

## **MOLECULES**

**Supplementary Information associated with the paper**

### **Synthesis and characterization of dihydouracil analogs utilizing Biginelli hybrids**

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6-phenyl-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2a**

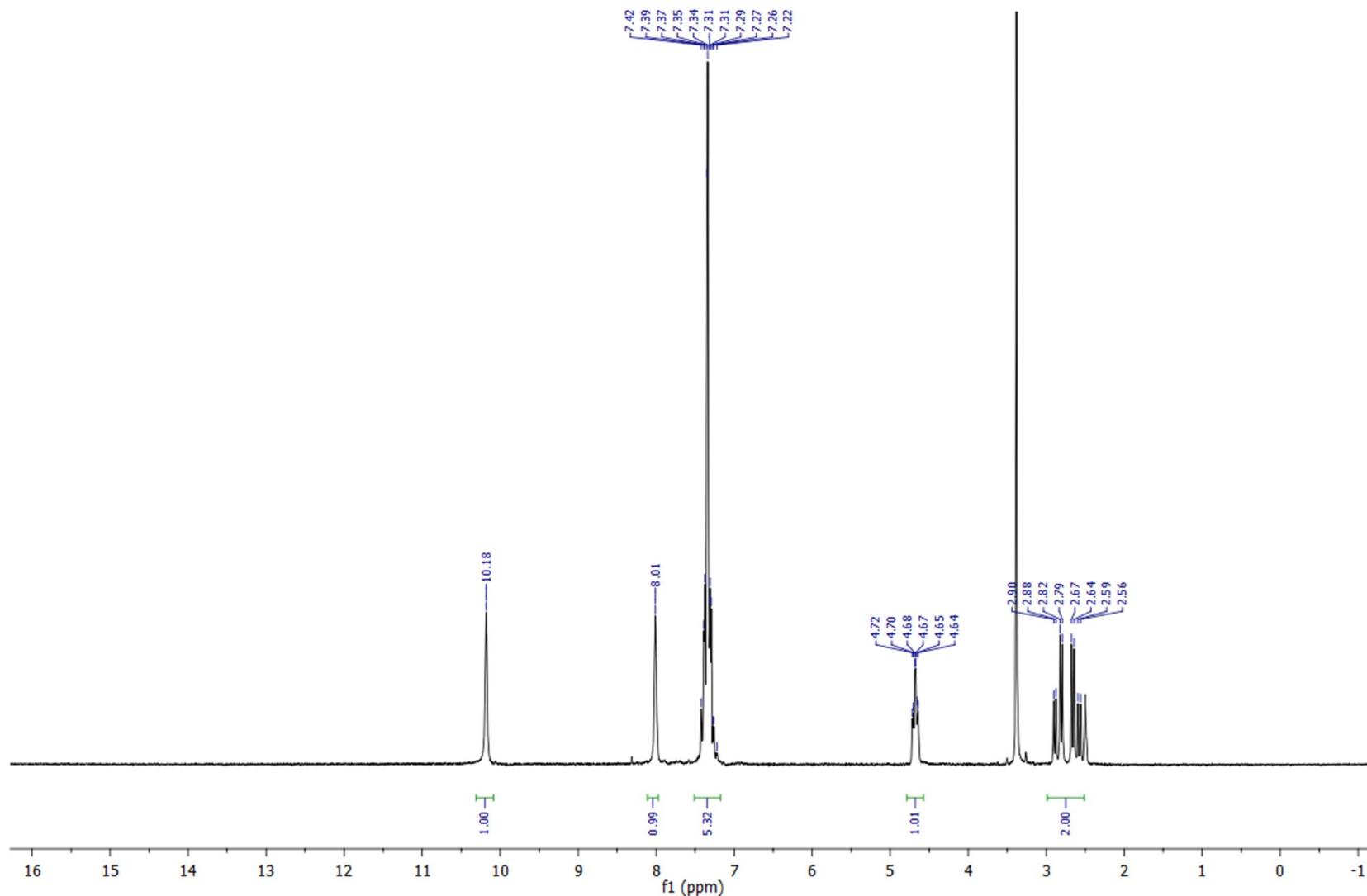
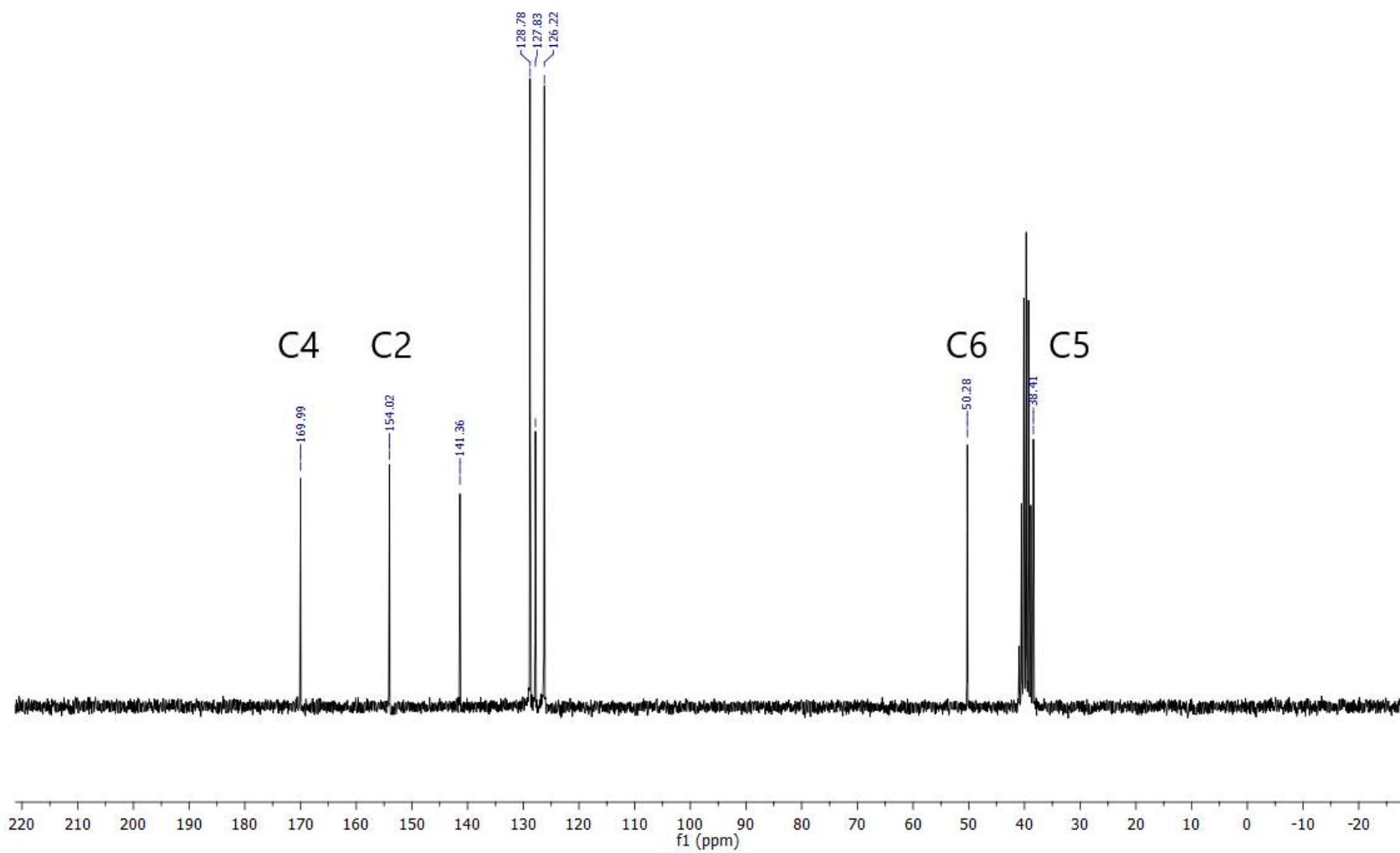
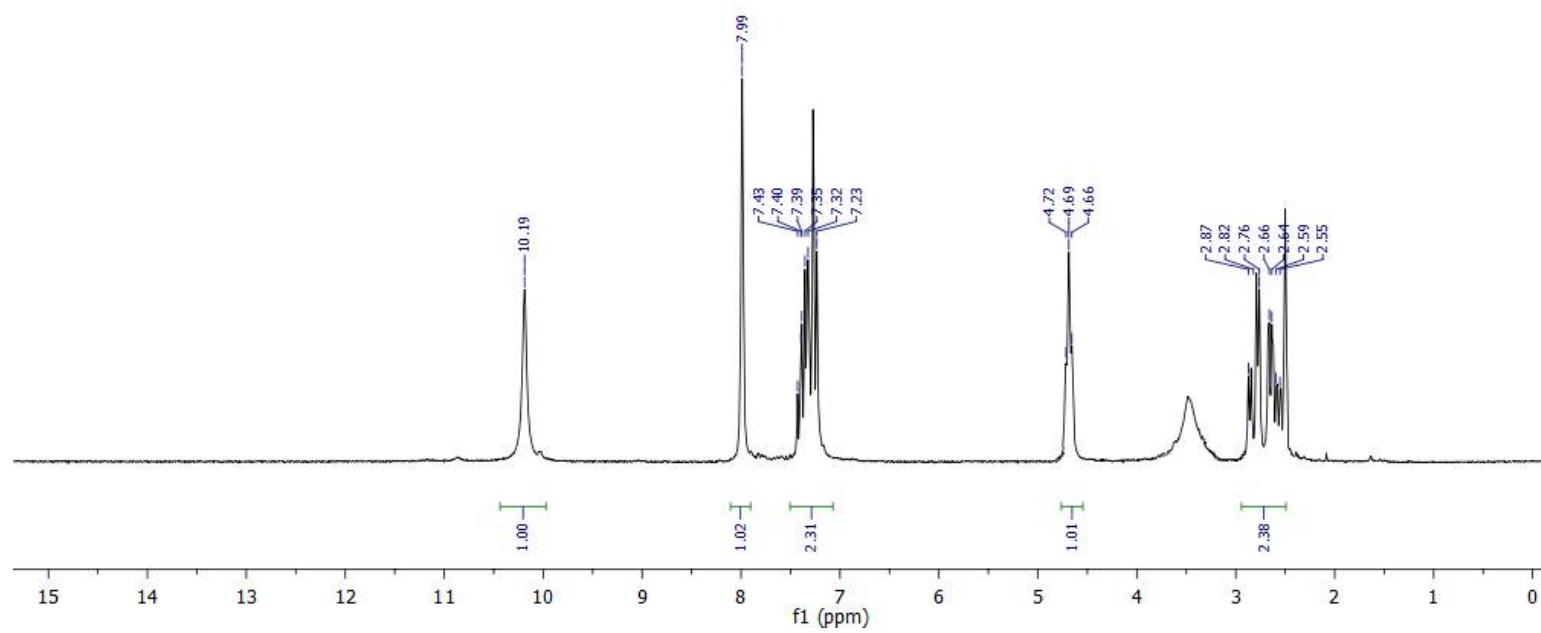


Figure S1. <sup>1</sup>H NMR spectrum of **2a**



**Figure S2.**  $^{13}\text{C}$  NMR spectrum of **2a**

dihydro-6-(3'-(hexahydro-2'',6''-dioxopyrimidin-4''-yl)phenyl)pyrimidine-2,4(1H,3H)-dione **2b**



**Figure S3.**  $^1\text{H}$  NMR spectrum of **2b**

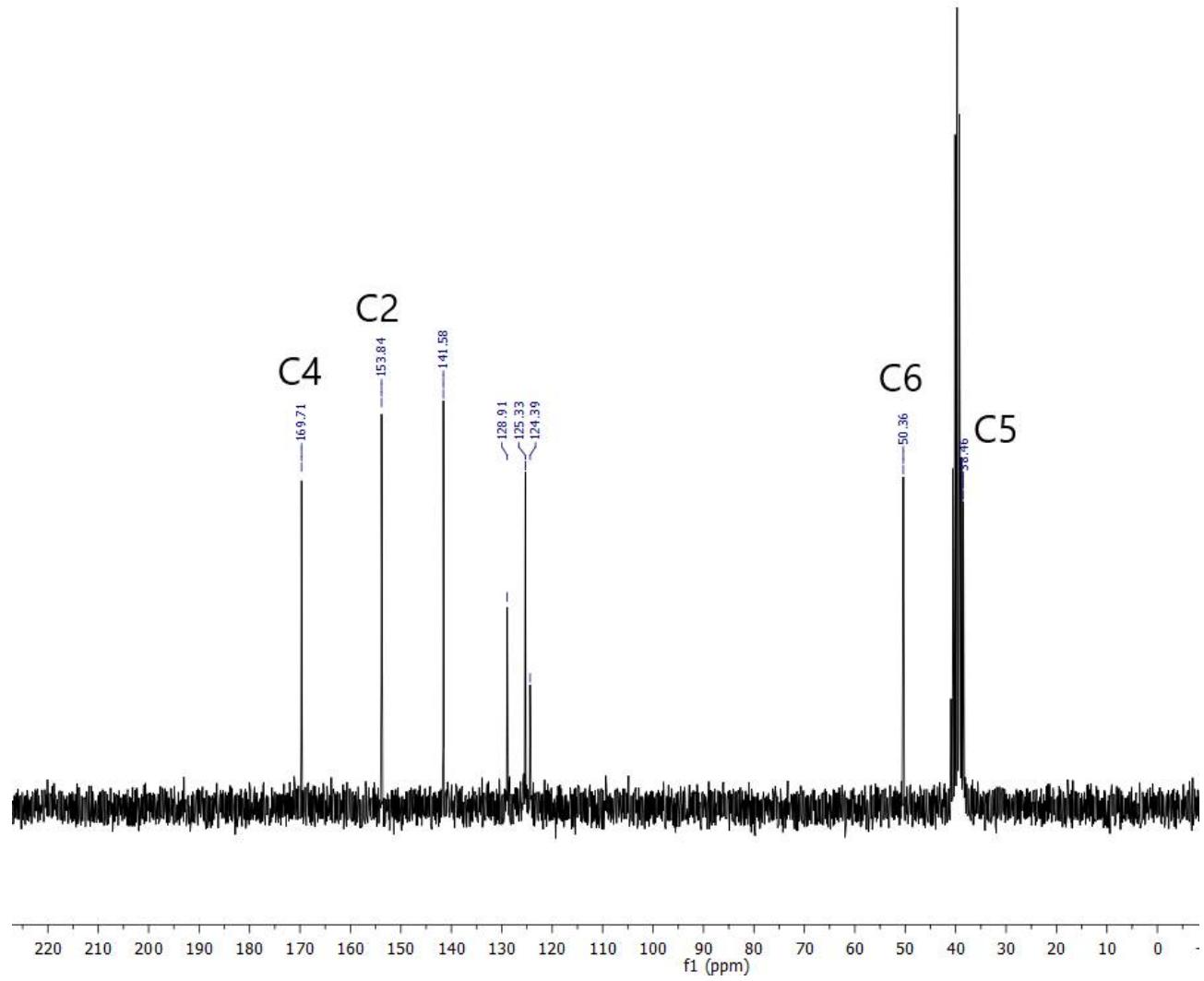
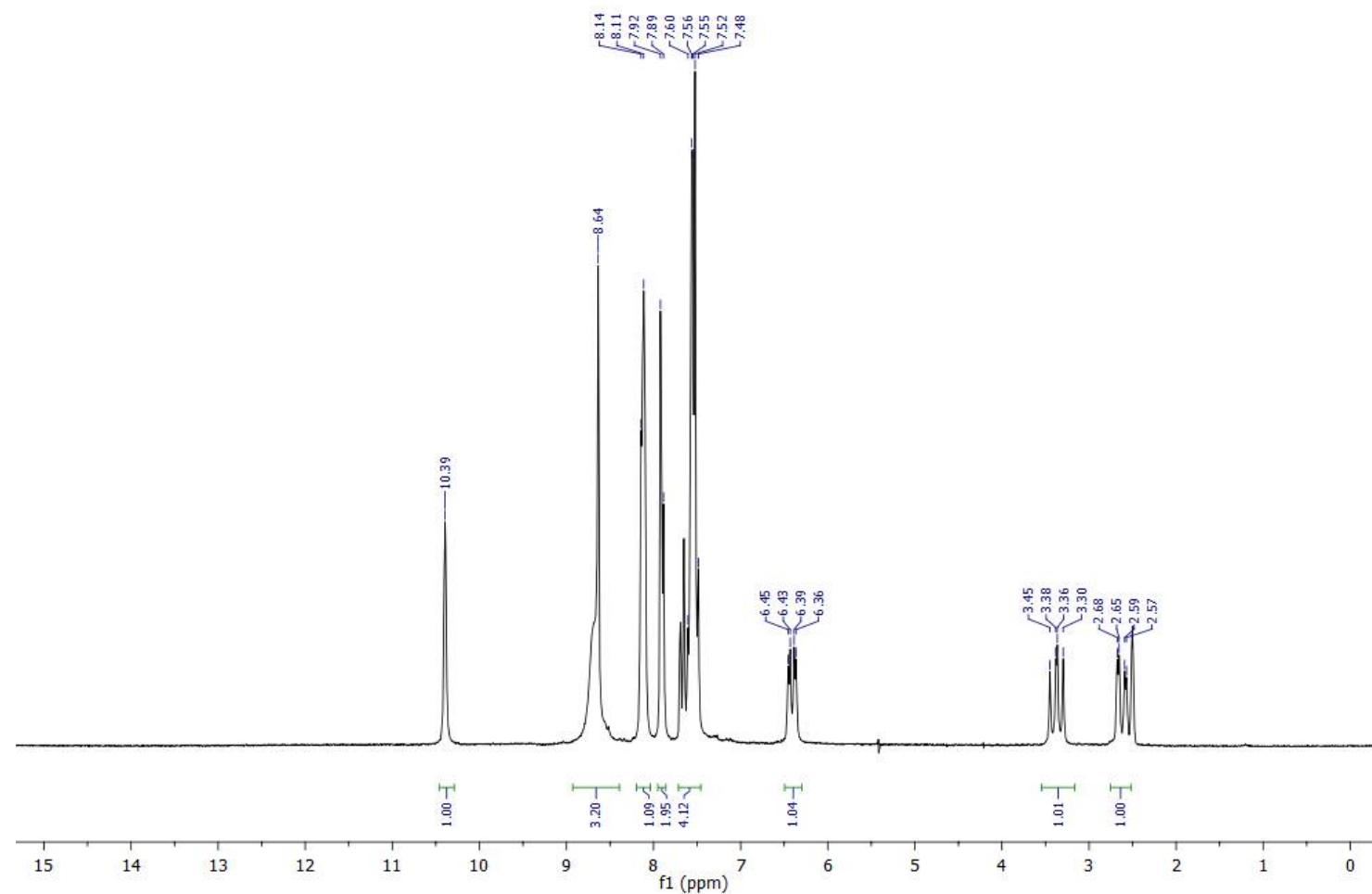
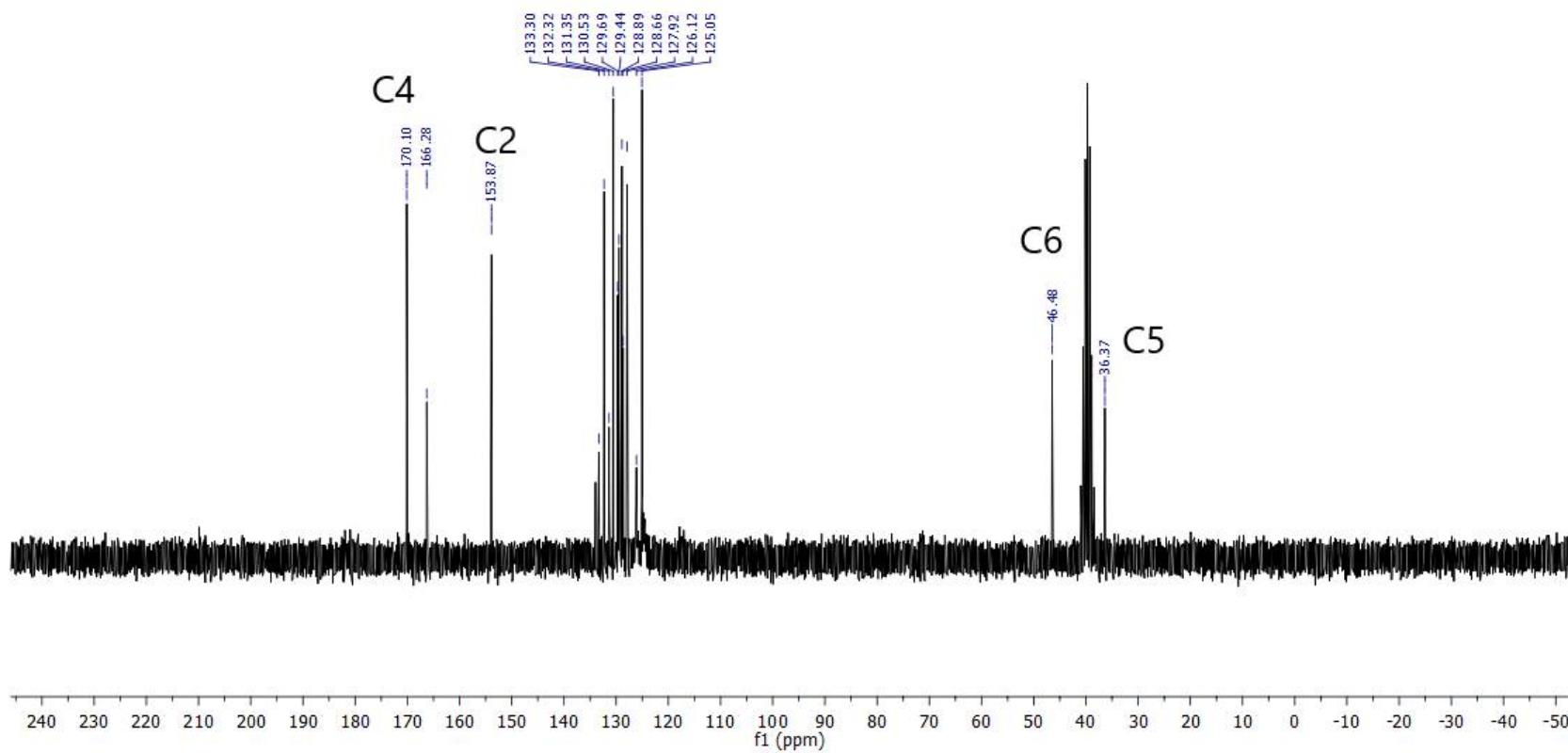


