Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

A series of tetraphenylethene-based benzimidazoles: syntheses, structures, aggregation-induced emission and reversible mechanochromism

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1. Crystal structure of compounds 2a-2d

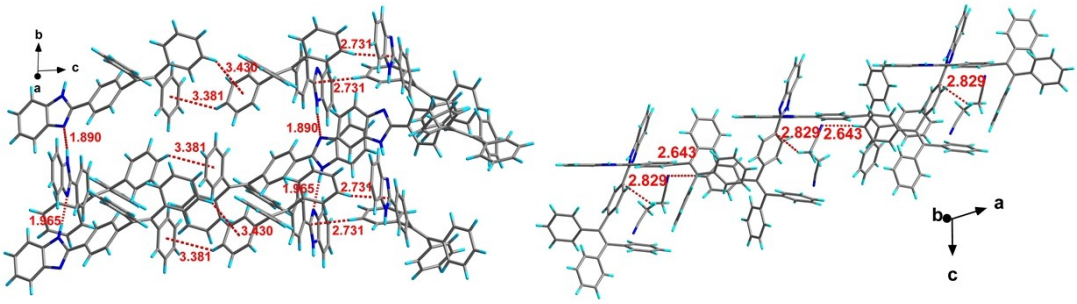


Fig. S1 Intermolecular C–H---π interactions and hydrogen bonds in the crystal structures of compound **2a**.

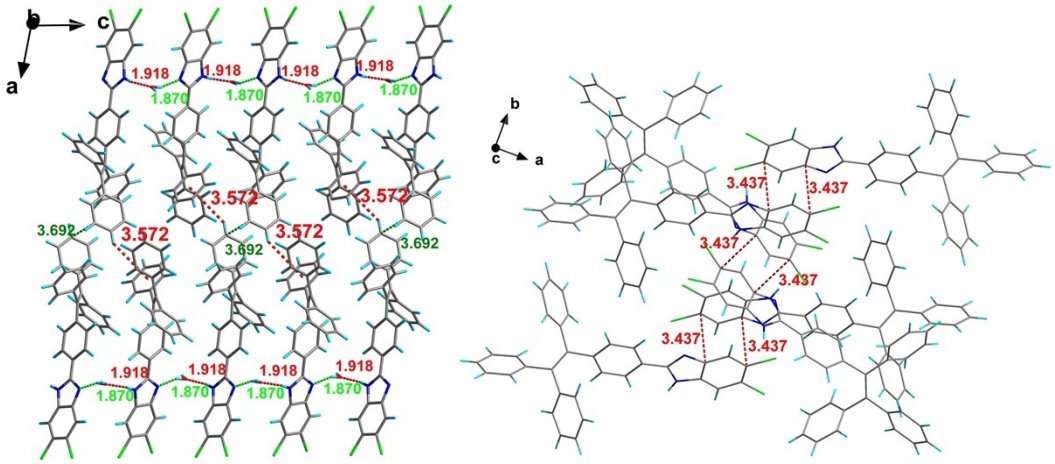


Fig. S2 Intermolecular C–H---π, π–π interactions and hydrogen bonds in the crystal structures of compound **2b**.

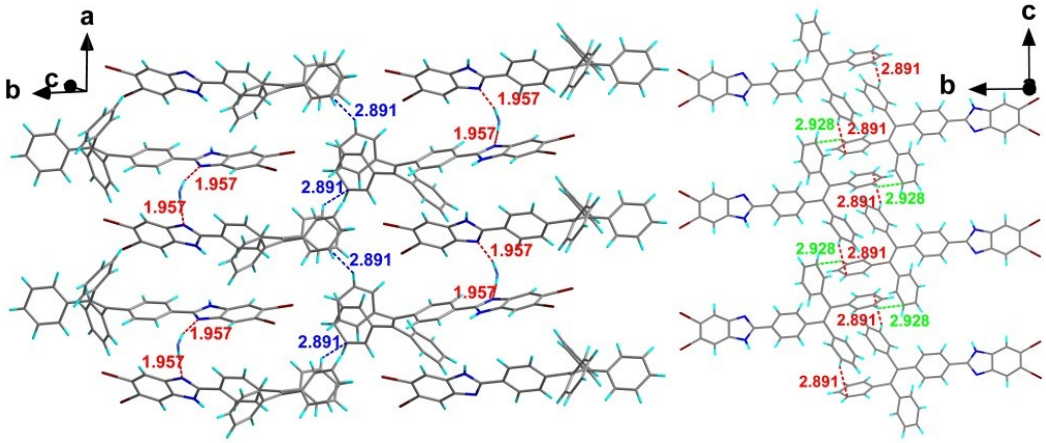


Fig. S3 Intermolecular C–H---π interactions and hydrogen bonds in the crystal structures of compound **2c**.

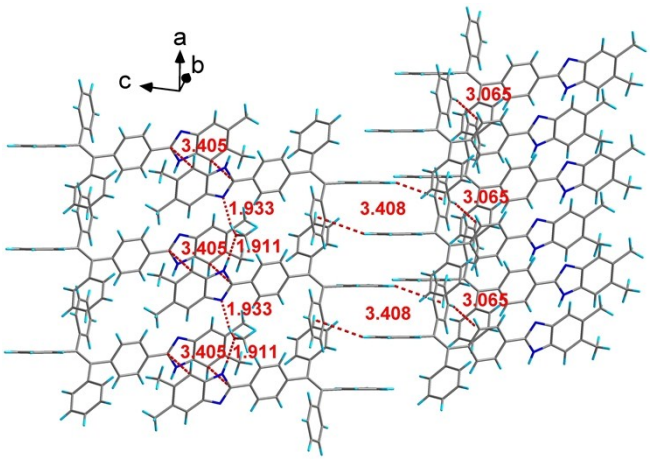


Fig. S4 Intermolecular C–H---π, π–π interactions and hydrogen bonds in the crystal structures of compound **2d**.

