

# Supplementary Materials

**Table S1.** Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

<b>S1A—C37A</b>	1.748 (6)	O2—C27	1.220 (3)
<b>S1A—O7A</b>	1.518 (3)	O3—C26	1.225 (3)
<b>S1A—C36A</b>	1.769 (3)	O4—N3	1.222 (3)
<b>S2—O6</b>	1.471 (2)	O5—N3	1.216 (3)
<b>S2—C35</b>	1.735 (5)	N1—C8	1.366 (3)
<b>S2—C34</b>	1.727 (6)	N1—C1	1.385 (3)
<b>S1B—C36B</b>	1.75 (3)	N2—C7	1.473 (3)
<b>S1B—C37B</b>	1.68 (3)	N2—C11	1.459 (3)
<b>S1B—O7B</b>	1.49 (3)	N3—C4	1.456 (3)
<b>O1—C8</b>	1.216 (3)		
<b>C36A—S1A—C37A</b>	99.2 (2)	N1—C1—C2	128.3 (2)
<b>O7A—S1A—C37A</b>	104.8 (2)	N3—C4—C5	118.7 (2)
<b>O7A—S1A—C36A</b>	107.06 (17)	N3—C4—C3	118.1 (2)
<b>O6—S2—C35</b>	110.2 (2)	N2—C7—C8	107.08 (17)
<b>C34—S2—C35</b>	97.3 (3)	N2—C7—C6	112.92 (17)
<b>O6—S2—C34</b>	107.1 (3)	N2—C7—C9	103.96 (16)
<b>C36B—S1B—C37B</b>	108.4 (19)	N1—C8—C7	107.15 (18)
<b>O7B—S1B—C36B</b>	110.9 (17)	O1—C8—N1	125.5 (2)
<b>O7B—S1B—C37B</b>	117 (2)	O1—C8—C7	127.2 (2)
<b>C1—N1—C8</b>	112.46 (18)	N2—C11—C12	112.29 (18)
<b>C7—N2—C11</b>	105.40 (17)	N2—C11—C10	107.19 (16)
<b>O4—N3—C4</b>	118.7 (2)	O3—C26—C10	125.82 (19)
<b>O4—N3—O5</b>	122.7 (2)	O3—C26—C25	126.1 (2)
<b>O5—N3—C4</b>	118.5 (2)	O2—C27—C28	120.8 (2)
<b>N1—C1—C6</b>	109.51 (19)	O2—C27—C9	121.1 (2)

**Table S2.** Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<b>D—H<math>\cdots</math>A</b>	<b>D—H</b>	<b>H<math>\cdots</math>A</b>	<b>D<math>\cdots</math>A</b>	<b>D—H<math>\cdots</math>A</b>
<b>N1—H1N1<math>\cdots</math>O7A<sup>i</sup></b>	0.84 (3)	1.97 (3)	2.779 (3)	162 (3)
<b>N2—H1N2<math>\cdots</math>O3<sup>ii</sup></b>	0.86 (3)	2.26 (3)	3.120 (2)	176 (2)
<b>C3—H3A<math>\cdots</math>O2<sup>iii</sup></b>	0.9300	2.6000	3.235 (3)	126.00
<b>C9—H9A<math>\cdots</math>O3</b>	0.9800	2.4800	2.992 (3)	112.00
<b>C11—H11A<math>\cdots</math>O1</b>	0.9800	2.5000	3.083 (3)	118.00
<b>C12—H12B<math>\cdots</math>O5<sup>ii</sup></b>	0.9700	2.4800	3.247 (3)	136.00
<b>C20—H20A<math>\cdots</math>O1</b>	0.9300	2.4300	3.241 (3)	145.00
<b>C25—H25A<math>\cdots</math>O6<sup>iv</sup></b>	0.9300	1.9000	2.800 (3)	161.00
<b>C31—H31A<math>\cdots</math>O7A<sup>v</sup></b>	0.9300	2.4900	3.364 (4)	156.00
<b>C37A—H37C<math>\cdots</math>O4<sup>vi</sup></b>	0.9600	2.4300	3.202 (6)	138.00

Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $-x+1, -y+1, -z$ ; (iii)  $-x+2, -y+1, -z$ ; (iv)  $x, y, z-1$ ; (v)  $x+1/2, -y+1/2, z-1/2$ ; (vi)  $x-1/2, -y+3/2, z+1/2$ .

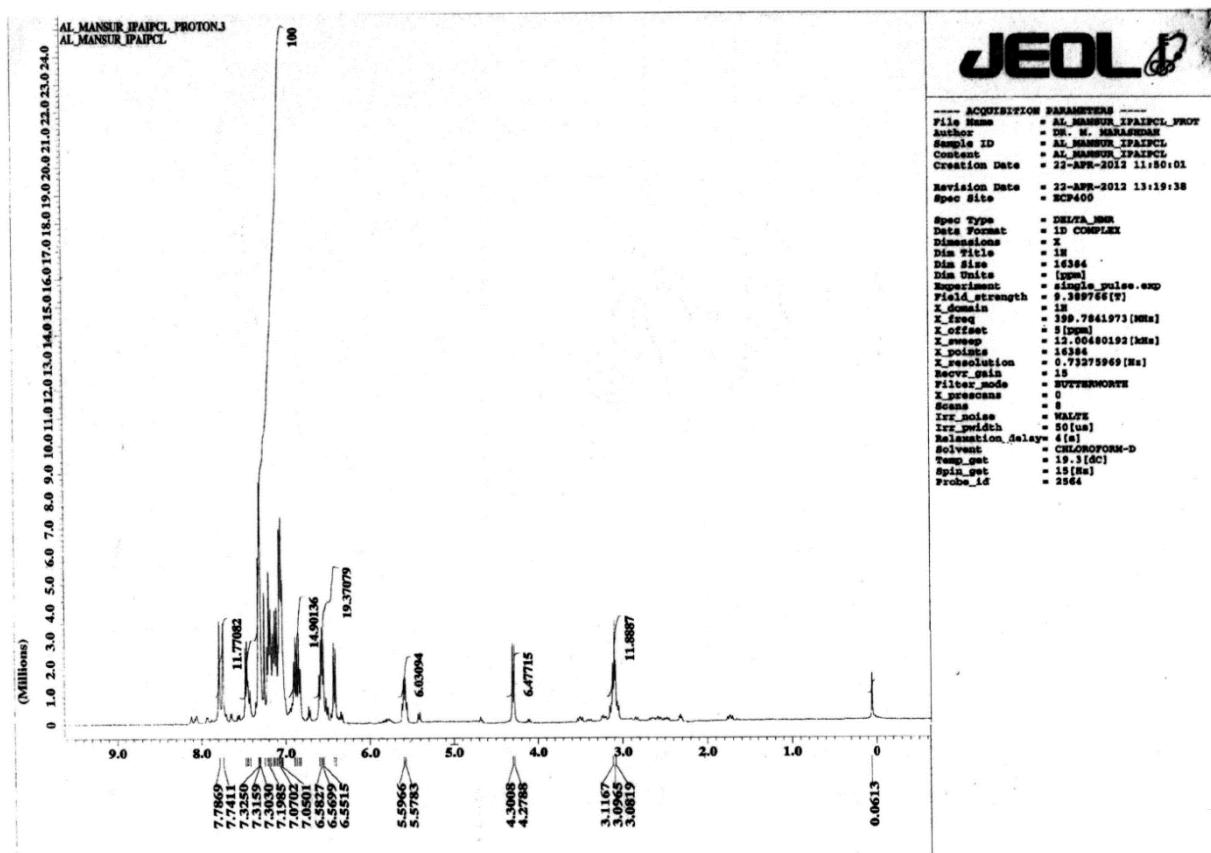


Figure S1.  $^1\text{H}$ -NMR spectrum of **5a**.

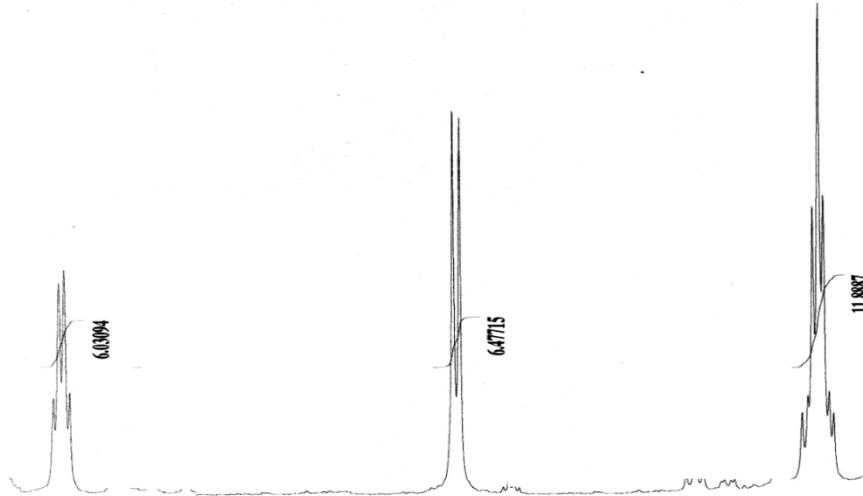


Figure S2. Expanded  $^1\text{H}$ -NMR spectrum of **5a**.

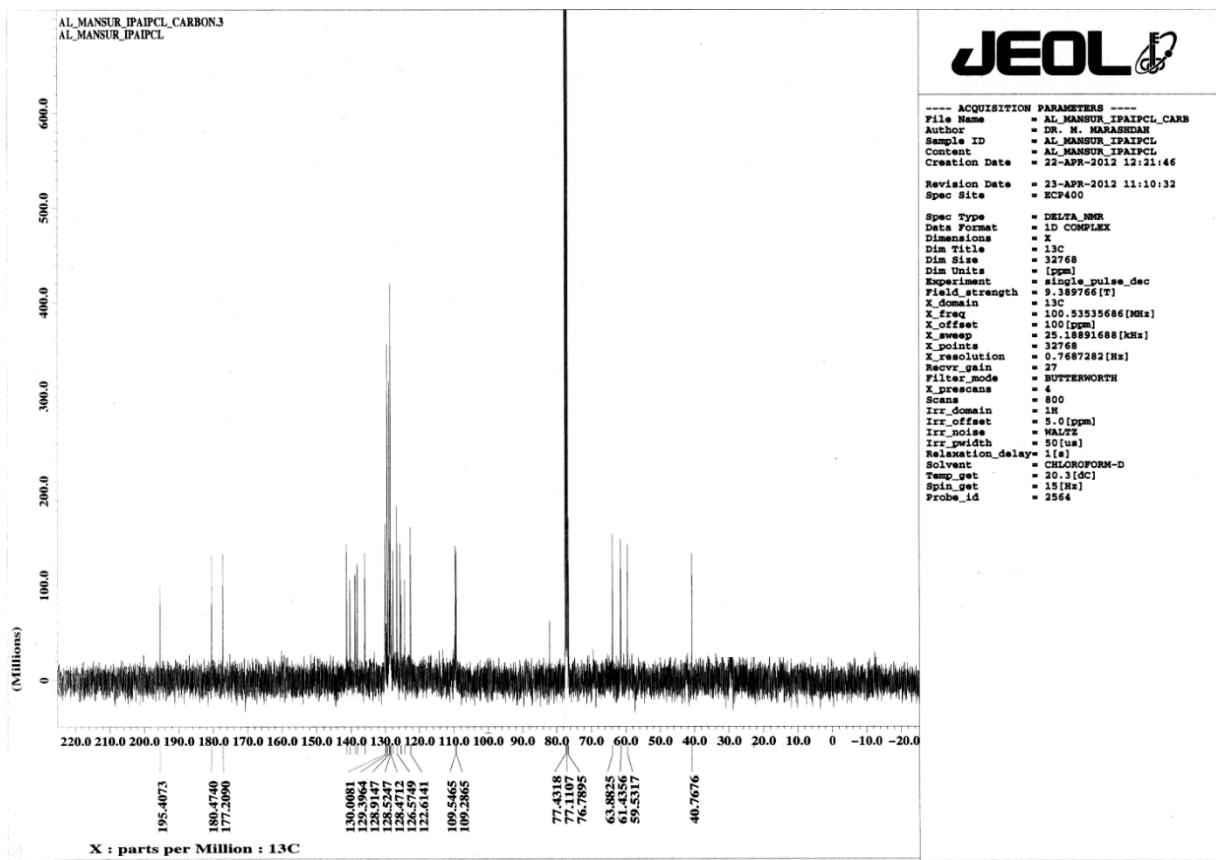
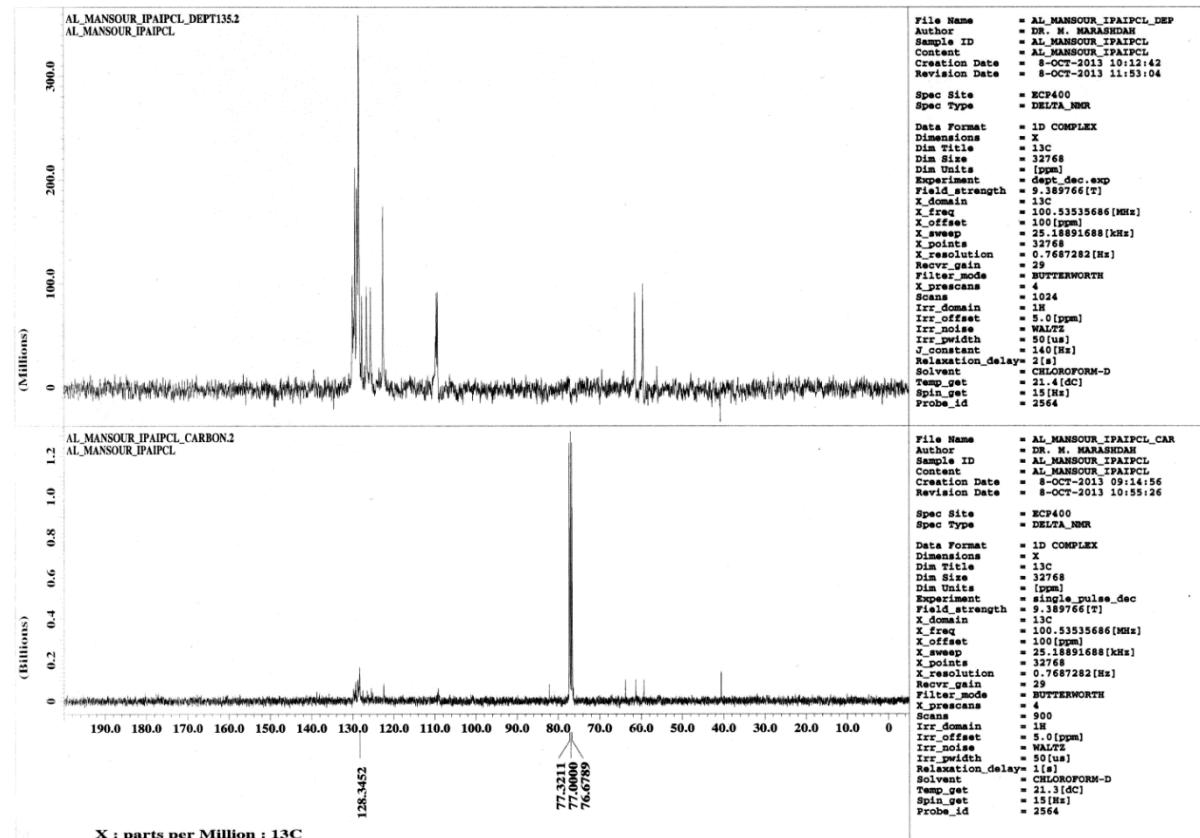
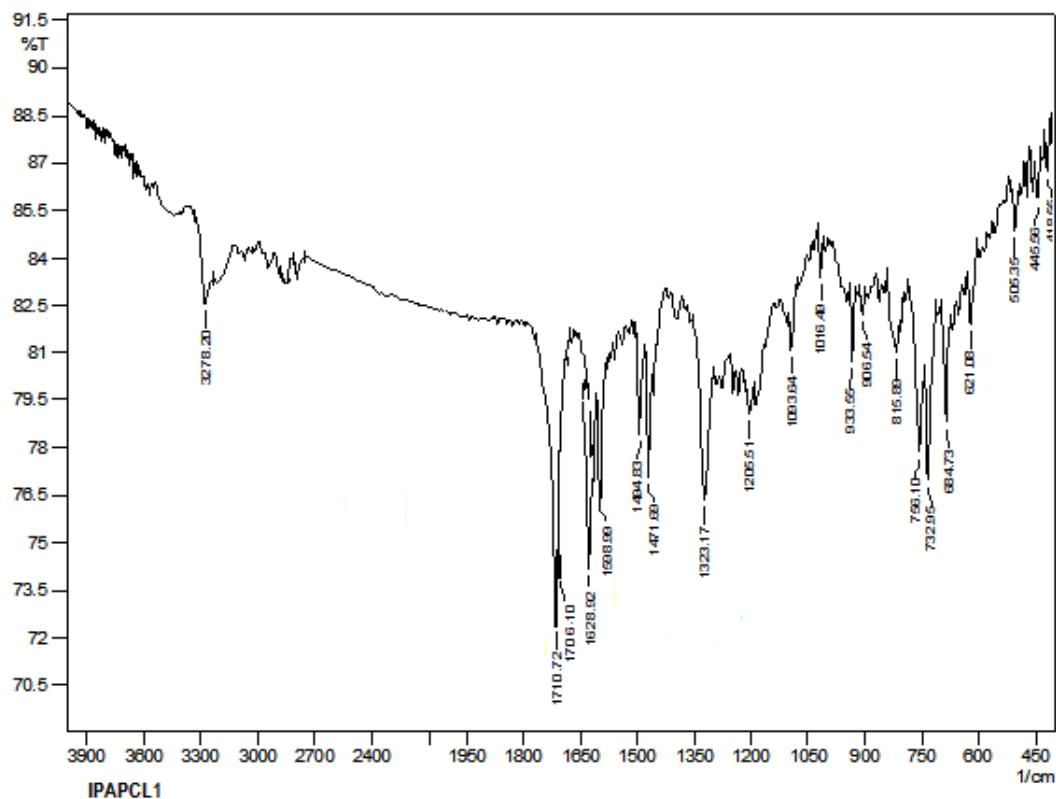
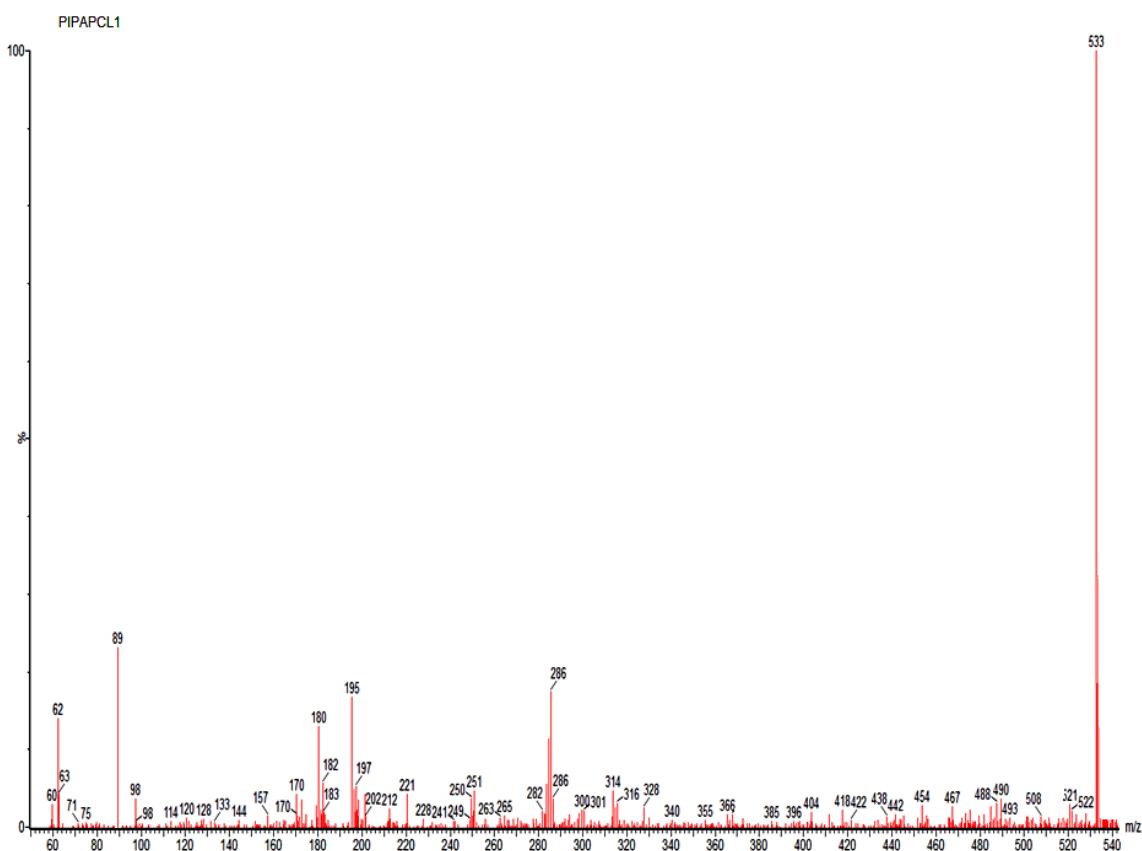
Figure S3.  $^{13}\text{C}$ -NMR spectrum of 5a.

