

*Supporting information for*

# Synthesis of Pyrrolyldipyrrinato BF<sub>2</sub> Complexes by Oxidative Nucleophilic Substitution of Boron Dipyrromethene with Pyrrole

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### 1. Figure S1 and Scheme S1-S3

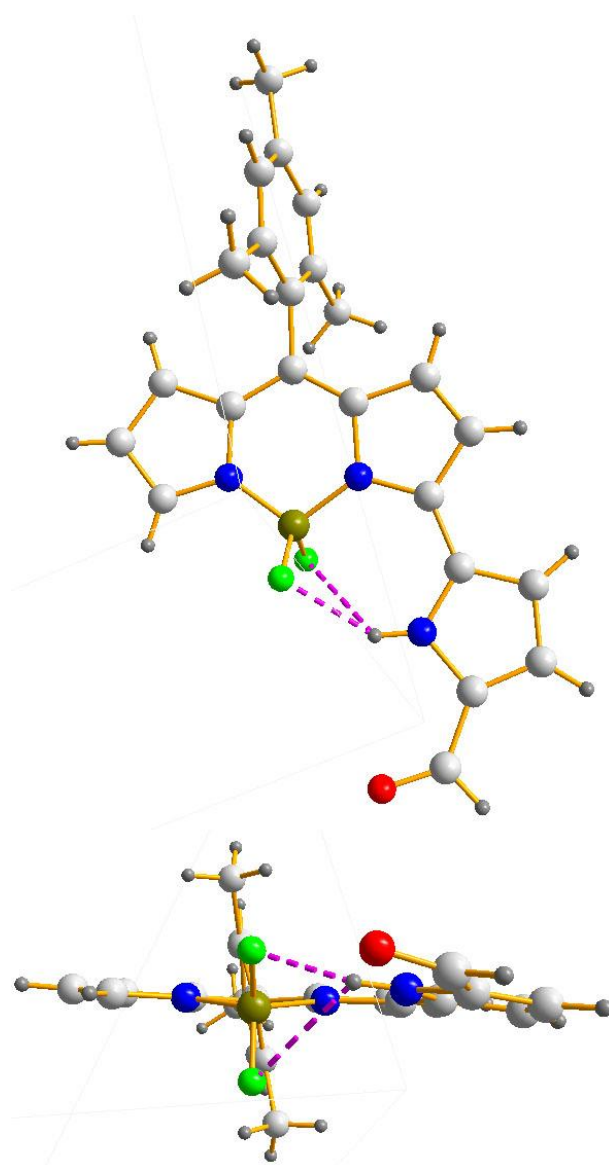
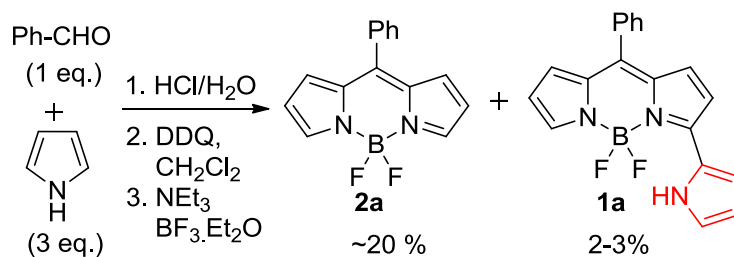
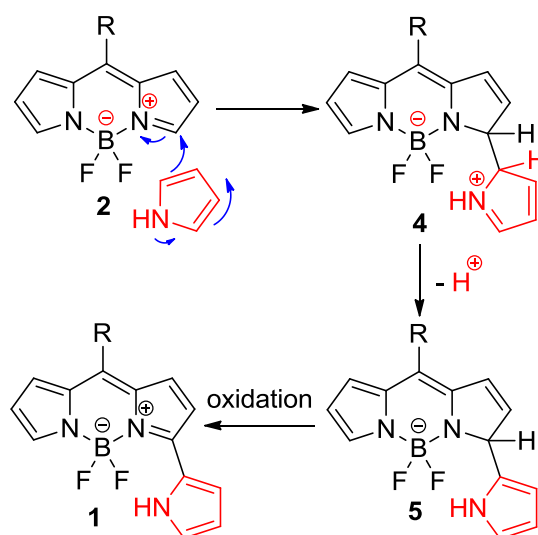


Figure S1. X-Ray structures of BODIPYs **6**. C grey, N blue, O red, B yellow, F bright-green.

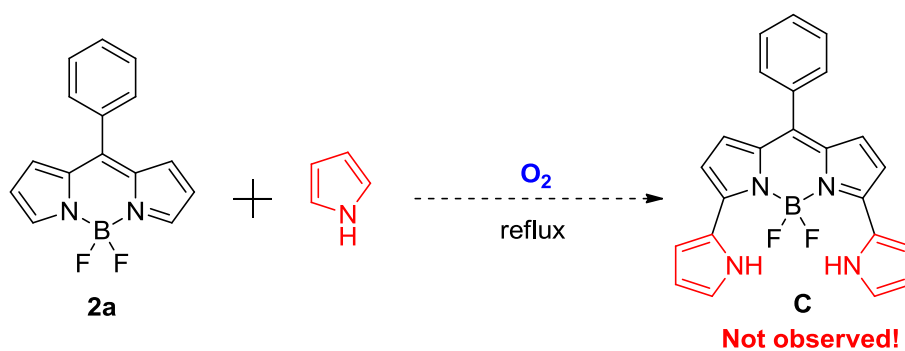
Scheme S1. One-pot synthesis of BODIPY **2a**.



Scheme S2. Possible mechanism for formation of BODIPY **1** via oxidative nucleophilic substitution.



Scheme S3. Failed attempt to synthesize the double-substituted BODIPY **C**.



## 2. Copies of $^1\text{H}$ NMR, $^{13}\text{C}$ NMR for all new compounds

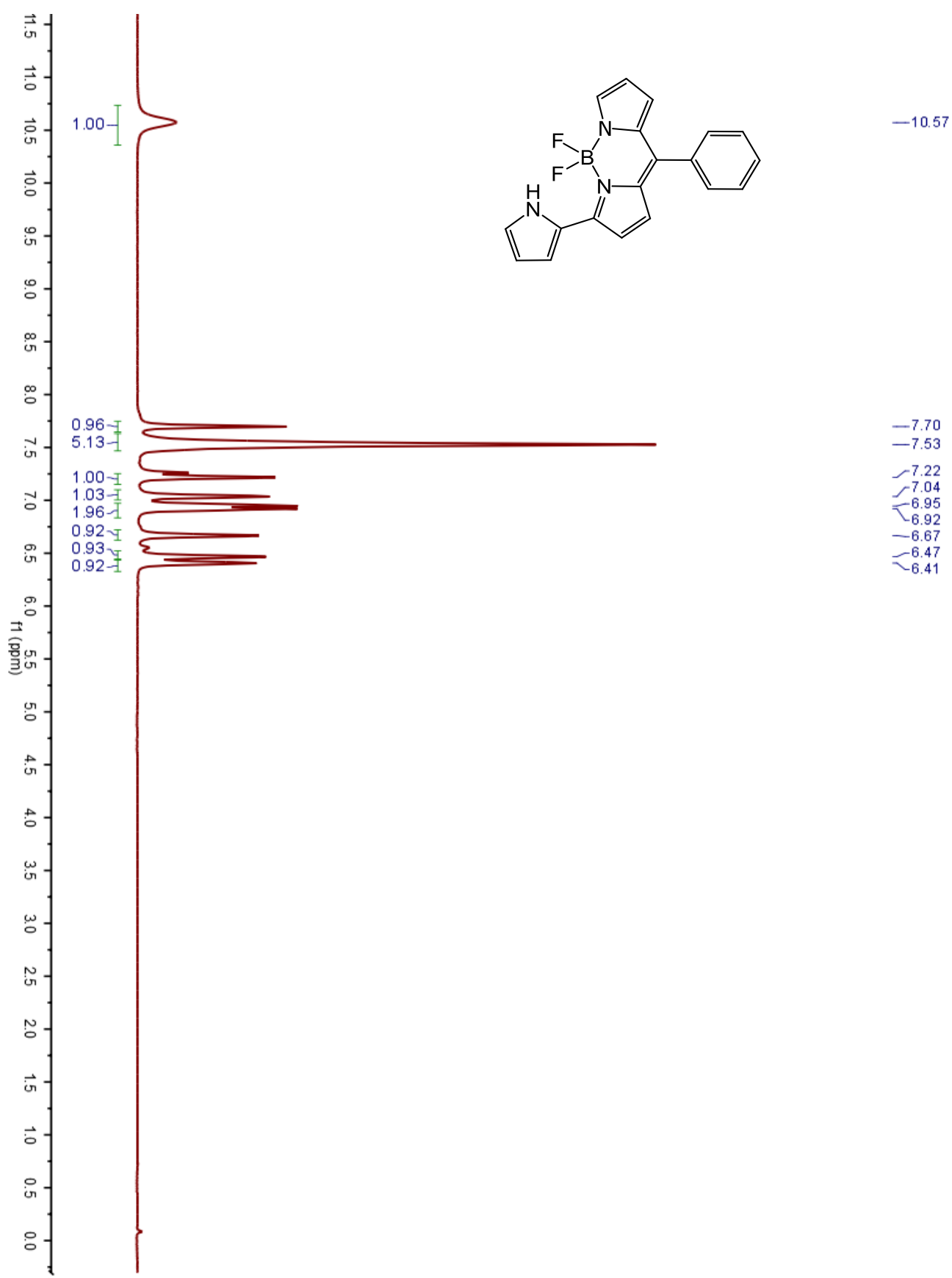


Figure S2.  $^1\text{H}$  NMR spectrum of BODIPY dye **1a** in  $\text{CDCl}_3$  solution

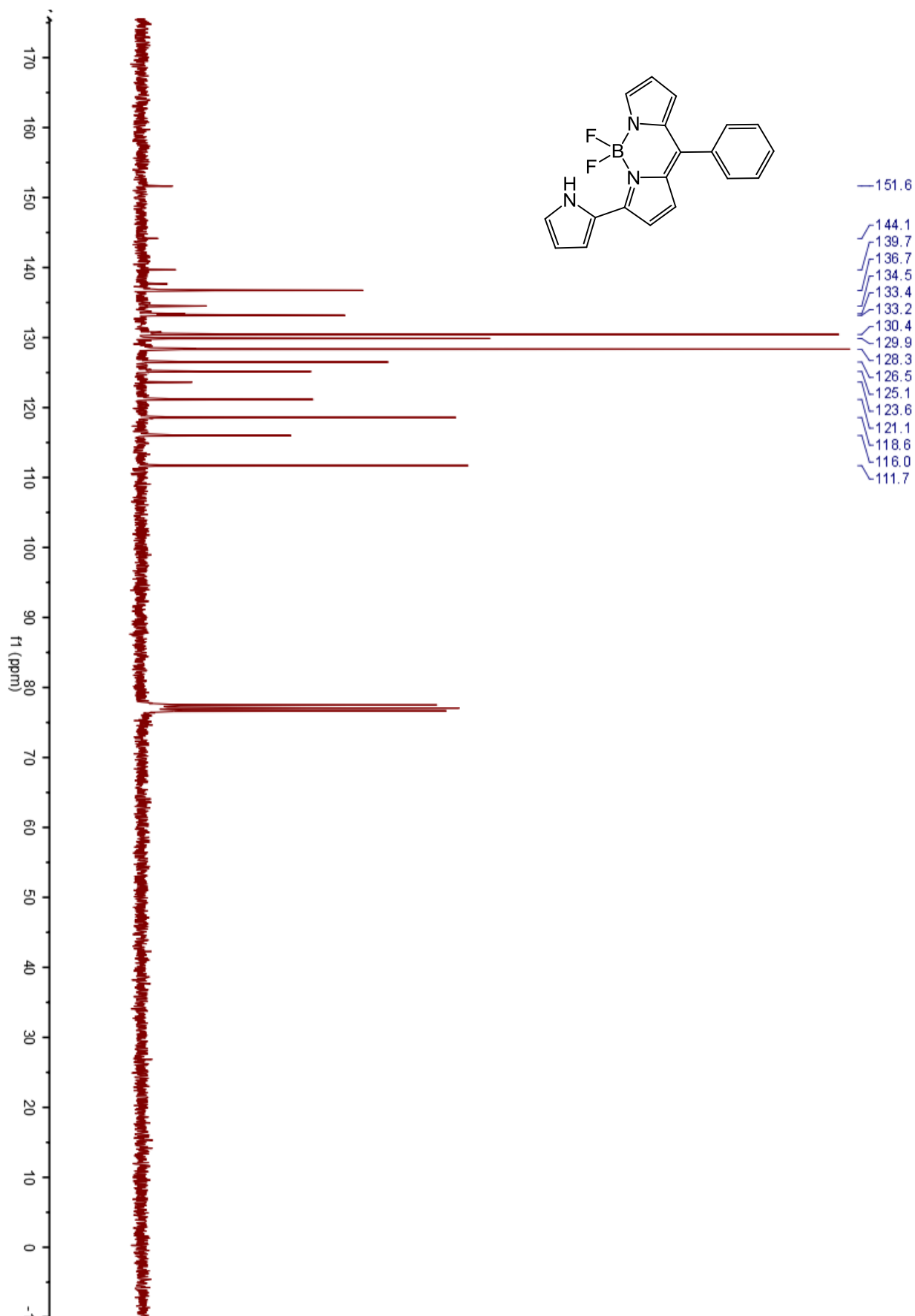


Figure S3.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1a** in  $\text{CDCl}_3$  solution

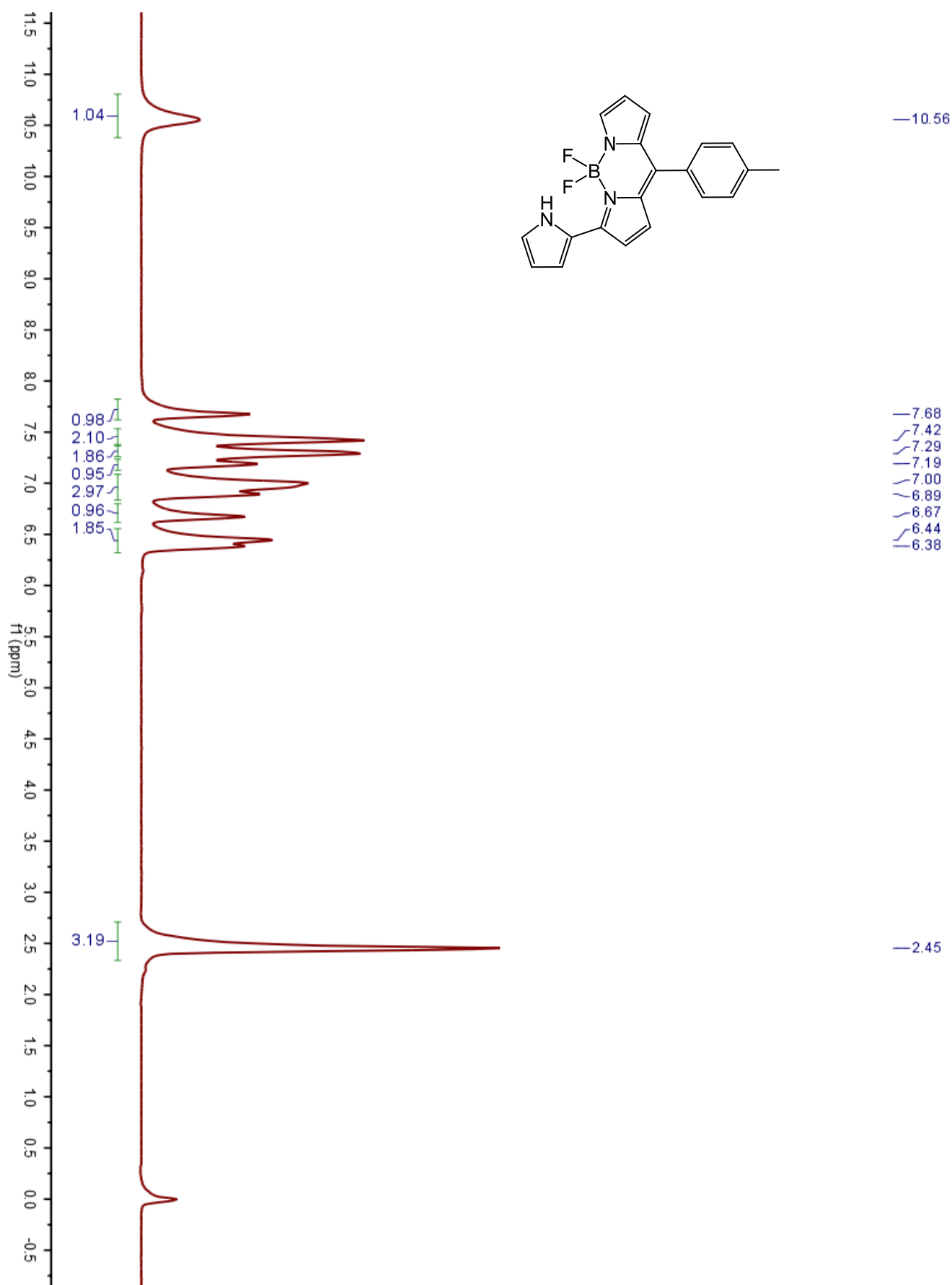


Figure S4. <sup>1</sup>H NMR spectrum of BODIPY dye **1b** in CDCl<sub>3</sub> solution

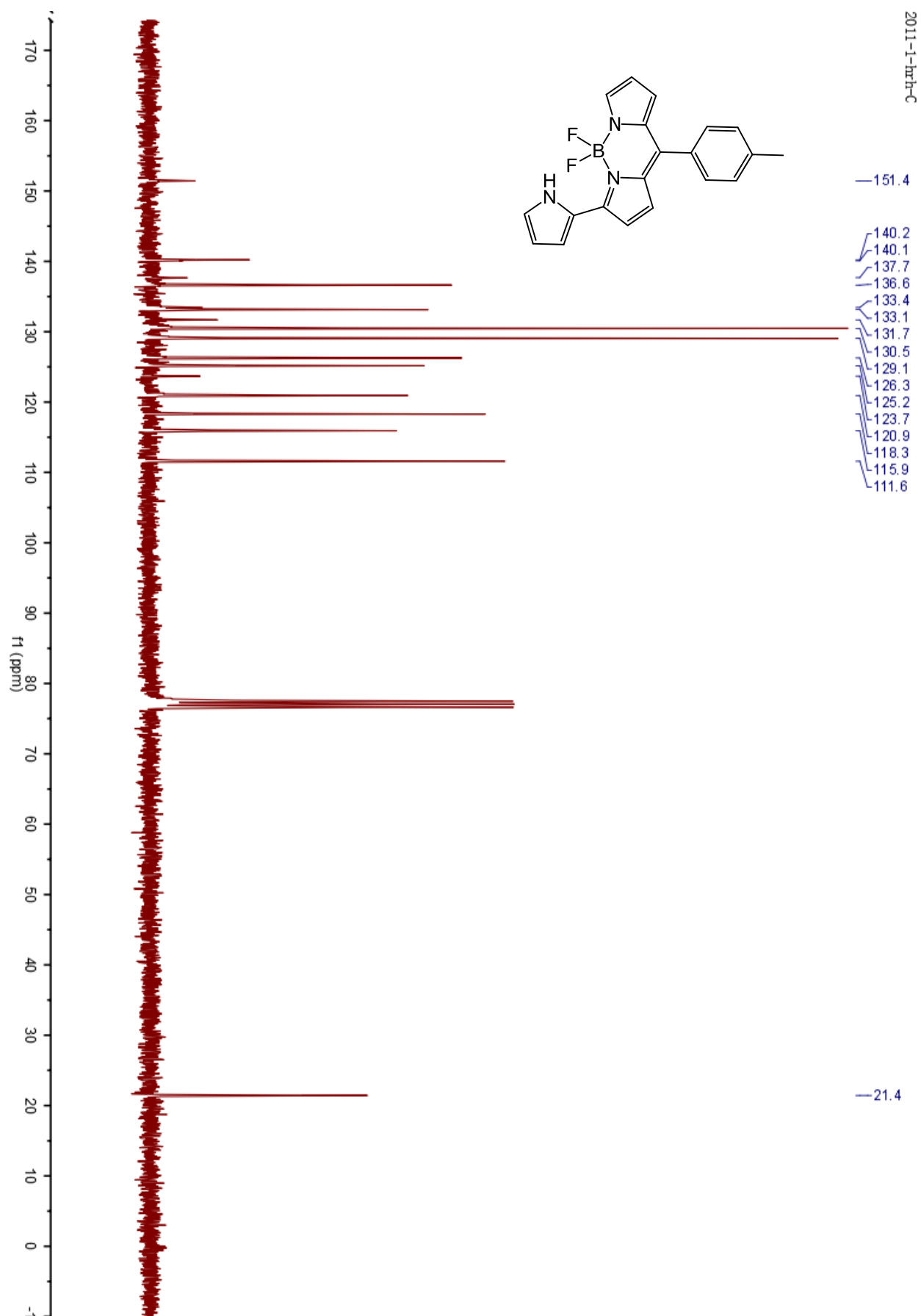


Figure S5.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1b** in  $\text{CDCl}_3$  solution