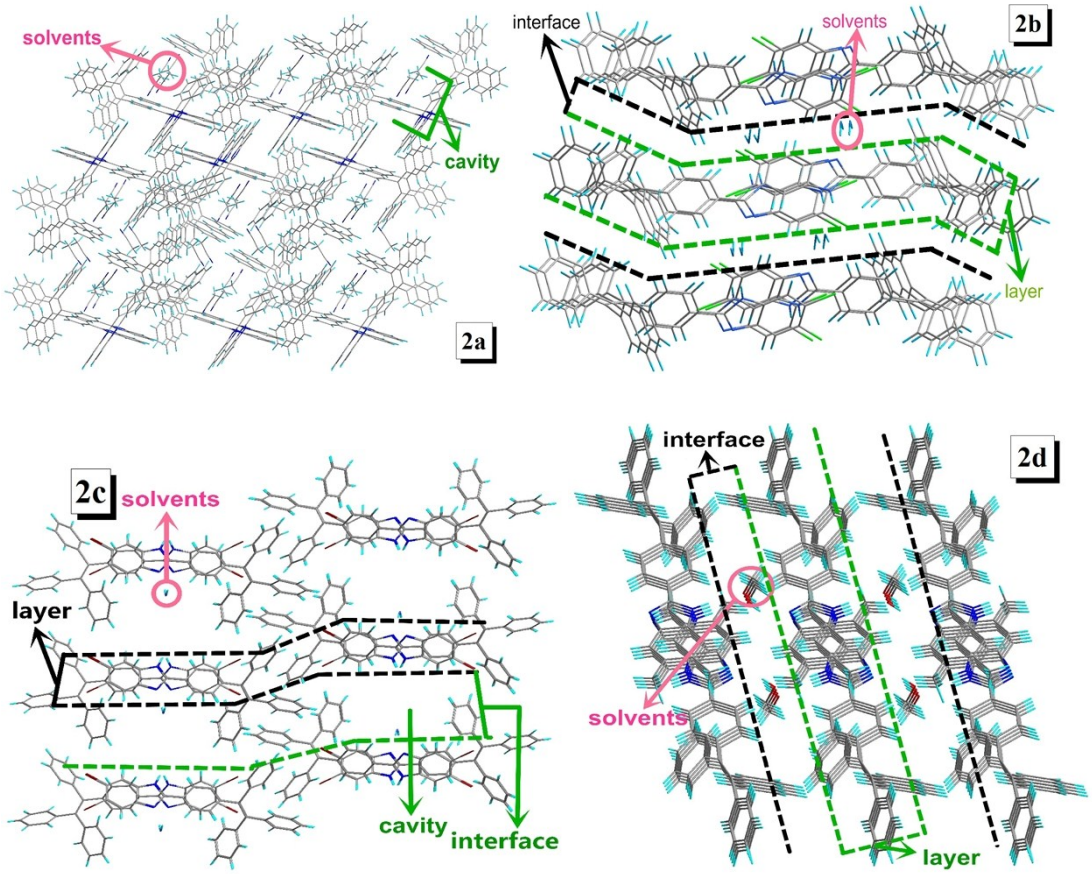


Fig. S5 3D molecules packing diagram of **2a**–**2d**. In all panels, the host atoms are represented as sticks and the guest solvents molecules inhabit in the 1-dimensional channels highlighted with a pink circle.

2. Crystal data of compounds 2a–2d

Table S1 Crystal data and structure refinement for **2a–2d**.

Parameter	2a	2b	2c	2d
Empirical formula	$C_{33}H_{24}N_2$	$C_{33}H_{22}Cl_2N_2$	$C_{33}H_{22}Br_2N_2$	$C_{35}H_{28}N_2$
Formula weight	448.56	517.45	606.35	476.23
Temperature	293(2)	293(2)	293(2)	293(2)
Wavelength(A)	0.71073	0.71073	0.71073	0.71073
Crystal system, space group	Monoclinic, I 2/a	Monoclinic, P 21/c	Orthorhombic, P 21 21 2	Triclinic, P -1
***a*/ (Å)**	27.518(12)	26.19(3)	9.581(3)	7.275(2)
***b*/ (Å)**	9.894(4)	9.313(10)	35.690(12)	9.280(3)
***c*/ (Å)**	45.122(19)	11.122(12)	9.867(3)	23.640(7)
α /(°)	90.00	90.00	90.00	83.829(6)
β/ (°)	106.22(2)	101.79(2)	90.00	88.466(6)
γ/ (°)	90.00	90.00	90.00	79.361(6)
Volume	11796(9)	2656(5)	3374.0(19)	1559.4(8)
Z	8	4	4	2
Calculated density (mg m^{-3})	1.149	1.339	1.211	1.117
Absorption coefficient /(mm^{-1})	0.068	0.274	2.424	0.068
F(000)	4304	1112	1236	558
Crystal size	0.29*0.27*0.23	0.23*0.17*0.14	0.24*0.19*0.17	0.14*0.12*0.10
***θ* range (deg)**	1.88-26.0	2.33-25.0	2.41-25.0	2.98-25.0
reflns collected	31604(R_{int}=0.0879)	13270(R_{int}=0.0805)	17206(R_{int}=0.1032)	7978(R_{int}=0.0602)
indep. reflns	11548	4672	5908	5429
Refns obs. [I＞2σ(I)]	4563	2383	2805	1951
GOF	1.007	0.971	0.991	0.986
R_1/wR_2 [I＞2σ(I)]	0.0619/0.1232	0.0563/0.1086	0.0728/0.1687	0.0733/0.1492
R_1/wR_2 (all data)	0.1743/0.1575	0.1290/0.1270	0.1745/0.1921	0.1851/ 0.1863
larg peak and hole(e /Å^{-3})	0.248/-0.196	0.197/-0.251	0.823/-0.404	0.460/ -0.267

3. **AIE properties of compounds 2b–2d**

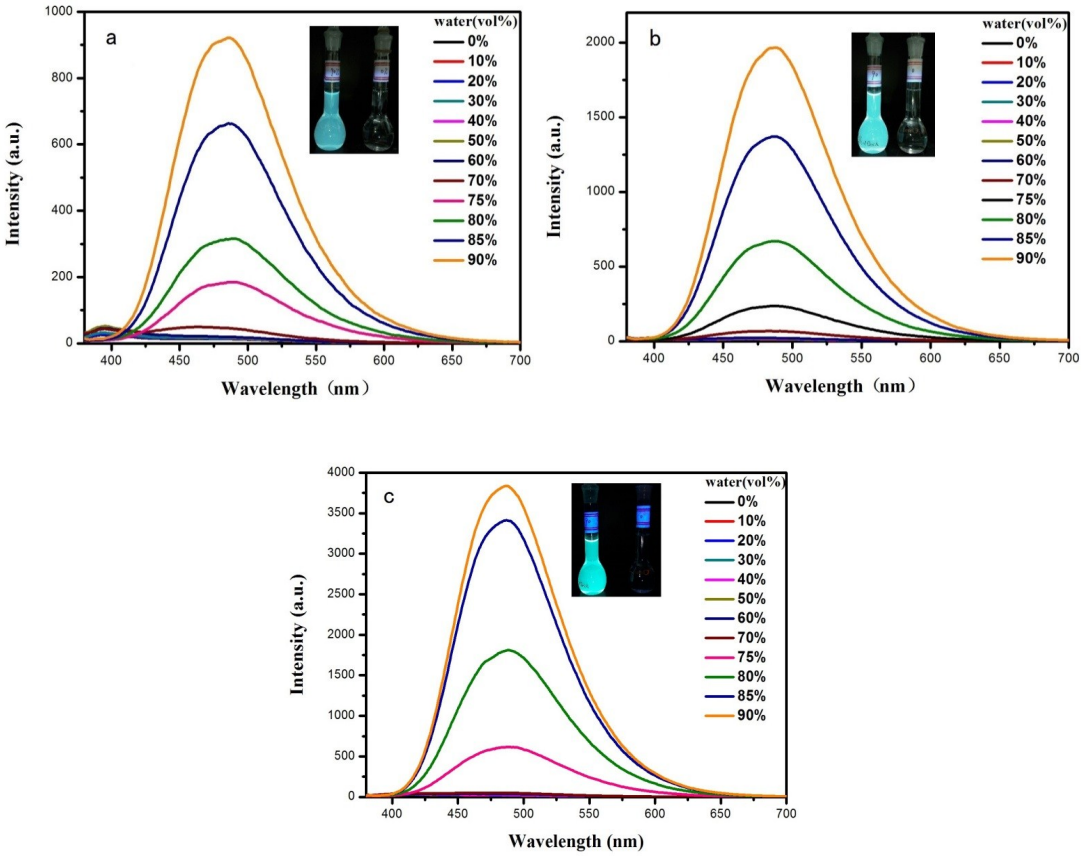


Fig. S6 Fluorescence spectra of compounds **2b** (a)**, 2c** (b) and **2d** (c) in THF/water mixtures with different water fractions, inset in panel: photos of compound in THF/water mixtures (f_w =0 and 90%) under 365 nm UV illumination.

