

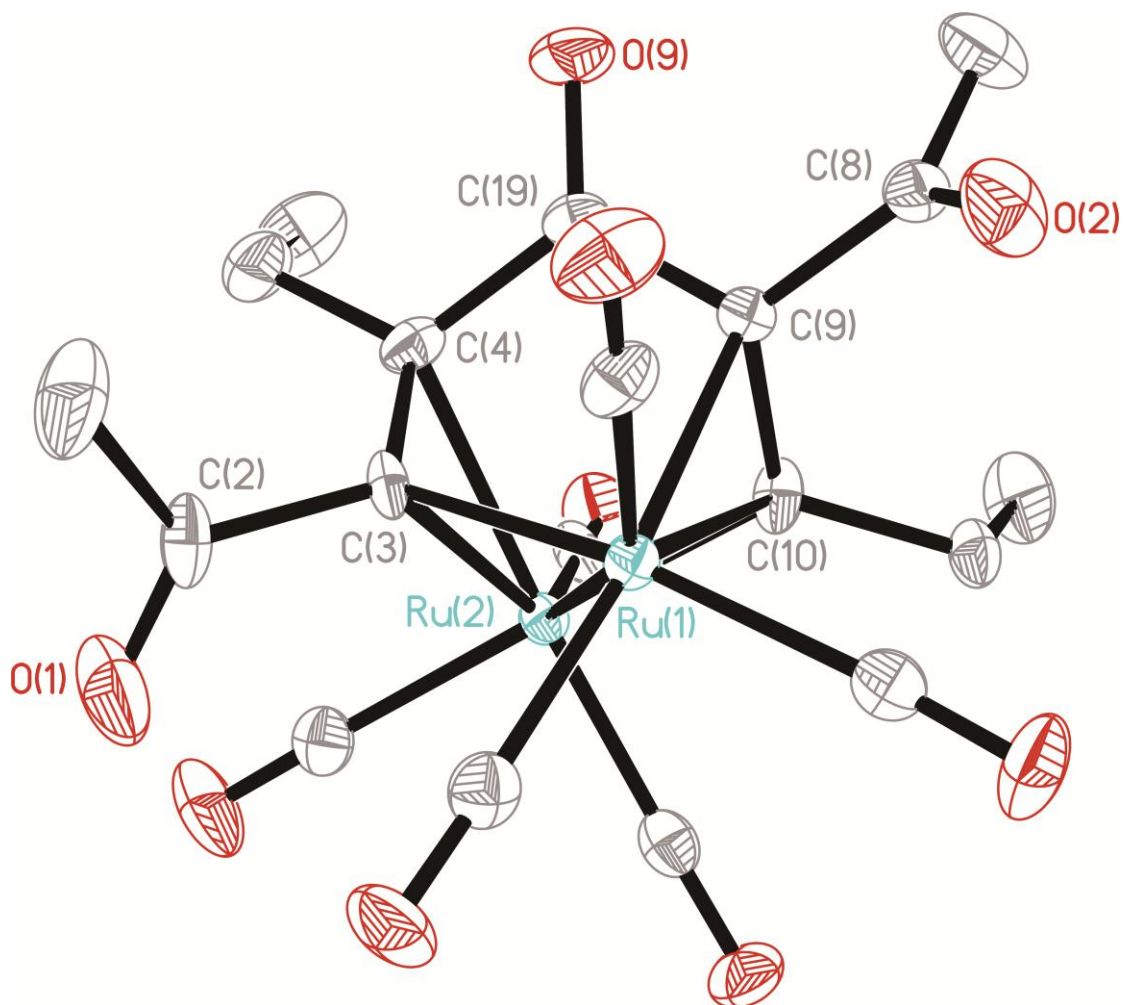
Unexpected formation and conversion: role of substituents on the reactivity and product distribution in reactions of 1,3-ynones with $\text{Ru}_3(\text{CO})_{12}$

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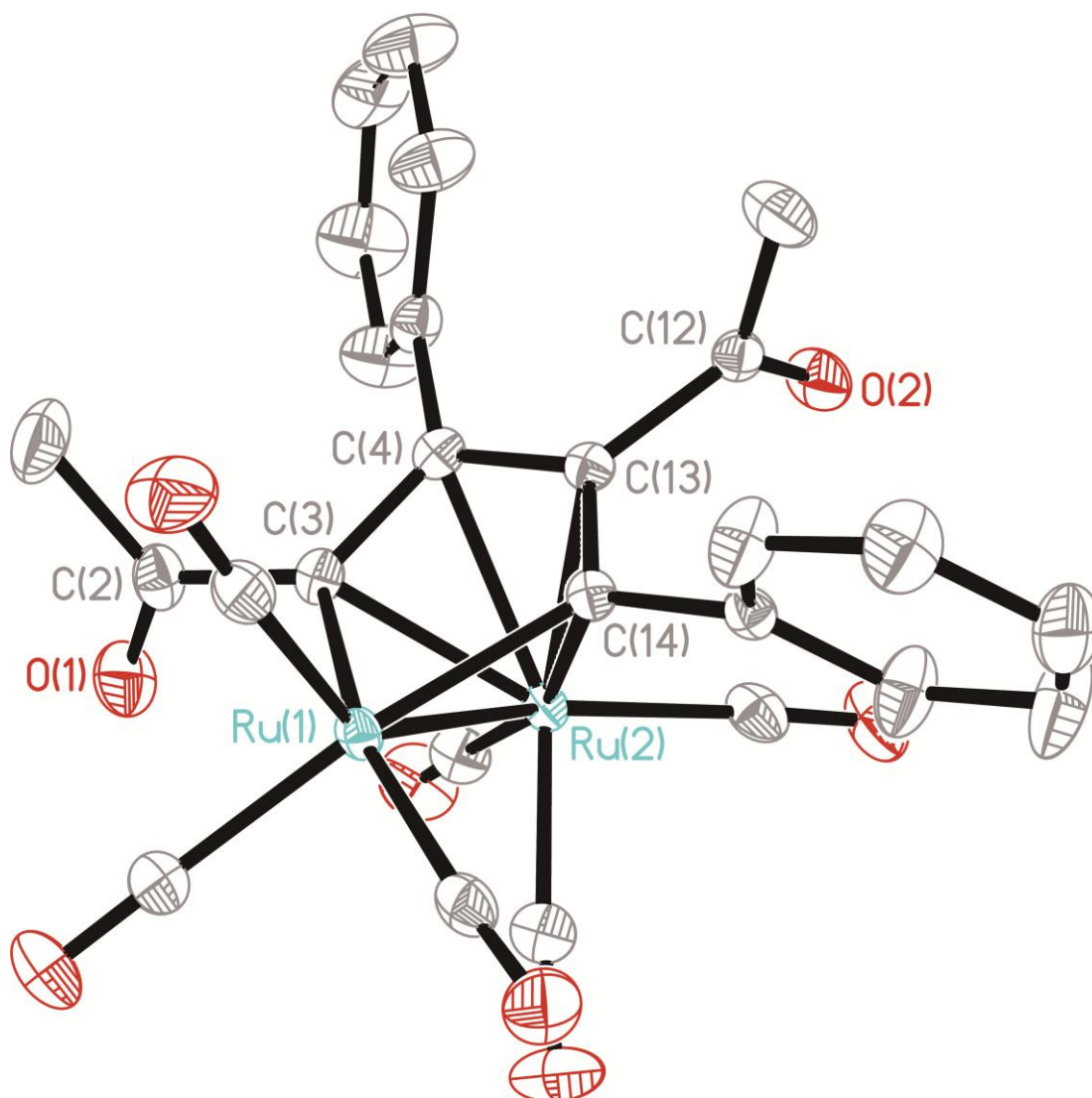
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Fig. S1. The crystal structure of compound 1c	S1
Fig. S2. The crystal structure of compound 2a	S2
¹ H NMR spectra of all new compounds.....	S3
¹³ C{ ¹ H} NMR spectra of all new compounds.....	S8
FT-IR spectra of all new compounds.....	S13



