

## Electronic Supplementary Information

### The influence of different *N*-substituted groups on the mechanochromic properties of 1,4-dihydropyridine derivatives with simple structure

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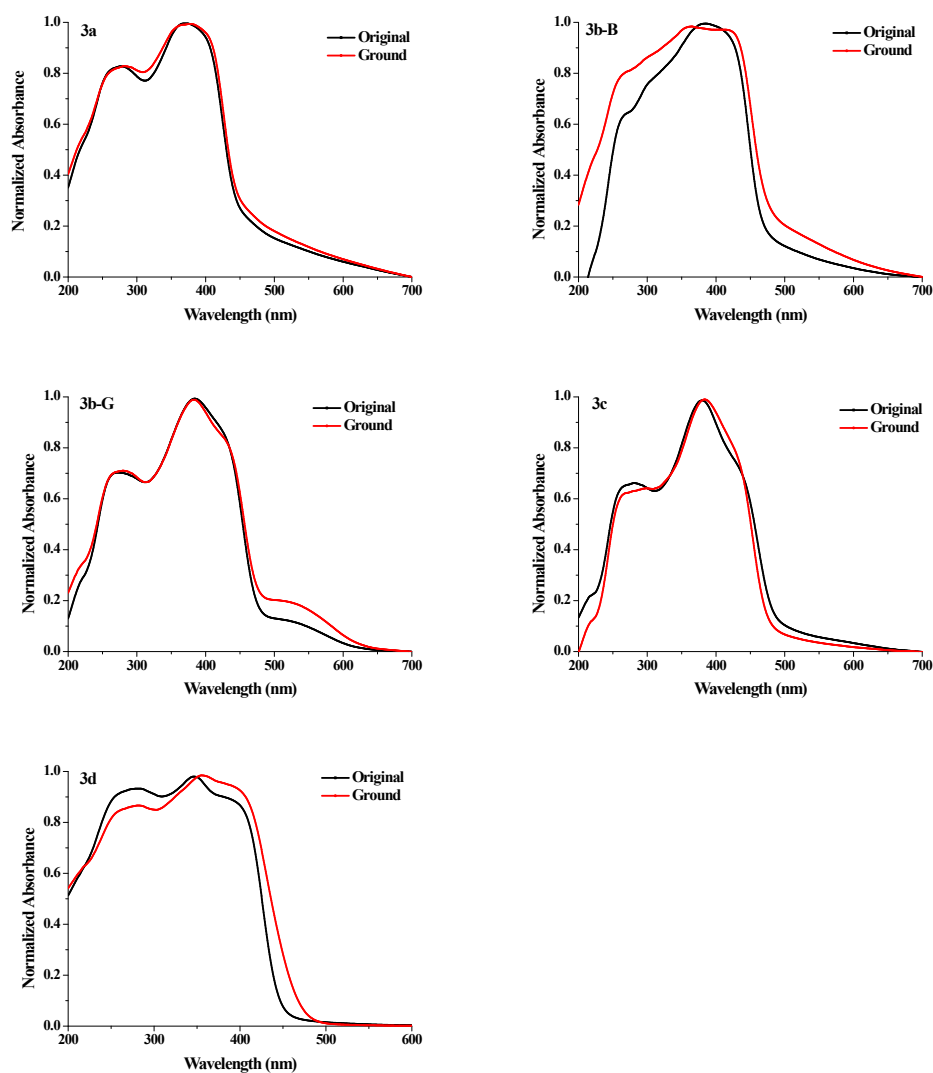
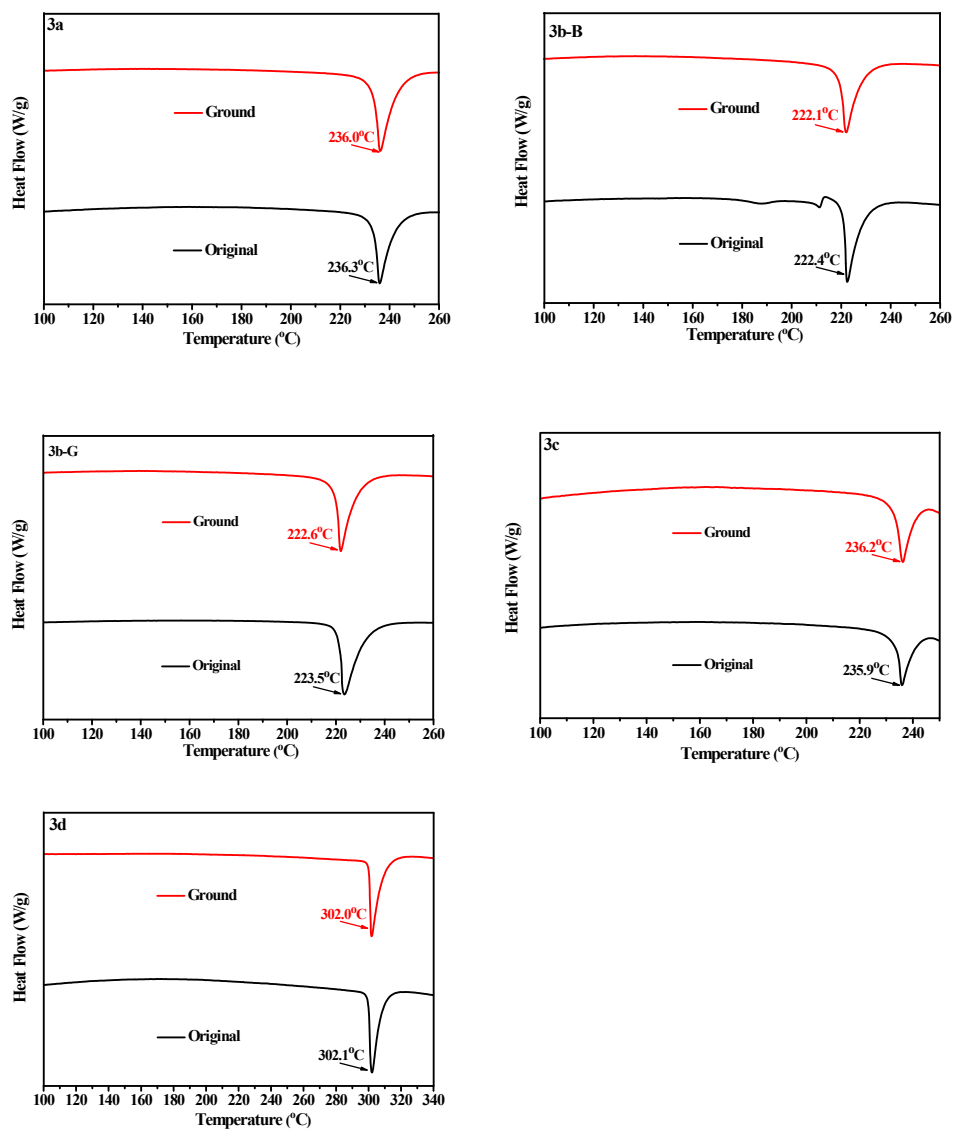
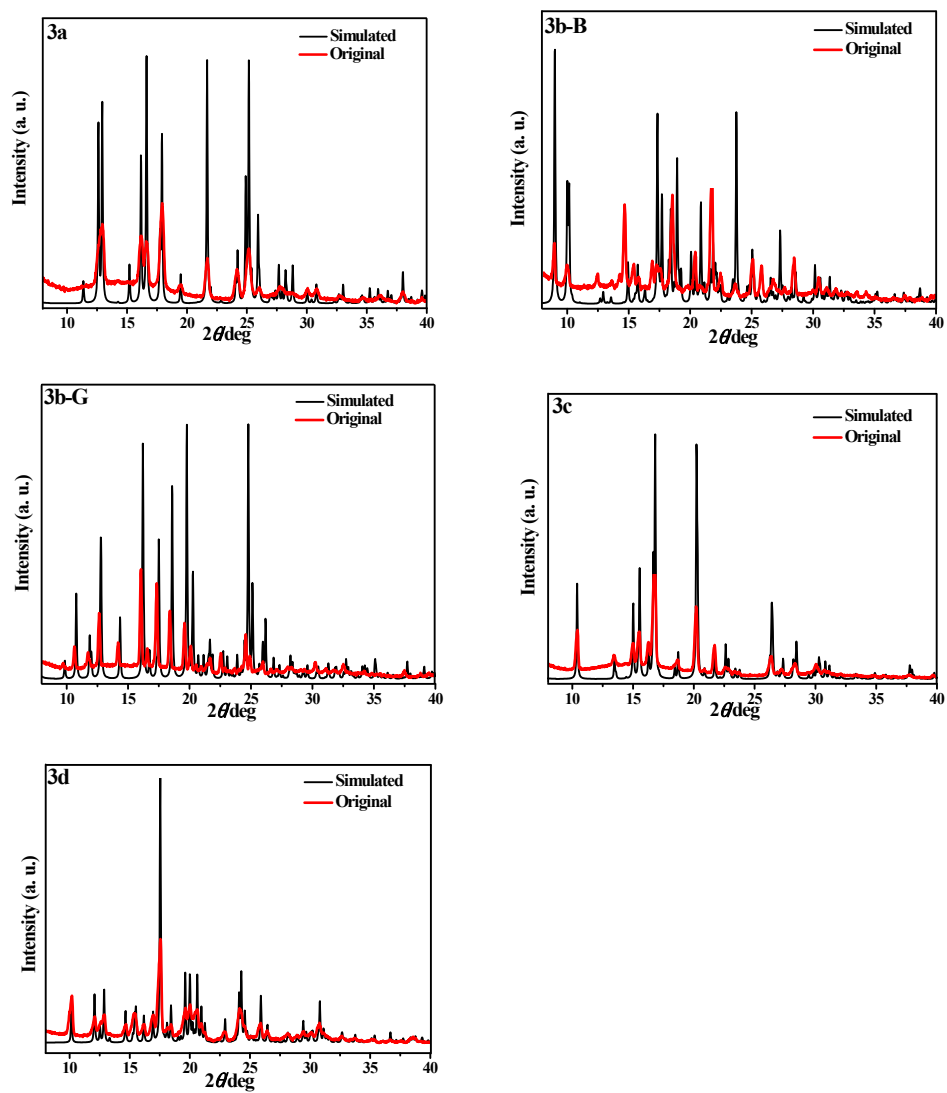


