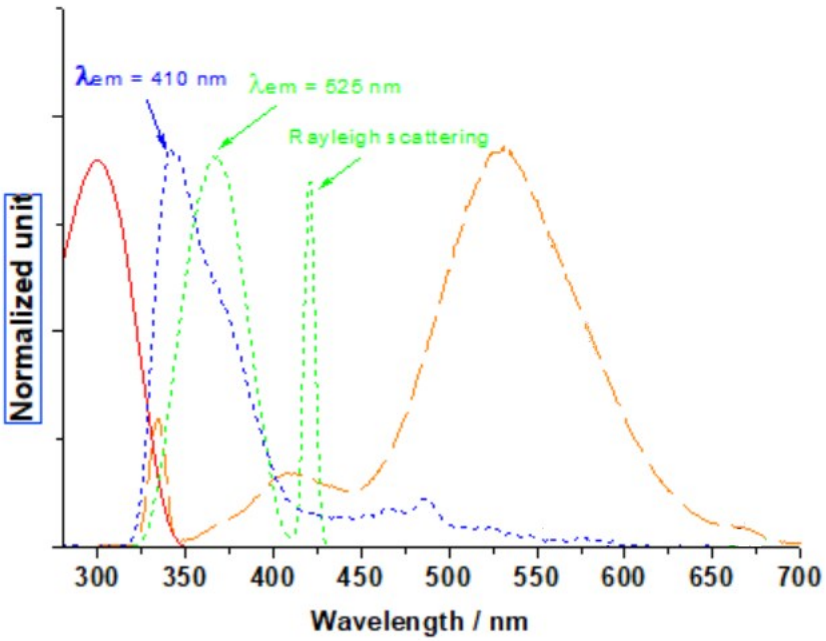


Fig. S10 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=330 nm) spectra of $\mathbf{V_{Am}}$ in acetone (500 μM)

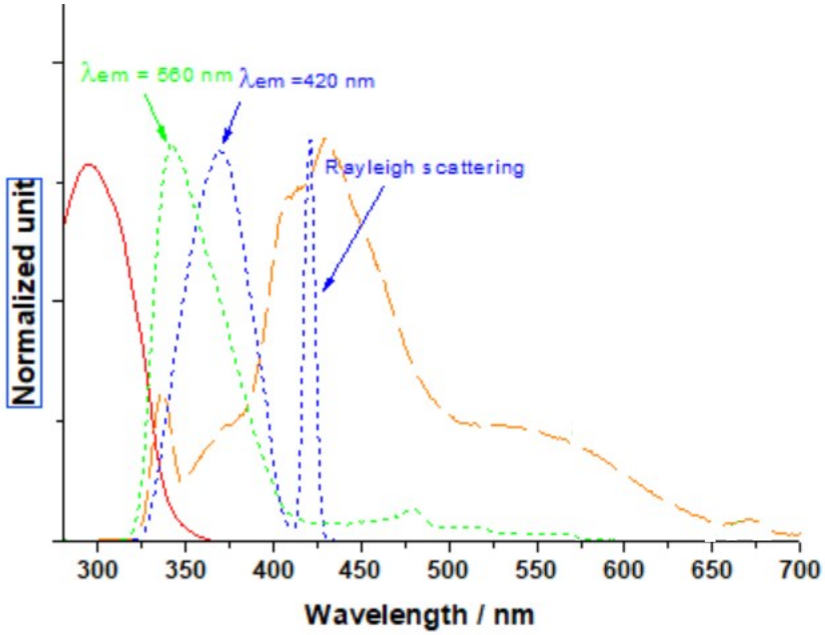


Fig. S11 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=330 nm) spectra of $\mathbf{V_{Bm}}$ in acetone (500 μM)

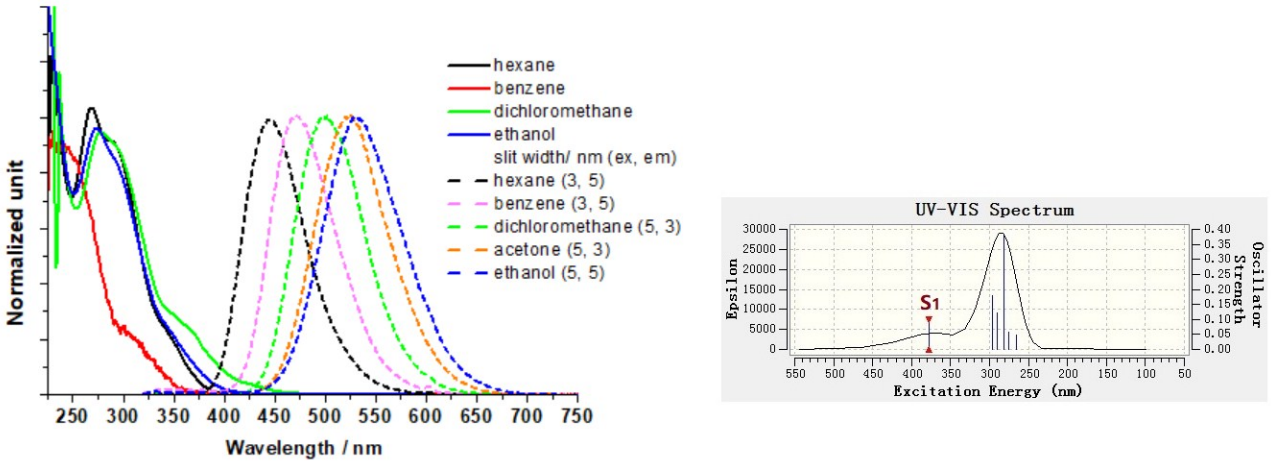


Fig. S12 Absorption (solid lines) and emission spectra (dash lines, λ_{ex}=350 nm) of compound **V** (50 μM) in different solvents [*inserted*: TD-DFT calculated UV-Vis spectrum at B3LYP/6-31G(d, p) level in gas phase]

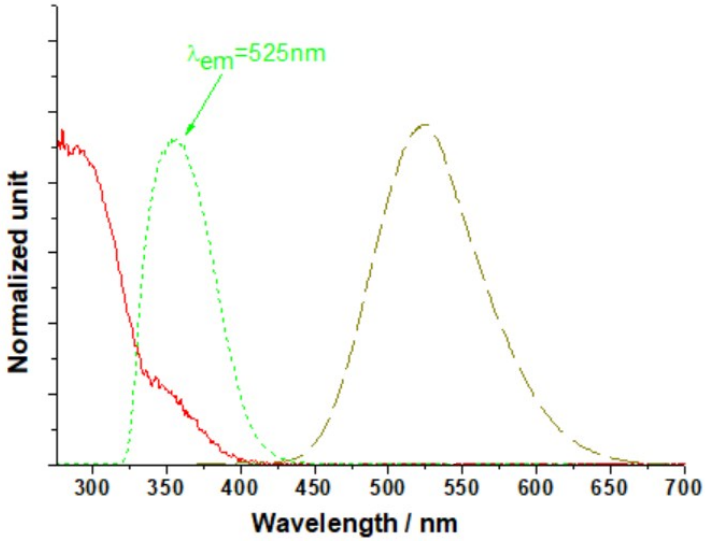


Fig. S13 Absorption (solid line), excitation (dot lines) and emission (dash line, λ_{ex}=350 nm) spectra of **V** (50 μM) in acetone

Table S1 Emission wavelengths of compounds in different solvents [a]

Compd.	*n*-hexane		benzene		dichloromethane		acetone		ethanol	
V	----[b]	*445*	----[b]	*471*	----[b]	*498*	----[b]	*522*	----[b]	*531*
$\mathbf{V_O}$	409	----[c]	410	*447*	426	*520*	430	*538*	430	----[c]
$\mathbf{V_{Am}}$	406	----[c]	392	*467*	406	*530*	414	*560*	416	----[c]
$\mathbf{V_{Ap}}$	412	----[c]	395	*487*	406	*526*	410	*558*	410	----[c]
$\mathbf{V_{Bm}}$	410	----[c]	392	*453*	413	*528*	424	*556*		
$\mathbf{V_{Bp}}$	402	----[c]	393	*489*	400	*532*	403	*565*	403	*575*

[a] underlined: LE emission; italic: TICT emission.
[b] not existent
[c] cannot be observable

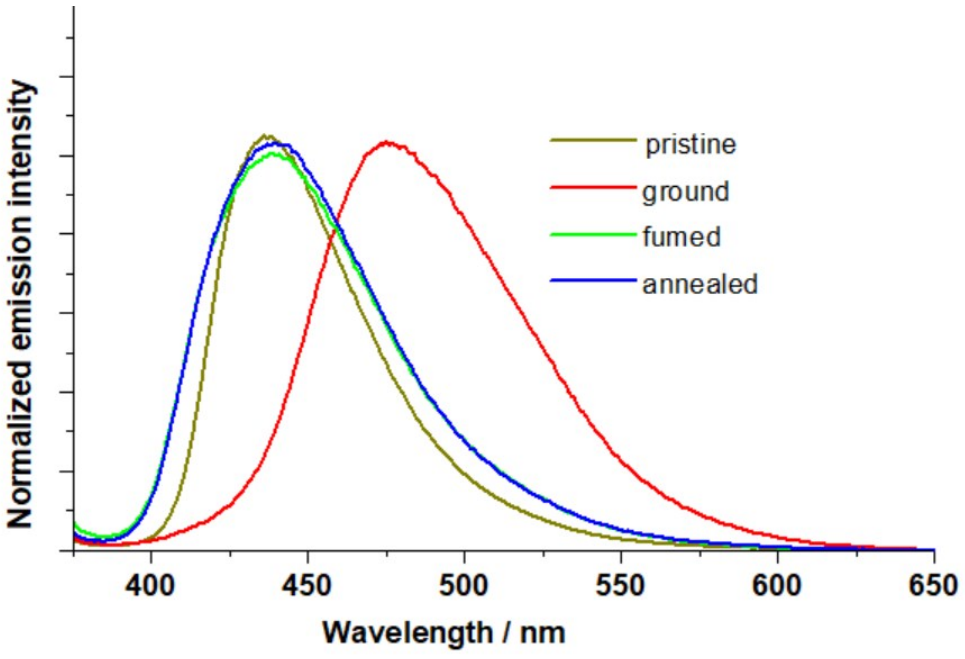


Fig. 14 Emission spectra (λ_{ex} =365 nm) of compound **V** under different solid-state conditions

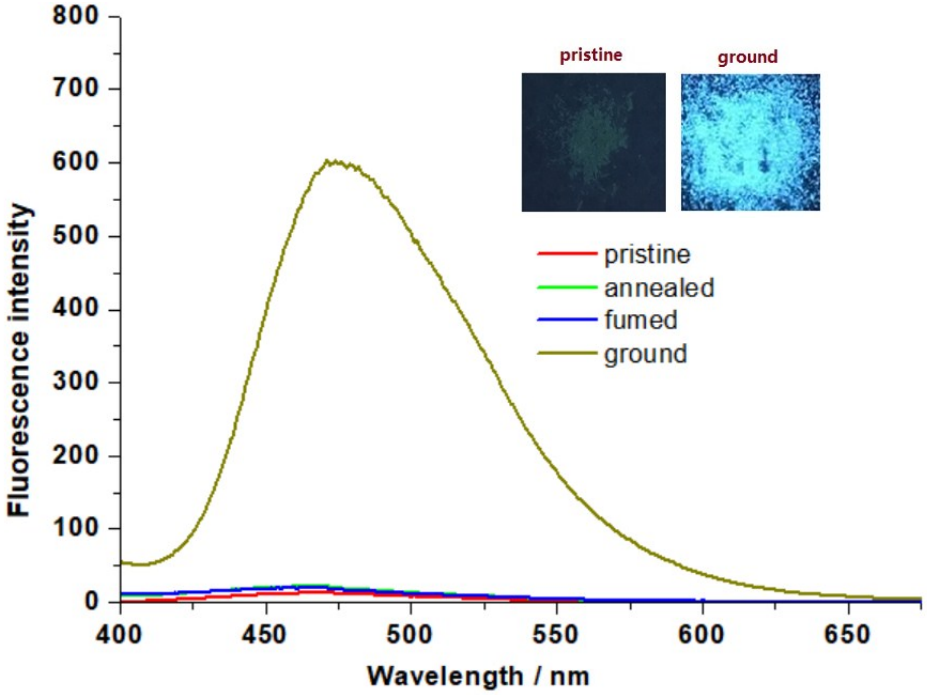


Fig. 15 Emission spectra (λ_{ex} =365 nm) and photos of compound $\mathbf{V_O}$ under different solid-state conditions (photos were taken under 365 nm UV light)

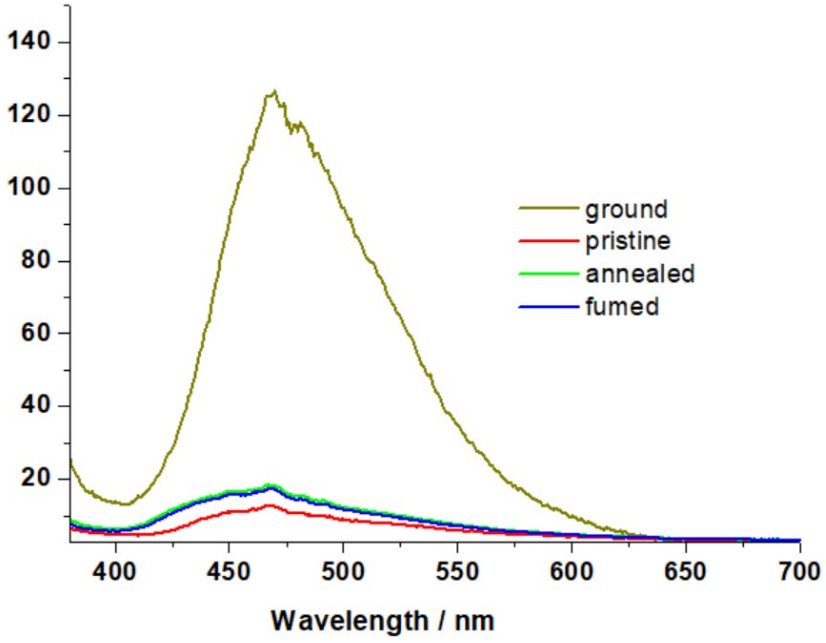


Fig. 16 Emission spectra(λ_{ex} =365 nm) of compound $\mathbf{V_{Am}}$ under different solid-state conditions

