

## Supporting Information

### One Pot Synthesis of Aryl Nitriles from Aromatic Aldehydes in the Water Environment

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## <sup>1</sup>H NMR spectra of compound 1b-25b.

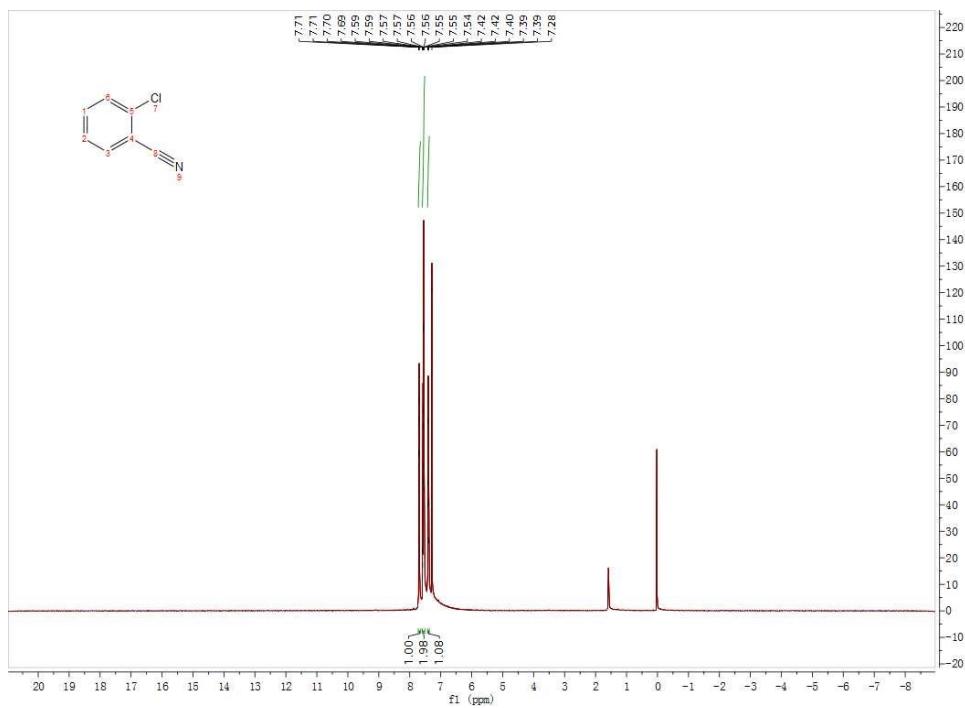


Figure S1 <sup>1</sup>H NMR spectra of compound 1b

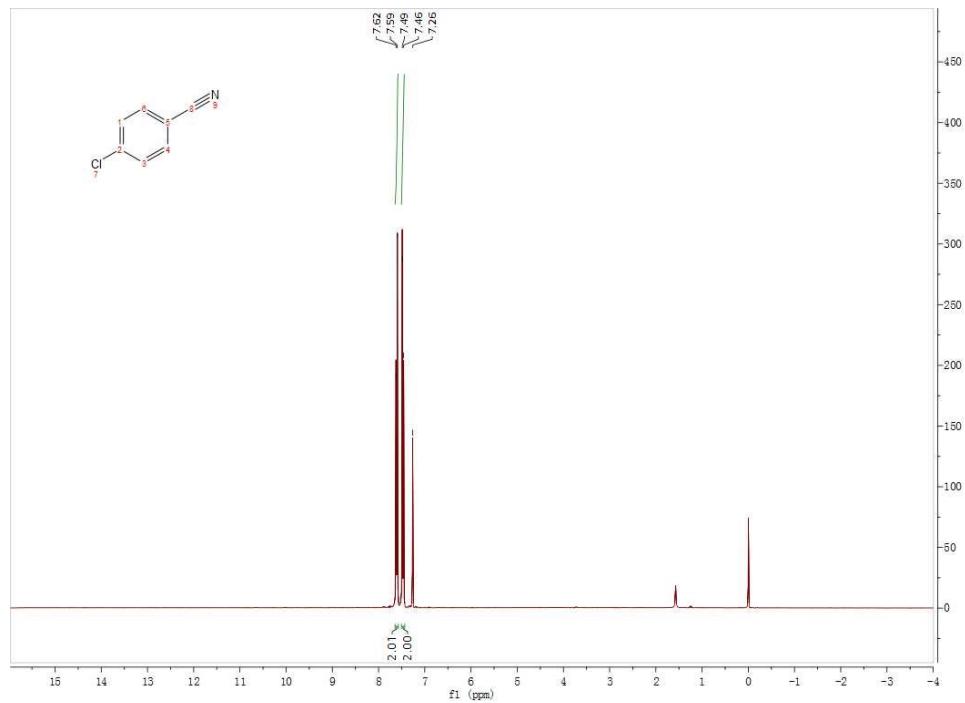


Figure S2 <sup>1</sup>H NMR spectra of compound 2b

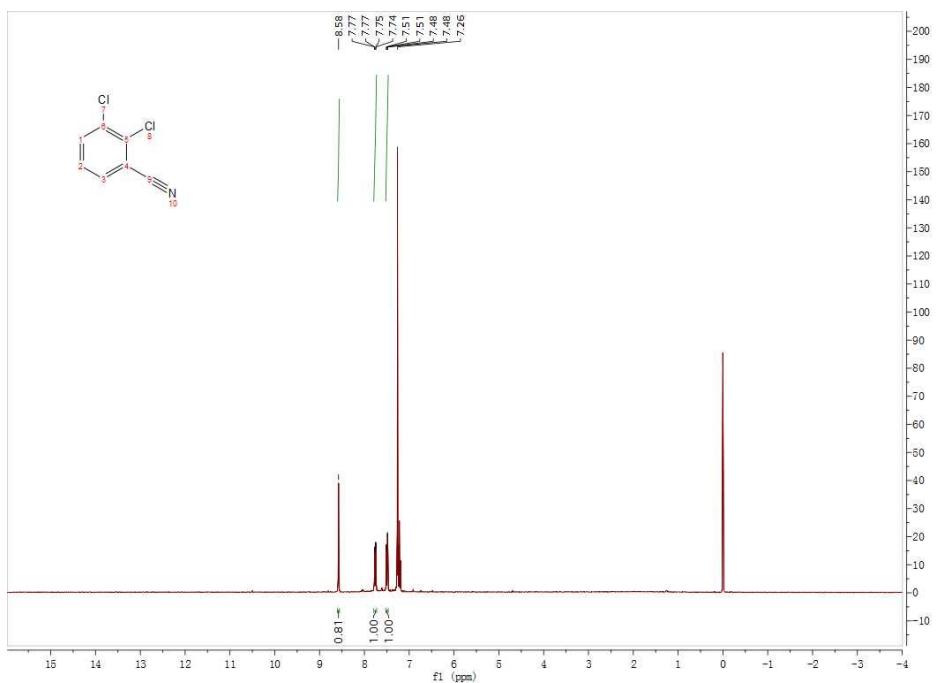


Figure S3 <sup>1</sup>H NMR spectra of compound 3b

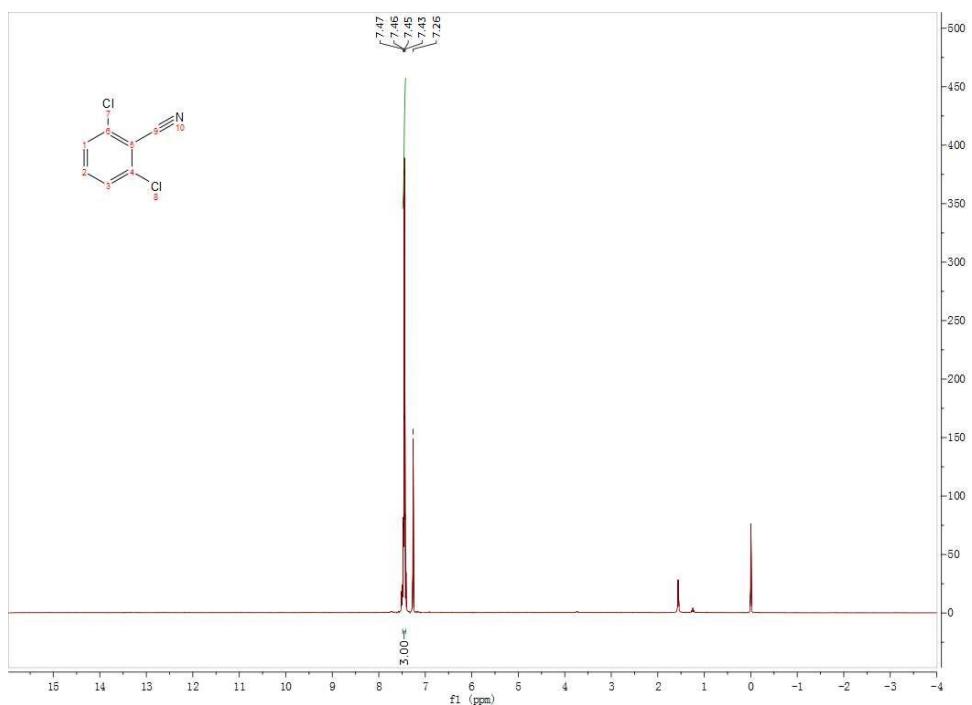


Figure S4 <sup>1</sup>H NMR spectra of compound 4b

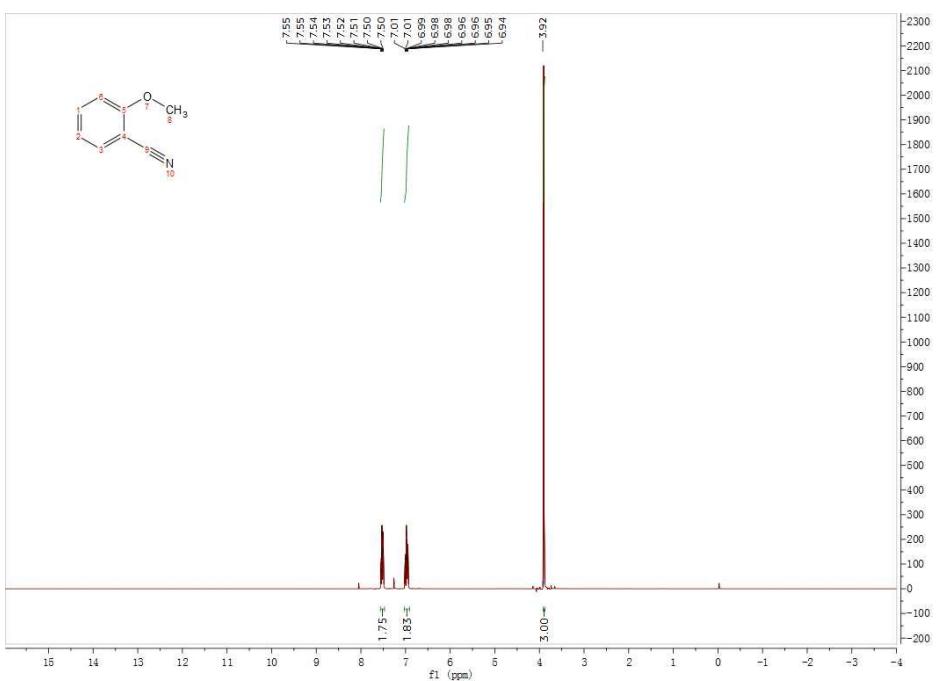


Figure S5 <sup>1</sup>H NMR spectra of compound 5b

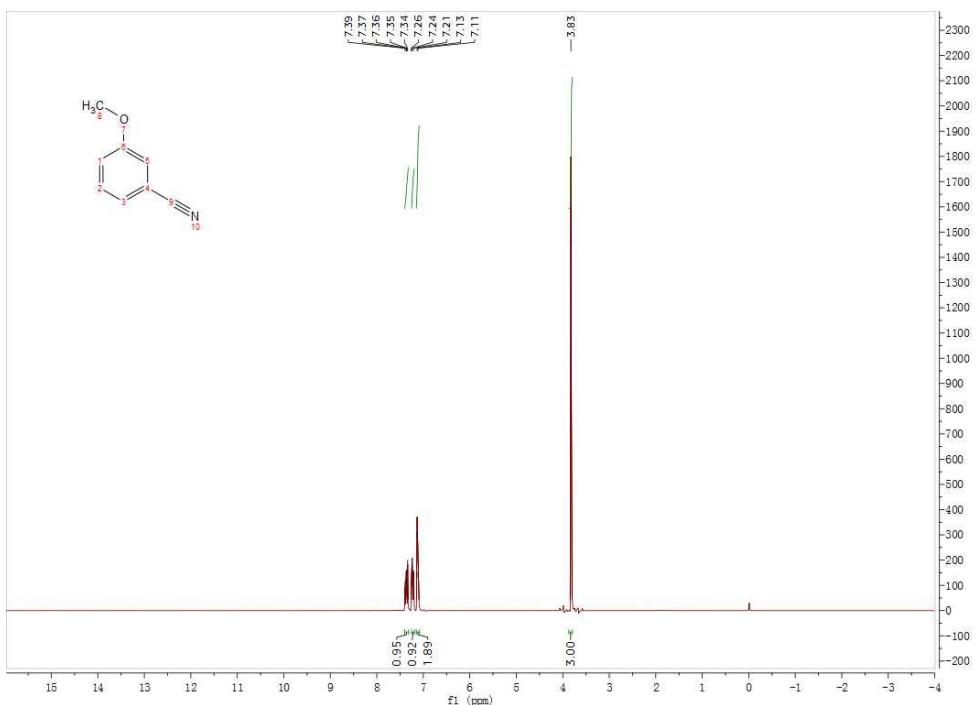


Figure S6 <sup>1</sup>H NMR spectra of compound 6b