4. **Theoretical calculations**

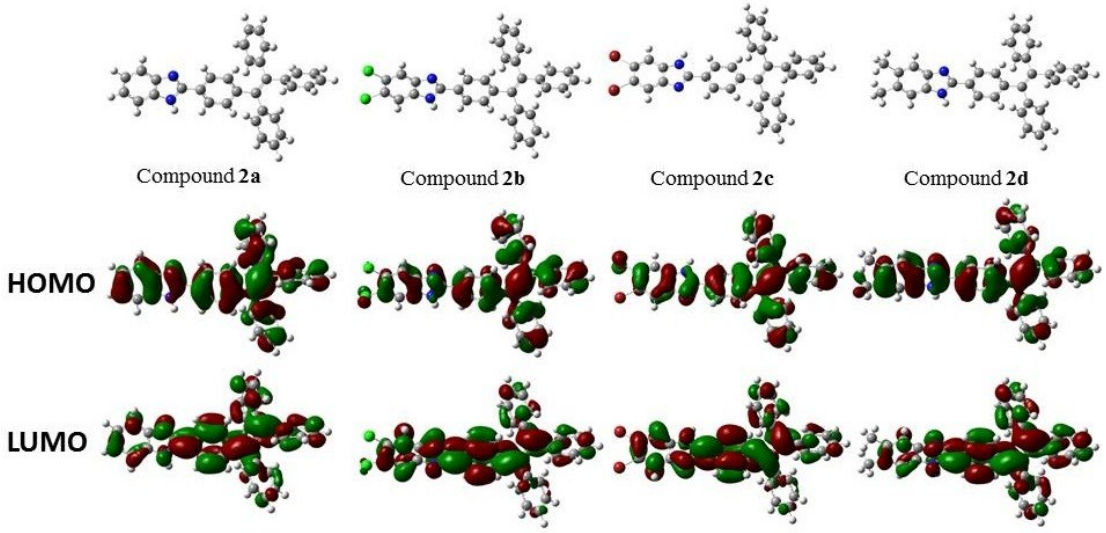


Fig. S7 Optimized molecular structures, and molecular orbital amplitude plots of HOMO and LUMO of **2a–2d** calculated using B3LYP/6-31G (d, p) basis set.

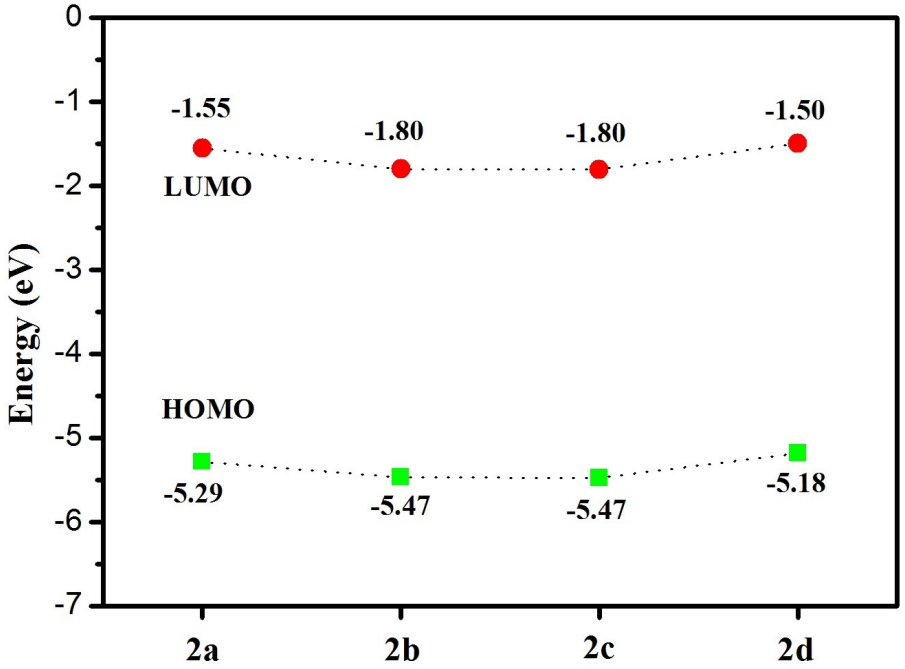


Fig. S8 Calculated HOMO and LUMO energy levels of compounds **2a**–**2d** using B3LYP/6-31G (d, p) basis set.