Fig. S1 Normalized absorption spectra of the solid samples of **3a-3d** before and after grinding.



**Fig. S2** Comparison of DSC curves of the original samples of **3a-3d** before and after grinding.



**Fig. S3** Comparison of XRD curves of the original samples of **3a-3d** and the corresponding simulated curves obtained from the single crystals.

**Table S1** The selected crystal data of compounds **3a-3d**.

	<b>3a</b>	<b>3b-B</b>	<b>3b-G</b>	<b>3c</b>	<b>3d</b>
Empirical formula	C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>	C <sub>44</sub> H <sub>58</sub> N <sub>2</sub> O <sub>8</sub>	C <sub>22</sub> H <sub>25</sub> NO <sub>2</sub>	C <sub>23</sub> H <sub>27</sub> NO <sub>2</sub>	C <sub>23</sub> H <sub>27</sub> NO <sub>2</sub>
Formula weight	273.36	742.92	335.43	349.45	349.45
Temperature (K)	301.83	293(2)	293(2)	293(2)	293(2)
Crystal system	Orthorhombic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>Pna</i> 2 <sub>1</sub>	<i>P</i> 2(1)/ <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2(1)/ <i>c</i>
<i>Z</i>	4	4	2	2	4
<i>D</i> <sub>calcd</sub> [Mg/m <sup>3</sup> ]	1.222	1.218	1.221	1.183	1.196
<i>F</i> (000)	592	1600	360	376	752
$\theta$ range [°]	3.500-25.999	1.048-24.999	2.270-24.999	1.661-25.490	2.052-24.997
<i>R</i> <sub>1</sub> [I>2 $\sigma$ (I)]	0.0859	0.0683	0.0776	0.0575	0.0487
<i>wR</i> <sub>2</sub> [I>2 $\sigma$ (I)]	0.2017	0.1687	0.2184	0.1551	0.1263
<i>a</i> [Å]	8.1907(5)	19.4307(19)	8.6562(3)	6.7838(11)	17.439(3)
<i>b</i> [Å]	24.8299(16)	17.6059(16)	9.3060(3)	11.793(2)	12.082(2)
<i>c</i> [Å]	7.3077(5)	11.8488(12)	12.0490(4)	12.664(2)	9.2298(16)
$\alpha$ [deg]	90	90	83.1427(10)	90	90
$\beta$ [deg]	90	91.348(2)	77.2334(10)	104.498(4)	93.491(4)
$\gamma$ [deg]	90	90	75.0473(11)	90	90
<i>V</i> [Å <sup>3</sup> ]	1486.20(17)	4052.3(7)	912.55(5)	980.9	1941.2(6)
GOF	1.025	1.020	1.052	1.040	1.013
R(int)	0.0872	0.0516	0.0366	0.0254	0.0382
No. of reflns collected	6521	22198	23873	5676	10438
No. of unique reflns	2769	7122	3190	3466	3412
<i>R</i> <sub>1</sub> (all data)	0.1116	0.1144	0.0888	0.0683	0.0682
<i>wR</i> <sub>2</sub> (all data)	0.2239	0.1990	0.2333	0.1650	0.1411

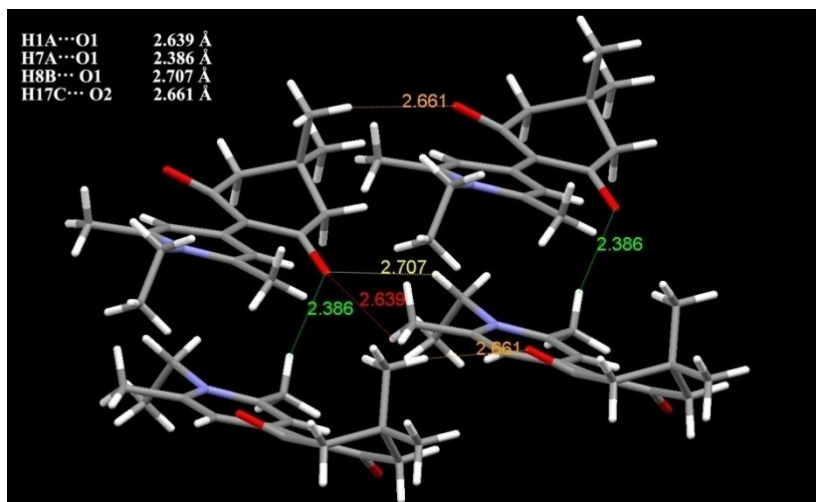


Fig. S4 The intermolecular interactions in the crystals of **3a**.

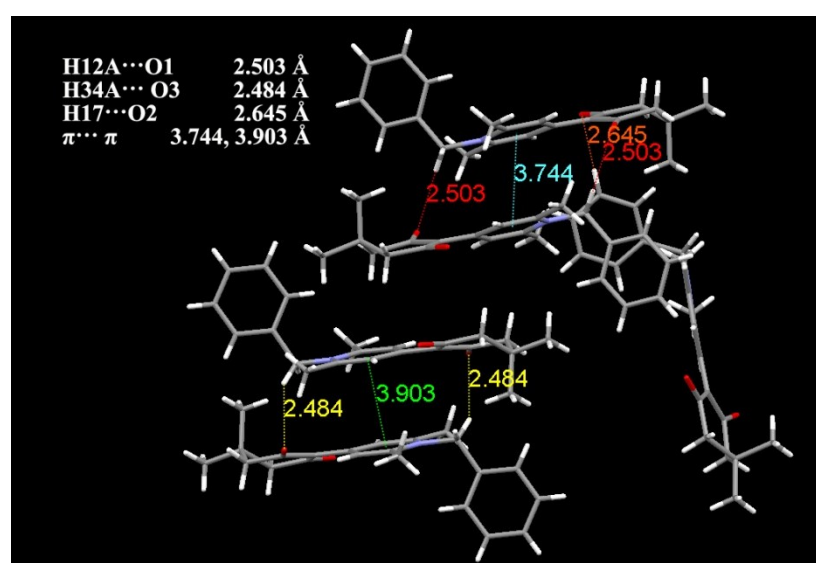


Fig. S5 The intermolecular interactions in the crystals of **3b-B**.

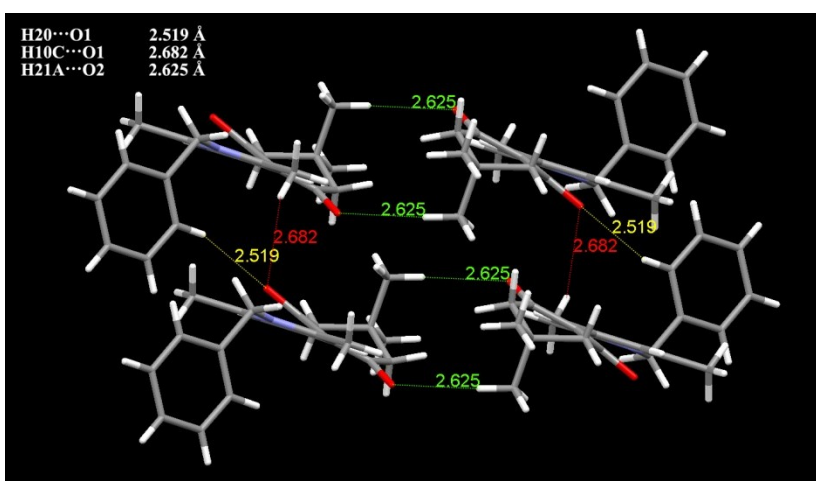


Fig. S6 The intermolecular interactions in the crystals of **3b-G**.