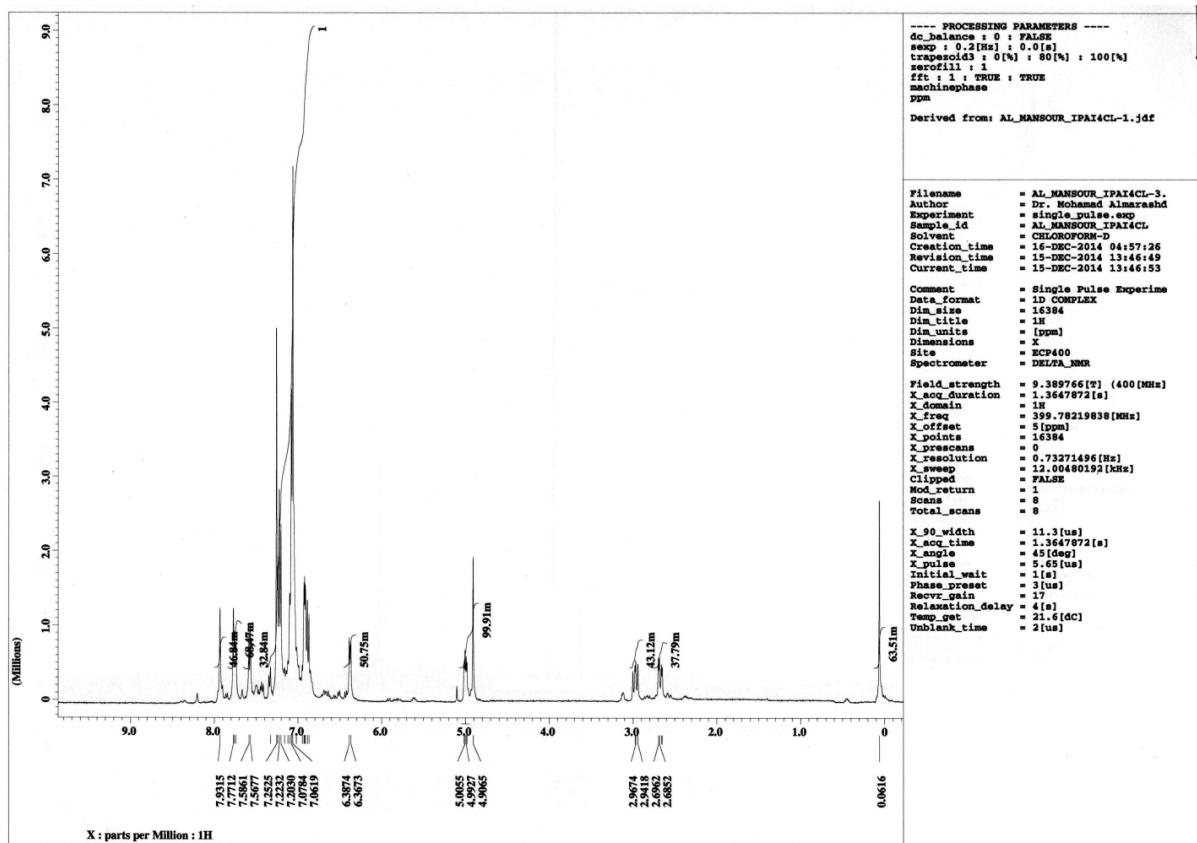
Figure S4. DEPT-135 spectrum of 5a.



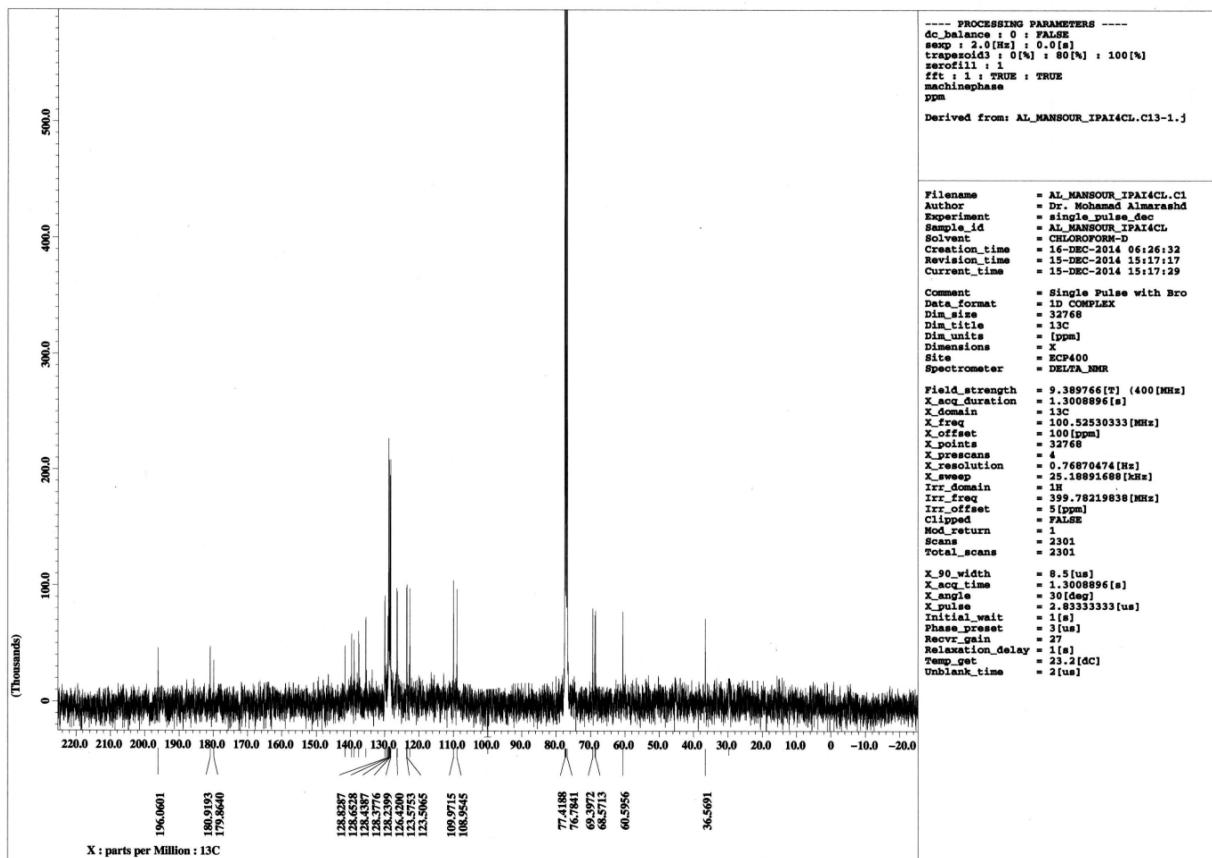
**Figure S5.** IR spectrum of **5a**.



**Figure S6.** Mass spectrum of **5a**.



**Figure S7.**  $^1\text{H}$ -NMR spectrum of **6a**.



**Figure S8.**  $^{13}\text{C}$ -NMR spectrum of **6a**.

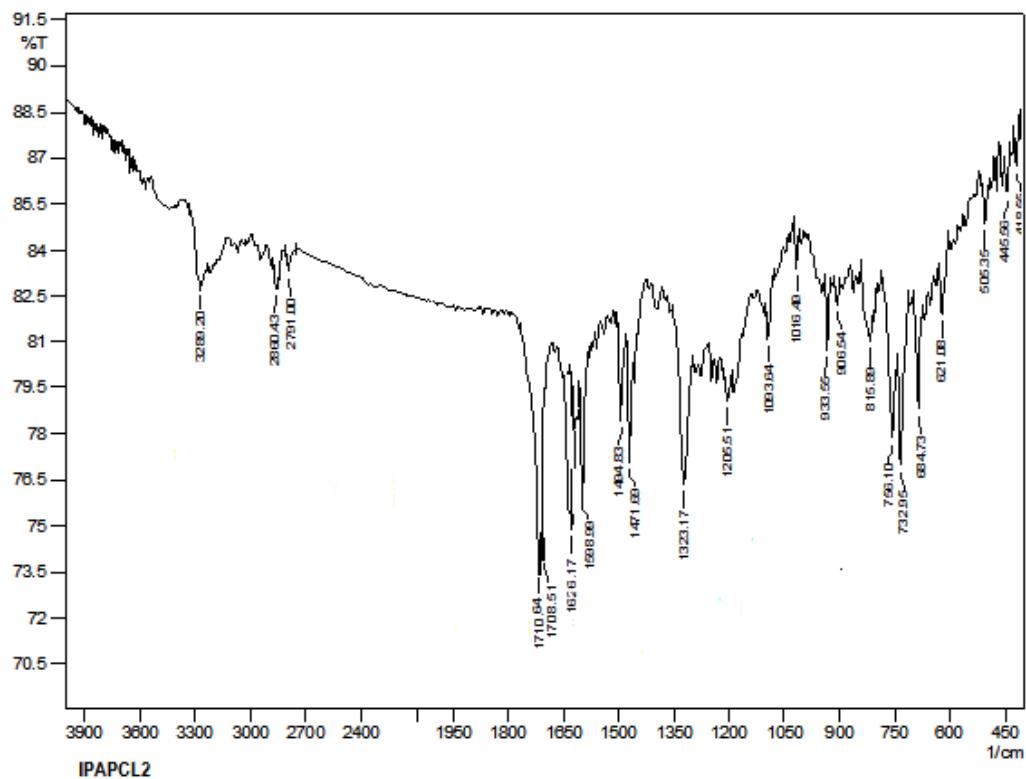


Figure S9. IR spectrum of 6a.

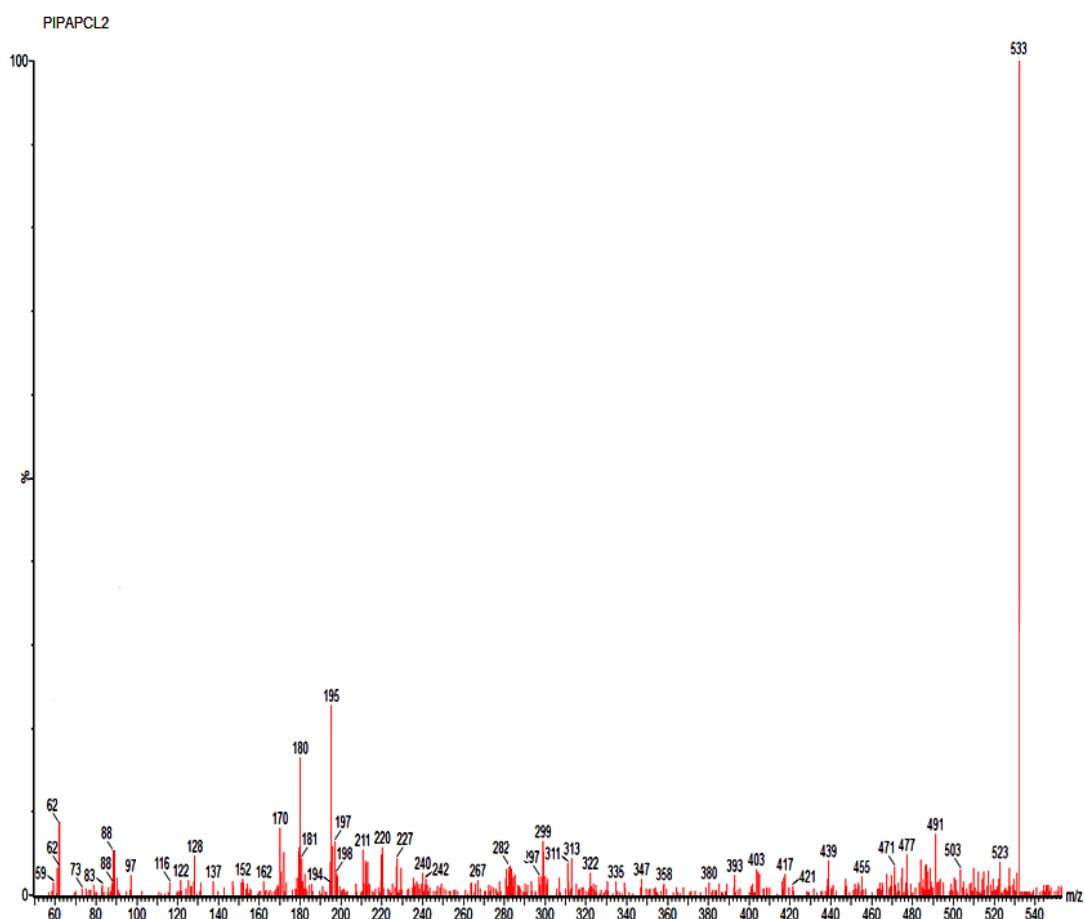
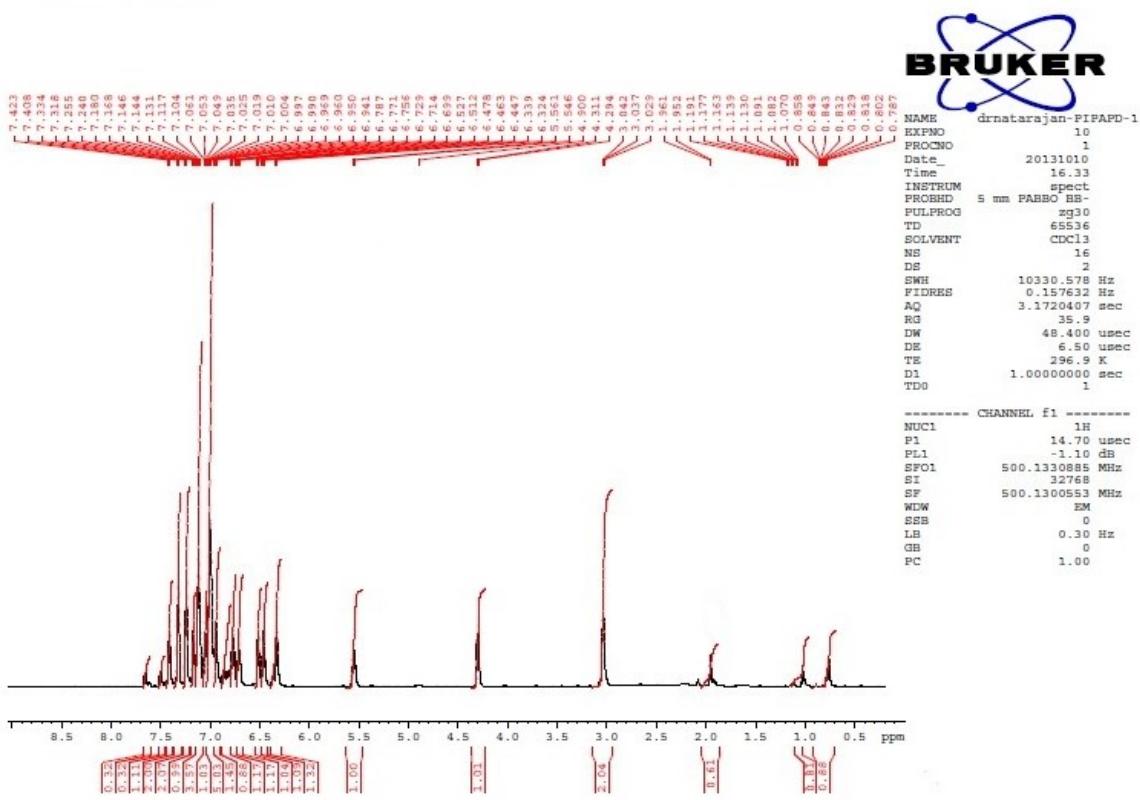


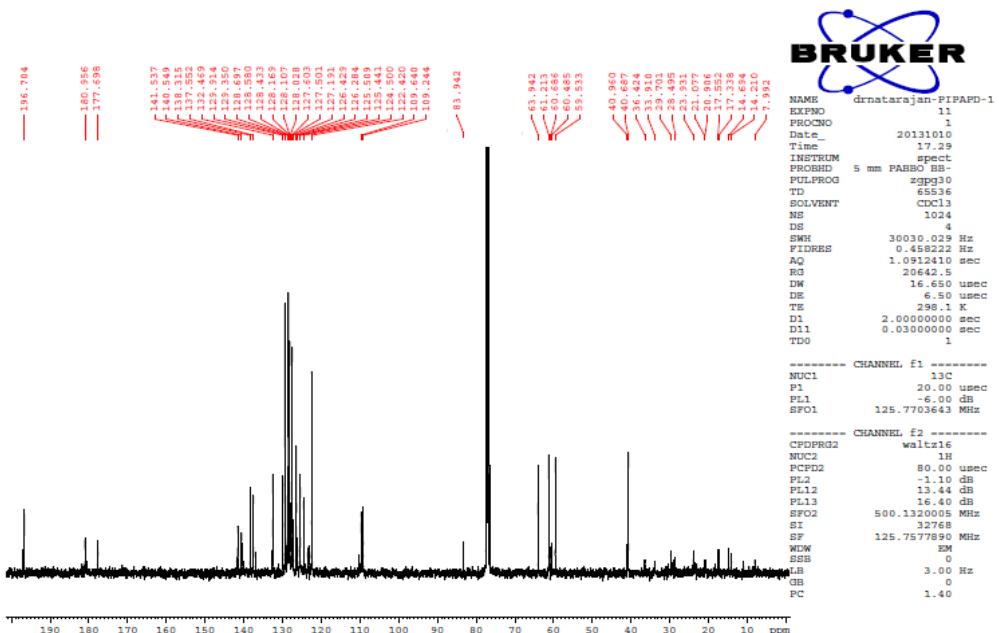
Figure S10. Mass spectrum of 6a.

