

Supplementary Information

Synthesis and *In Vivo* Evaluation of 5-Chloro-5-benzobarbiturates as New Central Nervous System Depressants

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Collection of ¹H NMR, ¹³C NMR and IR spectra of compounds **6a** to **6f**, and Tables S1 and S2 with the assignment of the ¹H and ¹³C NMR signals, respectively.

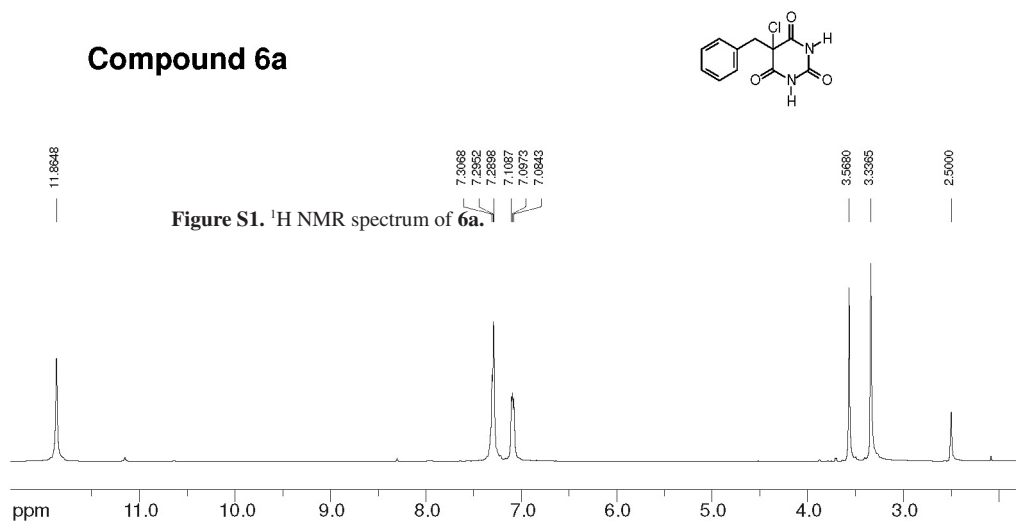


Figure S1. ¹H NMR spectrum of **6a**.