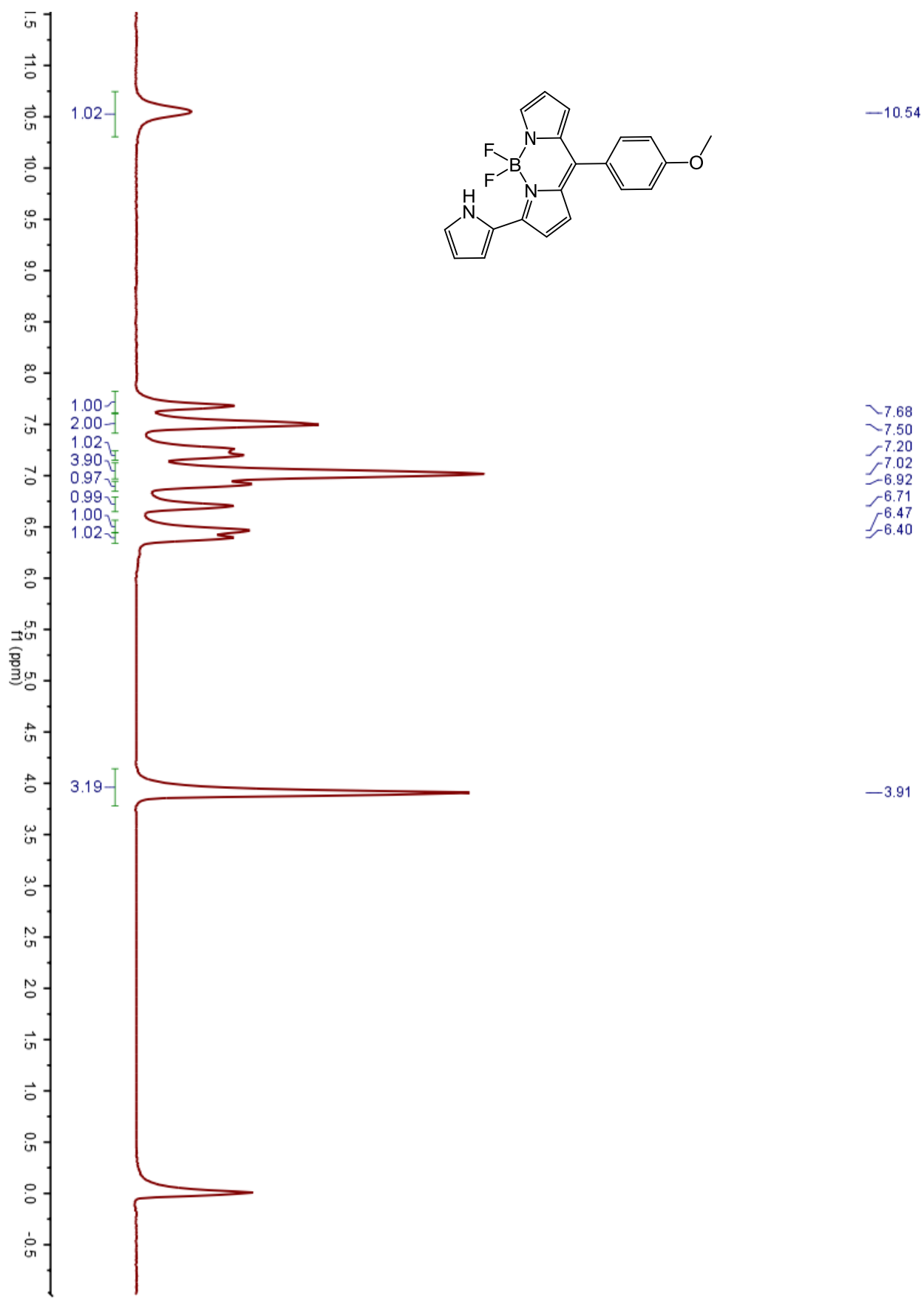


Figure S6. <sup>1</sup>H NMR spectrum of BODIPY dye **1c** in CDCl<sub>3</sub> solution



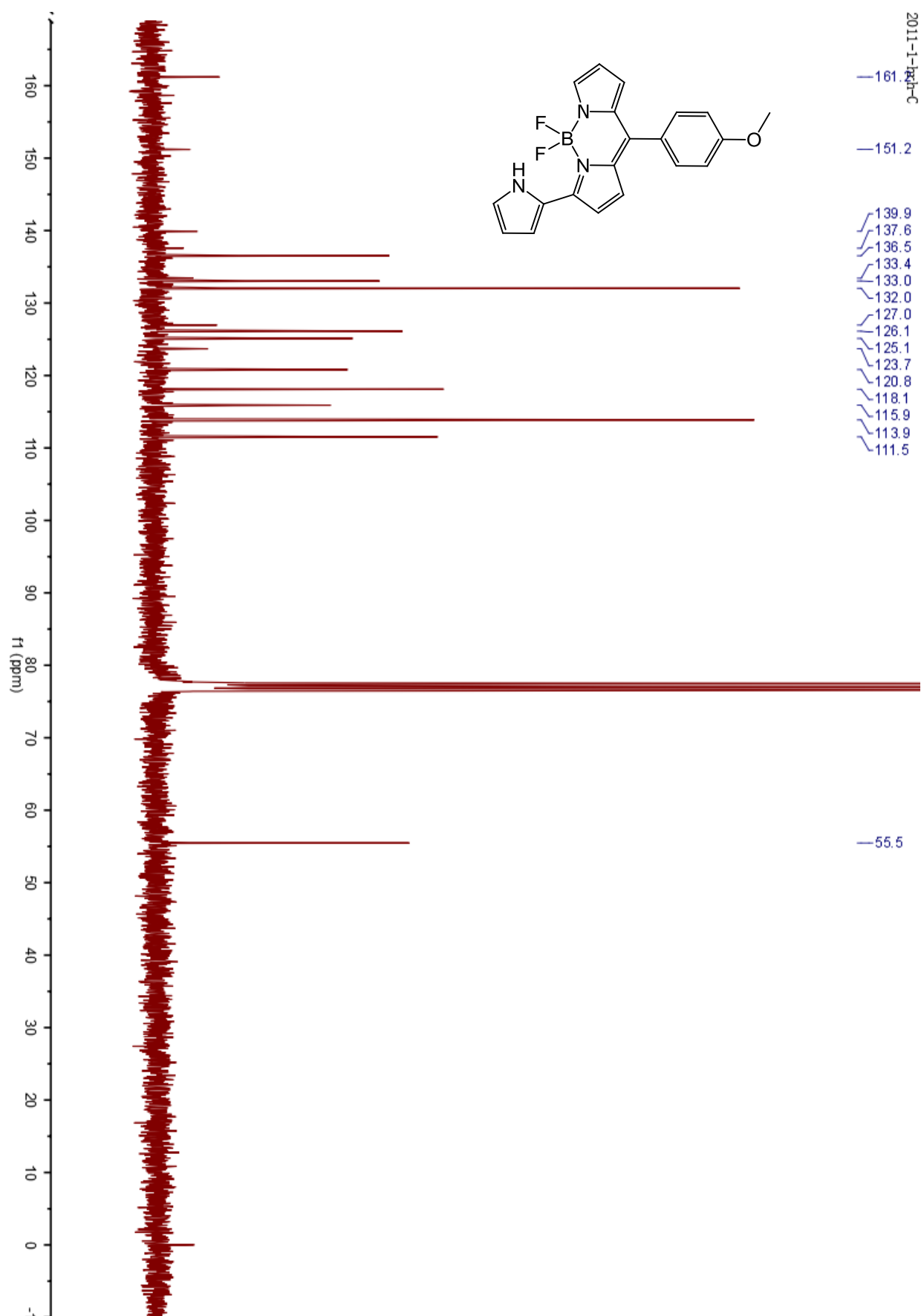


Figure S7.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1c** in  $\text{CDCl}_3$  solution

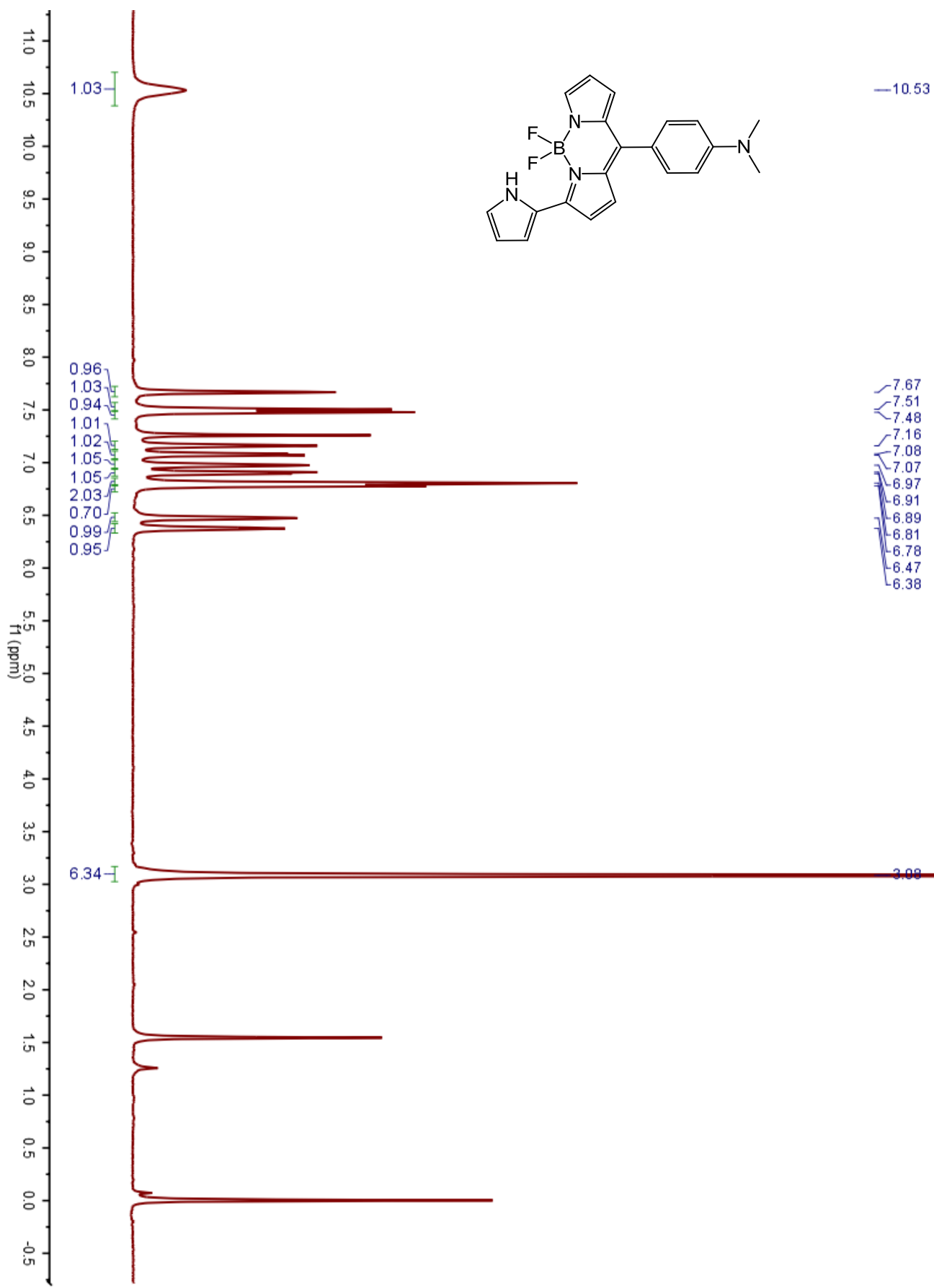


Figure S8. <sup>1</sup>H NMR spectrum of BODIPY dye **1d** in CDCl<sub>3</sub> solution

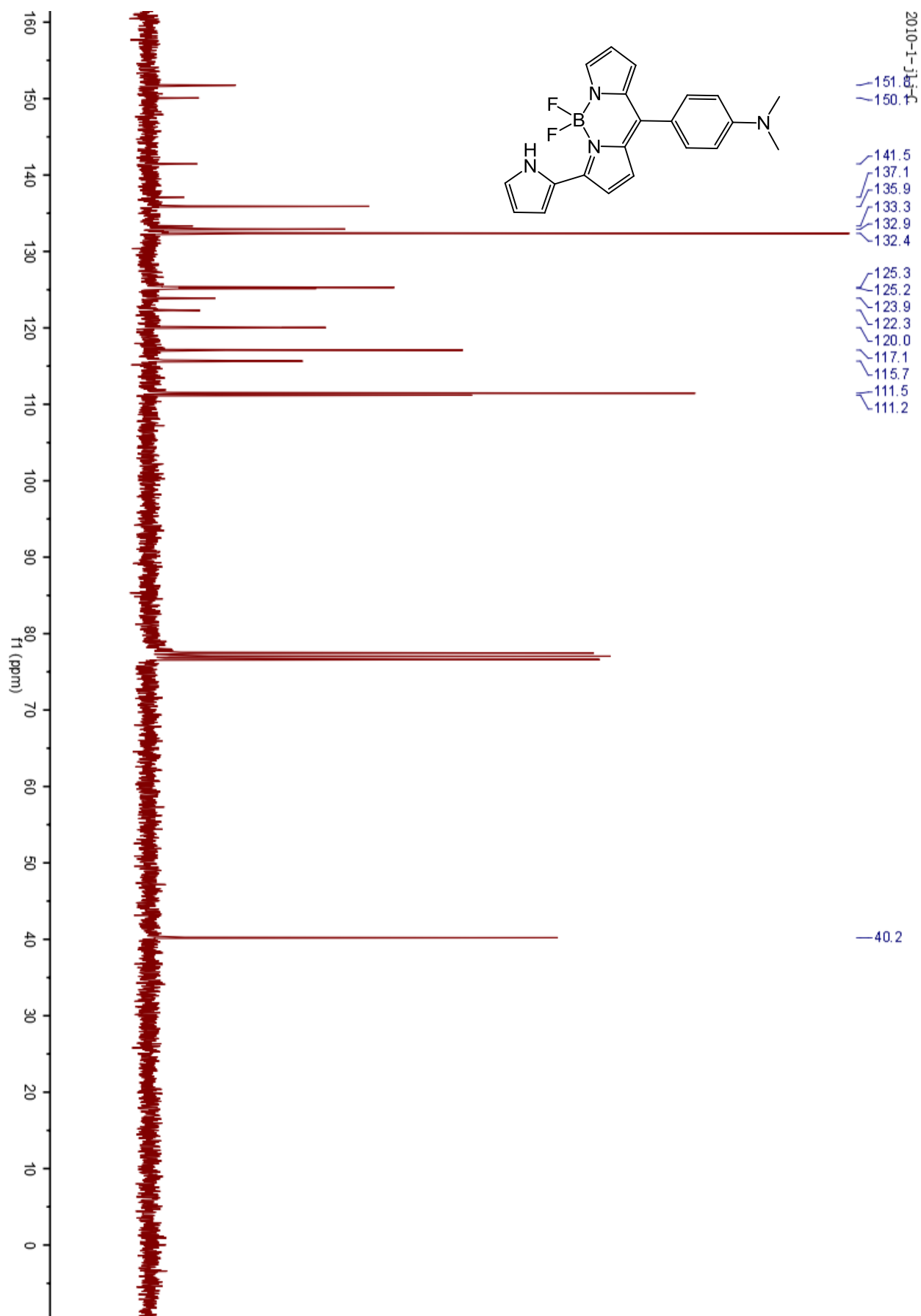


Figure S9.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1d** in  $\text{CDCl}_3$  solution

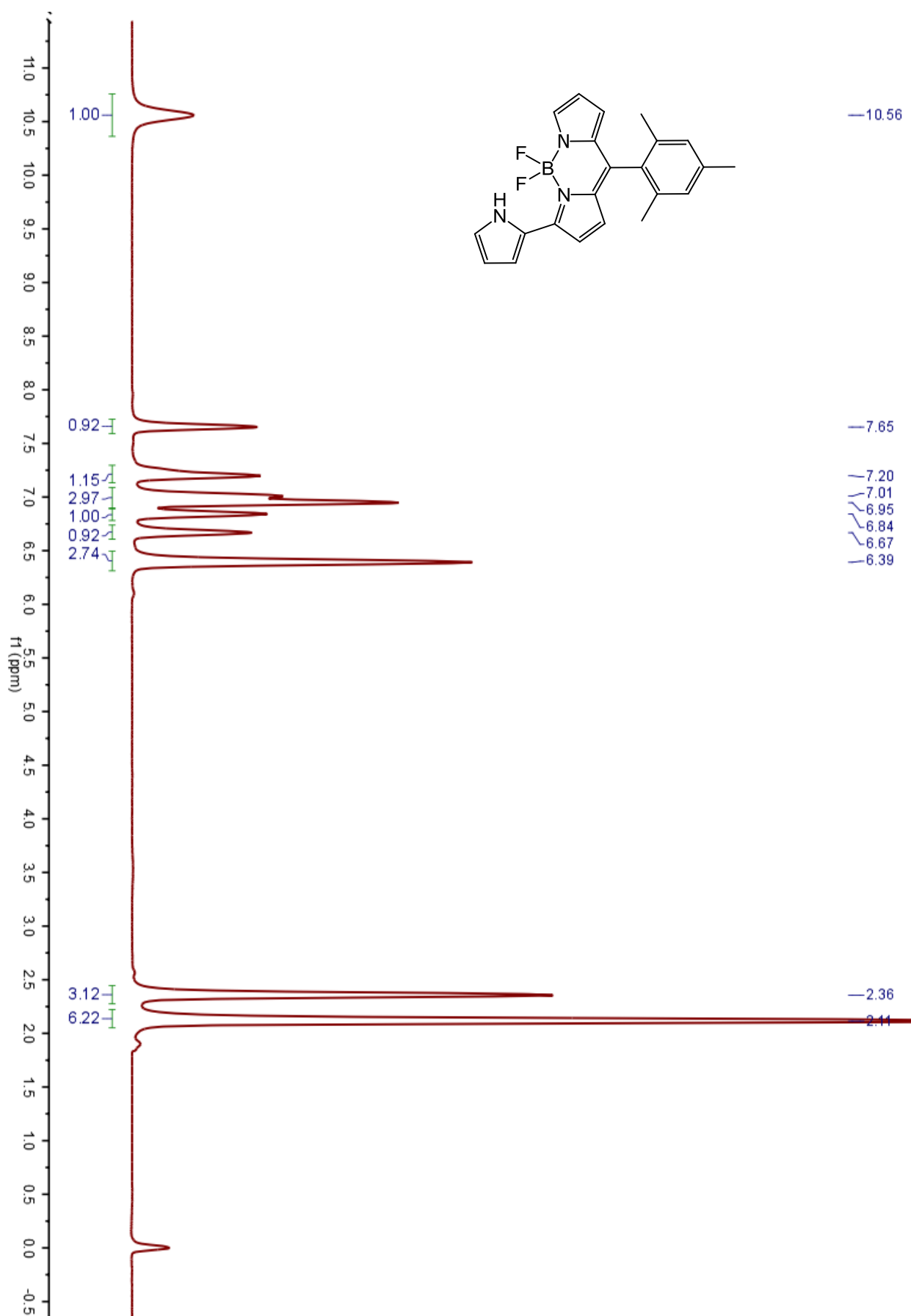


Figure S10. <sup>1</sup>H NMR spectrum of BODIPY dye **1e** in CDCl<sub>3</sub> solution

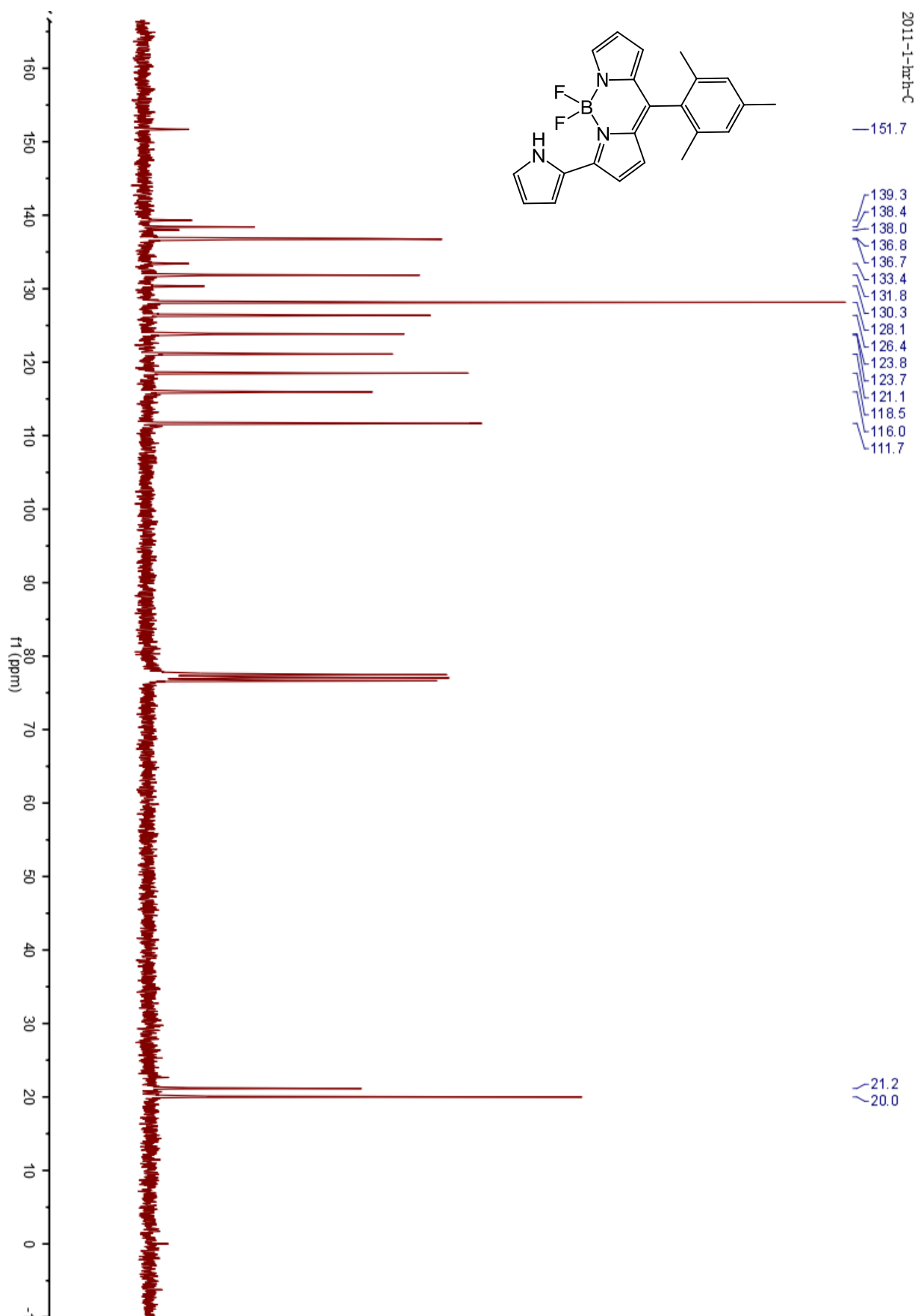


Figure S11.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1e** in  $\text{CDCl}_3$  solution