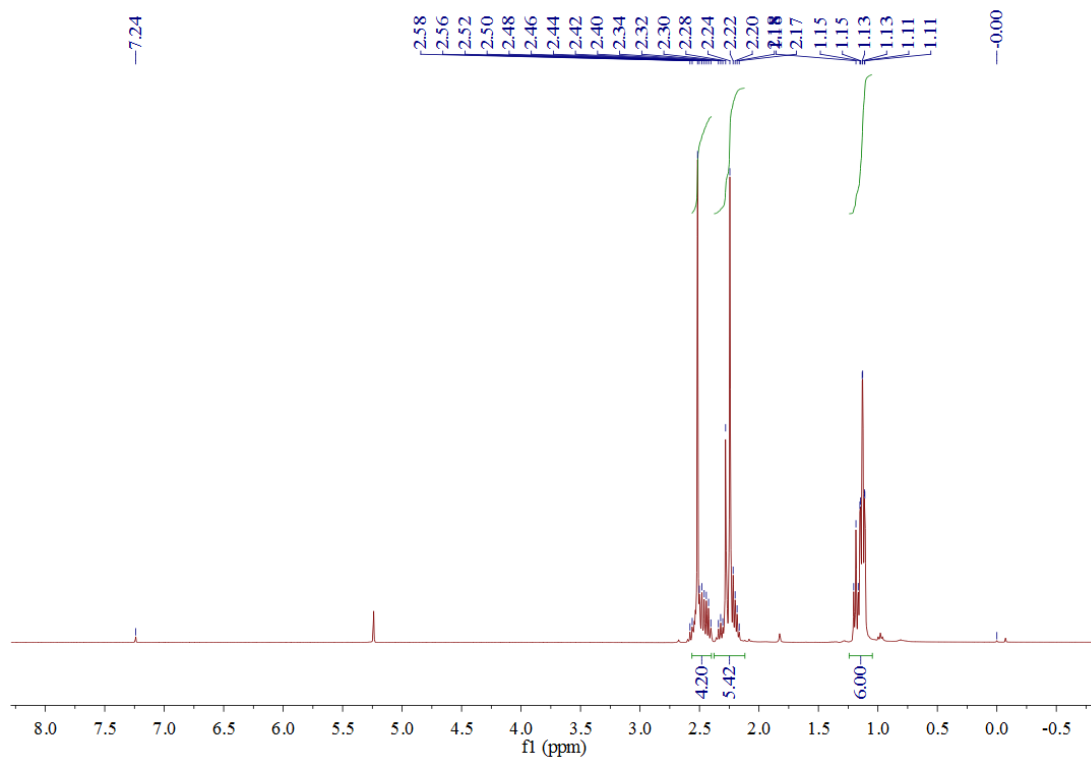
ORTEP view of cluster **1c** showing 50% ellipsoids. Selected bond lengths (Å) and bond angles (°):
 Ru1-Ru2 = 2.7567(5), Ru1-C10 = 2.2167(5), Ru1-C9 = 2.2708(6), Ru1-C3 = 2.0285(5), Ru2-C3 = 2.1936(5), Ru2-C4 = 2.2903(5), Ru2-C10 = 2.0670(5), C3-C4 = 1.4522(4), C9-C10 = 1.4455(4), C4-C19 = 1.4966(3), C9-C19 = 1.4916(4), C2-C3 = 1.4893(4), C8-C9 = 1.5154(3), C2-O1 = 1.2185(2), C8-O2 = 1.2117(2), C19-O9 = 1.2197(3).

Fig. S1. The crystal structure of compound **1c**.