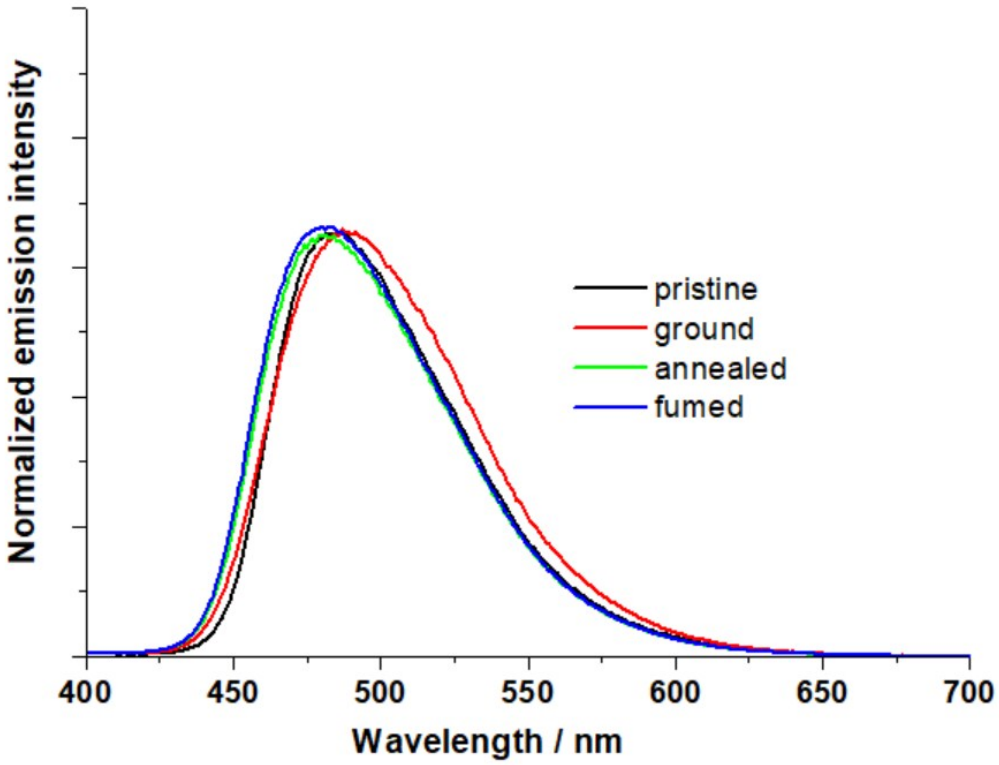


Fig. 17 Emission spectra (λ_{ex} =365 nm) of compound $\mathbf{V_{Bp}}$ under different solid-state conditions

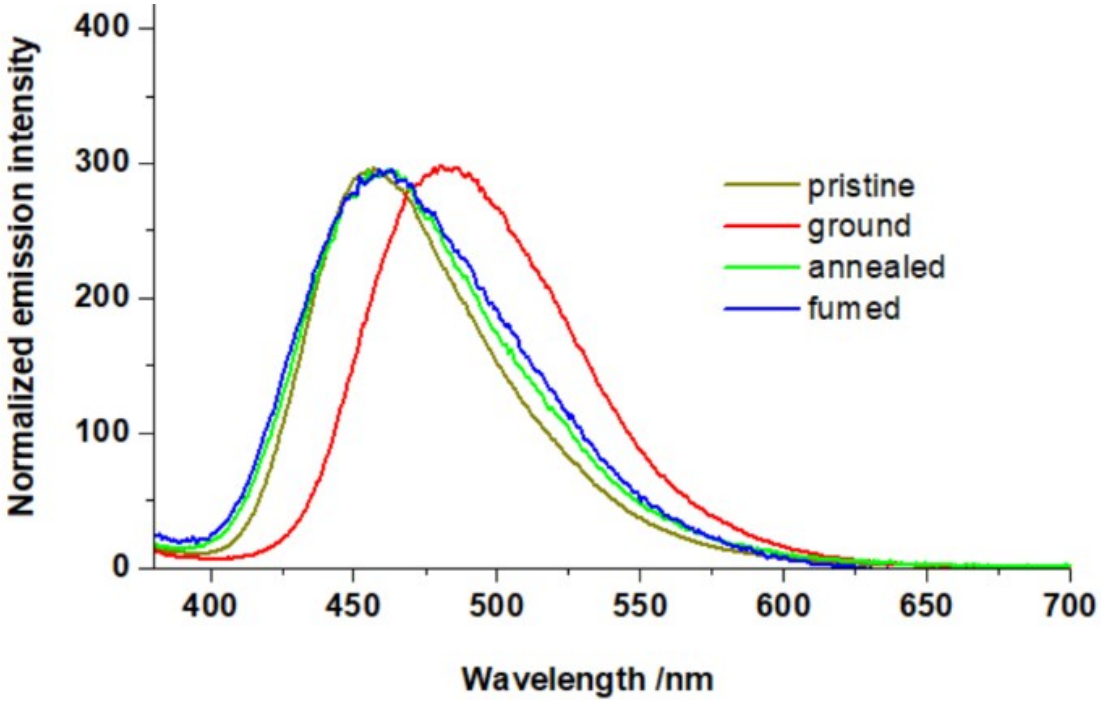


Fig. 18 Emission spectra (λ_{ex} =365 nm) of compound $\mathbf{V_{Ap}}$ under different solid-state conditions

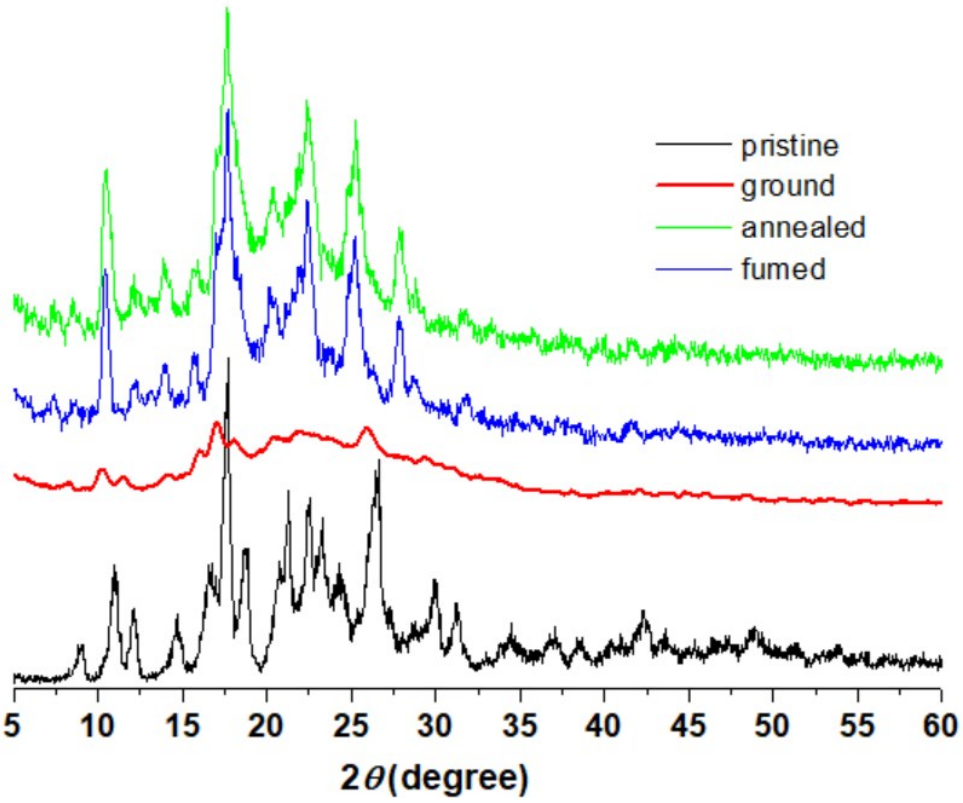


Fig. S19 PXRD patterns of compound $\mathbf{V_O}$ under different solid-state conditions

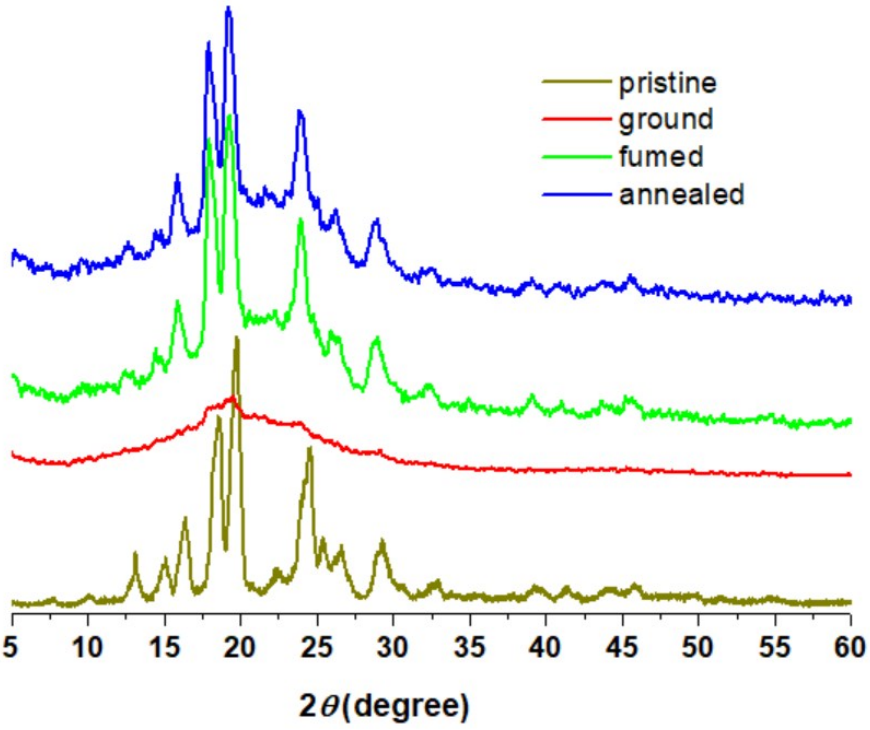


Fig. S20 PXRD patterns of compound $\mathbf{V_{Bp}}$ under different solid-state conditions

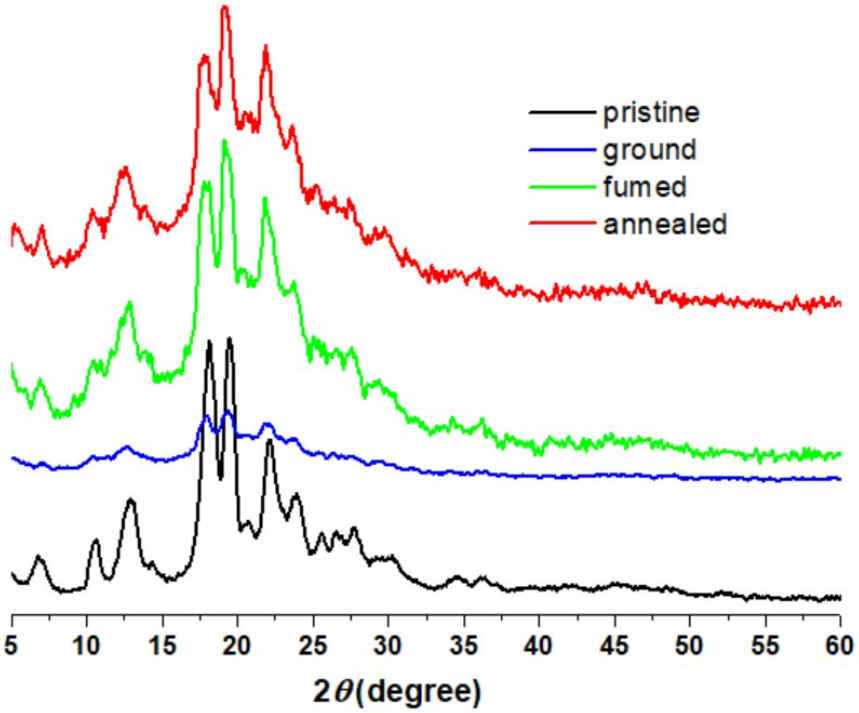


Fig. S21 PXRD patterns of compound $\mathbf{V_{Am}}$ under different solid-state condition

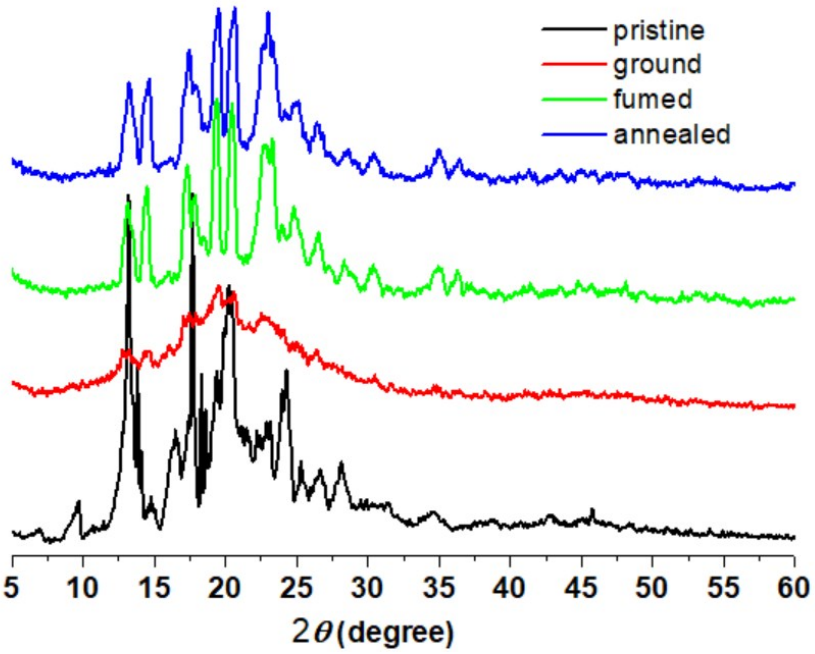


Fig. S22 PXRD patterns of compound $\mathbf{V_{Ap}}$ under different solid-state condition