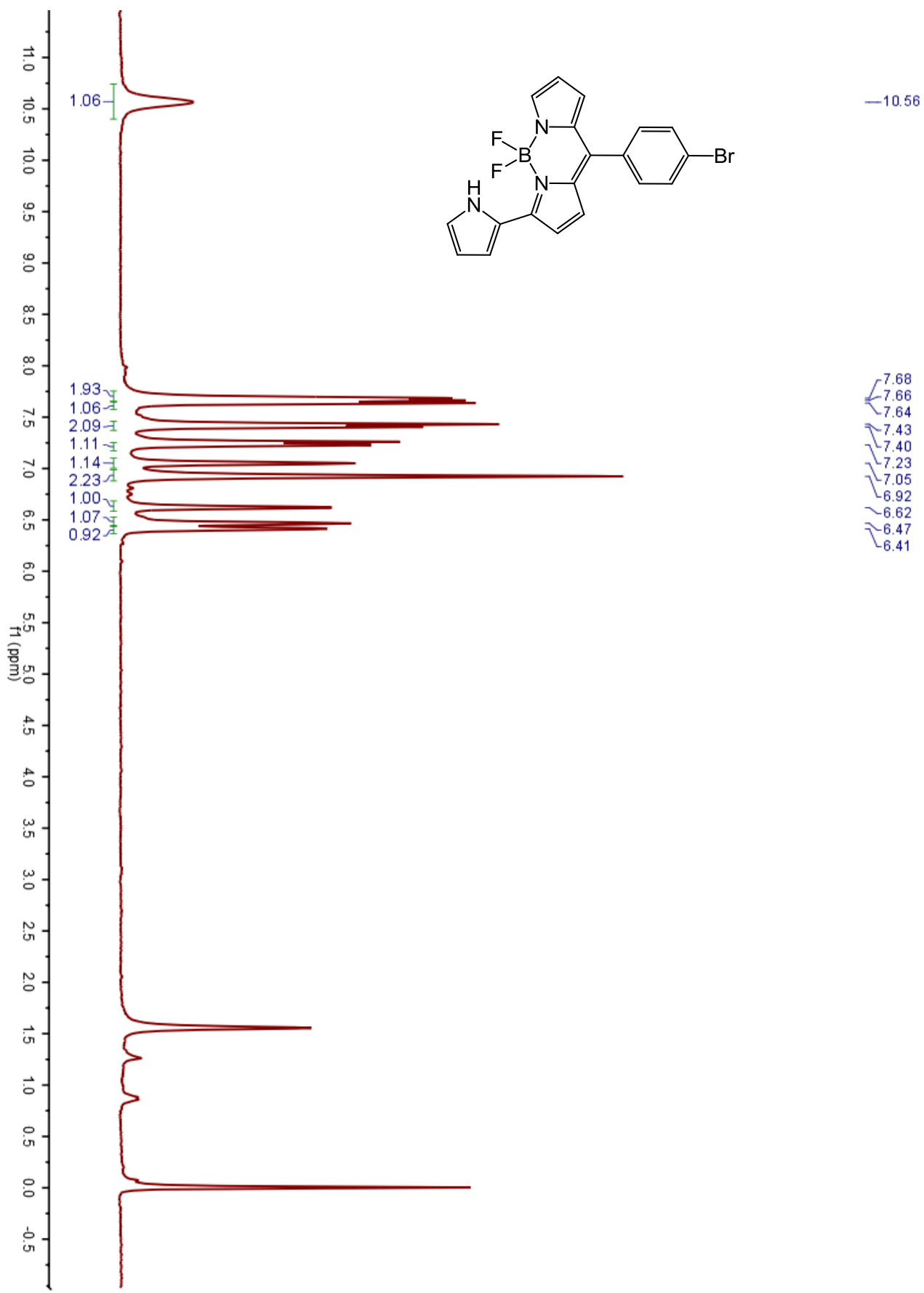


Figure S12.  $^1\text{H}$  NMR spectrum of BODIPY dye **1f** in  $\text{CDCl}_3$  solution

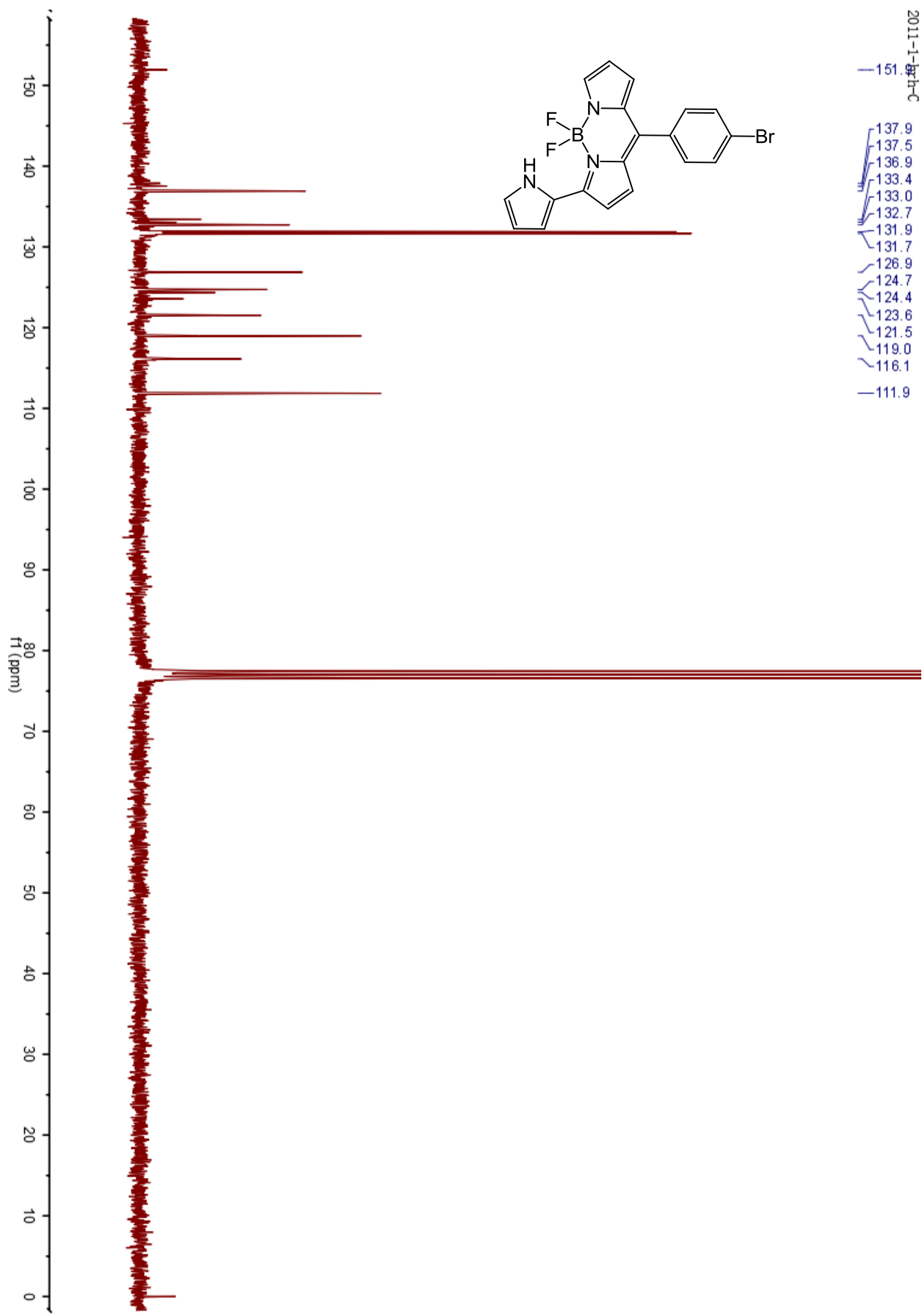


Figure S13.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1f** in  $\text{CDCl}_3$  solution

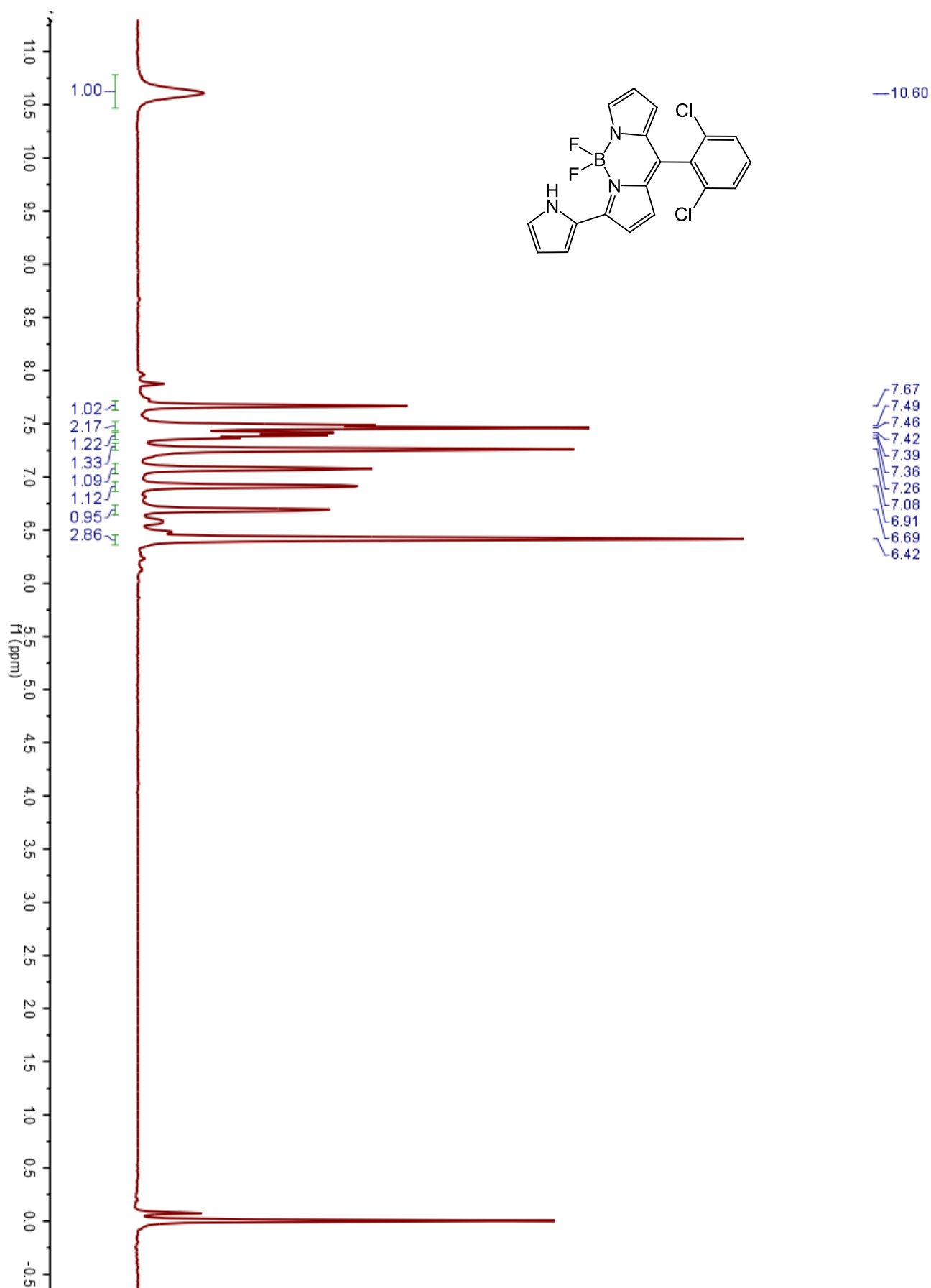


Figure S14.  $^1\text{H}$  NMR spectrum of BODIPY dye **1g** in  $\text{CDCl}_3$  solution



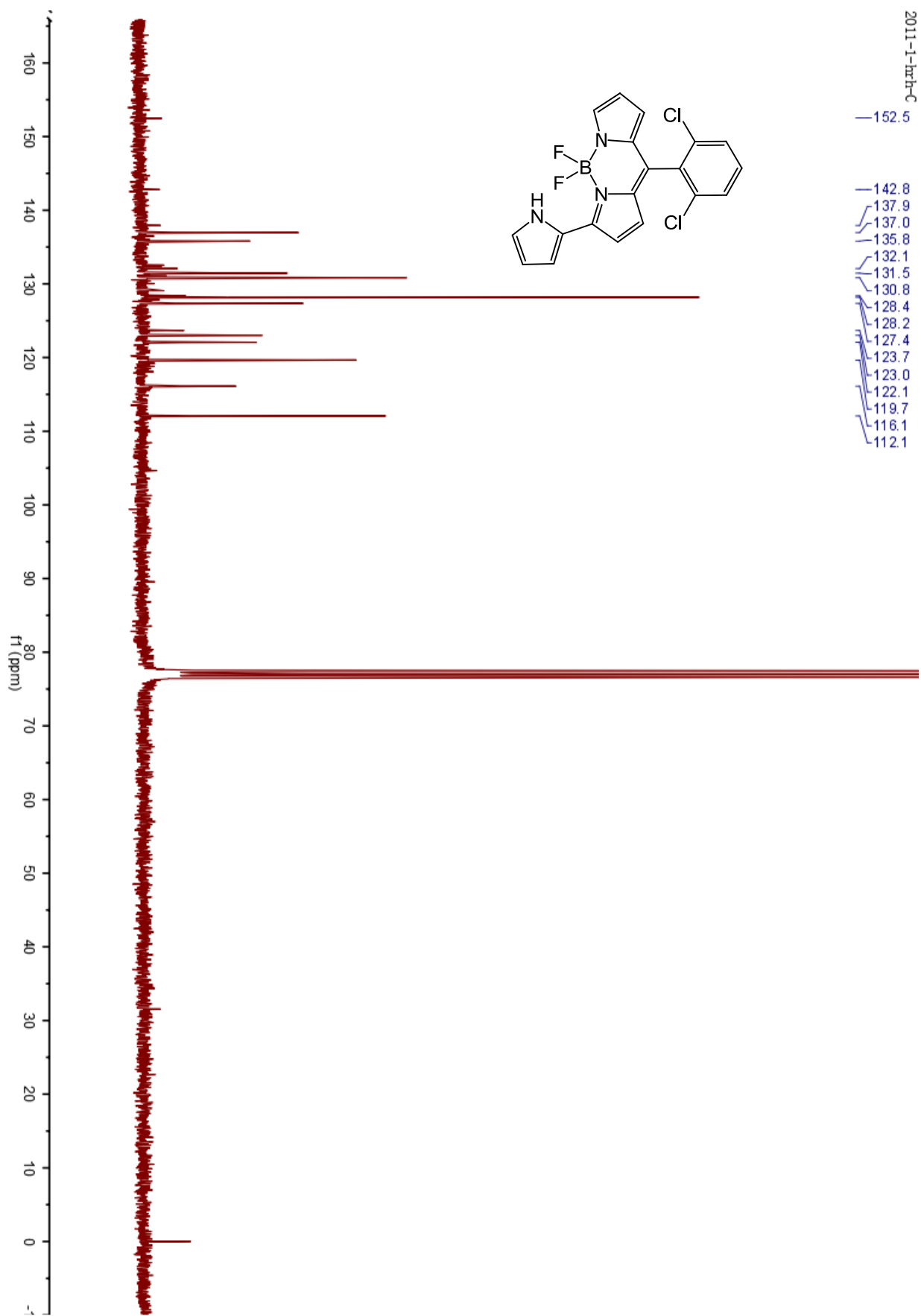


Figure S15.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1g** in  $\text{CDCl}_3$  solution

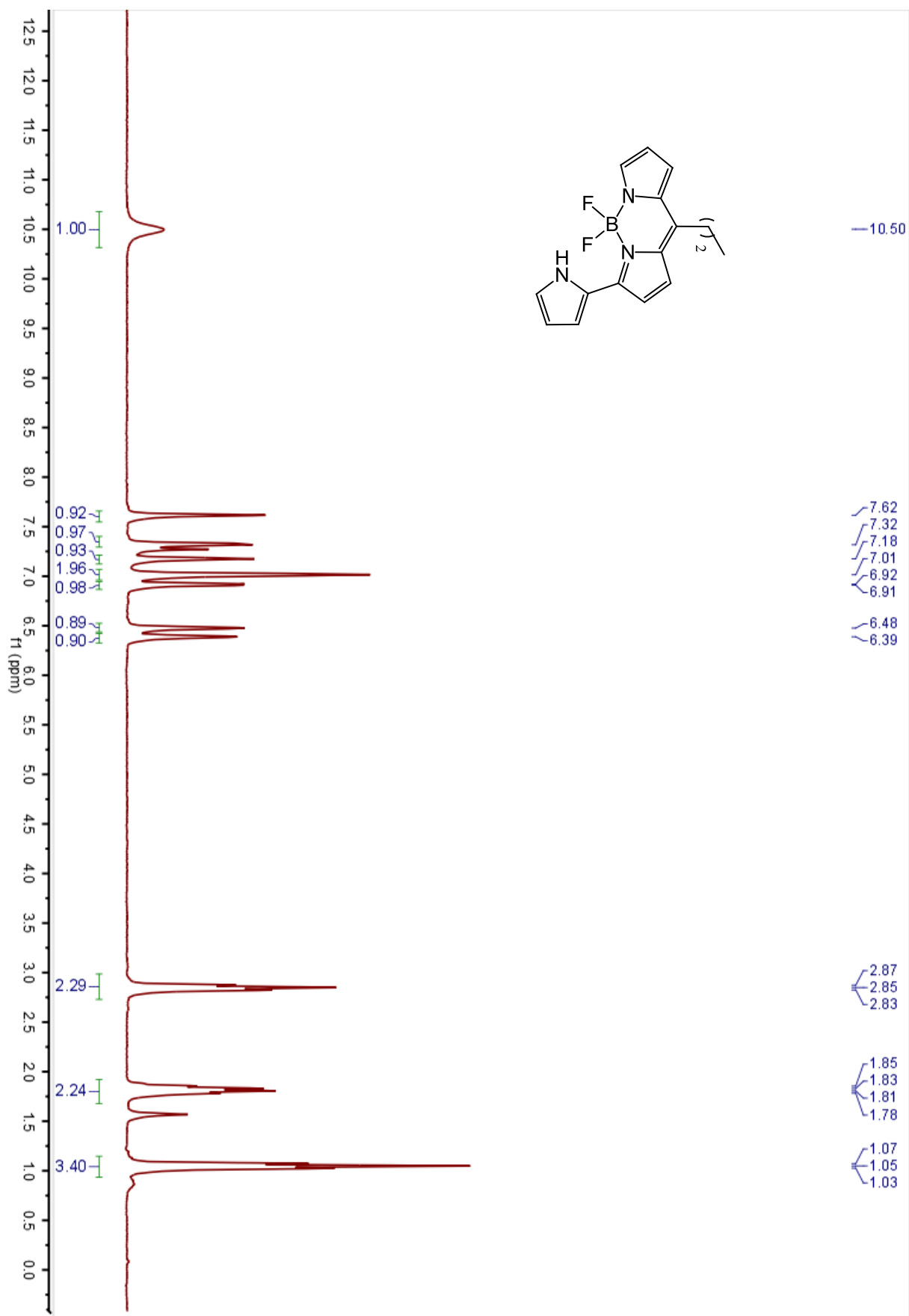


Figure S16. <sup>1</sup>H NMR spectrum of BODIPY dye **1h** in CDCl<sub>3</sub> solution

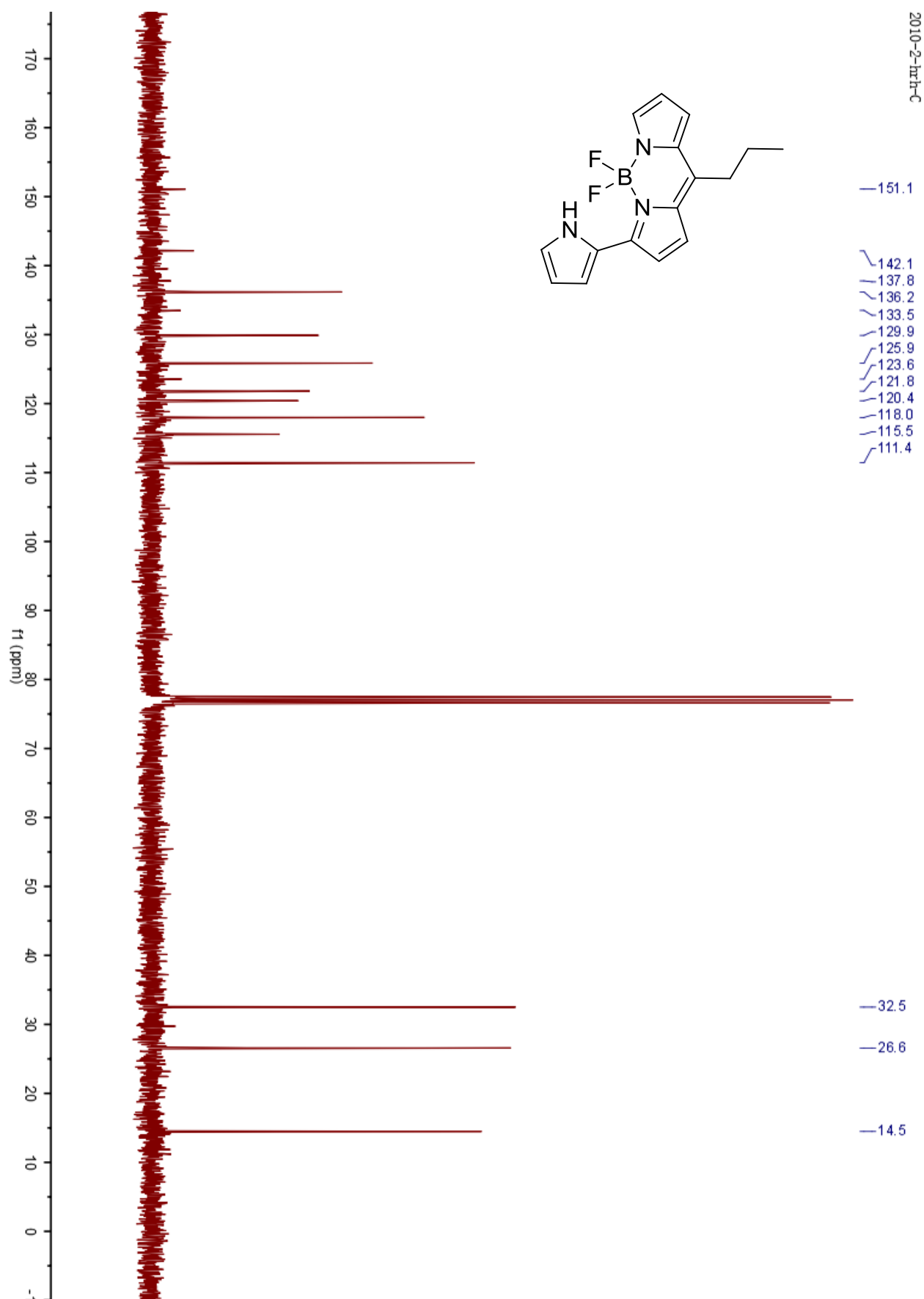


Figure S17.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **1h** in  $\text{CDCl}_3$  solution