N-BBO CDC13 D:\

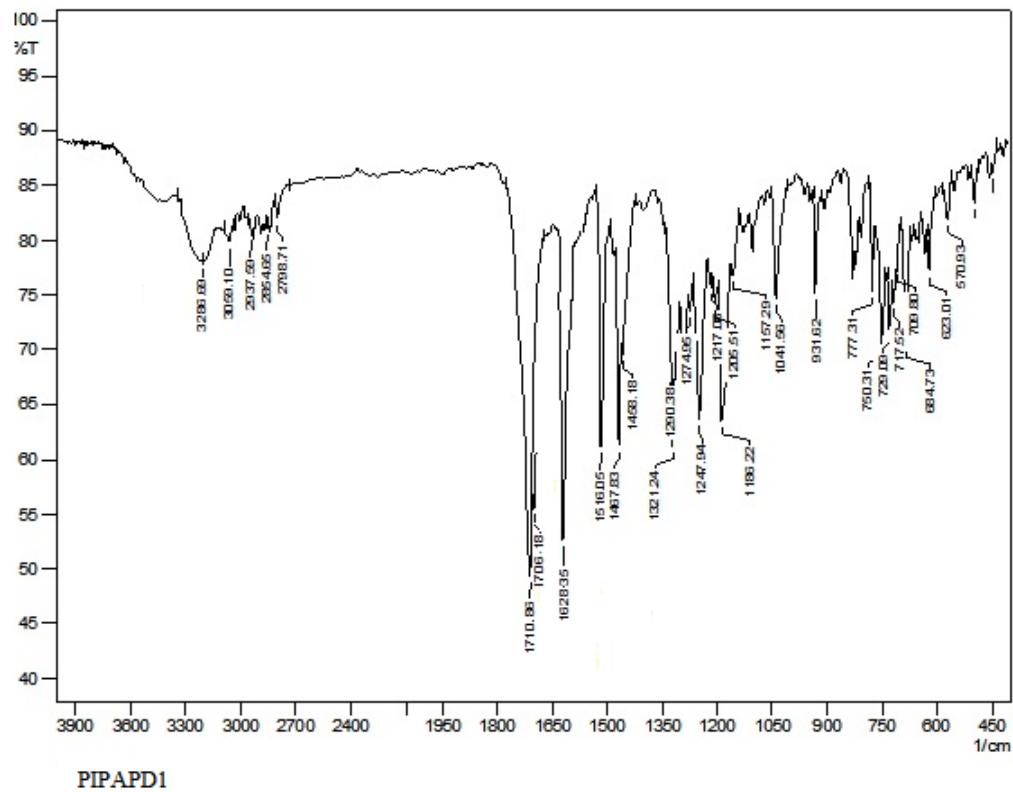


**Figure S11.**  $^1\text{H}$ -NMR spectrum of **5b**.

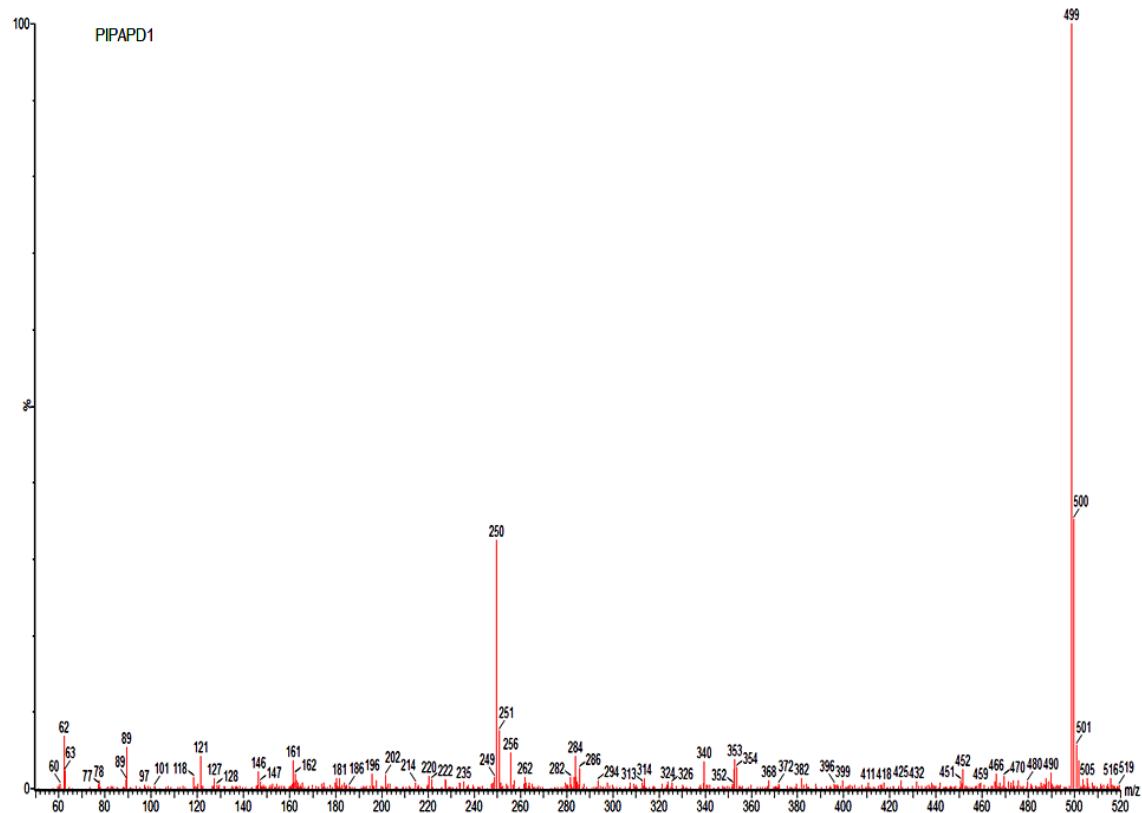
BBO CDC13 D:\\ al

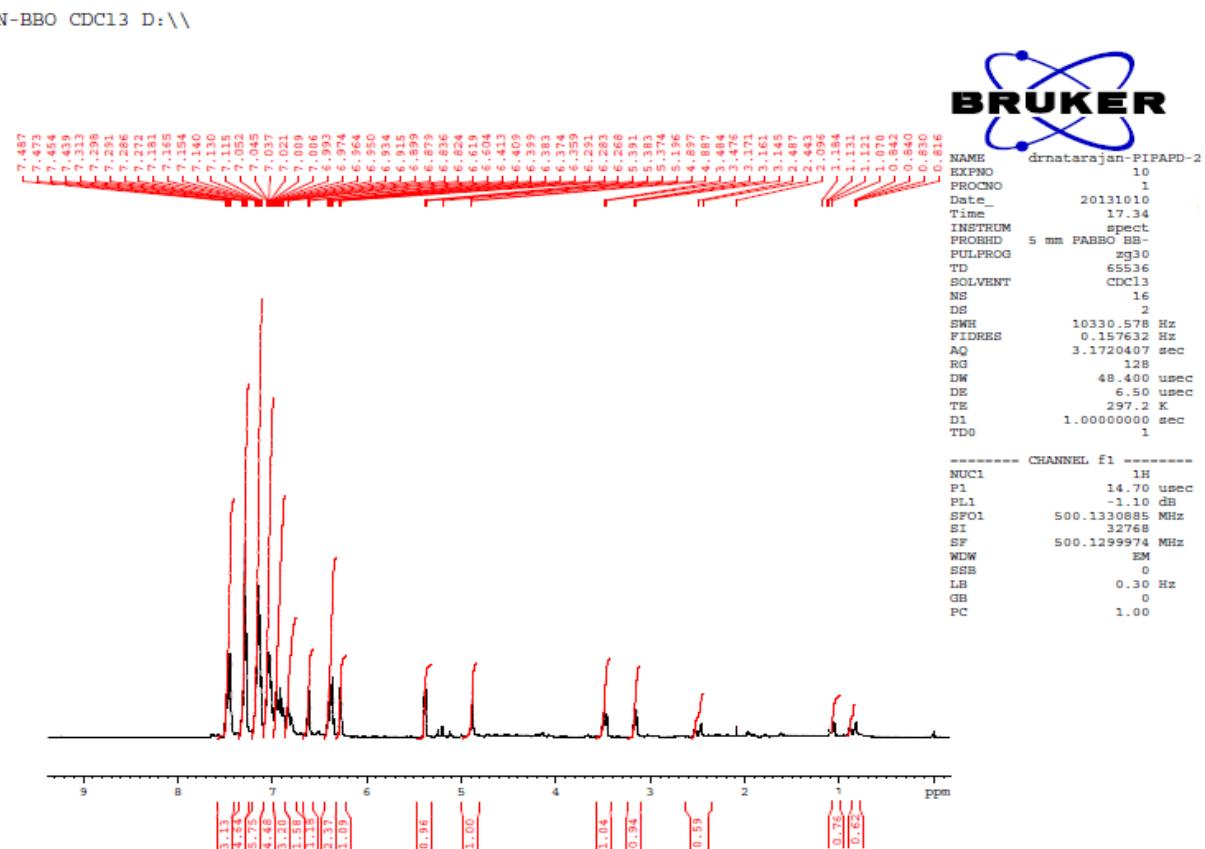


**Figure S12.**  $^{13}\text{C}$ -NMR spectrum of **5b**.

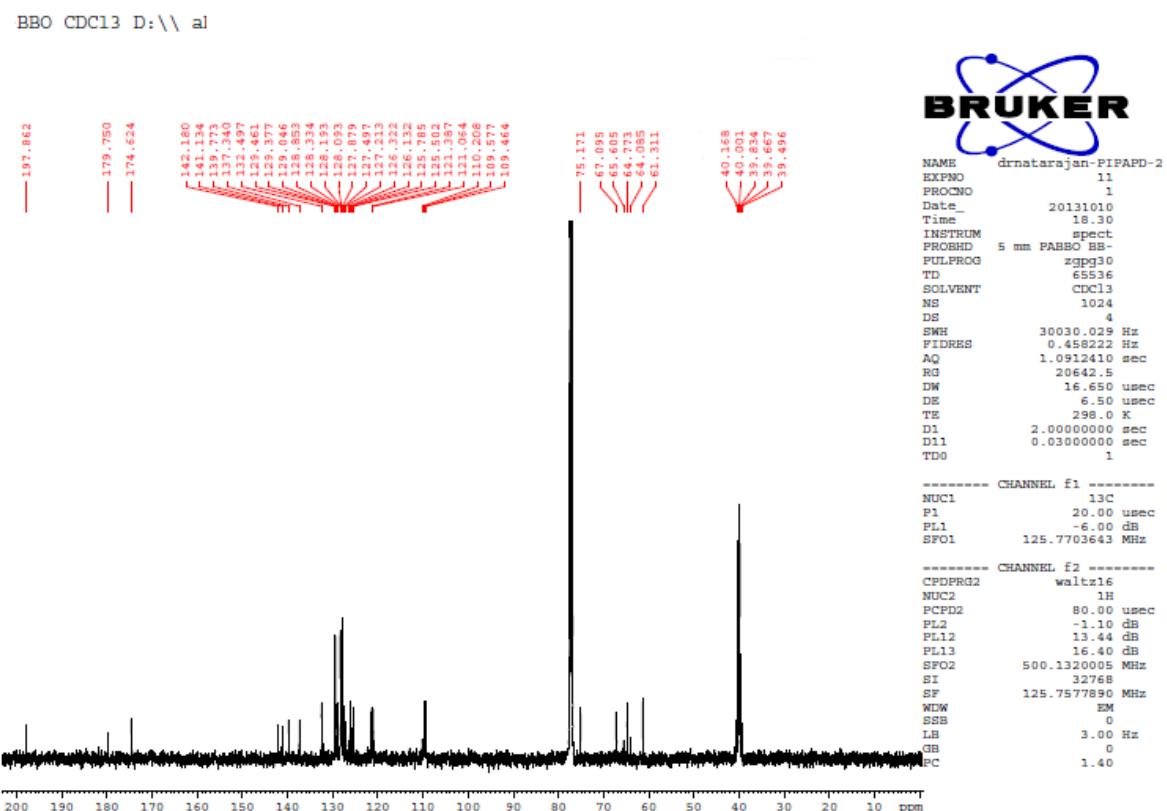


PIPAPD1

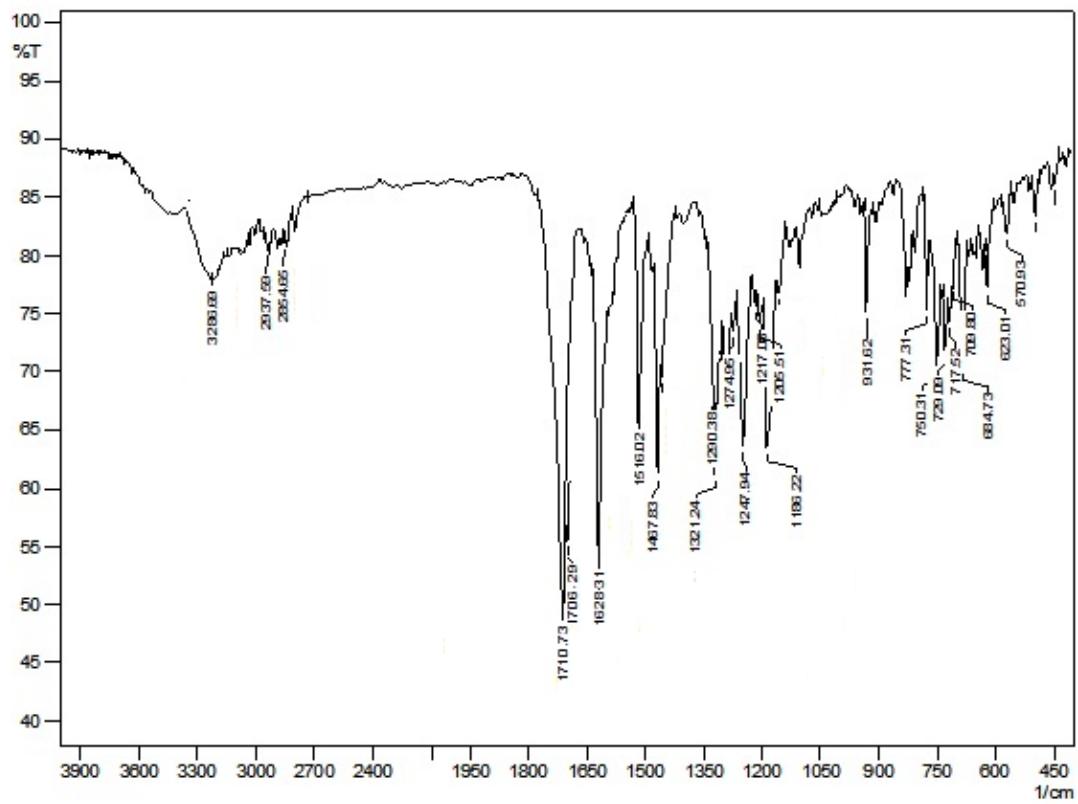
**Figure S13.** IR spectrum of **5b**.**Figure S14.** Mass spectrum of **5b**.



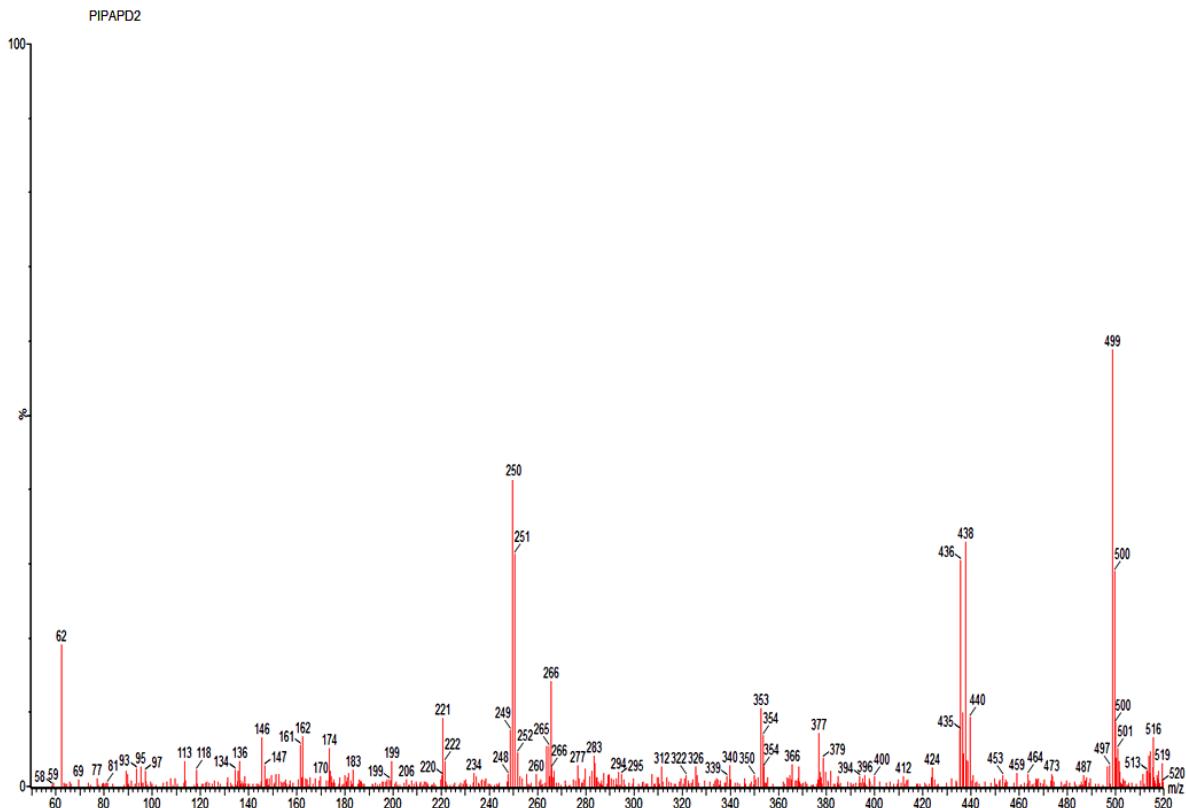
**Figure S15.**  $^1\text{H}$ -NMR spectrum of **6b**.