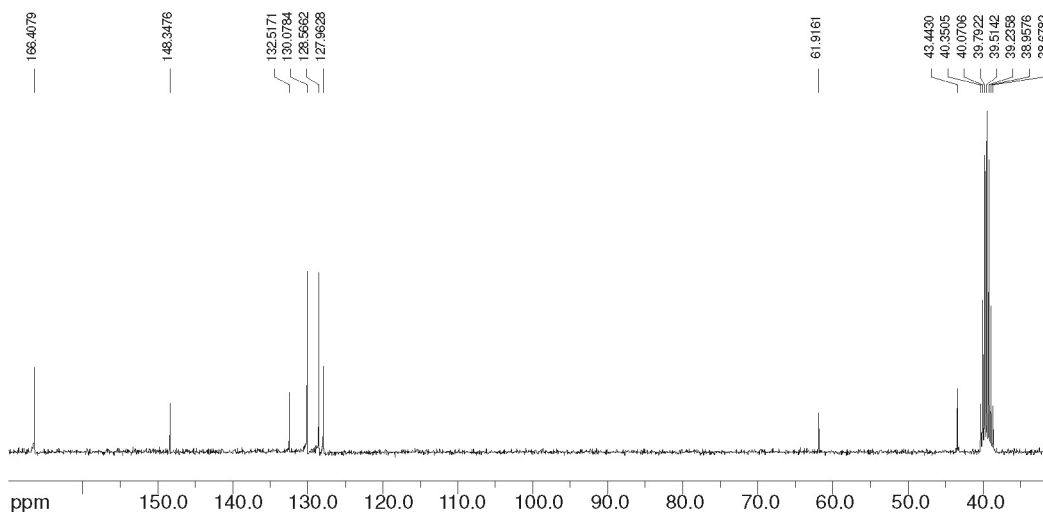
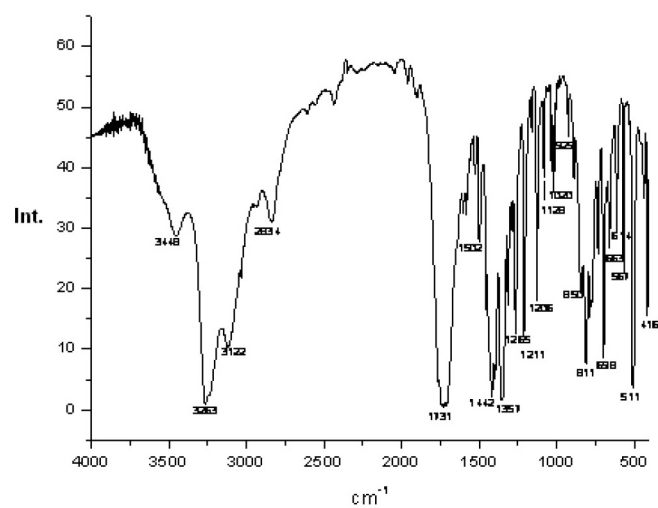
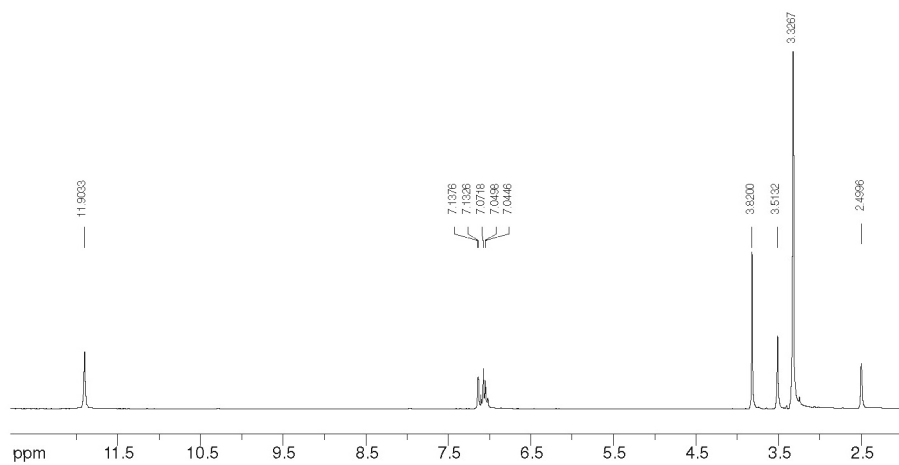
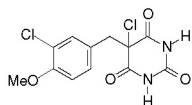


Figure S2. ¹³C NMR spectrum of **6a**.

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Figure S3. IR spectrum of **6a**.**Compound 6b**Figure 4. ¹H NMR spectrum of **6b**.

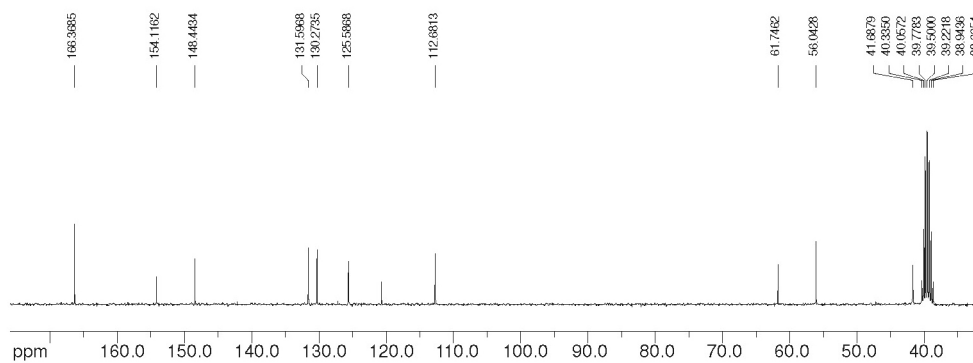


Figure S5. ¹³C NMR spectrum of 6b.