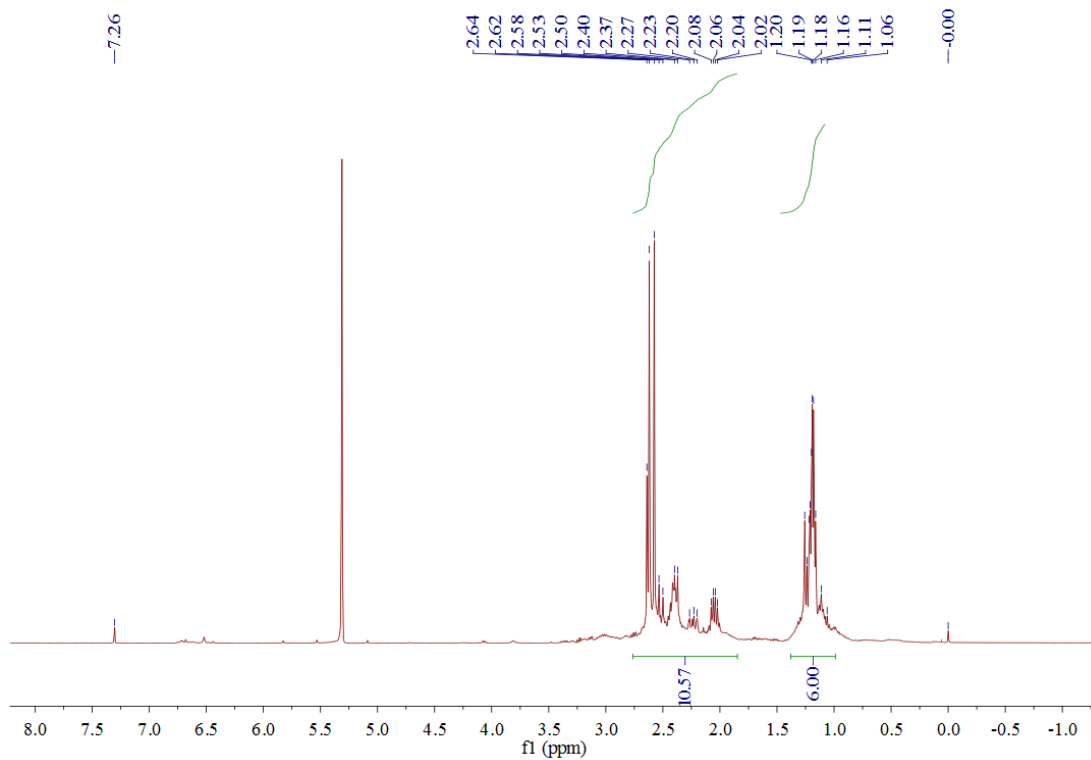


ORTEP view of cluster **2a** showing 50% ellipsoids. Selected bond lengths (Å) and bond angles (°):
 Ru1-Ru2 = 2.7253(4), Ru1-C3 = 2.0836(3), Ru1-C14 = 2.0852(3), Ru2-C3 = 2.2180(3), Ru2-C4 = 2.2768(3), Ru2-C13 = 2.2583(4), Ru2-C14 = 2.3012(4), C3-C4 = 1.4268(2), C4-C13 = 1.4432(2), C13-C14 = 1.4176(2), C2-C3 = 1.4911(2), C2-O1 = 1.2148(2), C12-C13 = 1.5195(2), C12-O2 = 1.2011(2).

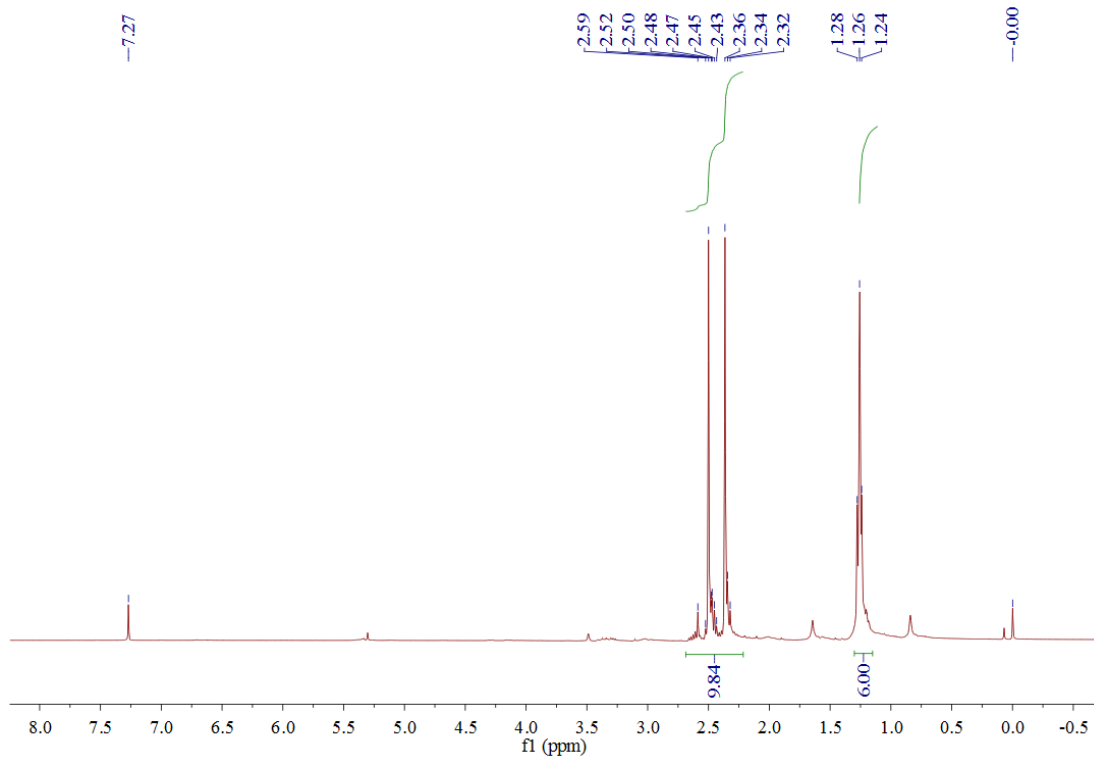
Fig. S2. The crystal structure of compound **2a**.



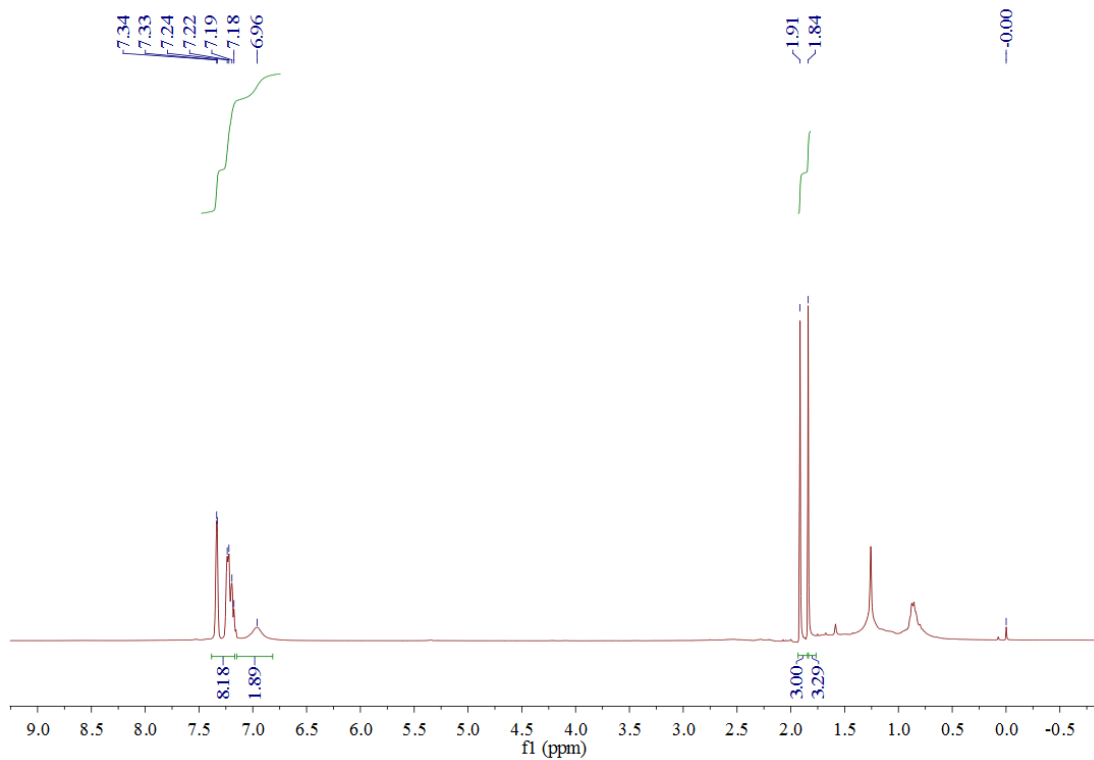
^1H NMR spectrum of compound **1a**.