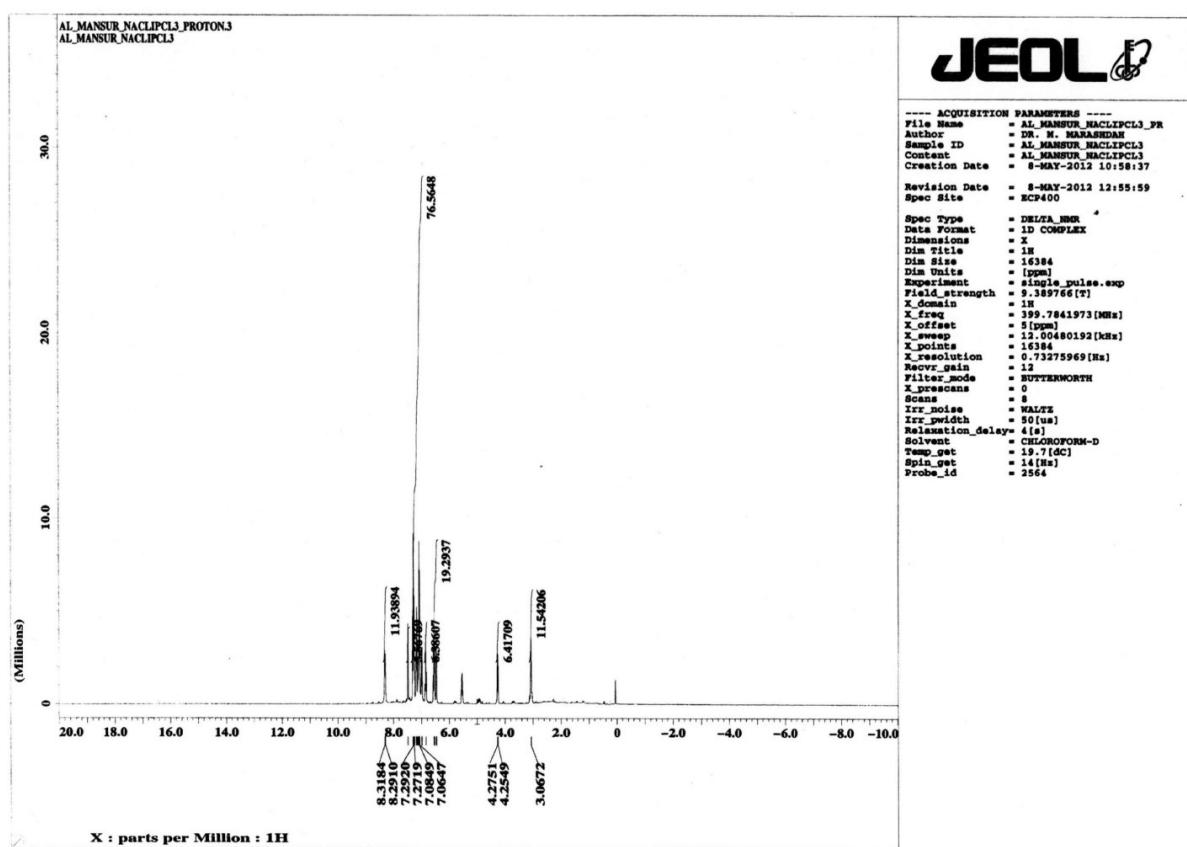
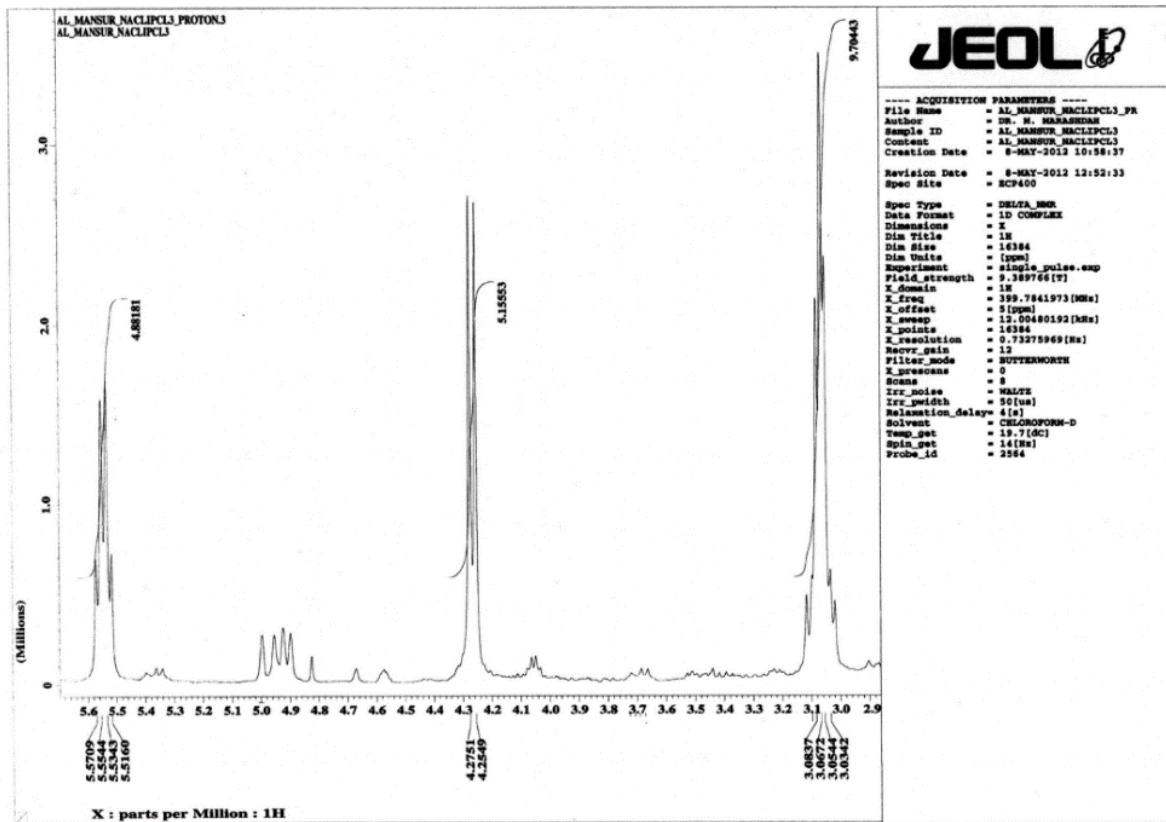


**Figure S16.**  $^{13}\text{C}$ -NMR spectrum of **6b**.



PIPAPD2

**Figure S17.** IR spectrum of **6b**.

Figure S19.  $^1\text{H}$ -NMR spectrum of 5c.Figure S20. Expanded  $^1\text{H}$ -NMR spectrum of 5c.

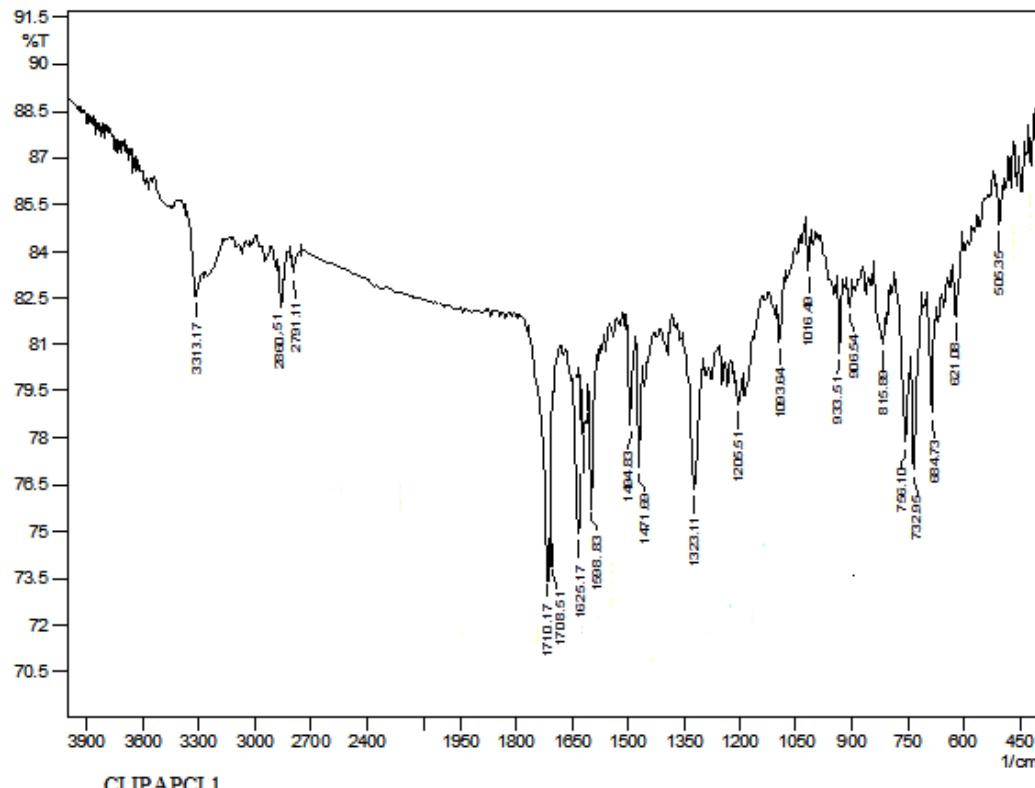
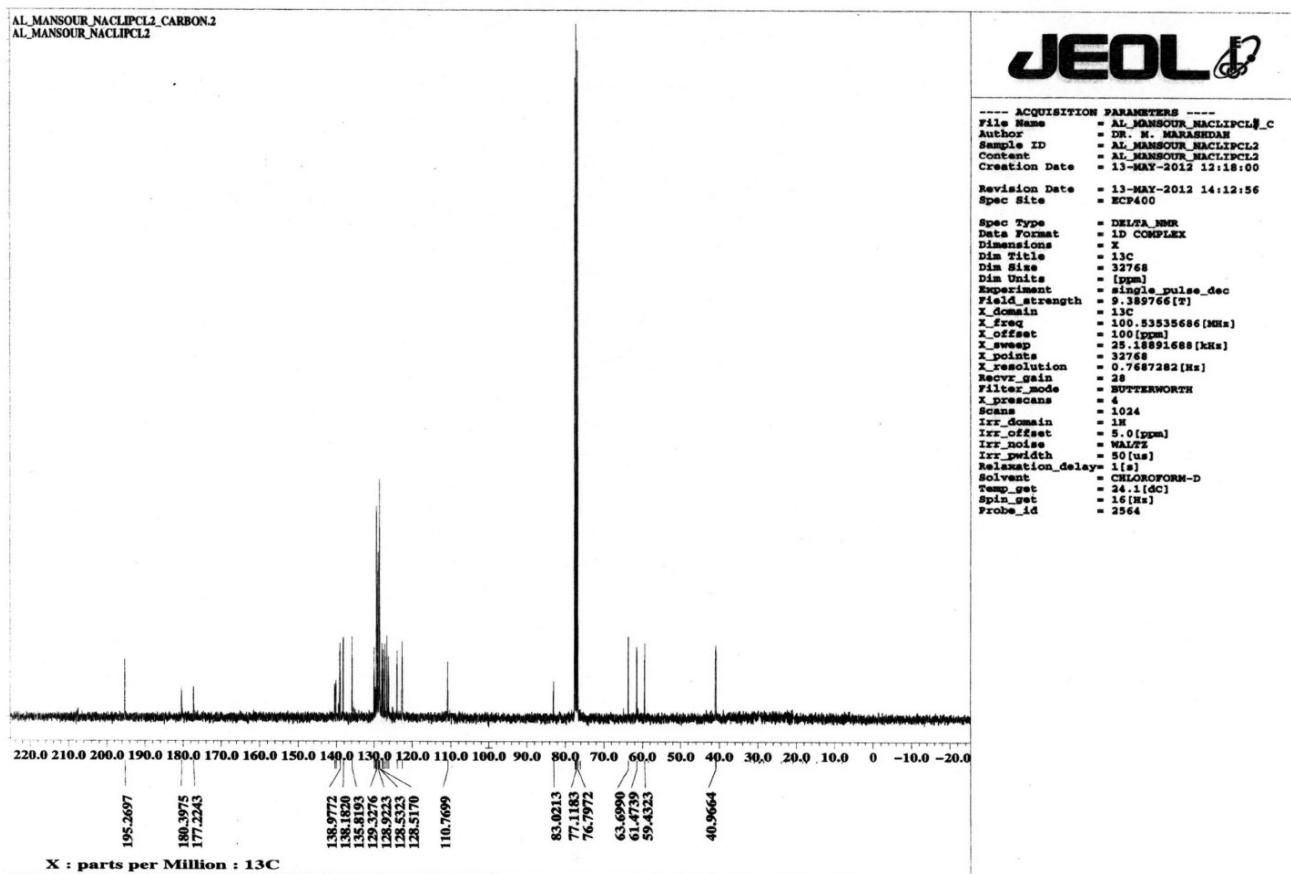


Figure S22. IR spectrum of **5c**.

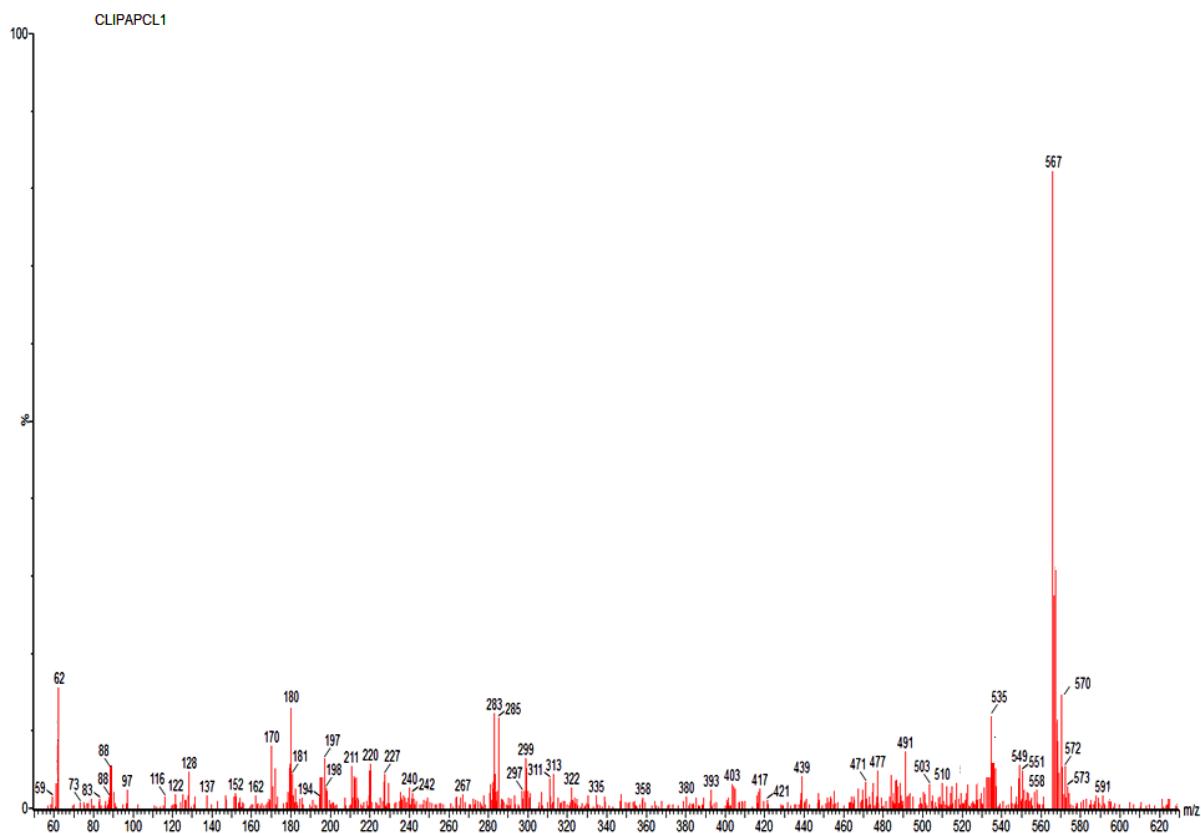
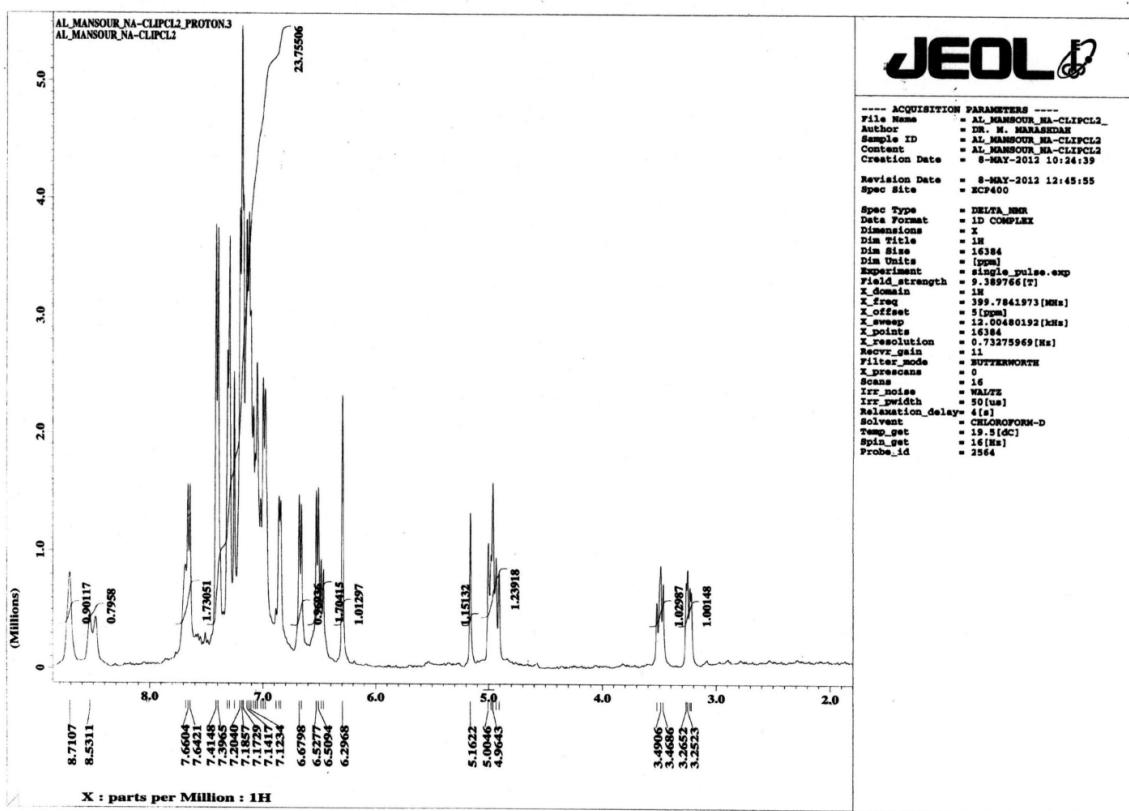


Figure S23. Mass spectrum of 5c.

Figure S24.  $^1\text{H}$ -NMR spectrum of 6c.

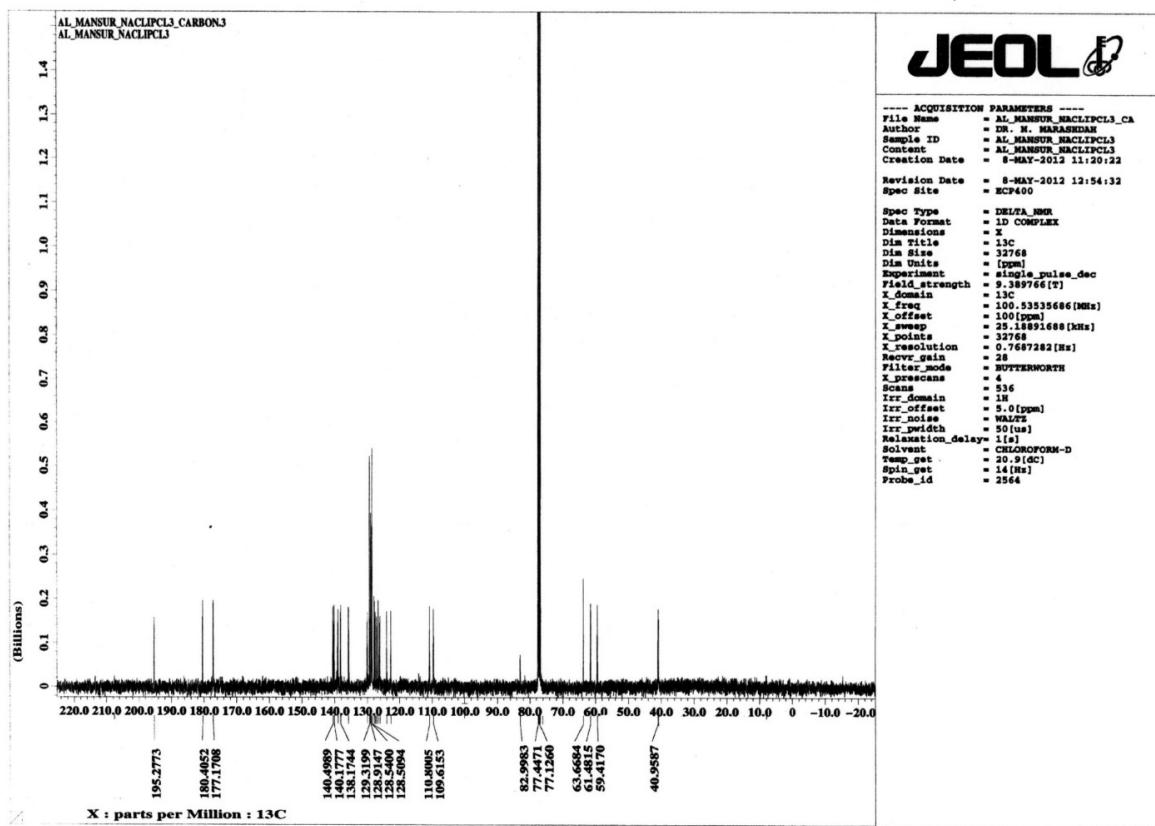


Figure S25.  $^{13}\text{C}$ -NMR spectrum of **6c**.