Figure S4.  $^{13}\text{C}$  NMR spectrum of **2b**

6-(anthracen-10'-yl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2c**



**Figure S5.** <sup>1</sup>H NMR spectrum of **2c** (aromatic protons in range 8.4-8.9 ppm originated from m-chlorobenzoic acid)



**Figure S6.**  $^{13}\text{C}$  NMR spectrum of **2c** [(carbonyl (COOH) at 166.3 ppm originated from m-chlorobenzoic acid)]

6-(4'-fluorophenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2d**

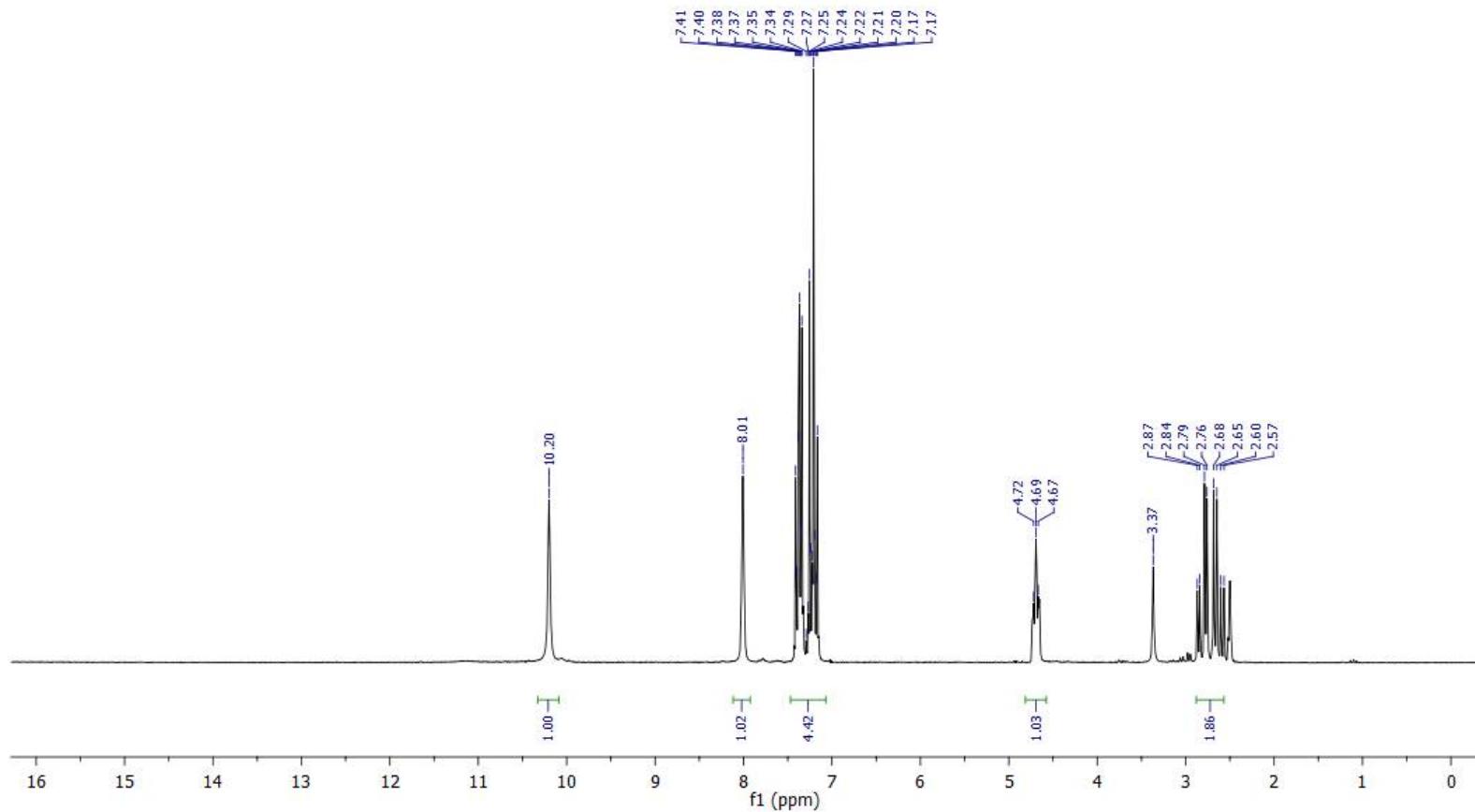
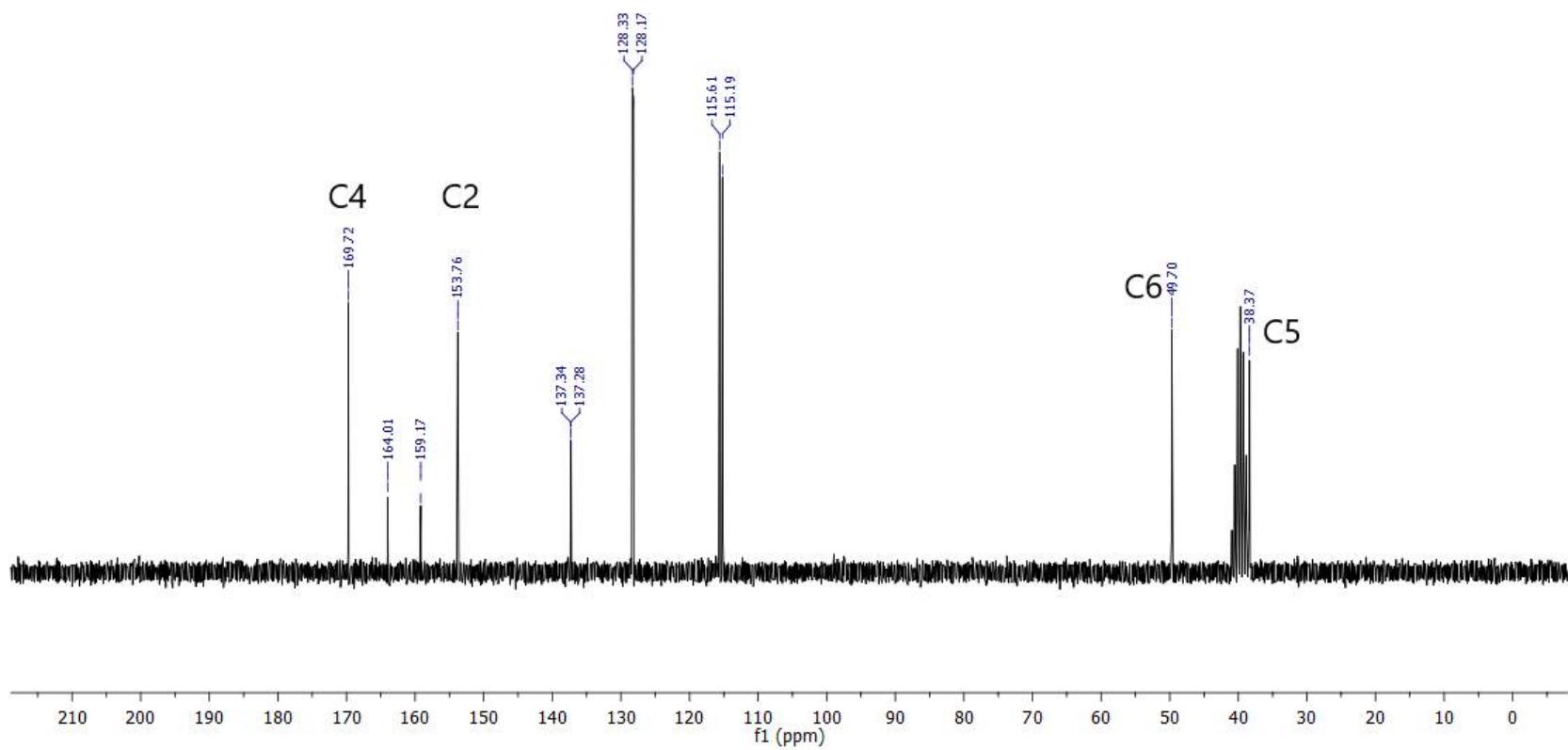


Figure S7. <sup>1</sup>H NMR spectrum of **2d**



**Figure S8.**  $^{13}\text{C}$  NMR spectrum of **2d**

6-(2'-chlorophenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2e**

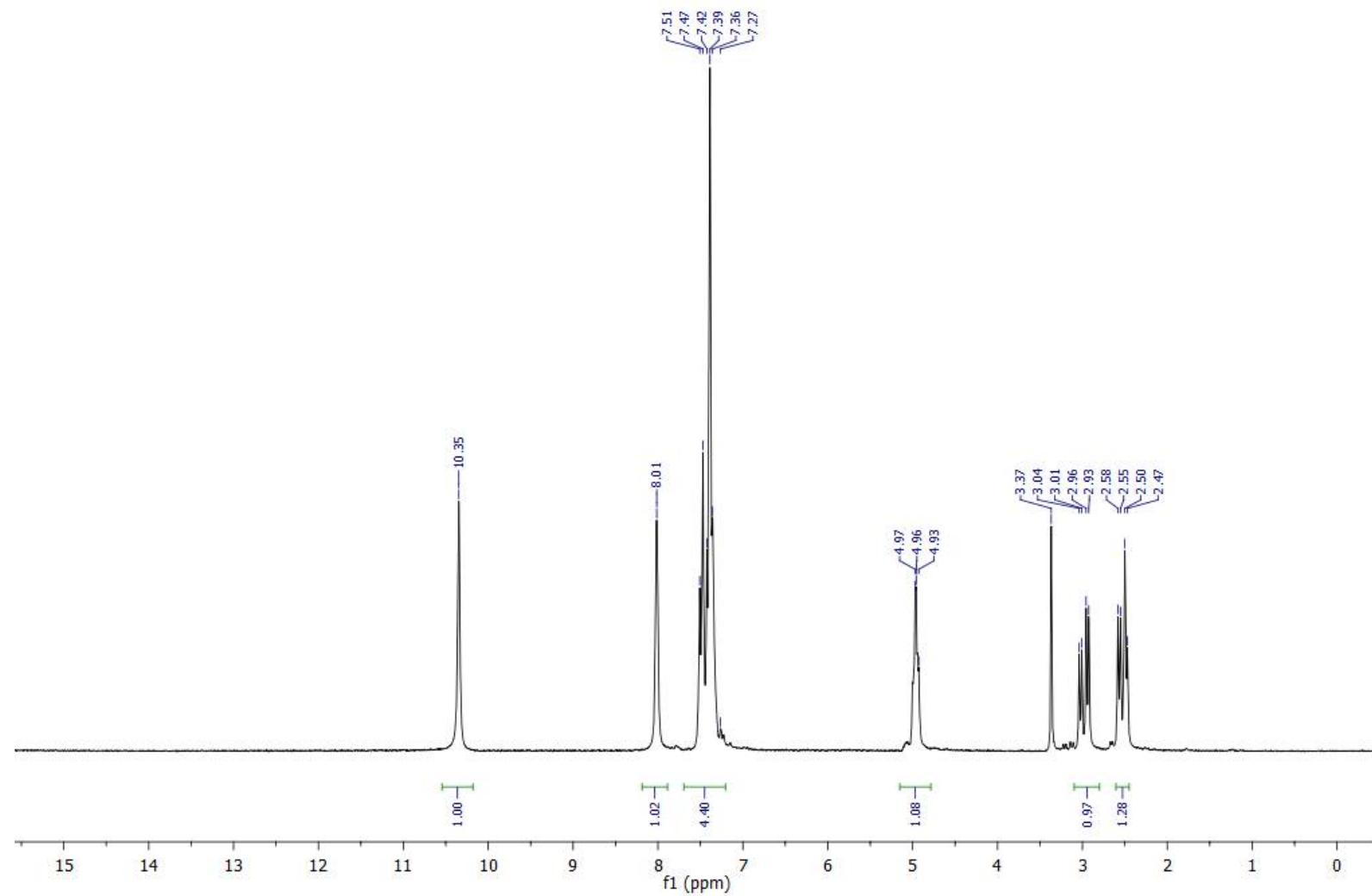
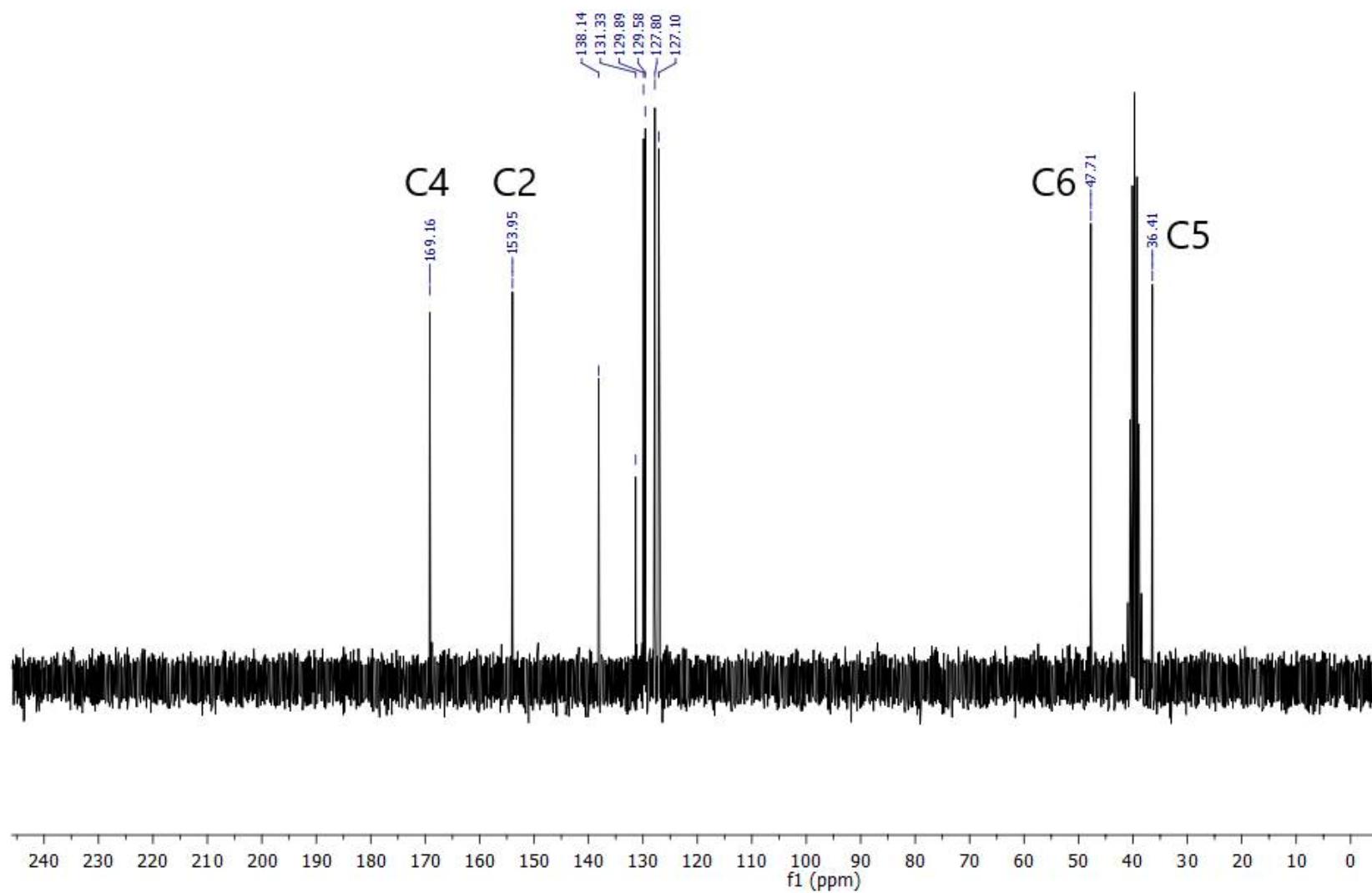
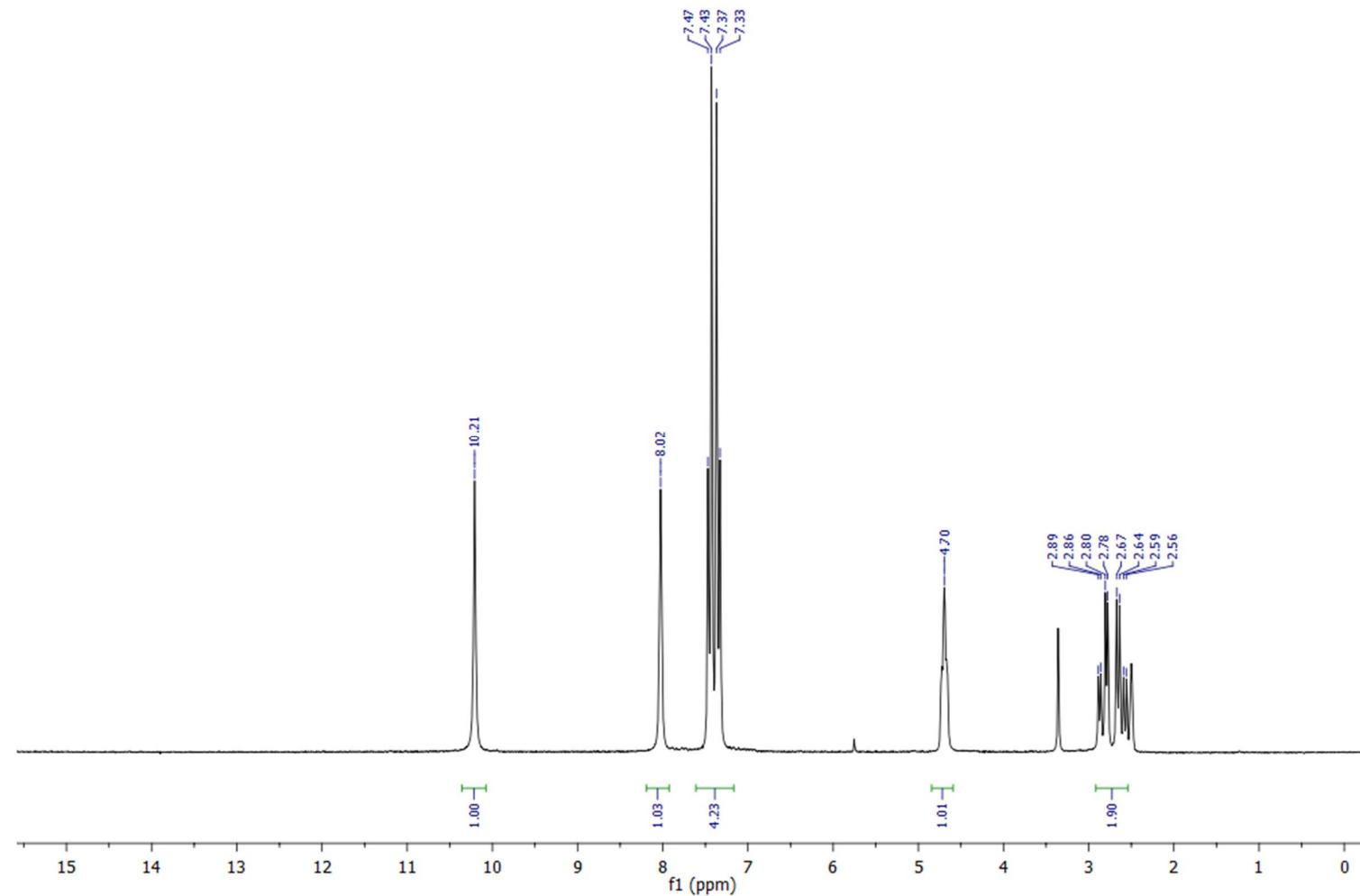