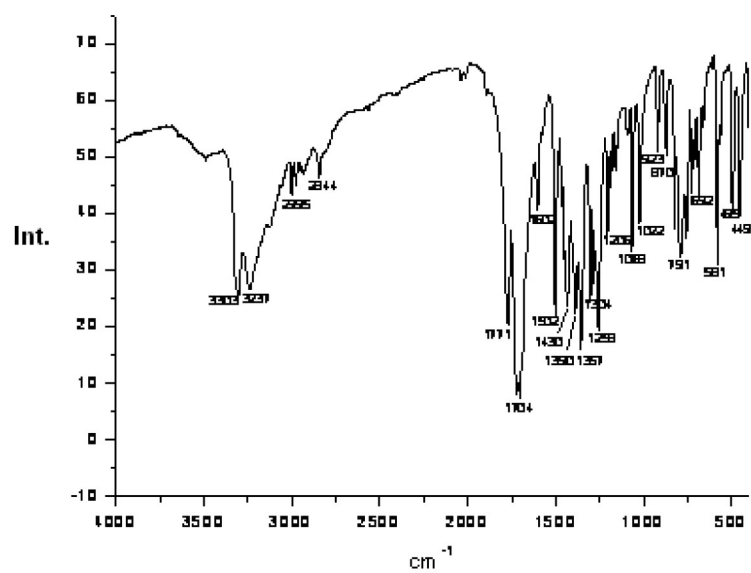
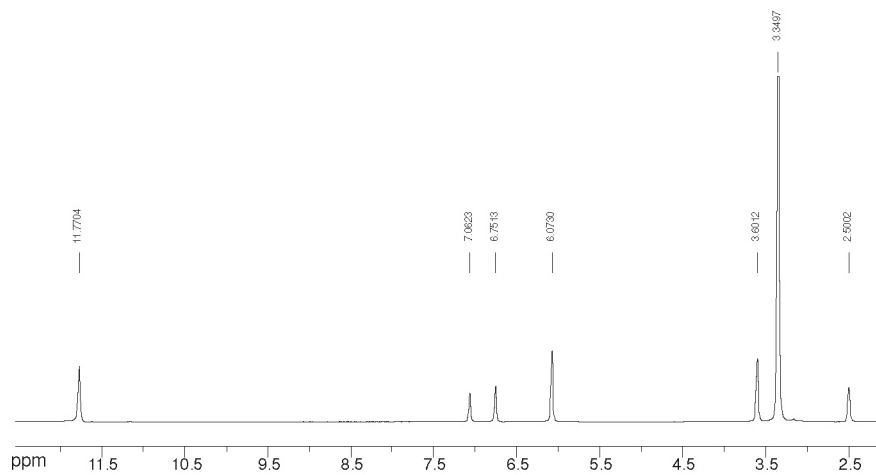
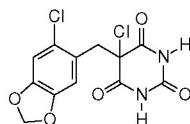