5. Thermal studies

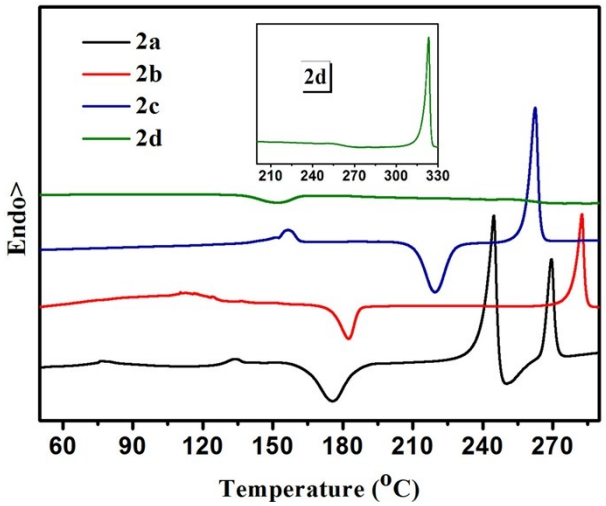
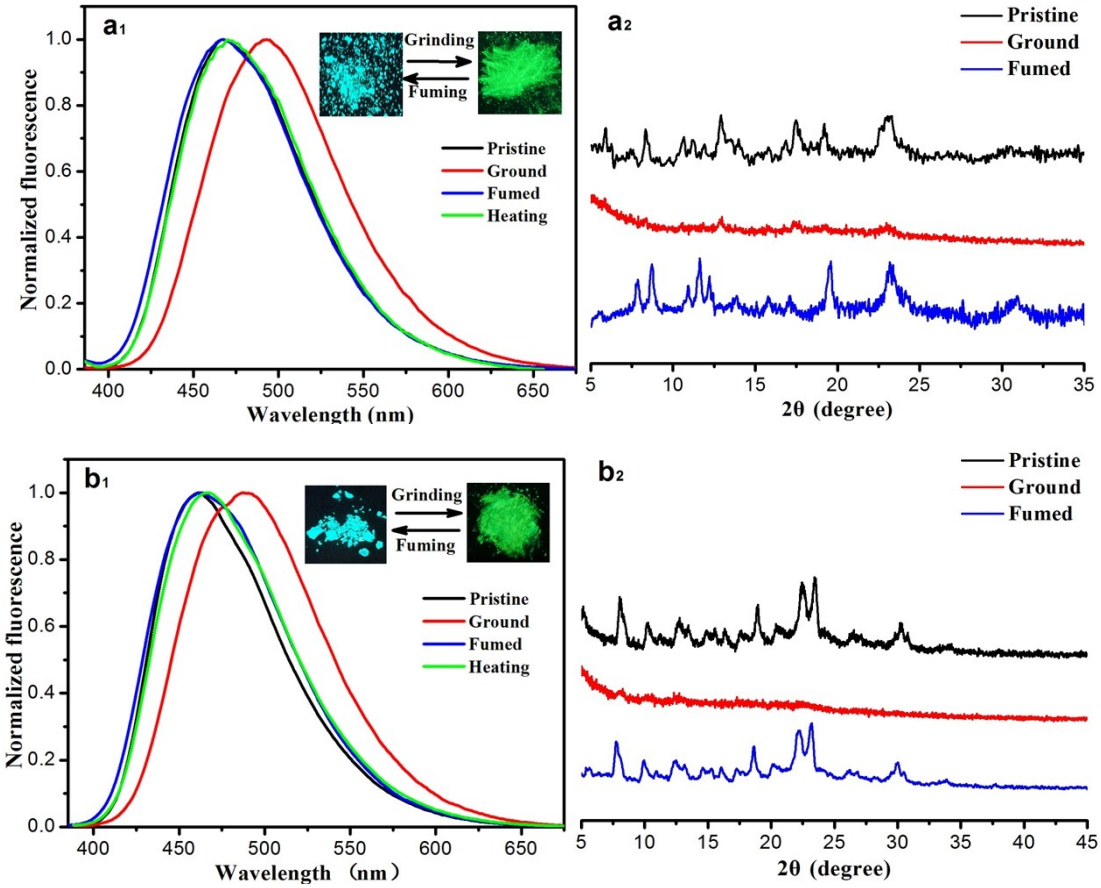


Fig. S9 DSC curves (first heating scan) of compounds **2a**–**2d** recorded under nitrogen at a heating rate of 10 °C min^{-1}.

6. **Mechanochromic properties of compounds 2b–2d**



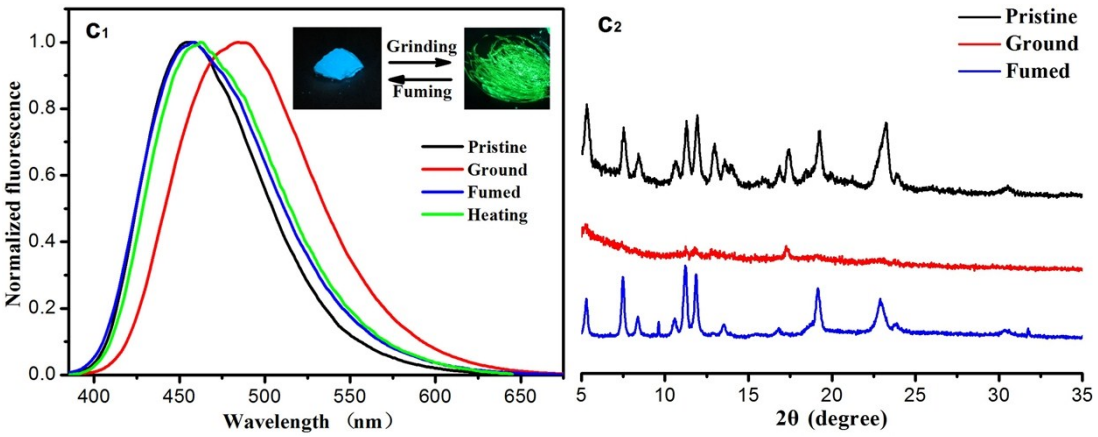


Fig. S10 Emission spectra of compounds **2b** (a_1)**, 2c** (b_1) and **2d** (c_1) as pristine, ground and fumed solids. inset in panel: photos of compounds in pristine (left) and ground (right) forms under 365 nm UV illumination.Powder X-ray diffraction patterns of compounds **2b** (a_2)**, 2c** (b_2) and **2d** (c_2) in pristine, ground and fumed forms.