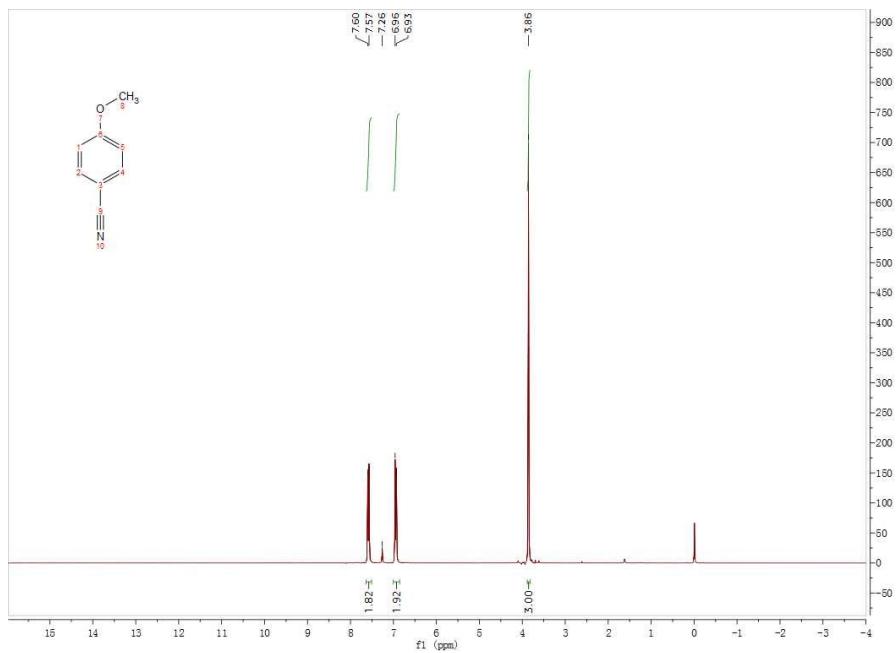


Figure S7 <sup>1</sup>H NMR spectra of compound 7b

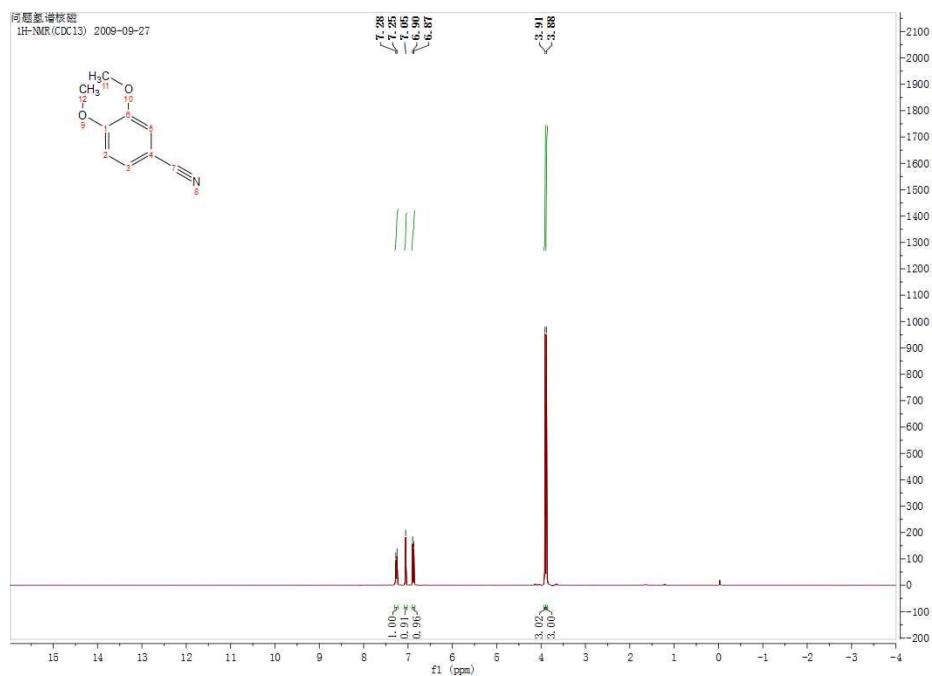


Figure S8 <sup>1</sup>H NMR spectra of compound 8b

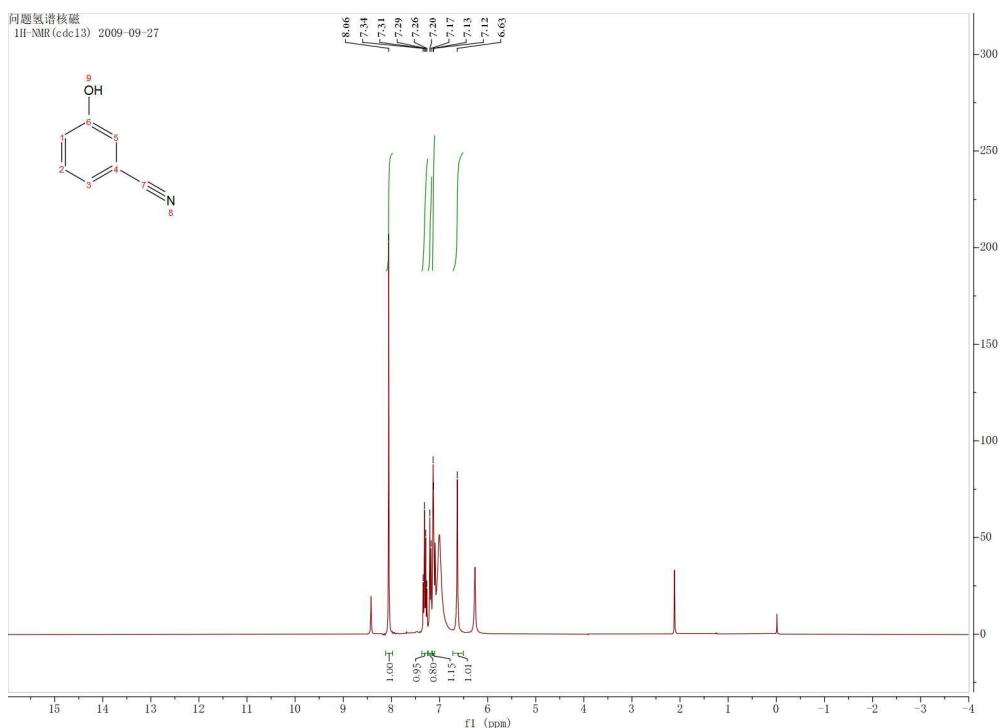


Figure S9 <sup>1</sup>H NMR spectra of compound 9b

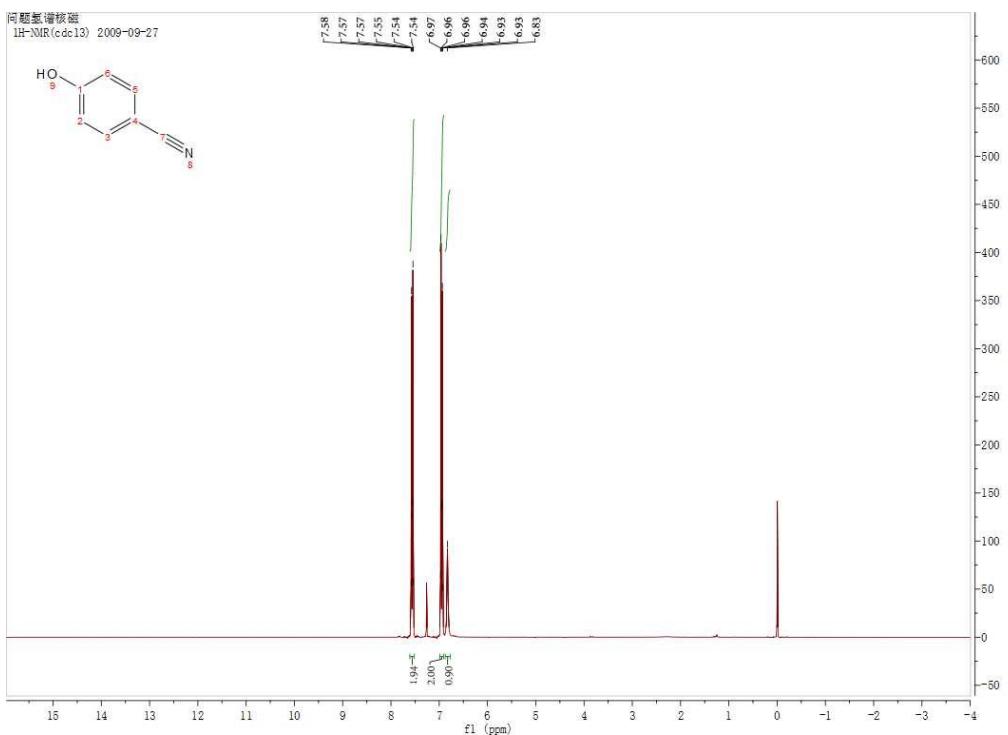


Figure S10 <sup>1</sup>H NMR spectra of compound 10b

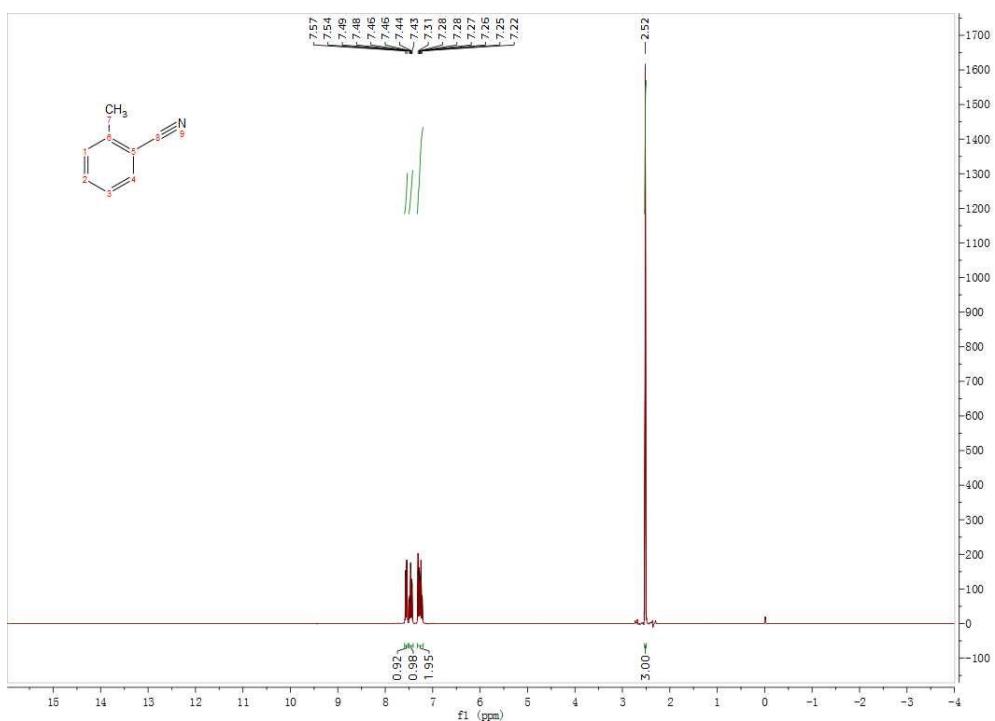


Figure S11  $^1\text{H}$  NMR spectra of compound 11b

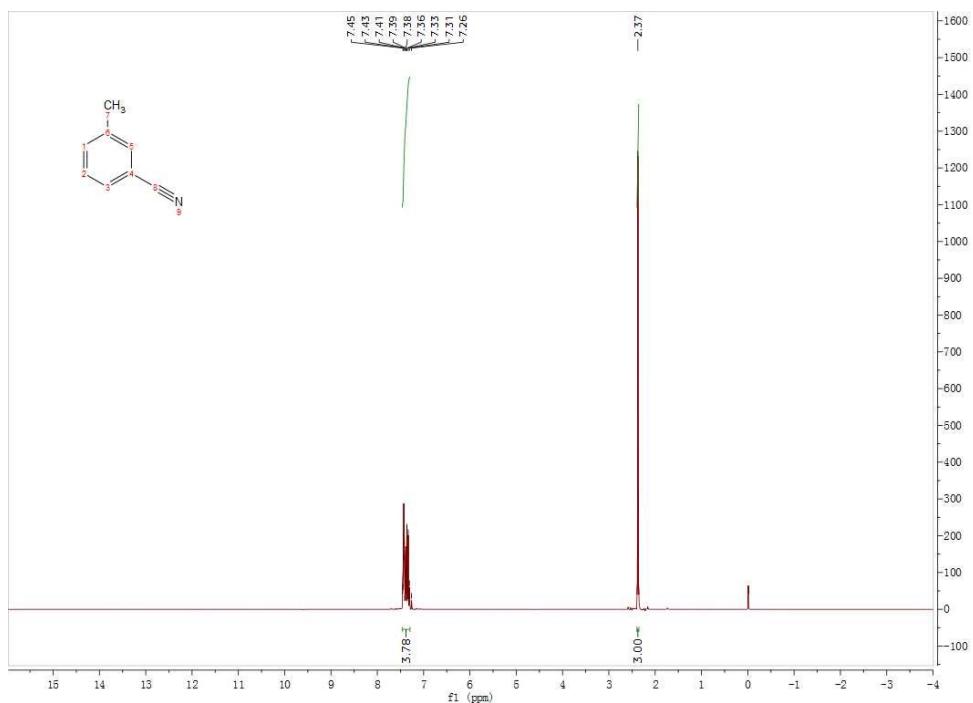


Figure S12  $^1\text{H}$  NMR spectra of compound 12b

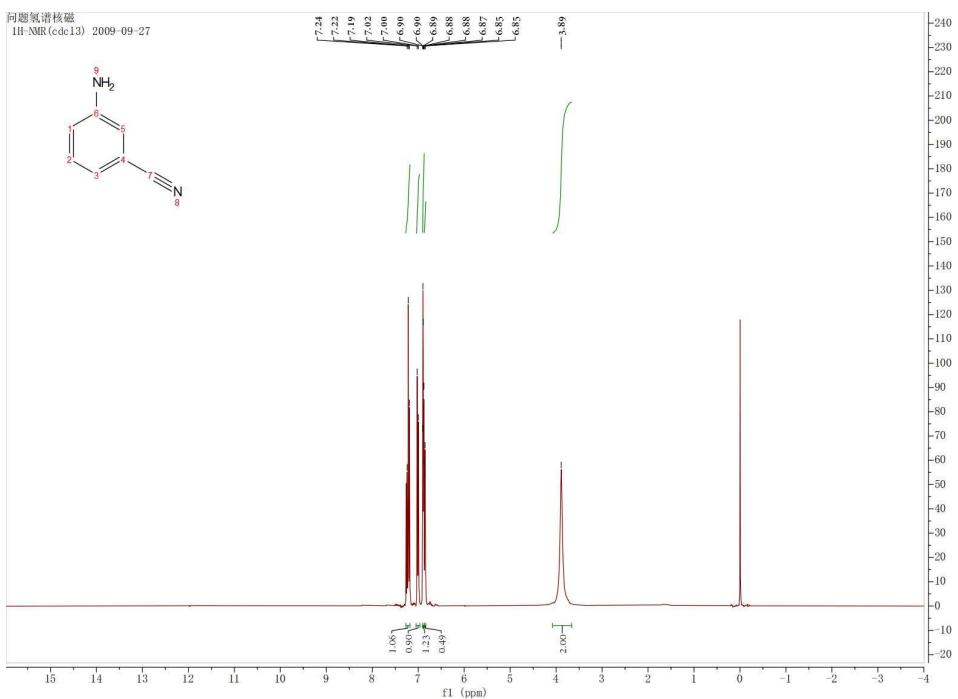


Figure S13  $^1\text{H}$  NMR spectra of compound 13b

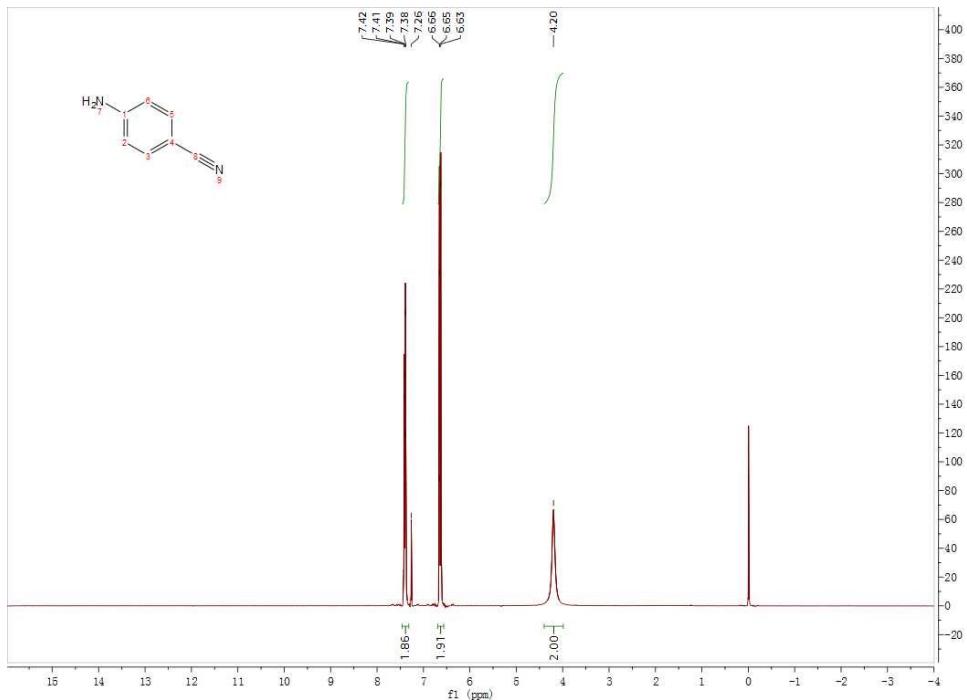
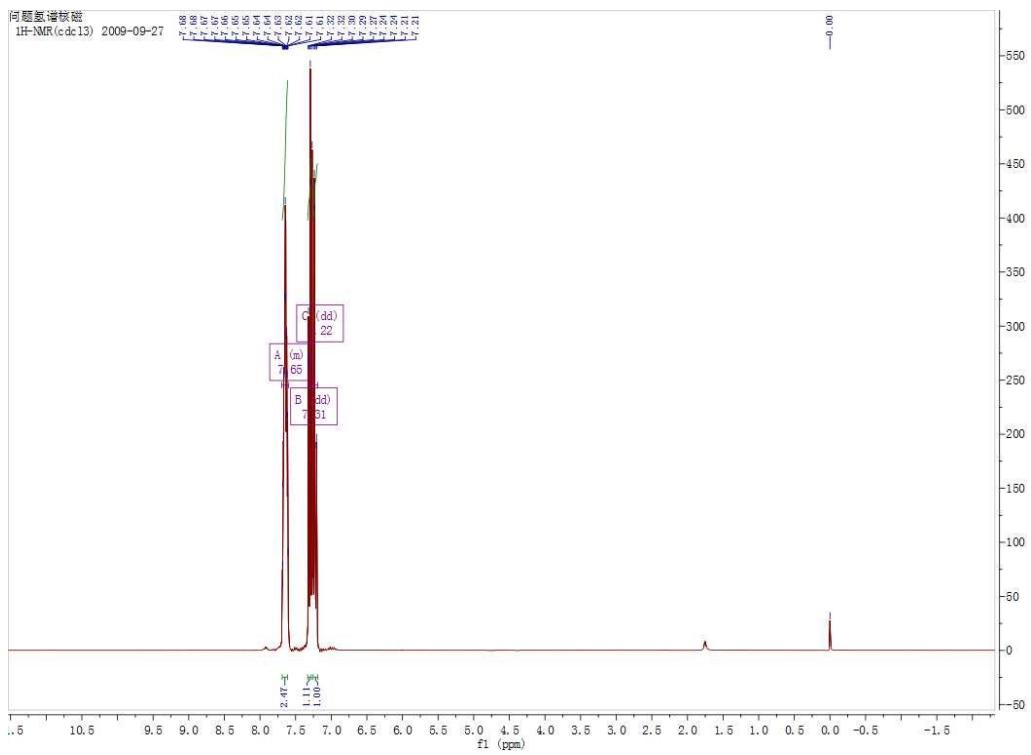