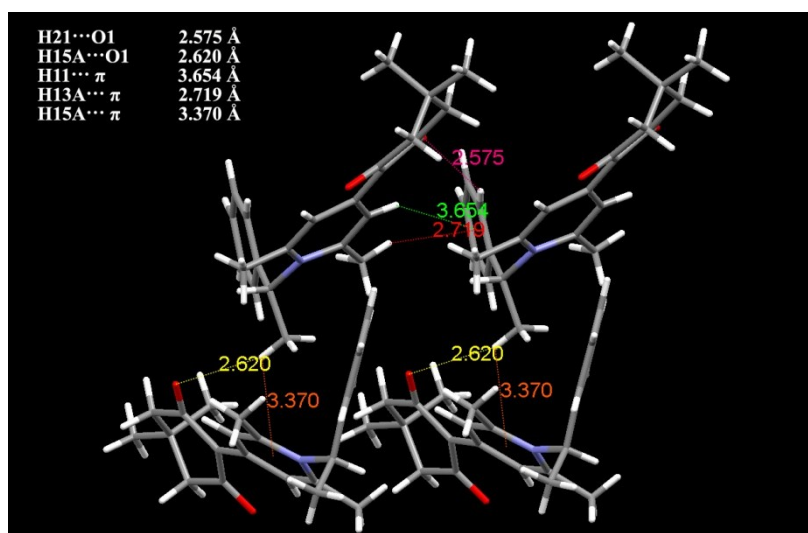


Fig. S7 The intermolecular interactions in the crystals of **3c**.

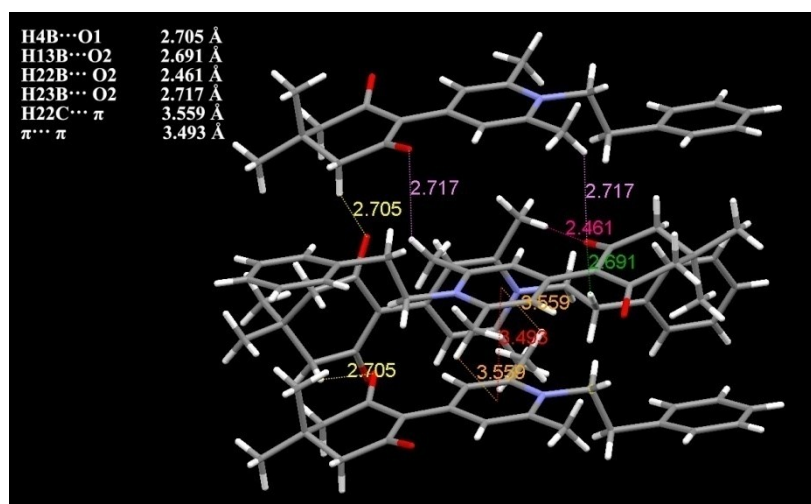


Fig. S8 The intermolecular interactions in the crystals of **3d**.

## NMR spectra of 3a-3d

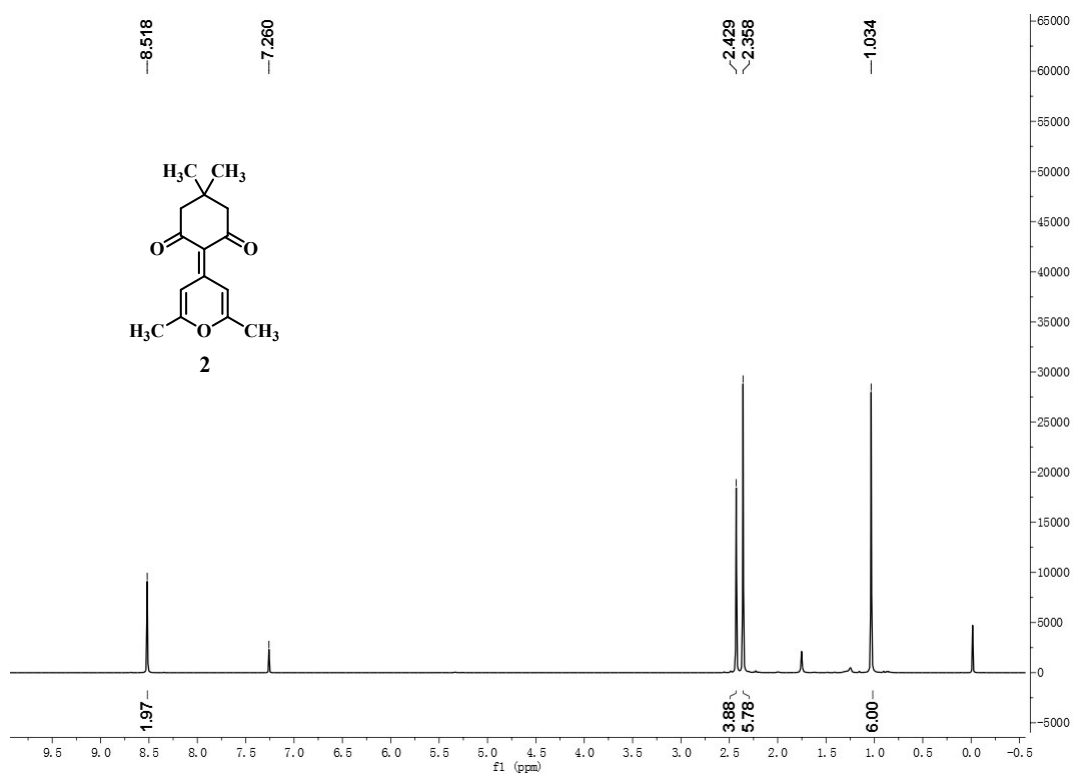


Fig. S9 <sup>1</sup>H NMR of compound 2 (CDCl<sub>3</sub>, 500 MHz).