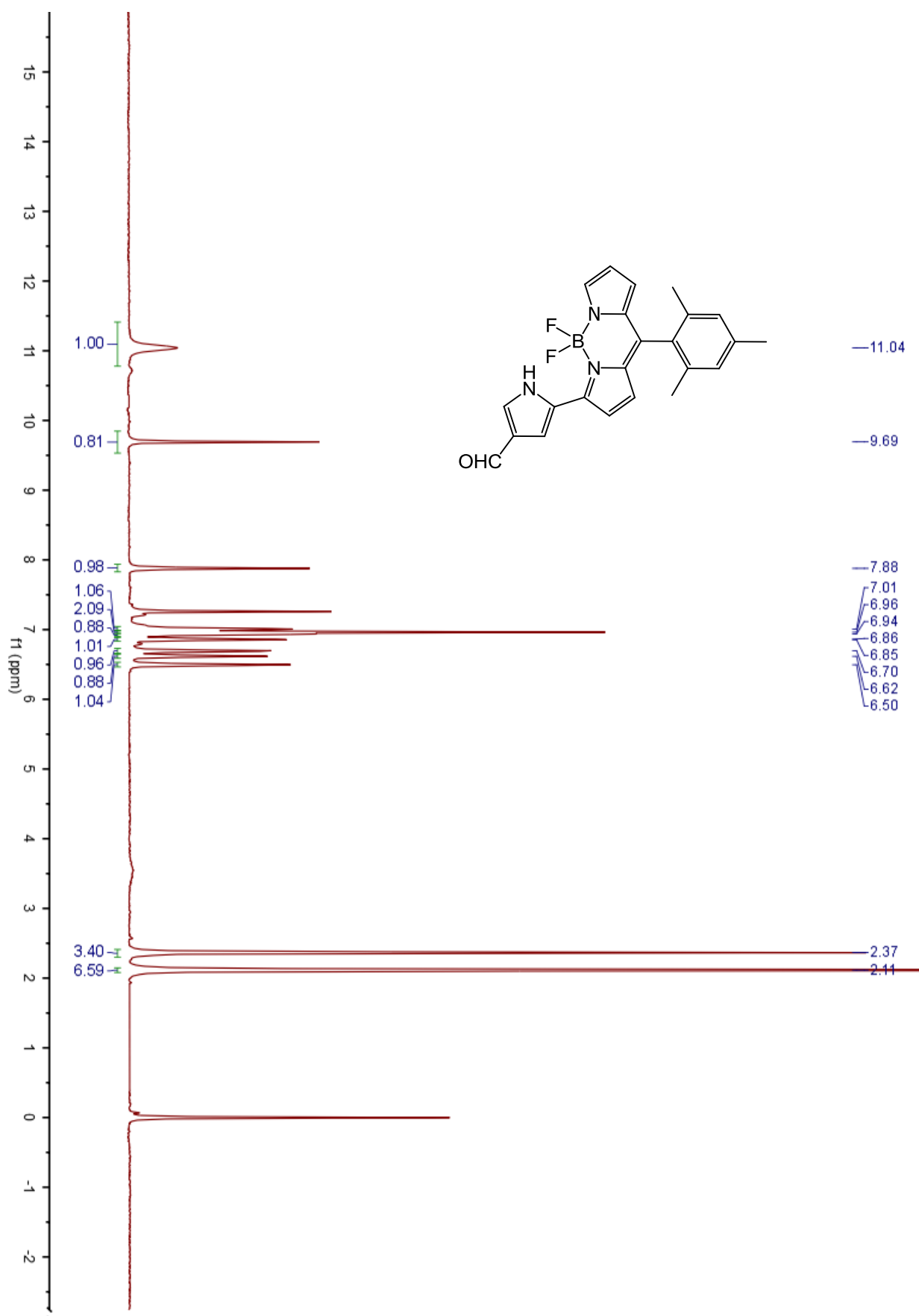


Figure S18. <sup>1</sup>H NMR spectrum of BODIPY dye **6** in CDCl<sub>3</sub> solution

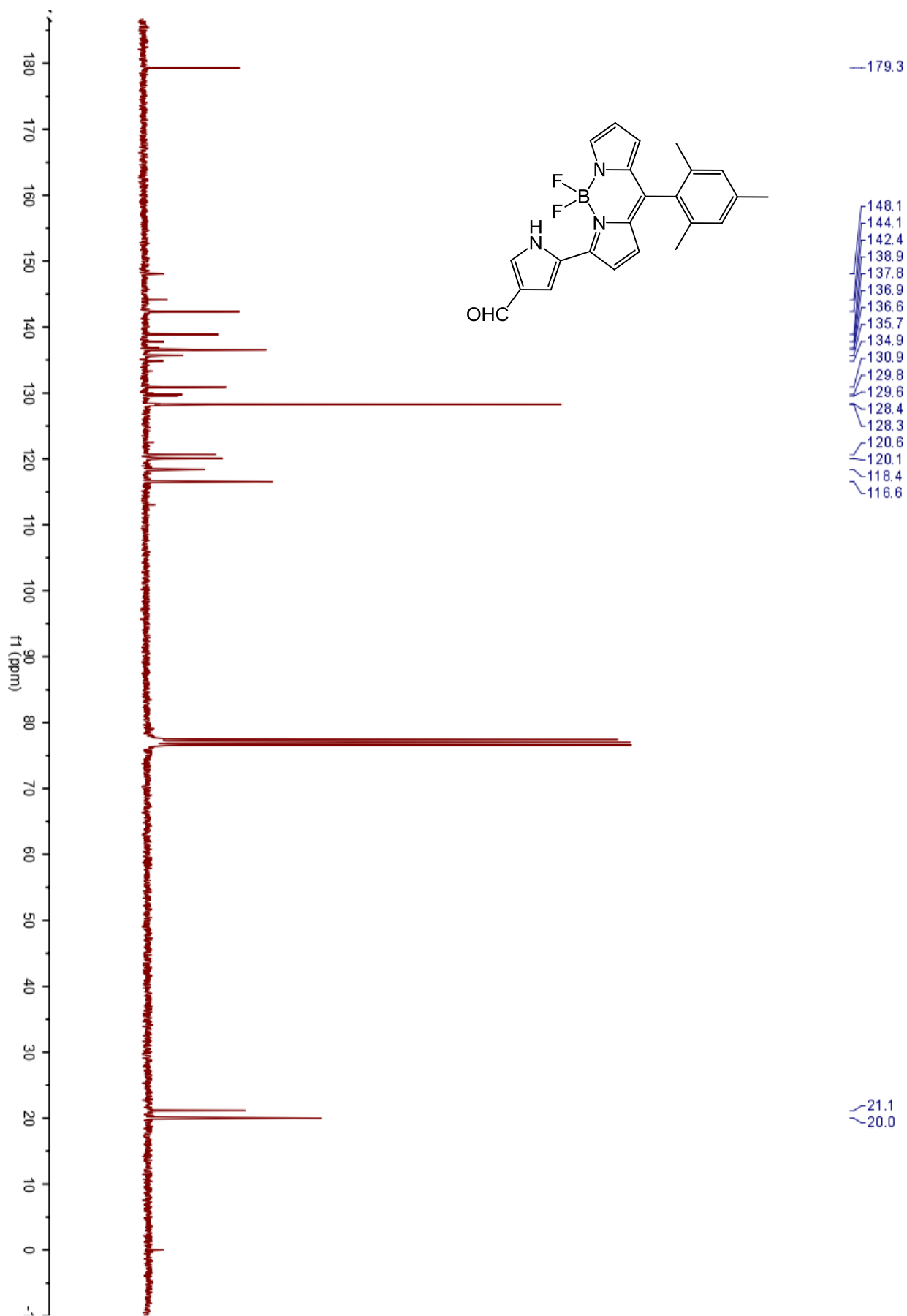


Figure S19.  $^{13}\text{C}$  NMR spectrum of BODIPY dye **6** in  $\text{CDCl}_3$  solution

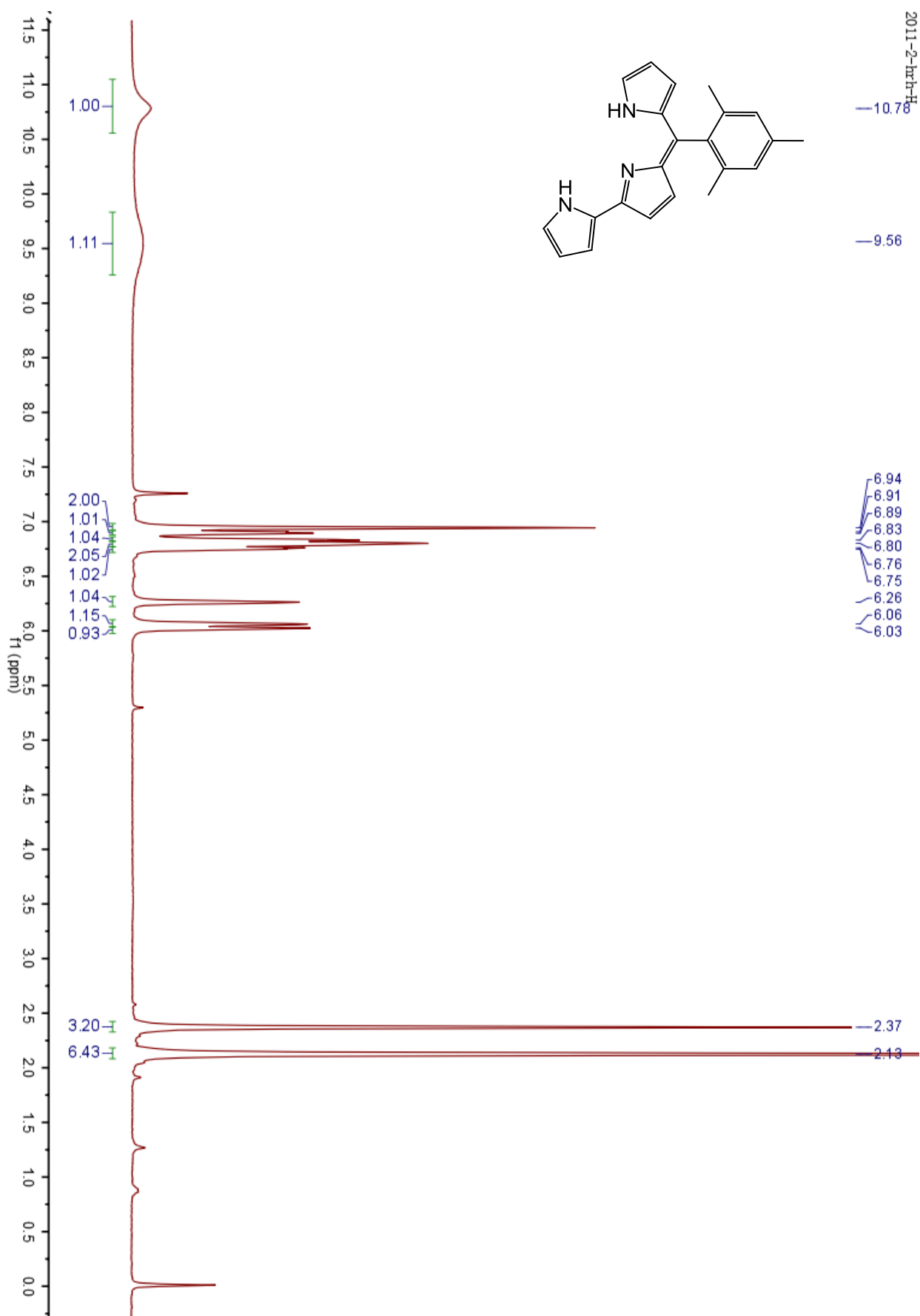


Figure S20. <sup>1</sup>H NMR spectrum of BODIPY dye 7 in CDCl<sub>3</sub> solution

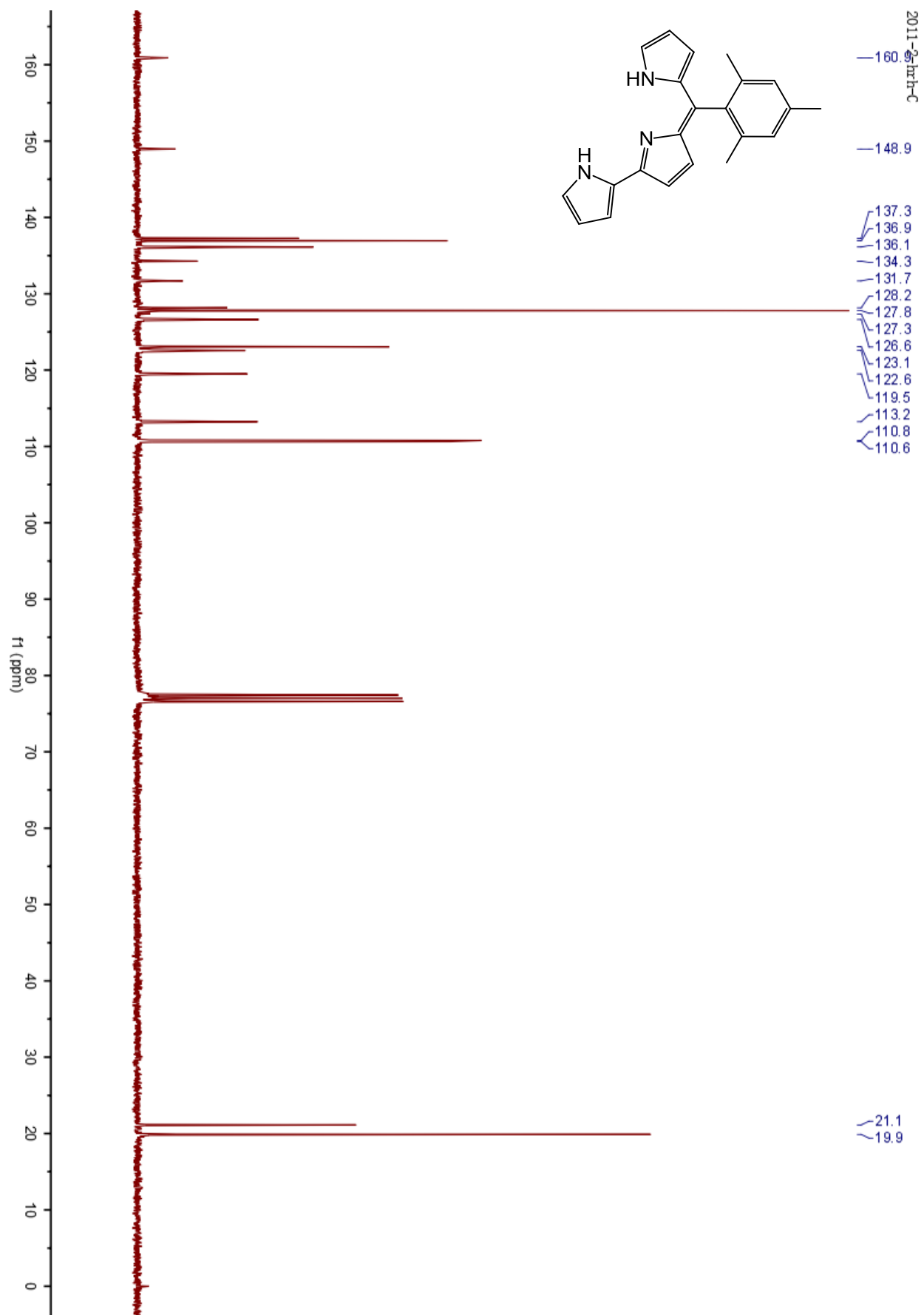
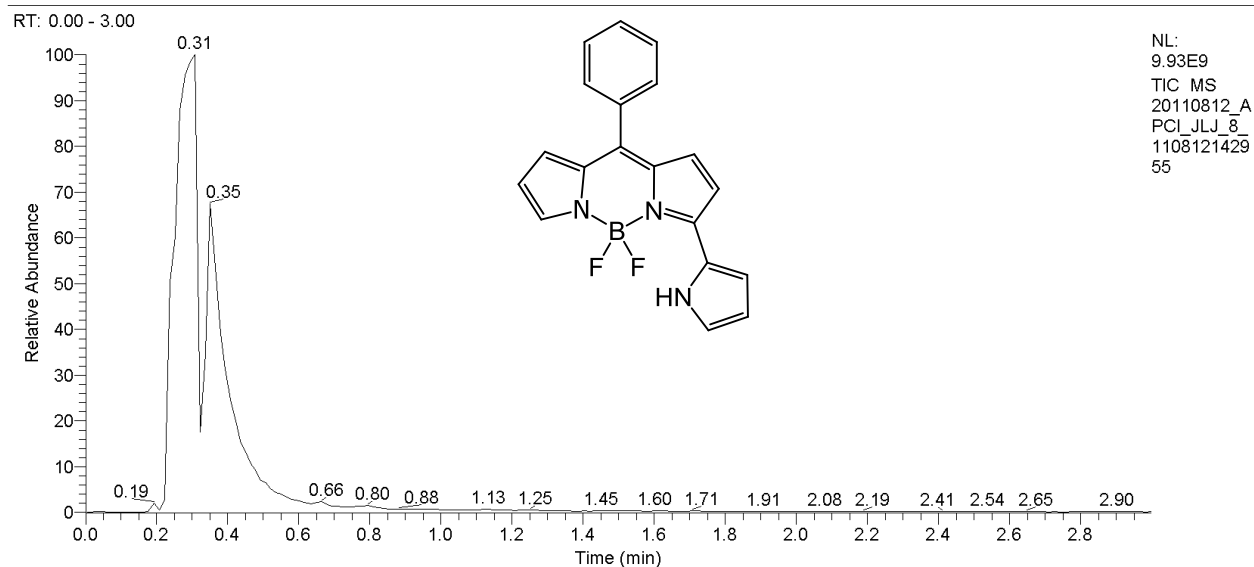


Figure S21.  $^{13}\text{C}$  NMR spectrum of BODIPY dye 7 in  $\text{CDCl}_3$  solution

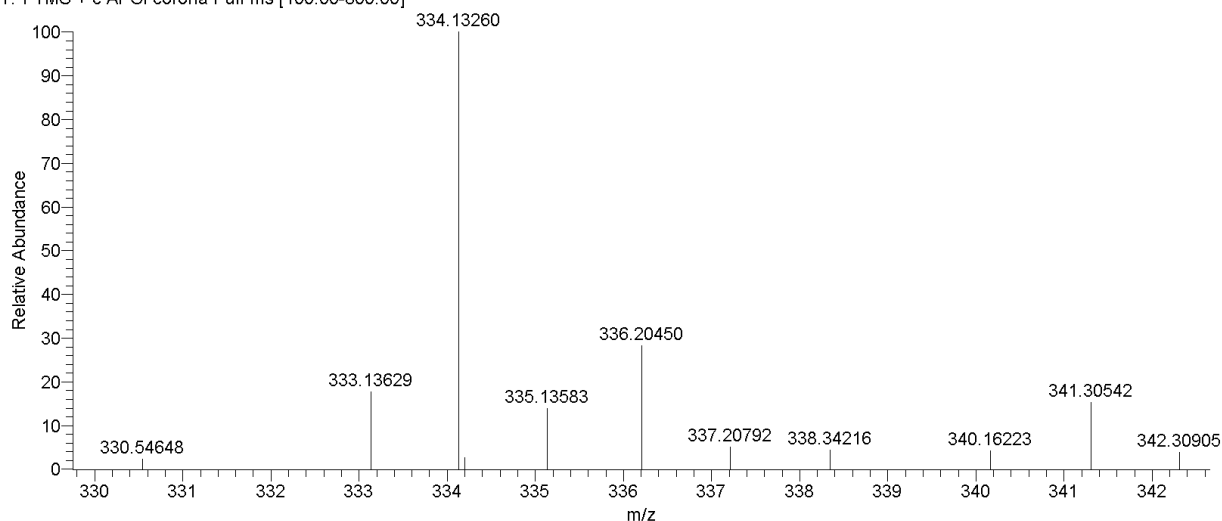
### 3. High resolution mass spectroscopies for all new compounds