Figure S14  $^1\text{H}$  NMR spectra of compound 14b



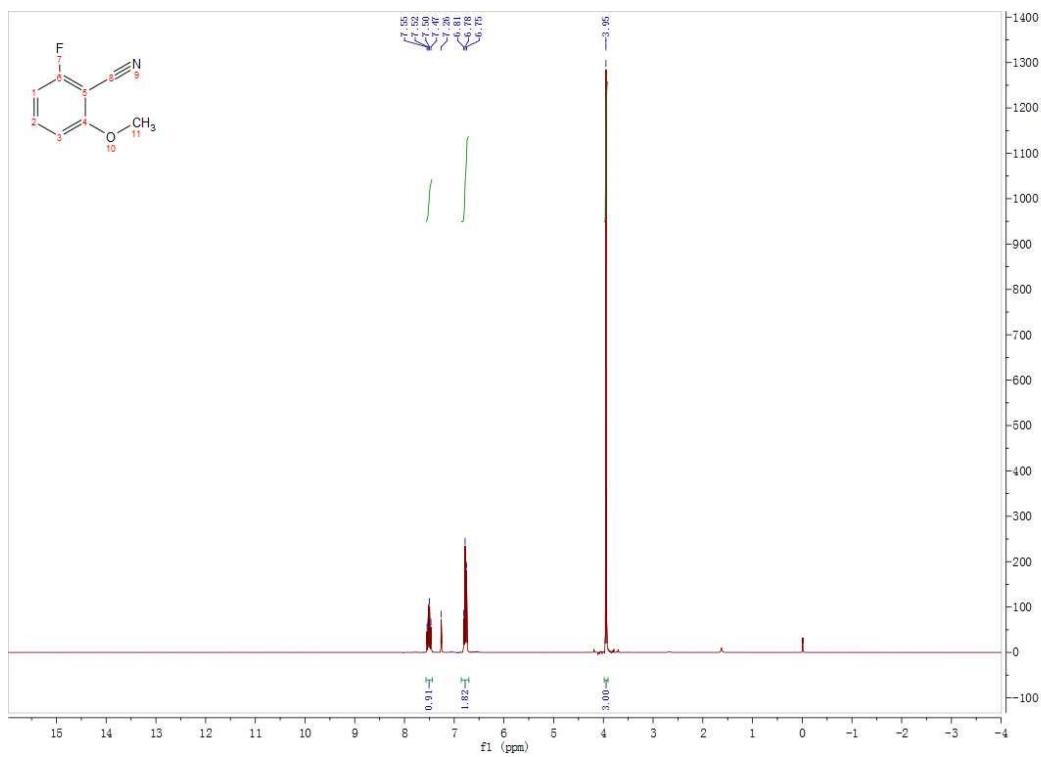


Figure S17 <sup>1</sup>H NMR spectra of compound 17b

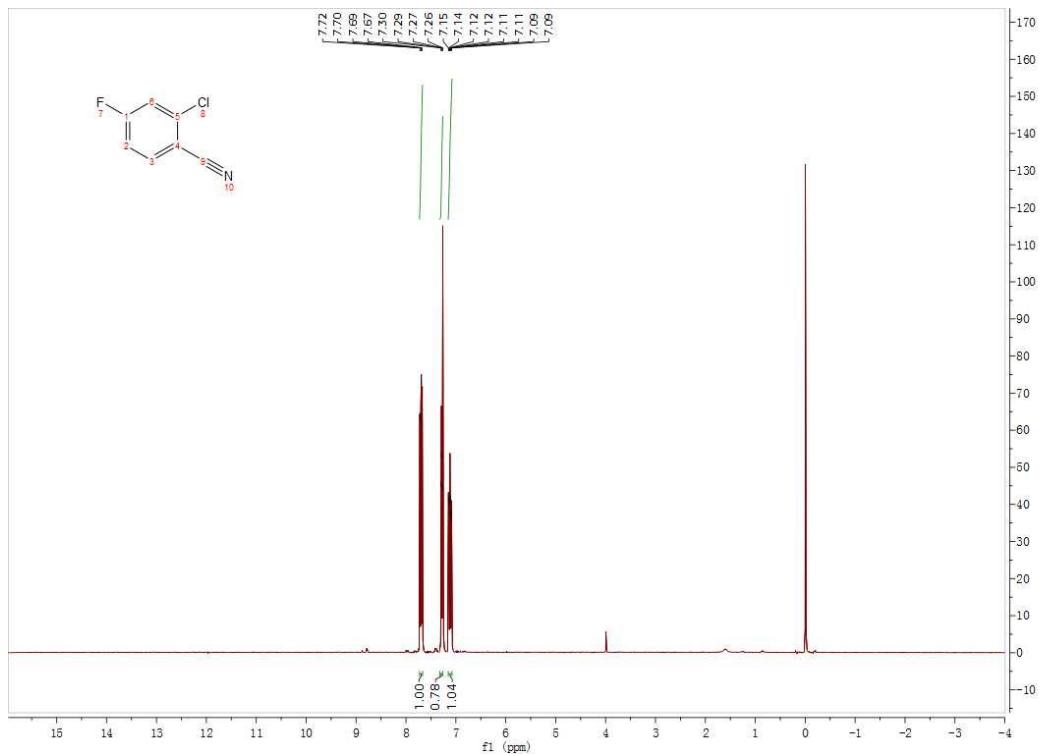


Figure S18 <sup>1</sup>H NMR spectra of compound 18b

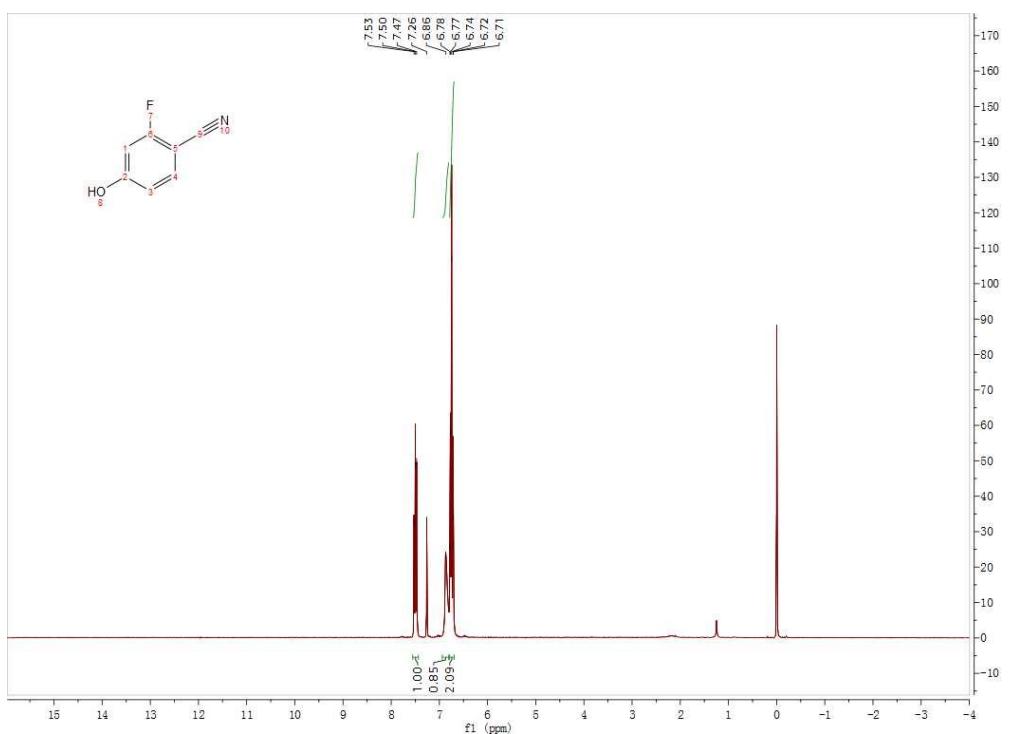


Figure S19 <sup>1</sup>H NMR spectra of compound 19b

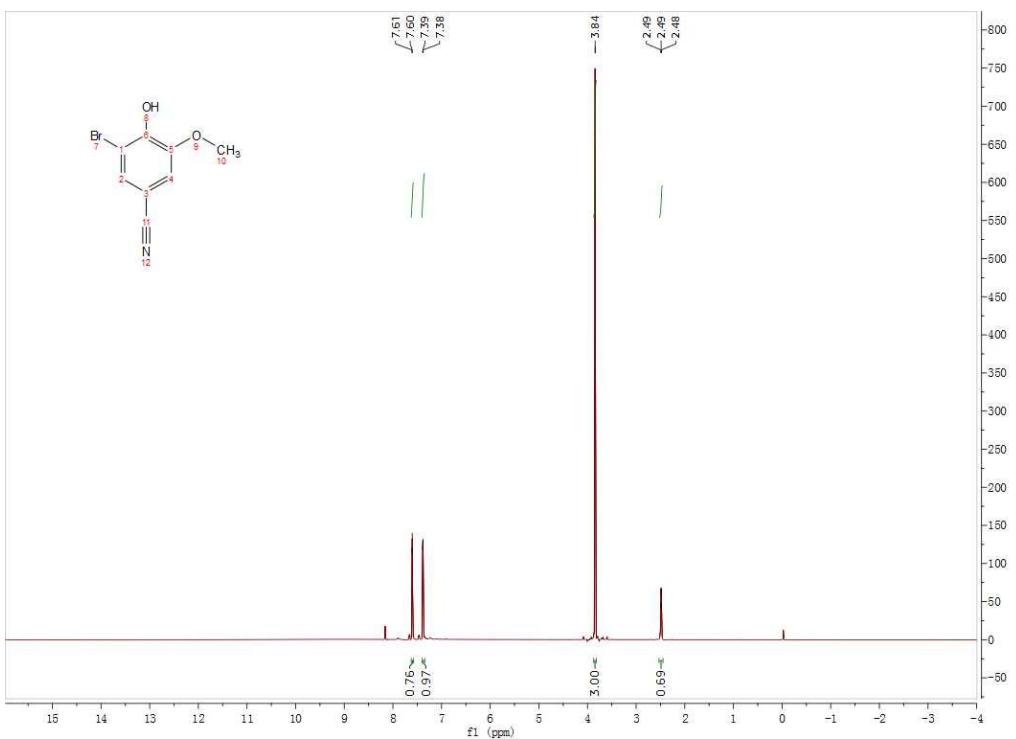


Figure S20 <sup>1</sup>H NMR spectra of compound 20b

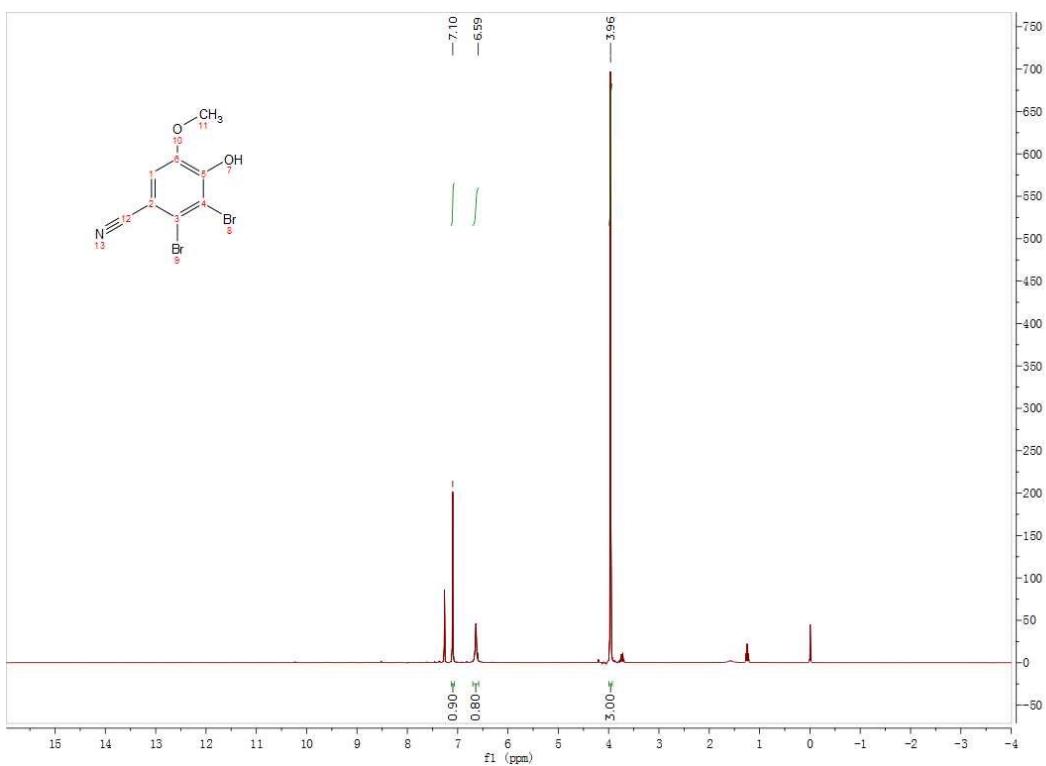


Figure S21 <sup>1</sup>H NMR spectra of compound 21b

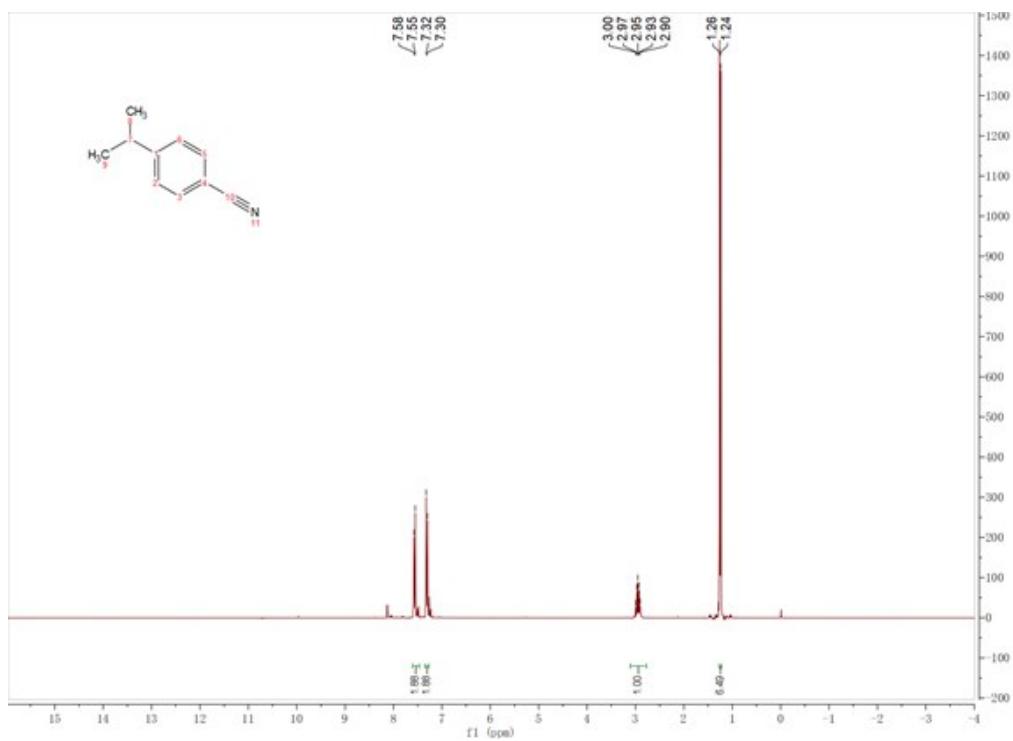


Figure S22 <sup>1</sup>H NMR spectra of compound 22b

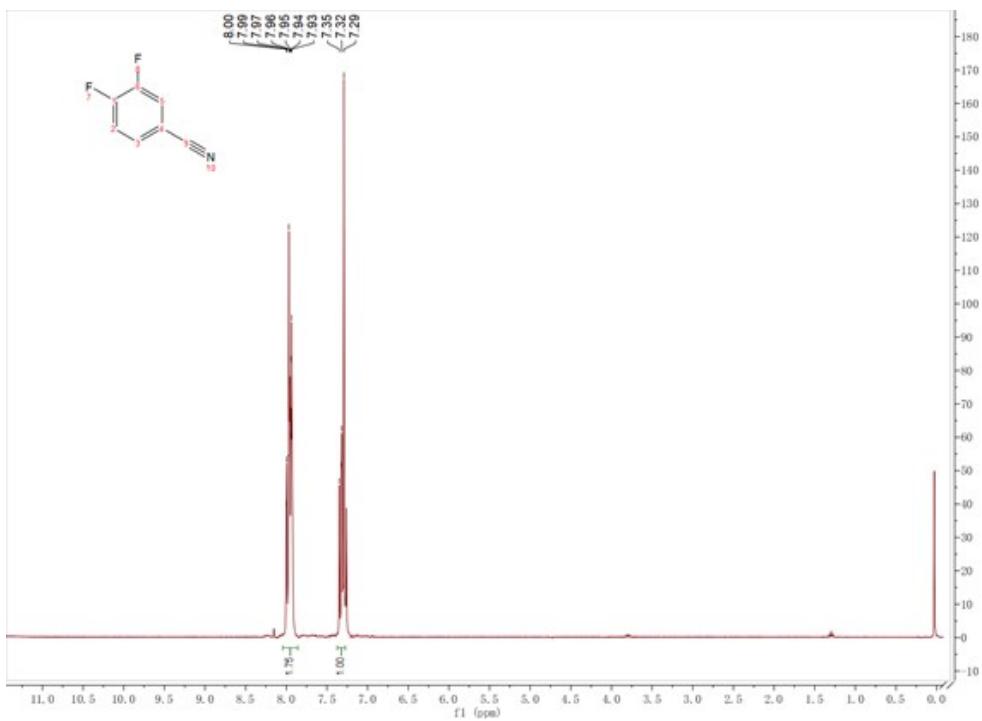