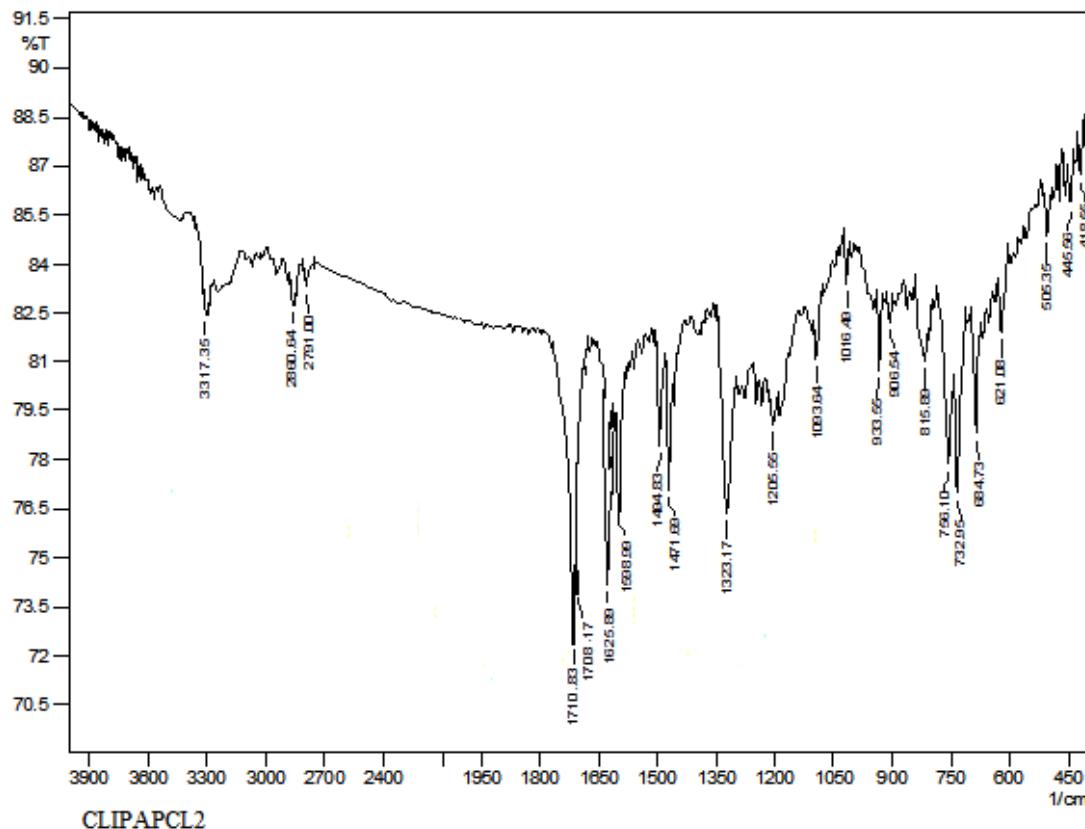
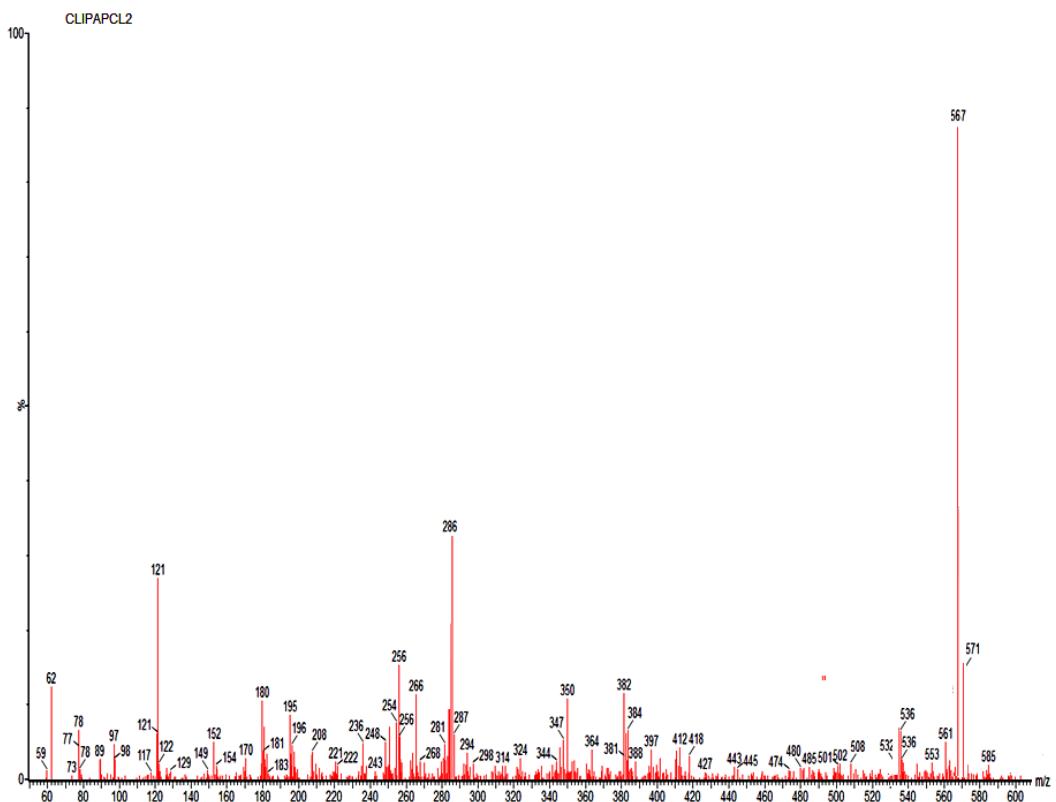
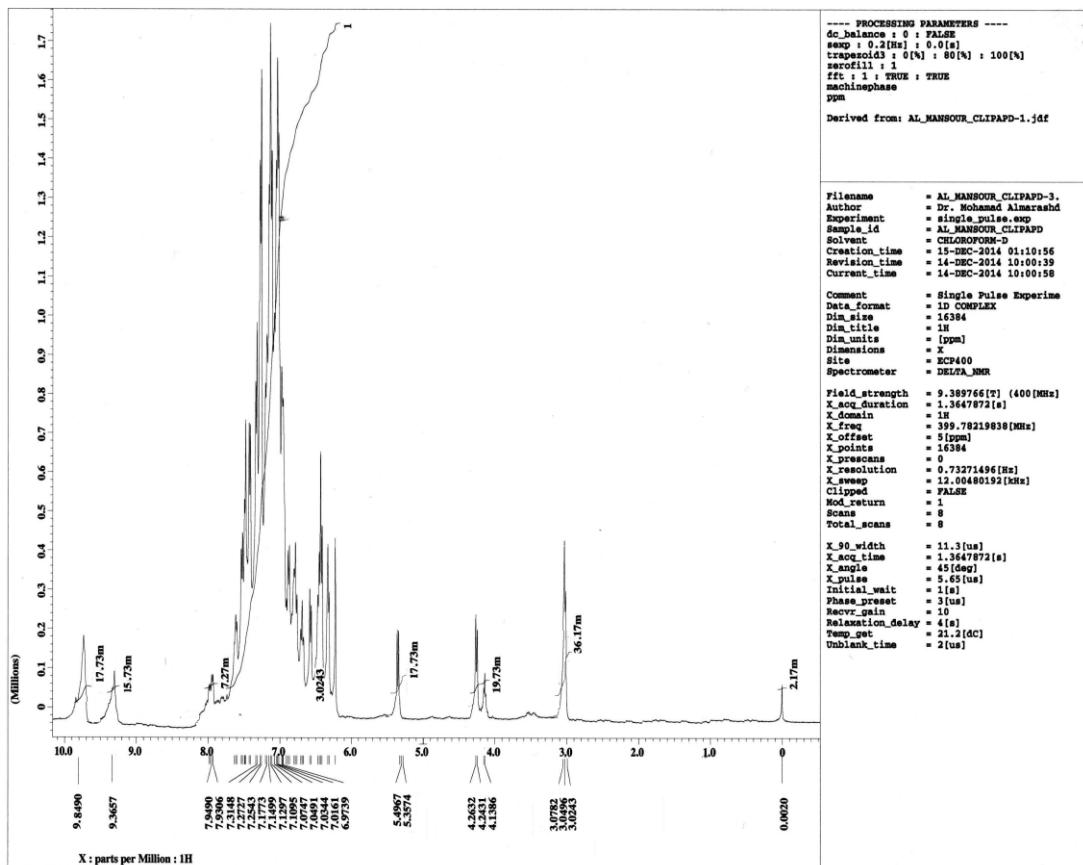


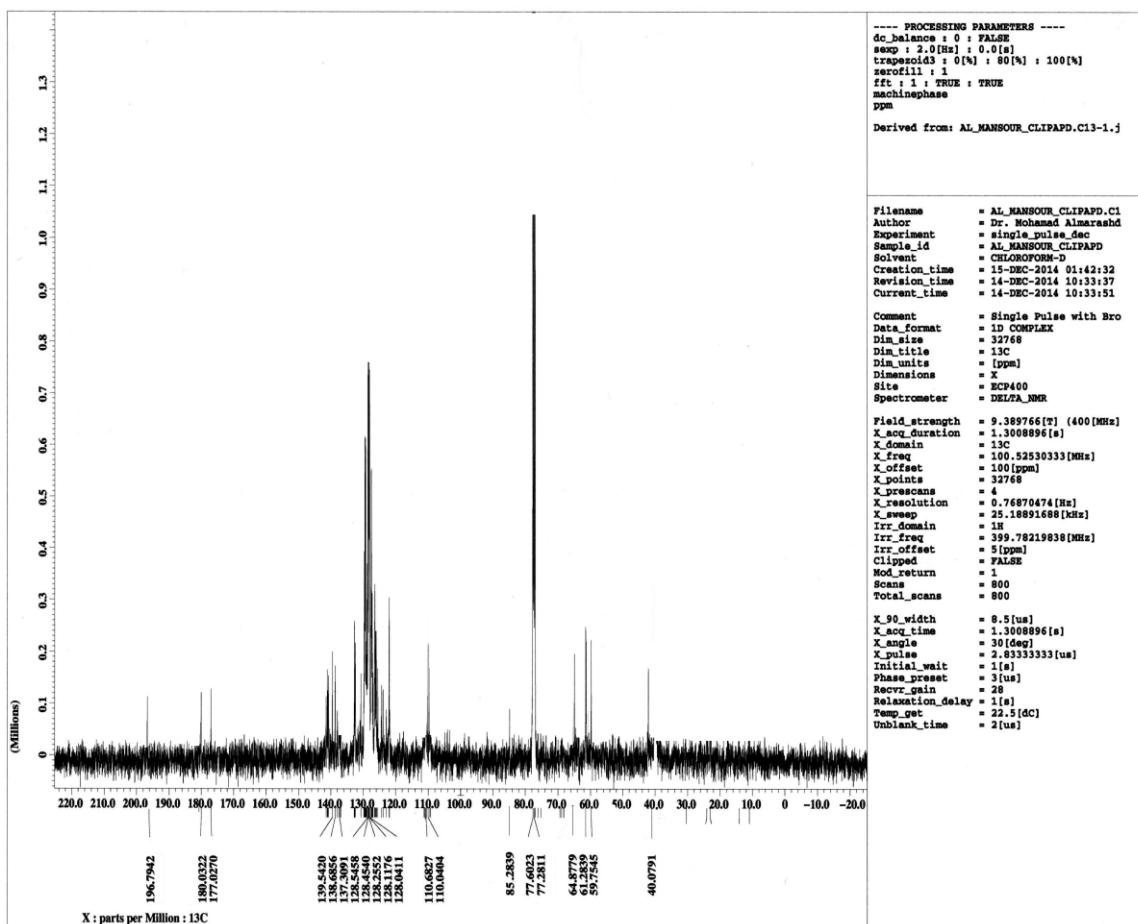
Figure S26. IR spectrum of **6c**.



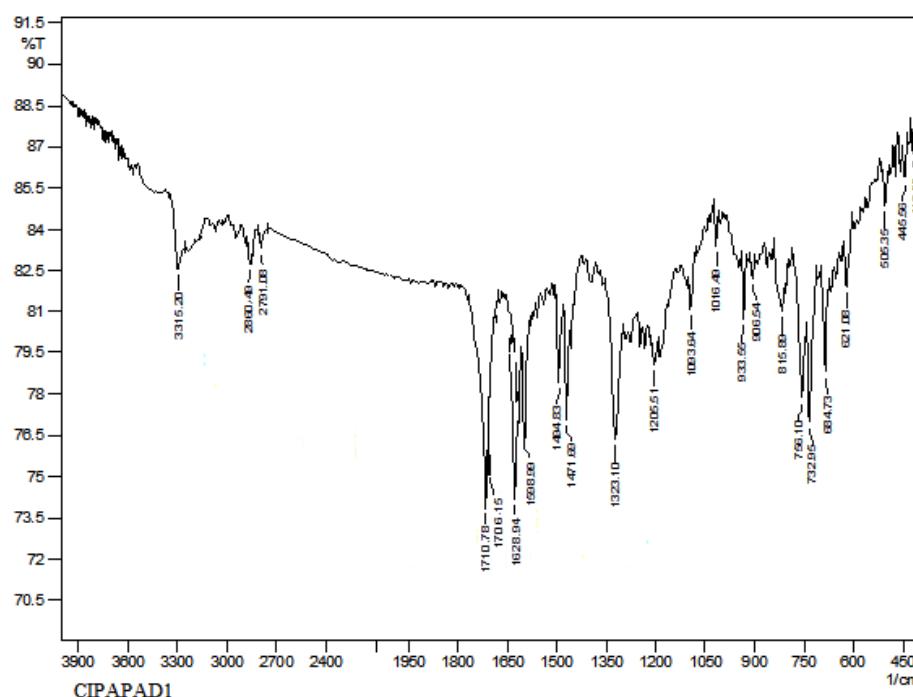
**Figure S27.** Mass spectrum of **6c**.