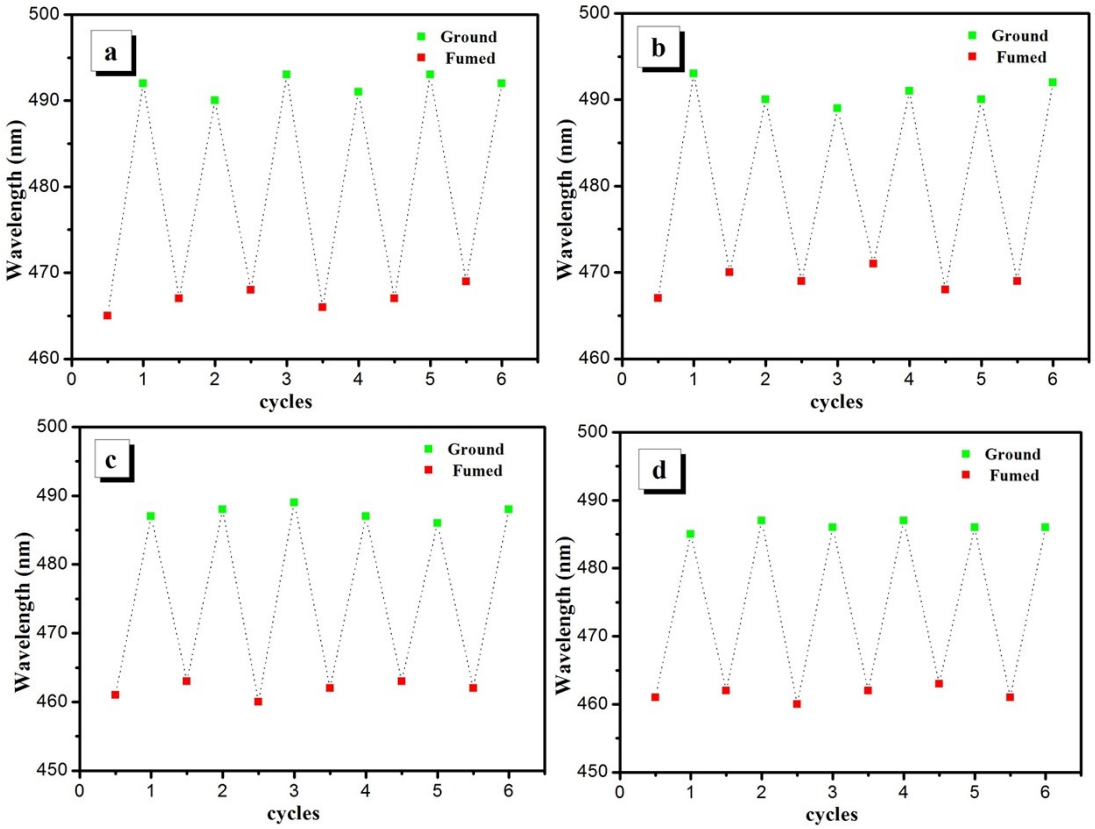
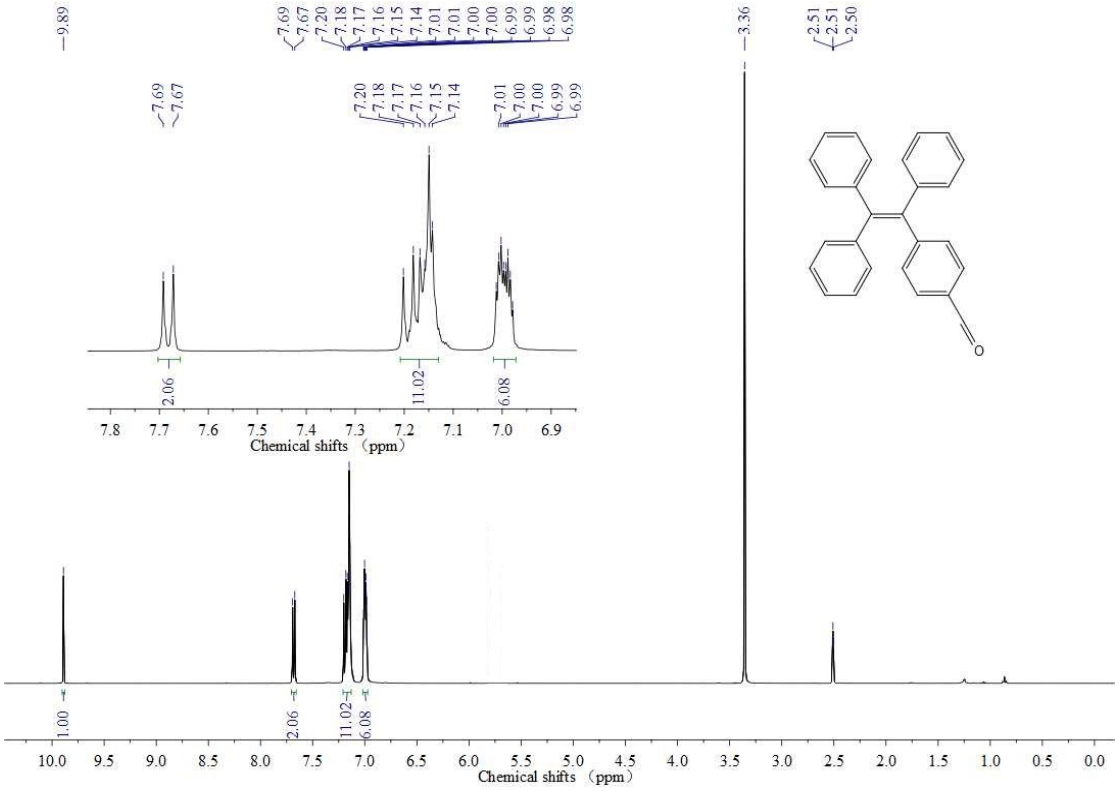