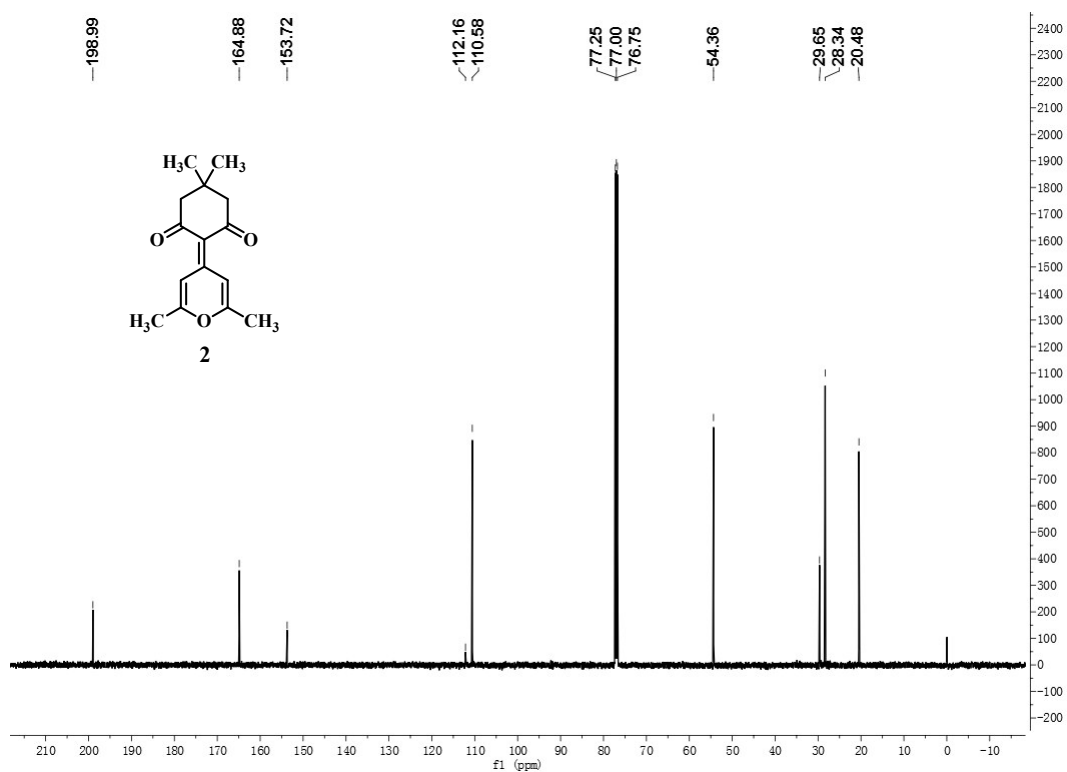
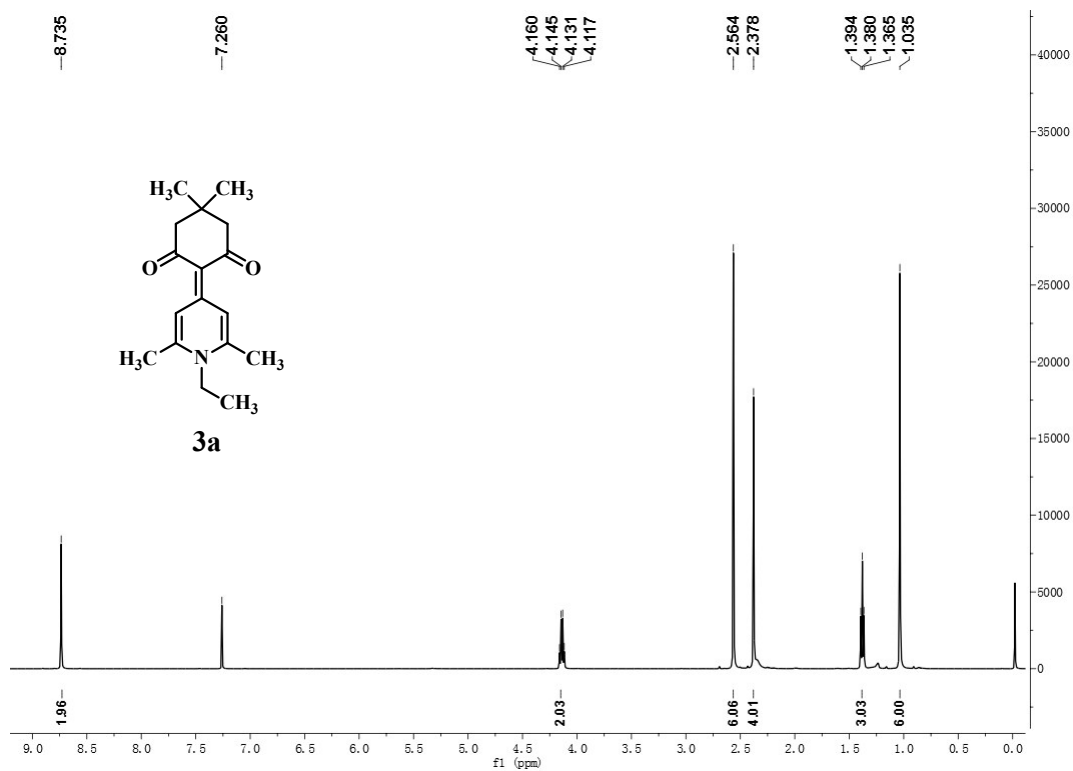
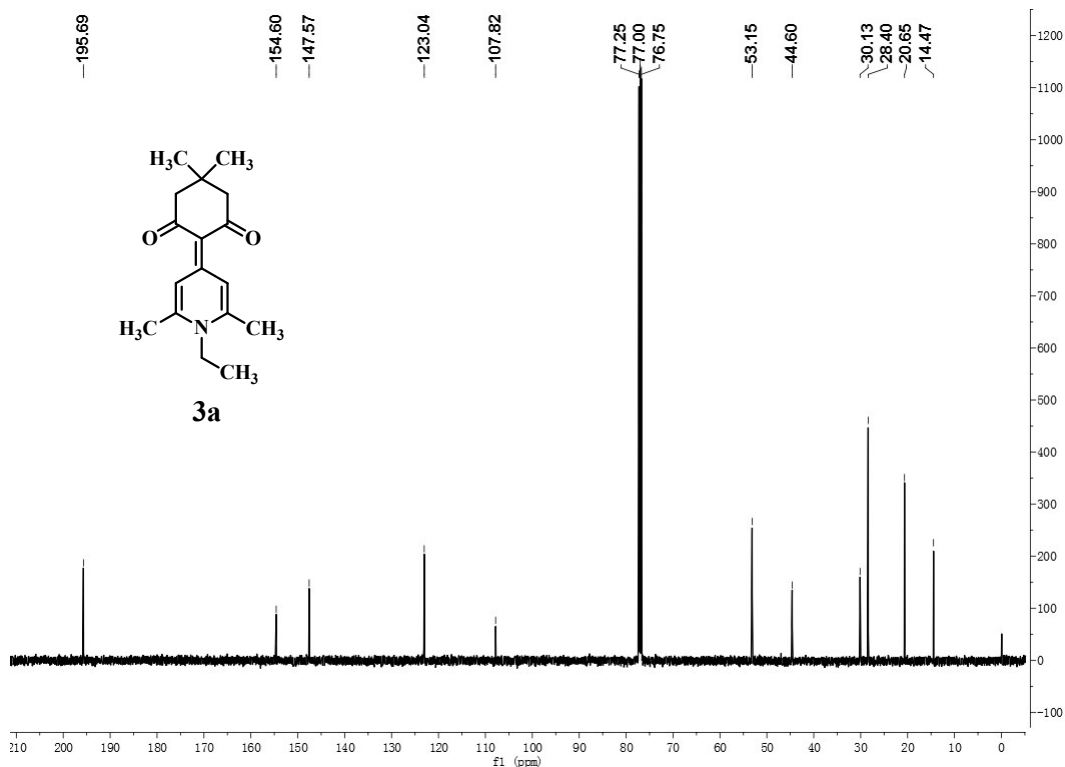