Figure S23 <sup>1</sup>H NMR spectra of compound 23b

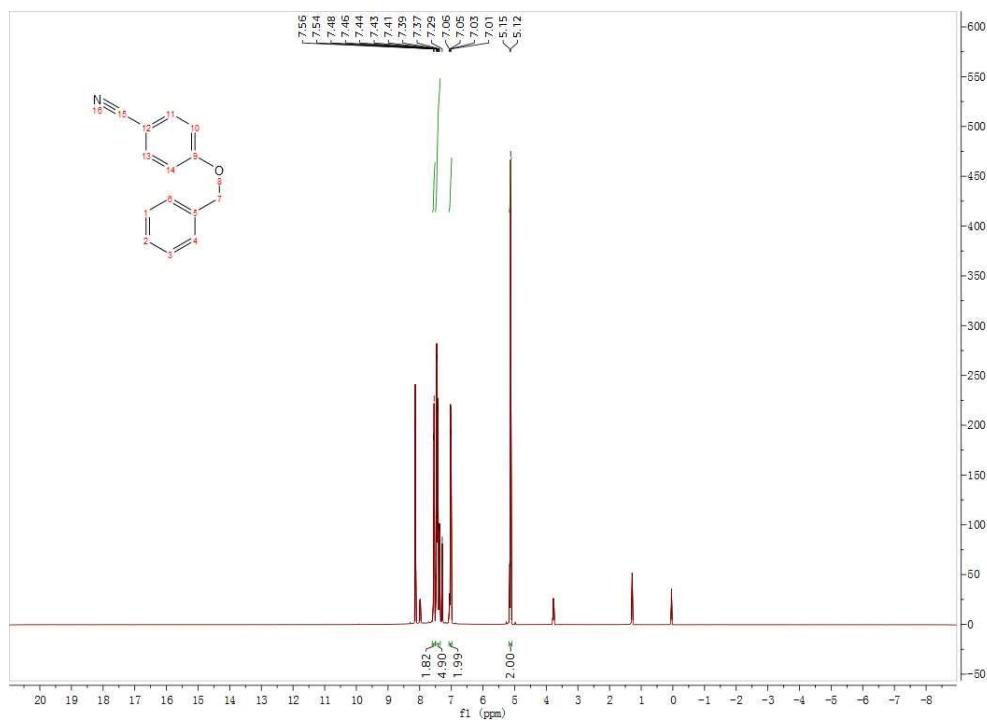


Figure S24 <sup>1</sup>H NMR spectra of compound 24b

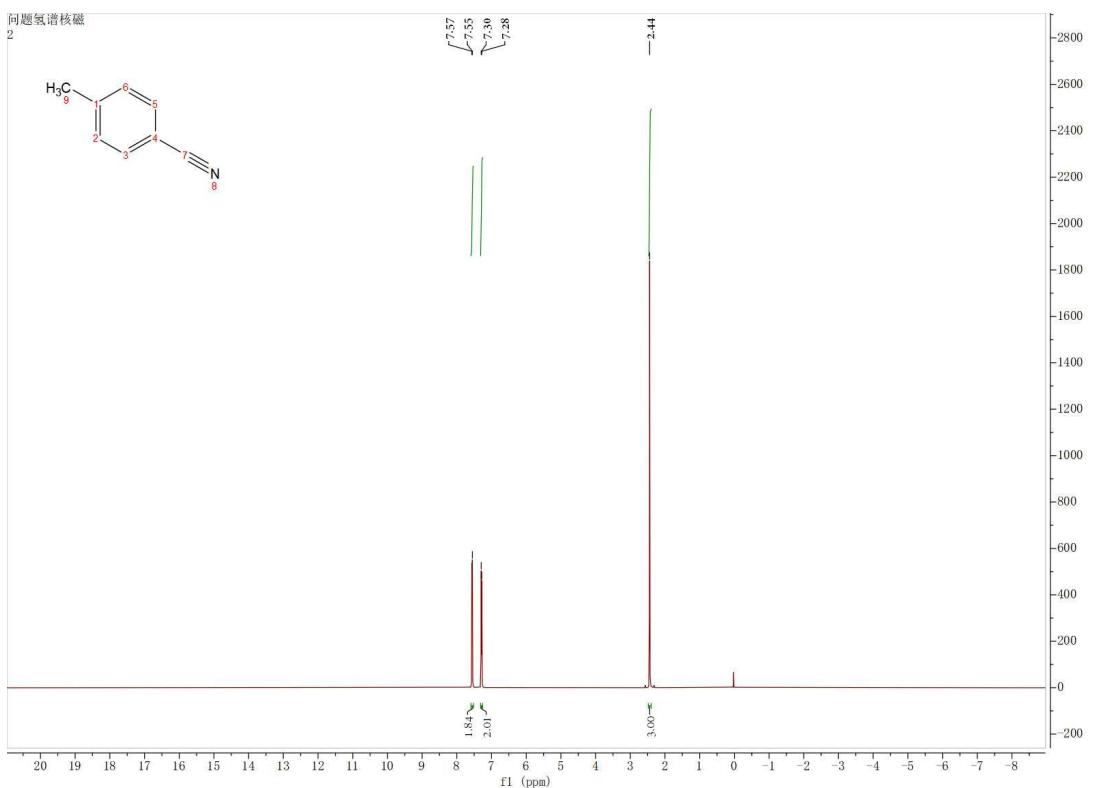


Figure S25  $^1\text{H}$  NMR spectra of compound 25b

### $^1\text{H}$ NMR spectra of the intermediate products.

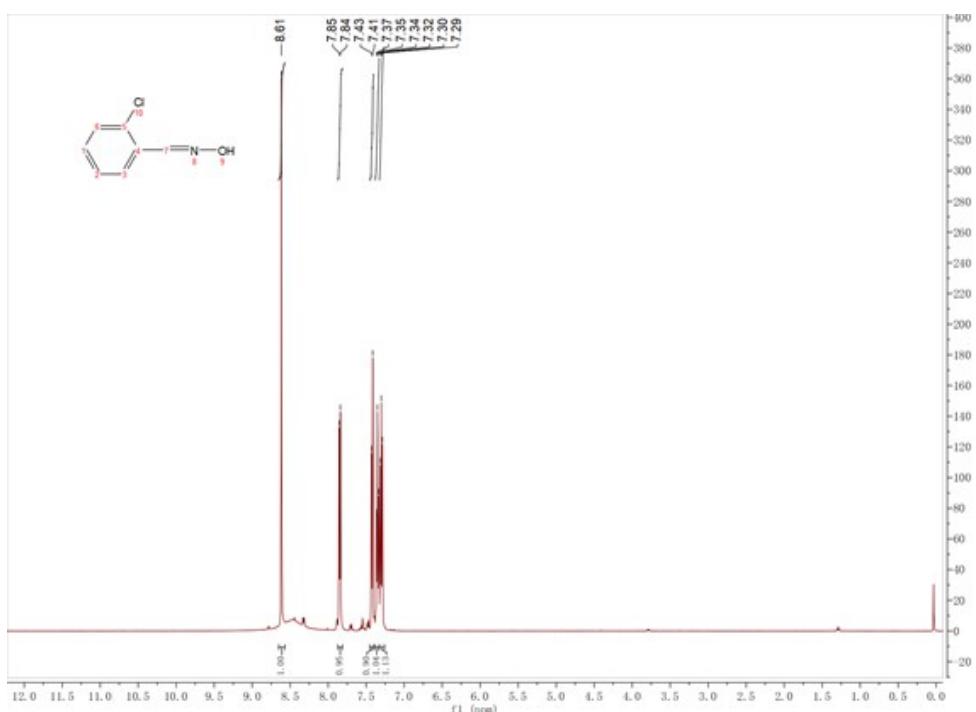


Figure S26  $^1\text{H}$  NMR spectra of 1A

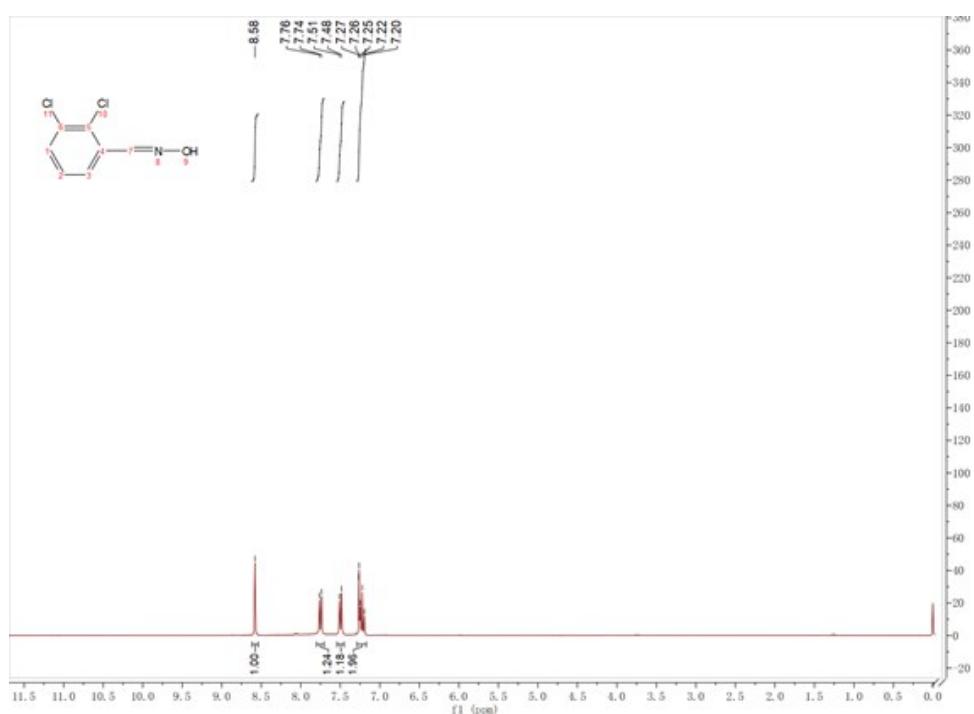


Figure S27 <sup>1</sup>H NMR spectra of 3A

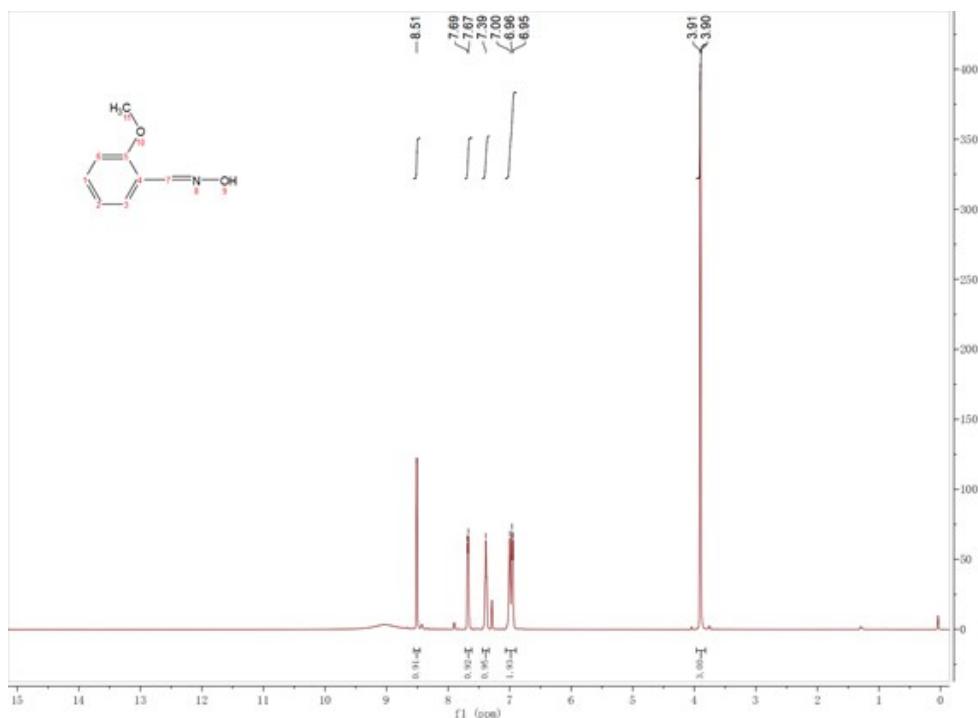


Figure S28 <sup>1</sup>H NMR spectra of 5A

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### **<sup>13</sup>C NMR spectra of compound 1b-25b.**