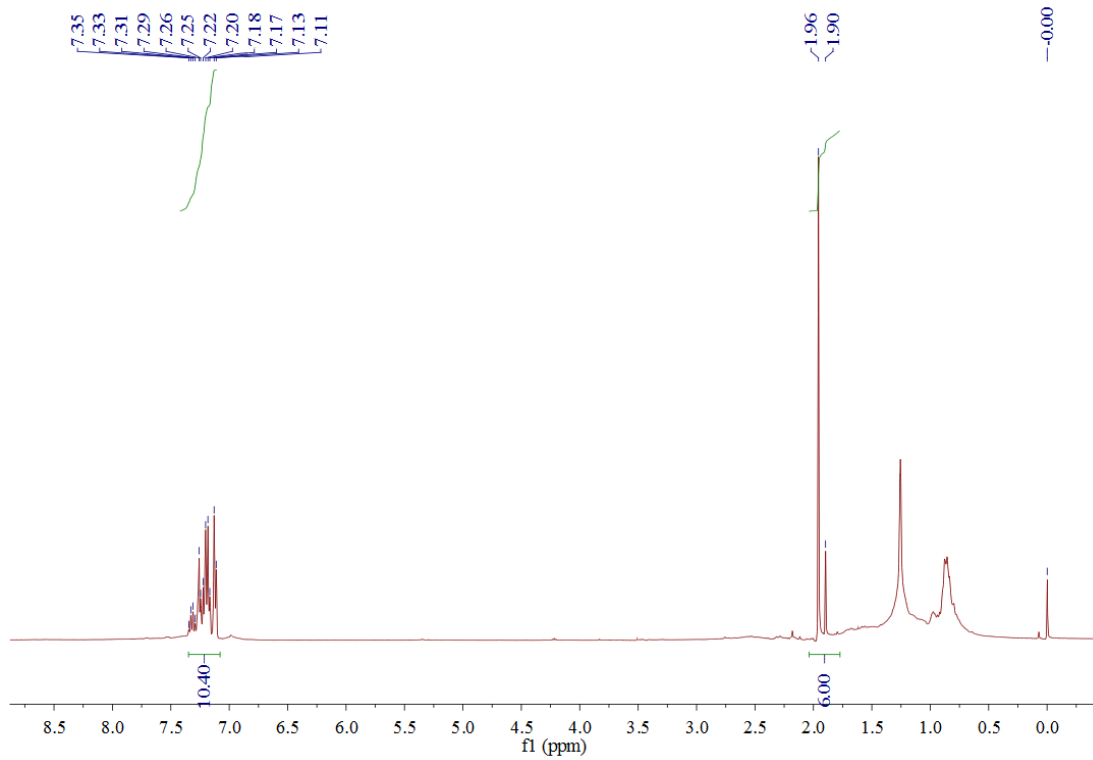
^1H NMR spectrum of compound **1b**.



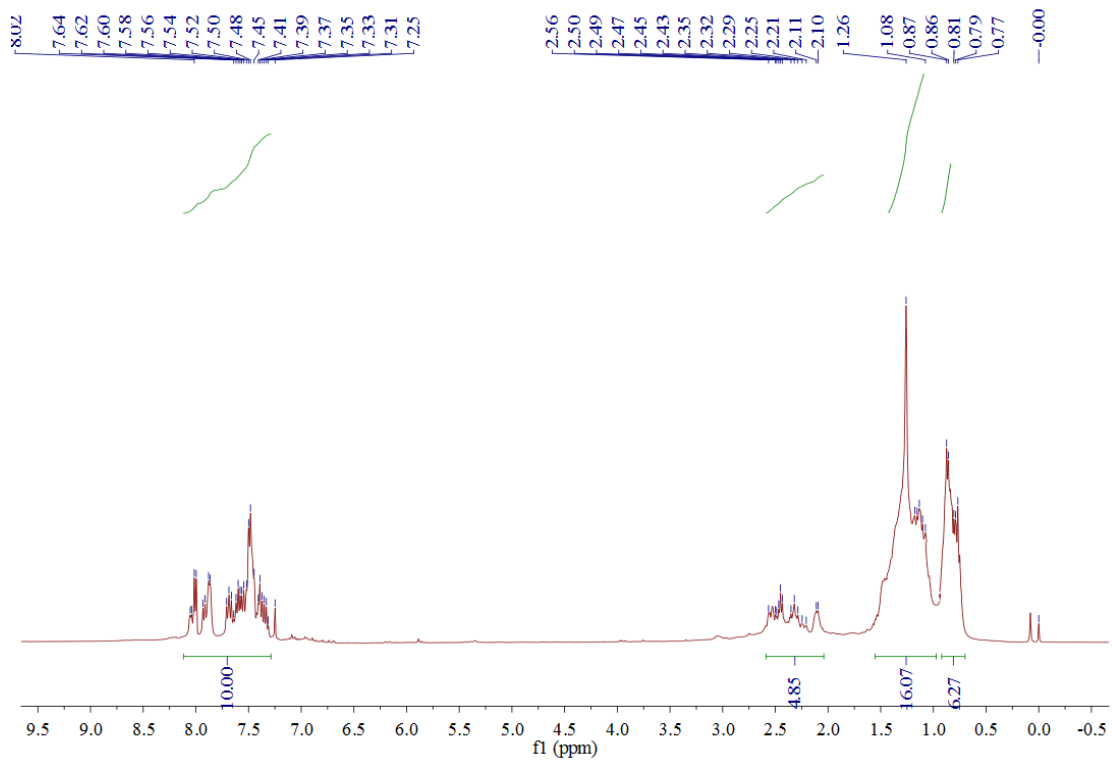
¹H NMR spectrum of compound **1c**.