Fig. S10 <sup>13</sup>C NMR of compound 2 (CDCl<sub>3</sub>, 125 MHz).



**Fig. S11** <sup>1</sup>H NMR of compound **3a** (CDCl<sub>3</sub>, 500 MHz).



**Fig. S12** <sup>13</sup>C NMR of compound **3a** (CDCl<sub>3</sub>, 125 MHz).



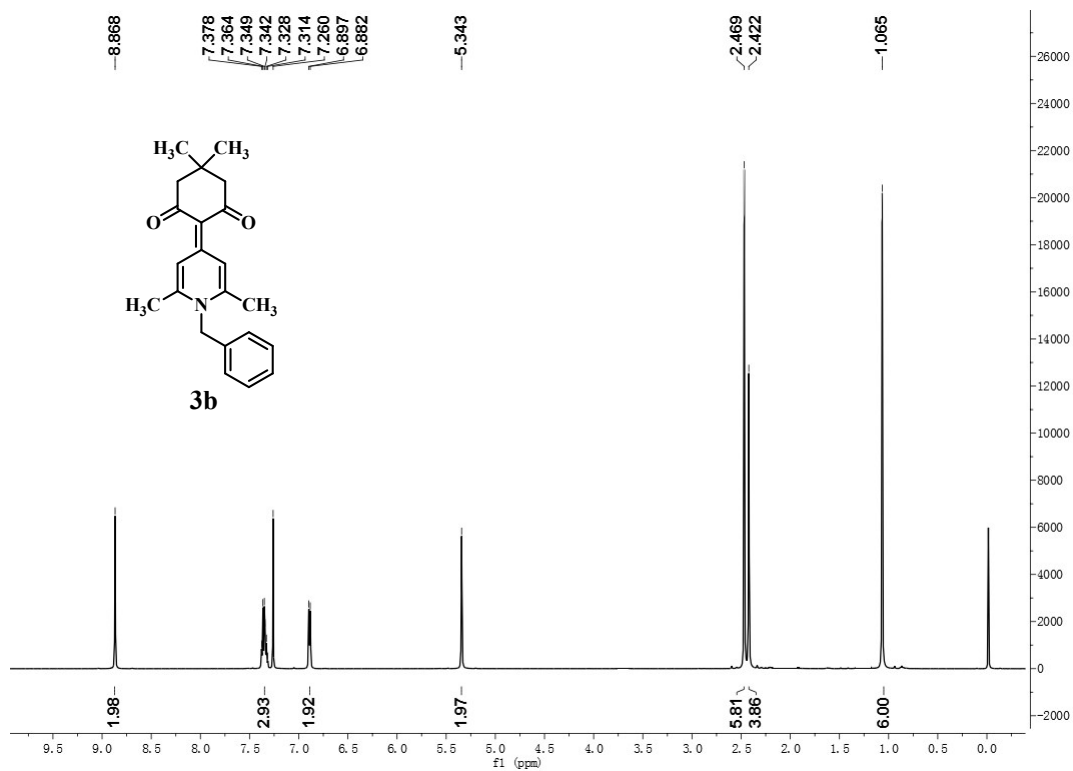


Fig. S13  $^1\text{H}$  NMR of **3b** ( $\text{CDCl}_3$ , 500 MHz).