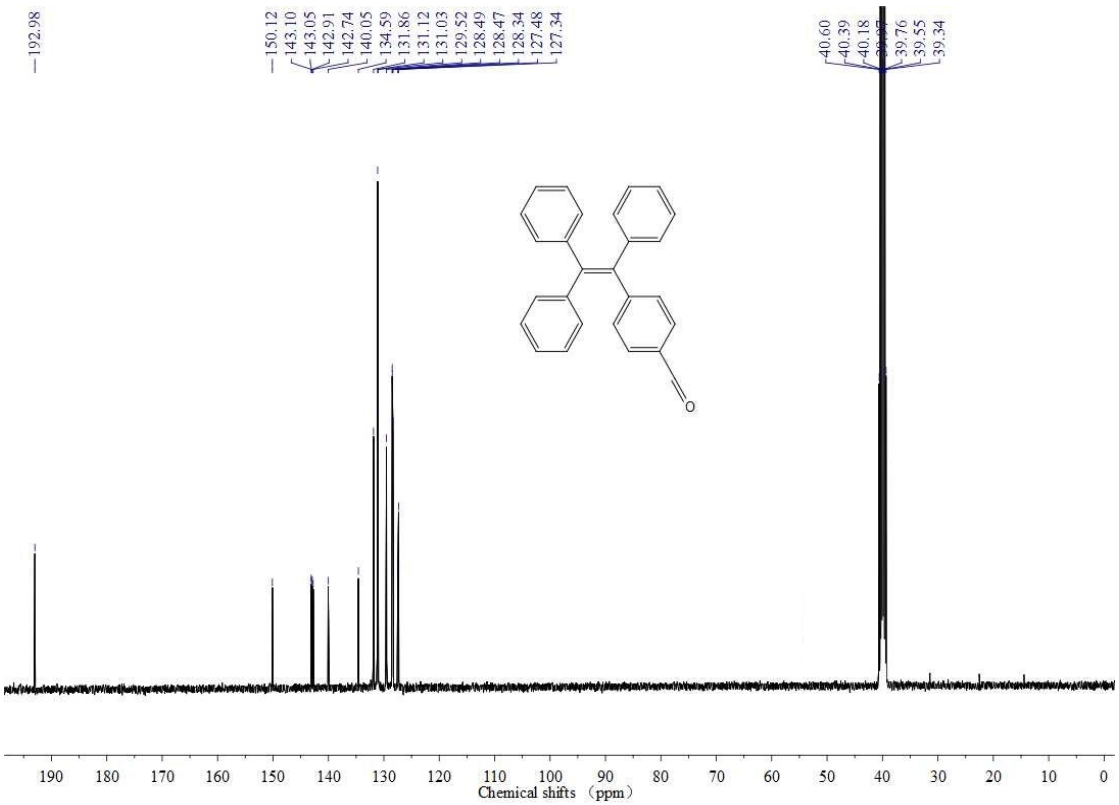
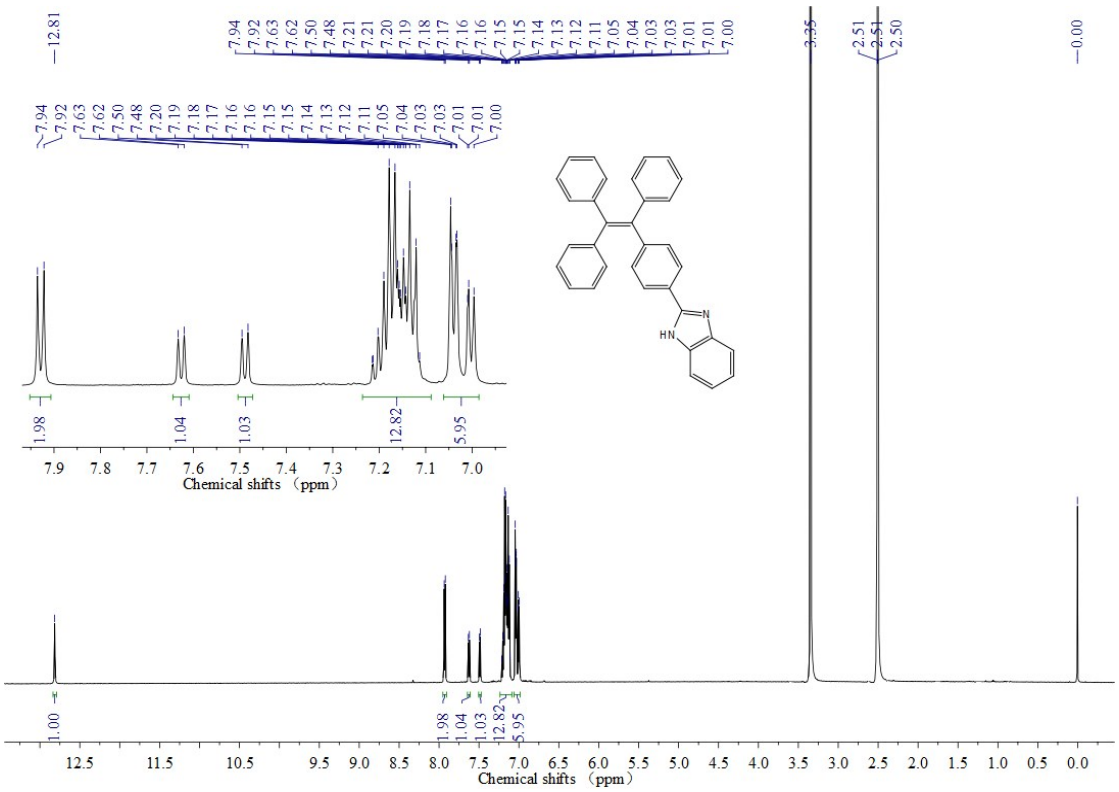