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2011-8-12 14:29:55



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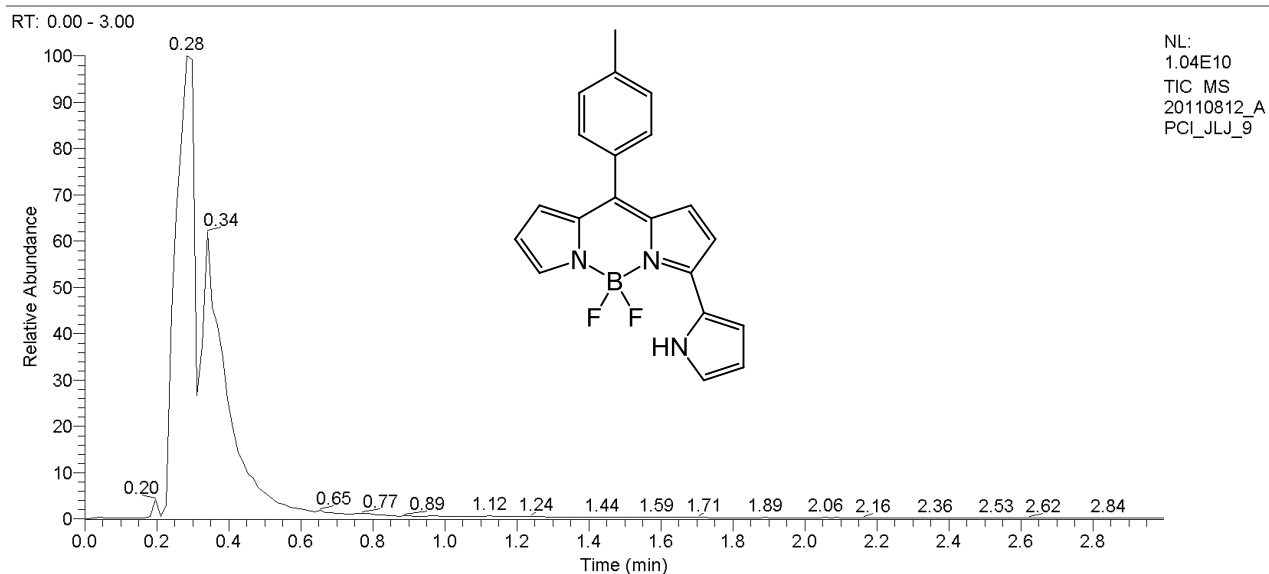
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m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
333.13629	7715913.5	0.20	333.13691	-0.62	C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> B F <sub>2</sub>
334.13260	43326648.0	1.11	334.13216	0.44	C <sub>19</sub> H <sub>15</sub> N <sub>3</sub> B F <sub>2</sub>
334.19949	1175933.3	0.03	334.20091	-1.42	C <sub>16</sub> H <sub>23</sub> N <sub>5</sub> B F <sub>2</sub>
335.13583	6008603.5	0.15	335.13999	-4.15	C <sub>19</sub> H <sub>16</sub> N <sub>3</sub> B F <sub>2</sub>
336.20450	12272509.0	0.31	336.20398	0.52	C <sub>15</sub> H <sub>23</sub> N <sub>6</sub> B F <sub>2</sub>
337.20792	2225465.3	0.06	337.21181	-3.89	C <sub>15</sub> H <sub>24</sub> N <sub>6</sub> B F <sub>2</sub>
338.34216	1880872.9	0.05	338.30096	41.21	C <sub>13</sub> H <sub>35</sub> N <sub>7</sub> B F <sub>2</sub>
340.16223	1846292.9	0.05	340.16654	-4.30	C <sub>18</sub> H <sub>19</sub> N <sub>4</sub> B F <sub>2</sub>
341.30542	6645545.0	0.17	341.30599	-0.57	C <sub>20</sub> H <sub>38</sub> N B F <sub>2</sub>
342.30905	1717402.6	0.04	342.31381	-4.76	C <sub>20</sub> H <sub>39</sub> N B F <sub>2</sub>
345.14404	3169334.8	0.08	345.14278	1.26	C <sub>13</sub> H <sub>14</sub> N <sub>9</sub> B F <sub>2</sub>
346.09192	3134744.5	0.08	346.09443	-2.51	C <sub>17</sub> H <sub>9</sub> N <sub>6</sub> B F <sub>2</sub>
346.15268	6581354.0	0.17	346.15060	2.07	C <sub>13</sub> H <sub>15</sub> N <sub>9</sub> B F <sub>2</sub>

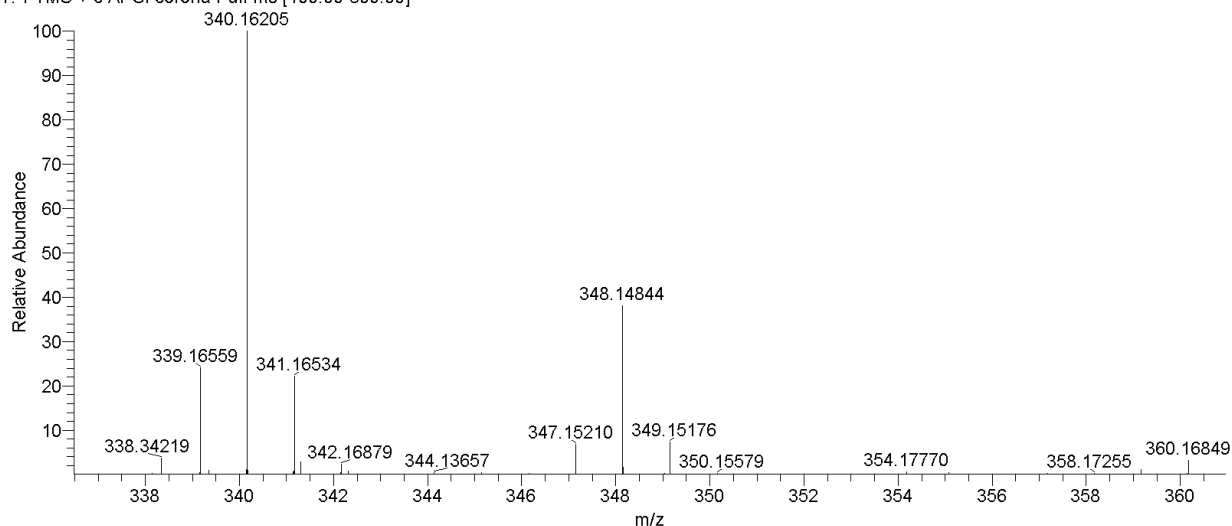


E:\data\20110812\20110812\_APCI\_JLJ\_9

2011-8-12 13:03:56



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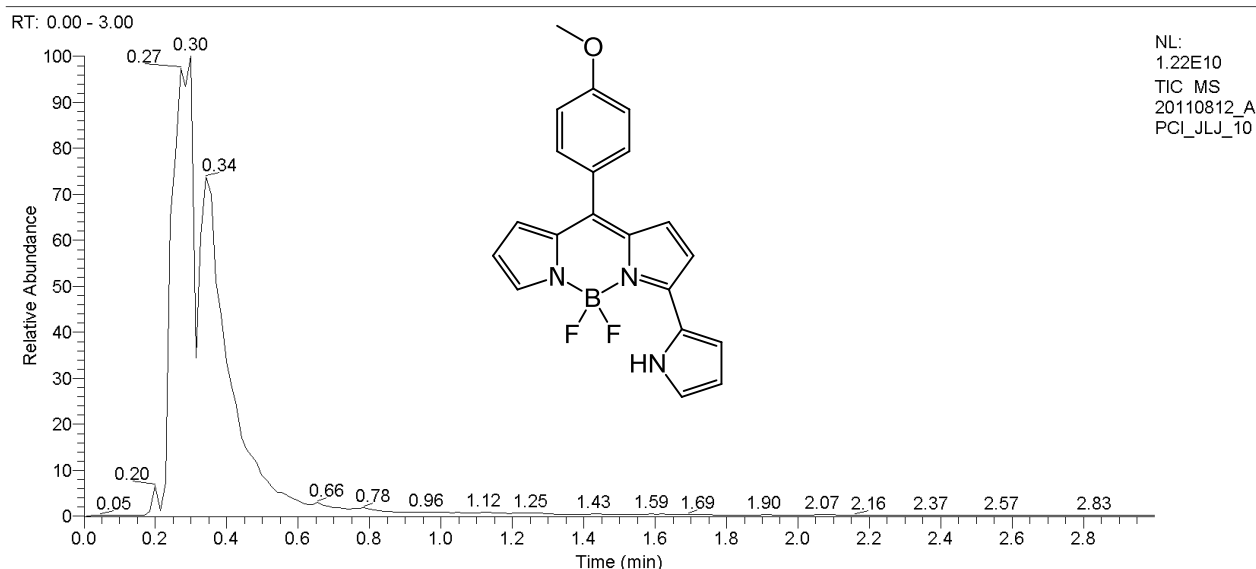


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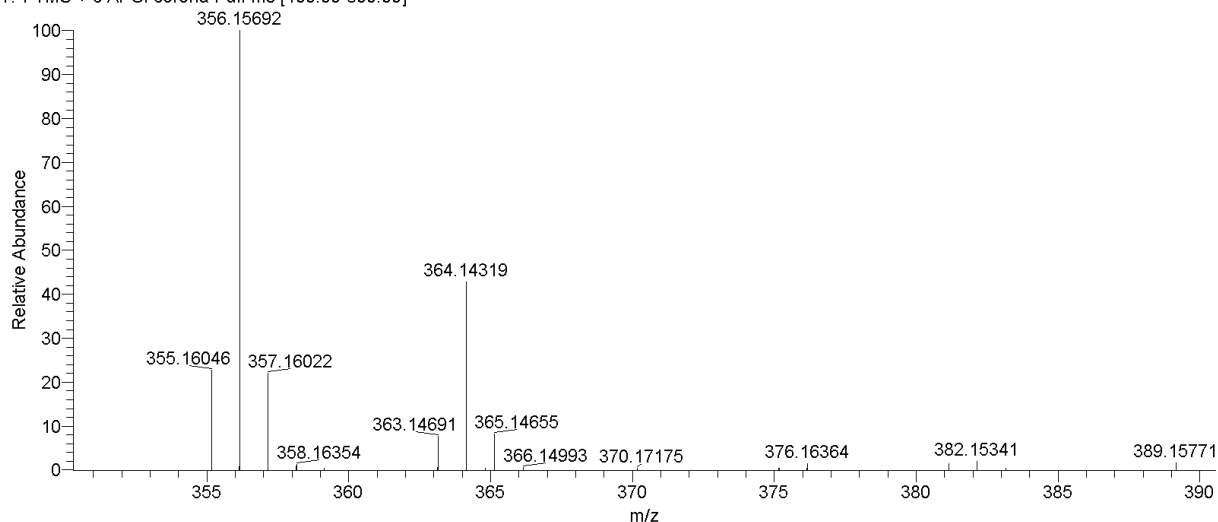
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
347.15210	9852960.0	0.35	347.15256	-0.46	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> B F <sub>2</sub>
348.14844	55039516.0	1.95	348.14781	0.63	C <sub>20</sub> H <sub>17</sub> N <sub>3</sub> B F <sub>2</sub>
348.15469	2428334.3	0.09	348.15551	-0.82	C <sub>11</sub> H <sub>20</sub> N <sub>8</sub> B Cl F <sub>2</sub>
349.15176	10634241.0	0.38	349.15144	0.32	C <sub>20</sub> H <sub>23</sub> B <sup>37</sup> Cl F <sub>2</sub>
360.16849	4713010.0	0.17	360.16808	0.40	C <sub>13</sub> H <sub>22</sub> N <sub>7</sub> B Cl F <sub>2</sub>
447.33340	2339721.8	0.08	447.33393	-0.53	C <sub>24</sub> H <sub>40</sub> N <sub>5</sub> B F <sub>2</sub>
448.33035	10349053.0	0.37	448.33101	-0.66	C <sub>22</sub> H <sub>44</sub> N <sub>4</sub> B Cl F <sub>2</sub>
449.33359	2973291.5	0.11	449.33281	0.77	C <sub>23</sub> H <sub>45</sub> N <sub>3</sub> B <sup>37</sup> Cl F <sub>2</sub>
468.33682	4643372.0	0.16	468.33729	-0.46	C <sub>20</sub> H <sub>44</sub> N <sub>7</sub> B <sup>37</sup> Cl F <sub>2</sub>
551.50470	3718662.0	0.13	551.47786	26.84	C <sub>30</sub> H <sub>58</sub> N <sub>6</sub> B F <sub>2</sub>
579.53589	16860522.0	0.60	579.48401	51.88	C <sub>30</sub> H <sub>58</sub> N <sub>8</sub> B F <sub>2</sub>
580.53918	5526243.0	0.20	580.49183	47.35	C <sub>30</sub> H <sub>59</sub> N <sub>8</sub> B F <sub>2</sub>
607.56738	11807922.0	0.42	607.49016	77.23	C <sub>30</sub> H <sub>58</sub> N <sub>10</sub> B F <sub>2</sub>

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2011-8-12 13:07:42



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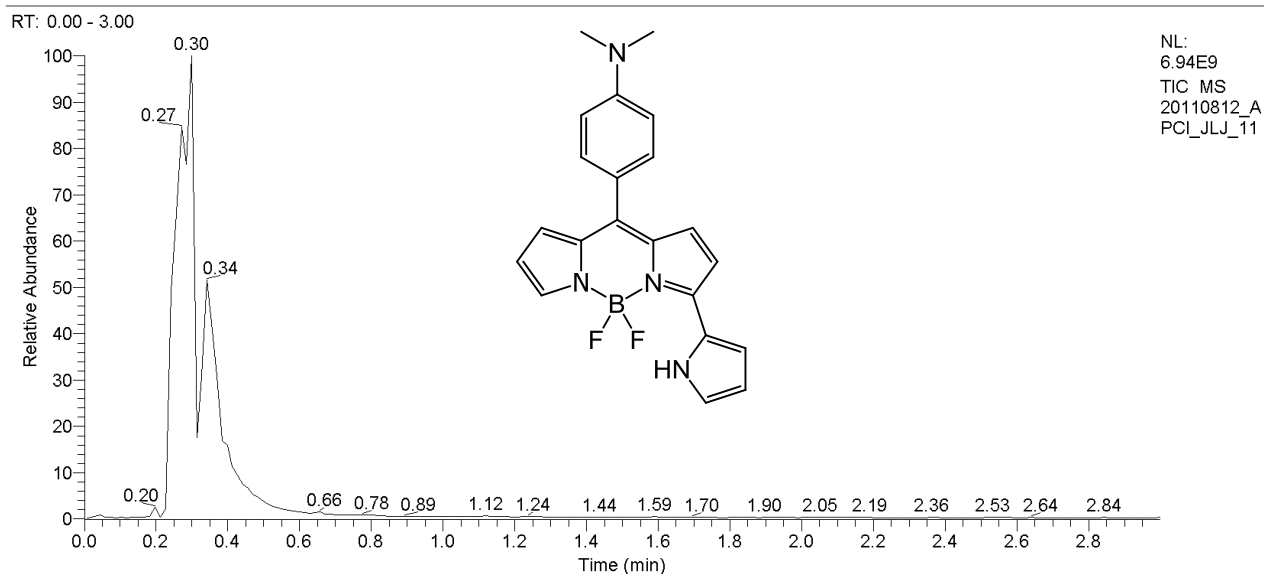


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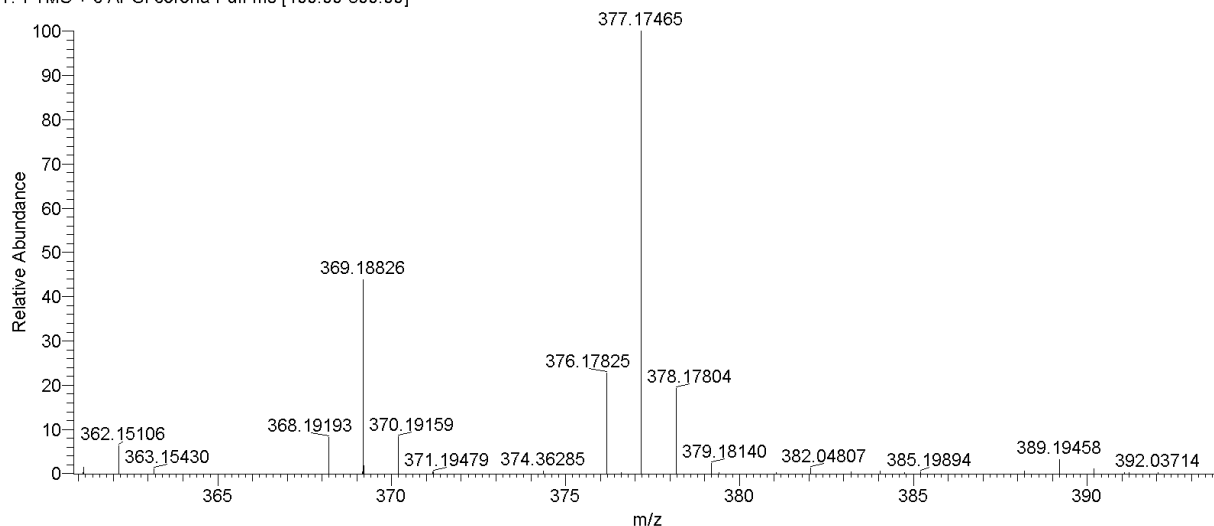
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
357.16022	49042756.0	1.20	357.16206	-1.85	C <sub>24</sub> H <sub>20</sub> B F <sub>2</sub>
363.14691	17309240.0	0.42	363.14748	-0.57	C <sub>21</sub> H <sub>18</sub> ON <sub>2</sub> B F <sub>2</sub>
364.14319	95541792.0	2.34	364.14273	0.46	C <sub>20</sub> H <sub>17</sub> ON <sub>3</sub> B F <sub>2</sub>
364.14978	4390581.5	0.11	364.14859	1.19	C <sub>12</sub> H <sub>15</sub> ON <sub>10</sub> B F <sub>2</sub>
365.14655	18386032.0	0.45	365.14921	-2.66	C <sub>18</sub> H <sub>16</sub> N <sub>6</sub> B F <sub>2</sub>
381.15689	3217123.5	0.08	381.15670	0.19	C <sub>19</sub> H <sub>18</sub> ON <sub>5</sub> B F <sub>2</sub>
382.15341	4360755.0	0.11	382.15195	1.46	C <sub>18</sub> H <sub>17</sub> ON <sub>6</sub> B F <sub>2</sub>
389.15771	3513491.5	0.09	389.15642	1.30	C <sub>14</sub> H <sub>16</sub> ON <sub>10</sub> B F <sub>2</sub>
409.16385	5107701.5	0.13	409.16285	1.00	C <sub>19</sub> H <sub>18</sub> ON <sub>7</sub> B F <sub>2</sub>
464.19464	4550421.0	0.11	464.19247	2.17	C <sub>21</sub> H <sub>21</sub> ON <sub>9</sub> B F <sub>2</sub>
551.50452	4992771.5	0.12	551.49765	6.87	C <sub>25</sub> H <sub>60</sub> ON <sub>9</sub> B F <sub>2</sub>
579.53577	13956922.0	0.34	579.48401	51.76	C <sub>30</sub> H <sub>58</sub> N <sub>8</sub> B F <sub>2</sub>
580.53864	7931231.5	0.19	580.49183	46.80	C <sub>30</sub> H <sub>59</sub> N <sub>8</sub> B F <sub>2</sub>

E:\data\20110812\20110812\_APCI\_JLJ\_11

2011-8-12 13:11:28



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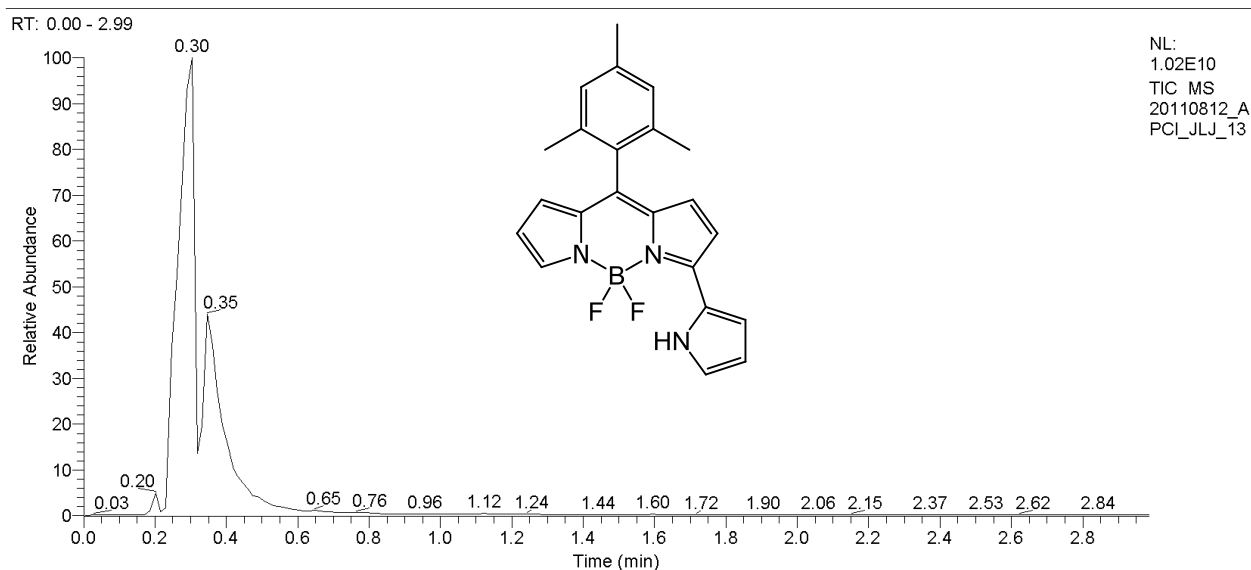