**Figure S28.**  $^1\text{H}$ -NMR spectrum of **5d**.



**Figure S29.** <sup>13</sup>C-NMR spectrum of 5d.



**Figure S30.** IR spectrum of 5d.

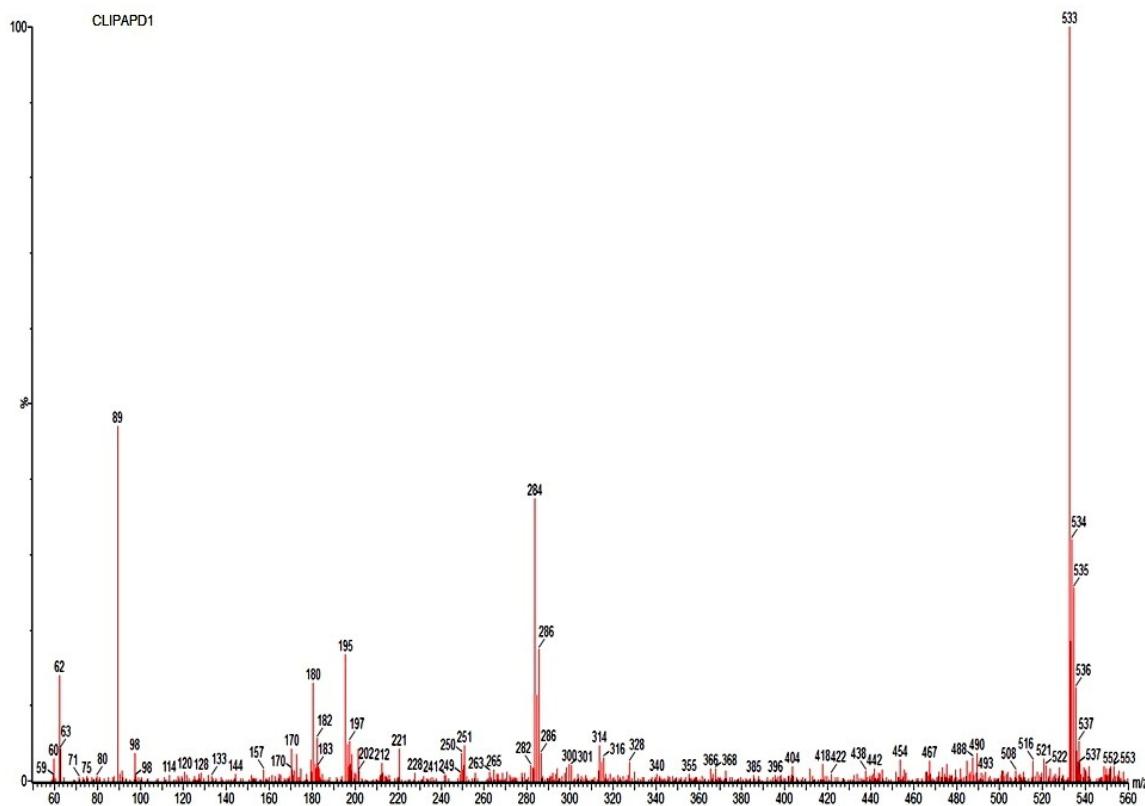
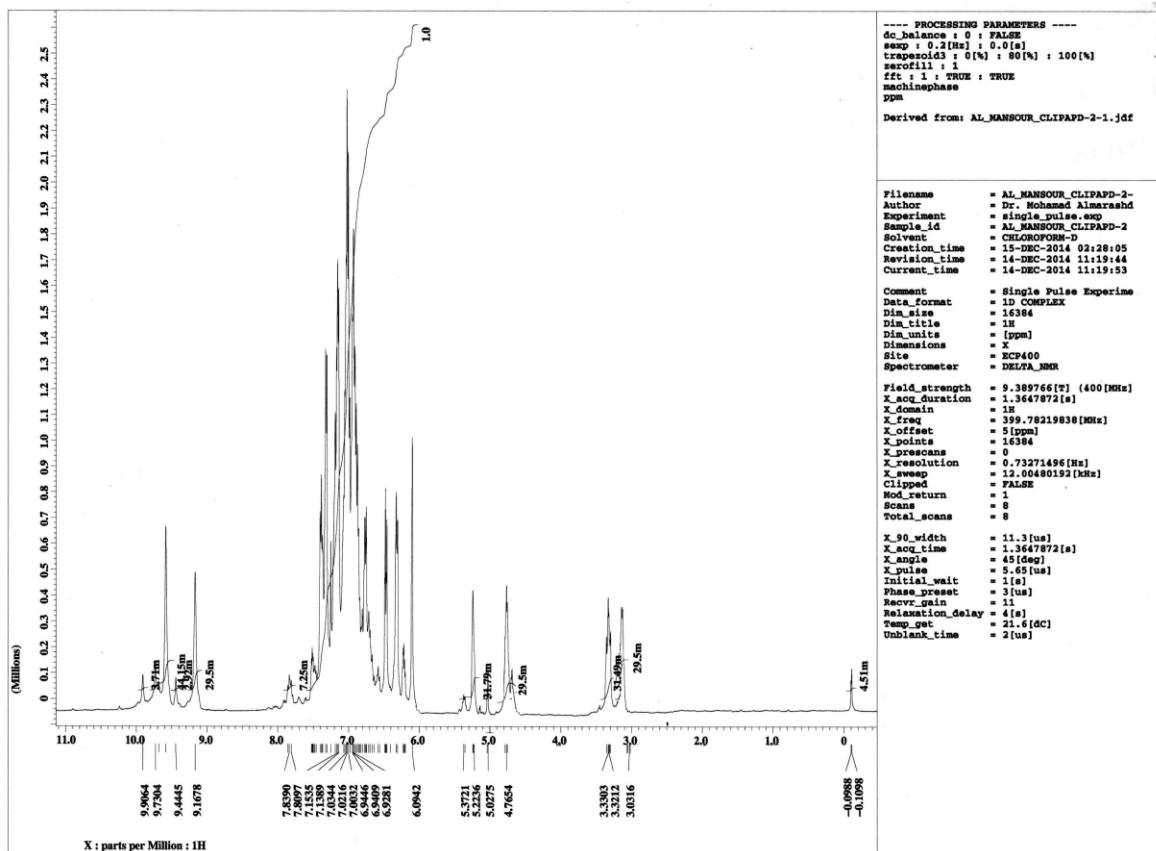
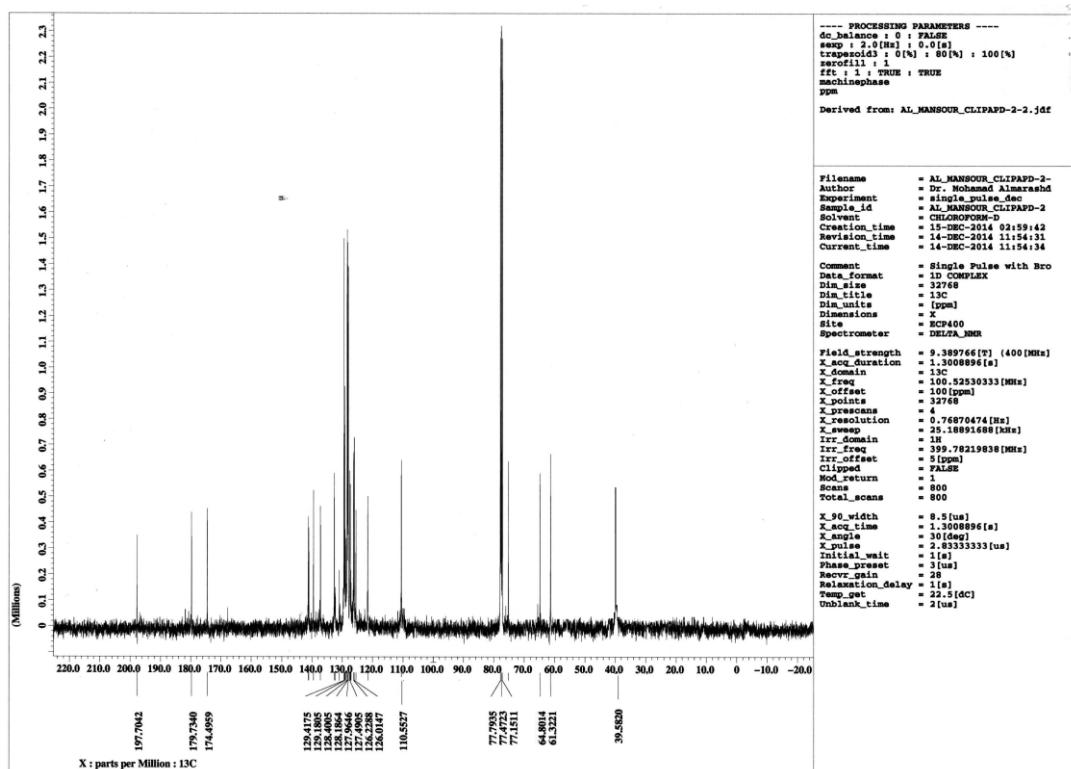
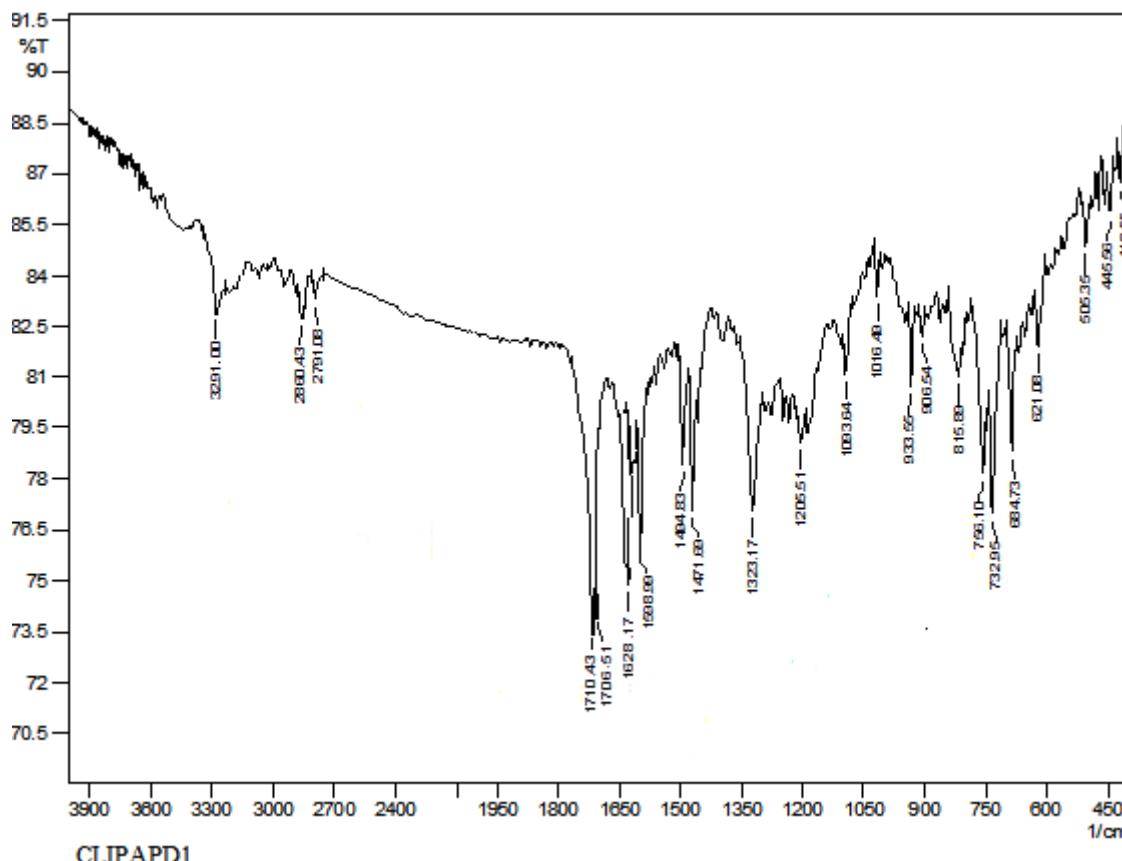


Figure S31. Mass spectrum of 5d.

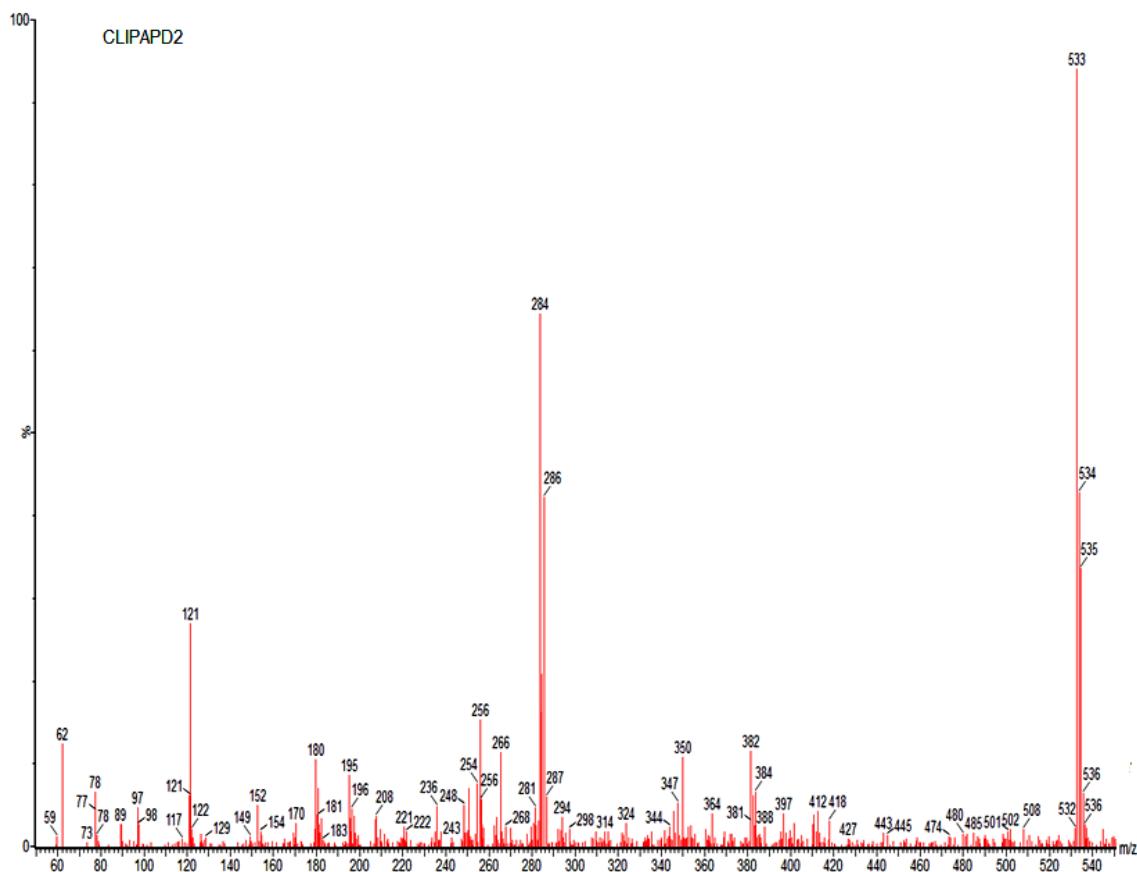
Figure S32.  $^1\text{H}$ -NMR spectrum of 6d.



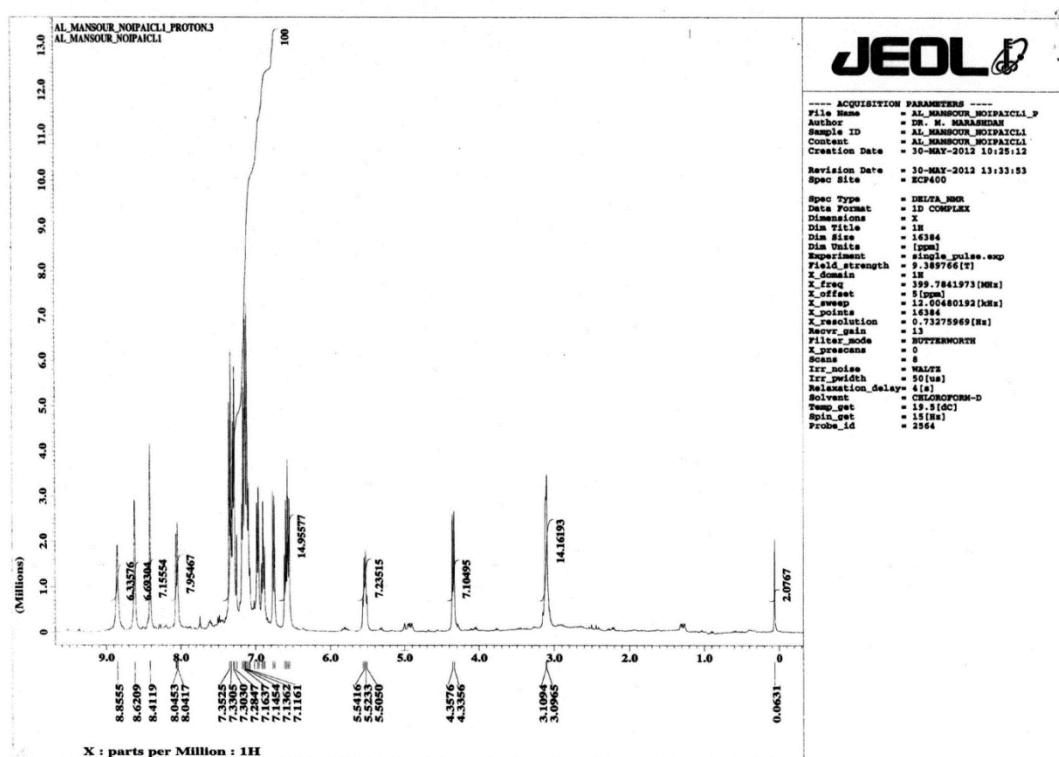
**Figure S33.**  $^{13}\text{C}$ -NMR spectrum of **6d**.



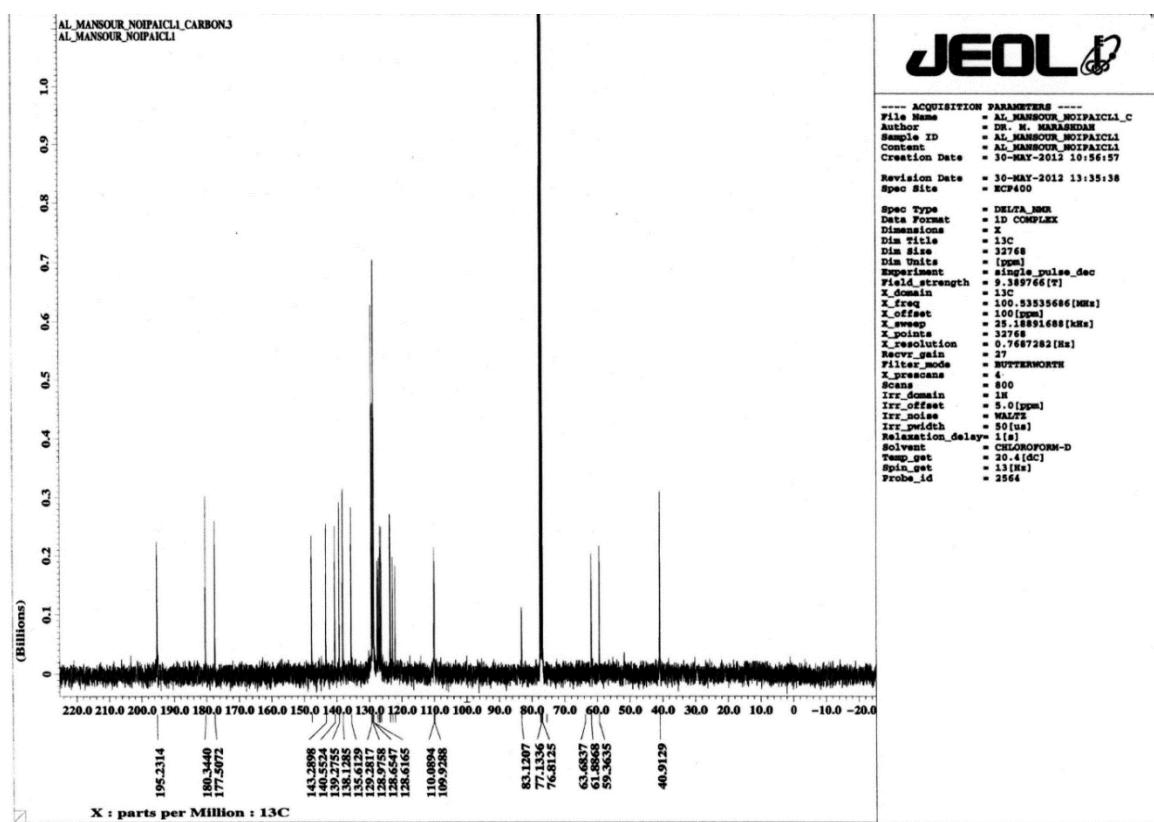
**Figure S34.** IR spectrum of **6d**.



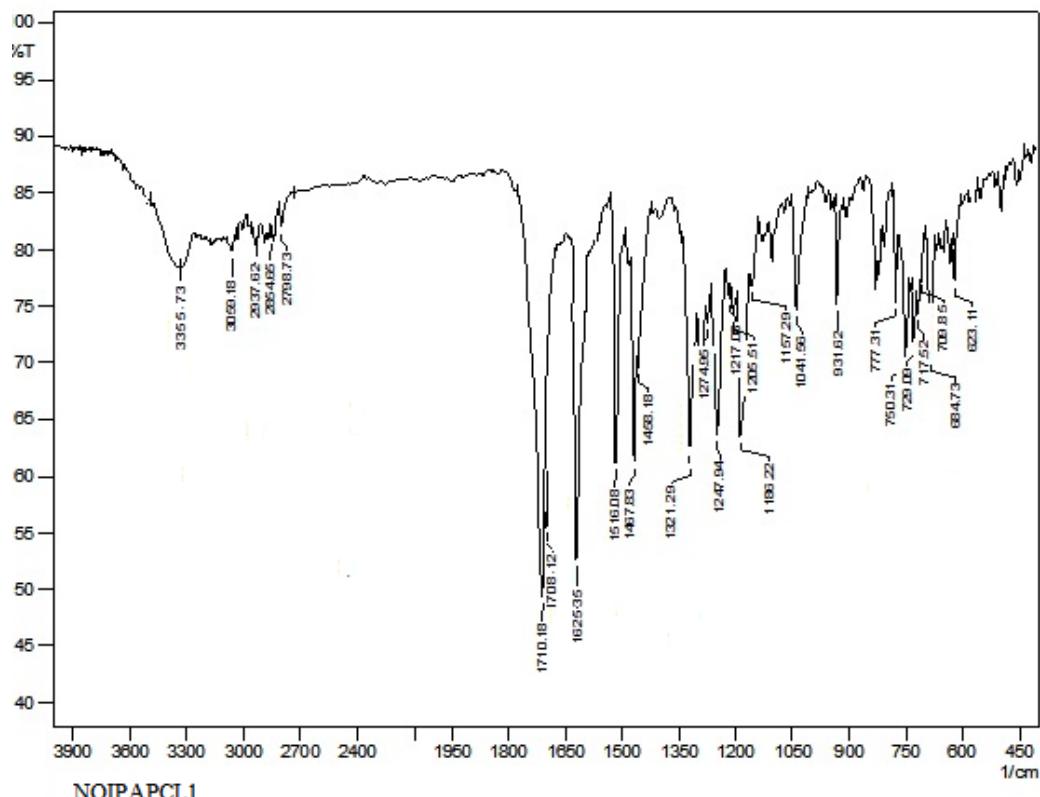
**Figure S35.** Mass spectrum of 6d.