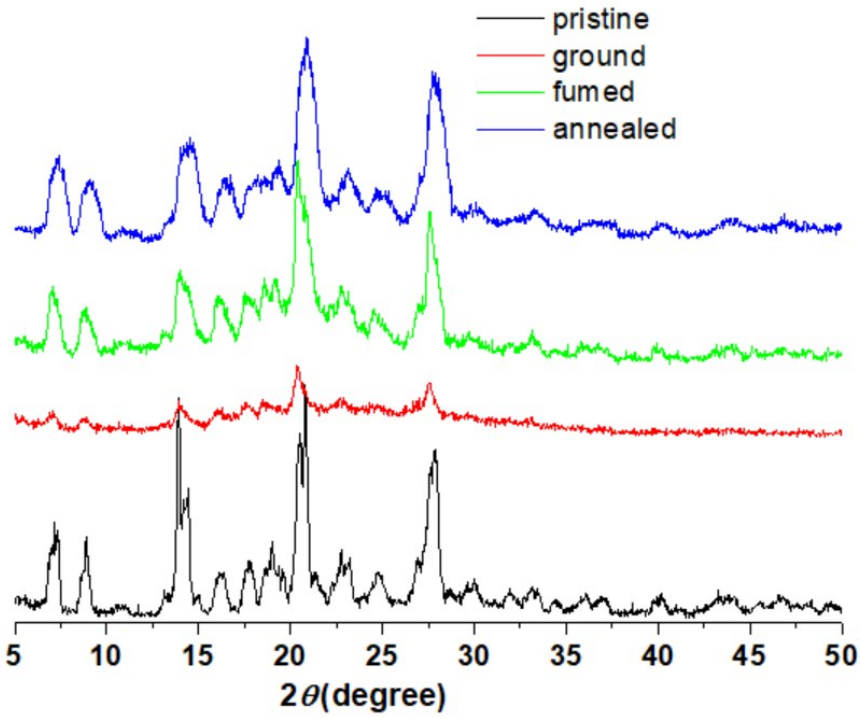


Fig. S23 PXRD patterns of compound **V** under different solid-state conditions

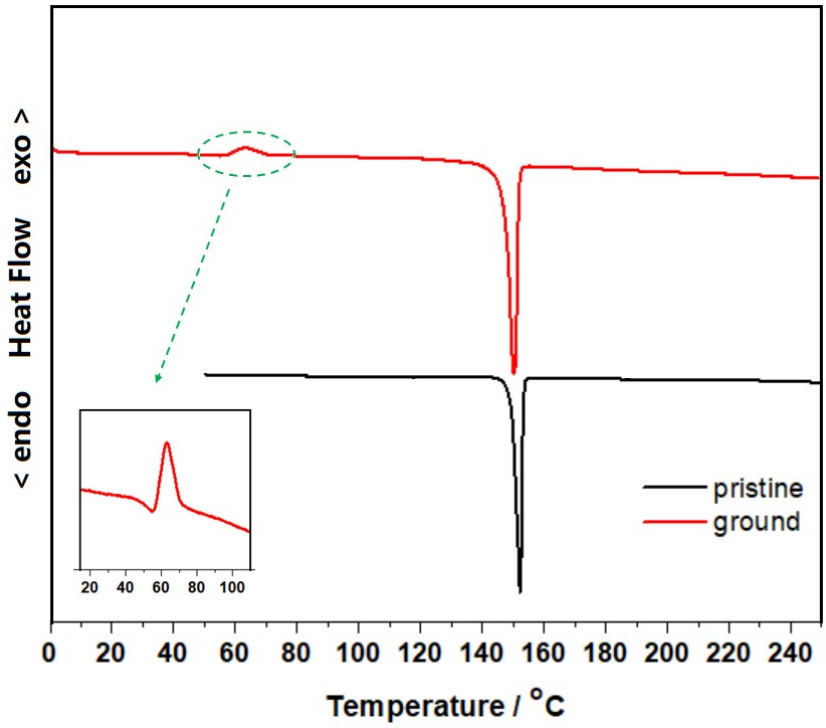


Fig. S24 Di□erential scanning calorimetry curves of $\mathbf{V_O}$ under different solid-state conditions

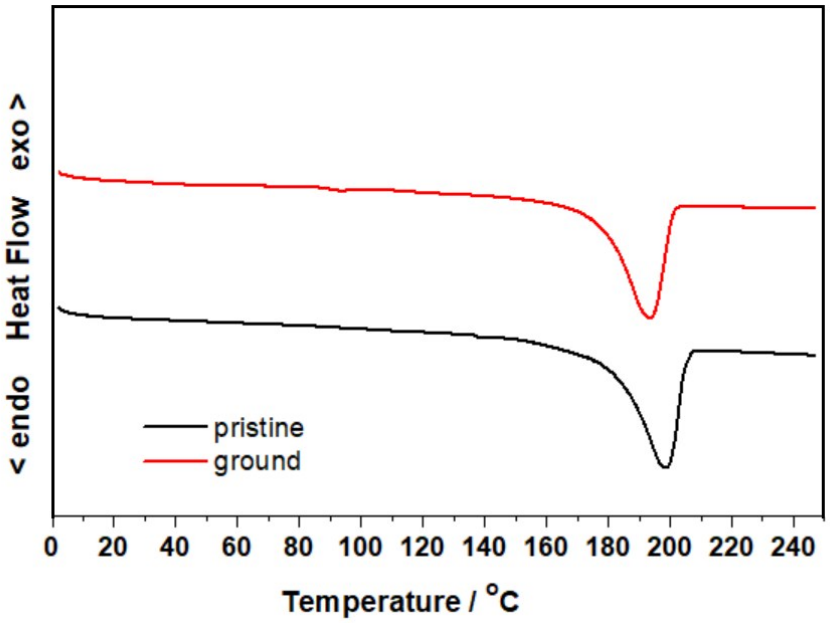


Fig. S25 Di□erential scanning calorimetry curves of $\mathbf{V_{Ap}}$ under different solid-state conditions

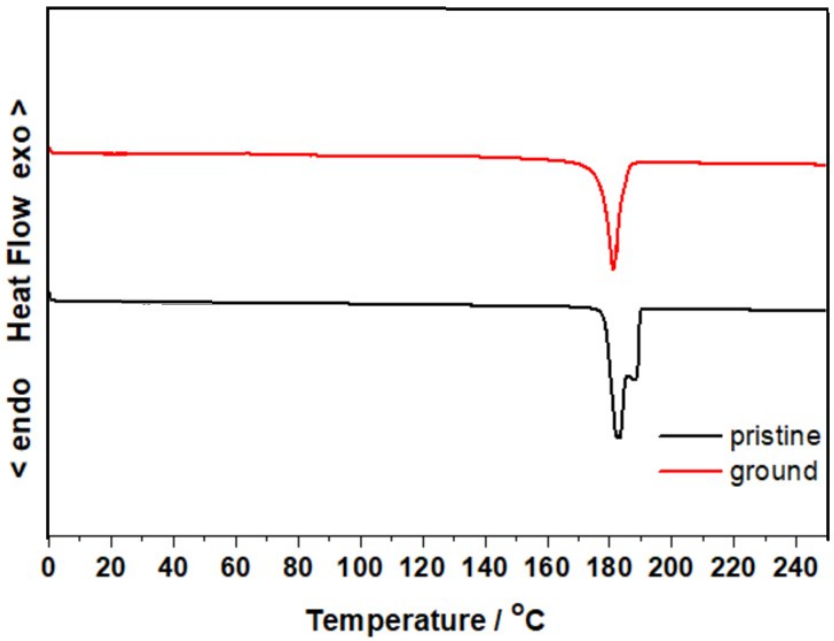


Fig. S26 Di□erential scanning calorimetry curves of $\mathbf{V_{Bp}}$ under different solid-state conditions

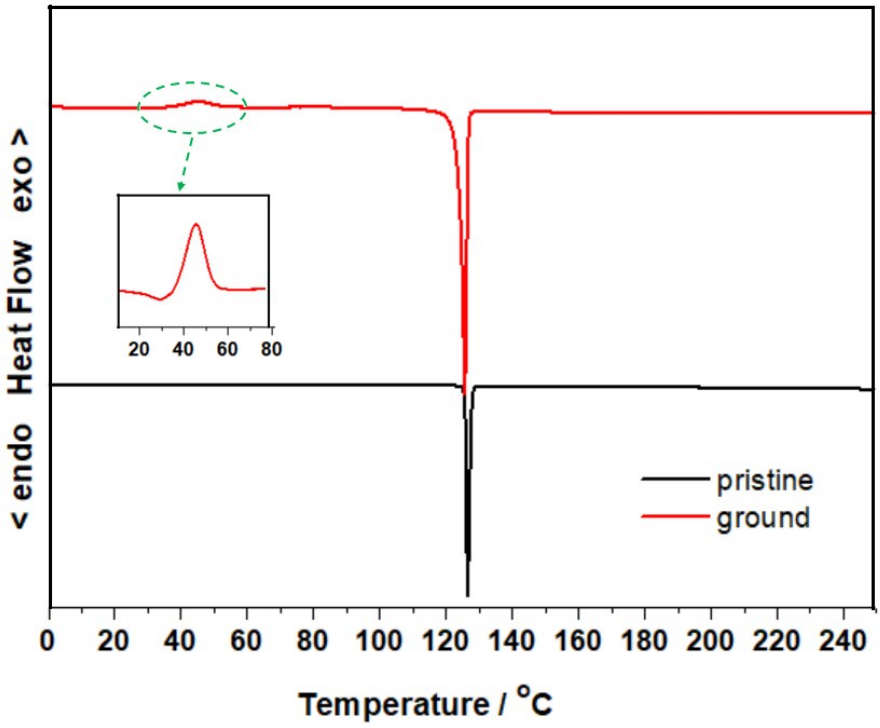


Fig. S27 Di□erential scanning calorimetry curves of **V** under different solid-state conditions