Figure S9.  $^1\text{H}$  NMR spectrum of **2e**

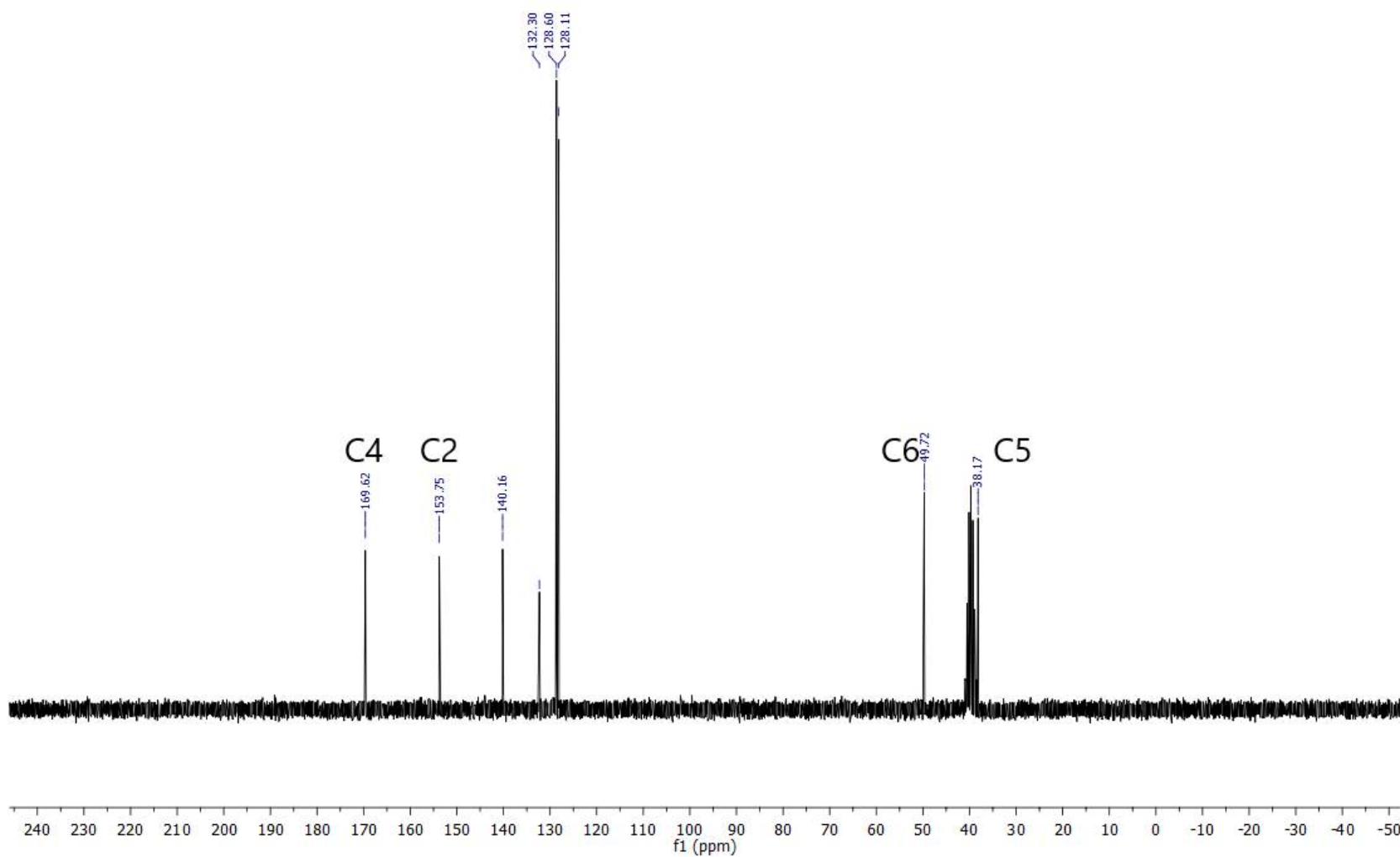


**Figure S10.**  $^{13}\text{C}$  NMR spectrum of **2e**

6-(4'-chlorophenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2f**



**Figure S11.**  $^1\text{H}$  NMR spectrum of **2f**



**Figure S12.**  $^{13}\text{C}$  NMR spectrum of **2f**

6-(4'-nitrophenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2g**

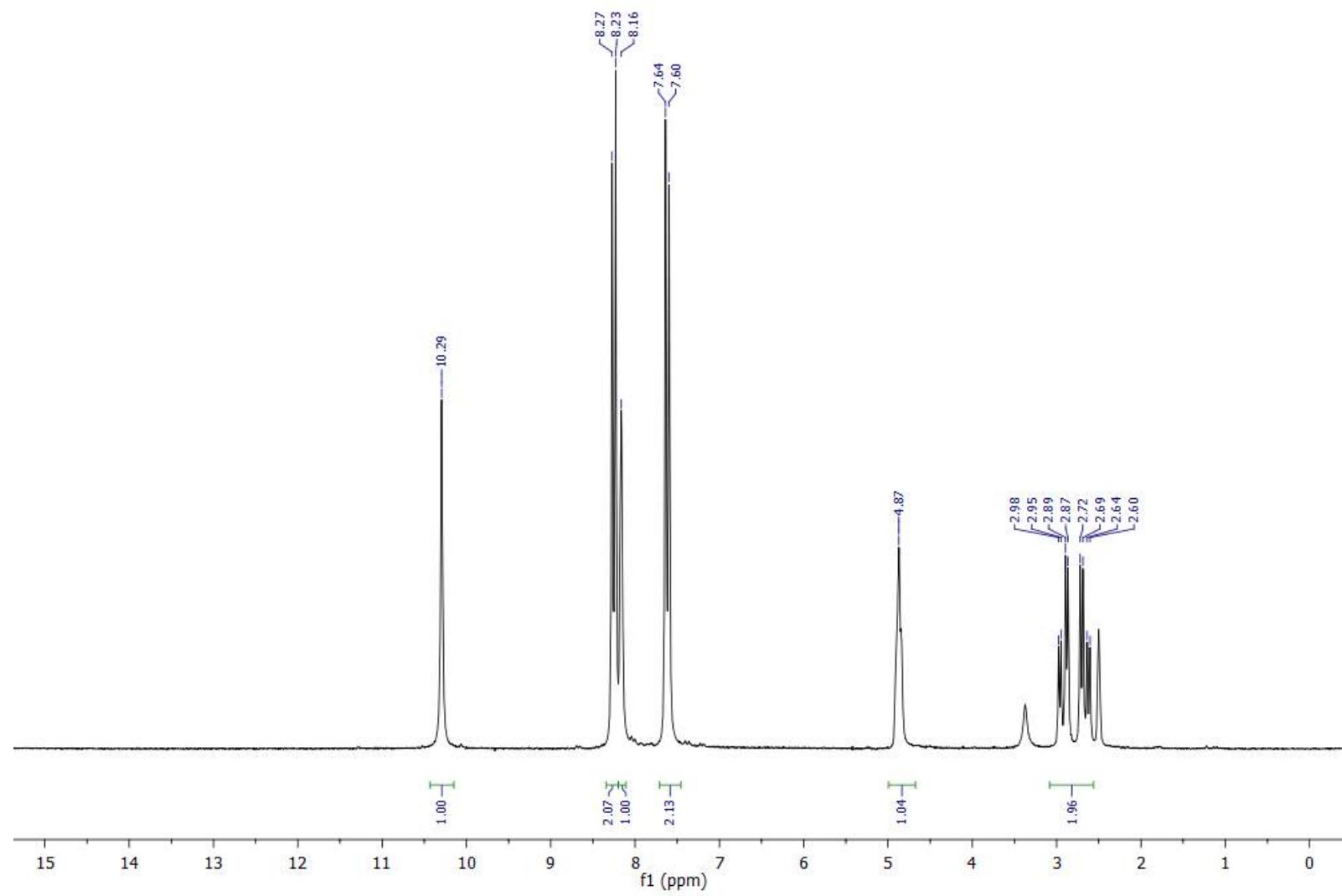


Figure S13. <sup>1</sup>H NMR spectrum of **2g**