Fig. S11 Emission wavelength of the repeated vapochromic behavior of compounds **2a** (a) **2b** (b), **2c** (c) and **2d** (d) by grinding and exposing to dichloromethane treatments.

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



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7.92
7.63
7.62
7.50
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7.16
7.16
7.15
7.15
7.14
7.13
7.12
7.11
7.05
7.04
7.03
7.03
7.01
7.01
7.00
3.35
2.51
2.51
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1.03
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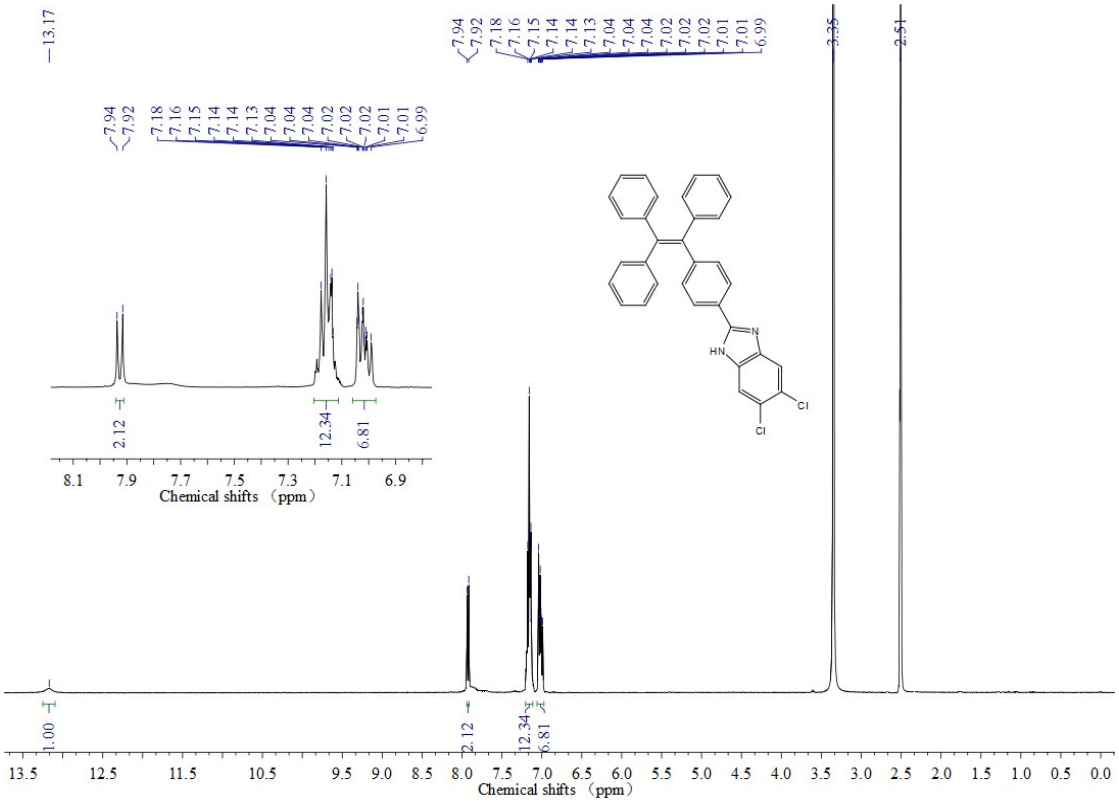
Chemical shifts (ppm)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7.15
7.14
7.14
7.13
7.04
7.04
7.04
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7.02
7.02
7.01
7.01
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HN
Cl
Cl
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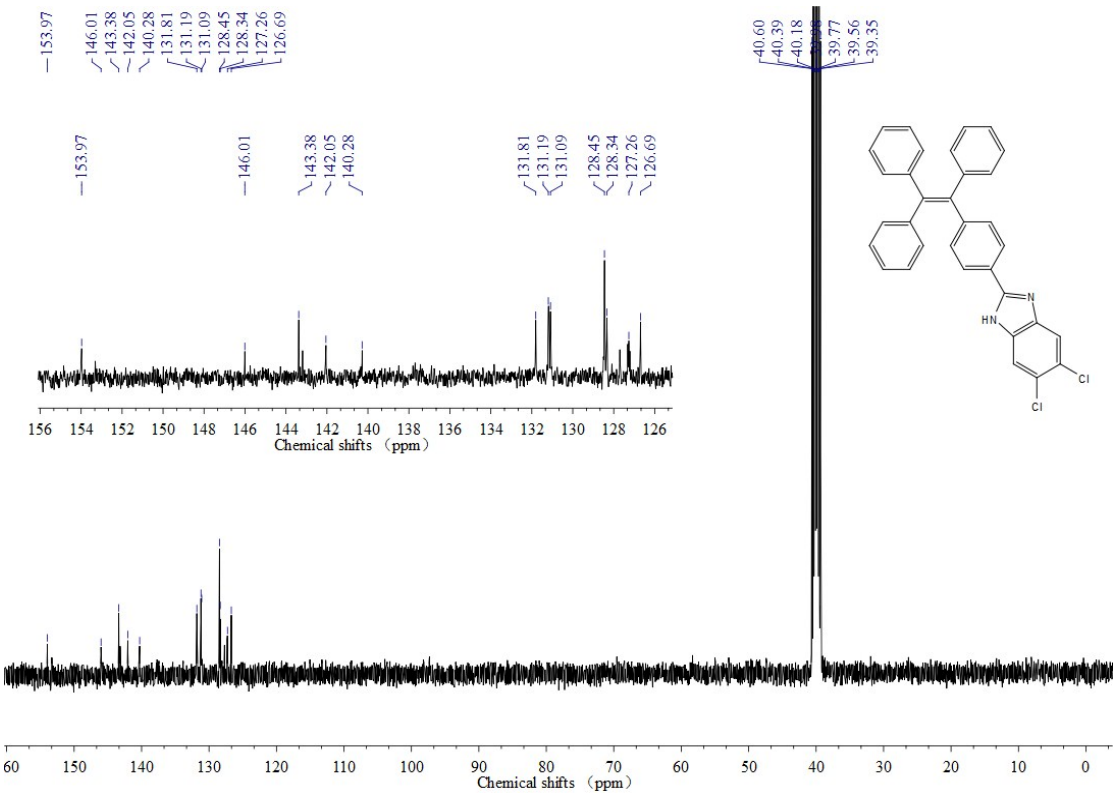
12.34
6.81
Chemical shifts (ppm)
1.00