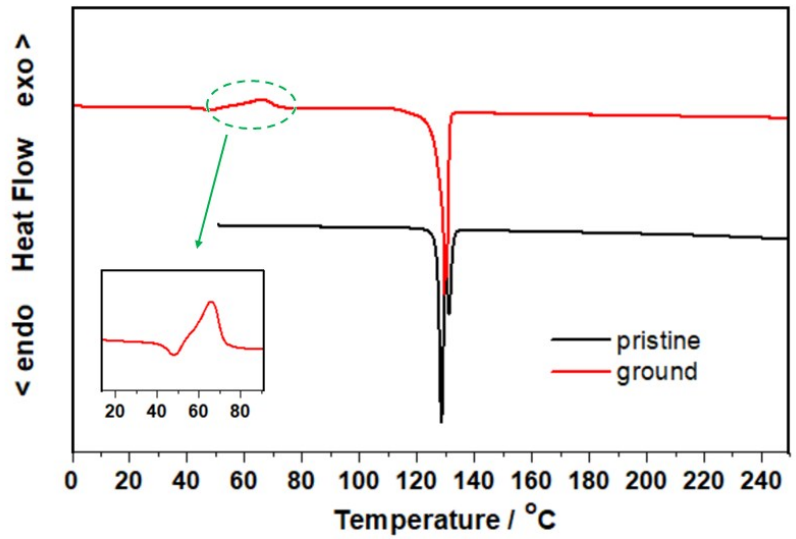
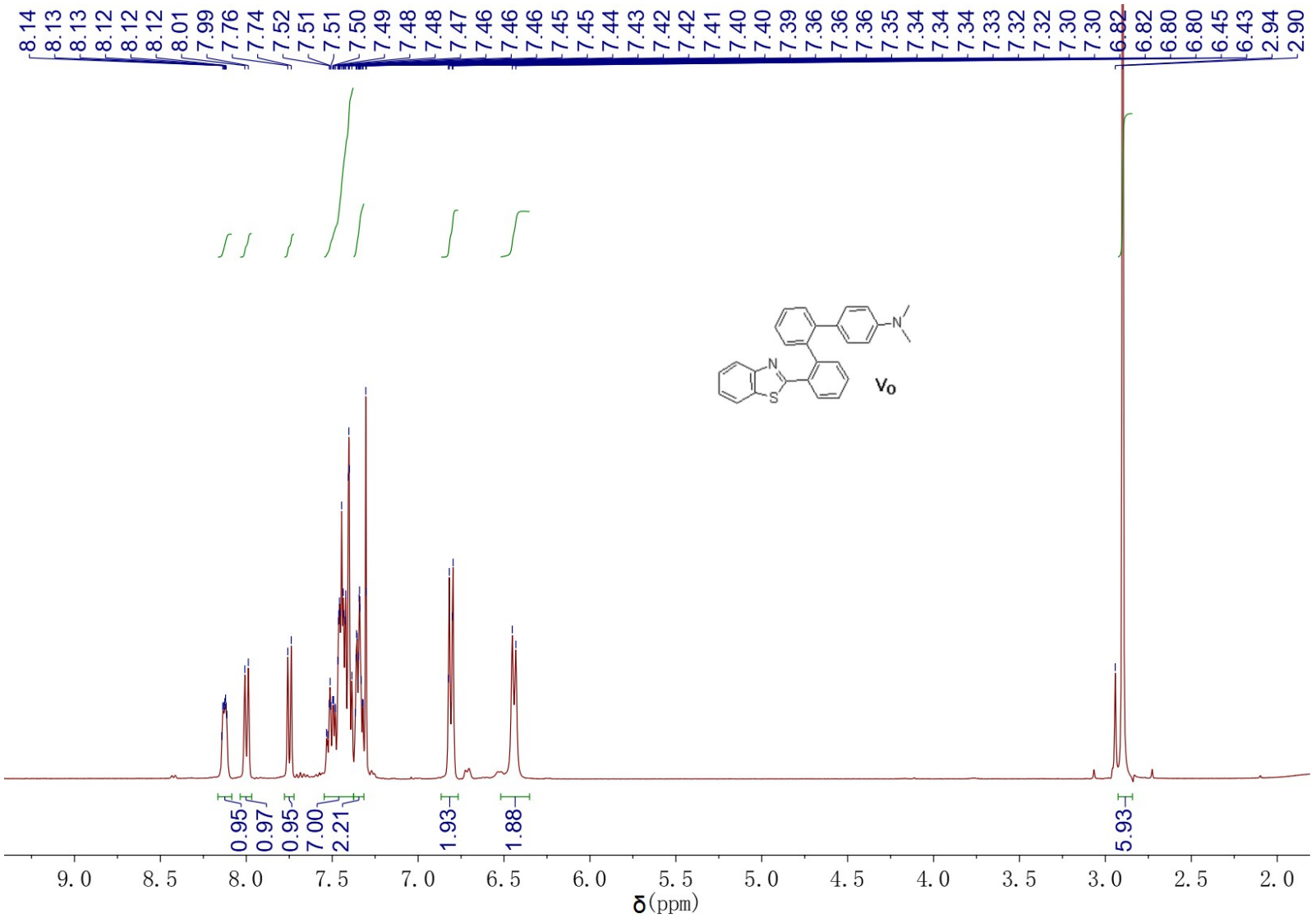
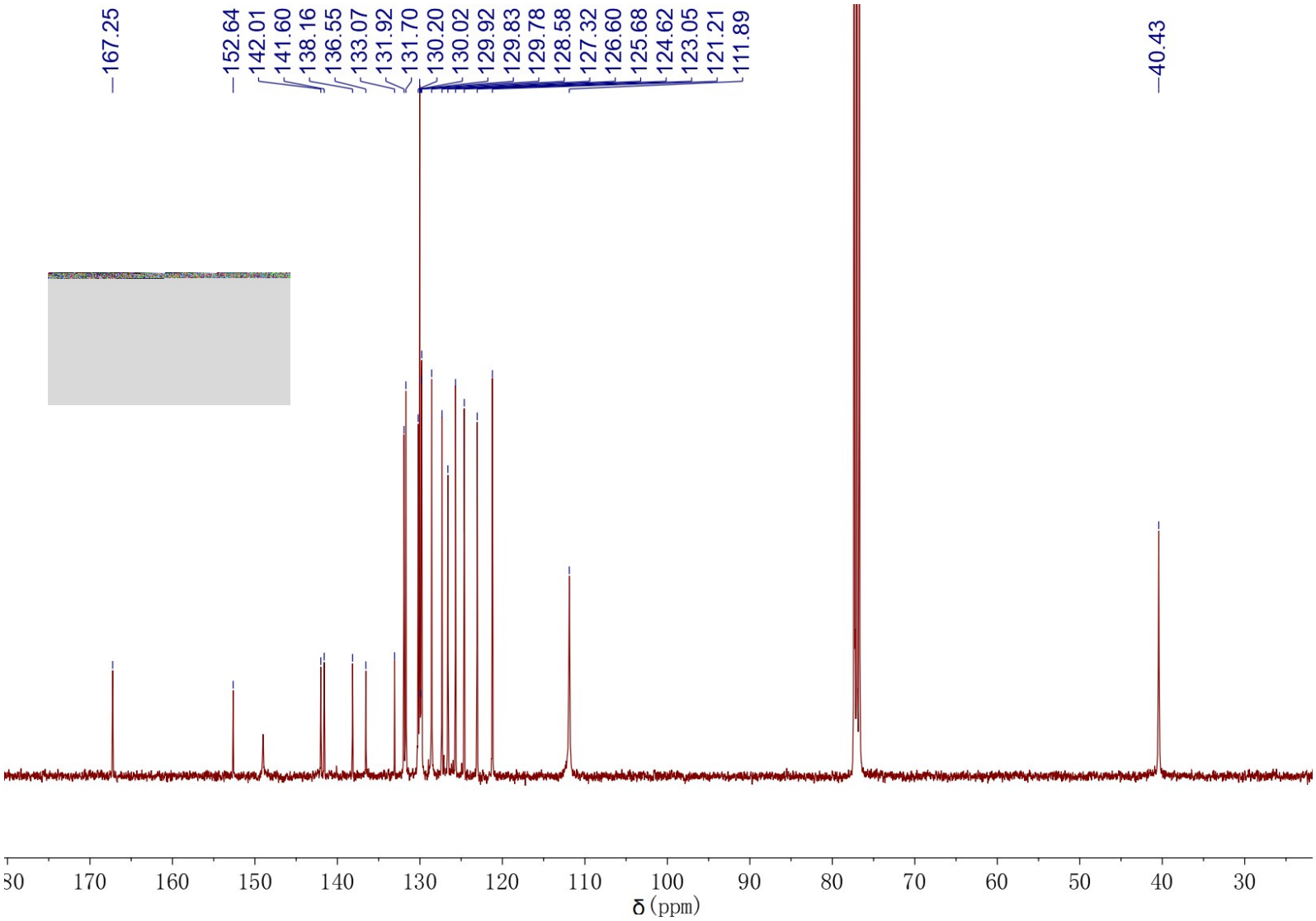
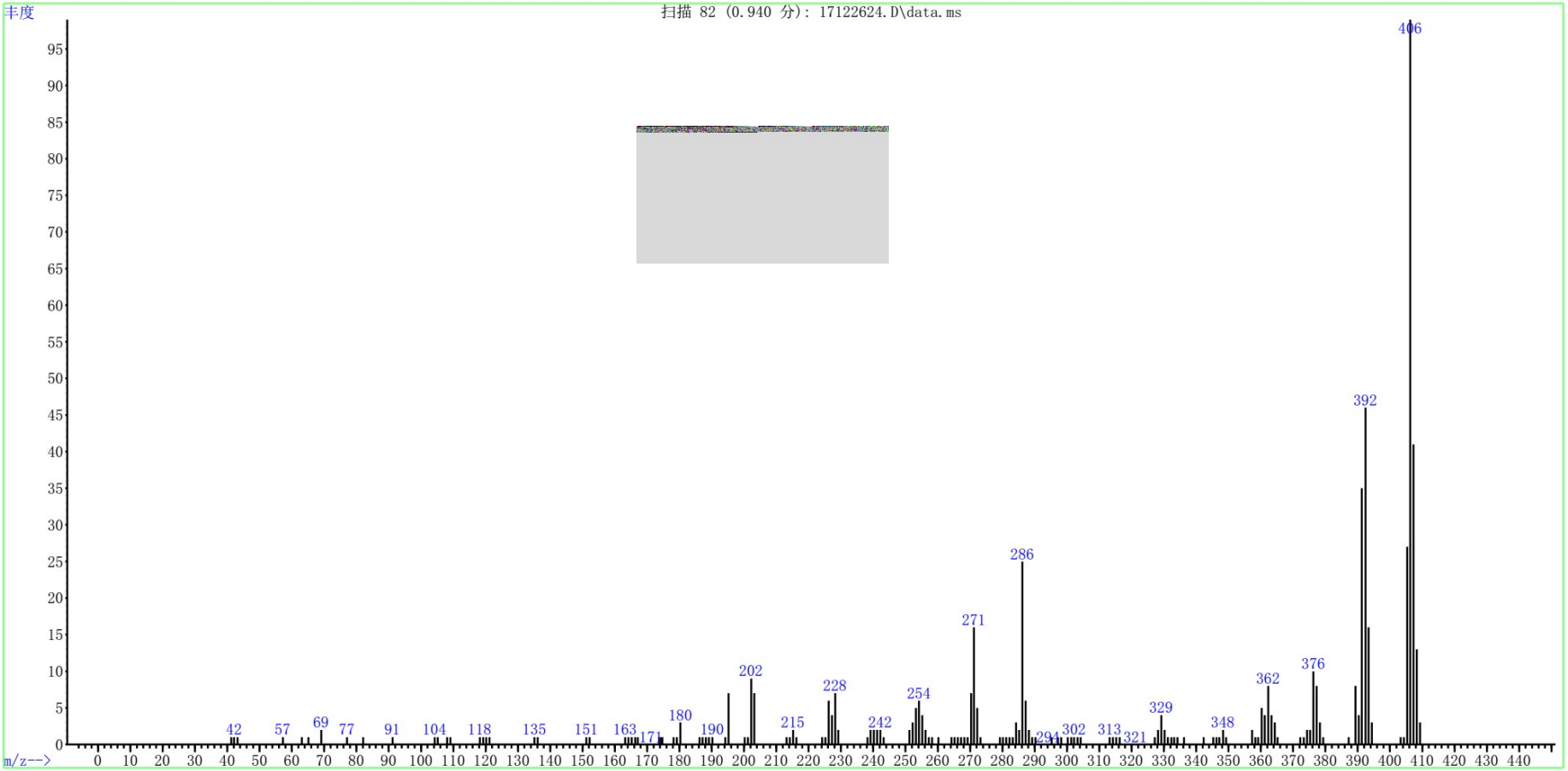


Fig. S28 Di□erential scanning calorimetry curves of $\mathbf{V_{Am}}$ under different solid-state conditions


8.14 8.13 8.13 8.12 8.12 8.12 8.01 7.99 7.76 7.74 7.52 7.51 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.43 7.42 7.42 7.41 7.40 7.40 7.39 7.36 7.36 7.36 7.35 7.34 7.34 7.34 7.33 7.32 7.32 7.30 7.30 6.82 6.82 6.80 6.80 6.45 6.43 2.94 2.90
N
S
V0
0.95 0.97 0.95 7.00 2.21 1.93 1.88 5.93
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
δ(ppm)


167.25
152.64
142.01
141.60
138.16
136.55
133.07
131.92
131.70
130.20
130.02
129.92
129.83
129.78
128.58
127.32
126.60
125.68
124.62
123.05
121.21
111.89
40.43
δ (ppm)


丰度
扫描 82 (0.940 分): 17122624.D\data.ms
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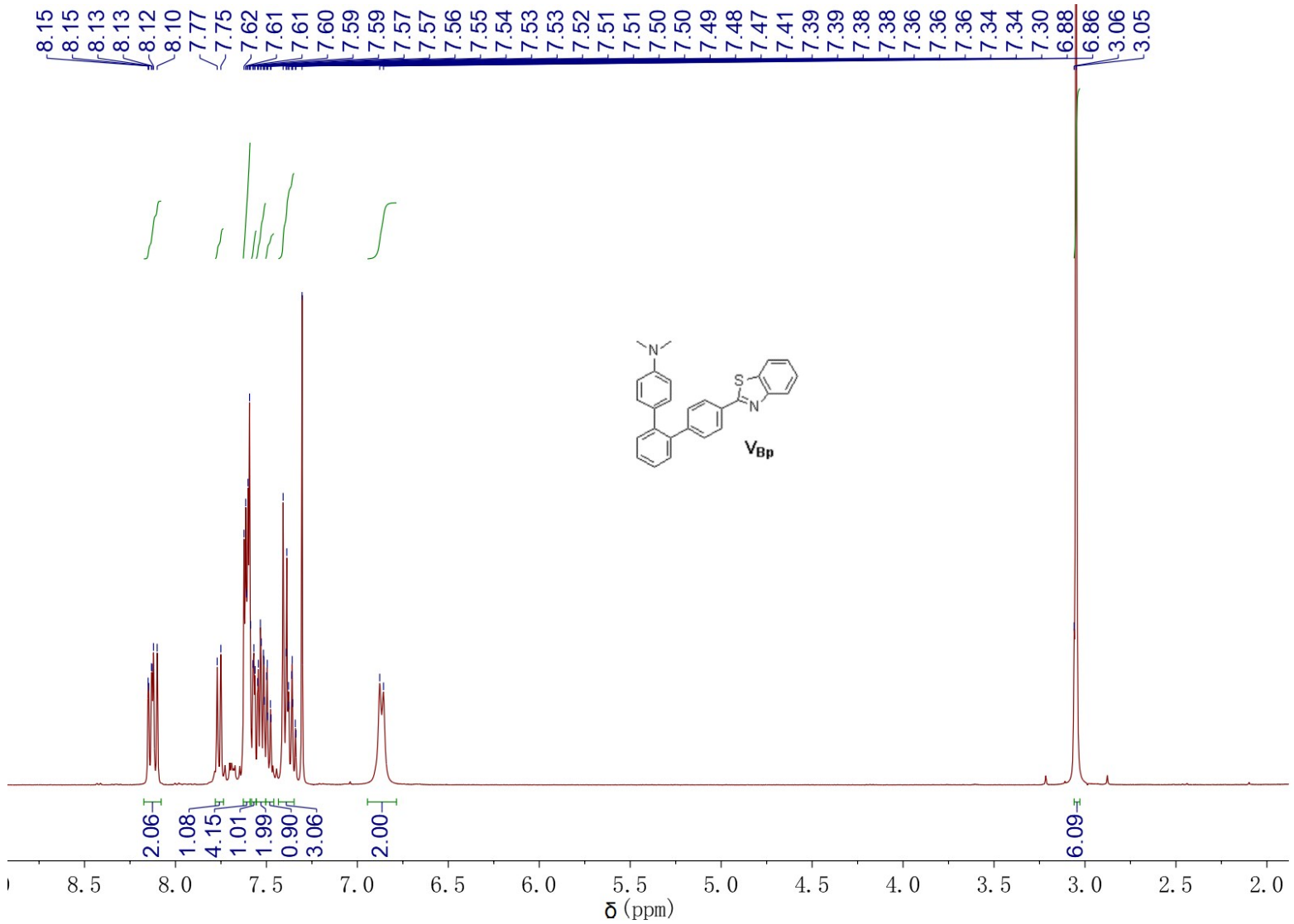
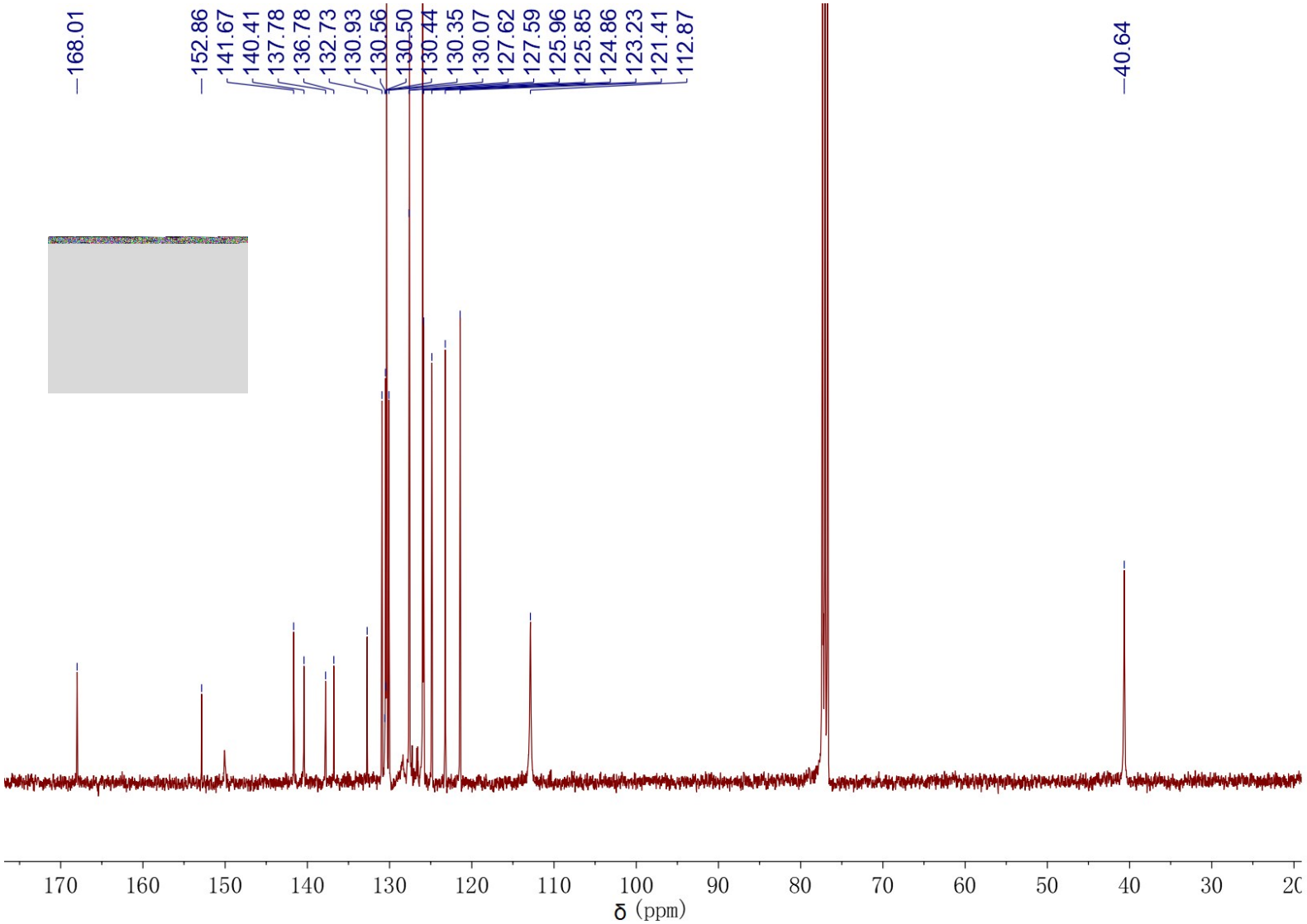
392
286
271
202
228
254
376
362
329
348
180
42
57
69
77
91
104
118
135
151
163
171
190
215
242
294
302
313
321