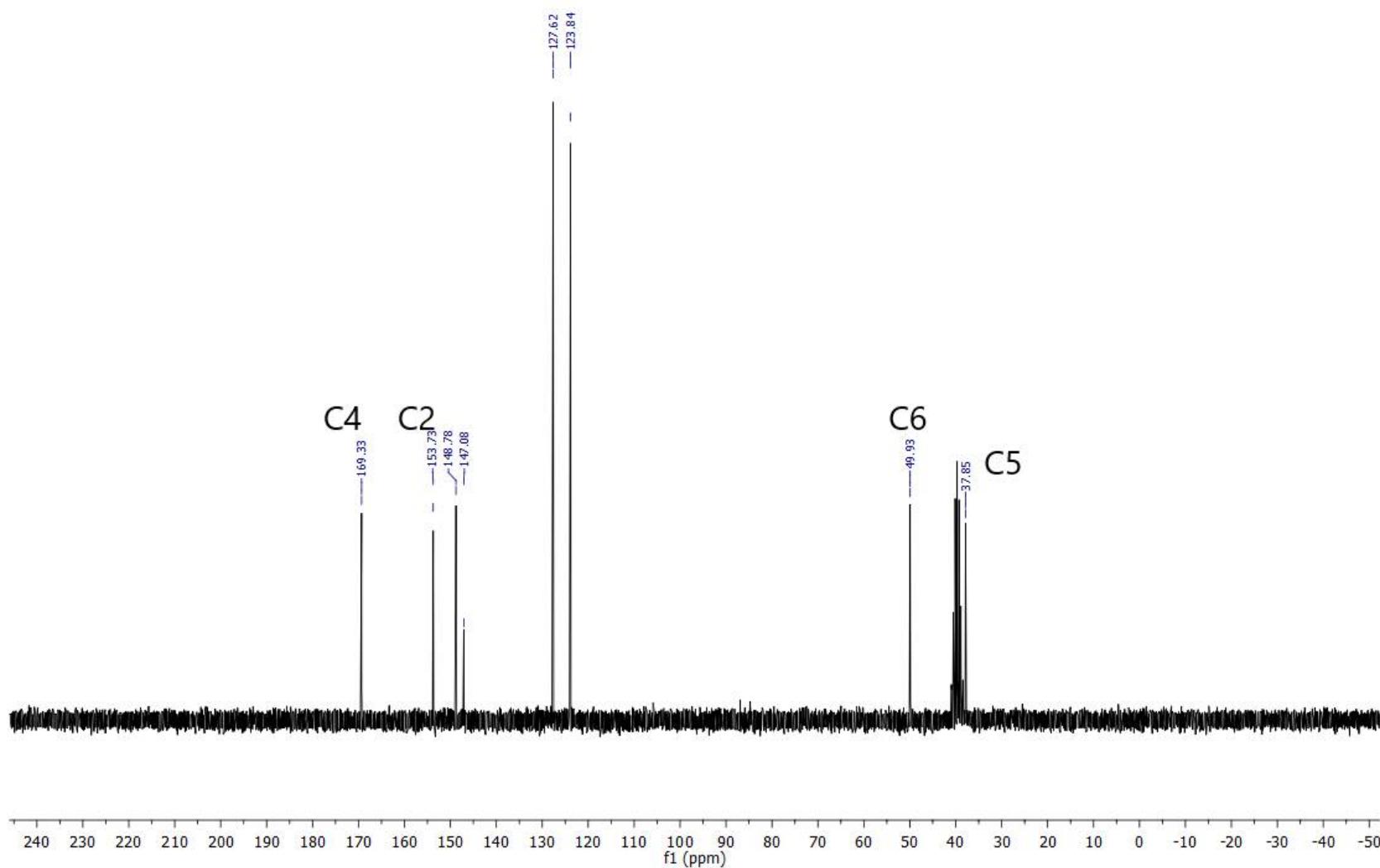


Figure S14.  $^{13}\text{C}$  NMR spectrum of **2g**

6-(4'-benzyloxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2h**

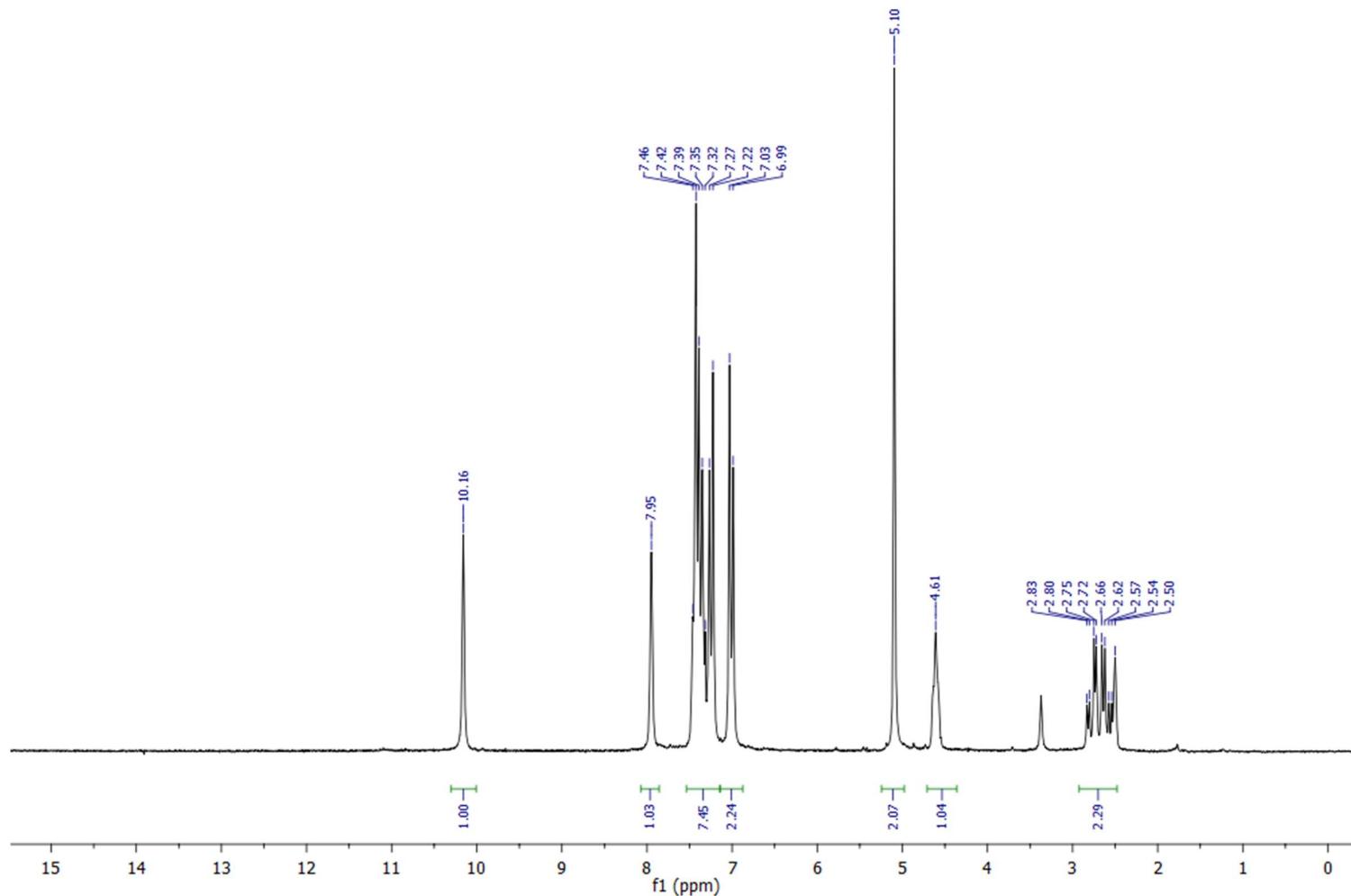
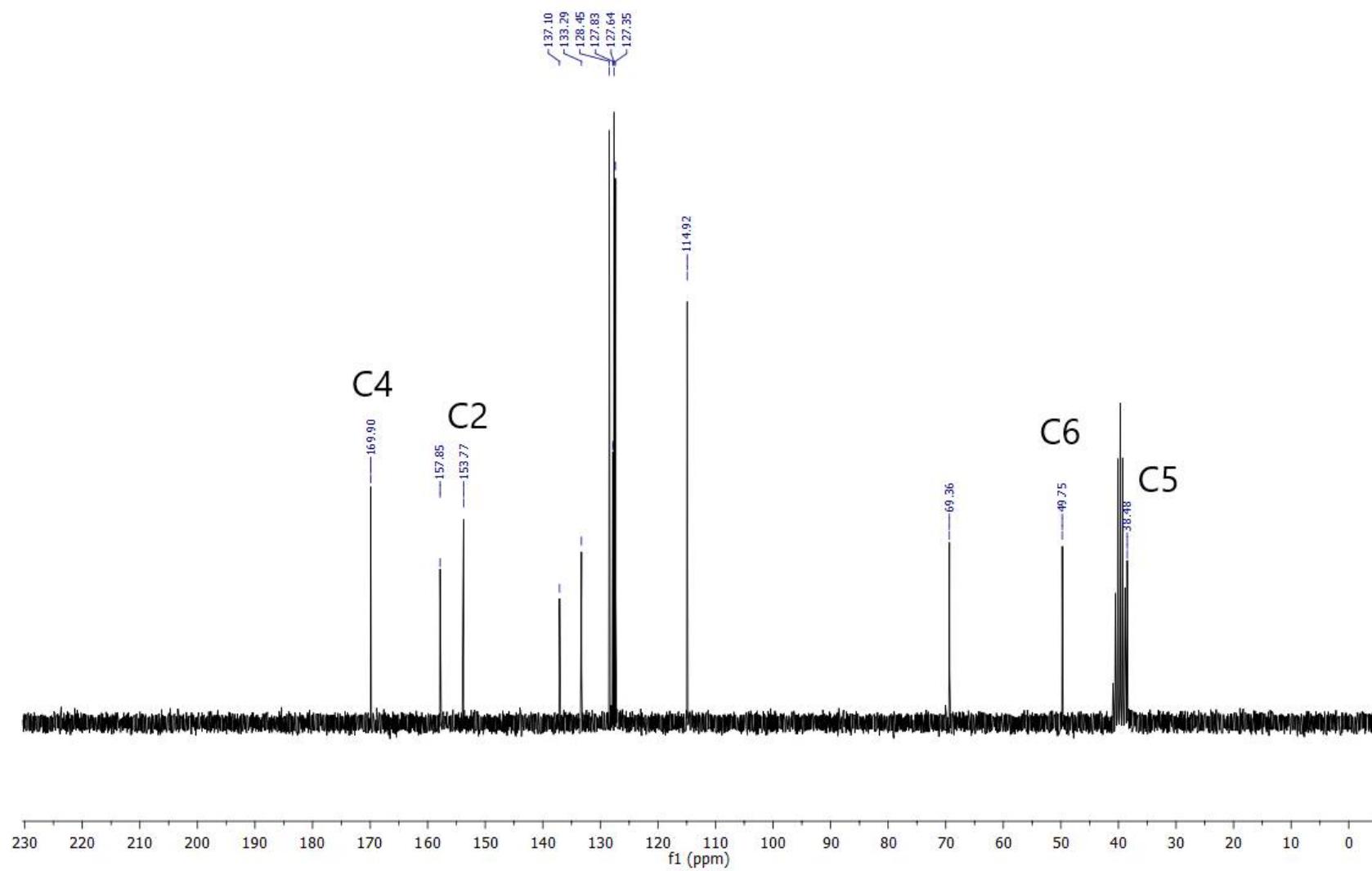
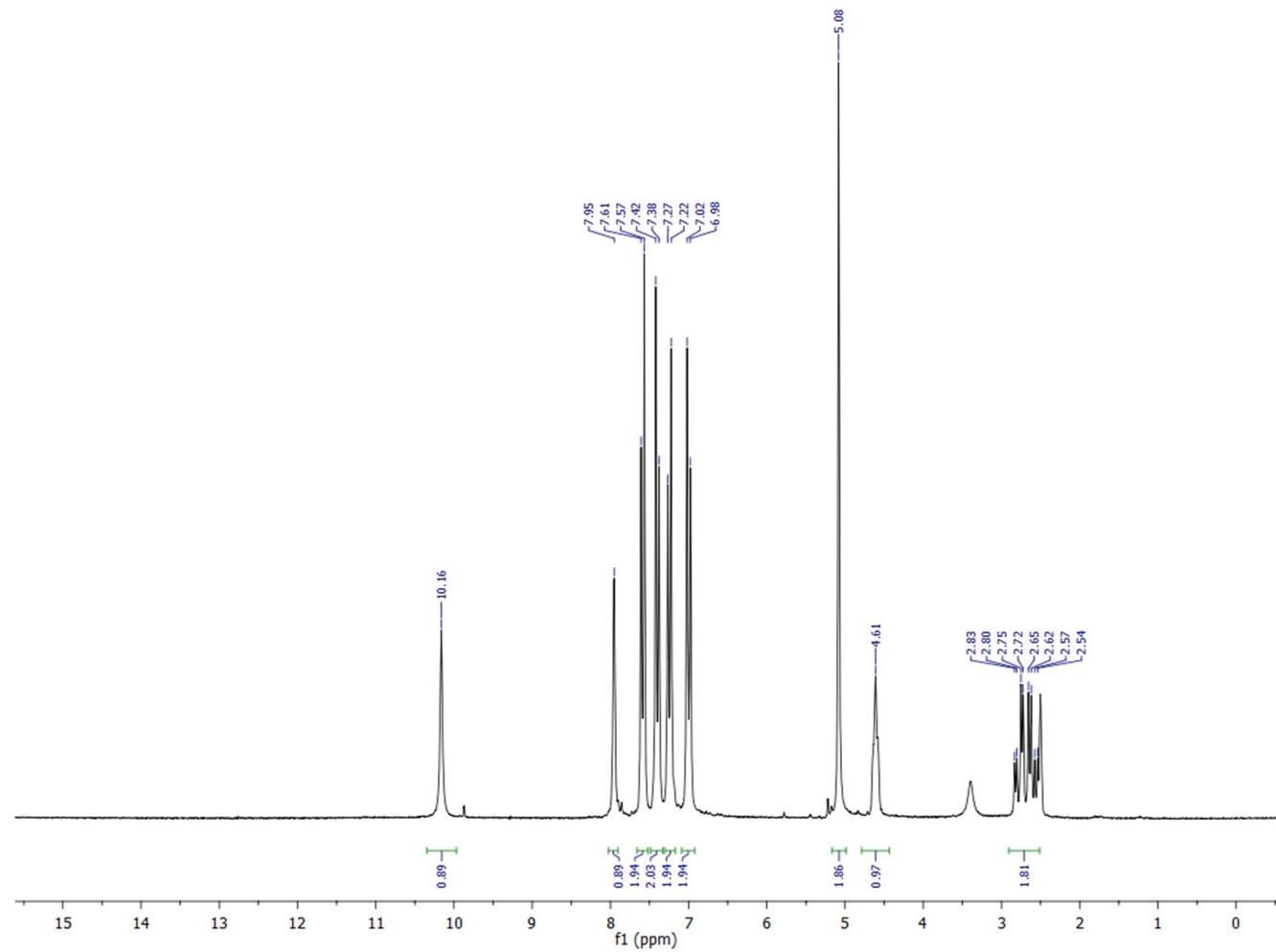


Figure S15.  $^1\text{H}$  NMR spectrum of **2h**

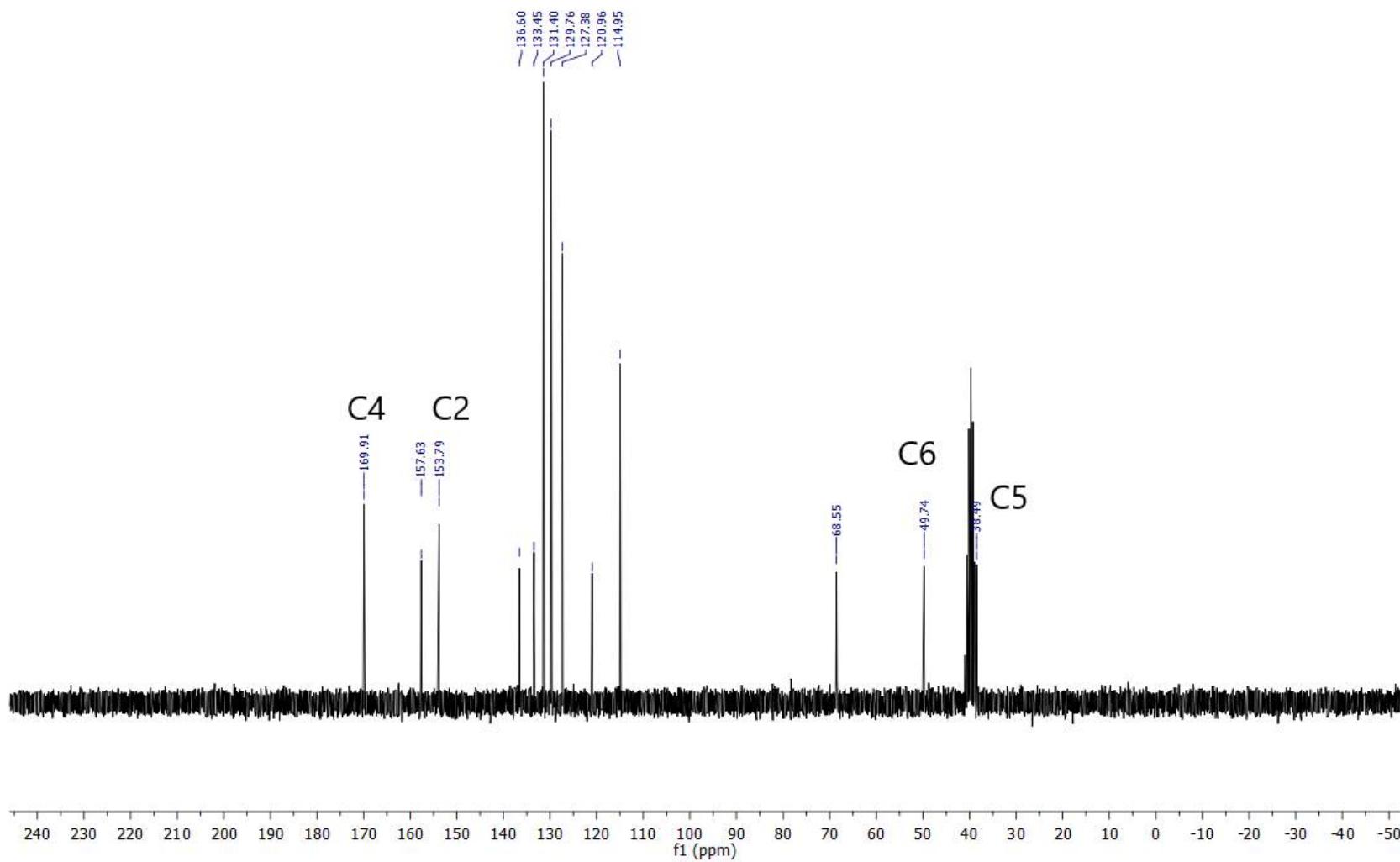


**Figure S16.**  $^{13}\text{C}$  NMR spectrum of **2h**

6-(4'-(4''-bromobenzyl)oxy)phenyl-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2i**