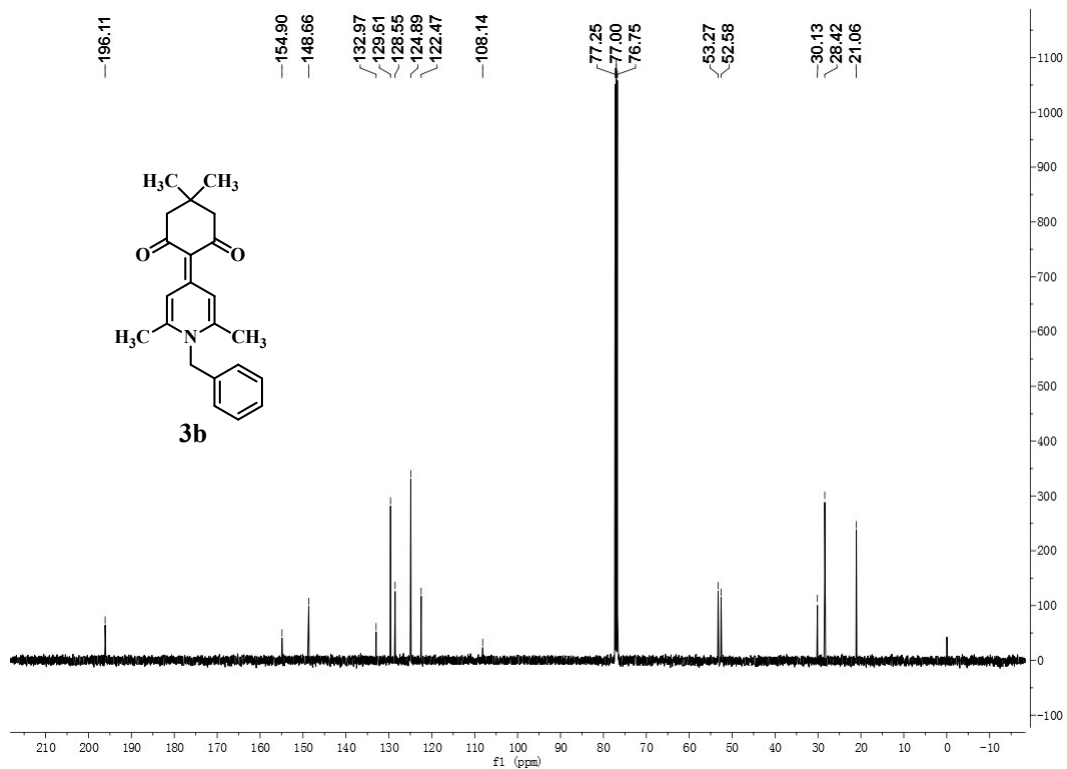


Fig. S14  $^{13}\text{C}$  NMR of **3b** ( $\text{CDCl}_3$ , 125 MHz).

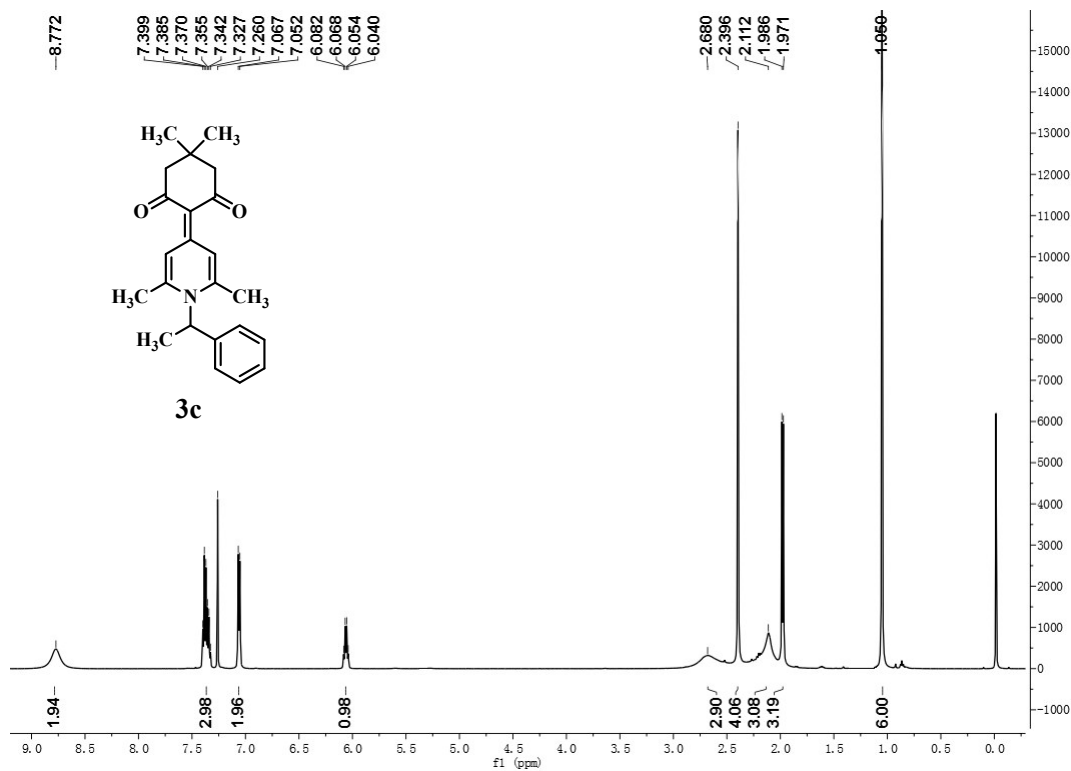


Fig. S15  $^1\text{H}$  NMR of **3c** ( $\text{CDCl}_3$ , 500 MHz).