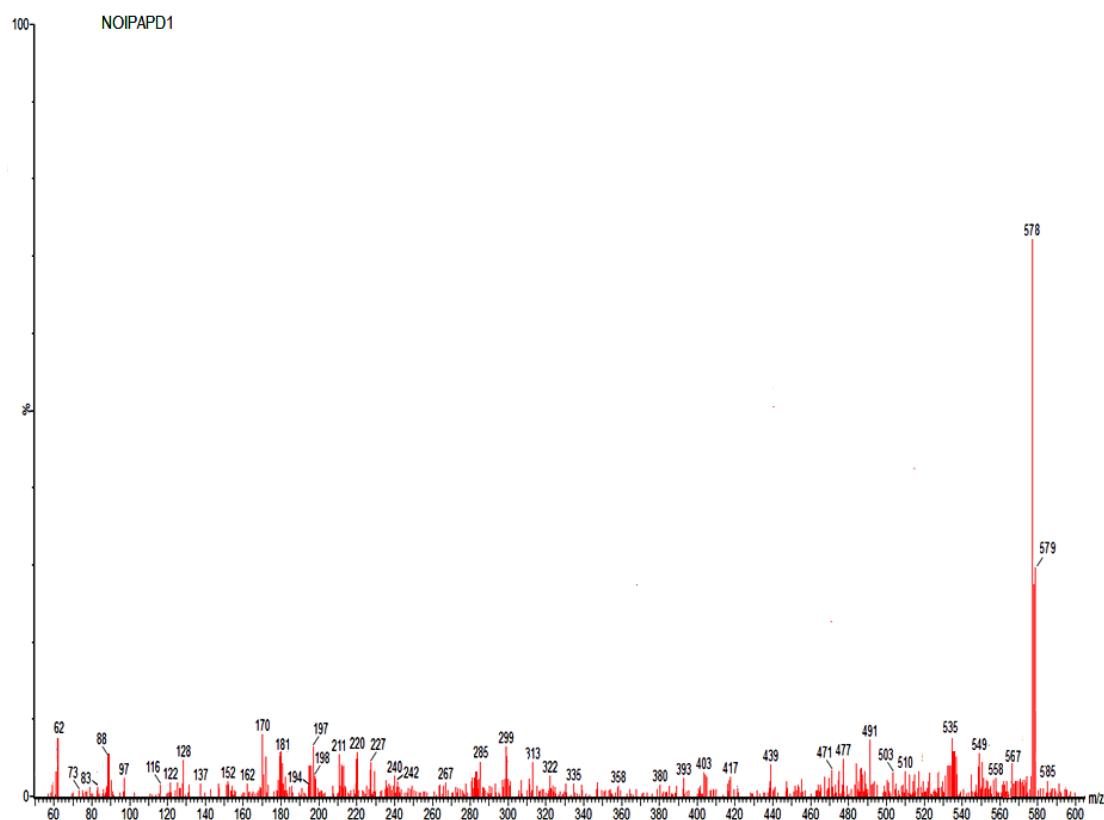
**Figure S36.**  $^1\text{H}$ -NMR spectrum of 5e.



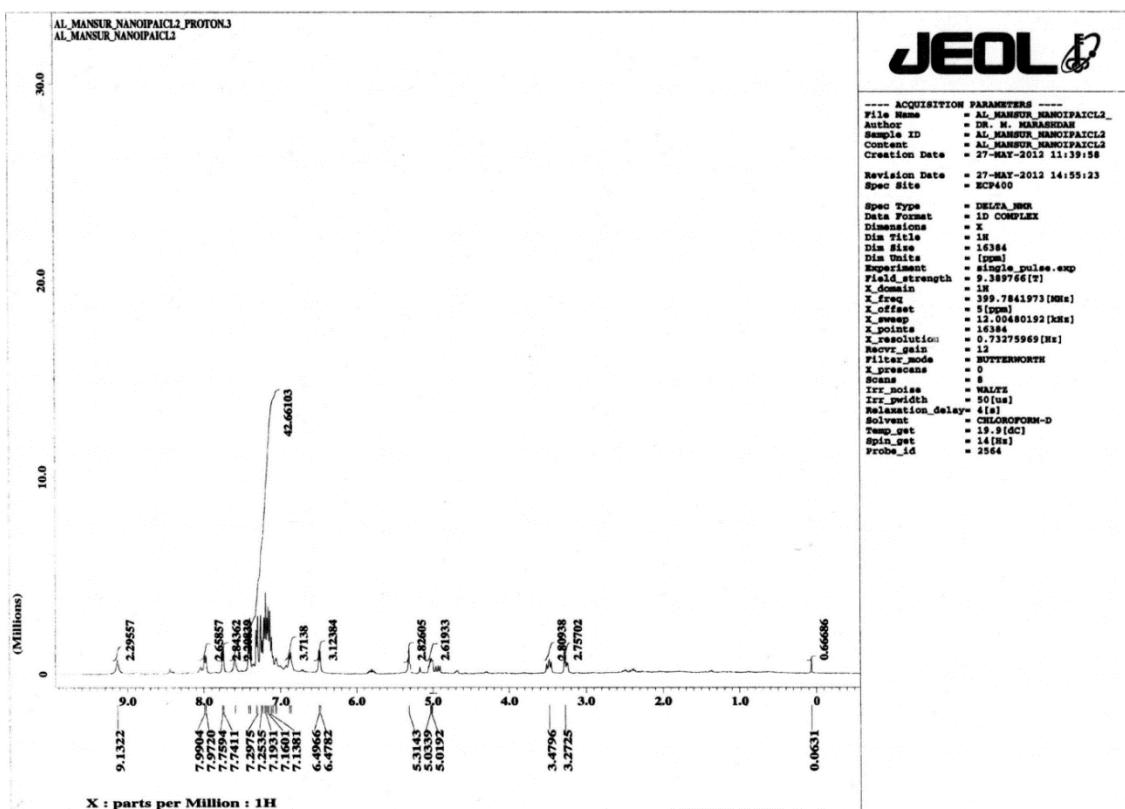
**Figure S37.**  $^{13}\text{C}$ -NMR spectrum of **5e**.



**Figure S38.** IR spectrum of **5e**.



**Figure S39.** Mass spectrum of 5e.



**Figure S40.**  $^1\text{H}$ -NMR spectrum of **6e**.

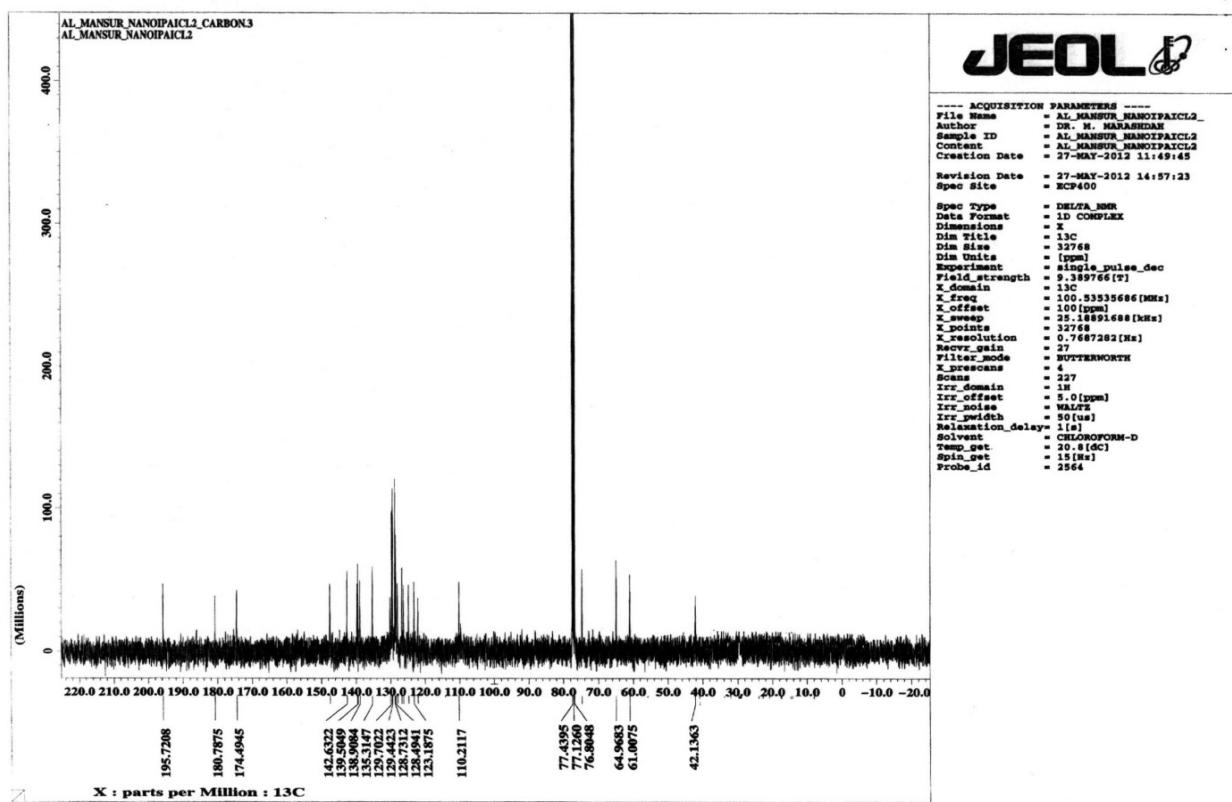


Figure S41.  $^{13}\text{C}$ -NMR spectrum of 6e.

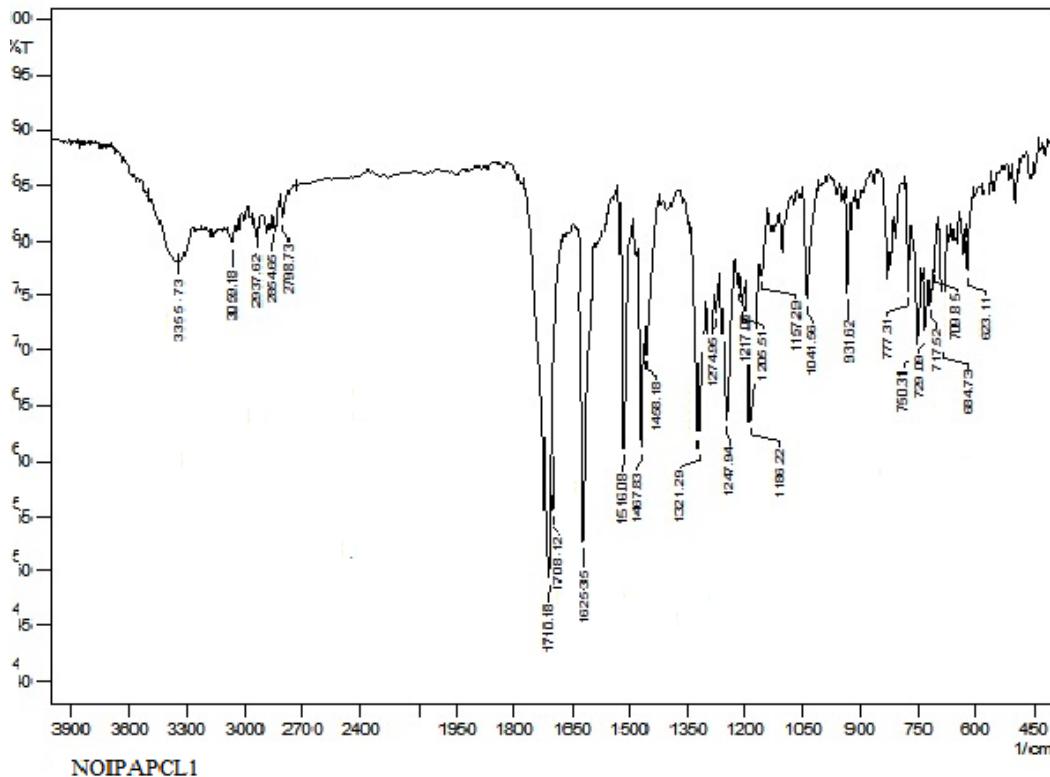
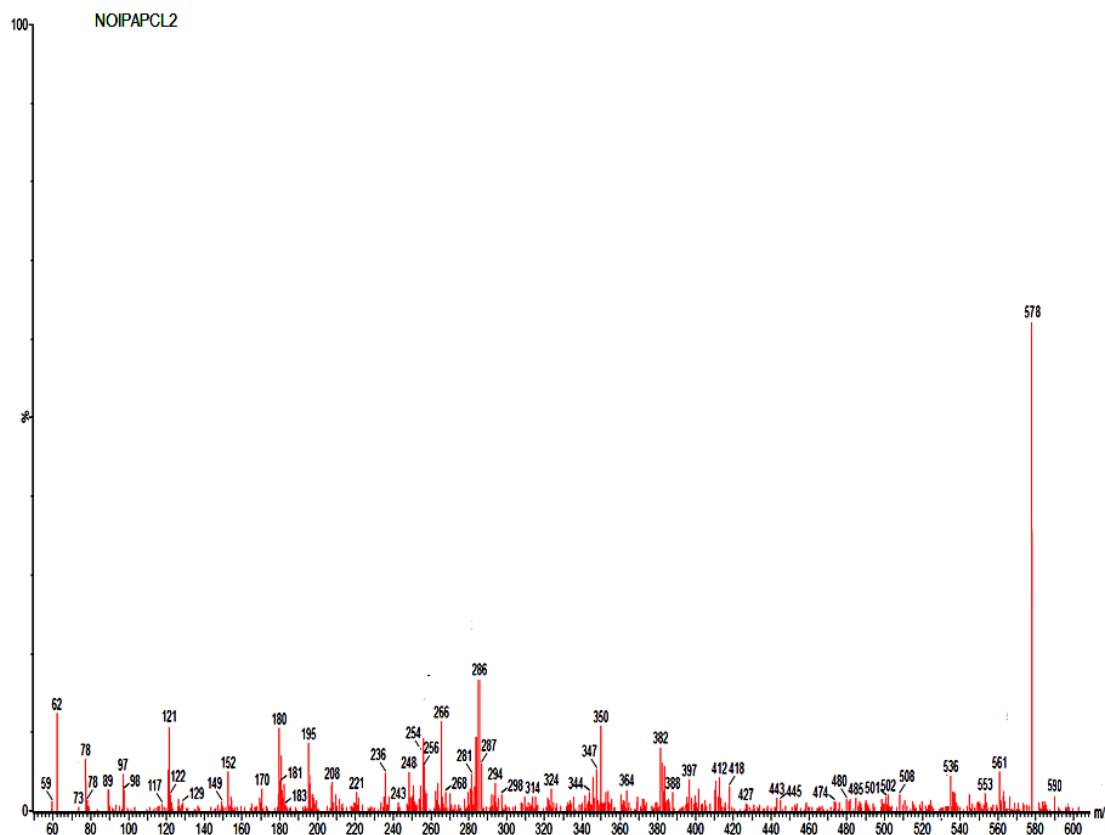
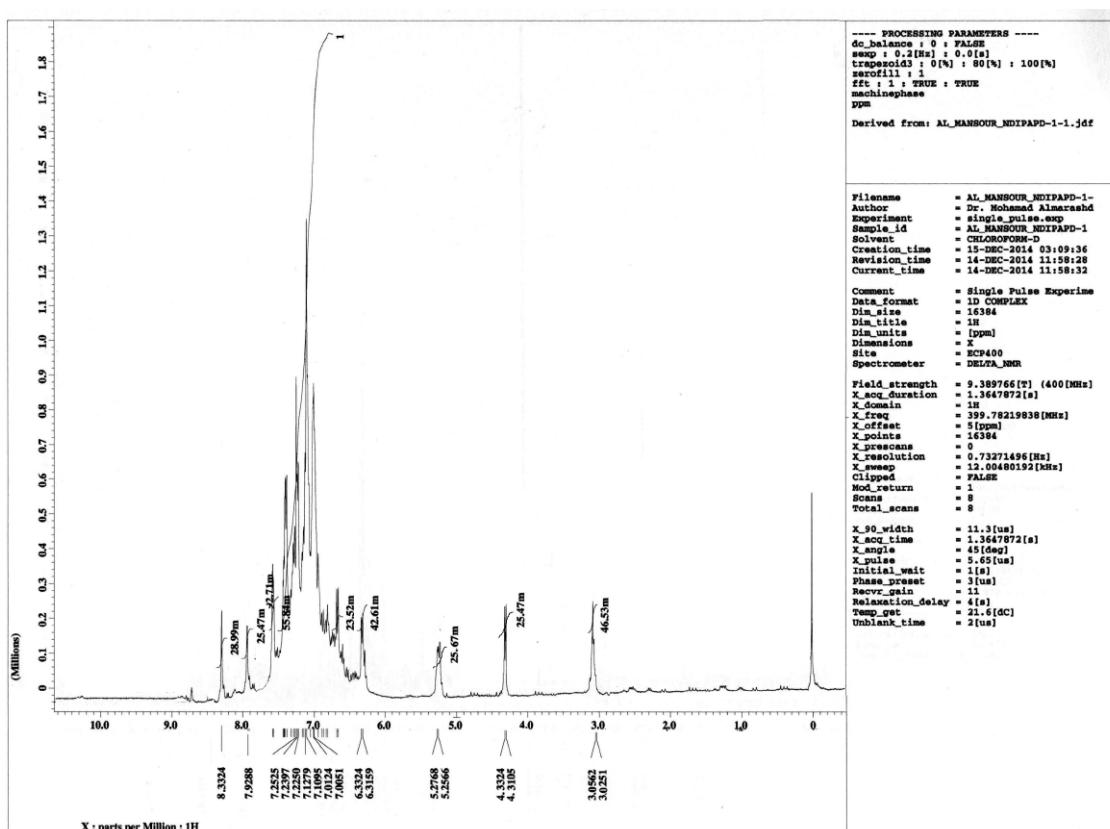


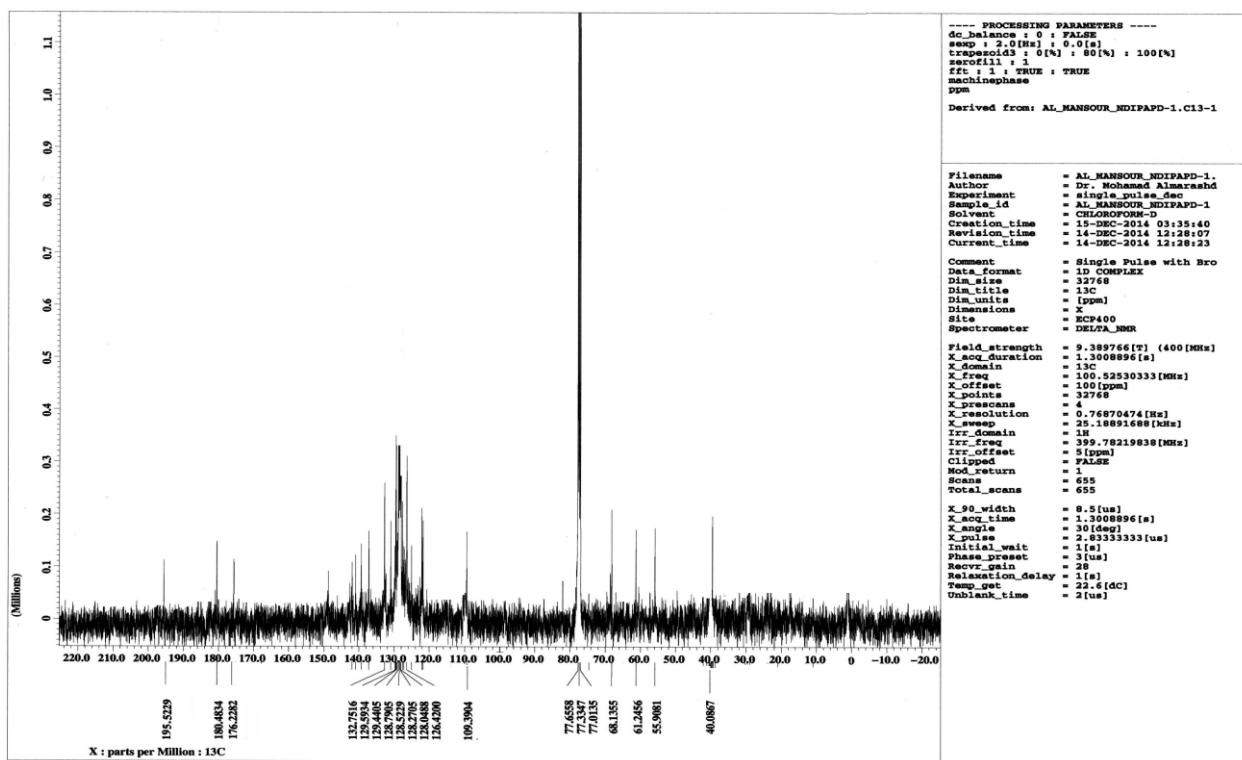
Figure S42. IR spectrum of 6e.