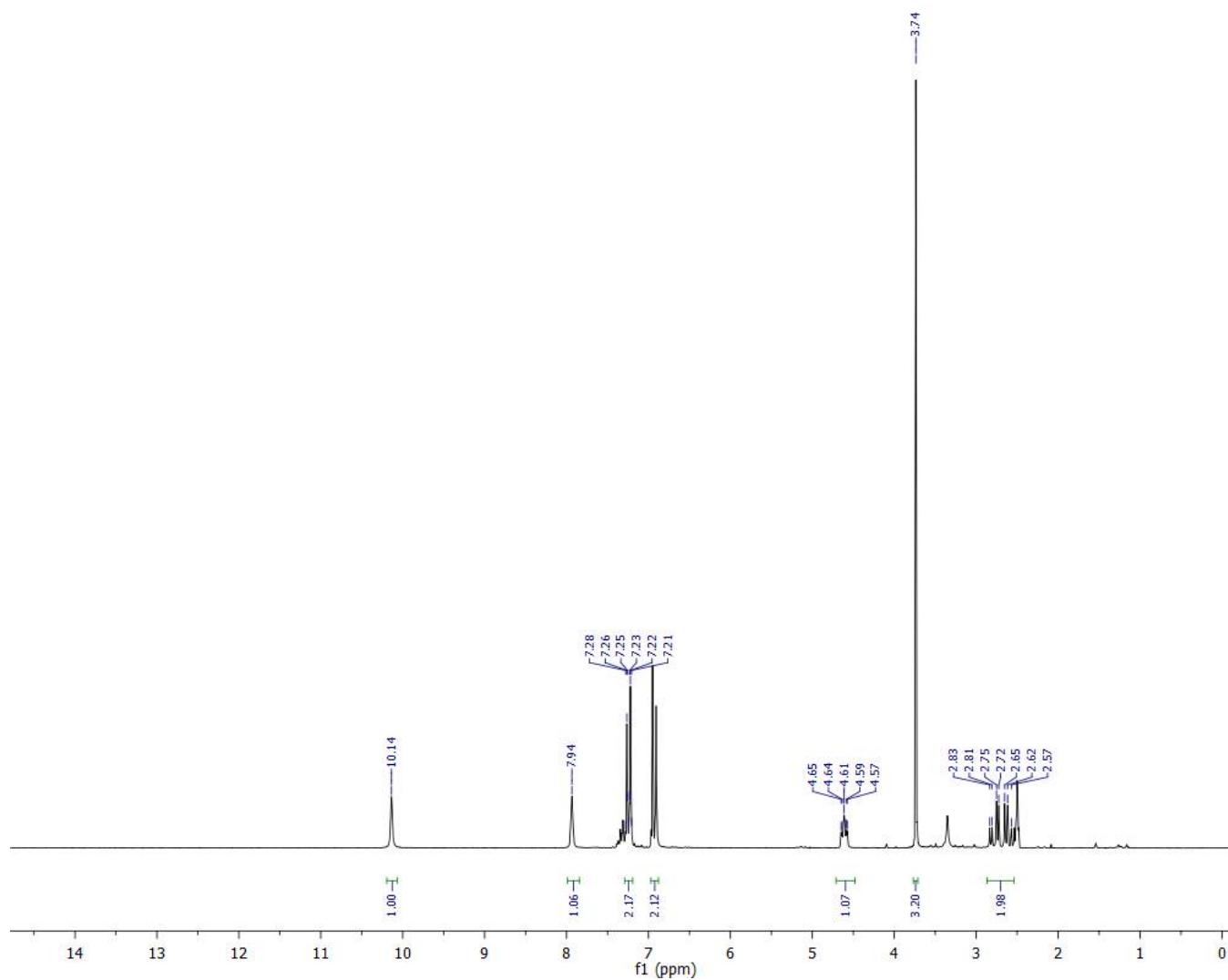


**Figure S17.**  $^1\text{H}$  NMR spectrum of **2i**

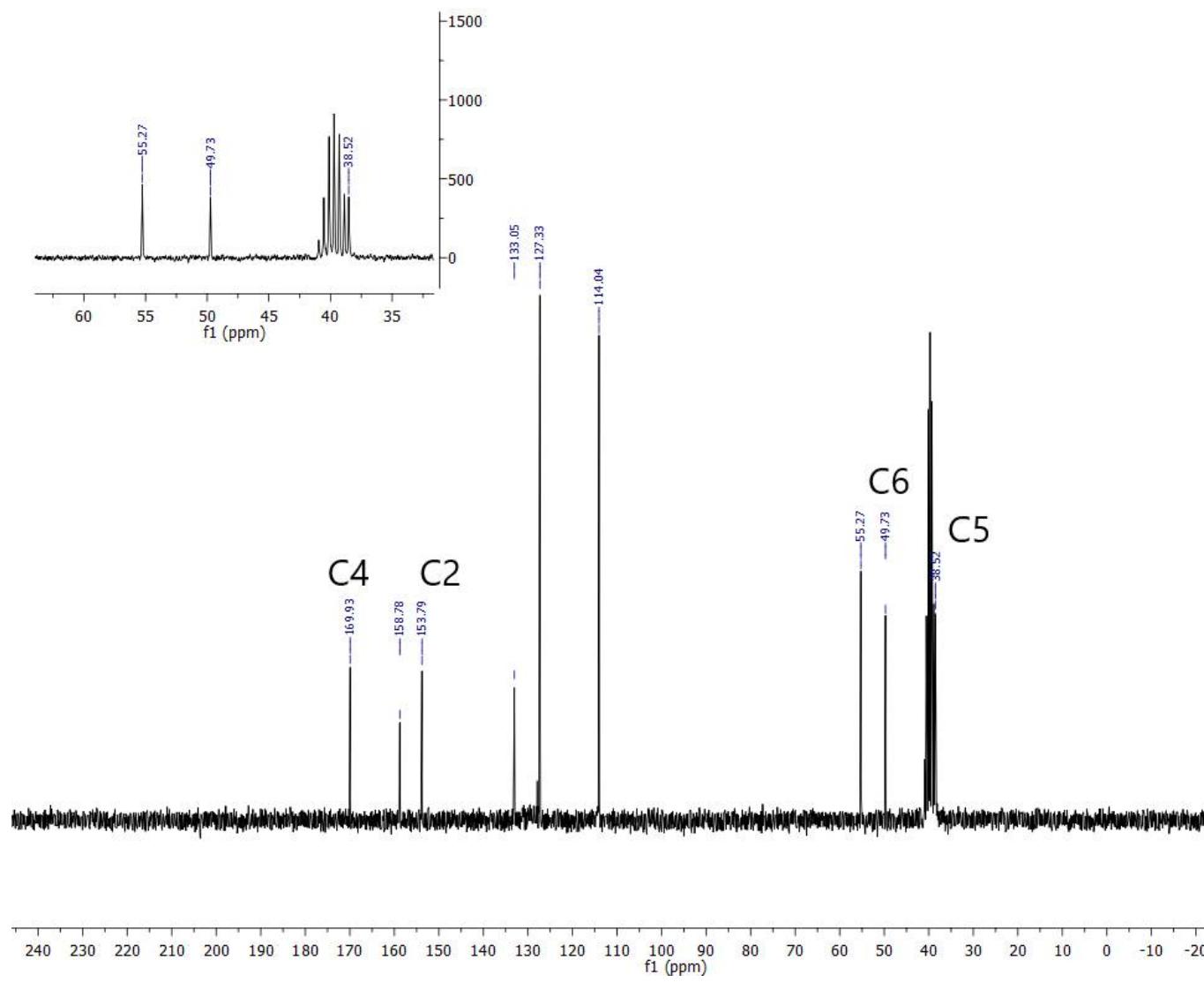


**Figure S18.**  $^{13}\text{C}$  NMR spectrum of **2i**

dihydro-6-(4'-methoxyphenyl)pyrimidine-2,4(1H,3H)-dione **2j**



**Figure S19.** <sup>1</sup>H NMR spectrum of **2j**



**Figure S20.**  $^{13}\text{C}$  NMR spectrum of **2j**

6-(3',4'-dimethoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2k**

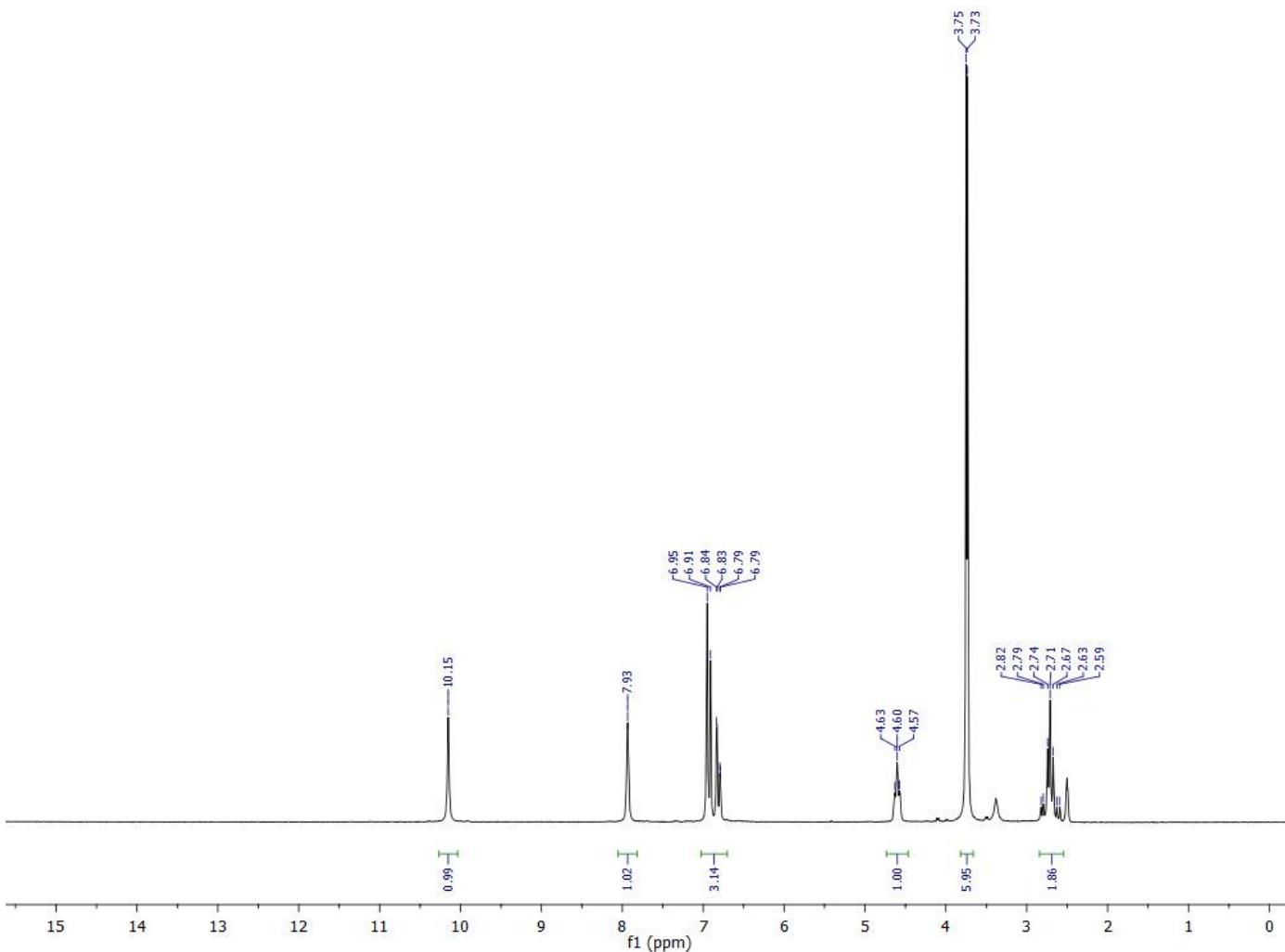
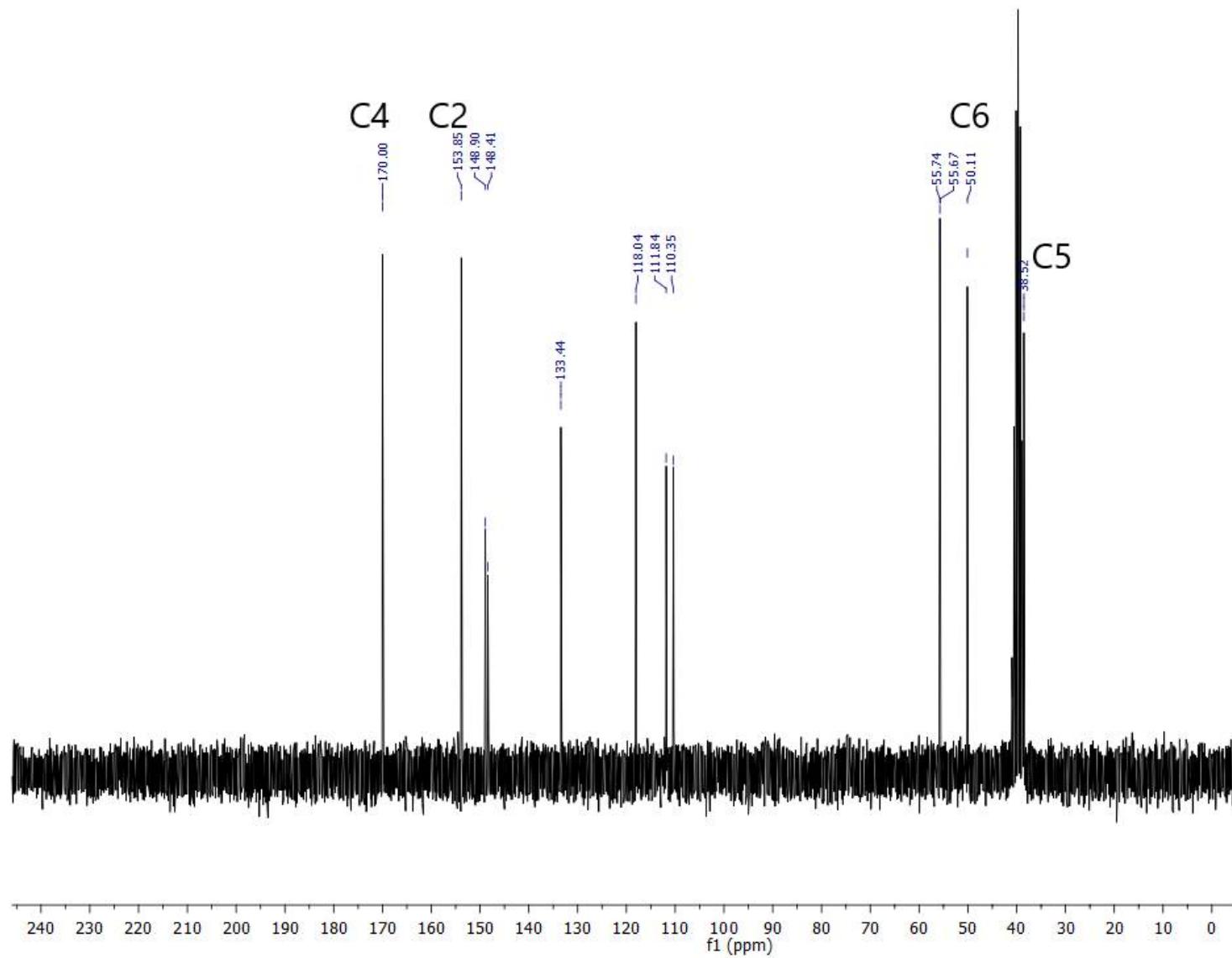


Figure S21. <sup>1</sup>H NMR spectrum of **2k**



**Figure S22.**  $^{13}\text{C}$  NMR spectrum of **2k**

dihydro-6-(3',4',5'-trimethoxyphenyl)pyrimidine-2,4(1H,3H)-dione **2l**

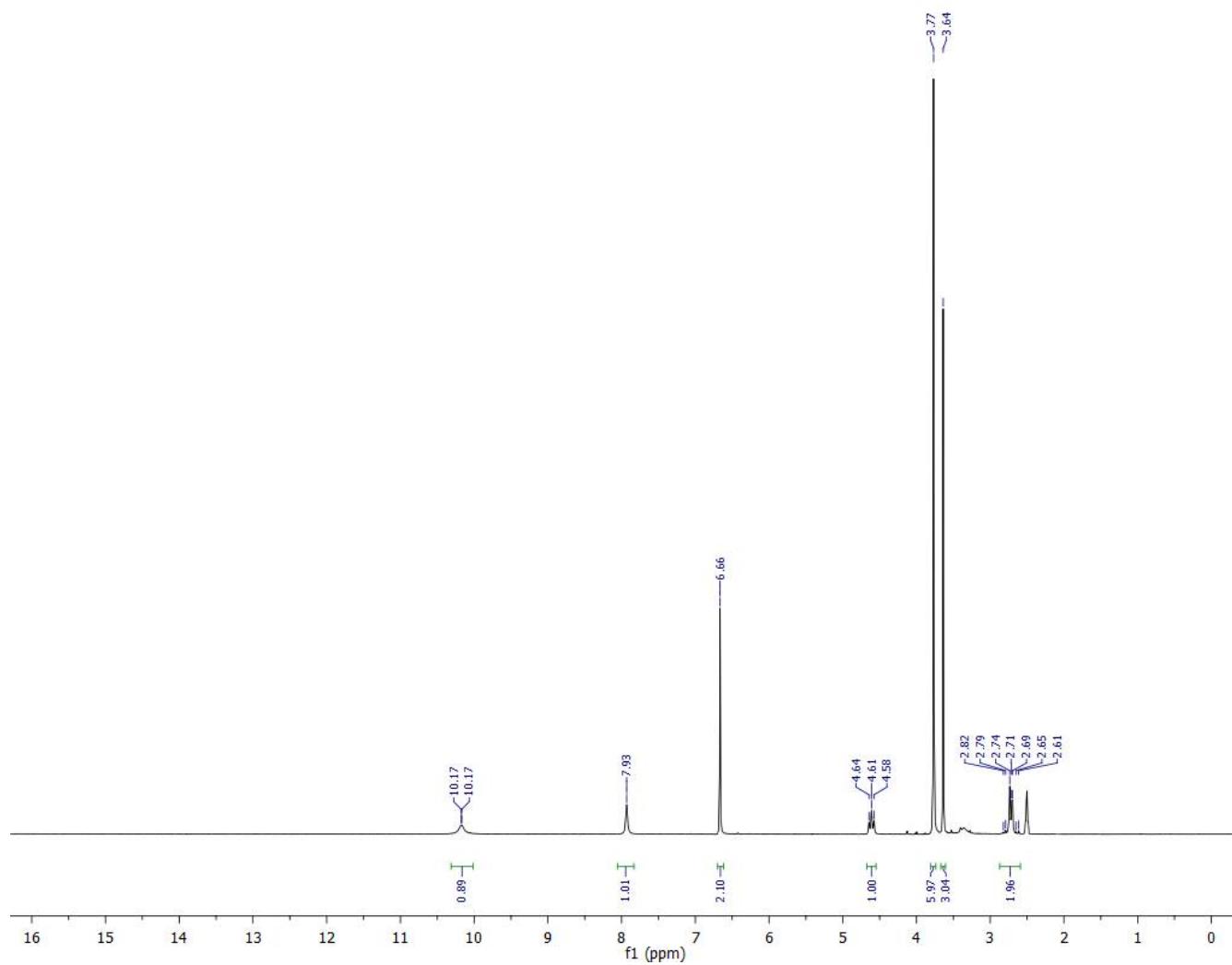
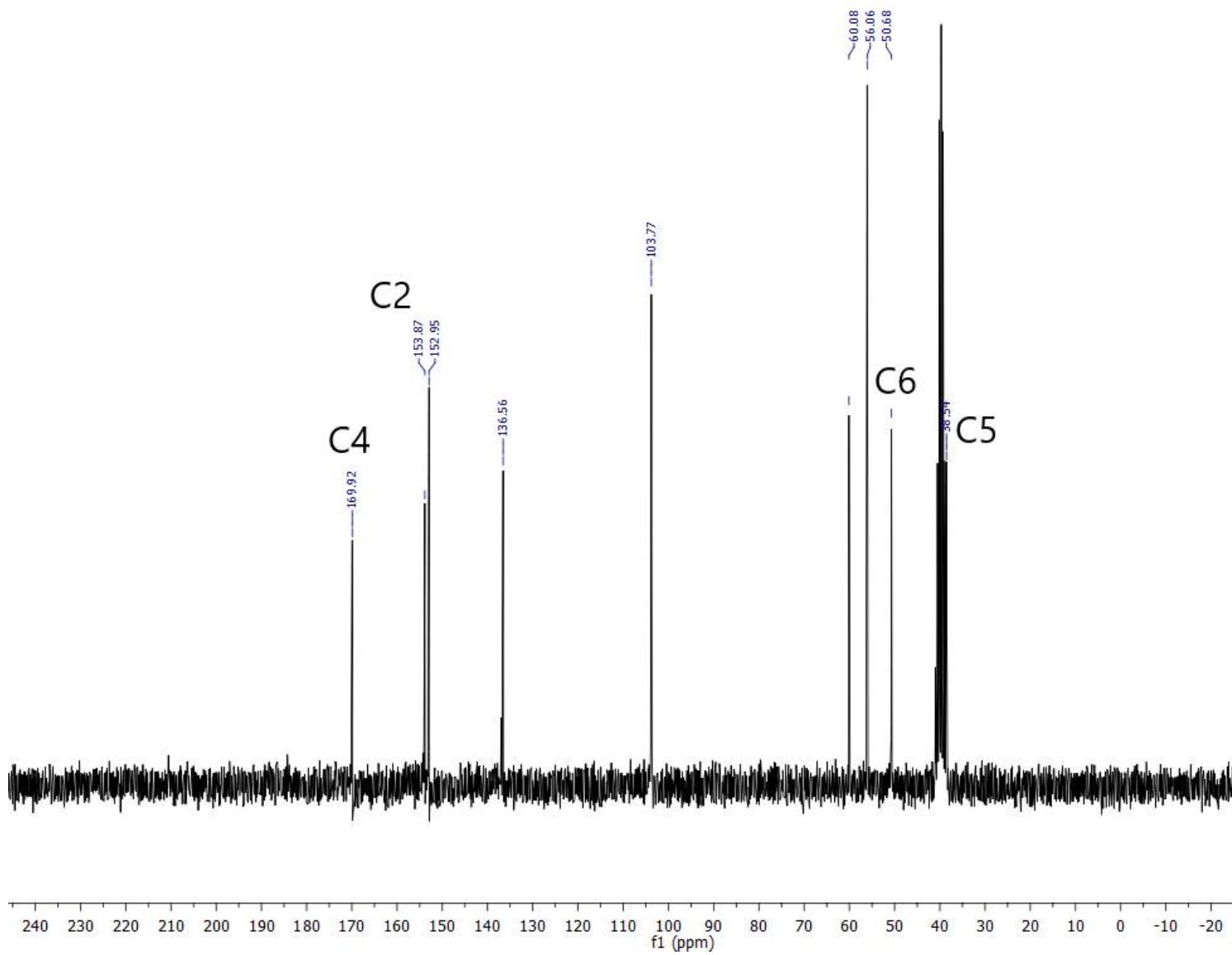