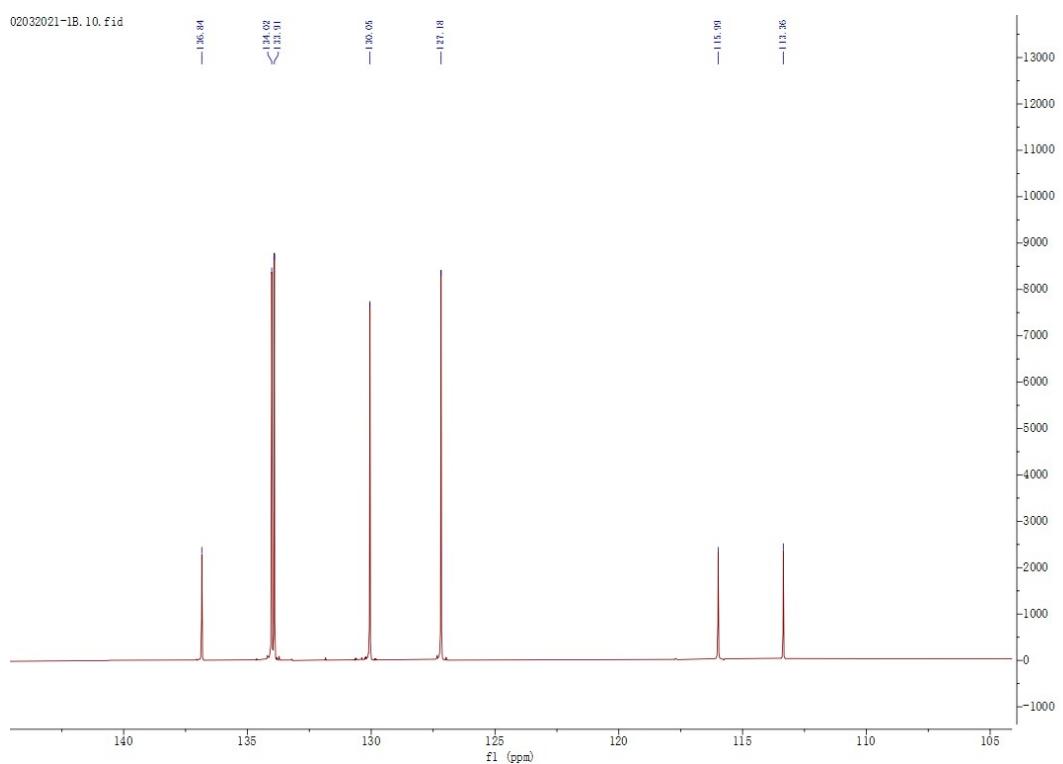


Figure S29 <sup>13</sup>C NMR spectra of compound 1b

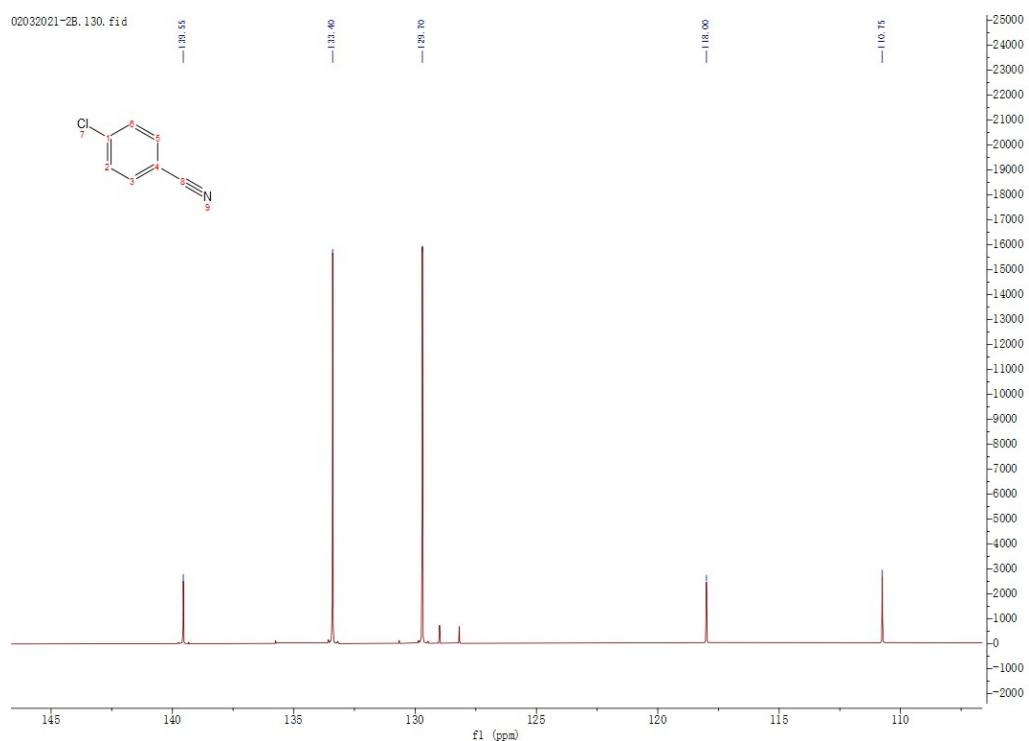


Figure S30 <sup>13</sup>C NMR spectra of compound 2b

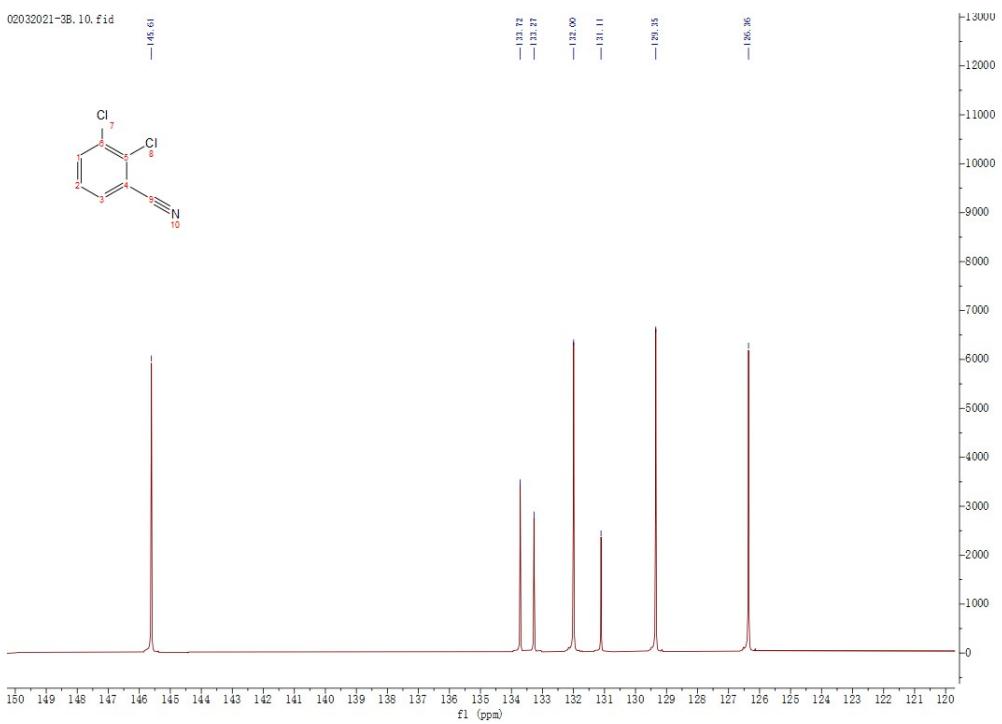


Figure S31  $^{13}\text{C}$  NMR spectra of compound 3b

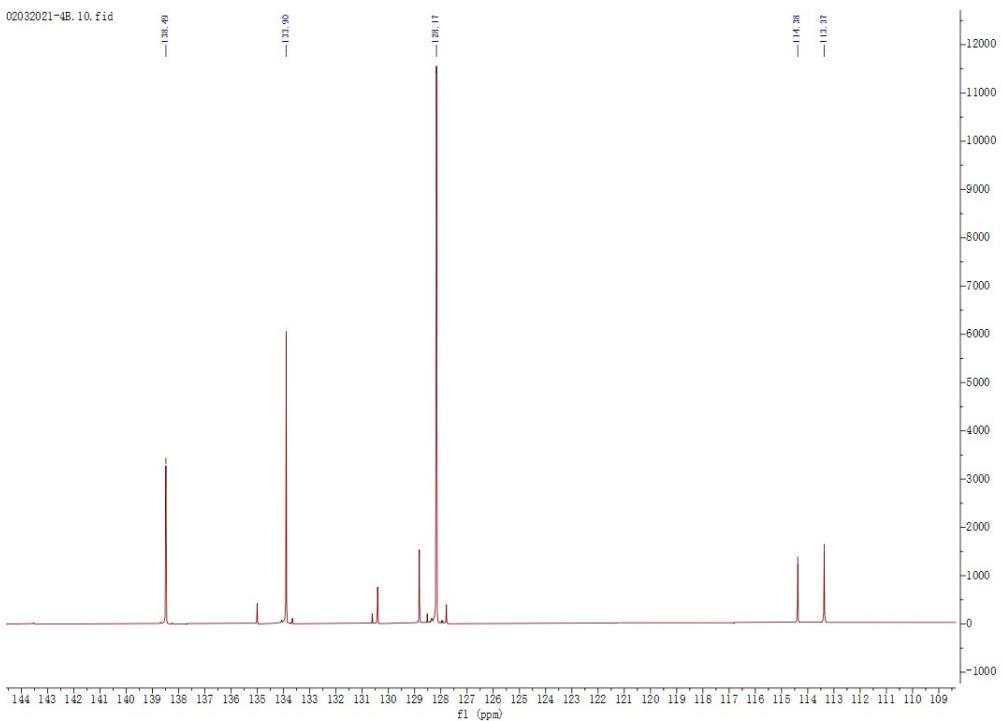


Figure S32  $^{13}\text{C}$  NMR spectra of compound 4b

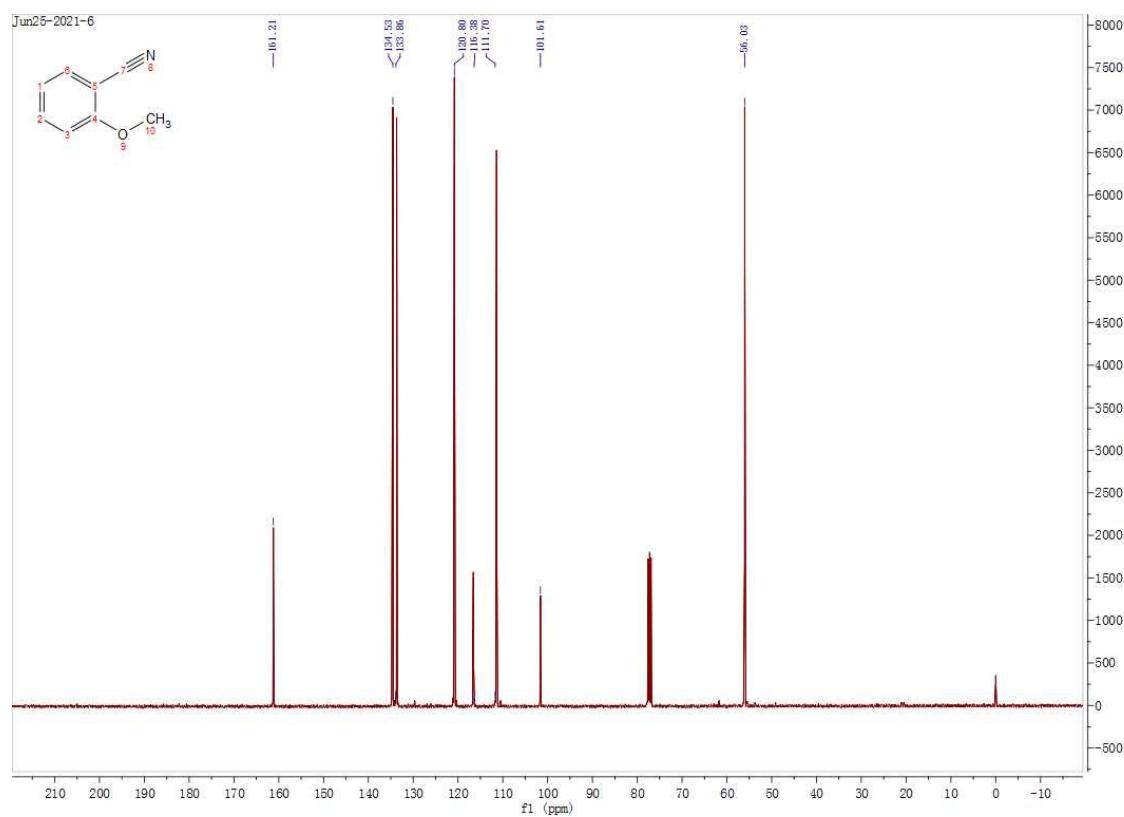


Figure S33  $^{13}\text{C}$  NMR spectra of compound 5b

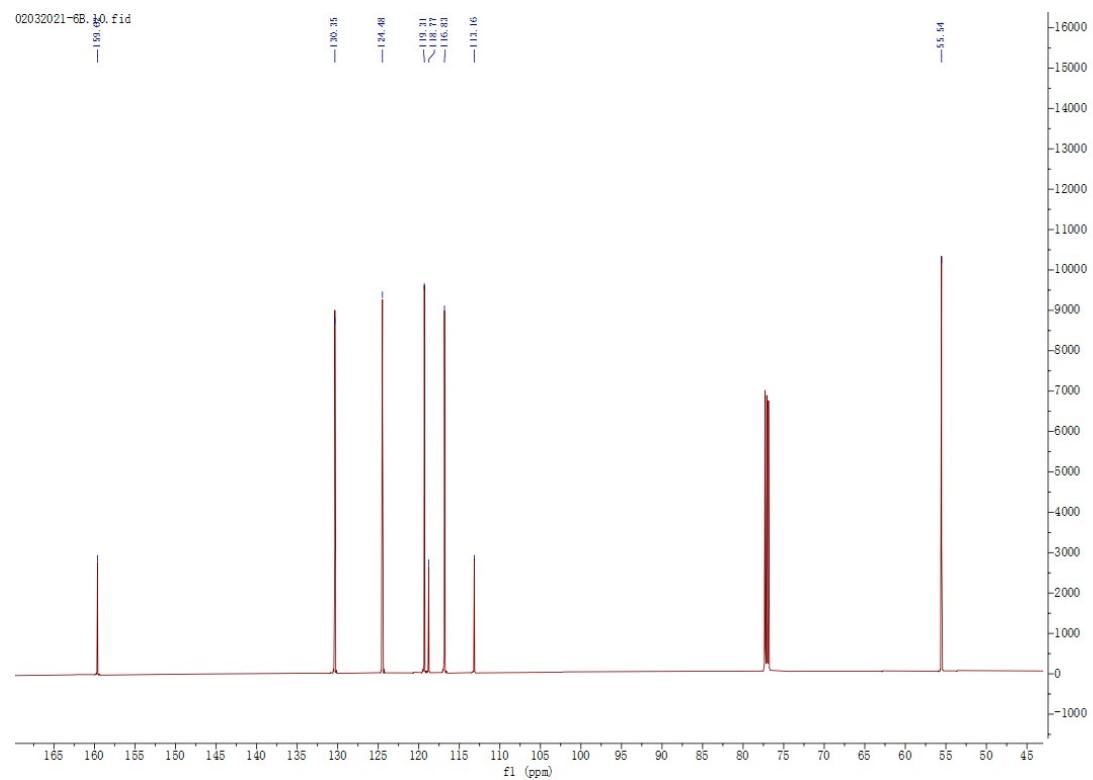


Figure S34  $^{13}\text{C}$  NMR spectra of compound 6b

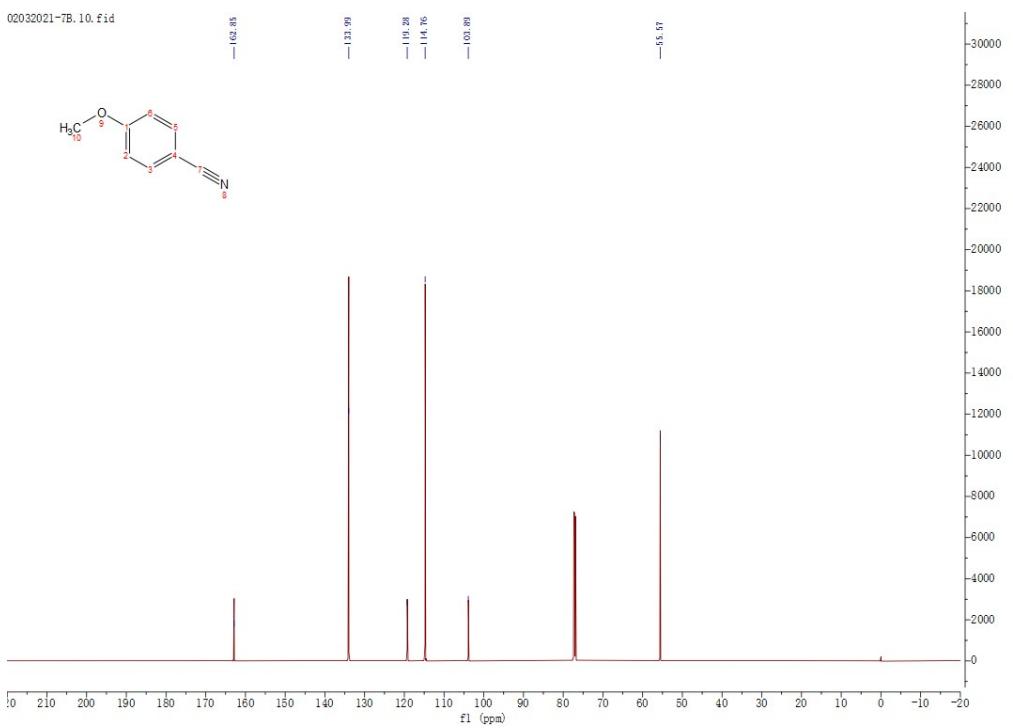


Figure S35  $^{13}\text{C}$  NMR spectra of compound 7b

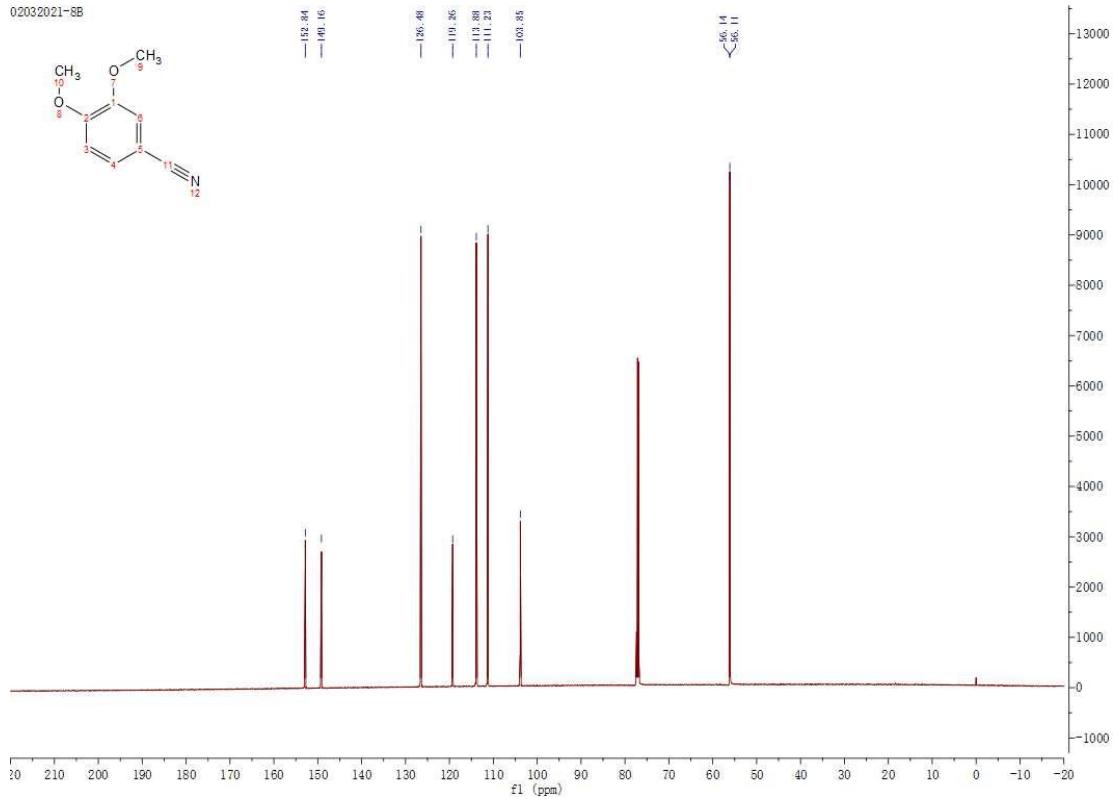


Figure S36  $^{13}\text{C}$  NMR spectra of compound 8b

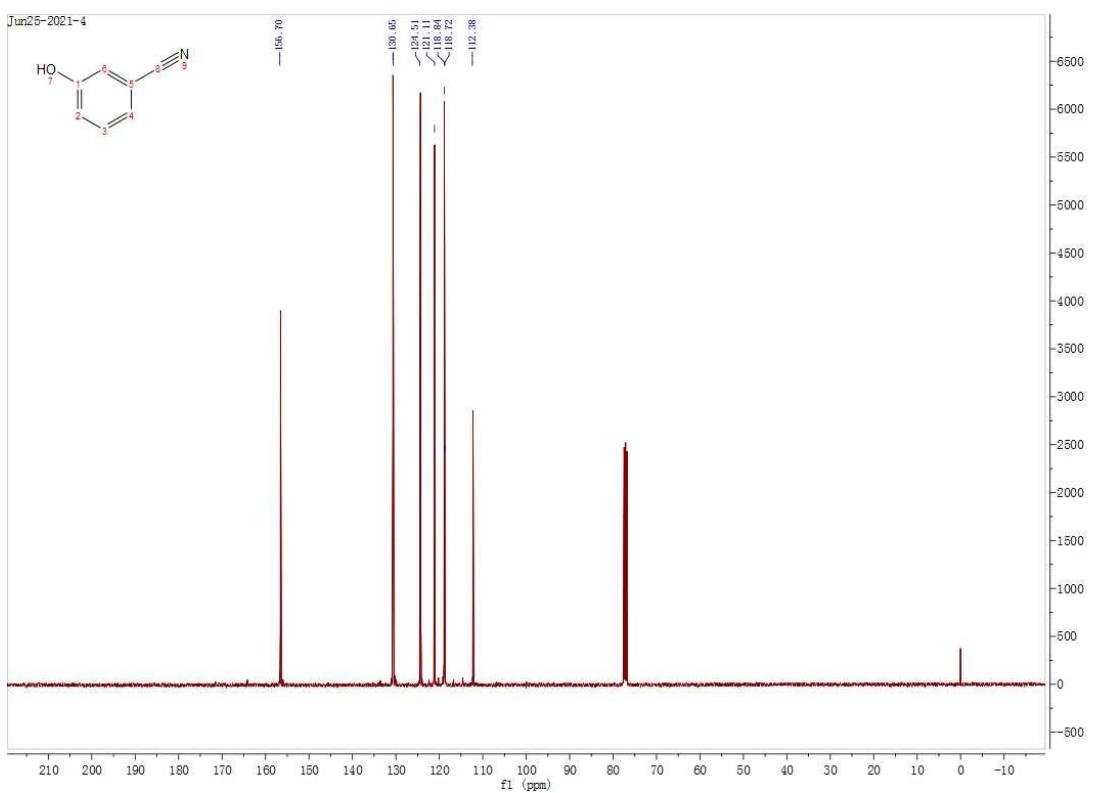