20110812\_APCI\_JLJ\_11 #32 RT: 0.46  
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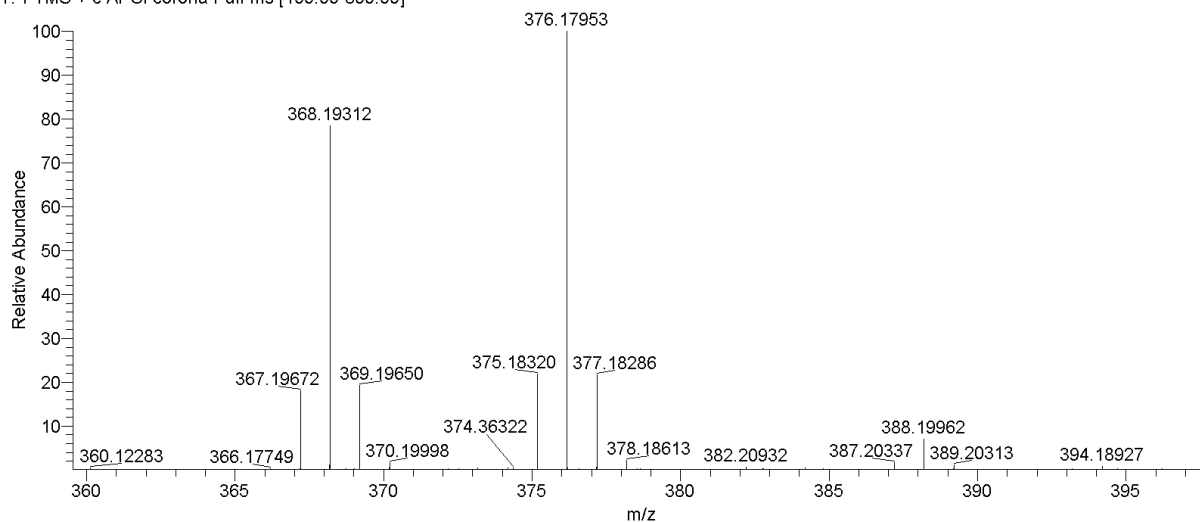
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
355.17273	9536859.0	5.12	355.17207	0.66	C <sub>11</sub> H <sub>18</sub> ON <sub>10</sub> BF <sub>2</sub>
356.17209	43249304.0	23.21	356.17268	-0.59	C <sub>17</sub> H <sub>19</sub> N <sub>6</sub> BF <sub>2</sub>
357.16833	186376256.0	100.00	357.16793	0.40	C <sub>16</sub> H <sub>18</sub> N <sub>7</sub> BF <sub>2</sub>
358.17136	41370000.0	22.20	358.16989	1.47	C <sub>24</sub> H <sub>21</sub> BF <sub>2</sub>
369.18790	5700902.5	3.06	369.18772	0.18	C <sub>12</sub> H <sub>20</sub> ON <sub>10</sub> BF <sub>2</sub>
377.17429	10598561.0	5.69	377.17436	-0.07	C <sub>21</sub> H <sub>20</sub> N <sub>4</sub> BF <sub>2</sub>
579.53461	6136140.5	3.29	579.48401	50.60	C <sub>30</sub> H <sub>58</sub> N <sub>8</sub> BF <sub>2</sub>
607.56592	5534480.5	2.97	607.49016	75.76	C <sub>30</sub> H <sub>58</sub> N <sub>10</sub> BF <sub>2</sub>

E:\data\20110812\20110812\_APCI\_JLJ\_13

2011-8-12 13:18:57



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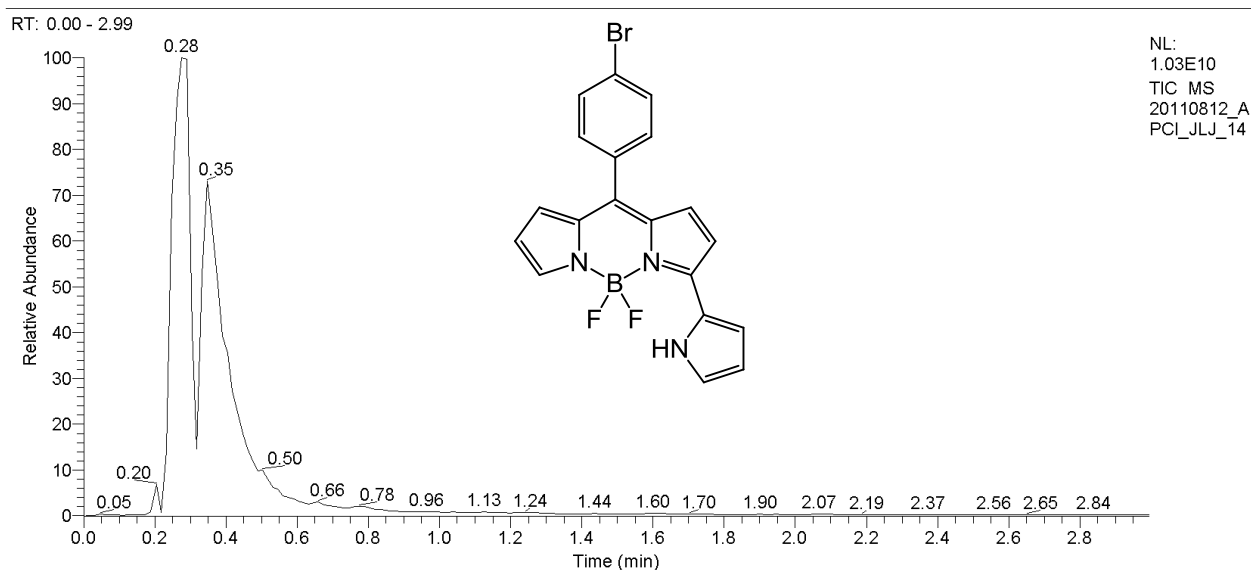


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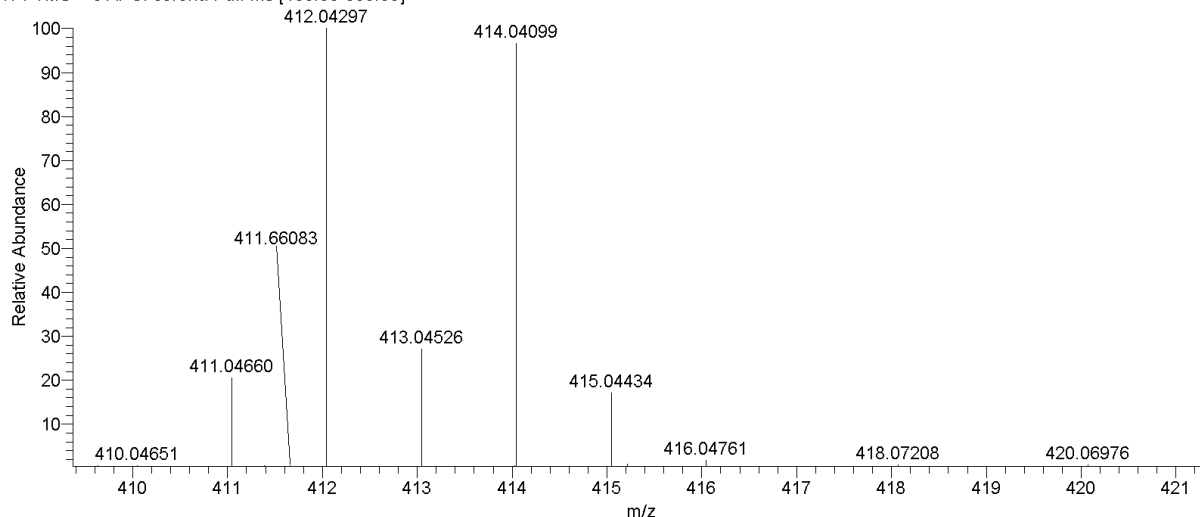
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
354.17776	17713906.0	6.35	354.17682	0.95	C <sub>12</sub> H <sub>19</sub> ON <sub>9</sub> B F <sub>2</sub>
355.17715	66948380.0	24.01	355.17743	-0.28	C <sub>18</sub> H <sub>20</sub> N <sub>5</sub> B F <sub>2</sub>
356.17334	278829120.0	100.00	356.17268	0.66	C <sub>17</sub> H <sub>19</sub> N <sub>6</sub> B F <sub>2</sub>
357.17636	63413432.0	22.74	357.18051	-4.15	C <sub>17</sub> H <sub>20</sub> N <sub>6</sub> B F <sub>2</sub>
358.17963	6736812.5	2.42	358.17710	2.53	C <sub>18</sub> H <sub>21</sub> ON <sub>4</sub> B F <sub>2</sub>
368.19287	11945678.0	4.28	368.19247	0.40	C <sub>13</sub> H <sub>21</sub> ON <sub>9</sub> B F <sub>2</sub>
376.17923	11848446.0	4.25	376.17911	0.12	C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> B F <sub>2</sub>

E:\data\20110812\20110812\_APCI\_JLJ\_14

2011-8-12 13:22:41



20110812\_APCI\_JLJ\_14 #18 RT: 0.26 AV: 1 NL: 1.07E8  
 T: FTMS + c APCI corona Full ms [100.00-800.00]

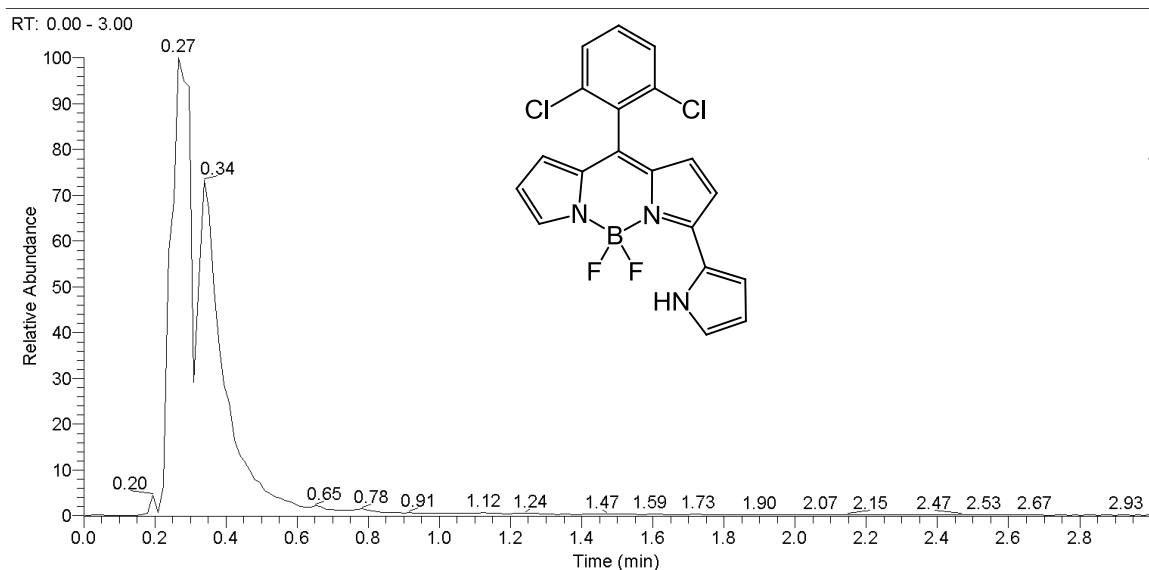


20110812\_APCI\_JLJ\_14#18 RT: 0.26  
 T: FTMS + c APCI corona Full ms [100.00-800.00]

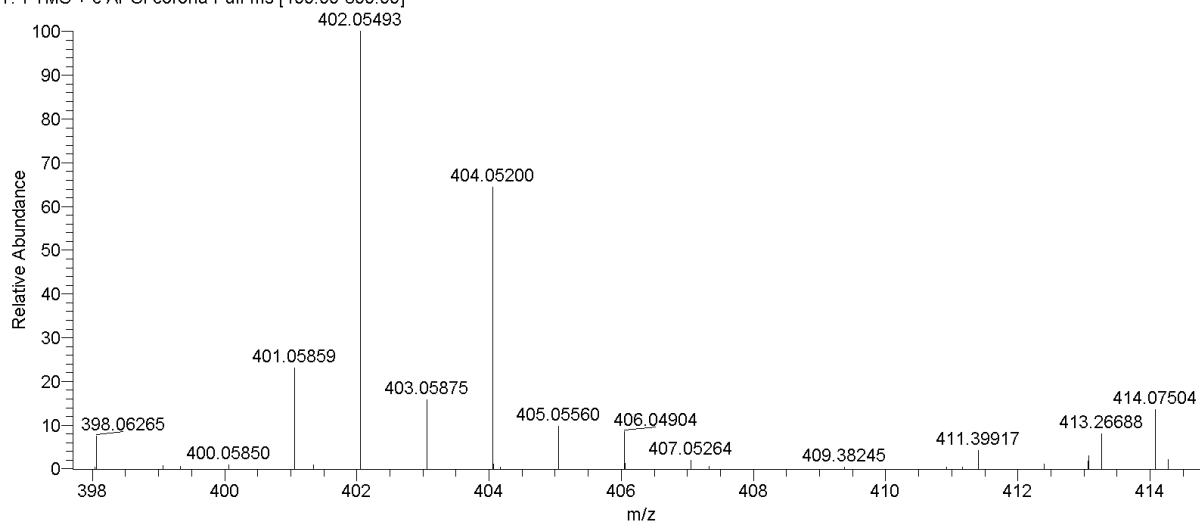
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
406.05460	137501168.0	5.88	406.05454	0.05	C <sub>13</sub> H <sub>27</sub> N <sub>3</sub> BBr <sup>81</sup> BrF <sub>2</sub>
407.05786	25009072.0	1.07	407.05866	-0.80	C <sub>27</sub> H <sub>6</sub> N <sub>2</sub> BF <sub>2</sub>
411.04660	22065392.0	0.94	411.04687	-0.27	C <sub>17</sub> H <sub>2</sub> ON <sub>10</sub> BF <sub>2</sub>
412.04297	107291080.0	4.59	412.04267	0.30	C <sub>19</sub> H <sub>14</sub> N <sub>3</sub> BBrF <sub>2</sub>
413.04526	29085526.0	1.24	413.04538	-0.12	C <sub>20</sub> H <sub>15</sub> N <sub>2</sub> B <sup>81</sup> BrF <sub>2</sub>
414.04099	103621720.0	4.43	414.04063	0.36	C <sub>19</sub> H <sub>14</sub> N <sub>3</sub> B <sup>81</sup> BrF <sub>2</sub>
415.04434	18327634.0	0.78	415.04364	0.70	C <sub>15</sub> H <sub>26</sub> BBr <sup>81</sup> BrF <sub>2</sub>
424.06308	4549271.5	0.19	424.06271	0.37	C <sub>23</sub> H <sub>18</sub> B <sup>81</sup> BrF <sub>2</sub>
426.06073	3692747.8	0.16	426.06041	0.32	C <sub>15</sub> H <sub>16</sub> ON <sub>6</sub> B <sup>81</sup> BrF <sub>2</sub>
430.05307	3987565.5	0.17	430.05324	-0.17	C <sub>19</sub> H <sub>16</sub> ON <sub>3</sub> BBrF <sub>2</sub>
457.06329	3325009.5	0.14	457.06279	0.50	C <sub>18</sub> H <sub>15</sub> N <sub>7</sub> BBrF <sub>2</sub>
551.50330	4572049.5	0.20	551.49765	5.65	C <sub>25</sub> H <sub>60</sub> ON <sub>9</sub> BF <sub>2</sub>
579.53534	19053504.0	0.82	579.48401	51.33	C <sub>30</sub> H <sub>58</sub> N <sub>8</sub> BF <sub>2</sub>

20110812\_APCI\_JLJ\_12\_110812143513

2011-8-12 14:35:13



20110812\_APCI\_JLJ\_12\_110812143513 #12 RT: 0.18 AV: 1 NL: 4.49E5  
 T: FTMS + c APCI corona Full ms [100.00-800.00]



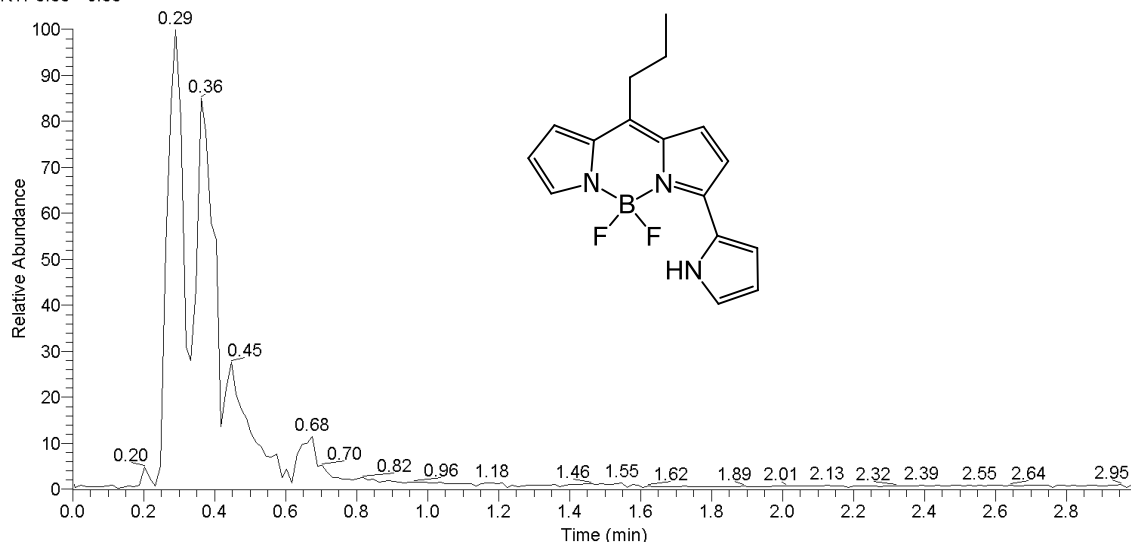
20110812\_APCI\_JLJ\_12\_110812143513 #12 RT: 0.18  
 T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
401.34171	3946.2	0.05	401.33701	4.70	C <sub>19</sub> H <sub>40</sub> N <sub>6</sub> B F <sub>2</sub>
402.05493	449063.5	5.14	402.05422	0.72	C <sub>19</sub> H <sub>13</sub> N <sub>3</sub> B Cl <sub>2</sub> F <sub>2</sub>
403.05875	71229.4	0.82	403.05952	-0.77	C <sub>11</sub> H <sub>22</sub> N <sub>4</sub> B Cl <sub>2</sub> <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>
404.05200	289416.0	3.31	404.05127	0.74	C <sub>19</sub> H <sub>13</sub> N <sub>3</sub> B Cl <sup>37</sup> Cl F <sub>2</sub>
404.06348	4765.8	0.05	404.06369	-0.21	C <sub>13</sub> H <sub>13</sub> N <sub>8</sub> B <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>
405.05560	43953.4	0.50	405.05490	0.71	C <sub>19</sub> H <sub>19</sub> B Cl <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>
406.04904	38352.2	0.44	406.04946	-0.42	C <sub>8</sub> H <sub>14</sub> N <sub>10</sub> B Cl <sub>2</sub> <sup>37</sup> Cl F <sub>2</sub>
406.05923	5725.5	0.07	406.05853	0.70	C <sub>18</sub> H <sub>8</sub> N <sub>7</sub> B Cl F <sub>2</sub>
407.05264	8902.0	0.10	407.05309	-0.45	C <sub>8</sub> H <sub>20</sub> N <sub>7</sub> B Cl <sub>2</sub> <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>
411.39917	18968.8	0.22	411.36495	34.22	C <sub>15</sub> H <sub>42</sub> N <sub>10</sub> B F <sub>2</sub>
412.40274	4697.0	0.05	412.31844	84.30	C <sub>18</sub> H <sub>42</sub> N <sub>5</sub> B Cl F <sub>2</sub>
413.06726	7799.7	0.09	413.06719	0.07	C <sub>15</sub> H <sub>19</sub> N <sub>4</sub> B Cl <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>
413.07858	13508.2	0.15	413.07794	0.64	C <sub>17</sub> H <sub>16</sub> N <sub>5</sub> B <sup>37</sup> Cl <sub>2</sub> F <sub>2</sub>

E:\data\20110812\20110812\_APCI\_JLJ\_2

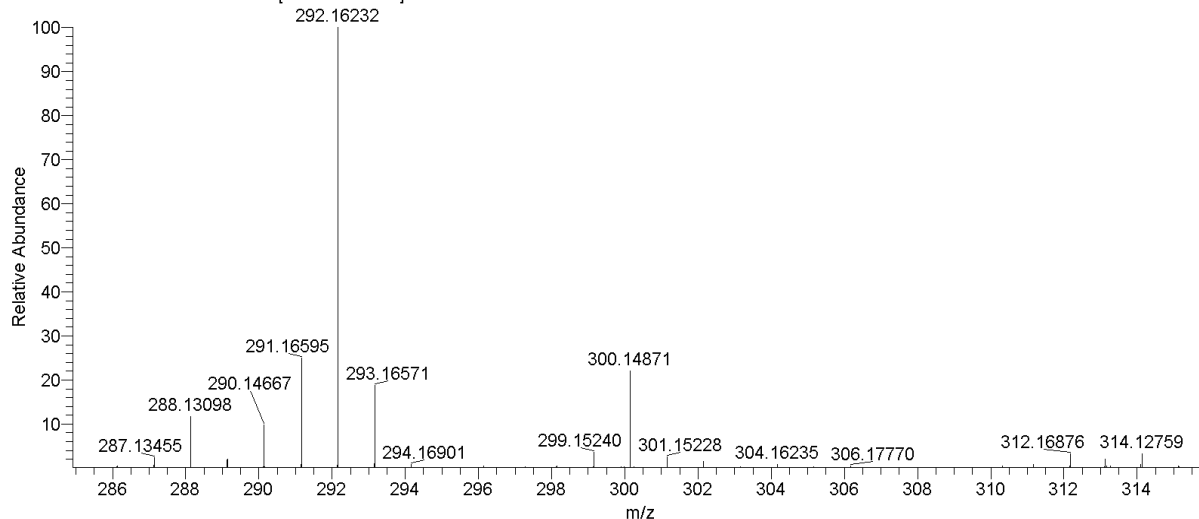
2011-8-12 12:37:54

RT: 0.00 - 3.00



NL:  
 8.57E9  
 TIC MS  
 20110812\_A  
 PCI\_JLJ\_2

20110812\_APCI\_JLJ\_2#20 RT: 0.28 AV: 1 NL: 1.55E8  
 T: FTMS + c APCI corona Full ms [100.00-800.00]