Figure S23. <sup>1</sup>H NMR spectrum of **2l**



**Figure S24.**  $^{13}\text{C}$  NMR spectrum of **2I**

6-(4'-ethoxy-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2m**

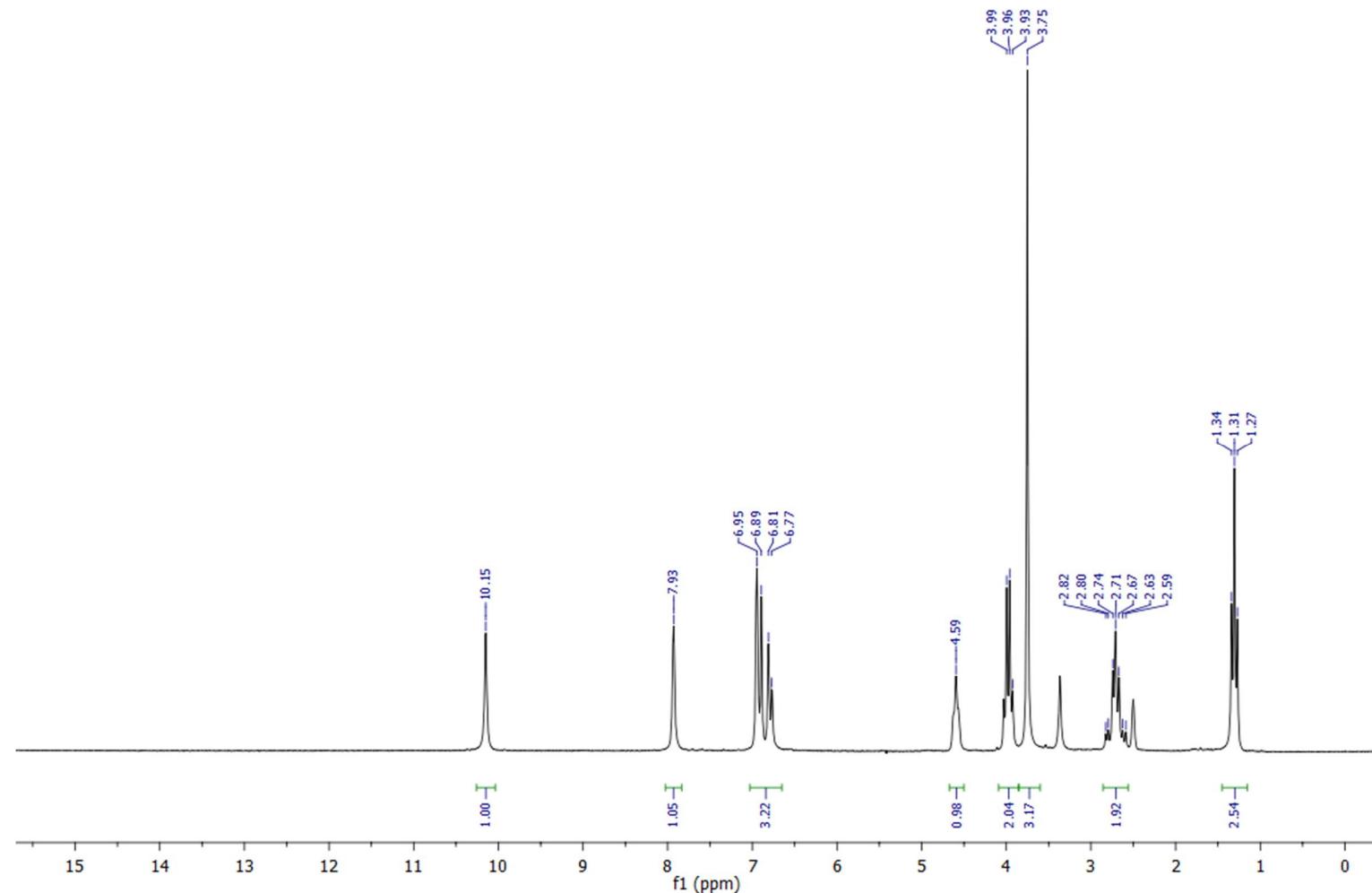
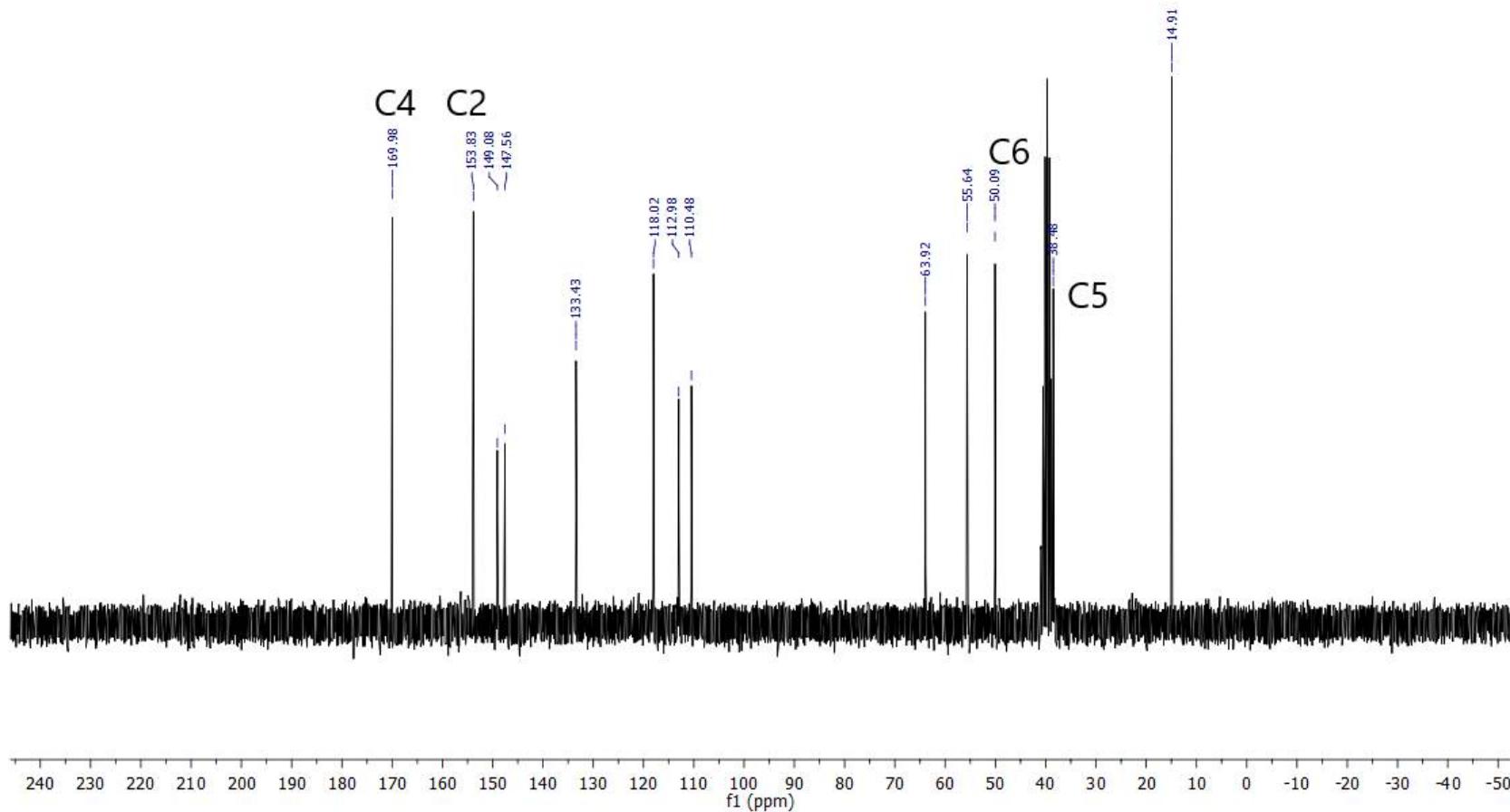
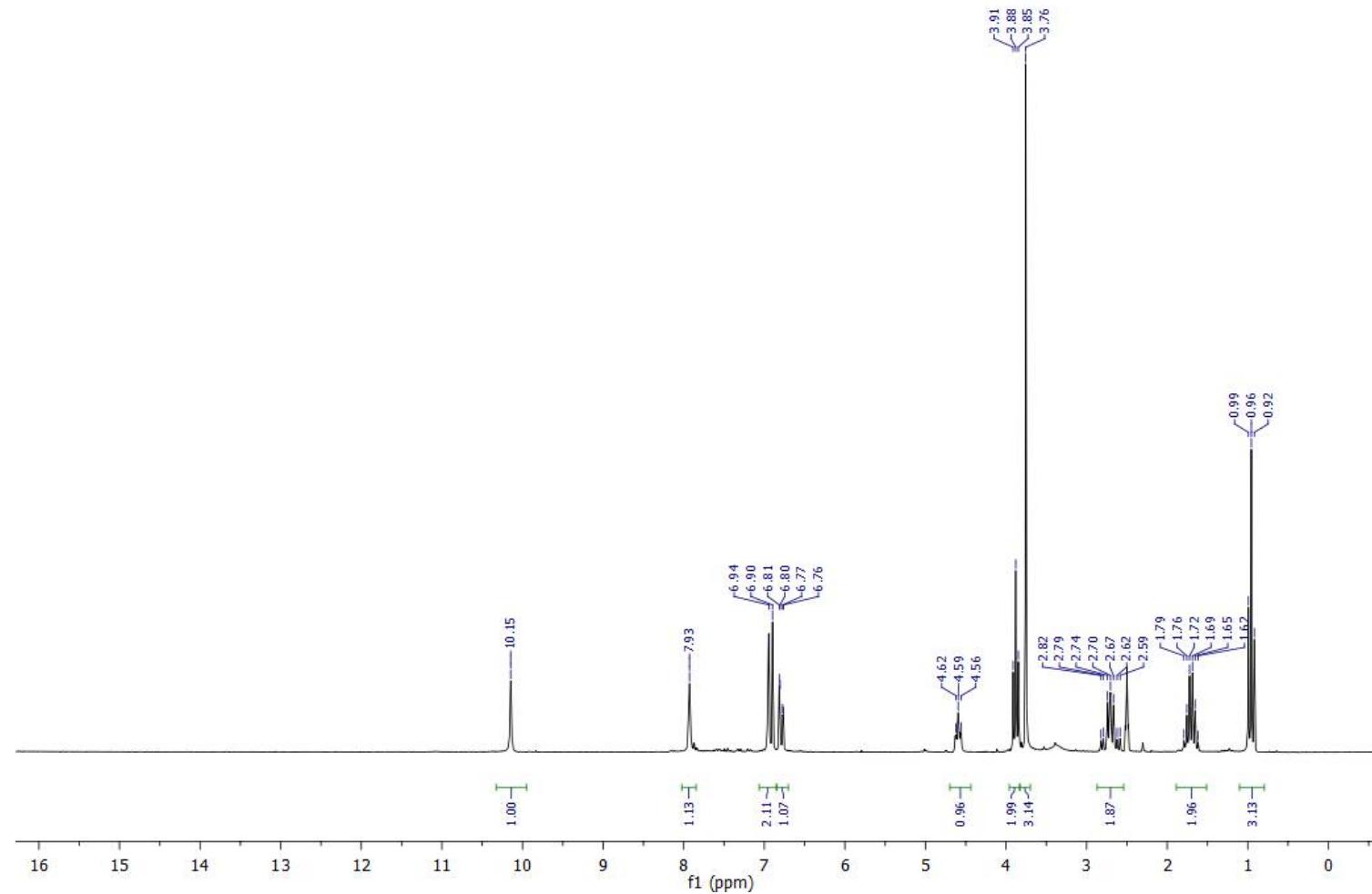