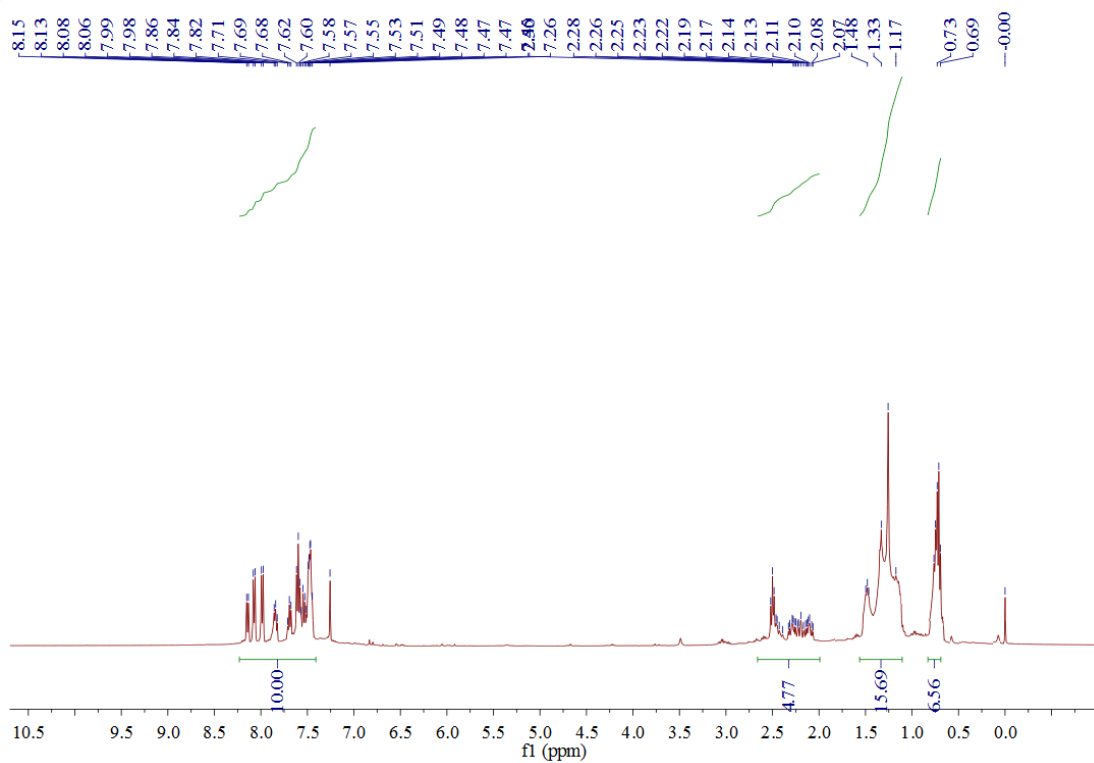
¹H NMR spectrum of compound **2a**.



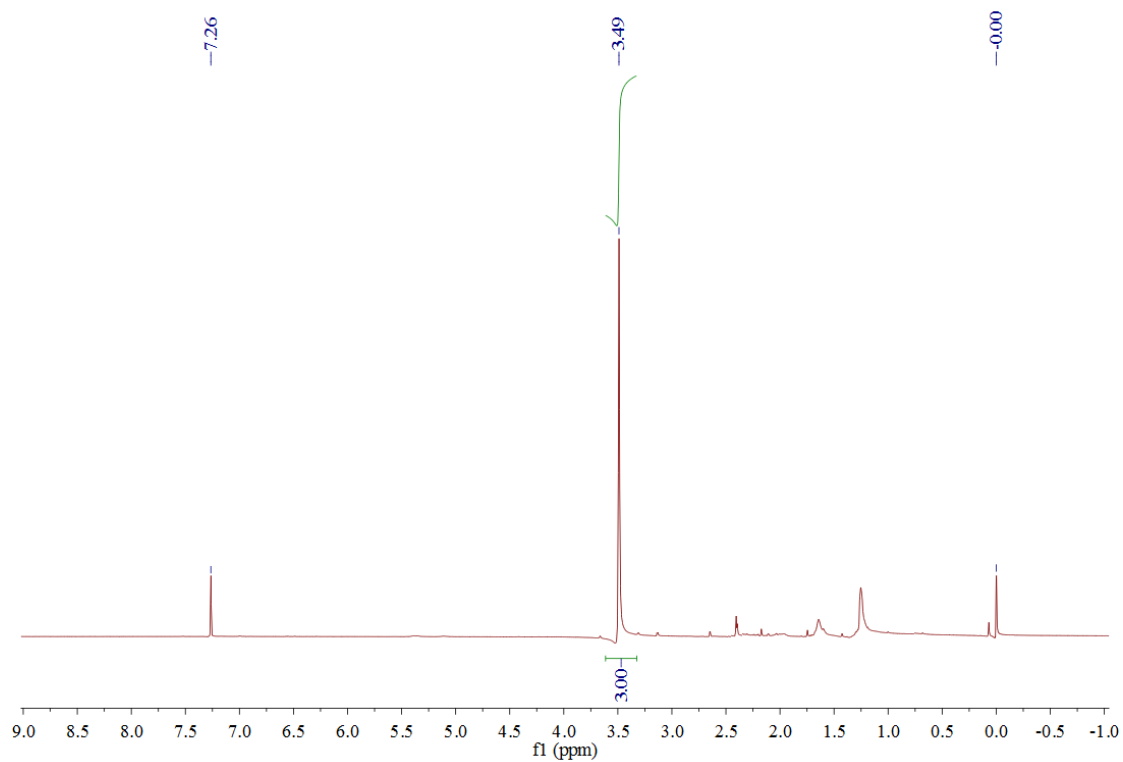
¹H NMR spectrum of compound **2b**.