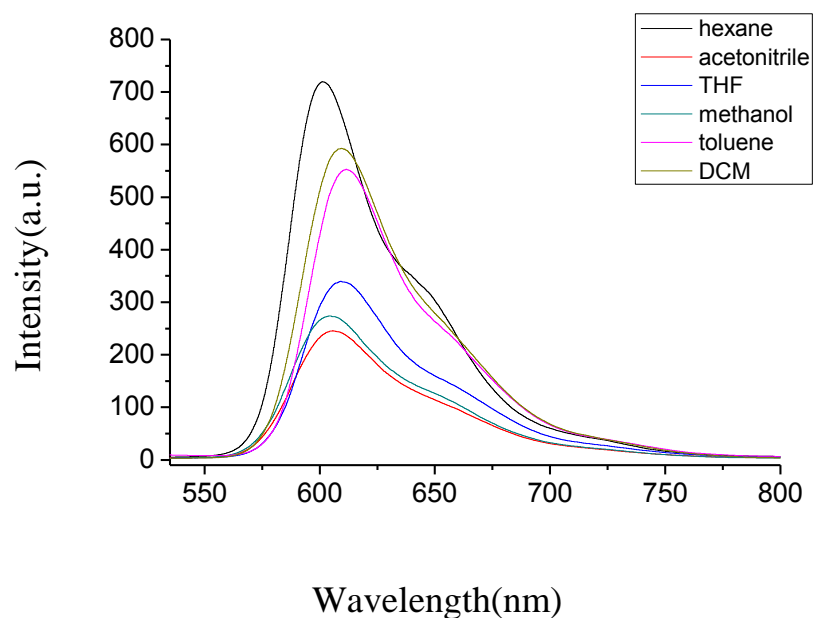
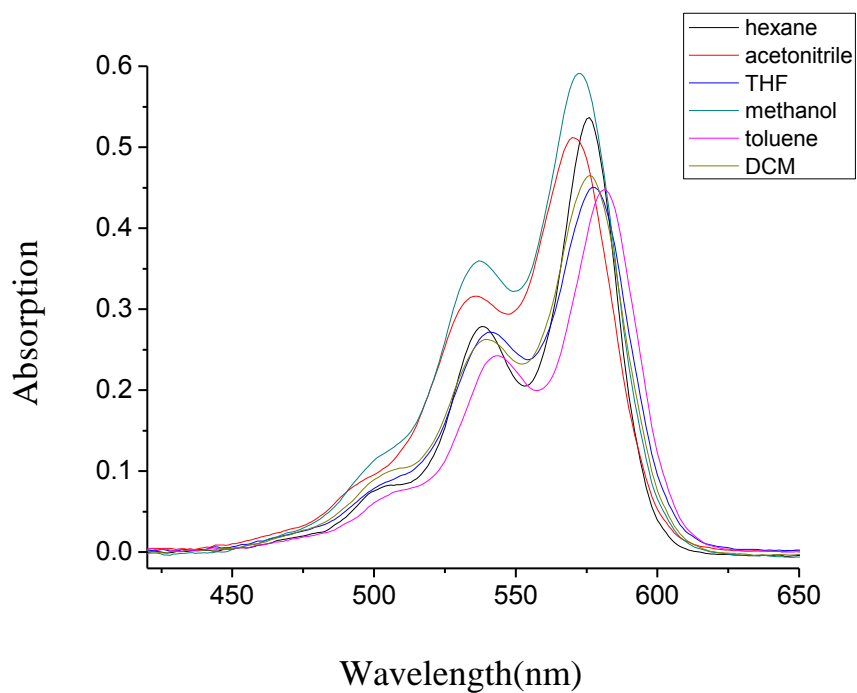


20110812\_APCI\_JLJ\_2#20 RT: 0.28

T: FTMS + c APCI corona Full ms [100.00-800.00]

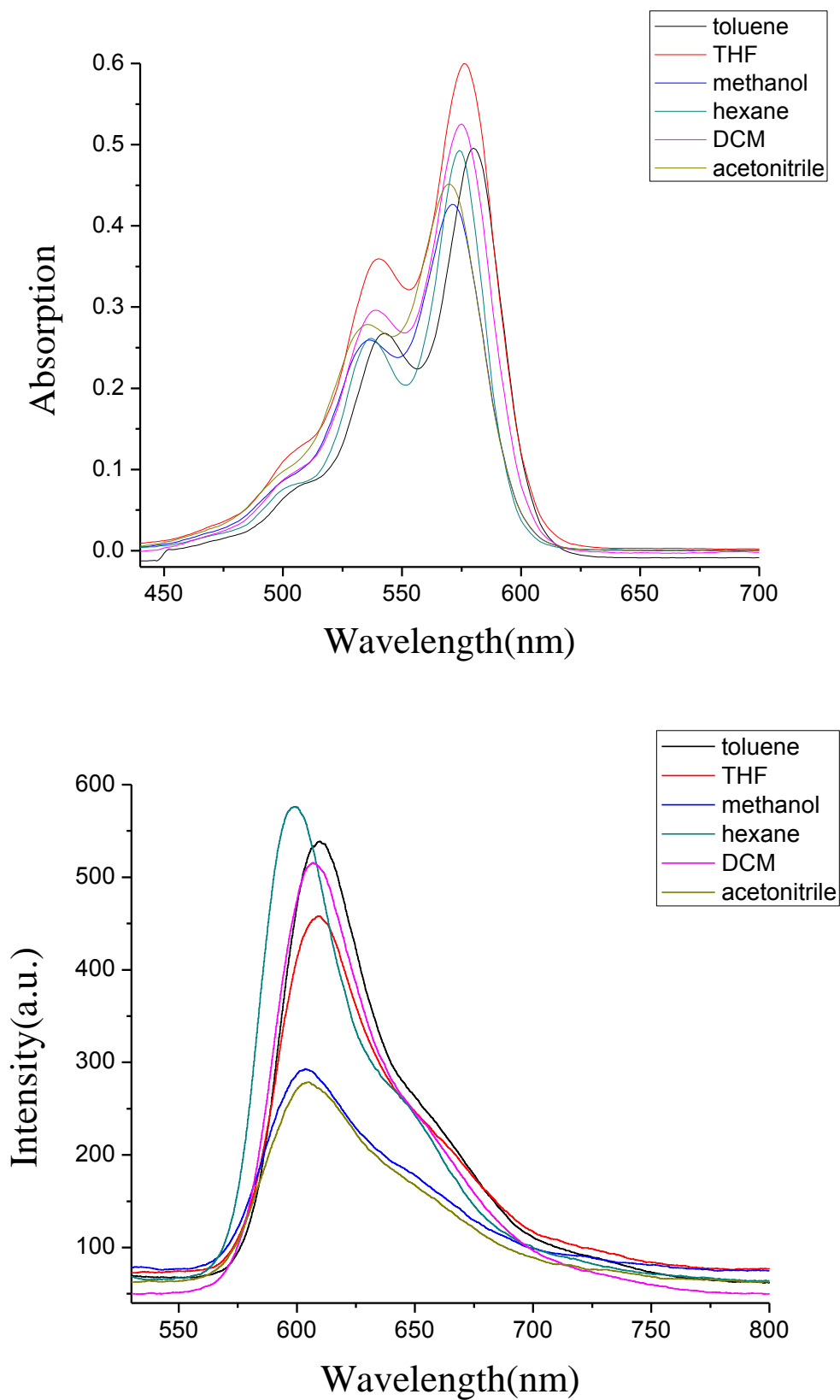
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
292.16232	155280976.0	6.72	292.16654	-4.21	C <sub>14</sub> H <sub>19</sub> N <sub>4</sub> B F <sub>2</sub>
292.16861	6068174.0	0.26	292.16654	2.07	C <sub>14</sub> H <sub>19</sub> N <sub>4</sub> B F <sub>2</sub>
293.16571	29188022.0	1.26	293.16178	3.93	C <sub>13</sub> H <sub>18</sub> N <sub>5</sub> B F <sub>2</sub>
299.15240	5688538.5	0.25	299.15843	-6.03	C <sub>9</sub> H <sub>16</sub> N <sub>9</sub> B F <sub>2</sub>
300.14871	34242248.0	1.48	300.14781	0.90	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> B F <sub>2</sub>
312.16876	4958324.0	0.21	312.16626	2.51	C <sub>10</sub> H <sub>17</sub> N <sub>9</sub> B F <sub>2</sub>
314.12759	5109665.5	0.22	314.12573	1.86	C <sub>14</sub> H <sub>13</sub> N <sub>6</sub> B F <sub>2</sub>
509.24442	4411931.0	0.19	509.24311	1.31	C <sub>29</sub> H <sub>28</sub> N <sub>6</sub> B F <sub>2</sub>
532.24792	10341207.0	0.45	532.22271	25.22	C <sub>30</sub> H <sub>25</sub> N <sub>7</sub> B F <sub>2</sub>
533.24438	23853666.0	1.03	533.23053	13.85	C <sub>30</sub> H <sub>26</sub> N <sub>7</sub> B F <sub>2</sub>
533.26733	7749823.5	0.34	533.28670	-19.37	C <sub>26</sub> H <sub>32</sub> N <sub>10</sub> B F <sub>2</sub>
534.24744	6750095.0	0.29	534.23836	9.08	C <sub>30</sub> H <sub>27</sub> N <sub>7</sub> B F <sub>2</sub>
534.26343	76023976.0	3.29	534.23836	25.07	C <sub>30</sub> H <sub>27</sub> N <sub>7</sub> B F <sub>2</sub>

4. UV-vis and Fluorescence data for all the new compounds (THF: Tetrahydrofuran; DCM: Dichloromethane).

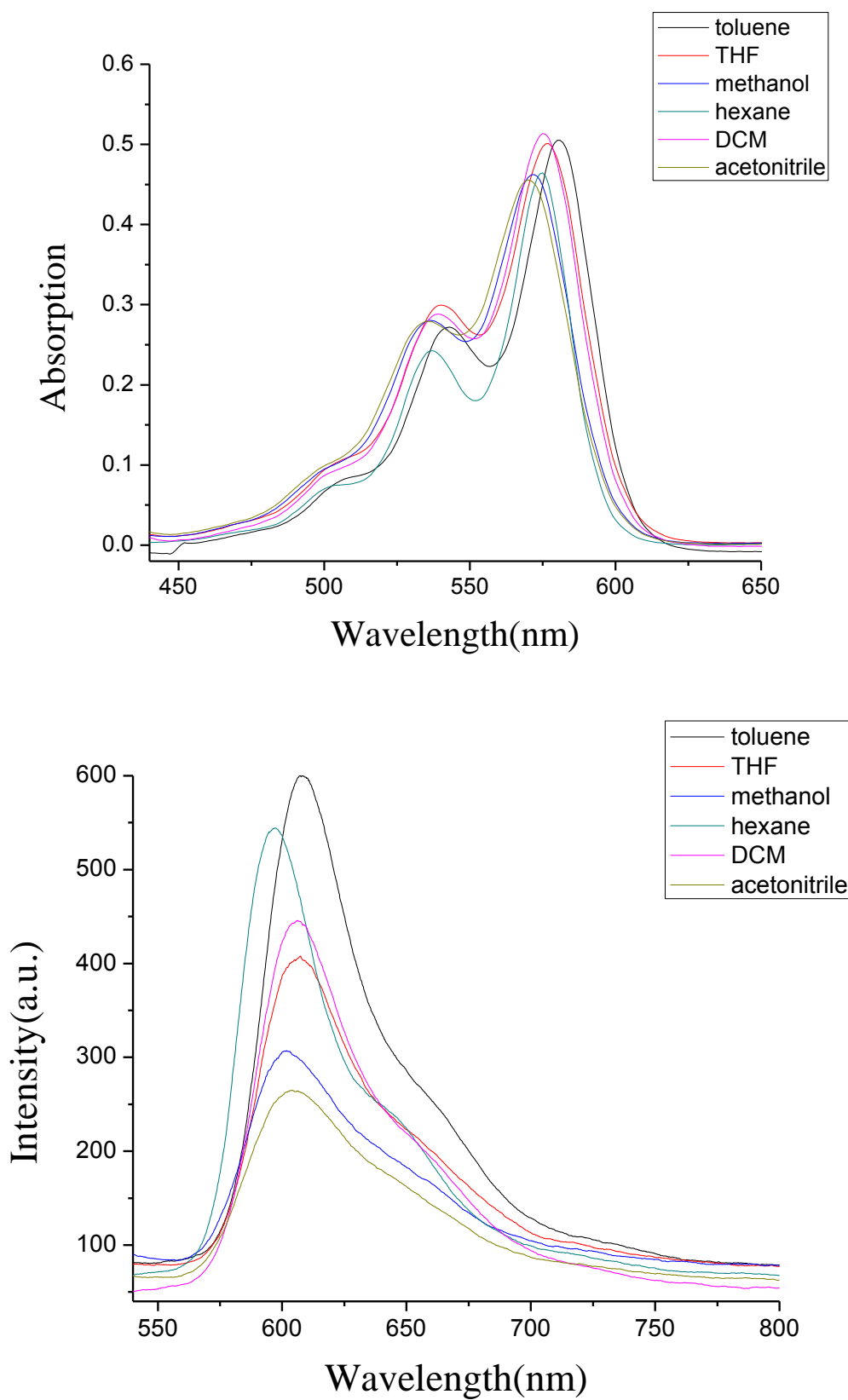


**Figure S22:** Absorption (top) and emission spectra (bottom) of BODIPY **1a** recorded in different solvents. Excited at 520 nm

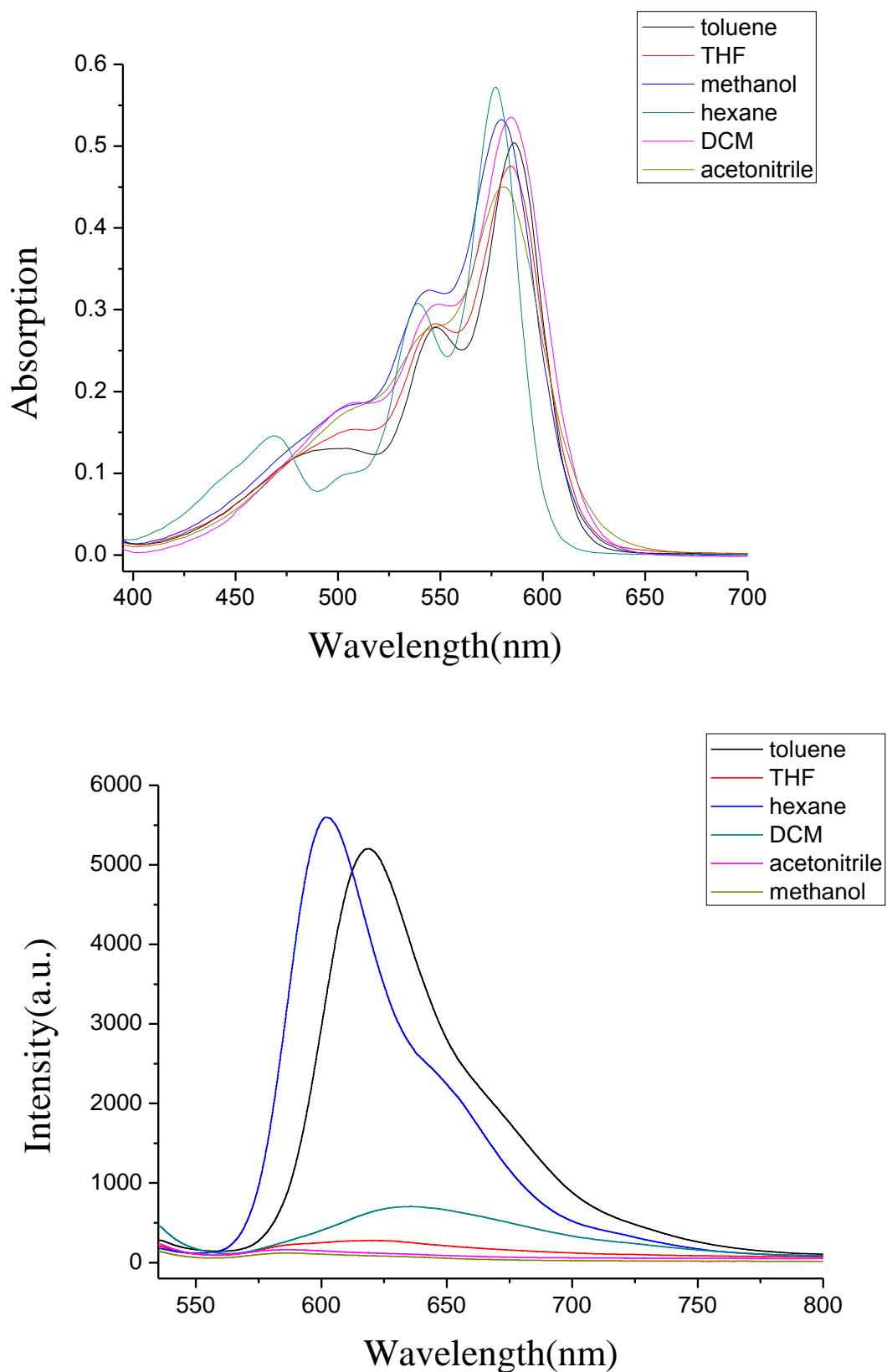




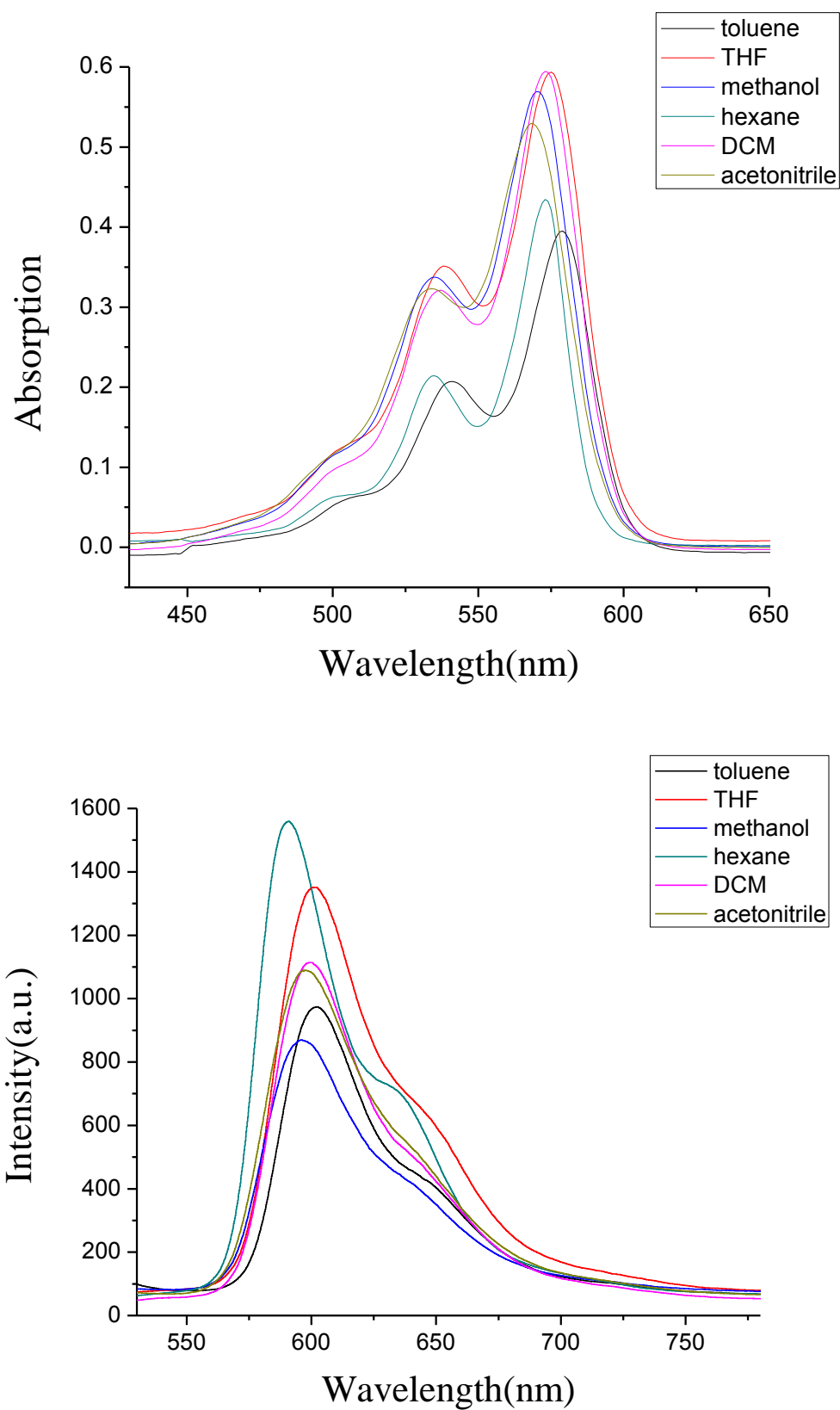
**Figure S23:** Absorption (top) and emission spectra (bottom) of BODIPY **1b** recorded in different solvents. Excited at 520 nm