Figure S25. <sup>1</sup>H NMR spectrum of **2m**

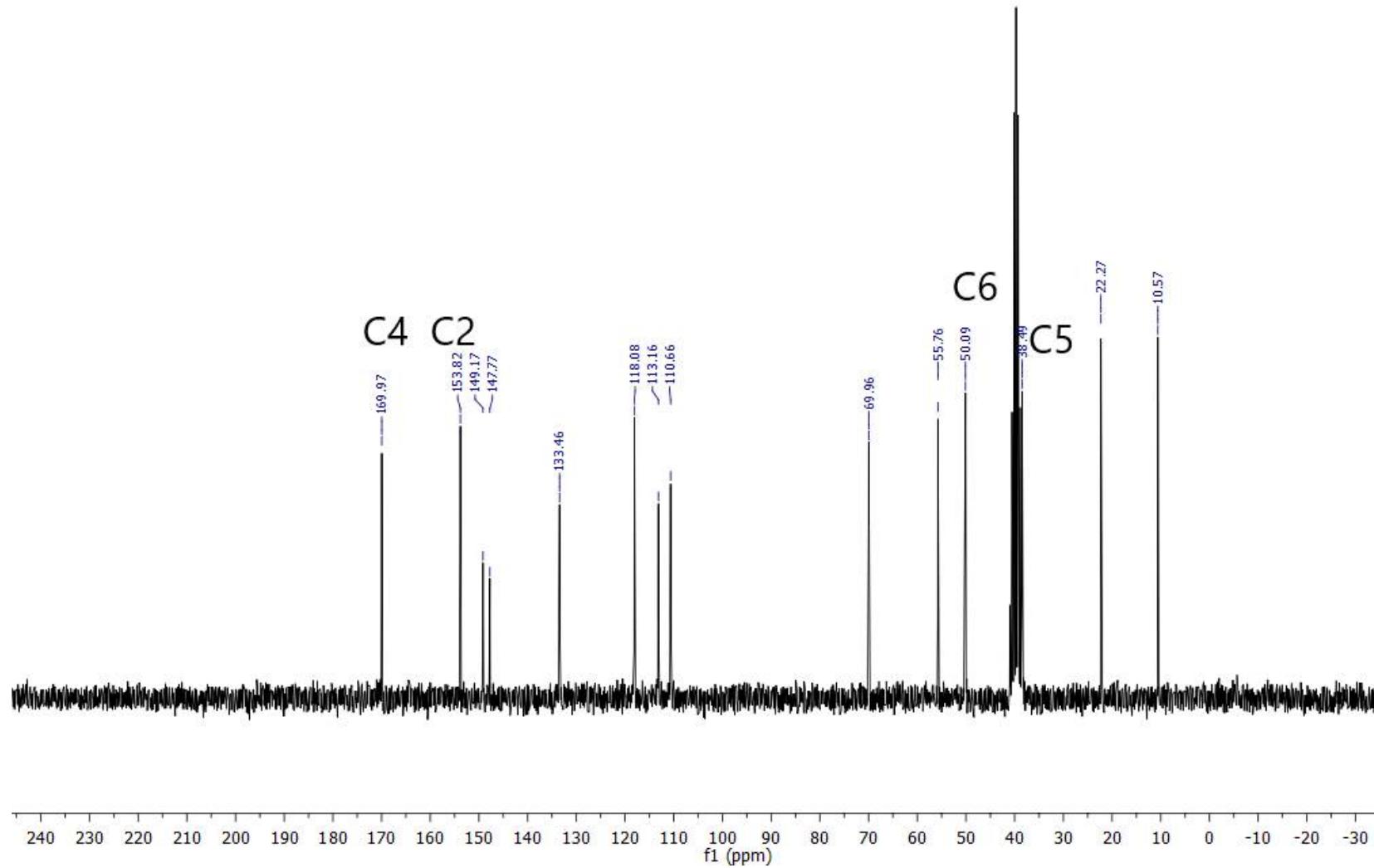


**Figure S26.**  $^{13}\text{C}$  NMR spectrum of **2m**

*6-(4'-propoxy-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2n***



**Figure S27.**  $^1\text{H}$  NMR spectrum of **2n**



**Figure S28.**  $^{13}\text{C}$  NMR spectrum of **2n**

6-(4'-butoxy-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2o**

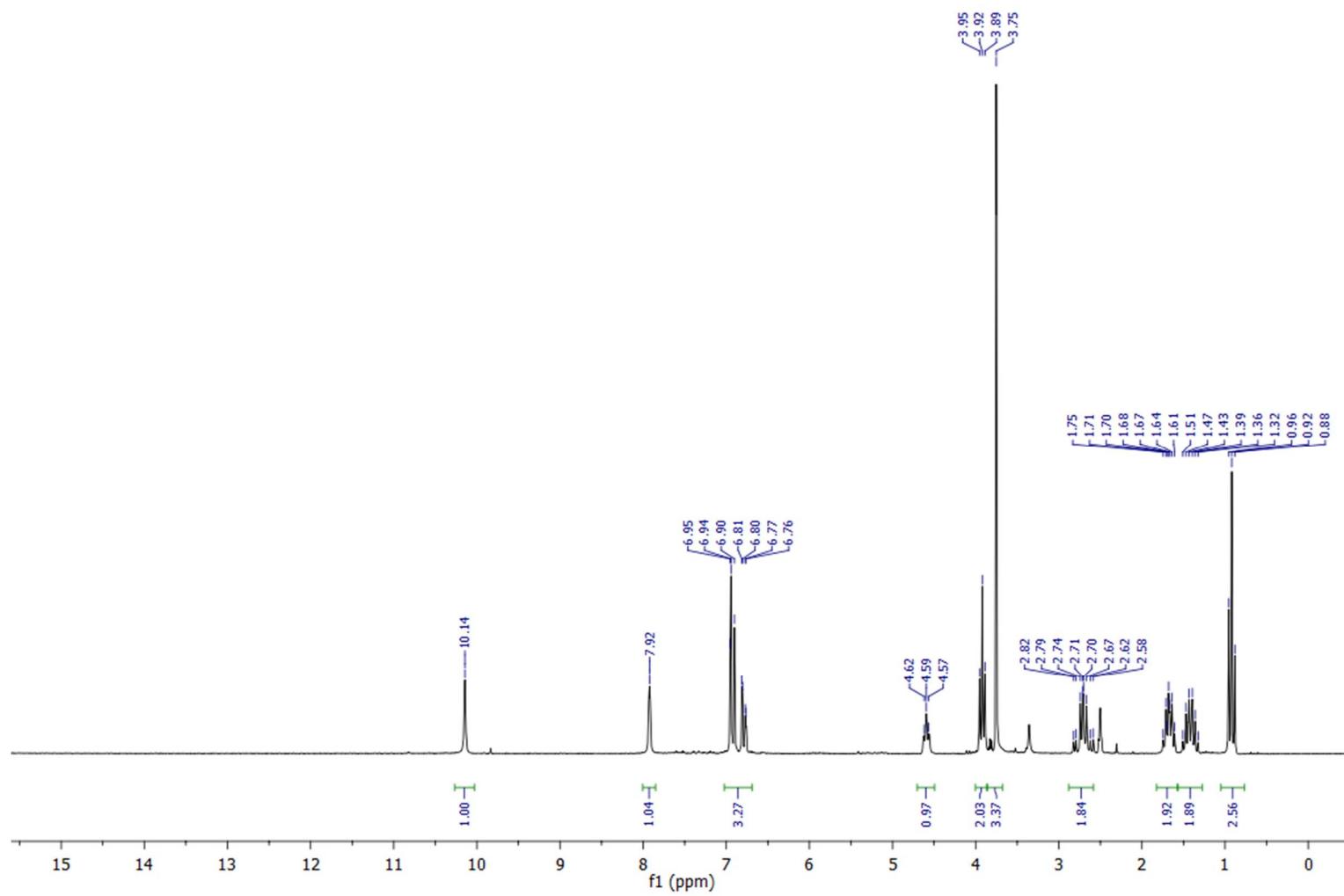
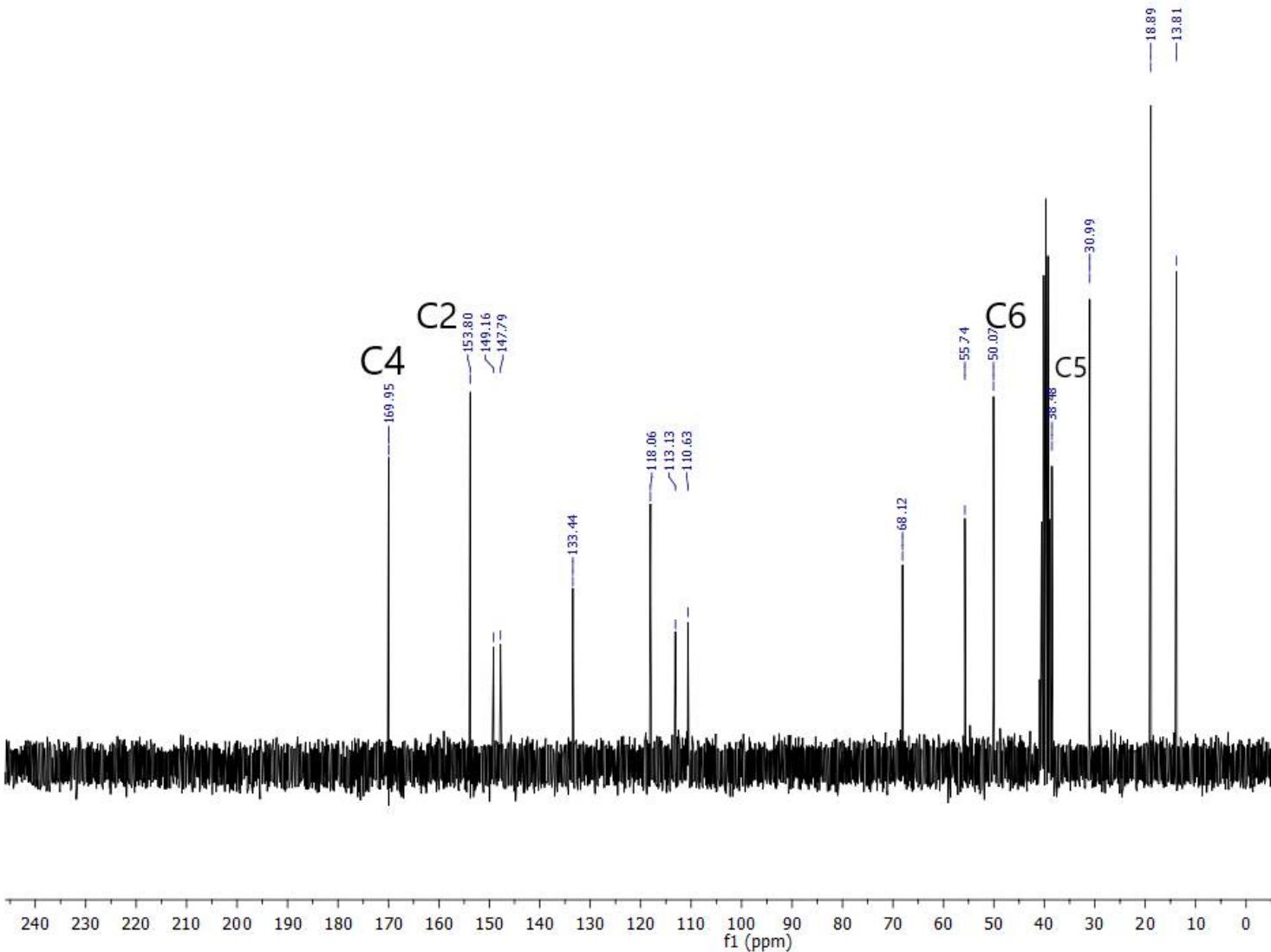


Figure S29. <sup>1</sup>H NMR spectrum of **2o**



**Figure S30.**  $^{13}\text{C}$  NMR spectrum of **2o**

6-(4'-benzyloxy-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2p**

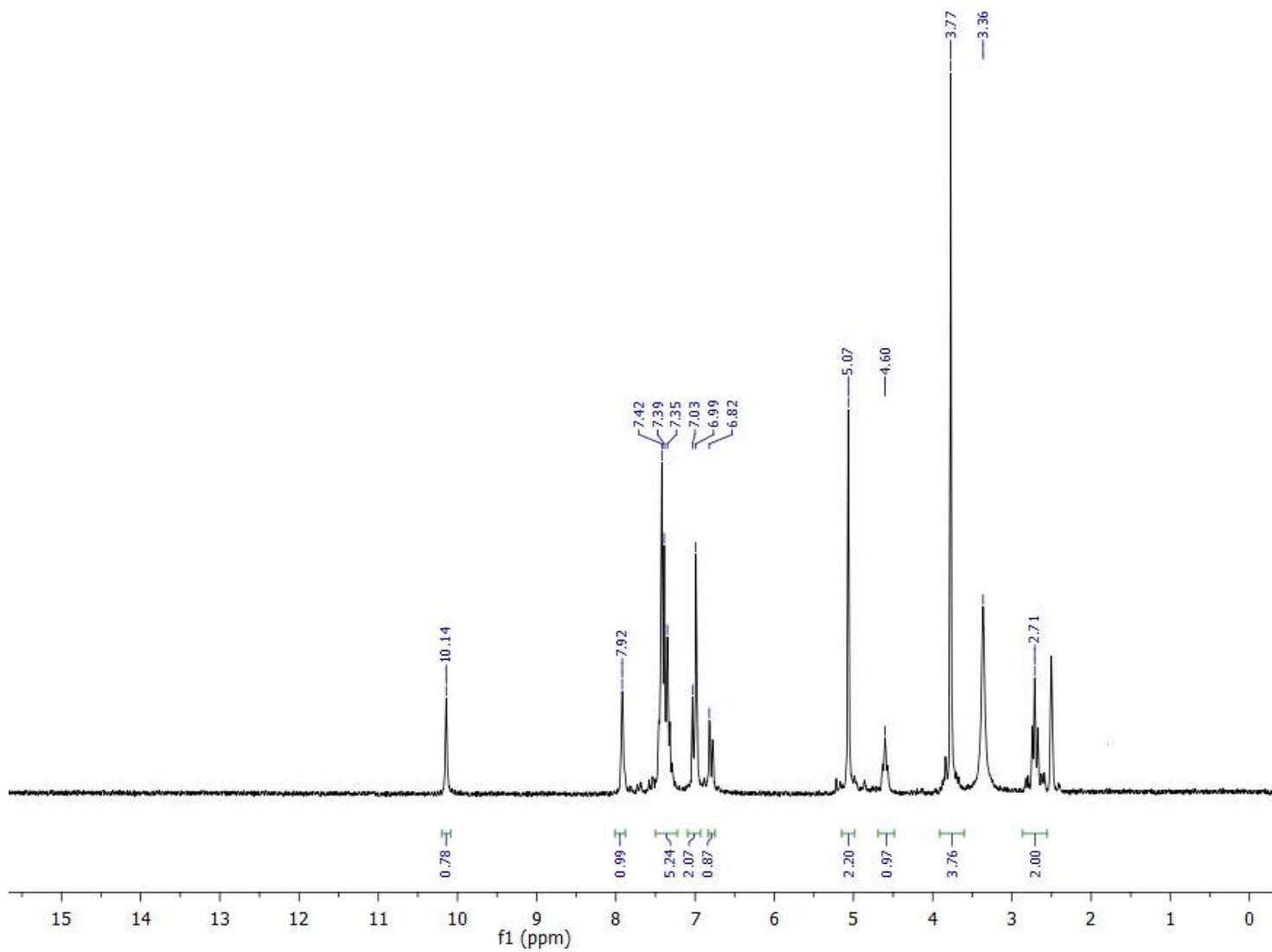
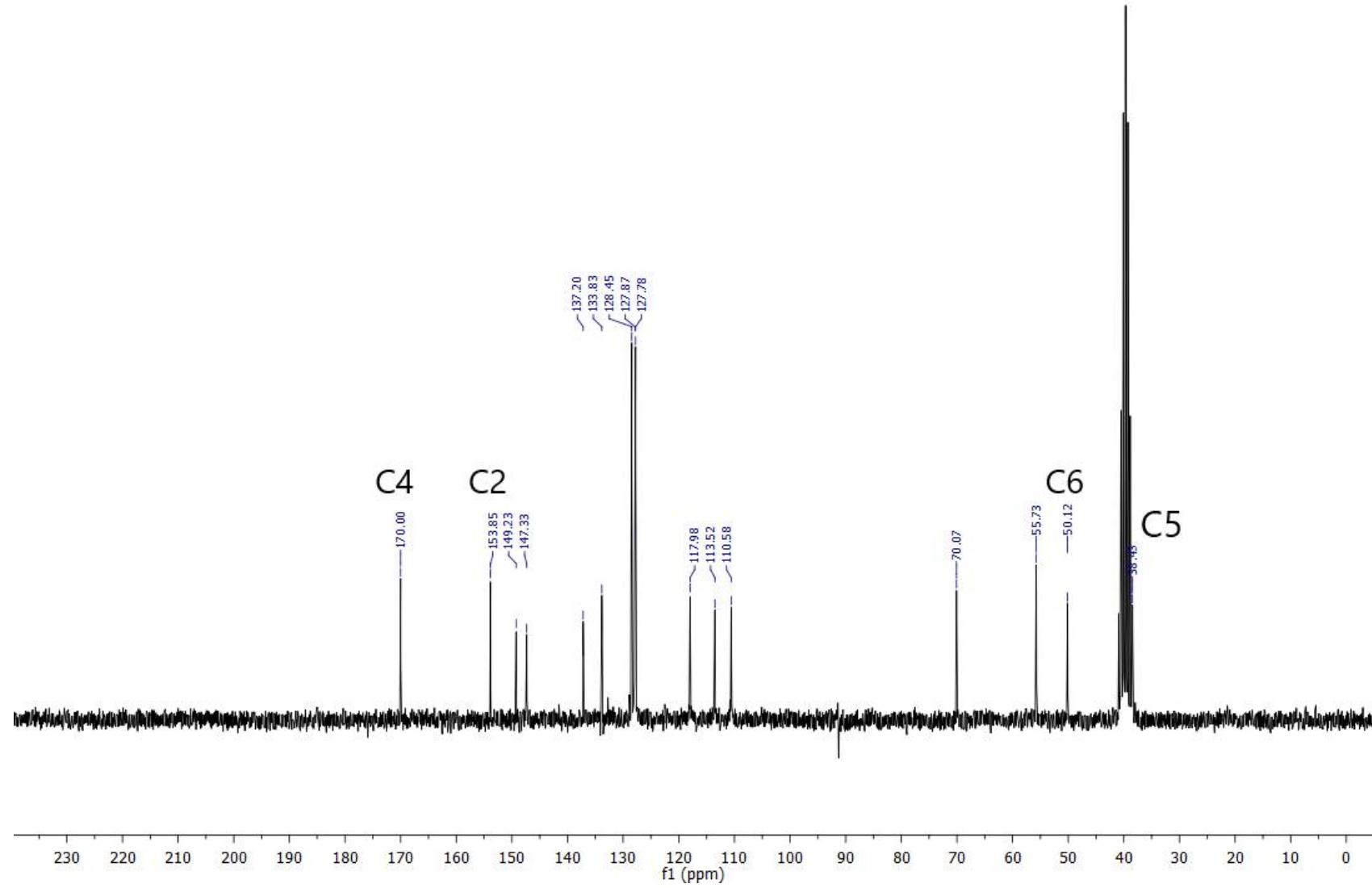


Figure S31. <sup>1</sup>H NMR spectrum of **2p**



**Figure S32.**  $^{13}\text{C}$  NMR spectrum of **2p**

6-(4'-(3''-methylbenzyloxy)-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2q**