8.15
8.15
8.13
8.13
8.12
8.10
7.77
7.75
7.62
7.61
7.61
7.60
7.59
7.59
7.57
7.57
7.56
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.48
7.47
7.41
7.39
7.39
7.38
7.38
7.36
7.36
7.36
7.34
7.34
7.30
6.88
6.86
3.06
3.05
N
S
N
VBp
2.06
1.08
4.15
1.01
1.99
0.90
3.06
2.00
6.09
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
δ (ppm)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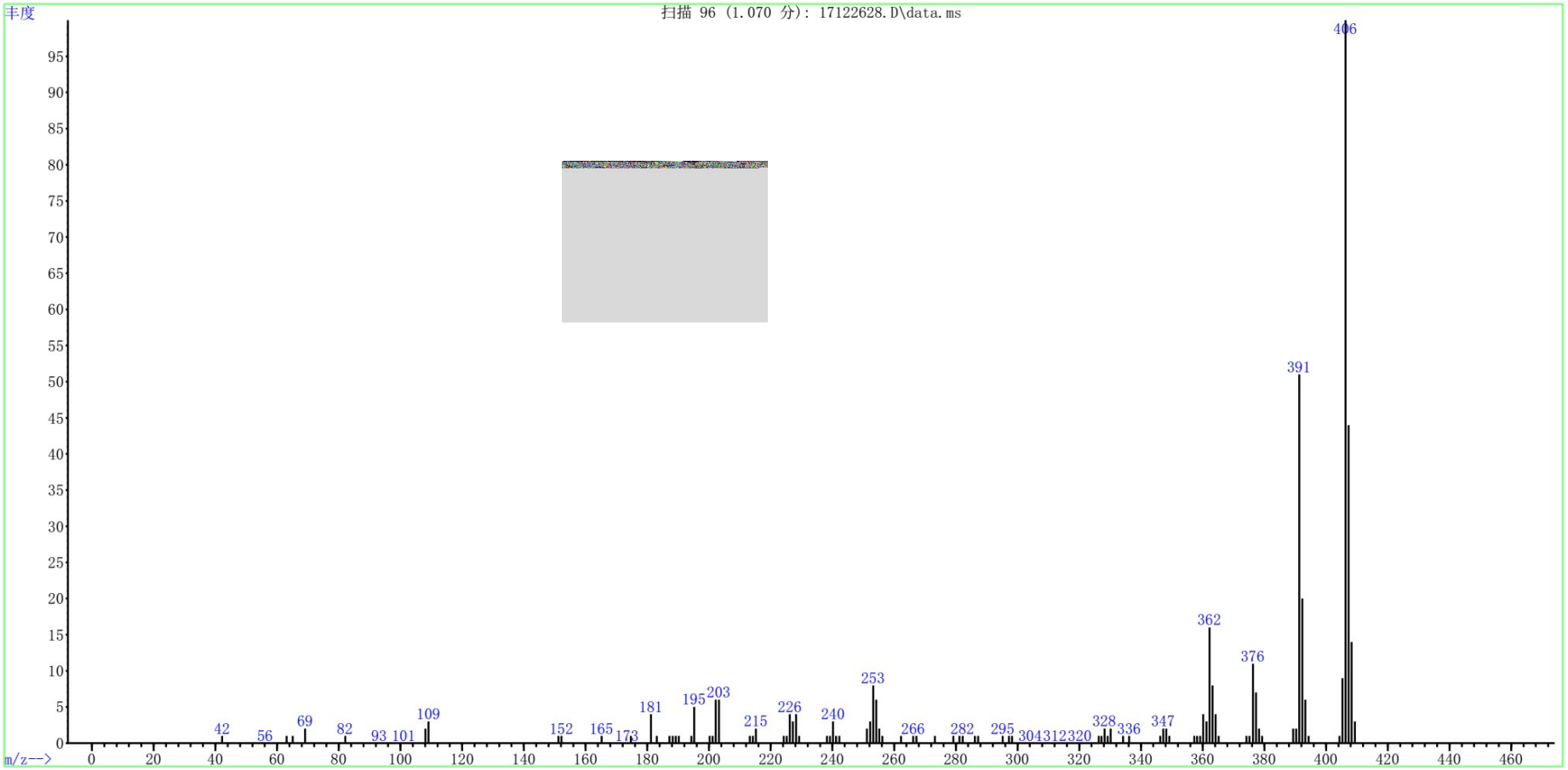
152.86
141.67
140.41
137.78
136.78
132.73
130.93
130.56
130.50
130.44
130.35
130.07
127.62
127.59
125.96
125.85
124.86
123.23
121.41
112.87
40.64
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
δ (ppm)


丰度
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362
376
253
203
195
181
109
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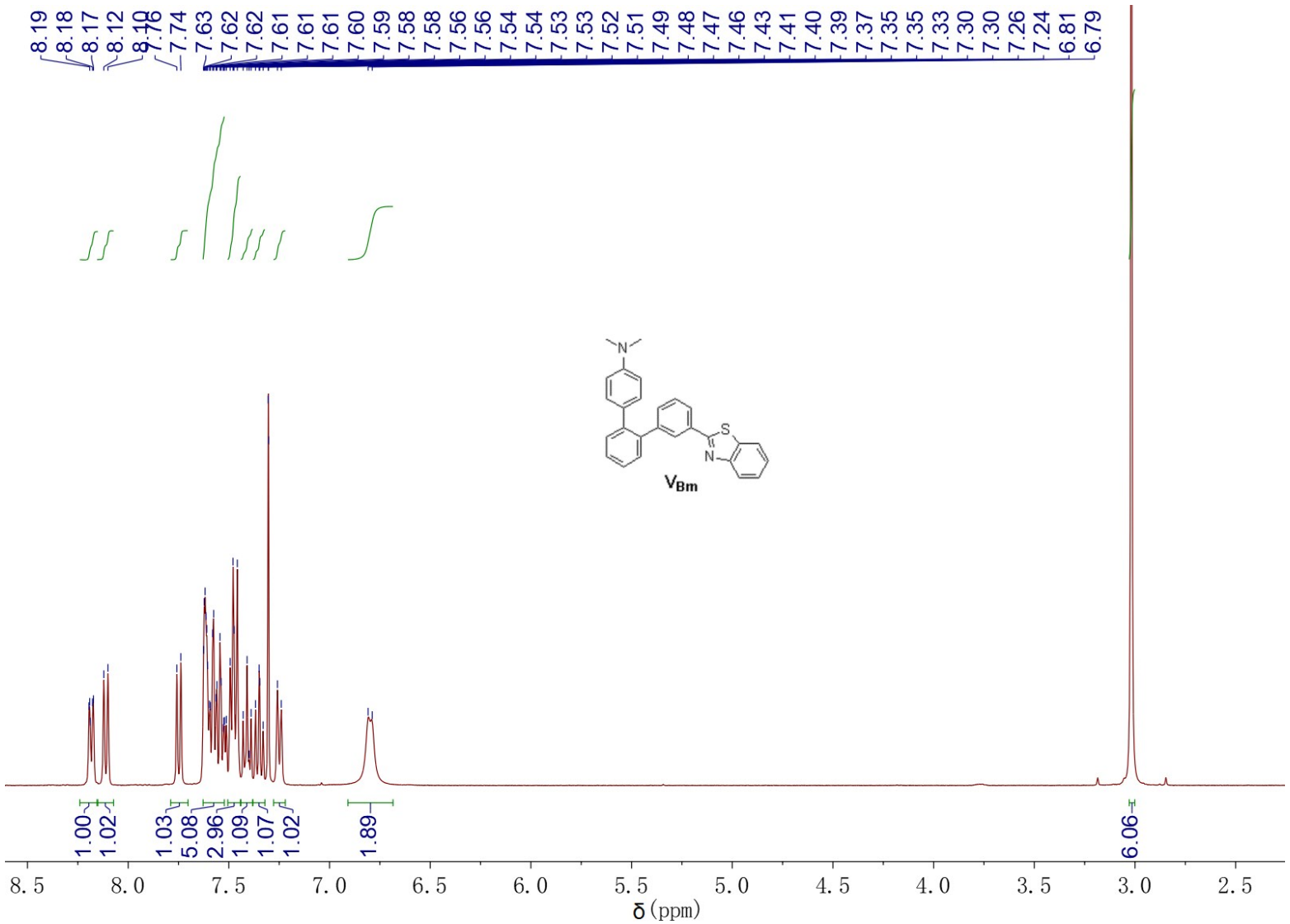
42
56
82
93
101
152
165
173
215
226
240
266
282
295
304
312
320
328
336
347
m/z-->
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0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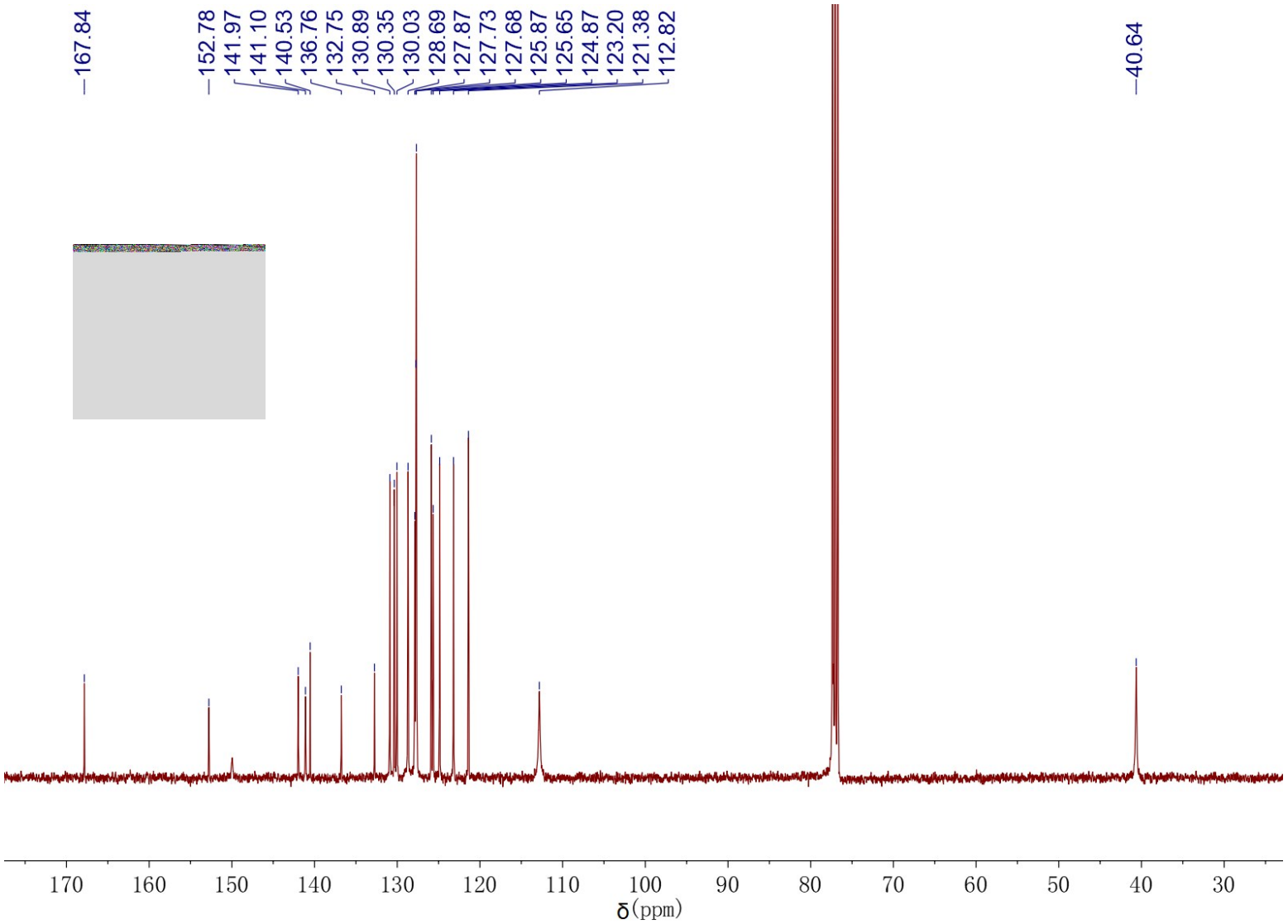
8.17
8.12
8.10
7.76
7.74
7.63
7.62
7.62
7.61
7.61
7.61
7.60
7.59
7.58
7.58
7.56
7.56
7.54
7.54
7.53
7.53
7.52
7.51
7.49
7.48
7.47
7.46
7.43
7.41
7.40
7.39
7.37
7.35
7.35
7.33
7.30
7.30
7.26
7.24
6.81
6.79
N
S
N
V_Bm
1.00
1.02
1.03
5.08
2.96
1.09
1.07
1.02
1.89
6.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
δ (ppm)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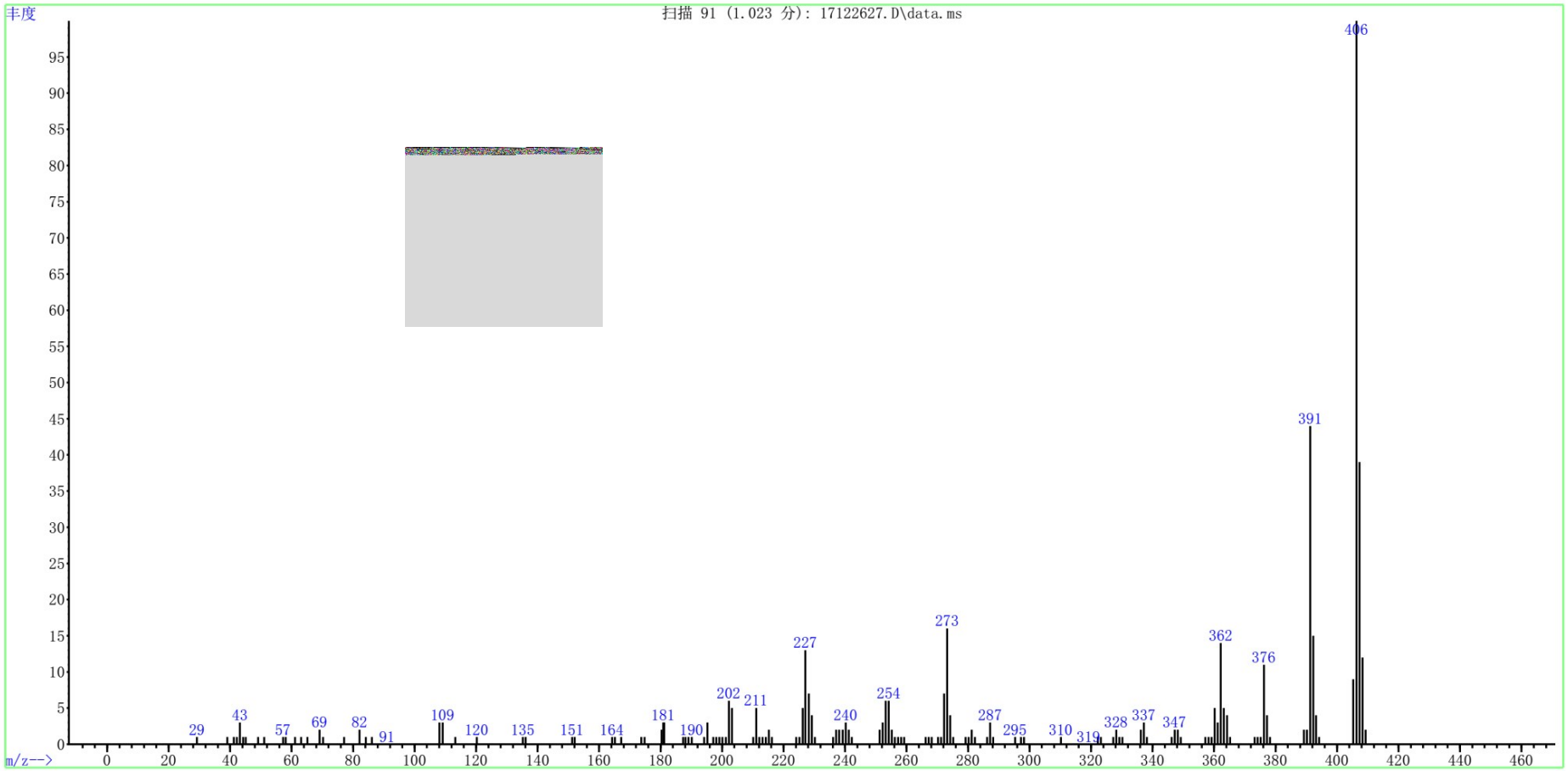
141.97
141.10
140.53
136.76
132.75
130.89
130.35
130.03
128.69
127.87
127.73
127.68
125.87
125.65
124.87
123.20
121.38
112.82
40.64
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
δ(ppm)