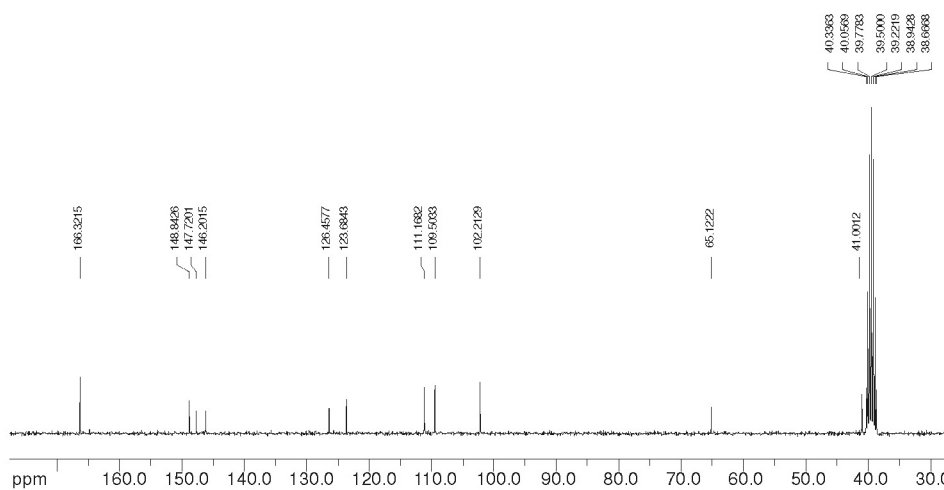
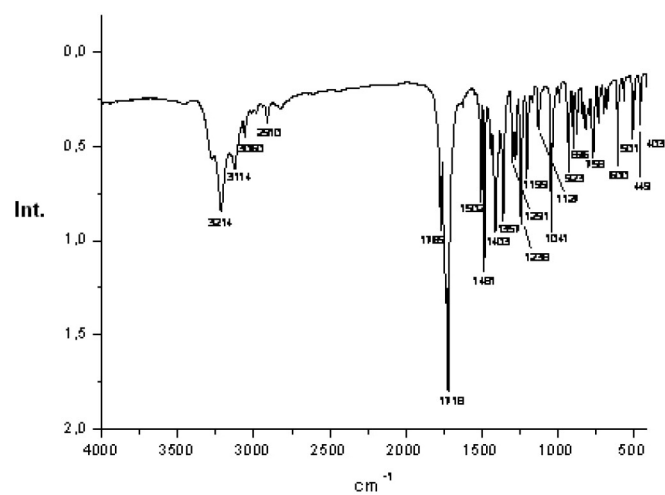
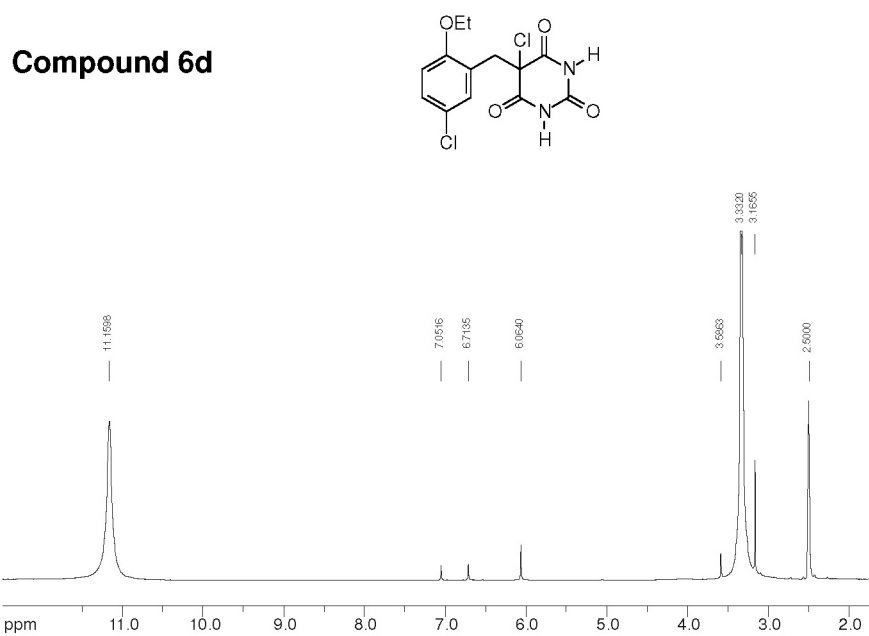