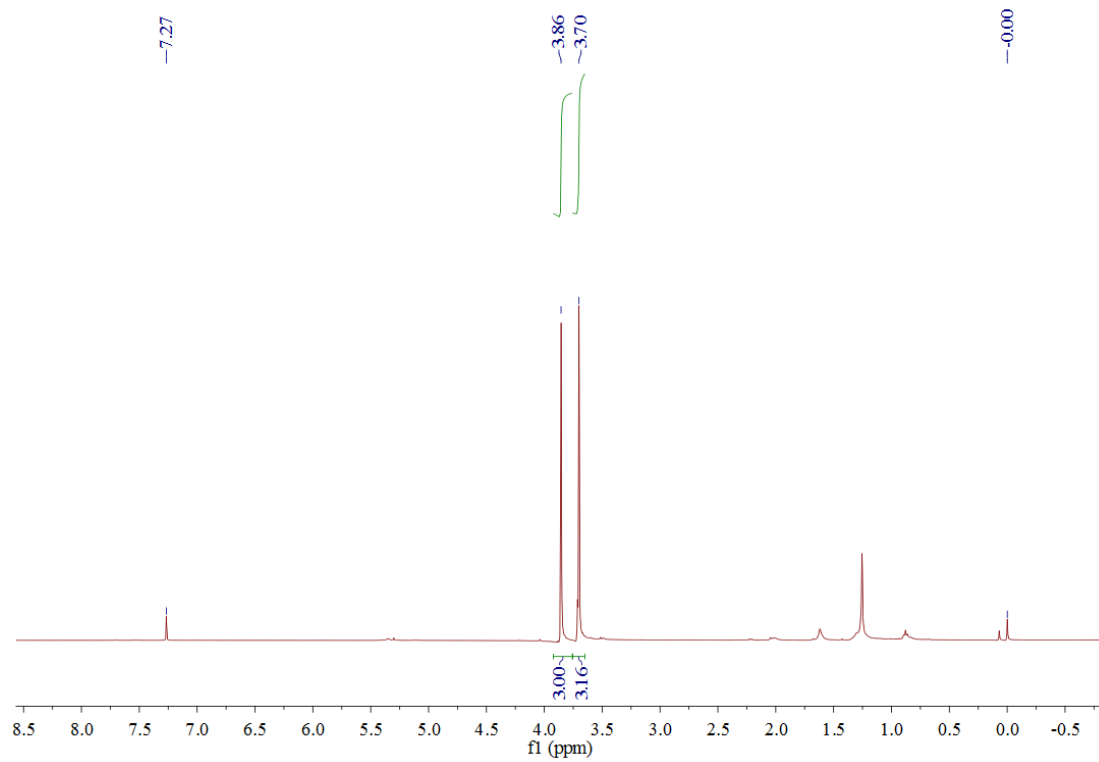
¹H NMR spectrum of compound **3a**.



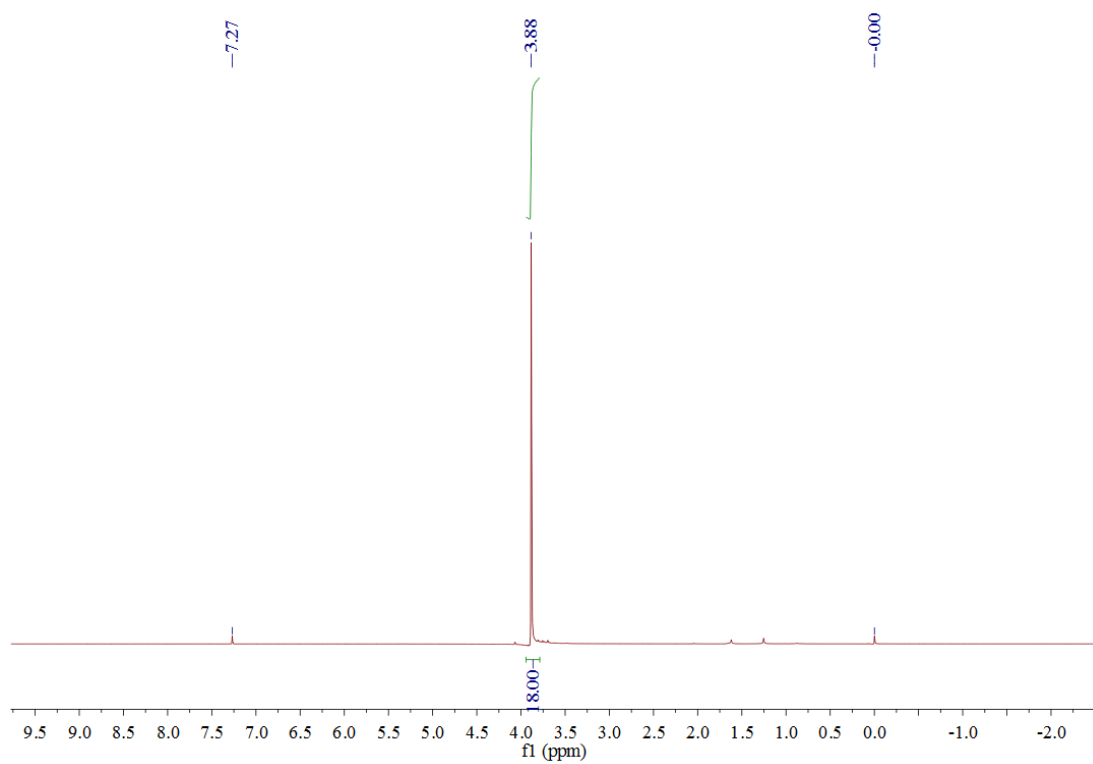
^1H NMR spectrum of compound **3c**.