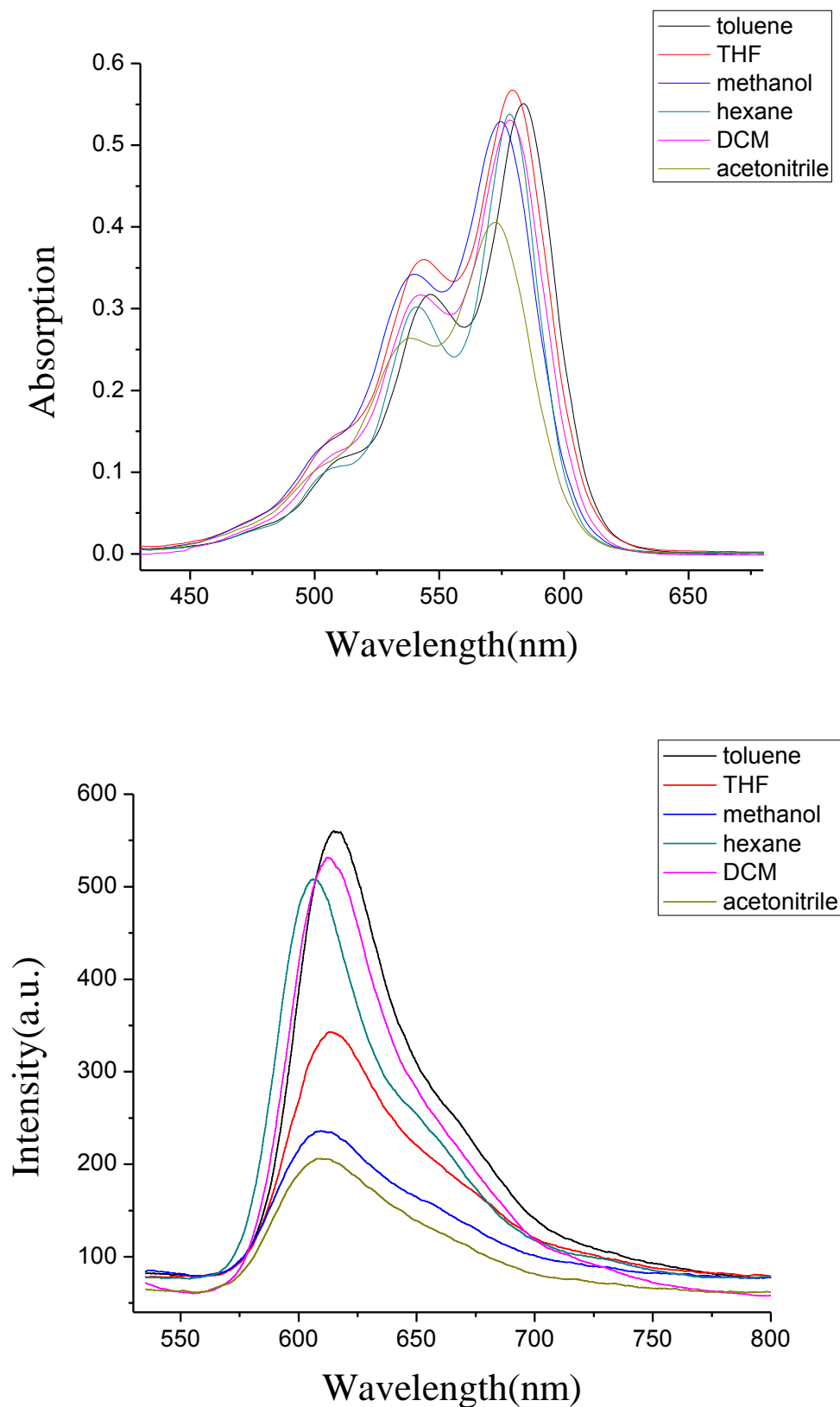
**Figure S24:** Absorption (top) and emission spectra (bottom) of BODIPY **1c** recorded in different solvents. Excited at 520 nm



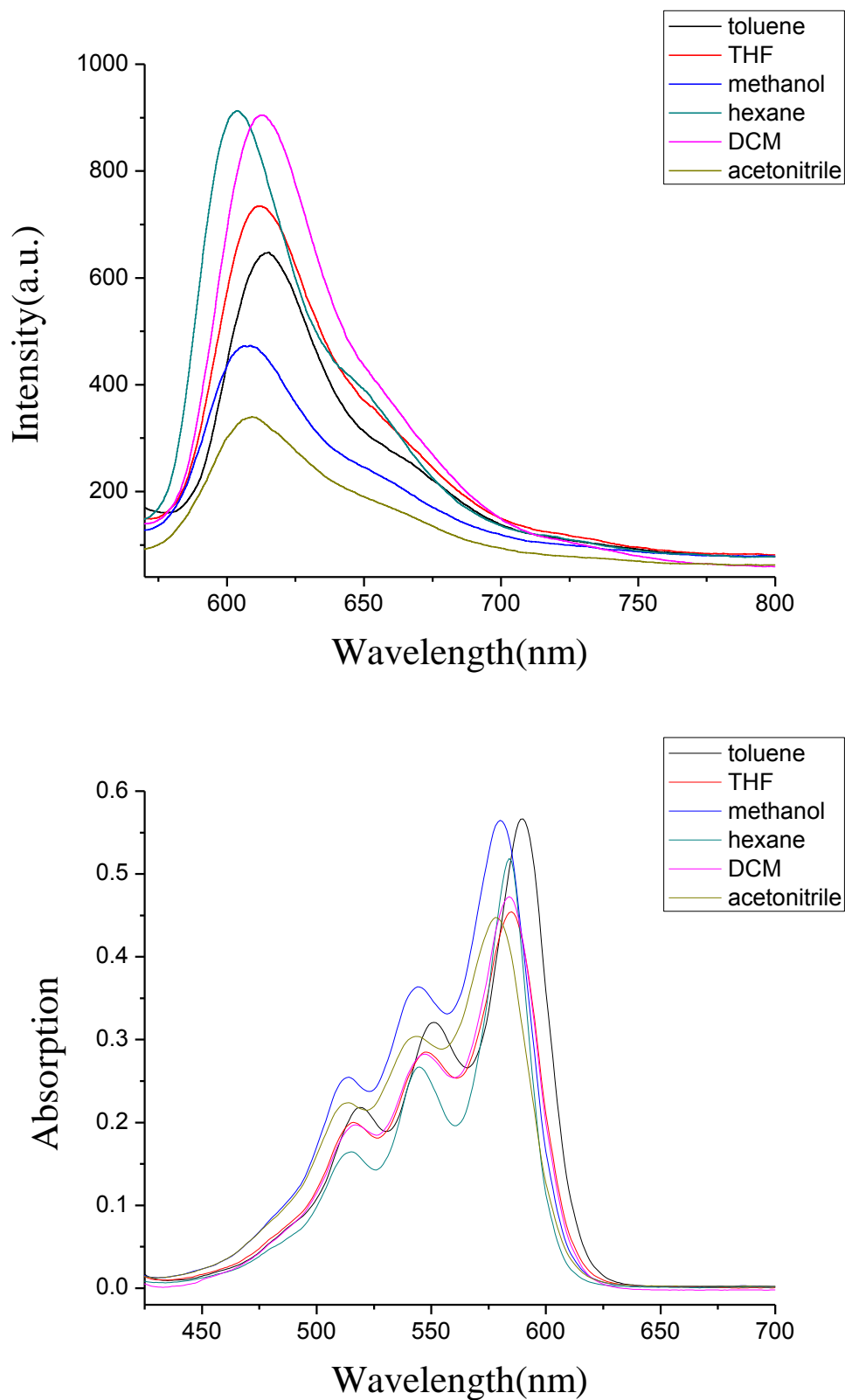
**Figure S25:** Absorption (top) and emission spectra (bottom) of BODIPY **1d** recorded in different solvents. Excited at 520 nm



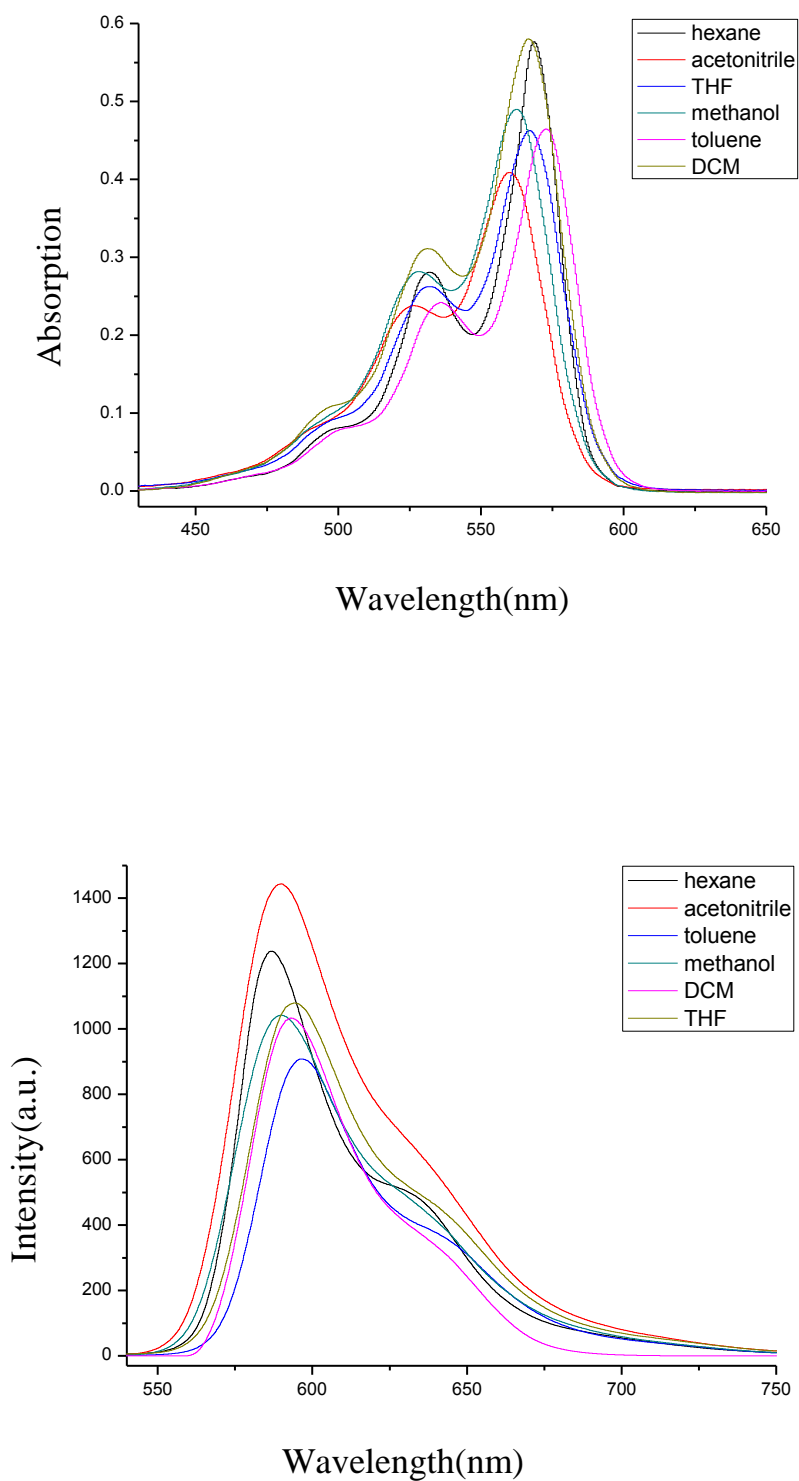
**Figure S26:** Absorption (top) and emission spectra (bottom) of BODIPY **1e** recorded in different solvents. Excited at 520 nm



**Figure S27:** Absorption (top) and emission spectra (bottom) of BODIPY **1f** recorded in different solvents. Excited at 520 nm

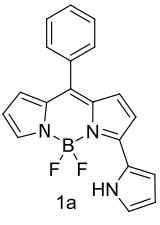
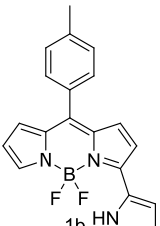
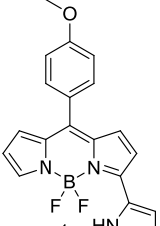
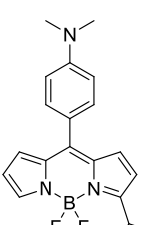
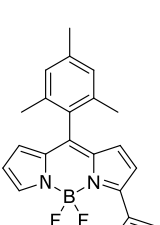


**Figure S28:** Absorption (top) and emission spectra (bottom) of BODIPY **1g** recorded in different solvents. Excited at 520 nm

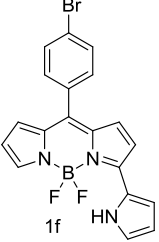
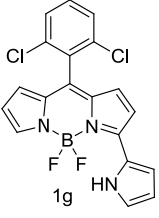
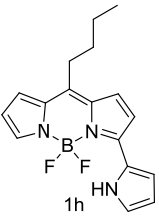


**Figure S29:** Absorption (top) and emission spectra (bottom) of BODIPY **1h** recorded in different solvents. Excited at 520 nm

**5. Table S1.** UV-vis and fluorescence properties of BODIPYs **1a-h** in various solvent at room temperature.

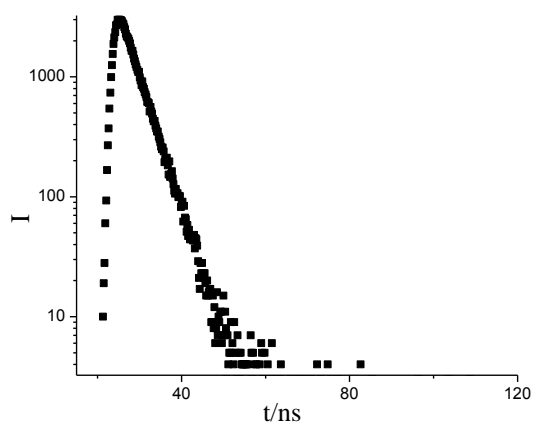
bodipys	solvent	$\lambda_{\text{abs}}$ (max)/nm	$\lambda_{\text{emiss}}$ (max)/nm	$\Phi^a$	Stokes Shift/ nm	Stokes Shift/cm <sup>-1</sup>
 1a	DCM <sup>b</sup>	576	609	0.24	33.4	952
	Toluene	581	612	0.29	30.4	856
	CH <sub>3</sub> CN	570	606	0.16	35.6	1031
	MeOH	573	604	0.16	31.2	901
	Hexane	576	601	0.26	25.0	722
	THF <sup>c</sup>	577	609	0.15	32.0	911
 1b	DCM	575	607	0.29	31.8	911
	Toluene	580	610	0.36	29.8	843
	CH <sub>3</sub> CN	570	605	0.23	34.8	1010
	MeOH	571	604	0.24	32.6	946
	Hexane	574	600	0.31	25.2	733
	THF	576	610	0.25	33.8	962
 1c	DCM	575	606	0.28	31.0	890
	Toluene	581	608	0.40	27.2	770
	CH <sub>3</sub> CN	570	604	0.18	34.2	993
	MeOH	572	602	0.23	29.8	866
	Hexane	575	597	0.30	22.0	641
	THF	577	607	0.32	30.2	862
 1d	DCM	585	636	0.05	50.8	1366
	Toluene	586	618	0.23	32.4	894
	CH <sub>3</sub> CN	581	622	0.01	40.8	1129
	MeOH	580	619	0.01	39.2	1092
	Hexane	577	602	0.26	24.8	714
	THF	584	620	0.02	36.0	994
 1e	DCM	573	600	0.60	26.6	774
	Toluene	579	602	0.57	23.0	660
	CH <sub>3</sub> CN	568	598	0.50	30.0	883
	MeOH	570	596	0.56	26.0	765
	Hexane	573	598	0.50	25.0	730
	THF	575	601	0.57	26.2	758



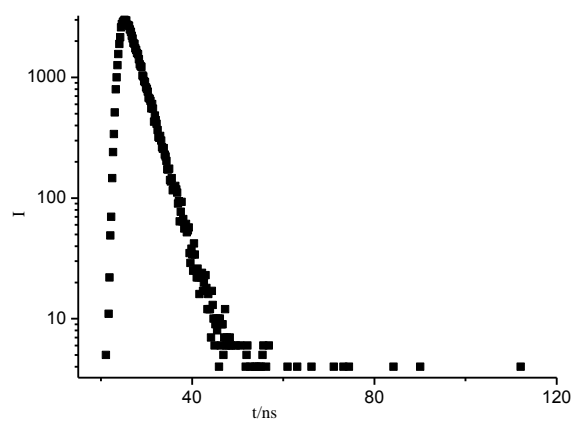
 1f	DCM	578	612	0.27	34.2	967
	Toluene	584	615	0.36	30.8	858
	CH <sub>3</sub> CN	572	609	0.21	36.8	1057
	MeOH	575	609	0.20	34.4	982
	Hexane	578	606	0.28	28.0	799
	THF	579	613	0.28	34.0	958
 1g	DCM	584	612	0.56	28.2	789
	Toluene	590	615	0.57	25.2	694
	CH <sub>3</sub> CN	578	609	0.35	31.0	881
	MeOH	580	608	0.33	28.2	799
	Hexane	584	604	0.68	19.6	556
	THF	585	612	0.55	17.2	480
 1h	DCM	567	593	0.34	26.0	773
	Toluene	573	597	0.45	23.4	685
	CH <sub>3</sub> CN	560	582	0.34	21.8	669
	MeOH	563	590	0.45	27.0	813
	Hexane	569	587	0.47	17.4	522
	THF	568	594	0.35	26.5	786

<sup>a</sup>the fluorescence quantum yields were calculated using Rhodamine B (0.49 in ethanol) as the reference. <sup>b</sup>Dichloromethane. <sup>c</sup>tetrahydrofuran.

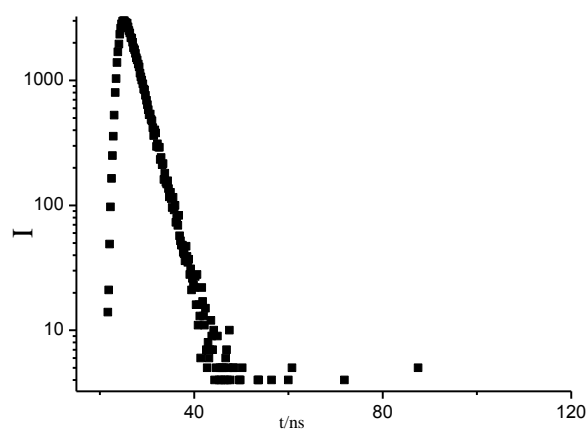
## 6. Experimental Fluorescence Decay Curve



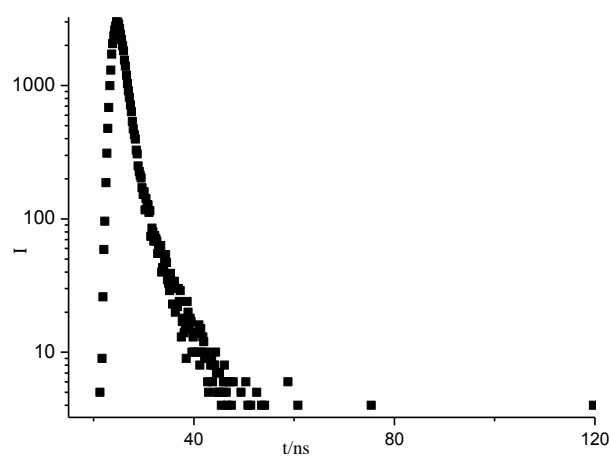
**Figure S30:** Experimental fluorescence decay Curve of BODIPYs **1a** in nondegassed DCM.



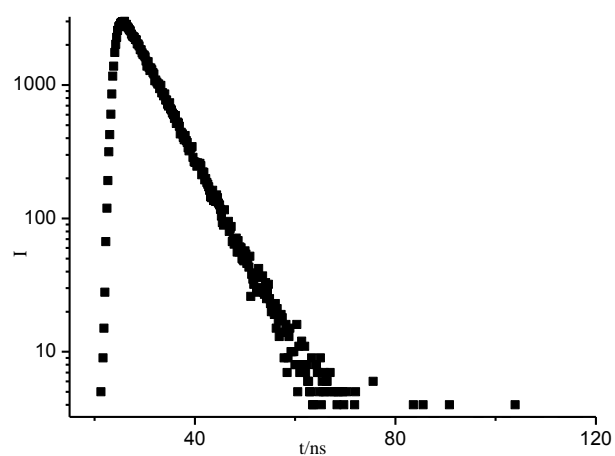
**Figure S31:** Experimental fluorescence decay Curve of BODIPYs **1b** in nondegassed DCM.



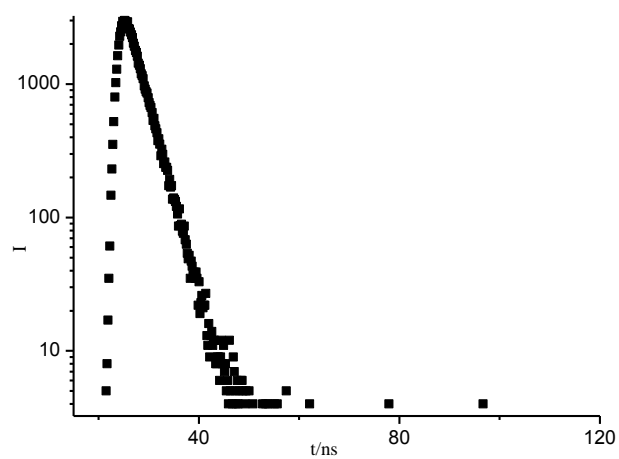
**Figure S32:** Experimental fluorescence decay Curve of BODIPYs **1c** in nondegassed DCM.



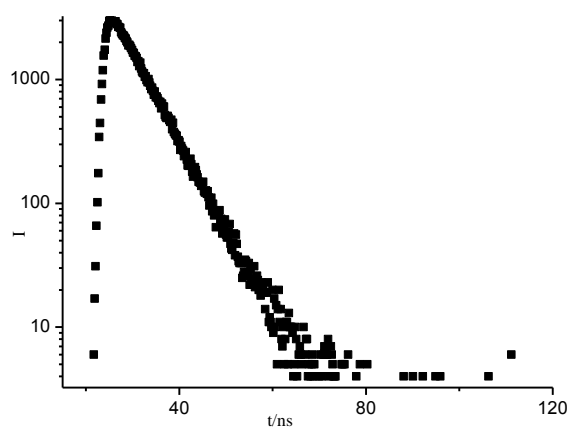
**Figure S33:** Experimental fluorescence decay Curve of BODIPYs **1d** in nondegassed DCM.



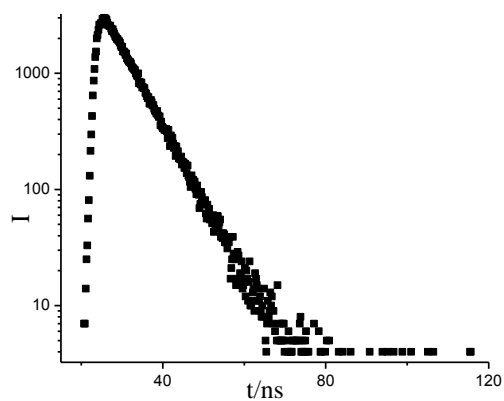
**Figure S34:** Experimental fluorescence decay Curve of BODIPYs **1e** in nondegassed DCM.



**Figure S35:** Experimental fluorescence decay Curve of BODIPYs **1f** in nondegassed DCM.



**Figure S36:** Experimental fluorescence decay Curve of BODIPYs **1g** in nondegassed DCM.



**Figure S37:** Experimental fluorescence decay Curve of BODIPYs **1h** in nondegassed DCM.