丰度
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227
362
376
202
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254
287
240
109
43
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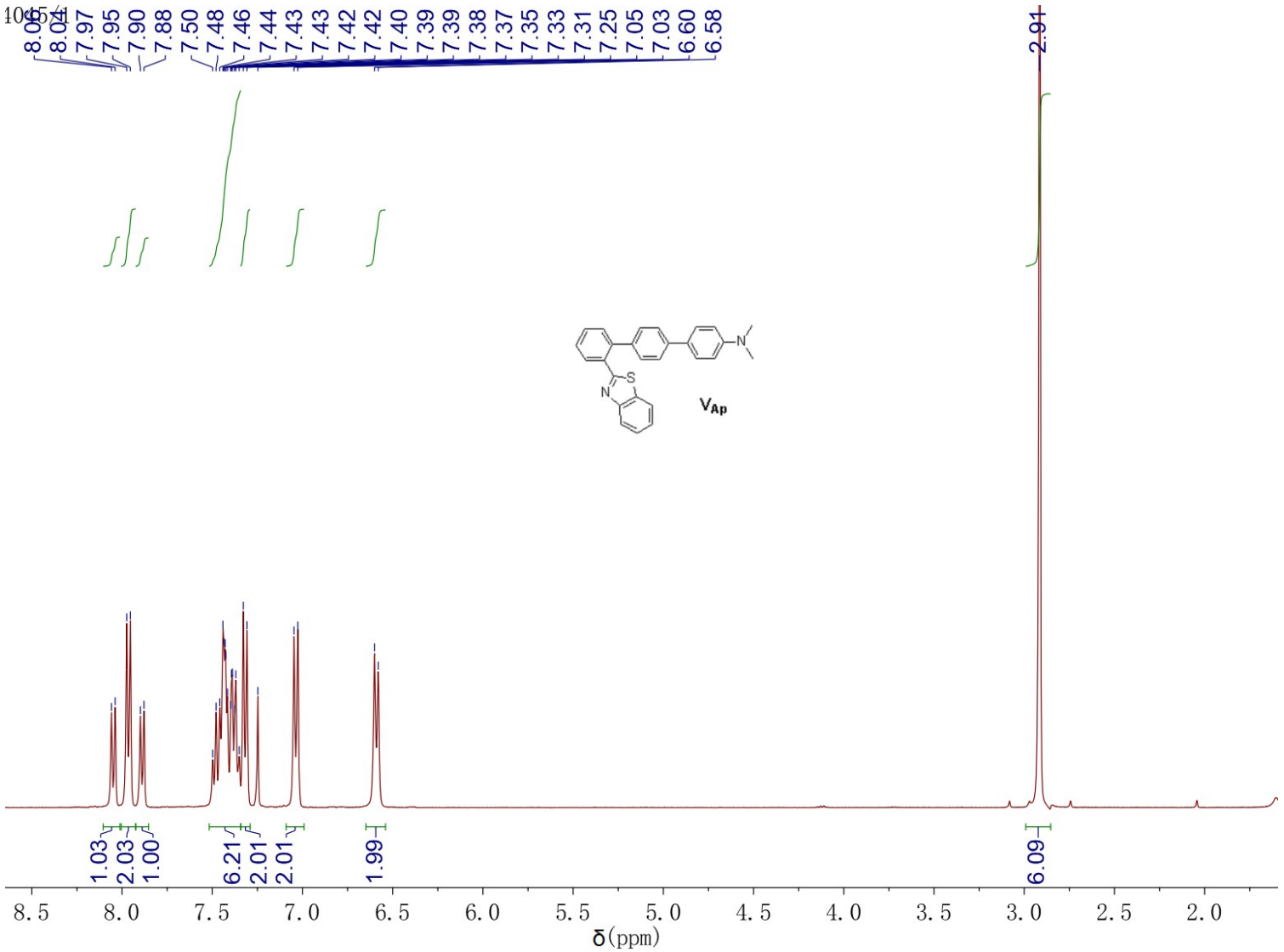
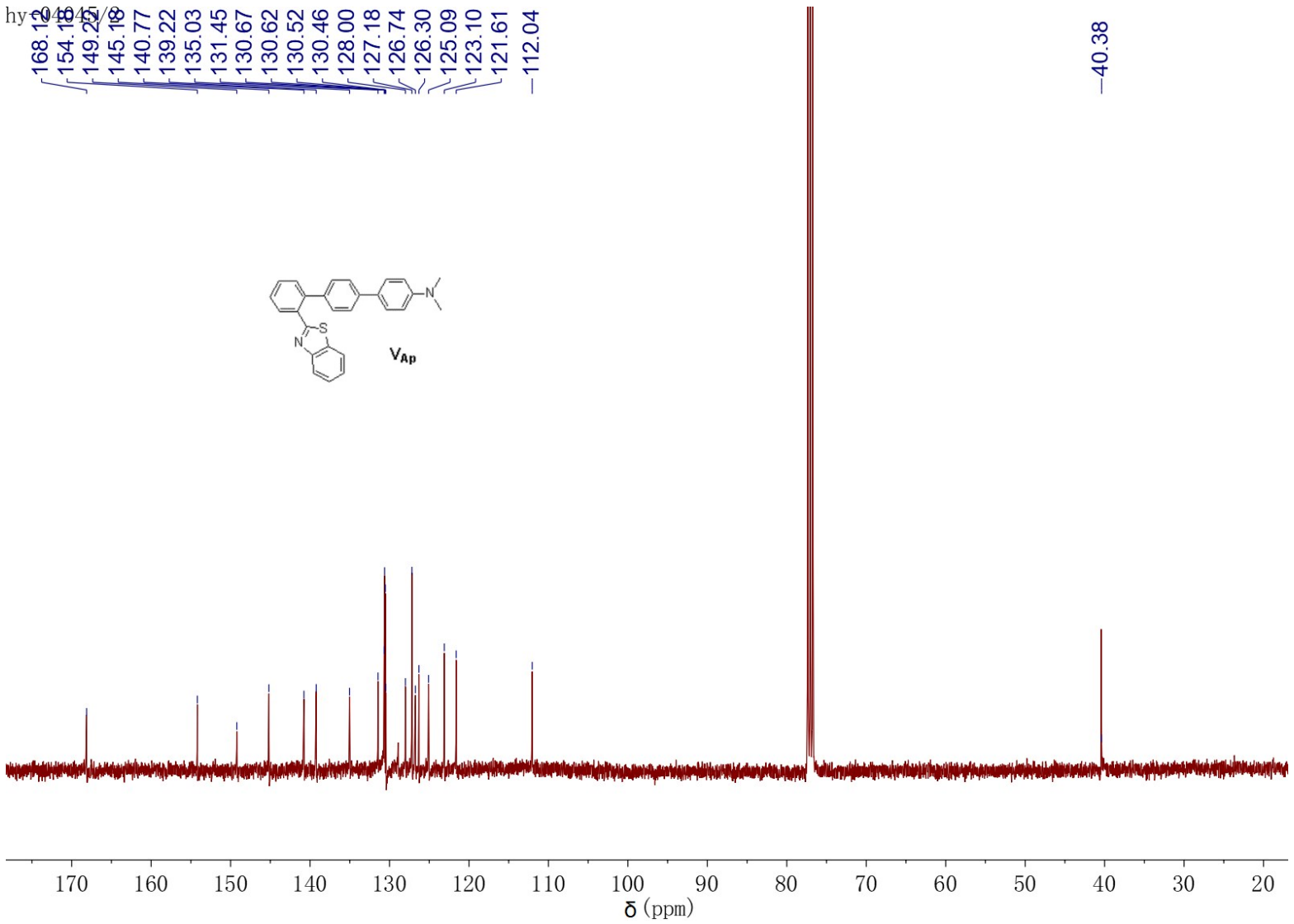
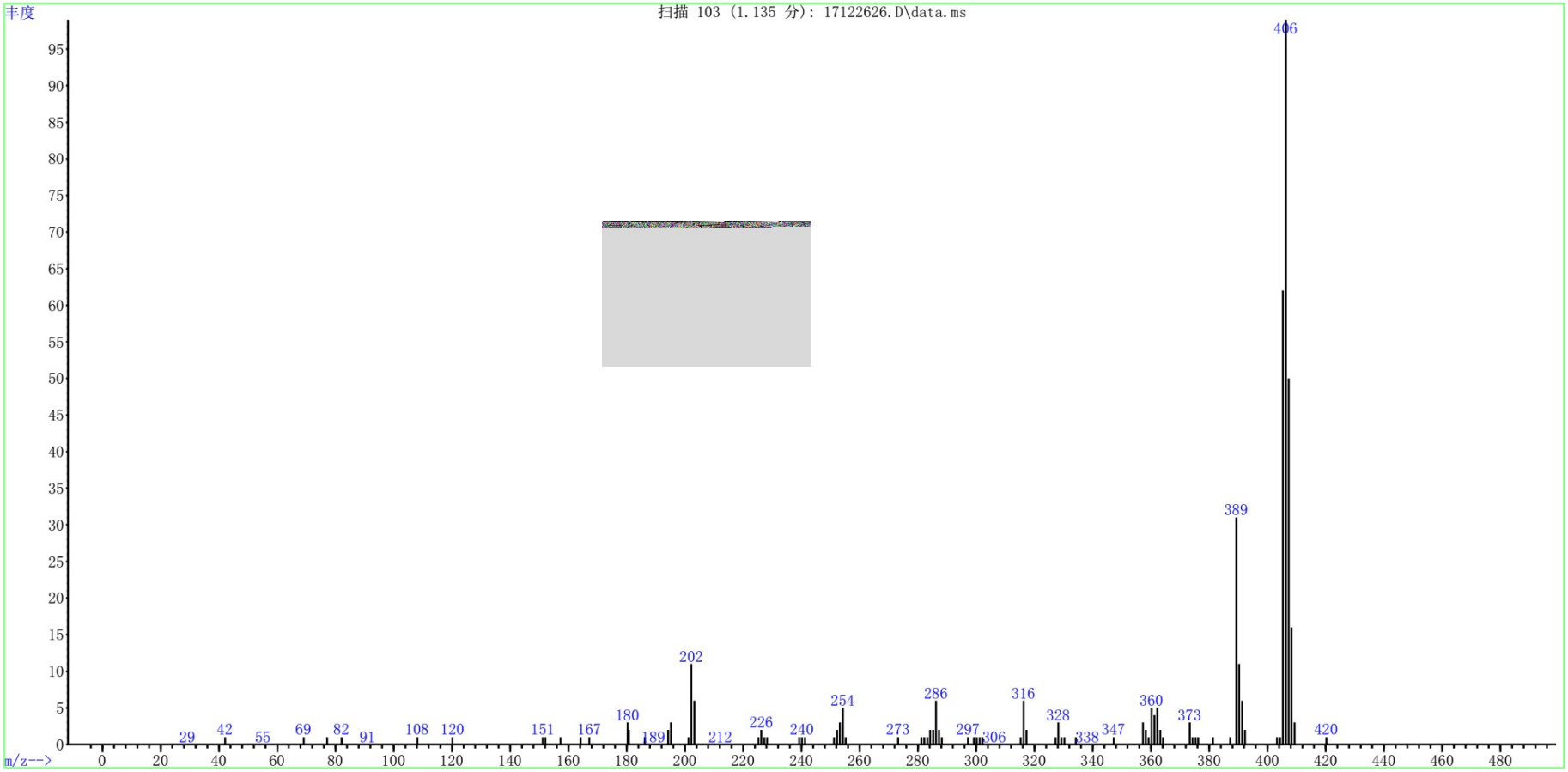
82
91
29
57
120
135
151
164
181
190
295
310
319
328
337
347