Figure S37  $^{13}\text{C}$  NMR spectra of compound 9b

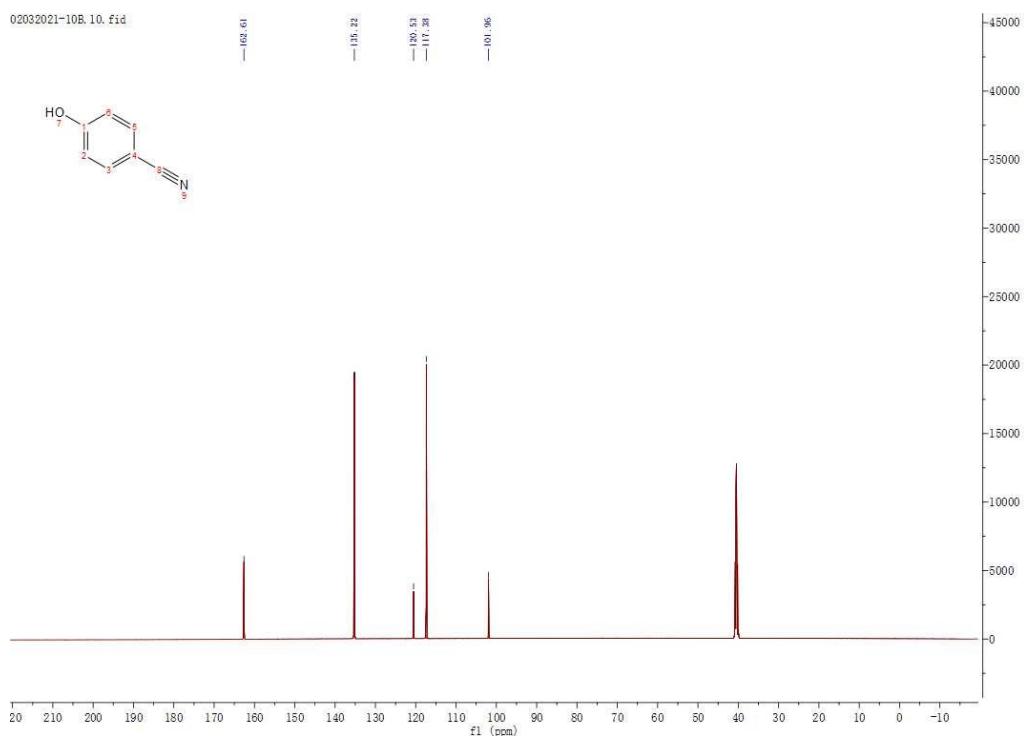


Figure S38  $^{13}\text{C}$  NMR spectra of compound 10b

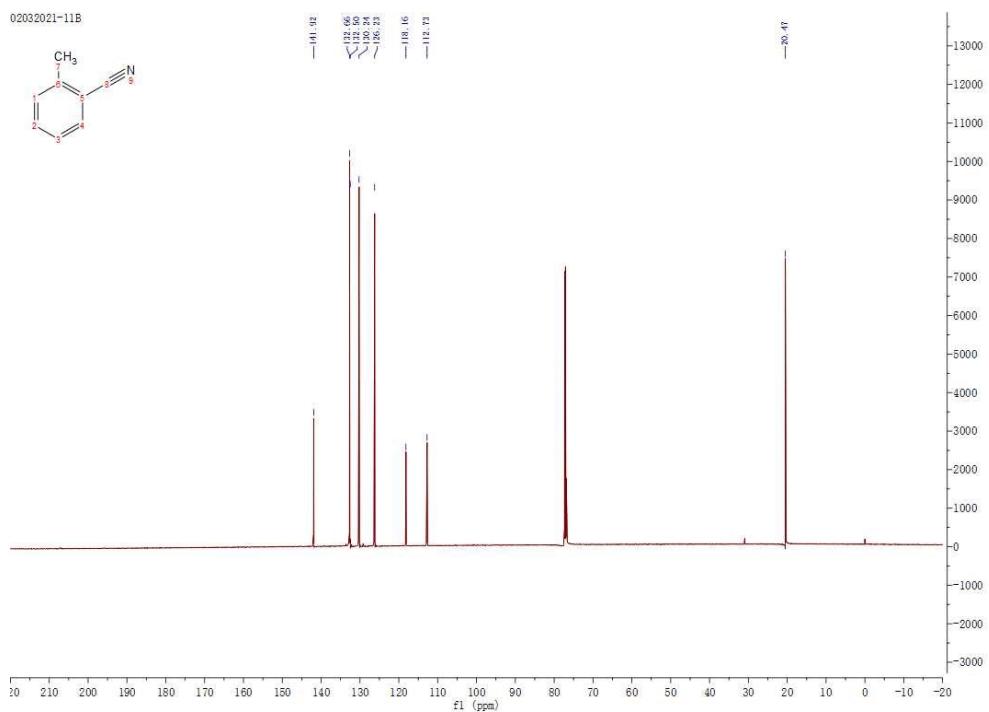


Figure S39  $^{13}\text{C}$  NMR spectra of compound 11b

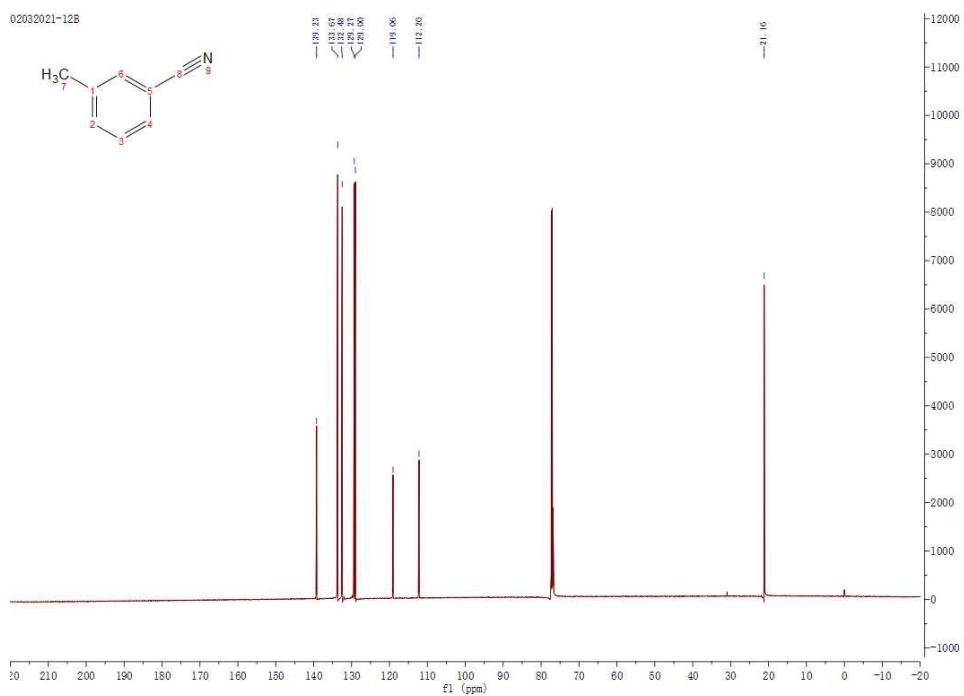


Figure S40  $^{13}\text{C}$  NMR spectra of compound 12b

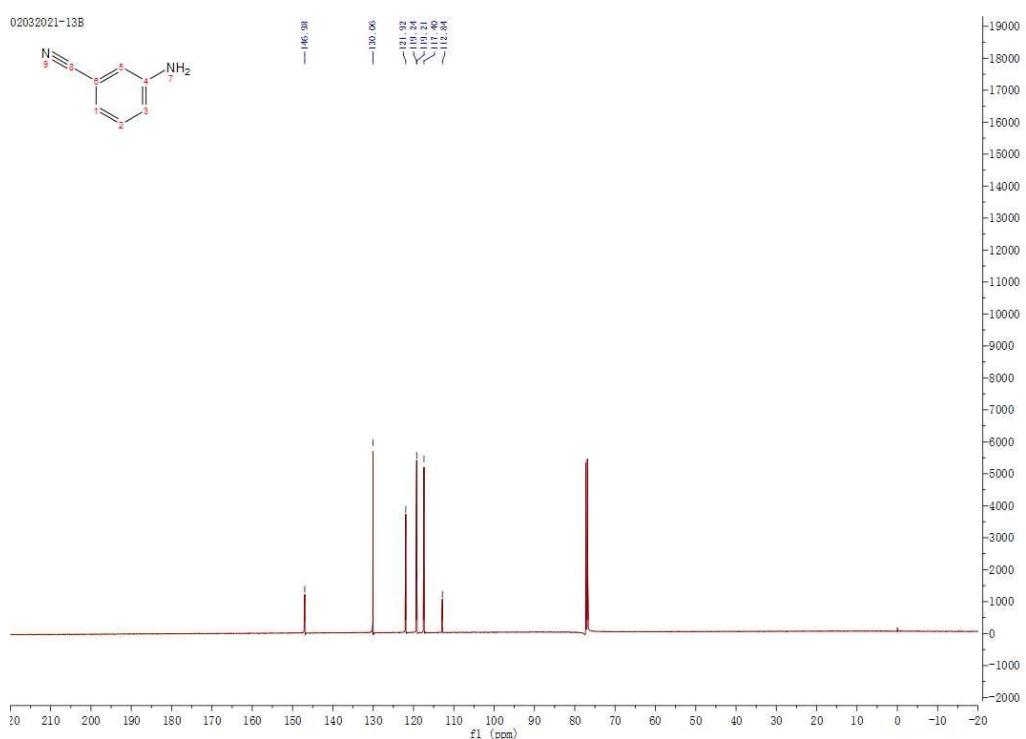


Figure S41  $^{13}\text{C}$  NMR spectra of compound 13b

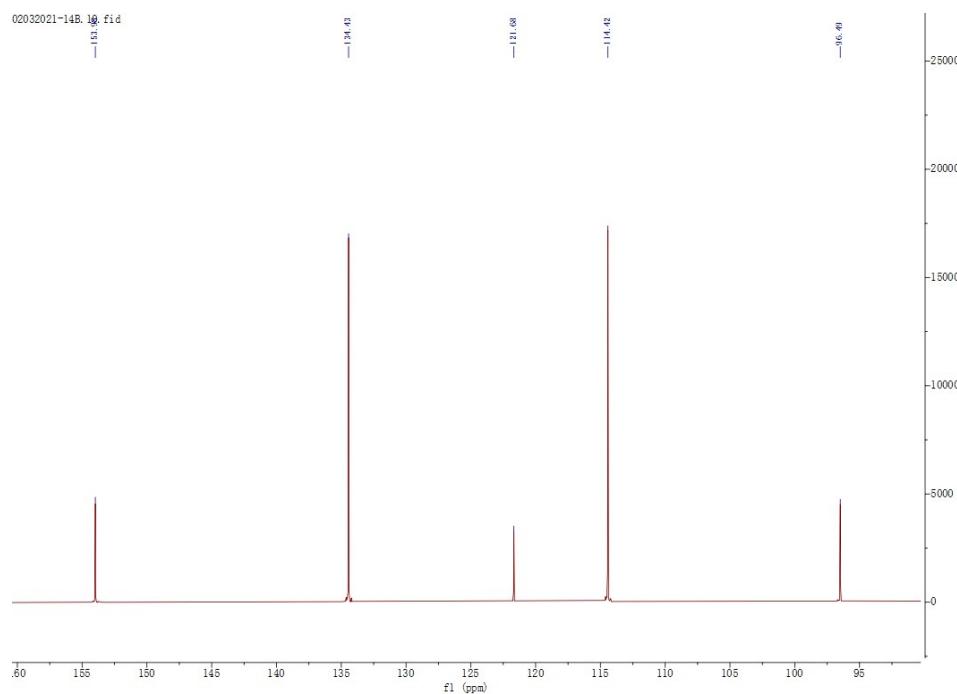


Figure S42  $^{13}\text{C}$  NMR spectra of compound 14b

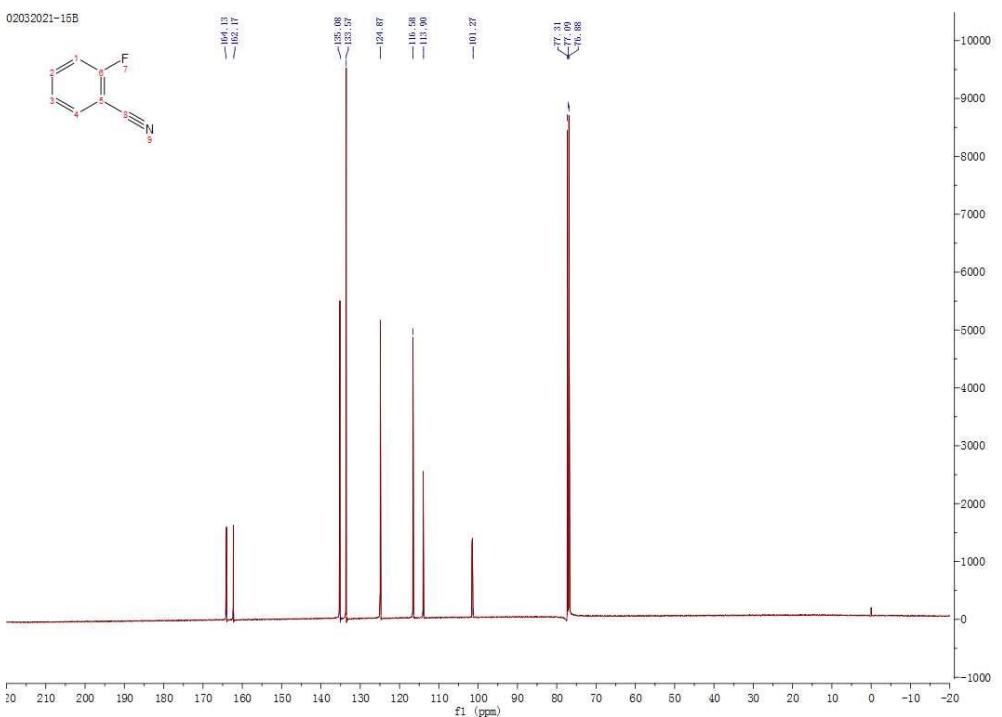


Figure S43  $^{13}\text{C}$  NMR spectra of compound 15b

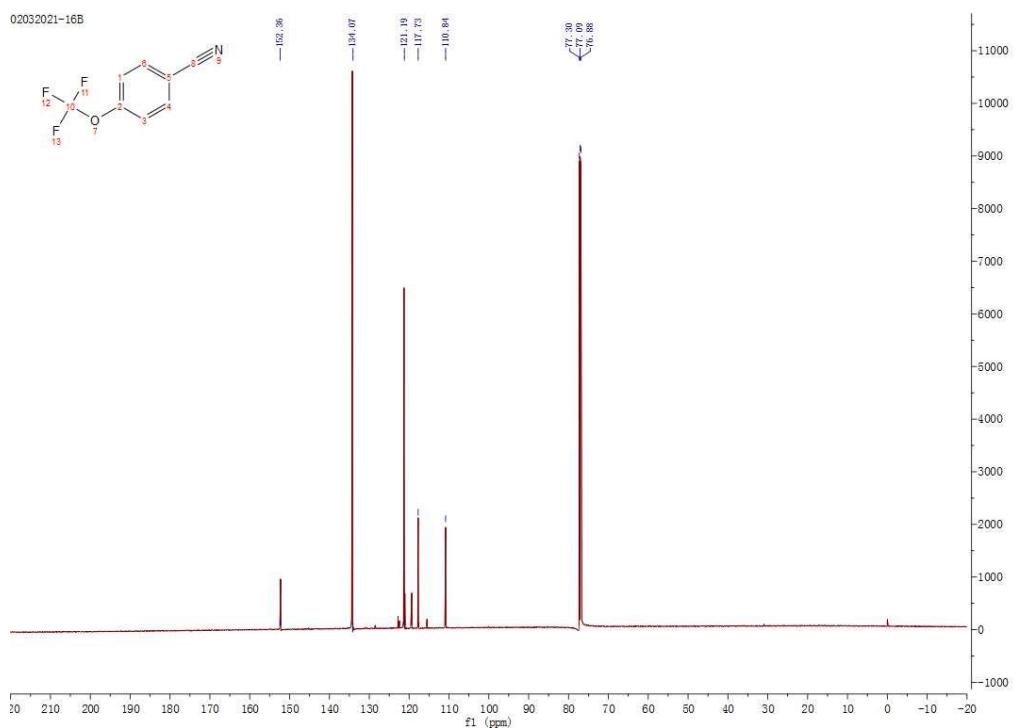


Figure S44  $^{13}\text{C}$  NMR spectra of compound 16b

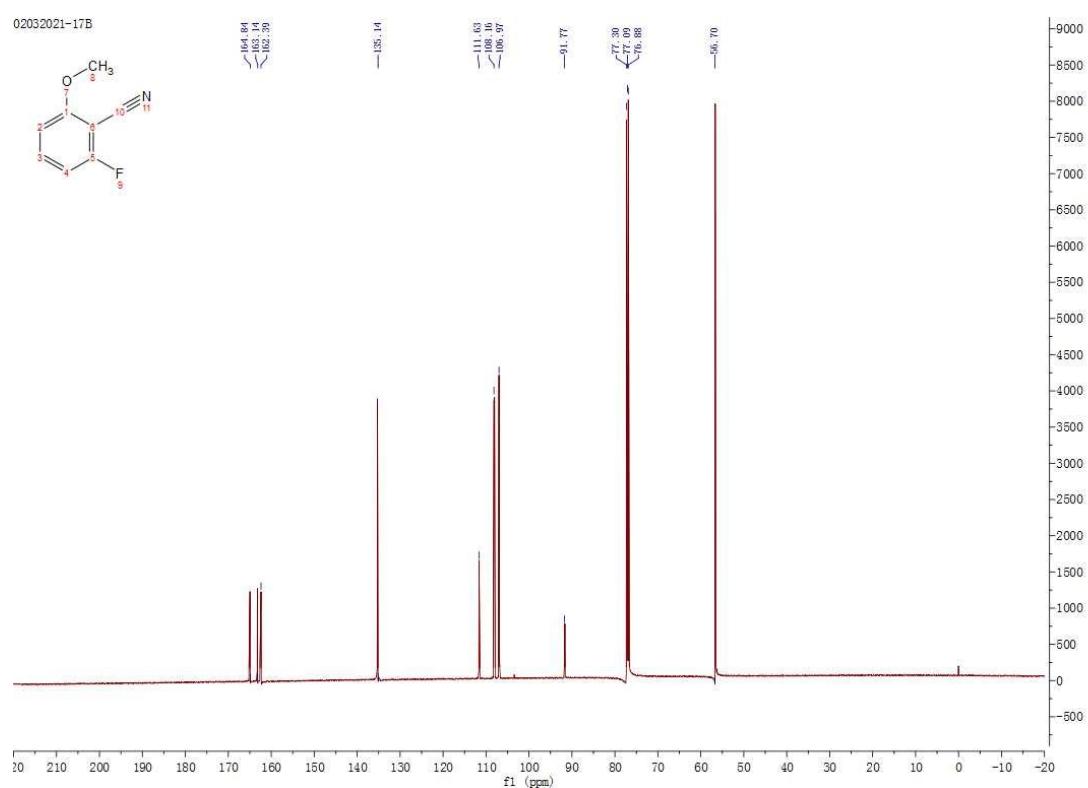


Figure S45  $^{13}\text{C}$  NMR spectra of compound 17b