Figure S6. IR spectrum of 6b.

Compound 6c**Figure S7.** ¹H NMR spectrum of 6c.**Figure S8.** ¹³C NMR spectrum of 6c.

Figure S9. IR spectrum of **6c**.Figure S10. ¹H NMR spectrum of **6d**.

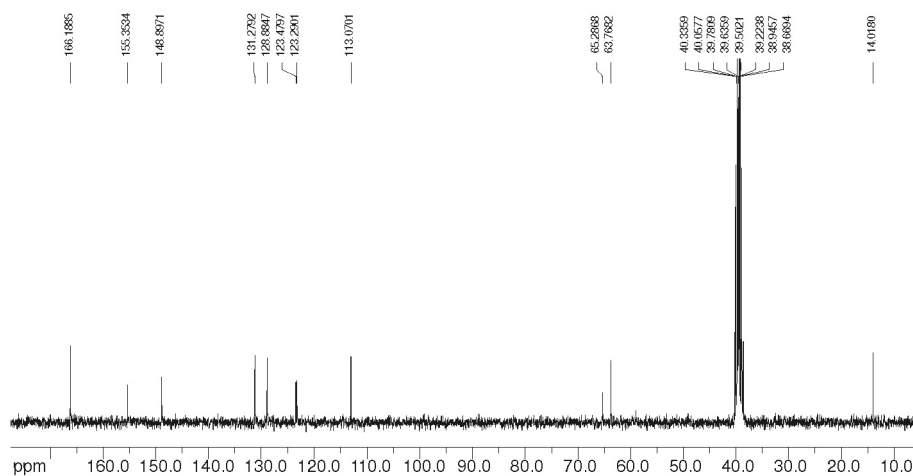
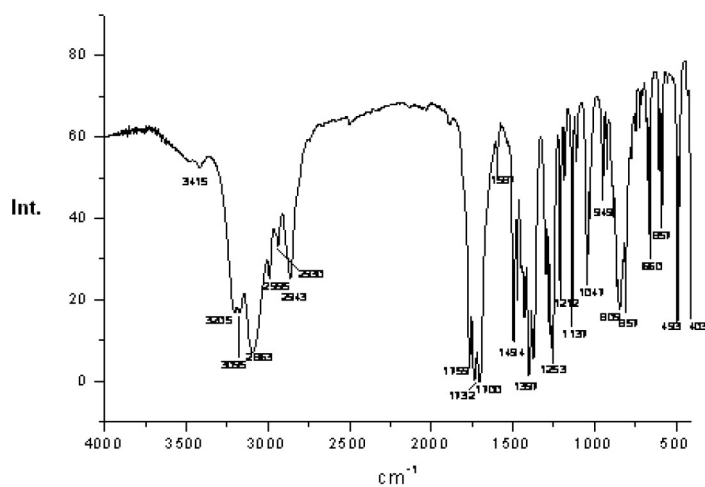