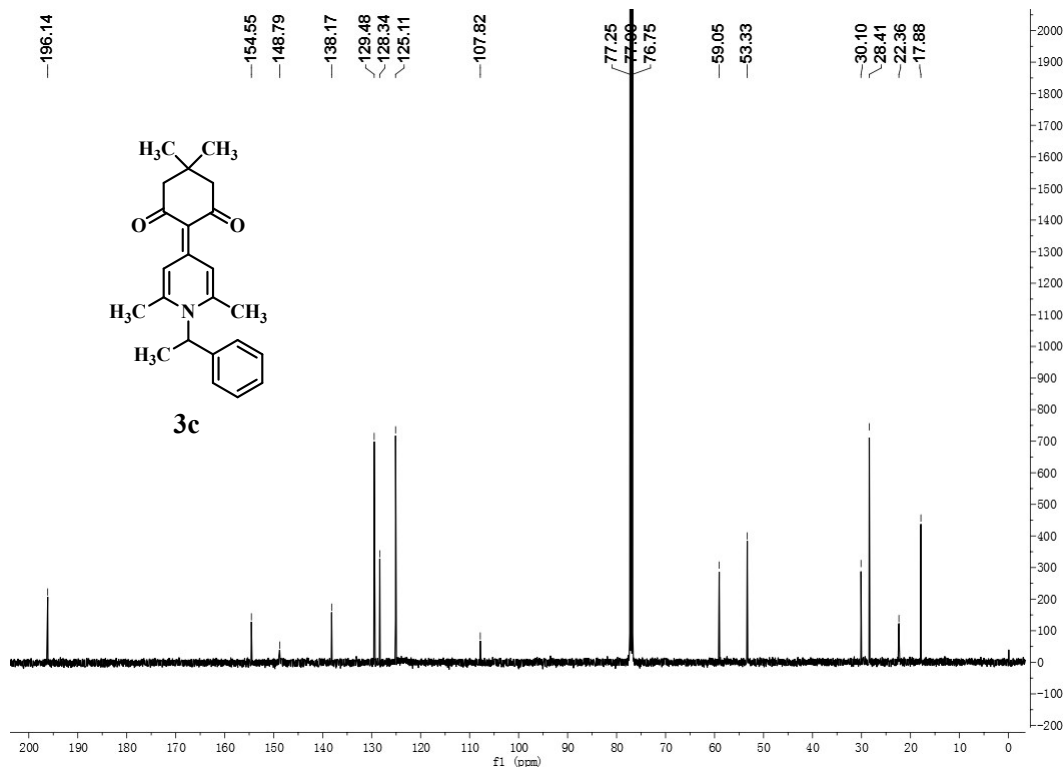


Fig. S16  $^{13}\text{C}$  NMR of **3c** ( $\text{CDCl}_3$ , 500 MHz).



Fig. S17 <sup>1</sup>H NMR of **3d** (CDCl<sub>3</sub>, 500 MHz).

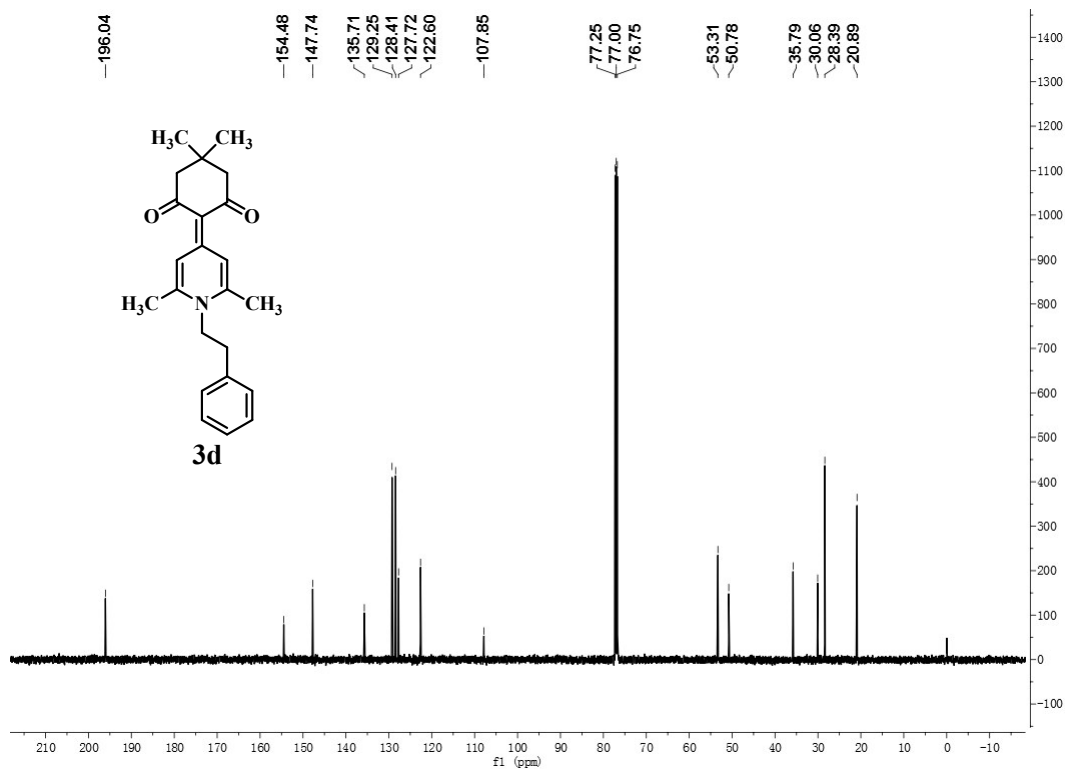


Fig. S18 <sup>13</sup>C NMR of **3d** (CDCl<sub>3</sub>, 125 MHz).