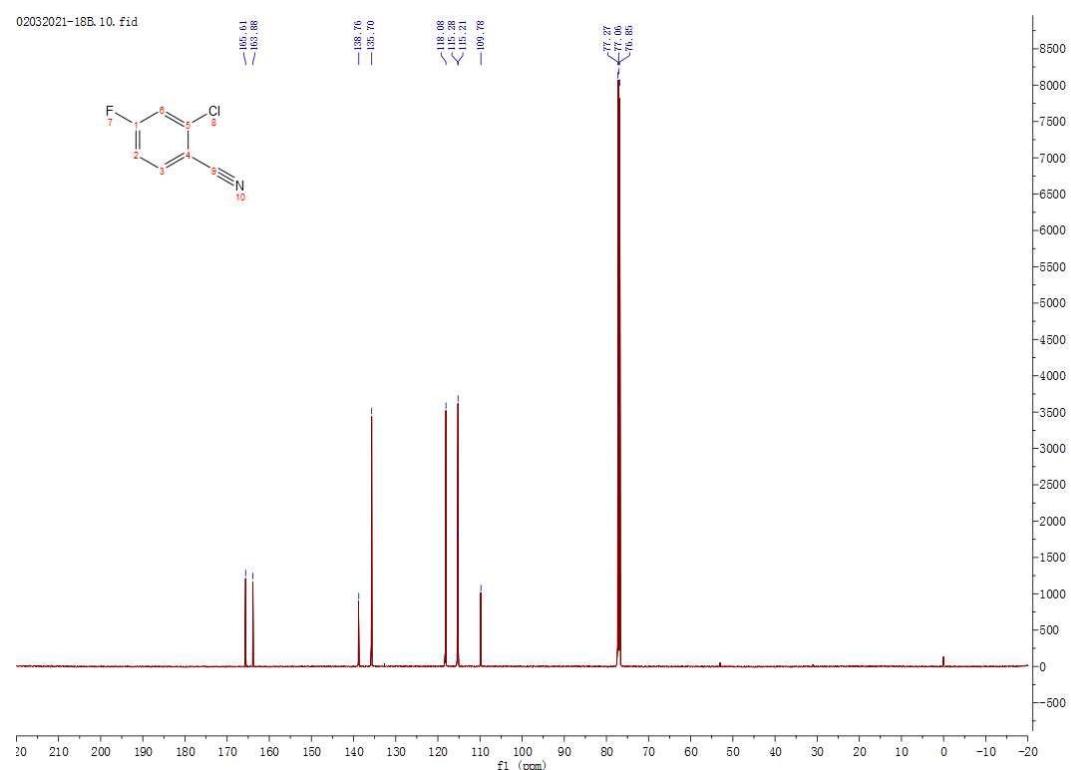


Figure S46  $^{13}\text{C}$  NMR spectra of compound 18b

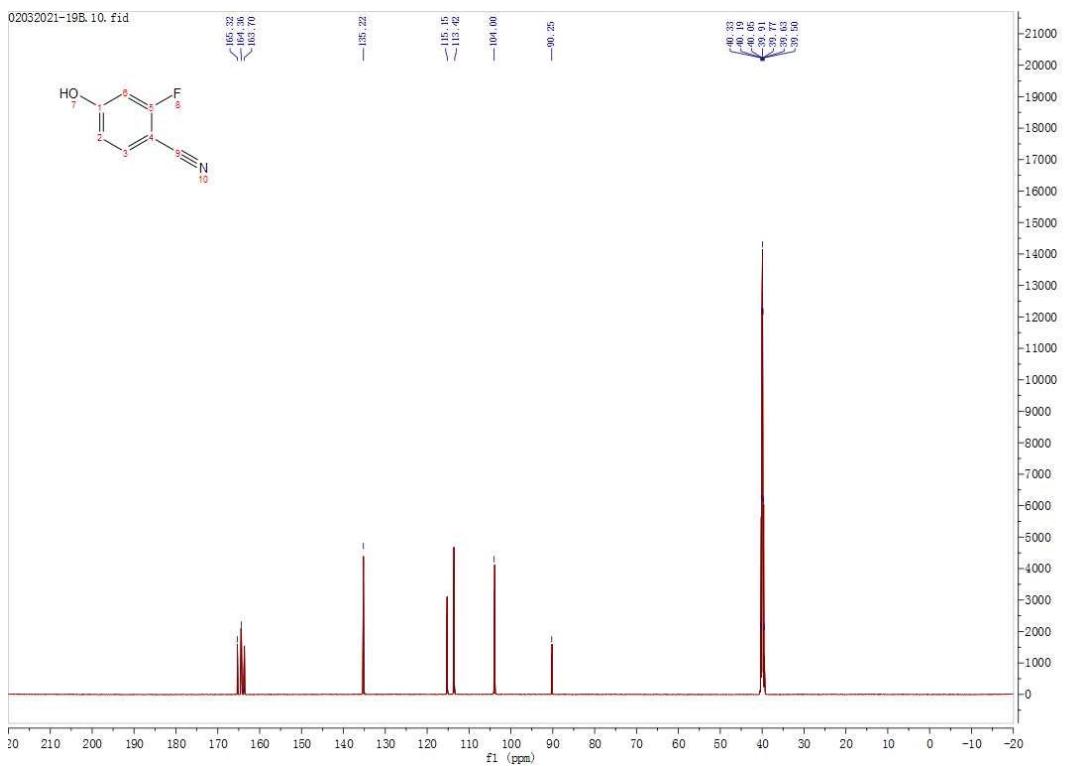


Figure S47  $^{13}\text{C}$  NMR spectra of compound 19b

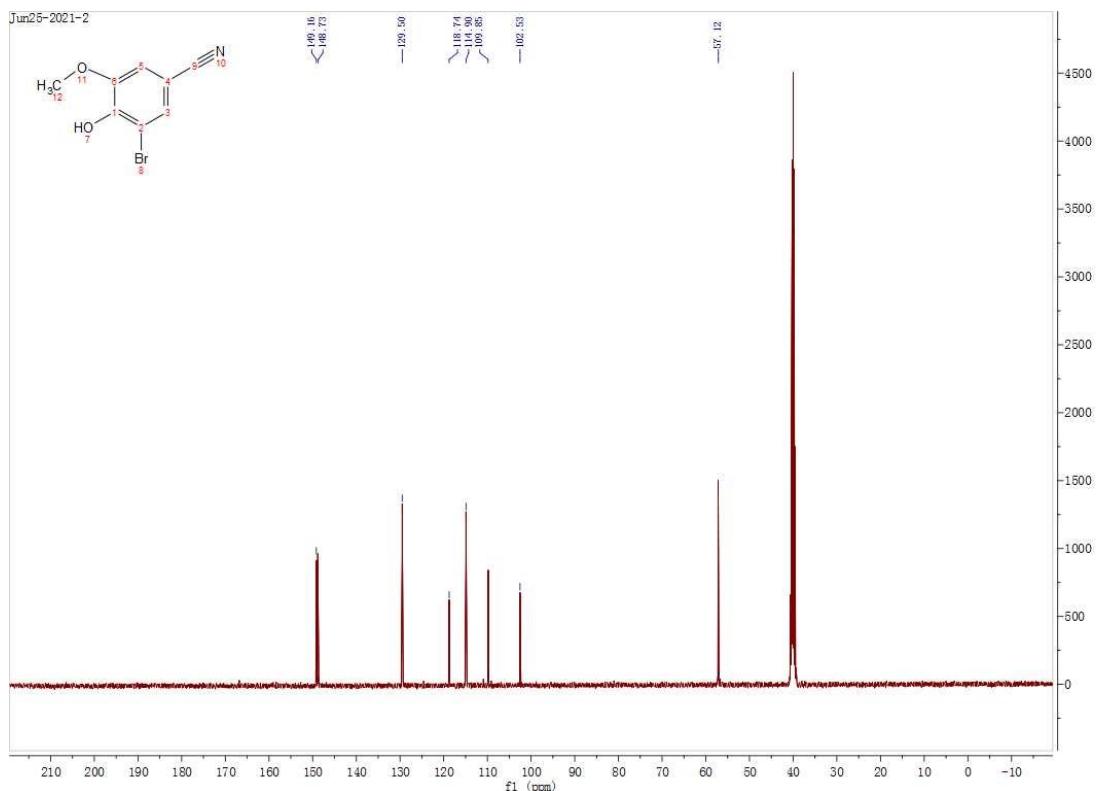


Figure S48  $^{13}\text{C}$  NMR spectra of compound 20b

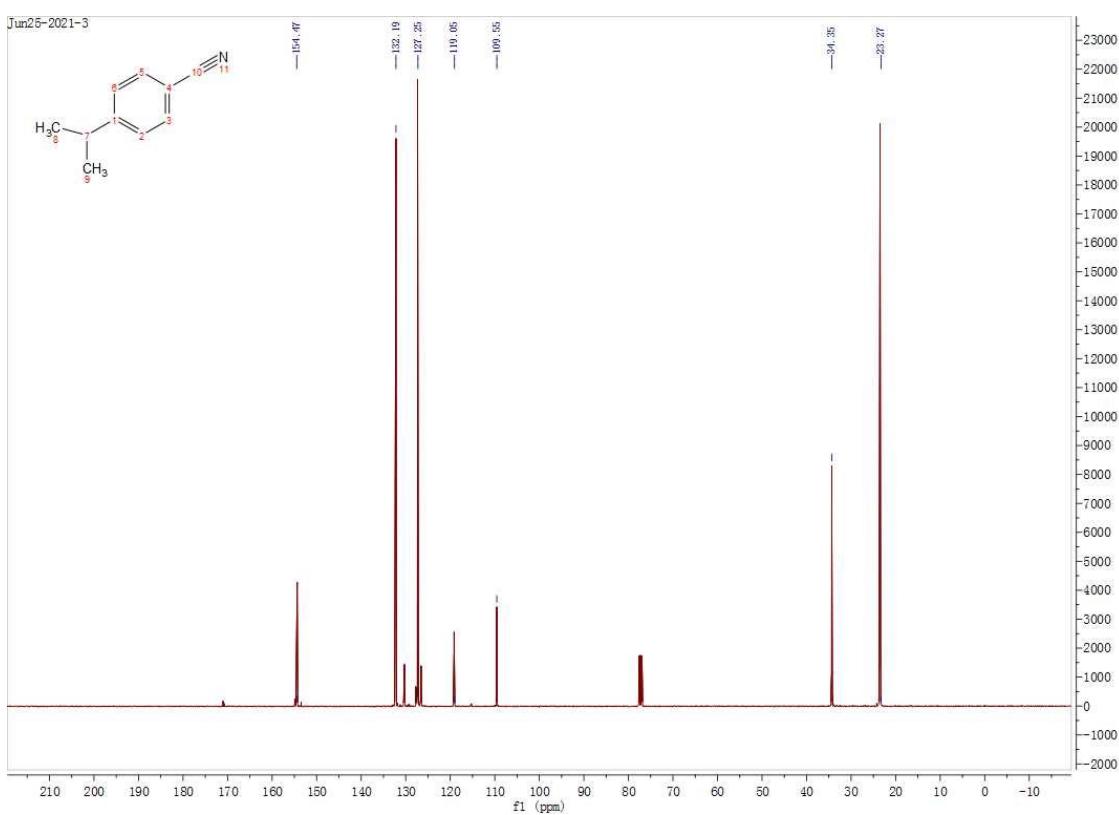


Figure S49 <sup>13</sup>C NMR spectra of compound 22b

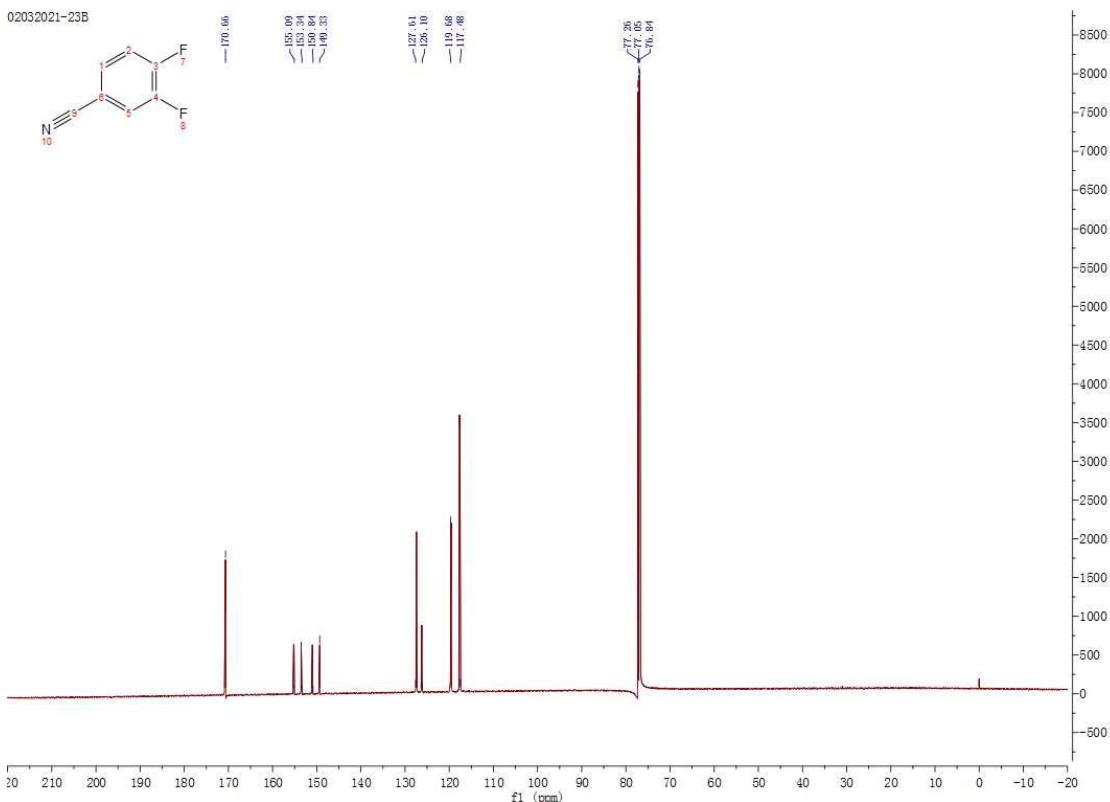


Figure S50 <sup>13</sup>C NMR spectra of compound 23b

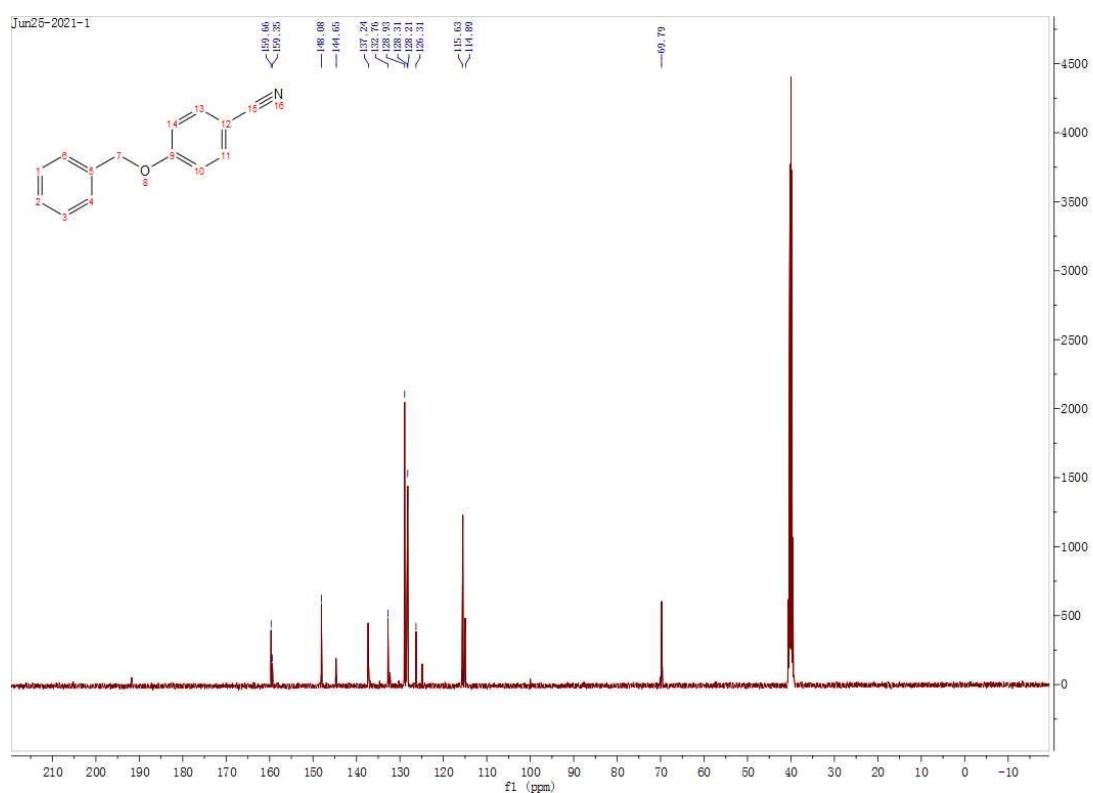


Figure S51  $^{13}\text{C}$  NMR spectra of compound 24b

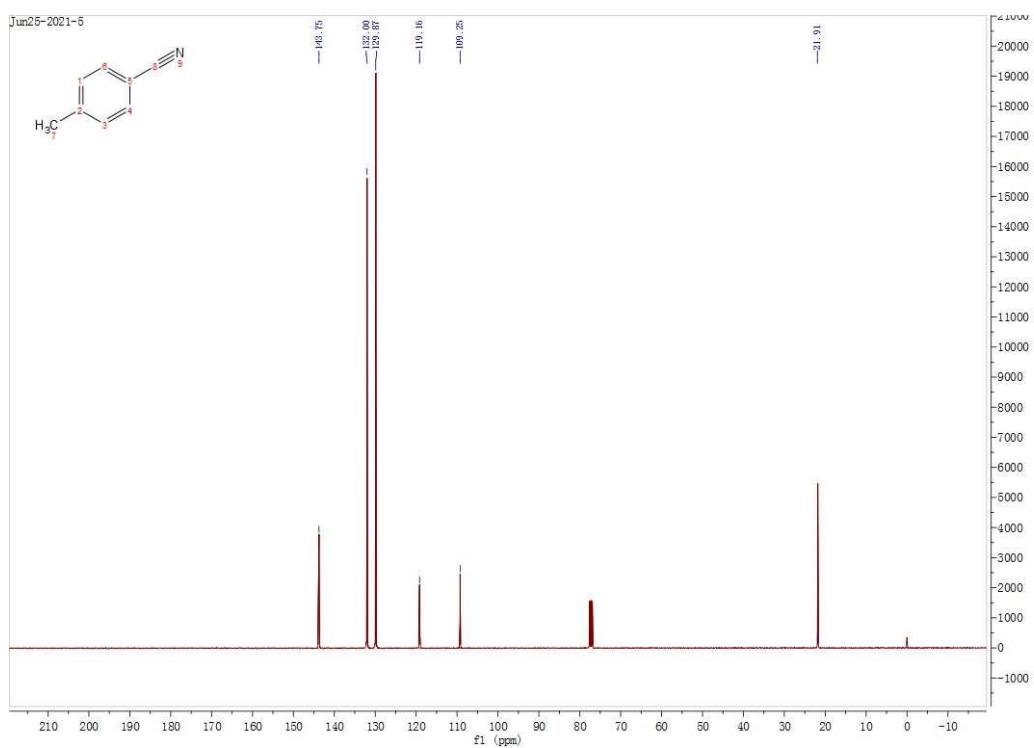


Figure S52  $^{13}\text{C}$  NMR spectra of compound 25b

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**<sup>19</sup>F NMR spectra of compound 15b, 16b, 17b, 18b, 19b and 23b**