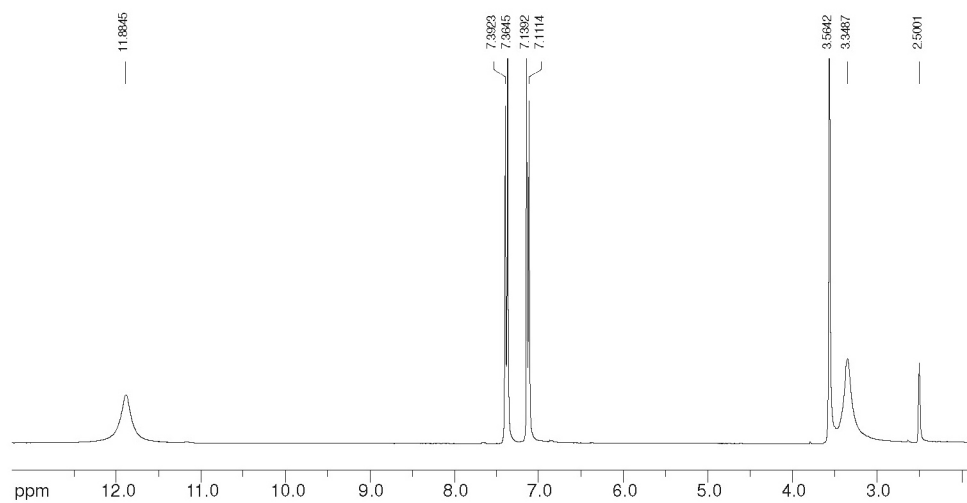
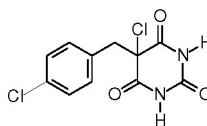
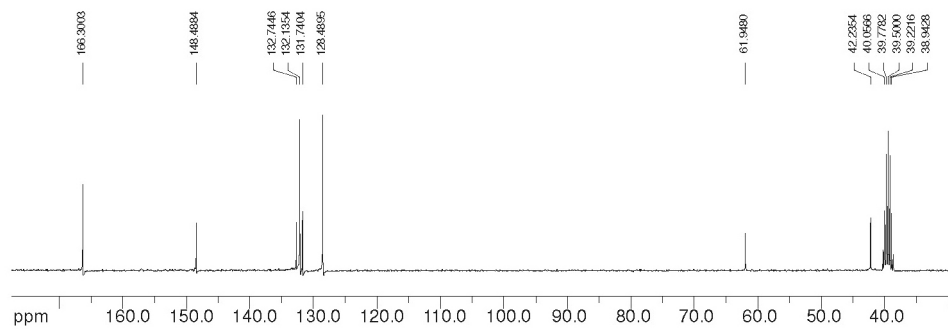
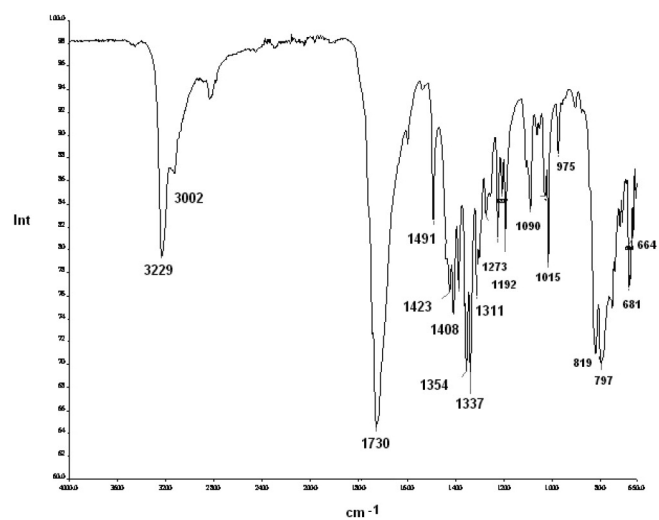
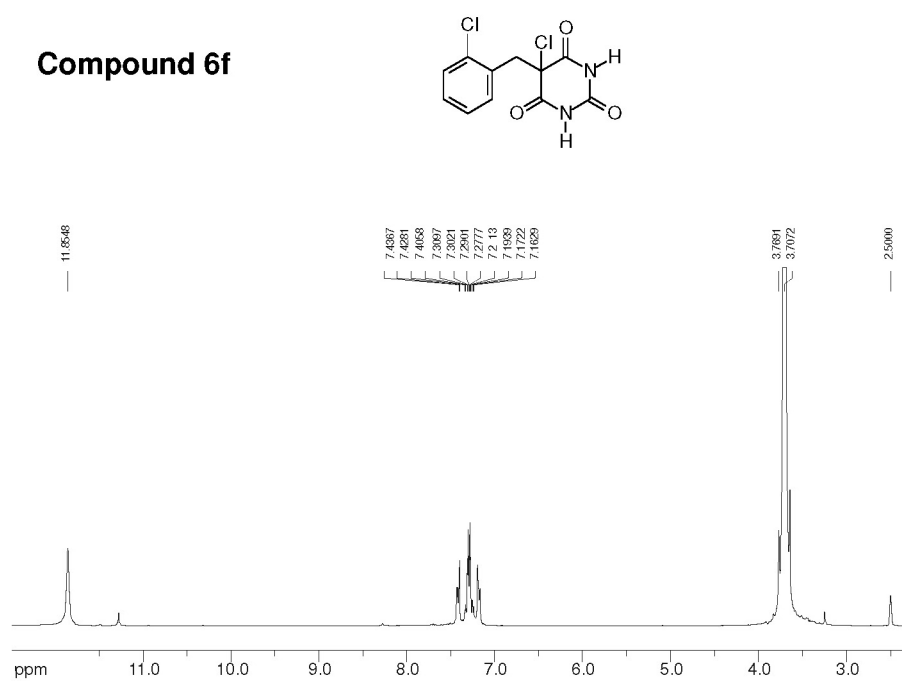
Figure S11. ¹³C NMR spectrum of 6d.