8.05
8.04
7.97
7.95
7.90
7.88
7.50
7.48
7.46
7.44
7.43
7.43
7.42
7.42
7.40
7.39
7.39
7.38
7.37
7.35
7.33
7.31
7.25
7.05
7.03
6.60
6.58
2.91
VAp
1.03
2.03
1.00
6.21
2.01
2.01
1.99
6.09
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
δ(ppm)


hy-04045/2
168.12
154.13
149.25
145.18
140.77
139.22
135.03
131.45
130.67
130.62
130.52
130.46
128.00
127.18
126.74
126.30
125.09
123.10
121.61
112.04
40.38
N
S
N
VAp
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
δ (ppm)


丰度
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406
389
202
m/z-->
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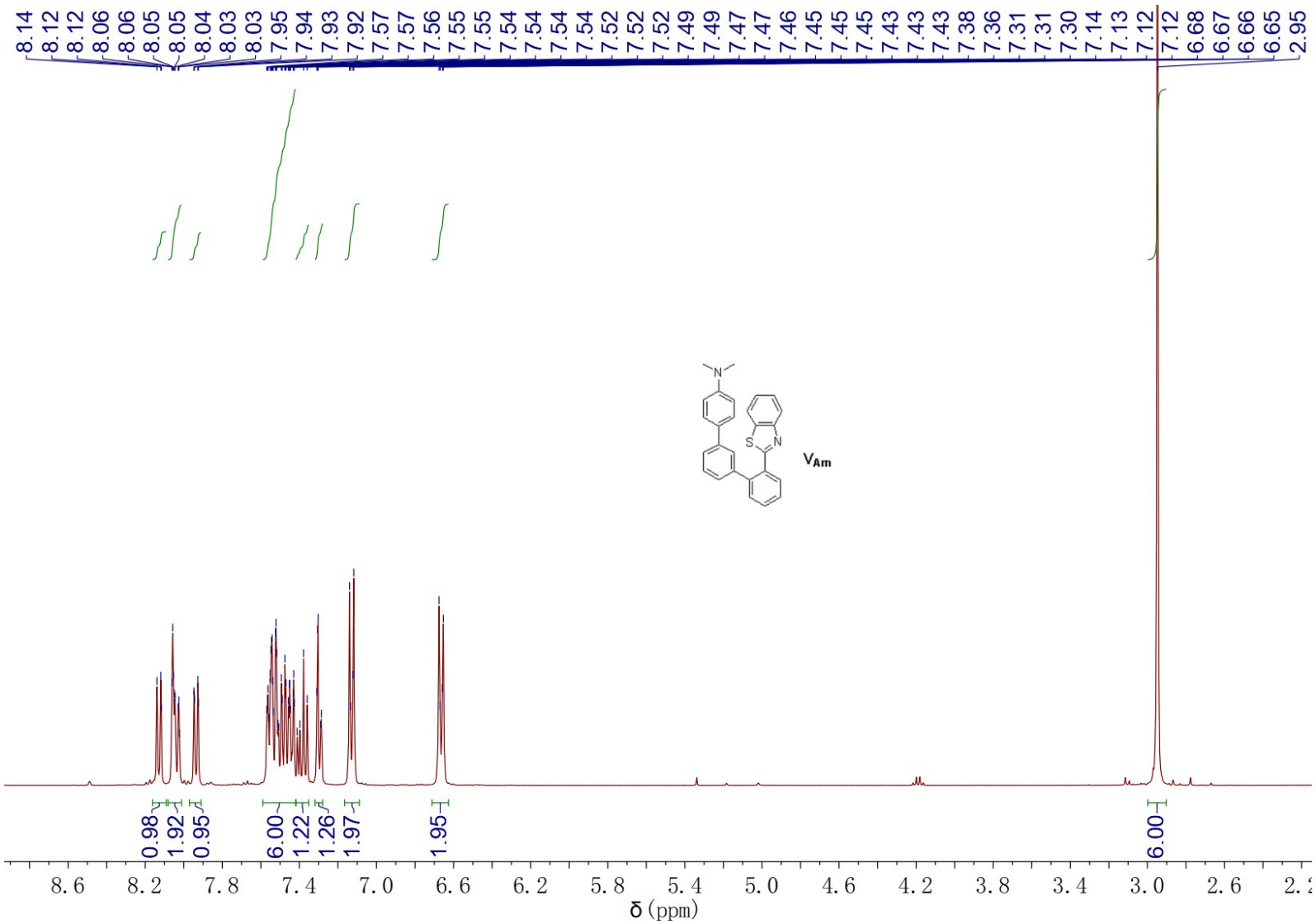
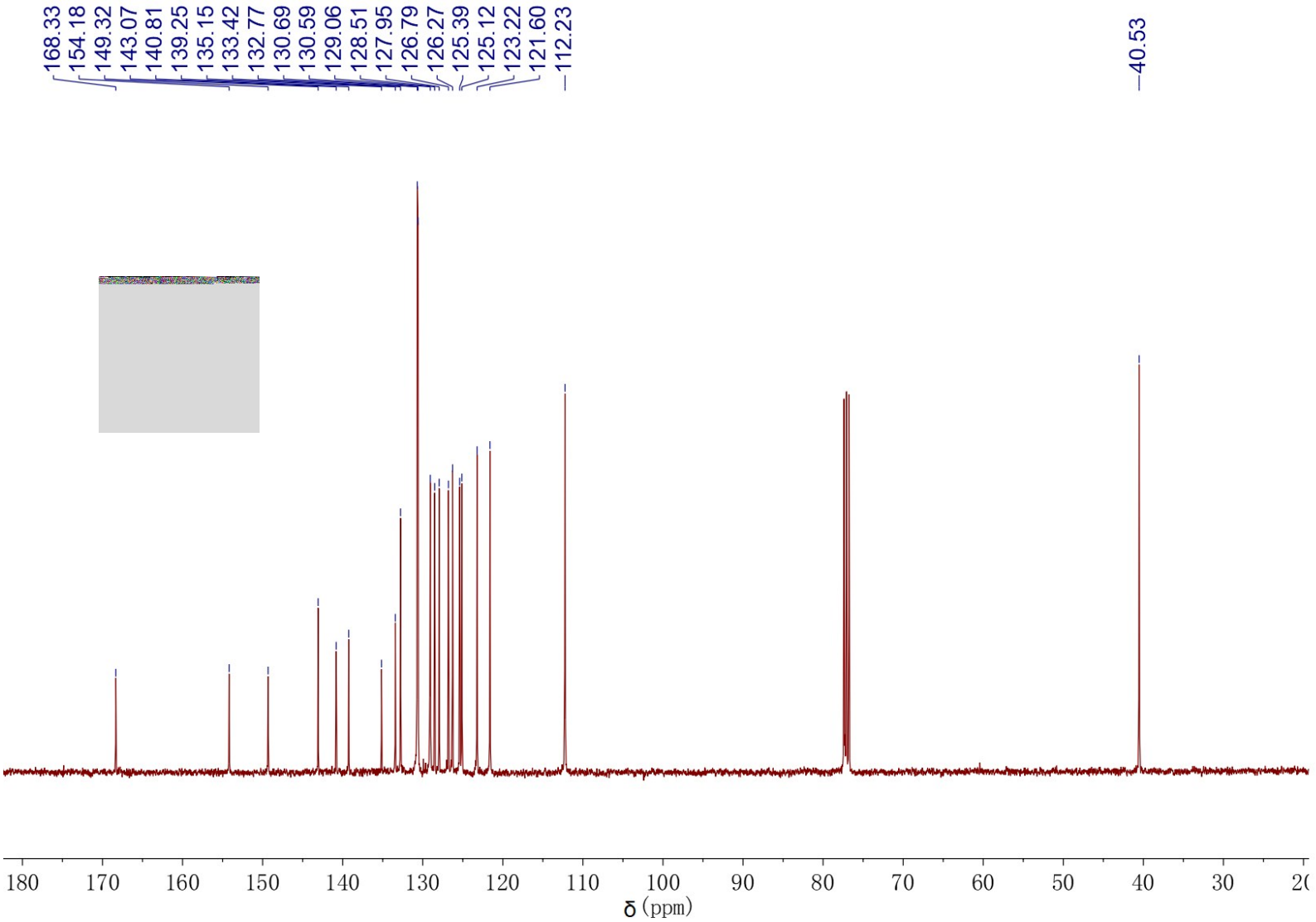
95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
29 42 55 69 82 91 108 120 151 167 180 189 212 226 240 254 273 286 297 306 316 328 338 347 360 373 420


8.14 8.12 8.12 8.06 8.06 8.05 8.05 8.04 8.03 8.03 7.95 7.94 7.93 7.92 7.57 7.57 7.56 7.55 7.55 7.54 7.54 7.54 7.54 7.52 7.52 7.52 7.49 7.49 7.47 7.47 7.46 7.45 7.45 7.45 7.43 7.43 7.43 7.38 7.36 7.31 7.31 7.30 7.14 7.13 7.12 7.12 6.68 6.67 6.66 6.65 2.95
N
S
N
VAm
0.98 1.92 0.95 6.00 1.22 1.26 1.97 1.95 6.00
8.6 8.2 7.8 7.4 7.0 6.6 6.2 5.8 5.4 5.0 4.6 4.2 3.8 3.4 3.0 2.6
δ (ppm)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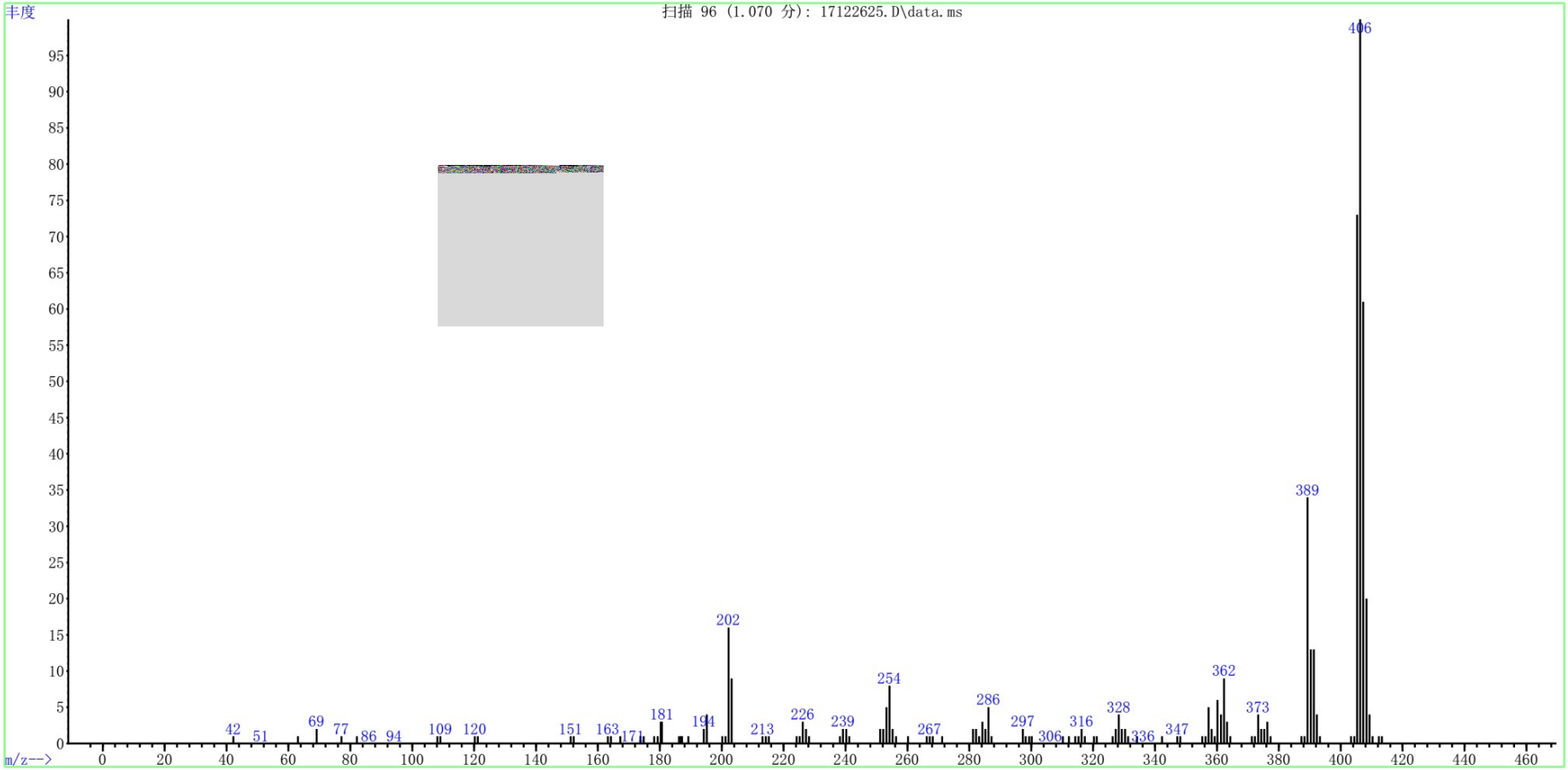
149.32
143.07
140.81
139.25
135.15
133.42
132.77
130.69
130.59
129.06
128.51
127.95
126.79
126.27
125.39
125.12
123.22
121.60
112.23
40.53
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
δ (ppm)