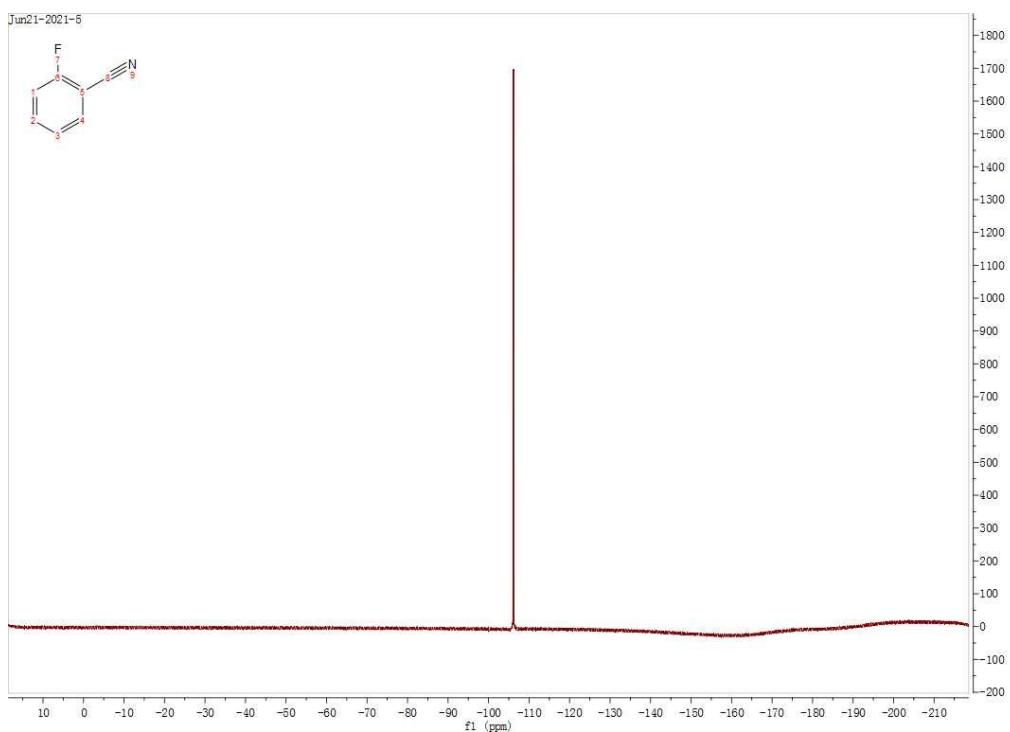


Figure S53 <sup>19</sup>F NMR spectra of compound 15b

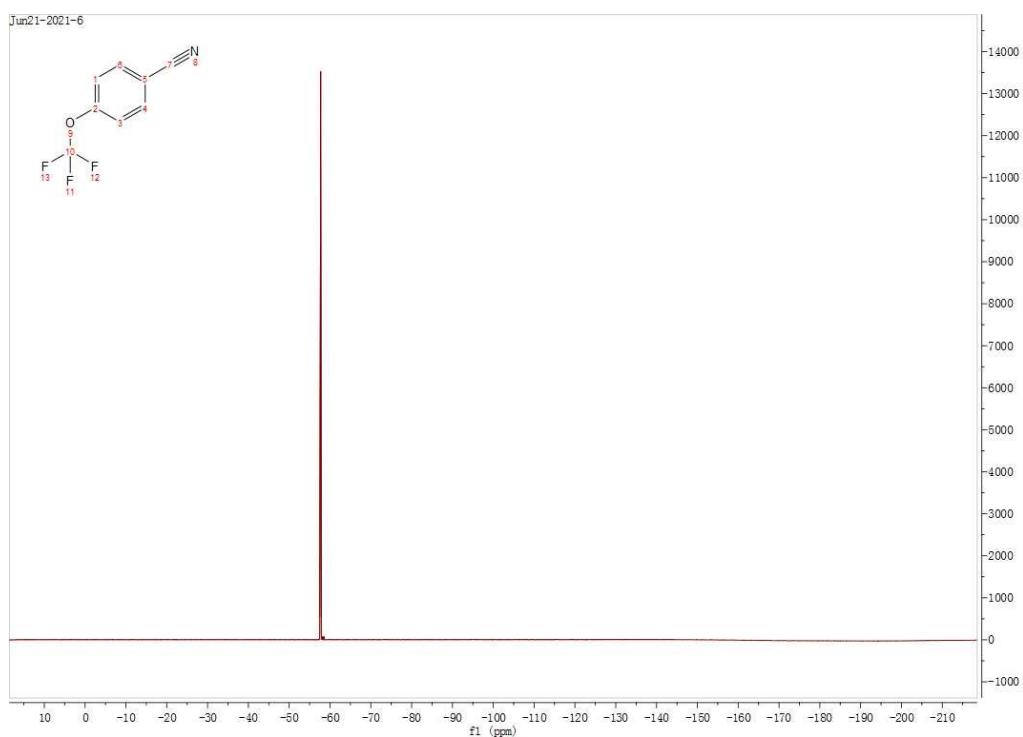


Figure S54 <sup>19</sup>F NMR spectra of compound 16b

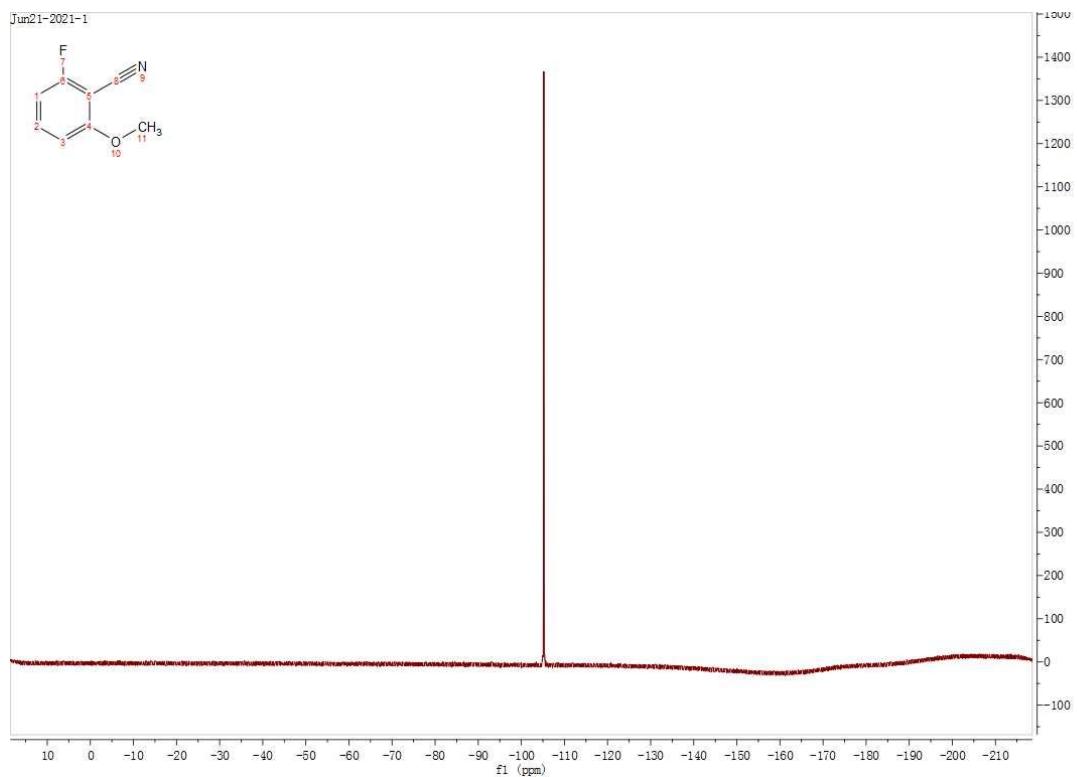


Figure S55 <sup>19</sup>F NMR spectra of compound 17b

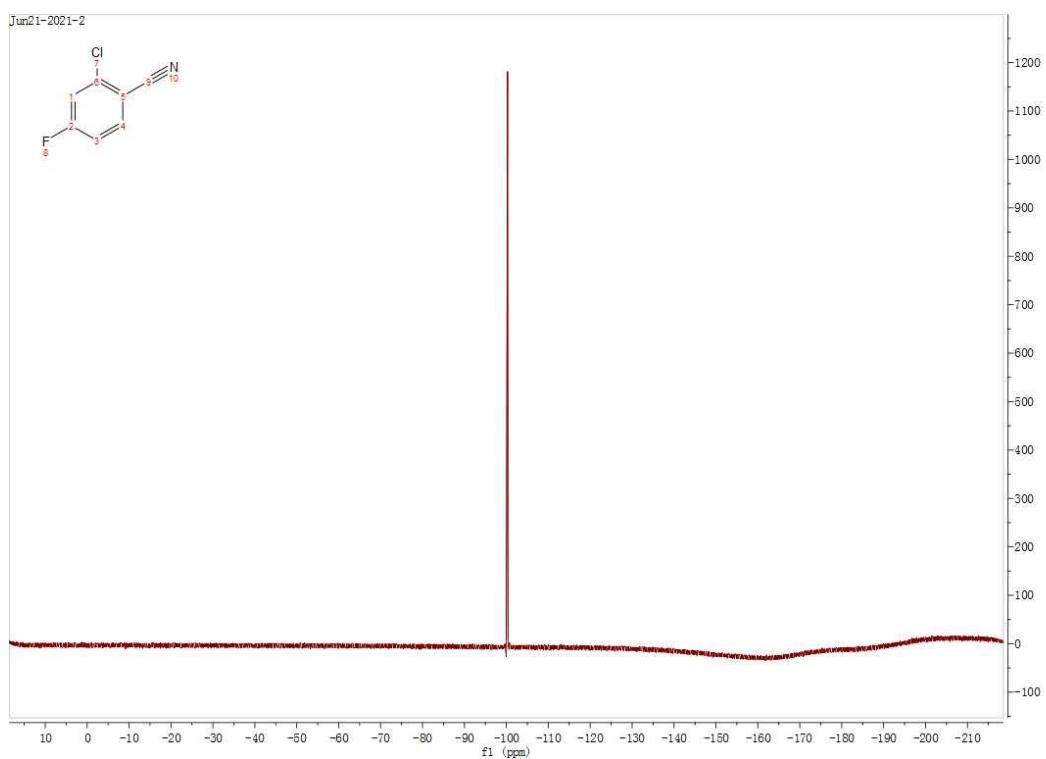


Figure S56 <sup>19</sup>F NMR spectra of compound 18b

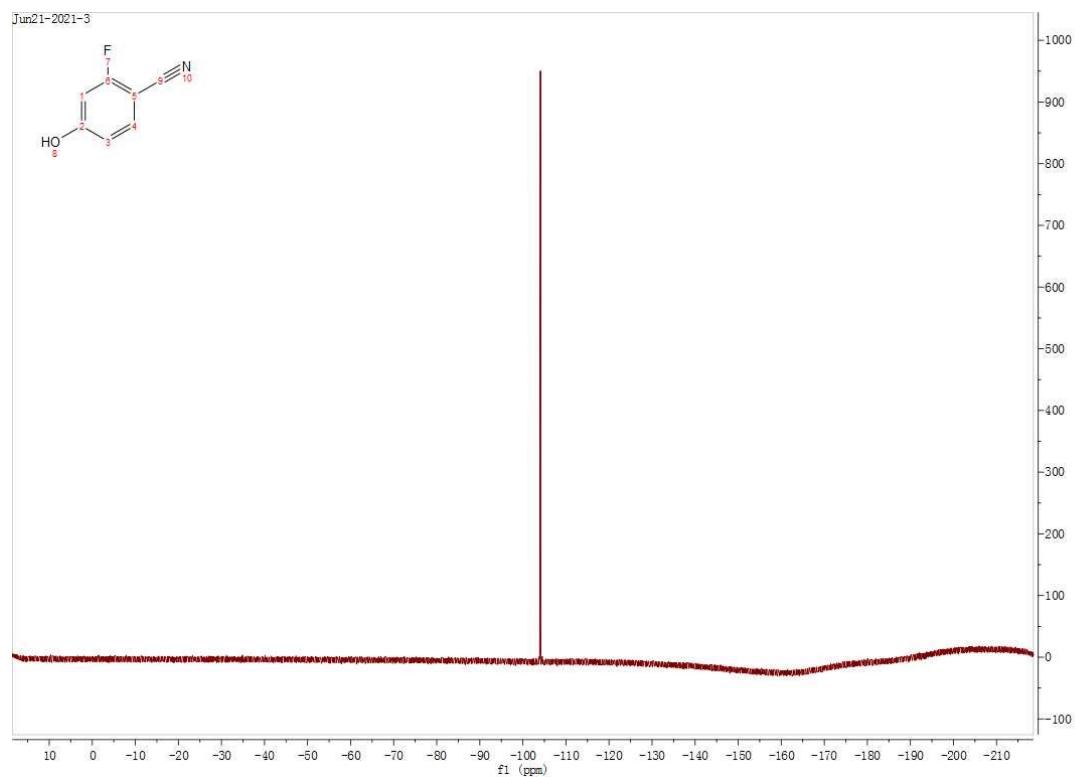


Figure S57  $^{19}\text{F}$  NMR spectra of compound 19b

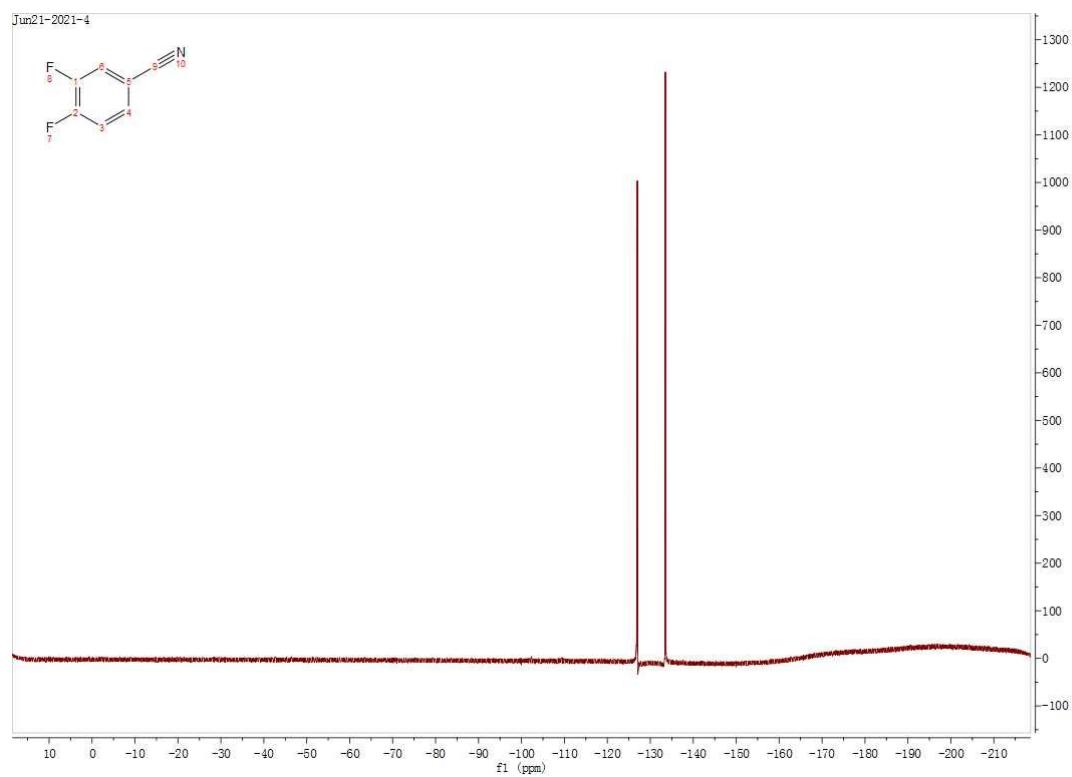


Figure S58  $^{19}\text{F}$  NMR spectra of compound 23b

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## Reference m.p. of compounds 1b-25b.

1b: 43-45 °C<sup>1</sup>  
2b: 90-93 °C<sup>2</sup>/ 92-94 °C<sup>3</sup>/ 91.2-93.1 °C<sup>4</sup>  
3b: 60-61 °C<sup>5</sup>/56-57 °C<sup>6</sup>/51-53.5 °C<sup>7</sup>  
4b: 144-145 °C<sup>8</sup>/140-143 °C<sup>9</sup>/144-145 °C<sup>10</sup>  
5b: 59 °C<sup>2</sup>/21.5-22 °C (ethanol)<sup>11</sup>/24.5 °C<sup>12</sup>  
6b: 24-25 °C<sup>13</sup>/23 °C<sup>14</sup>  
7b: 58-59 °C<sup>15</sup>/55-57 °C<sup>16</sup>/59.2-60.4 °C<sup>4</sup>/56-58 °C<sup>17</sup>/59-60 °C<sup>18</sup>  
8b: 68.6-70.5 °C<sup>4</sup>/65-67 °C<sup>19</sup>/66-67 °C<sup>20</sup>/62-65 °C/65-66 °C<sup>21</sup>/64.9-66.4 °C<sup>22</sup>  
9b: 74.8-77.2 °C<sup>23</sup>/57-59.5 °C<sup>24</sup>/78-80 °C<sup>25</sup>/68 °C<sup>26</sup>/76-78 °C<sup>27</sup>  
10b: 110-113 °C<sup>28</sup>/111-112 °C<sup>29</sup>/109-111 °C<sup>30</sup>/108.8-110.2 °C<sup>23</sup>/100.7-103.2 °C<sup>24</sup>/107-109 °C<sup>31</sup>  
11b: liquid  
12b: liquid  
13b: 52-54 °C<sup>32</sup>/50-52 °C<sup>33</sup>/50-54 °C<sup>34</sup>  
14b: 83-85 °C<sup>34, 35</sup>/83-86 °C<sup>34</sup>/85-87 °C<sup>32</sup>/85-86 °C<sup>30</sup>  
15b: liquid  
16b: liquid  
17b: 93-95 °C<sup>36</sup>  
18b: 63.0-65.0 °C<sup>33</sup>  
19b: 124-125 °C<sup>25</sup>/123.5 °C<sup>37</sup>/117-118 °C<sup>38</sup>  
20b: 159-160 °C<sup>39</sup>/134-136 °C<sup>40</sup>/144 °C<sup>41</sup>  
21b: 179 °C<sup>42</sup>  
22b: liquid  
23b: 51-53 °C<sup>43</sup>  
24b: 86 °C<sup>44</sup>/91-93 °C<sup>45</sup>/86 °C<sup>46</sup>/86-88 °C<sup>47</sup>/97-99 °C<sup>21</sup>/93-94 °C<sup>48</sup>/96-98 °C<sup>49</sup>  
25b: 26-28 °C<sup>28</sup>/26 °C<sup>50</sup>/27-29 °C<sup>51</sup>/28-29 °C(patent)/26-27 °C<sup>52</sup>/27.1-27.7 °C<sup>53</sup>

### References:

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6. Rahman, L. K. A.; Scrowston, R. M., 7-Substituted Benzo[B] Thiophenes and 1,2-Benzisothiazoles .2. Chloro and Nitro-Derivatives. *J Chem Soc Perk T 1* **1984**, (3): 385-390.
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