Figure S12. IR spectrum of 6d.

Compound 6e**Figure S13.** ^1H NMR spectrum of **6e**.**Figure S14.** ^{13}C NMR spectrum of **6e**.

Figure S15. IR spectrum of **6e**.Figure S16. ¹H NMR spectrum of **6f**.

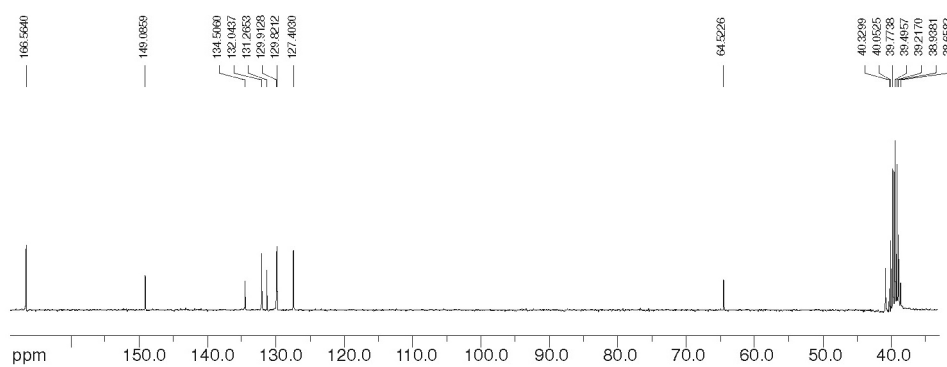
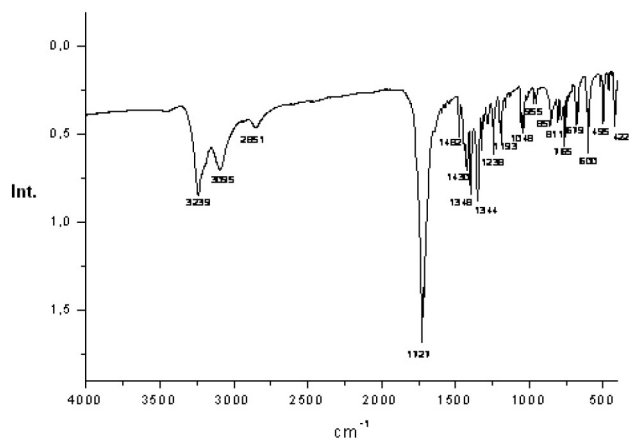
**Figure S17.** ^{13}C NMR spectrum of **6f**.**Figure S18.** IR spectrum of **6f**.

Table S1. ¹H NMR signal assignment for compounds **6a** to **6f**

Comp.	6a	6b	6c	6d	6e	6f
H1+H3	11.20(2H, s)	11.90(2H, s)	11.77(2H, s)	11.66(2H, s)	11.88(2H, s)	11.85(2H, s)
H7	3.57 (2H, s)	3.50(2H, s)	3.59(2H, s)	3.52(2H, s)	3.55(2H, s)	4.00(2H, s)
H9	7.09(2H, d, <i>J</i> 3.6 Hz)	7.11(1H, s);	7.05(1H, s)	-	7.11(2H, d, <i>J</i> 8.4 Hz)	-
H10	7.29(3H, t, <i>J</i> 3.6 Hz)	-	-	6.95(1H, d, <i>J</i> 4.3 Hz)	7.37(2H, d, <i>J</i> 8.4 Hz)	7.27(2H, t, <i>J</i> 3.2 Hz)
H11	7.29(3H, t, <i>J</i> 3.6 Hz)	-	-	7.28(1H, d, <i>J</i> 4.3 Hz)	-	7.27(2H, t, <i>J</i> 3.2 Hz)
H12	7.29(3H, t, <i>J</i> 3.6 Hz)	7.00(1H, d, <i>J</i> 6.0 Hz)	6.74(1H, s)	-	7.37(2H, d, <i>J</i> 8.4 Hz)	7.40(1H, d, <i>J</i> 3.8 Hz)
H13	7.09(2H, d, <i>J</i> 3.6 Hz)	7.05(1H, d, <i>J</i> 6.0 Hz);	-	7.11(1H, s);	7.11(2H, d, <i>J</i> 8.4 Hz)	7.17(1H, d, <i>J</i> 3.5 Hz)
Me	-	3.82(3H, s);	-	1.29(3H, t, <i>J</i> 5.0 Hz)	-	-
CH ₂	-	-	6.07(2H, s)	3.94(2H, q, <i>J</i> 4.5 Hz)	-	-

Table S2. ¹³C NMR signal assignment for compounds **6a** to **6f**

Comp.	6a	6b	6c	6d	6e	6f
C2	148.4	148.5	148.7	149.0	148.5	149.1
C4+C6	166.4	166.4	166.3	166.9	166.3	166.6
C5	61.9	61.8	65.2	65.3	61.9	64.3
C7	43.5	41.7	41.0	39.6	42.2	40.8
C8	132.5	120.7	126.2	123.3	131.7	131.3
C9	128.6	130.3	109.5	155.4	132.1	134.5
C10	130.1	125.6	146.1	113.1	128.5	132.1
C11	128.0	154.1	147.9	128.9	132.7	127.4
C12	130.1	112.7	111.2	123.5	128.5	129.8
C13	128.6	131.6	123.8	131.3	132.1	129.9
CH ₂	-	-	102.2	63.8	-	-
CH ₃	-	56.1	-	14.0	-	-