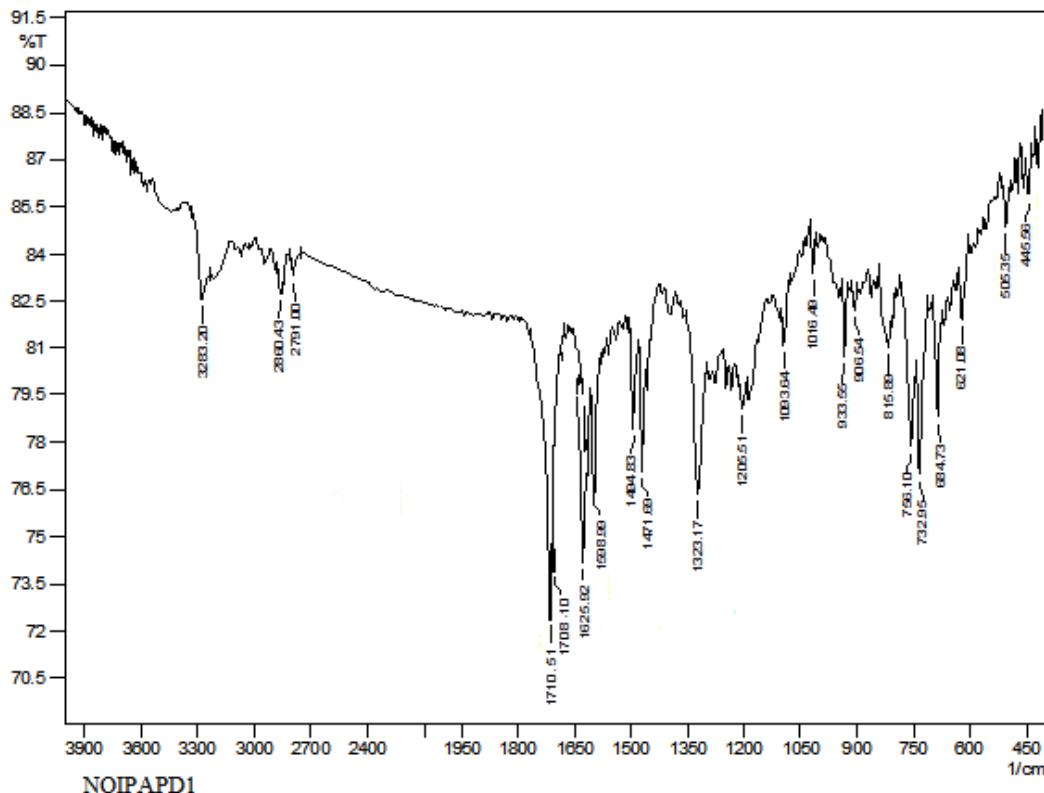
**Figure S43.** Mass spectrum of 6e.



**Figure S44.**  $^1\text{H}$ -NMR spectrum of 5f.



**Figure S45.**  $^{13}\text{C}$ -NMR spectrum of **5f**.



**Figure S46.** IR spectrum of **5f**.

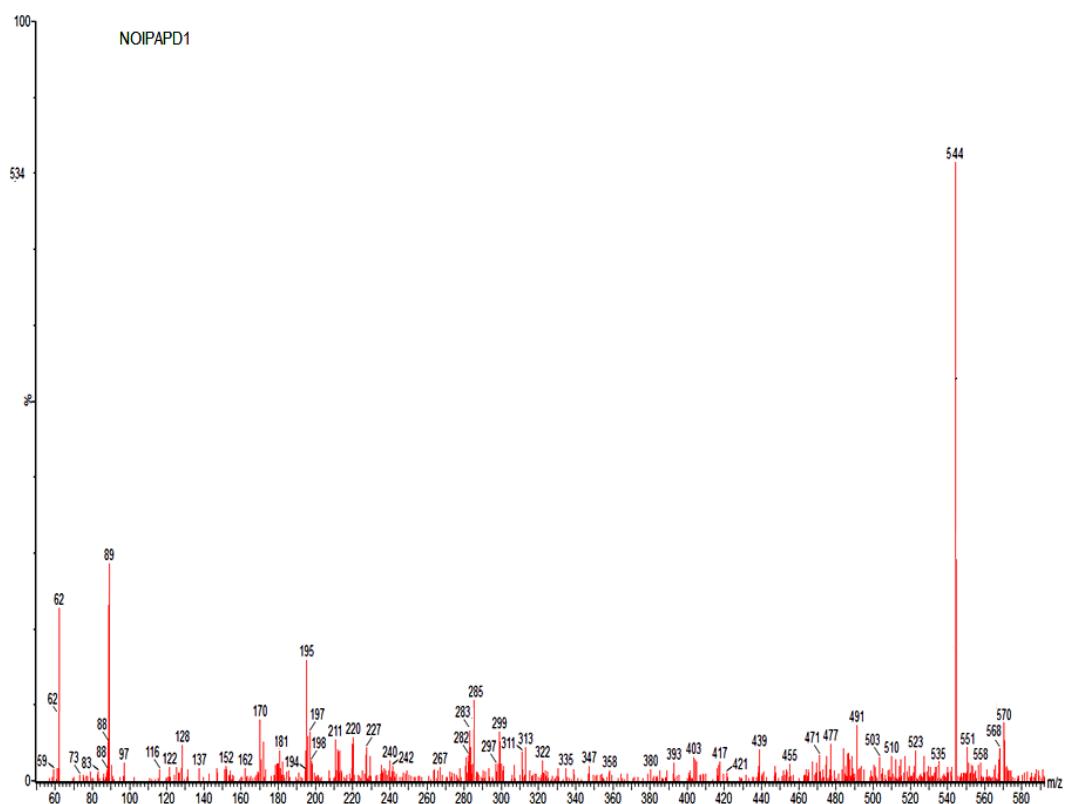
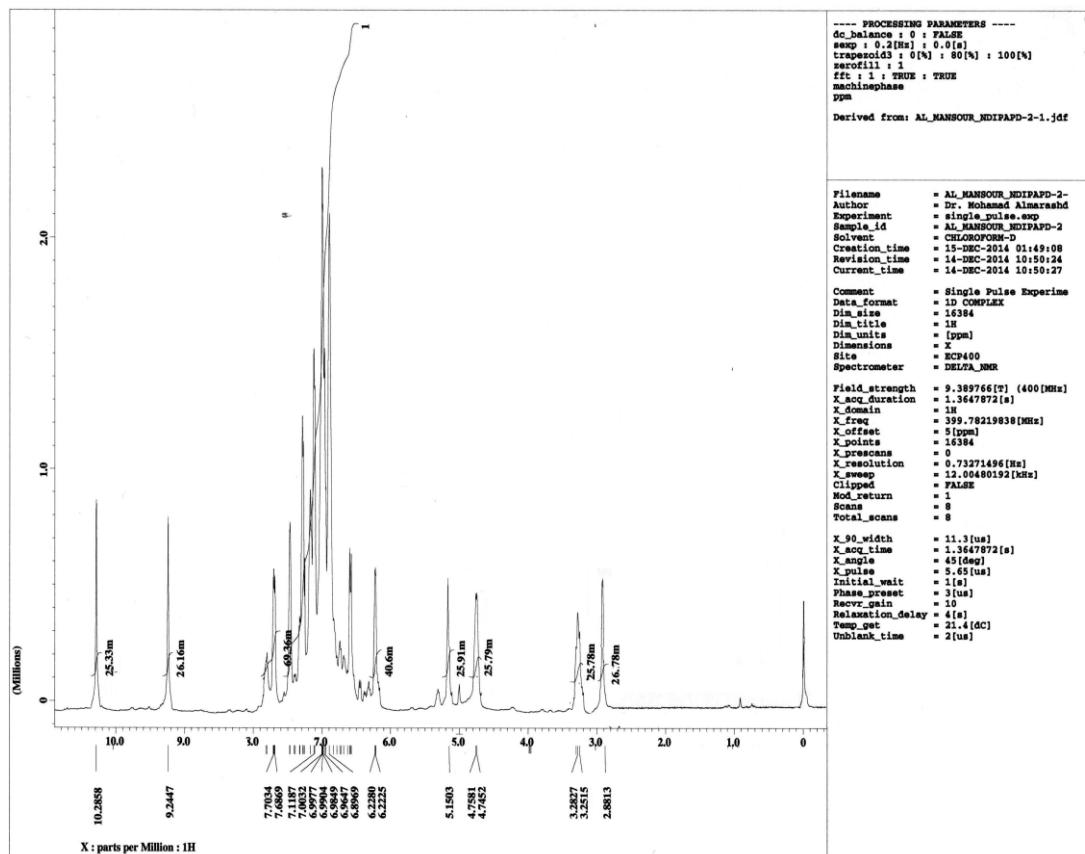
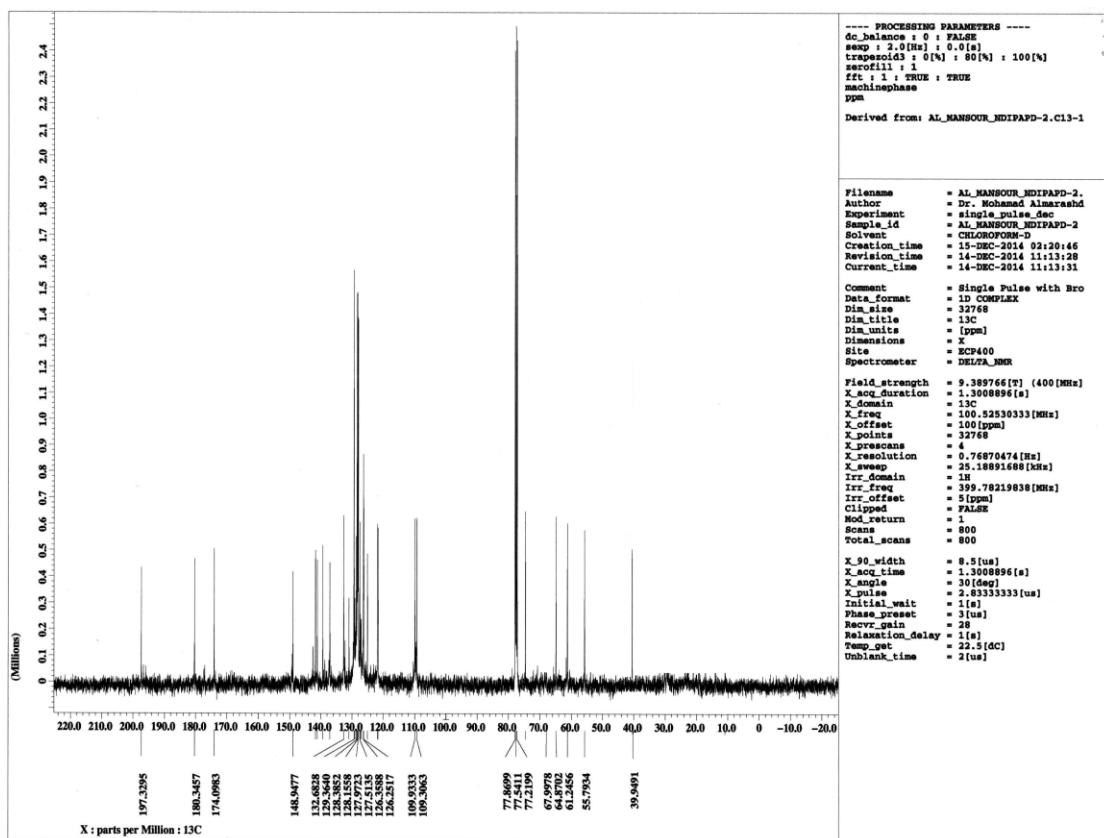
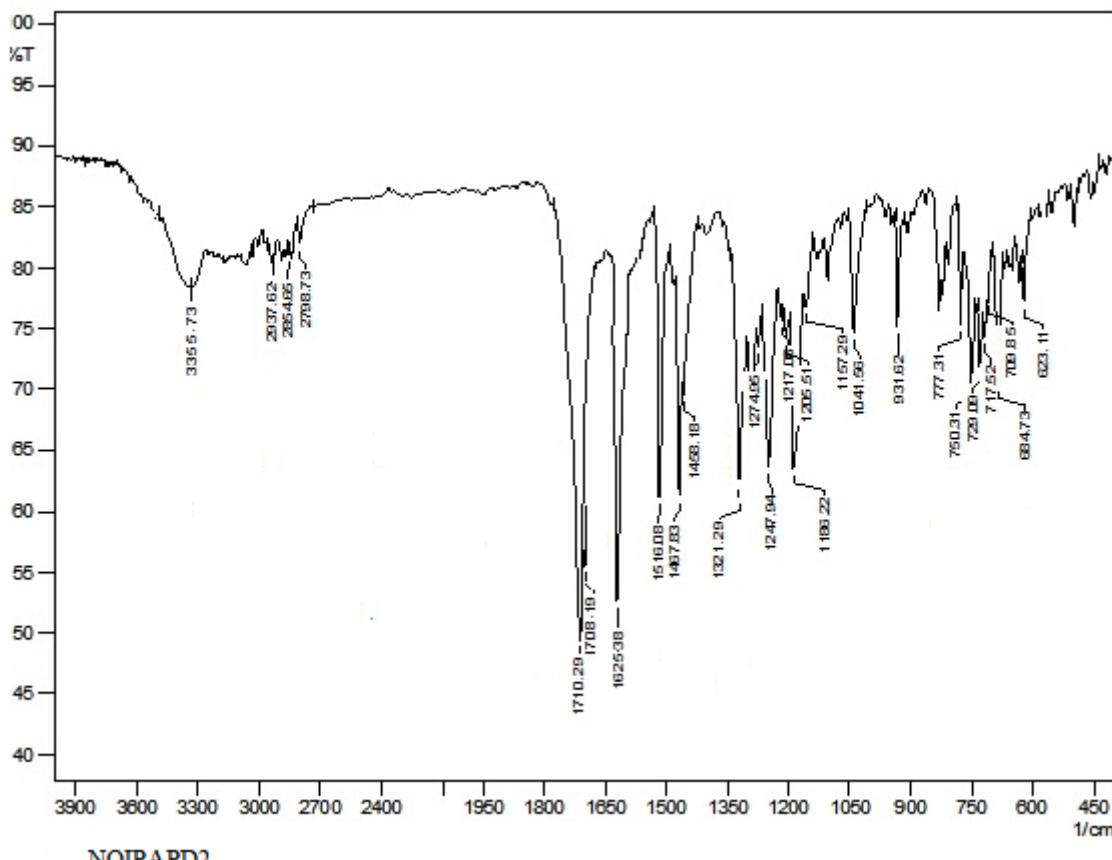


Figure S47. Mass spectrum of 5f.

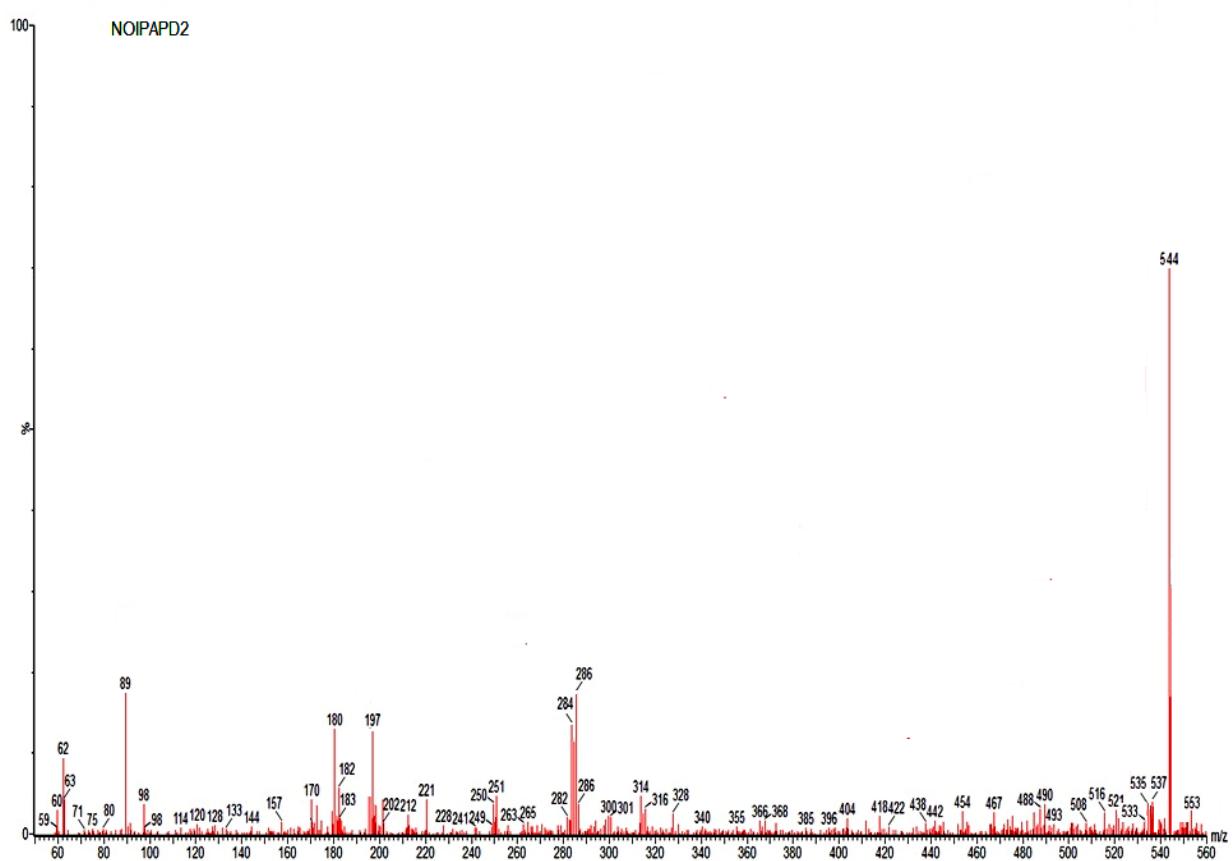
Figure S48.  $^1\text{H}$ -NMR spectrum of 6f.



**Figure S49.** <sup>13</sup>C-NMR spectrum of 6f.



**Figure S50.** IR spectrum of 6f.



**Figure S51.** Mass spectrum of **6f**.