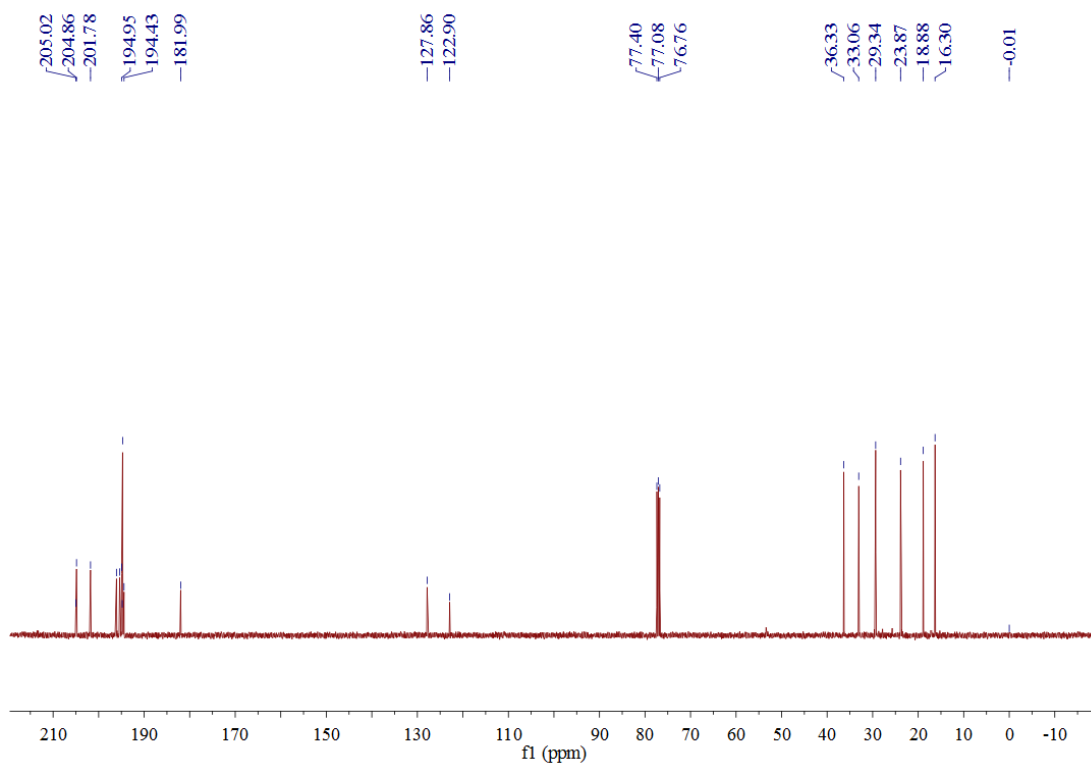
^1H NMR spectrum of compound **4a**.



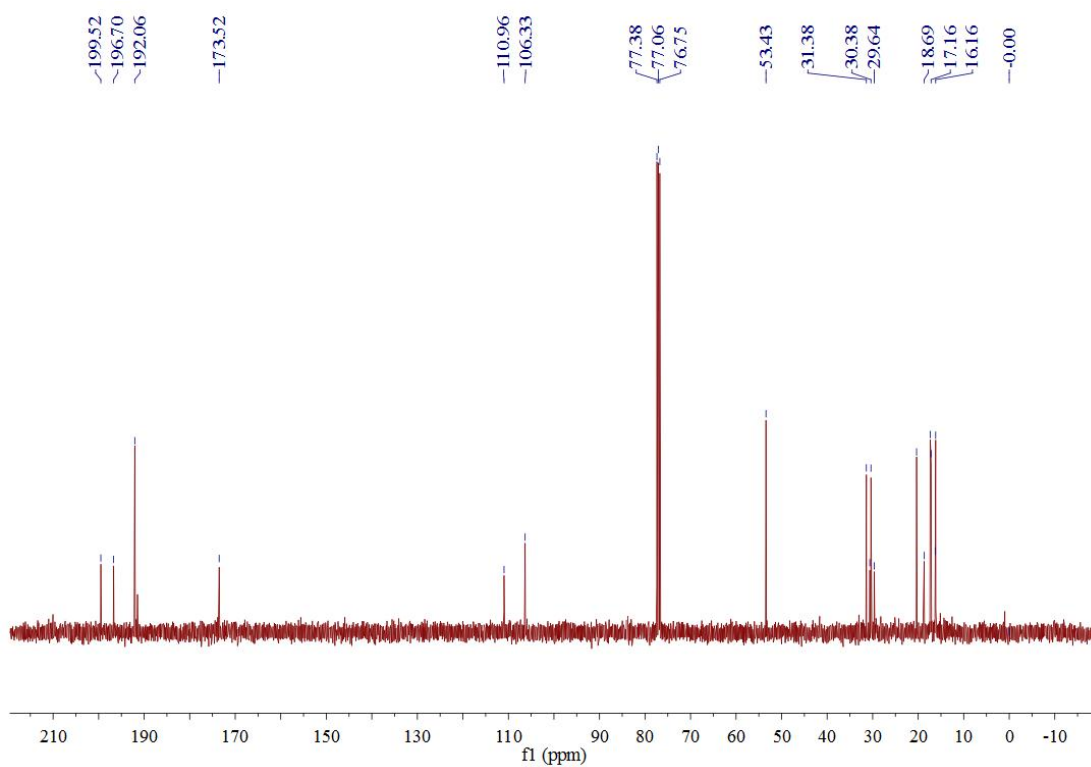
^1H NMR spectrum of compound **5a**.



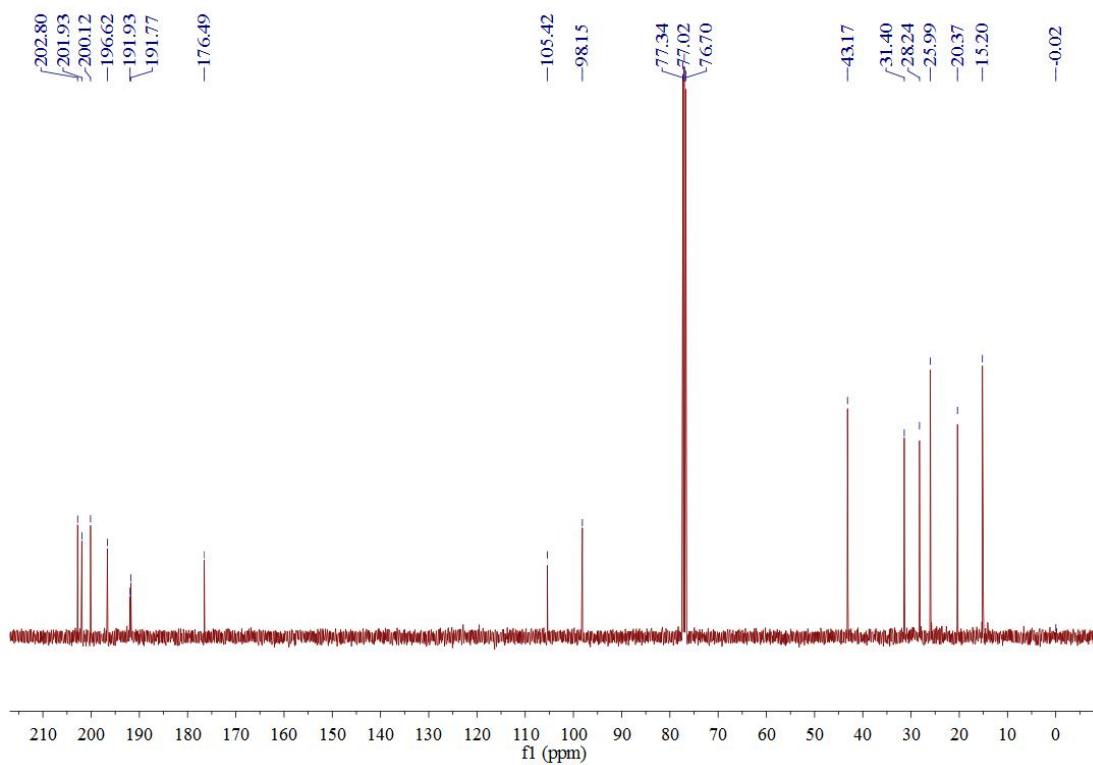
^1H NMR spectrum of compound **5b**.