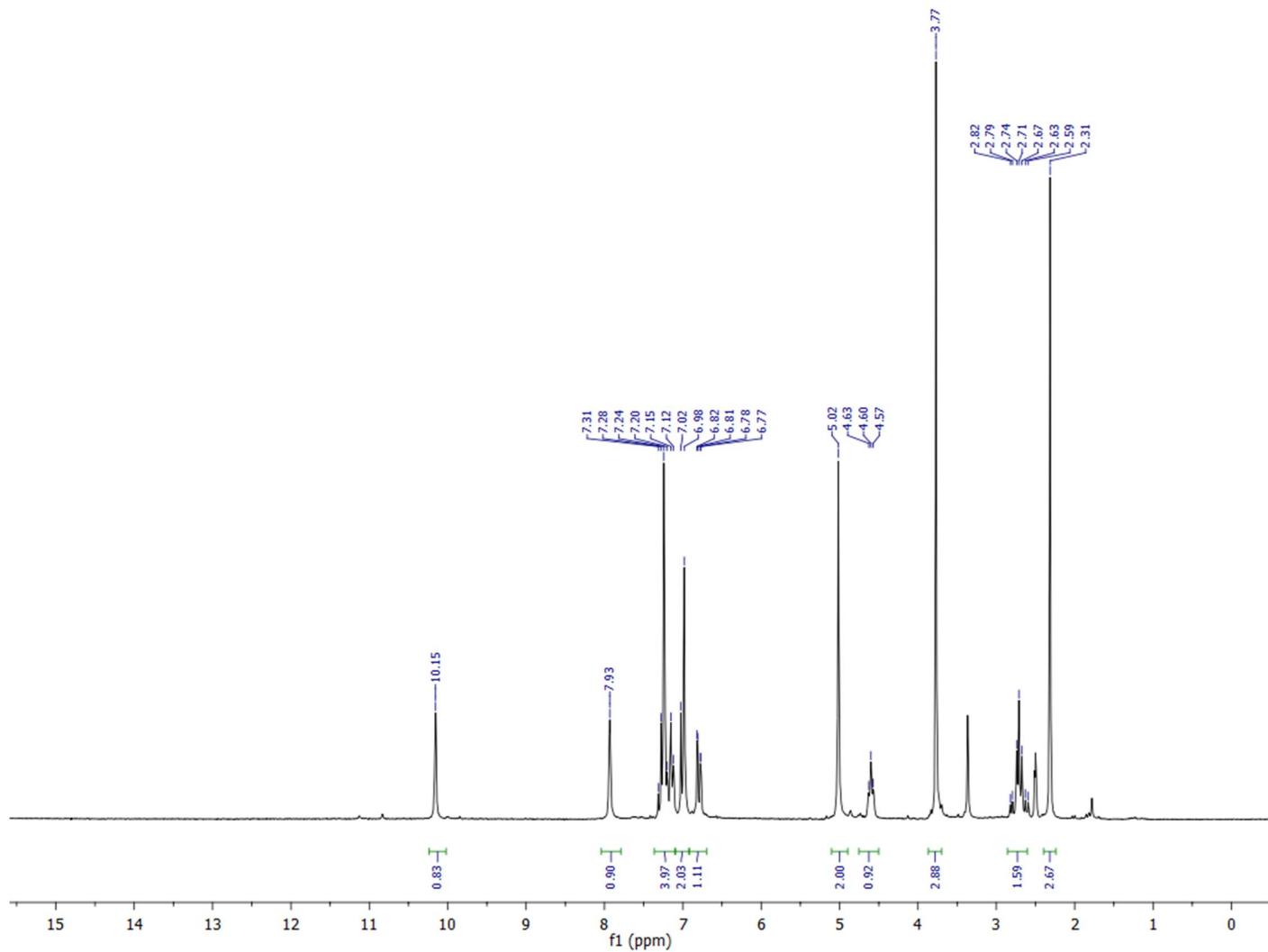
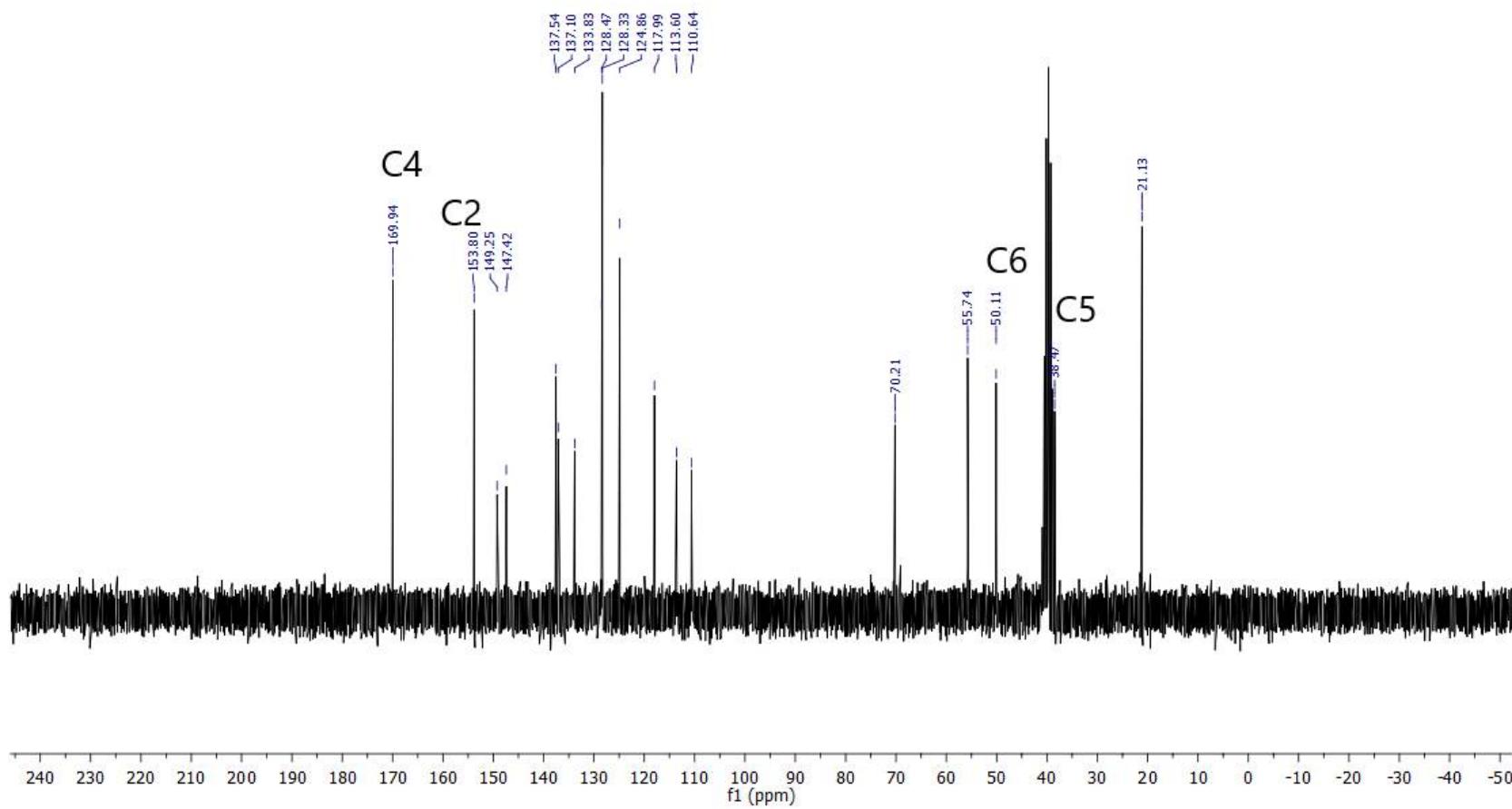
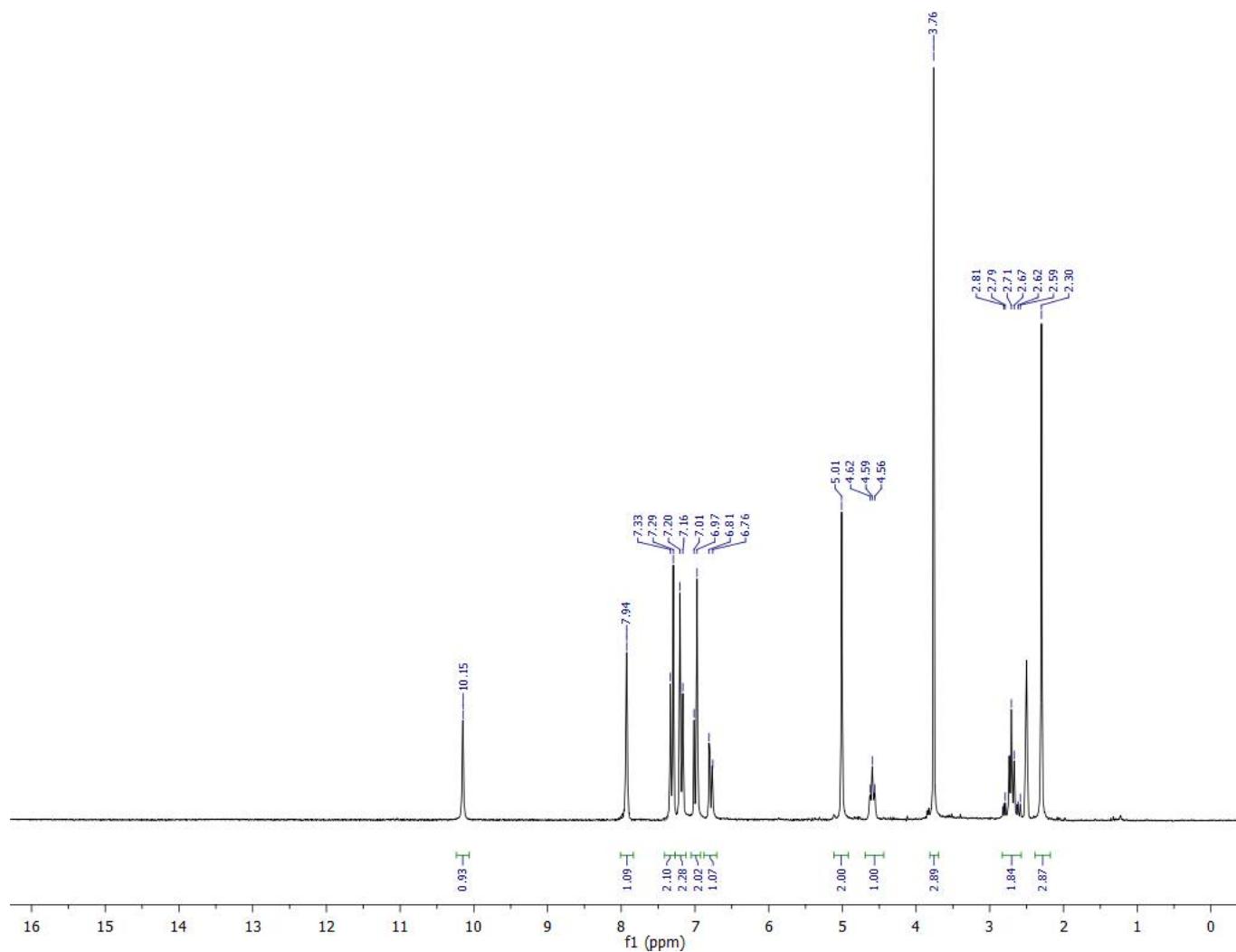


Figure S33.  $^1\text{H}$  NMR spectrum of **2q**

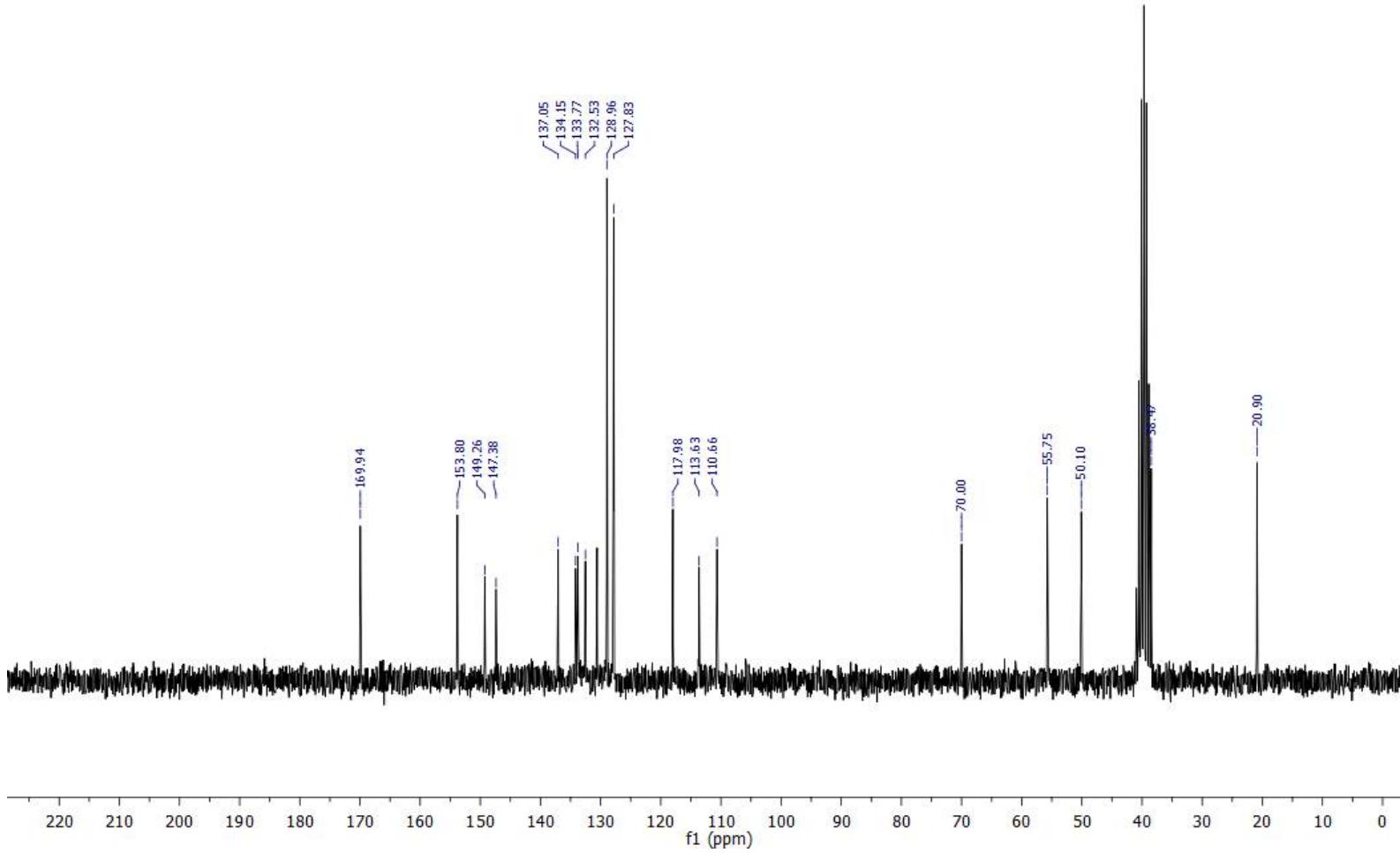


**Figure S34.**  $^{13}\text{C}$  NMR spectrum of **2q**

6-(4'-(4''-methylbenzyloxy)-3'-methoxyphenyl)-dihydropyrimidine-2,4(1H,3H)-dione **2r**



**Figure S35.** <sup>1</sup>H NMR spectrum of **2r**



**Figure S36.**  $^{13}\text{C}$  NMR spectrum of **2r**

6-(4'-acetoxy-3'-methoxyphenyl)-dihydropyrimidine-2,4(1*H*,3*H*)-dione **2s**

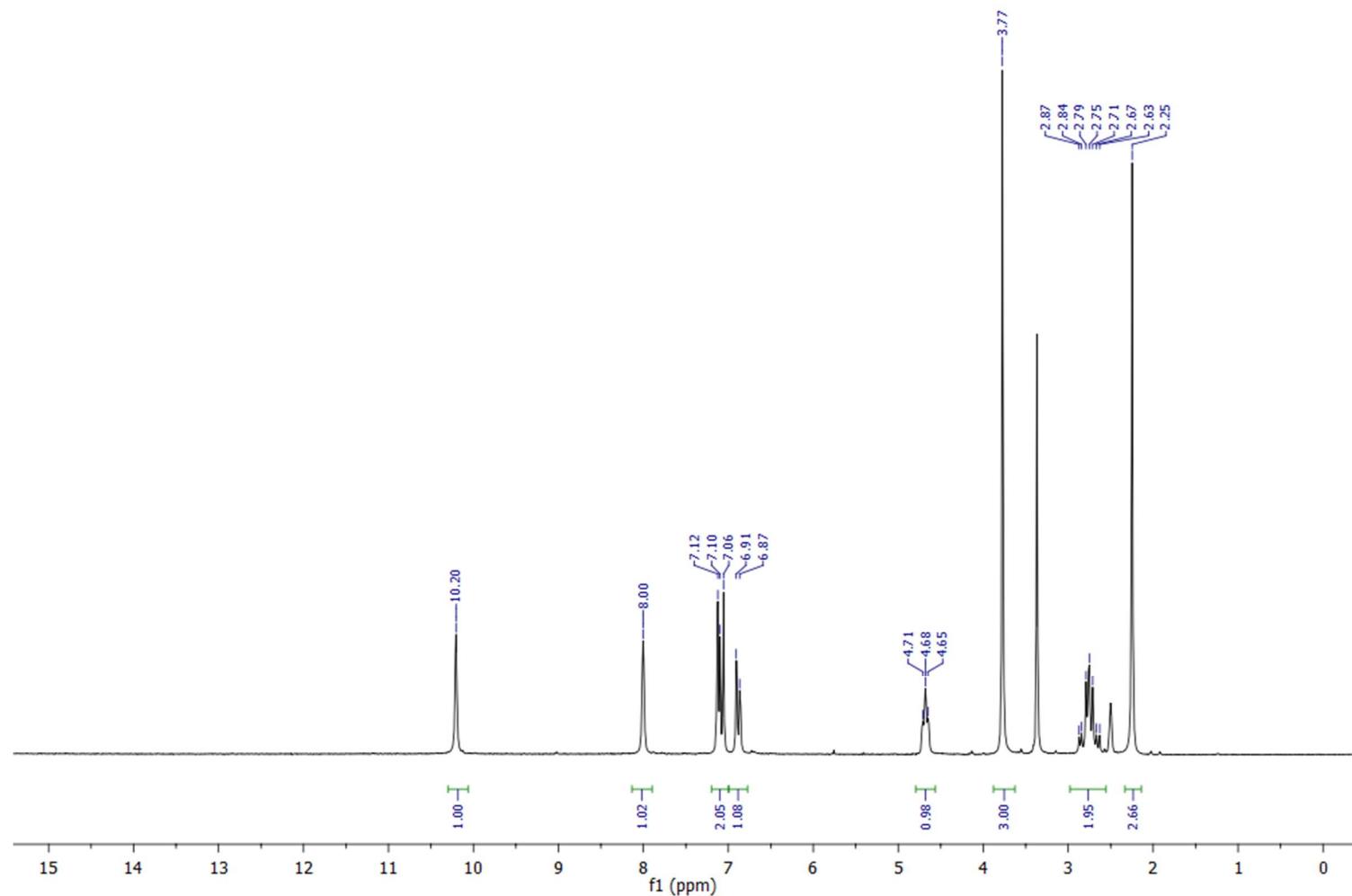
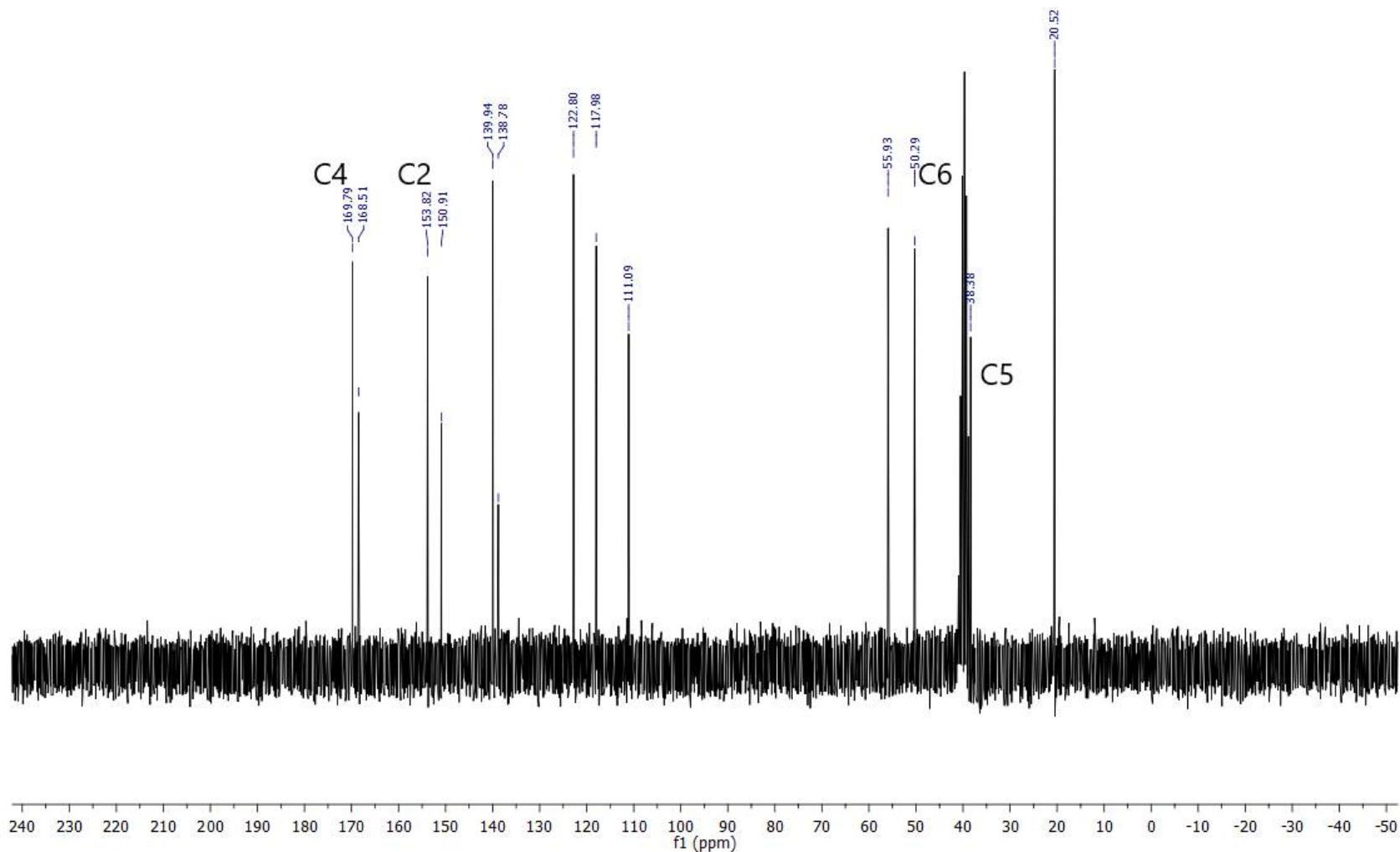


Figure S37.  $^1\text{H}$  NMR spectrum of **2s**



**Figure S38.**  $^{13}\text{C}$  NMR spectrum of **2s**