丰度
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202
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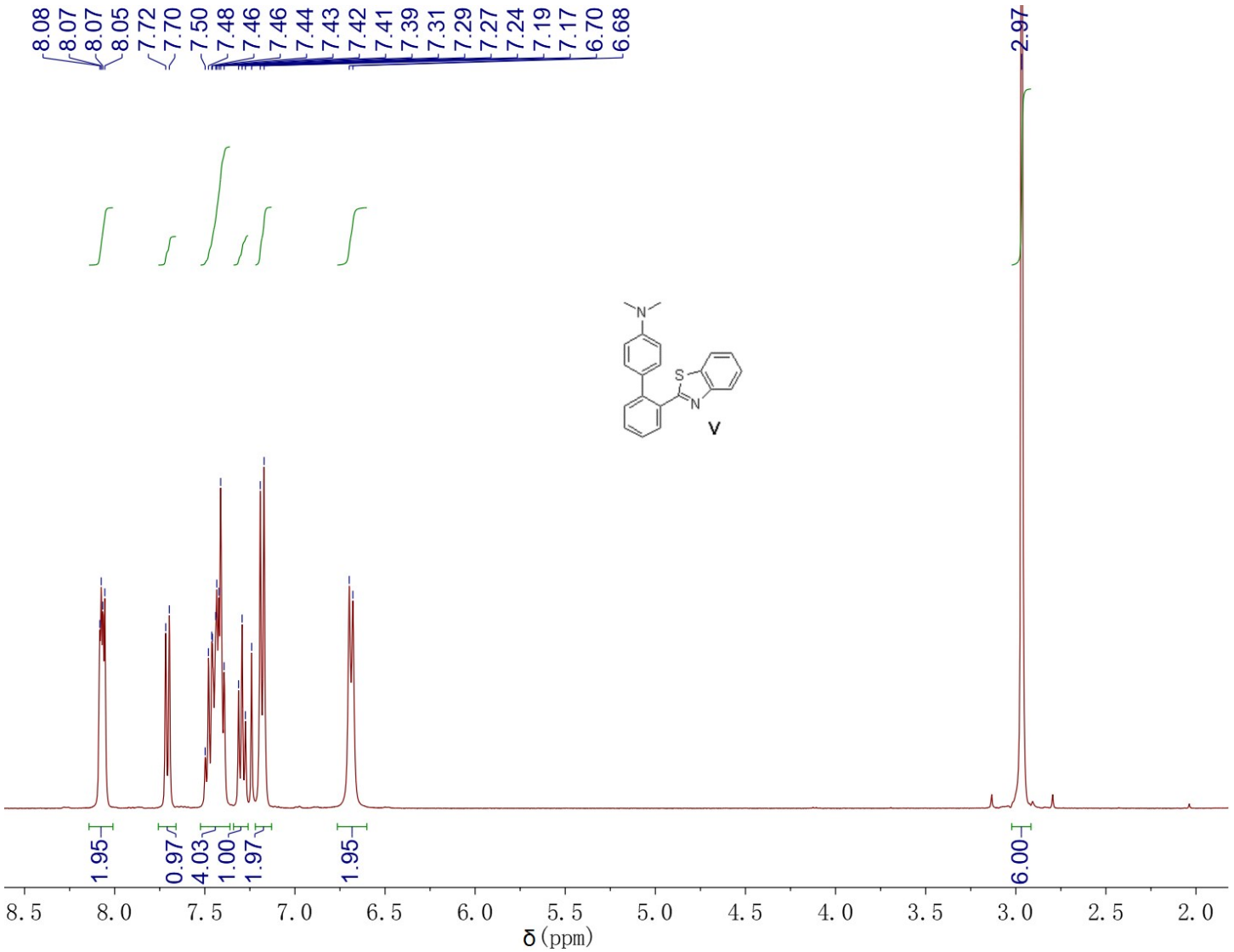
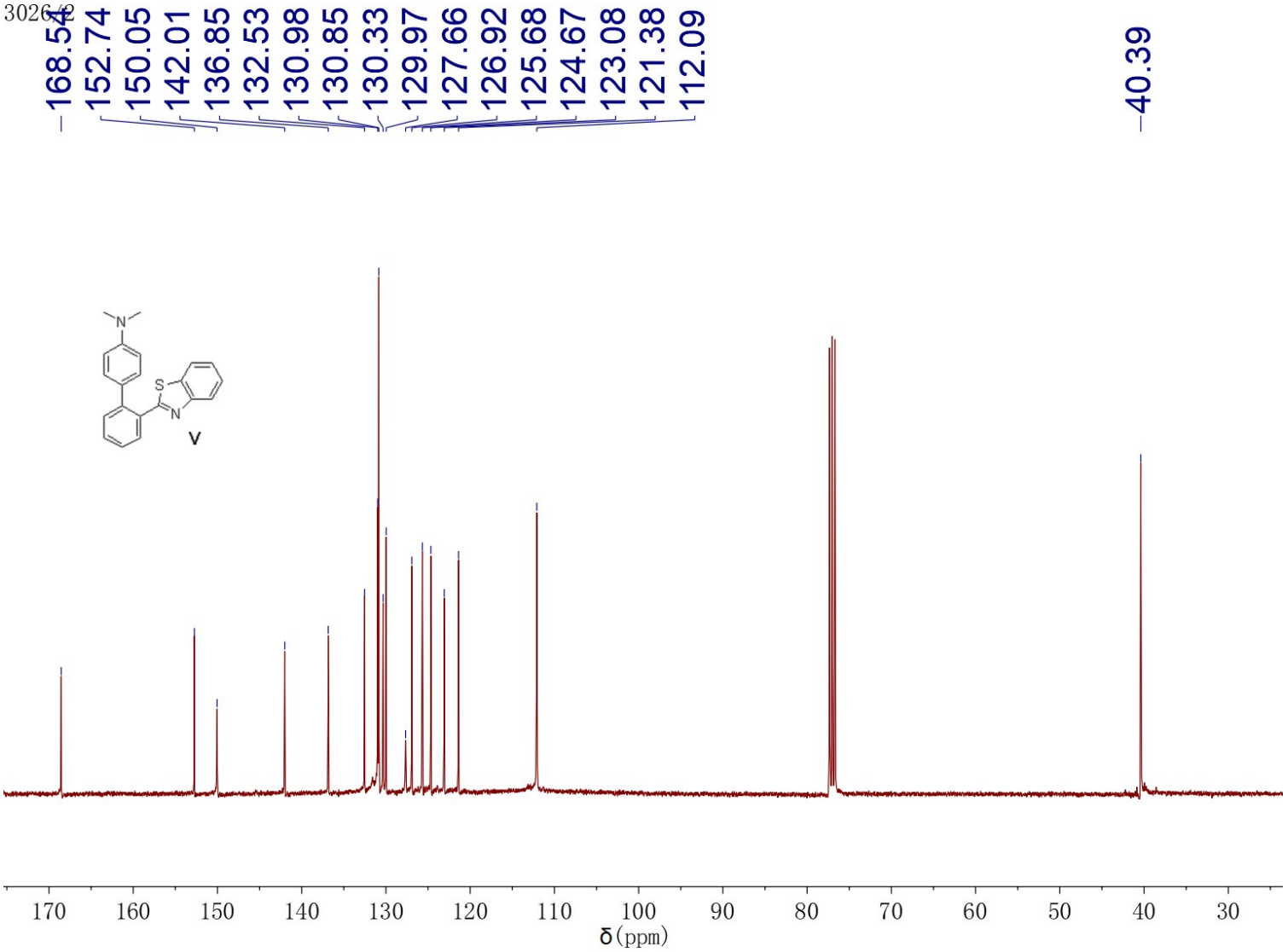
254
286
373
328
297
316
239
226
213
181
194
171
163
151
120
109
94
86
77
69
51
42
m/z-->
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460


8.08
8.07
8.07
8.05
7.72
7.70
7.50
7.48
7.46
7.46
7.44
7.43
7.42
7.41
7.39
7.31
7.29
7.27
7.24
7.19
7.17
6.70
6.68
2.97
N
S
N
V
1.95
0.97
4.03
1.00
1.97
1.95
6.00
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
δ(ppm)

3026-f2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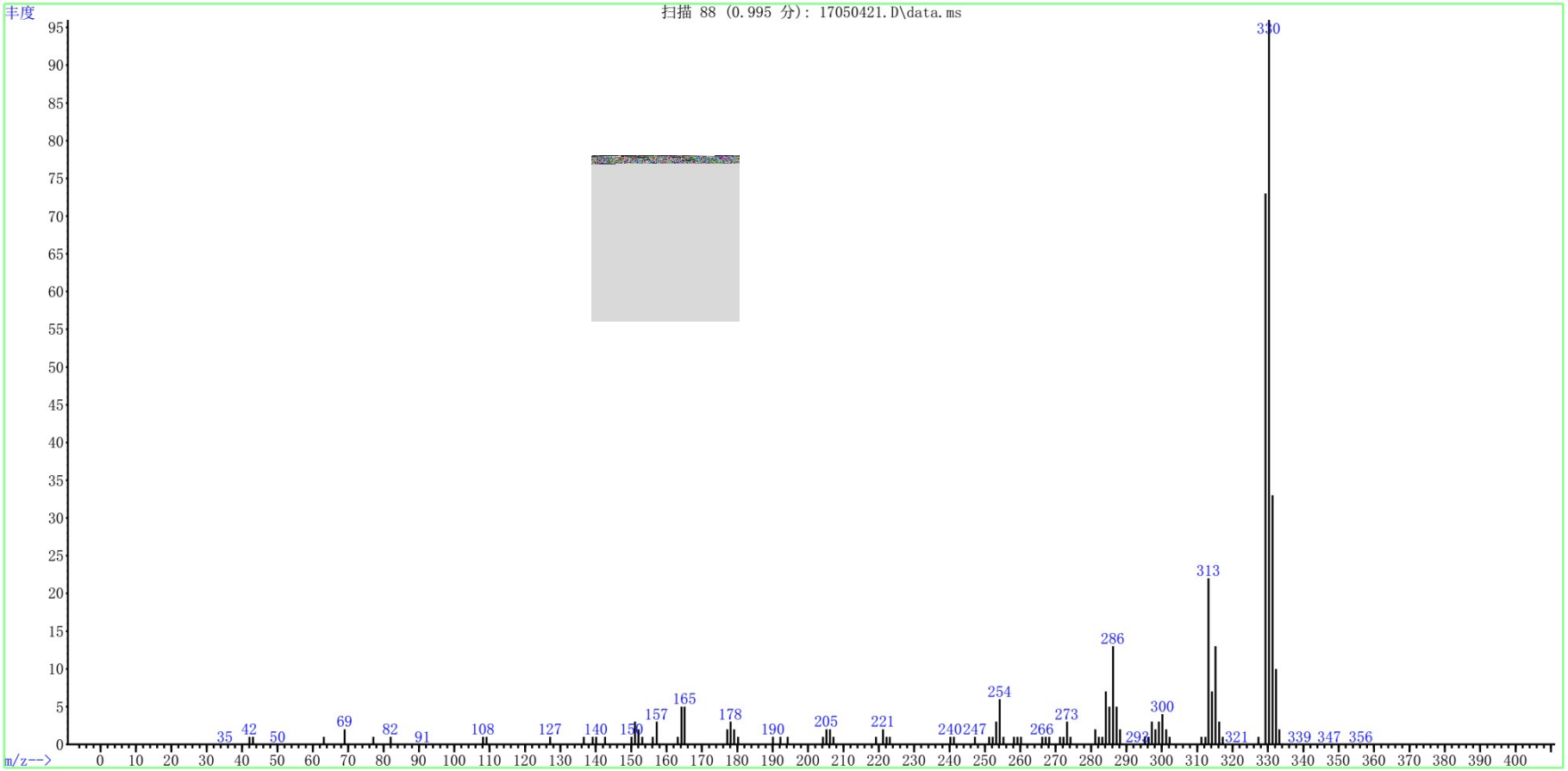
150.05
142.01
136.85
132.53
130.98
130.85
130.33
129.97
127.66
126.92
125.68
124.67
123.08
121.38
112.09
40.39
N
S
N
V
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
δ(ppm)


丰度
扫描 88 (0.995 分): 17050421.D\data.ms
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313
286
254
165
157
178
69
82
91
108
127
140
150
190
205
221
240
247
266
273
300
321
339
347
356