Chemical shifts (ppm)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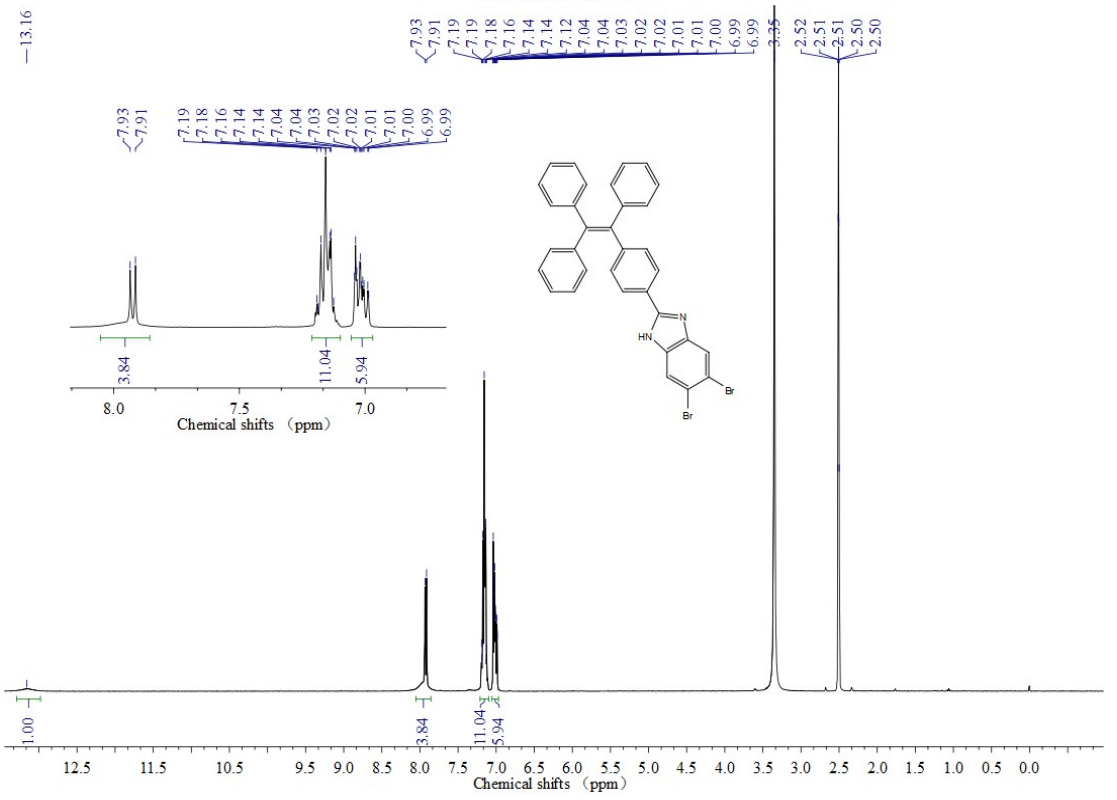
Chemical shifts (ppm)
Cl
Cl
HN
N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Chemical shifts (ppm)
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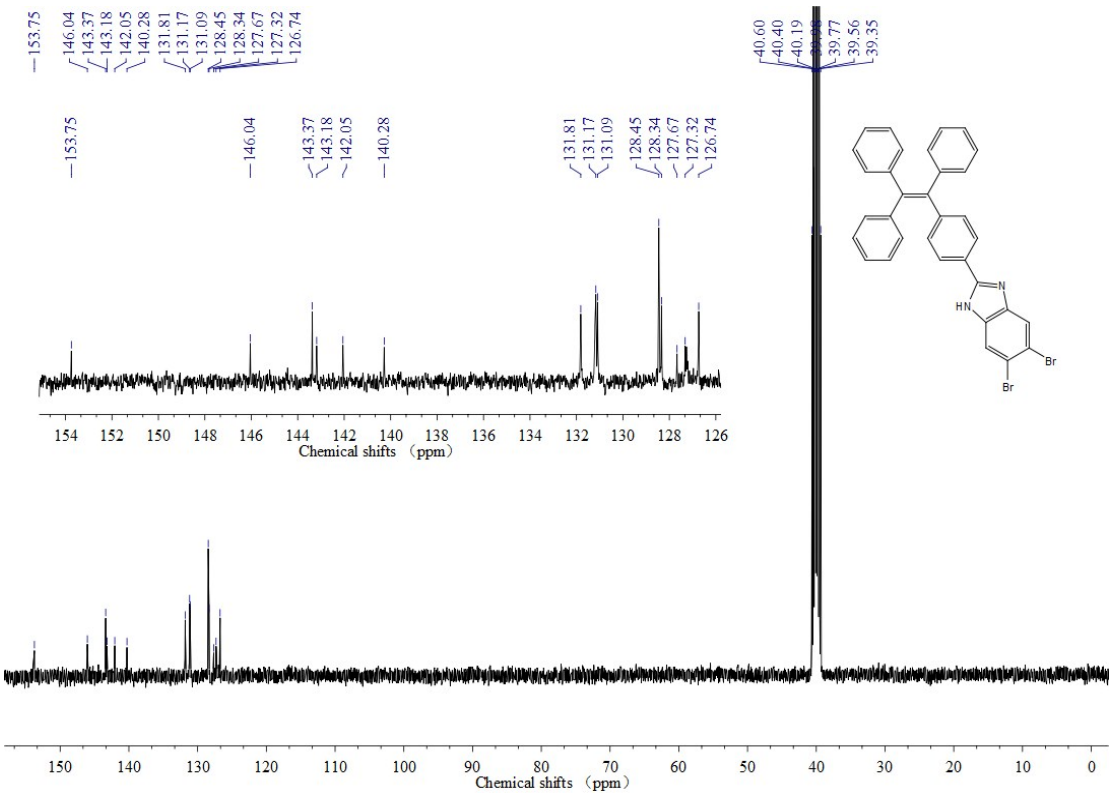
HN
N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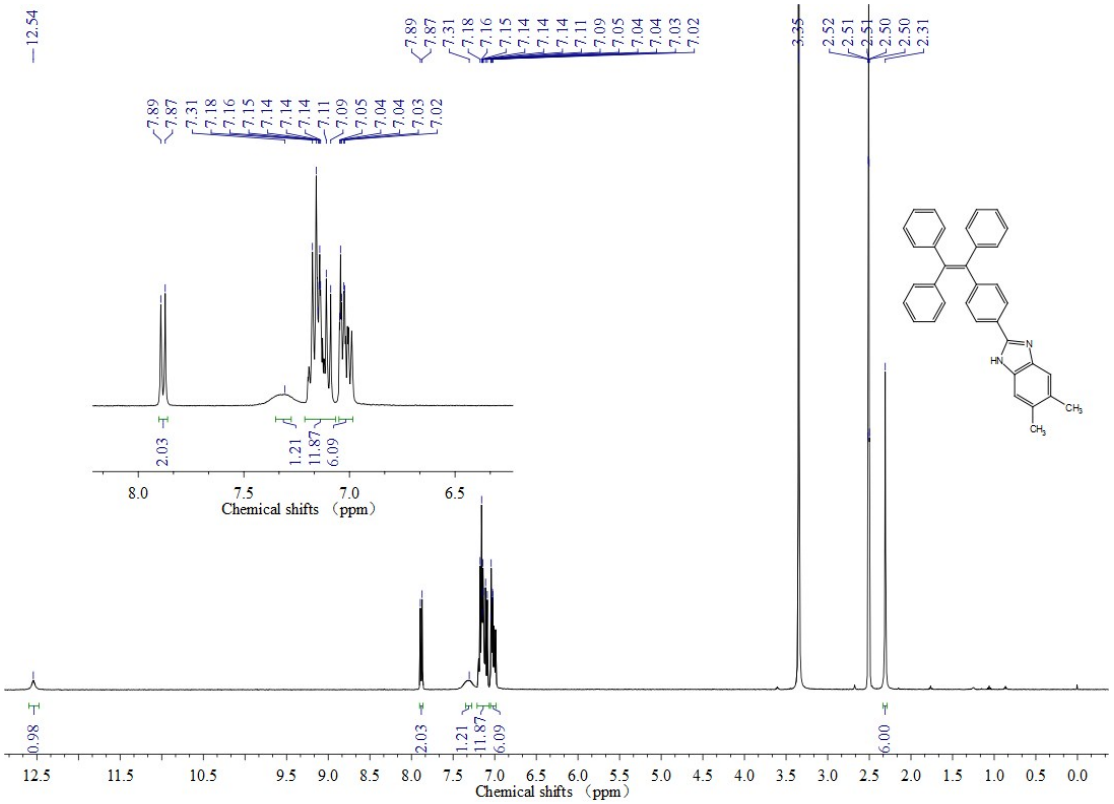
Chemical shifts (ppm)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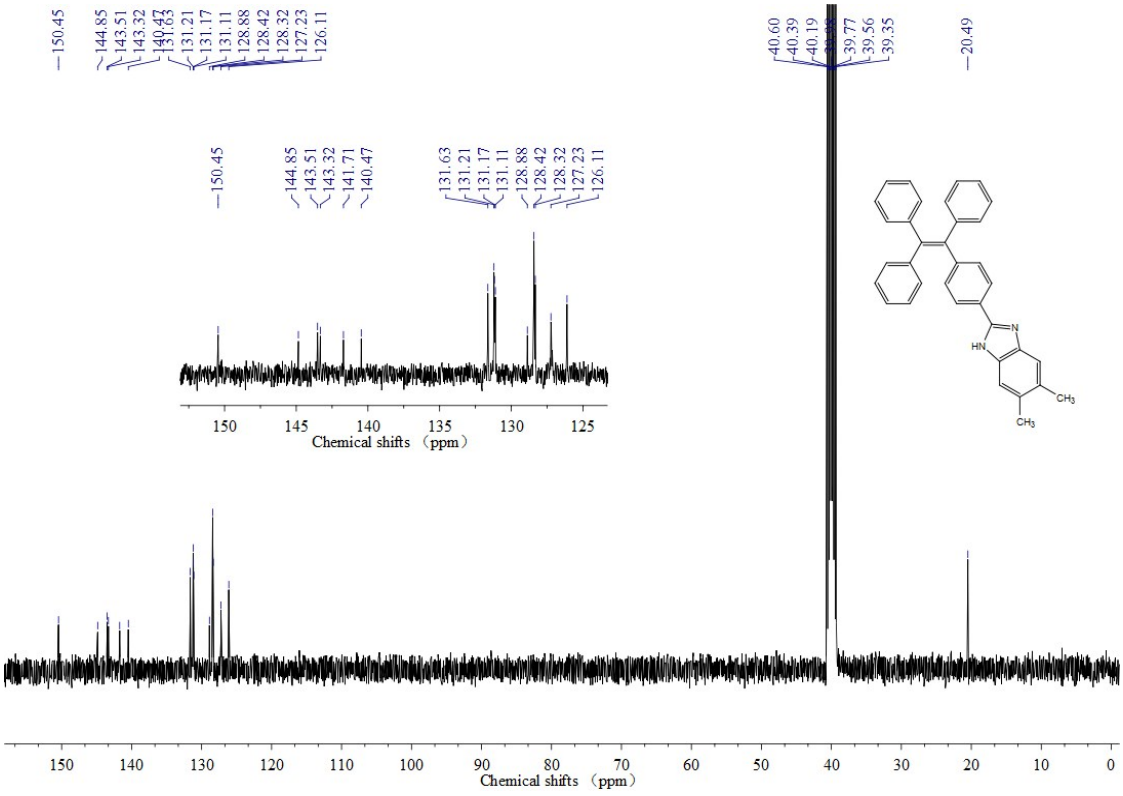
Chemical shifts (ppm)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131.17
131.11
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128.32
127.23
126.11
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140
135
130
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CH3
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130
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30
20
10
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Chemical shifts (ppm)