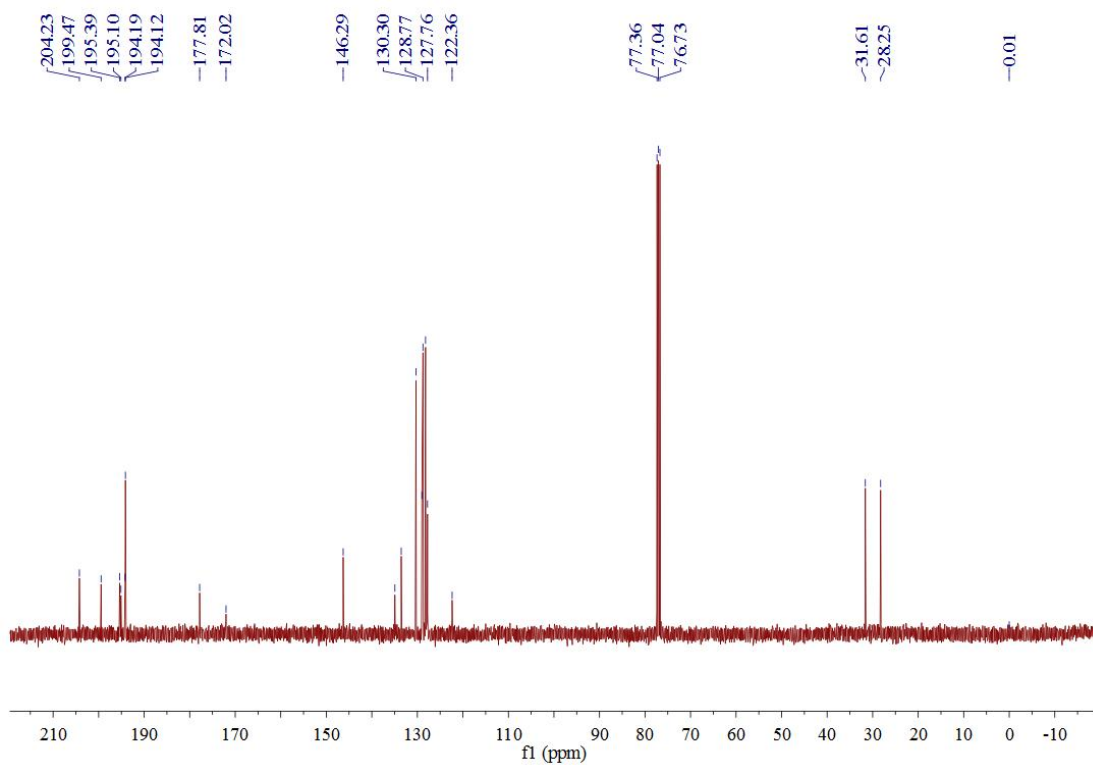
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **1a**.



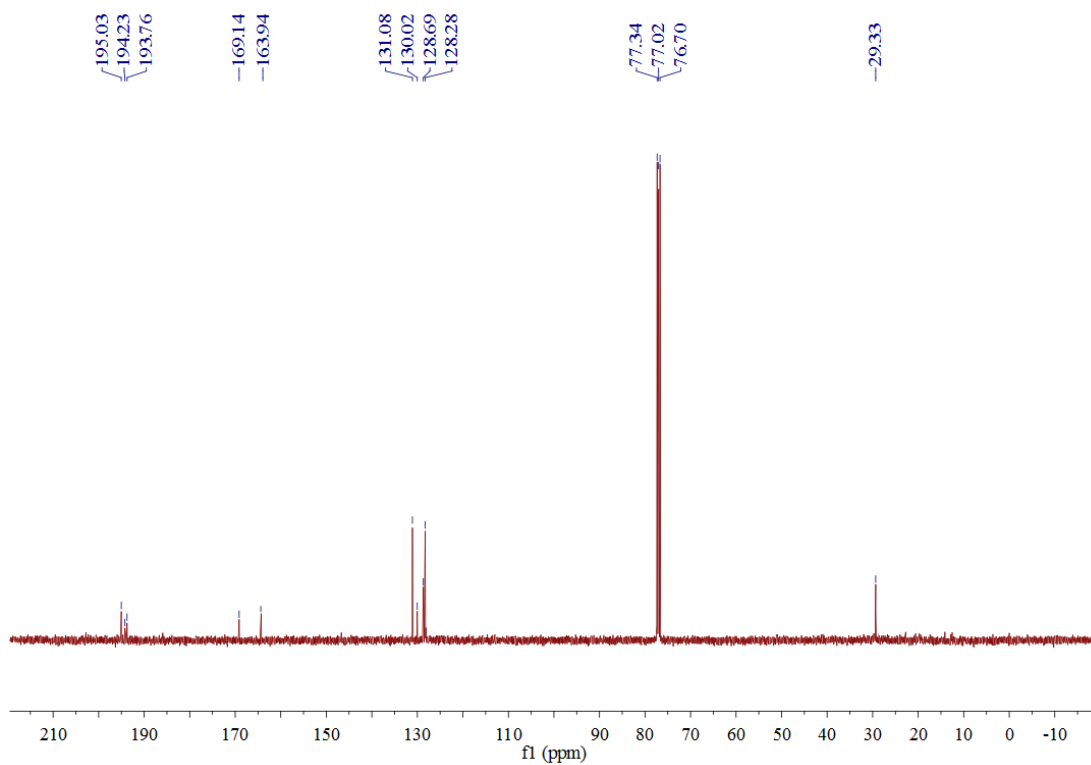
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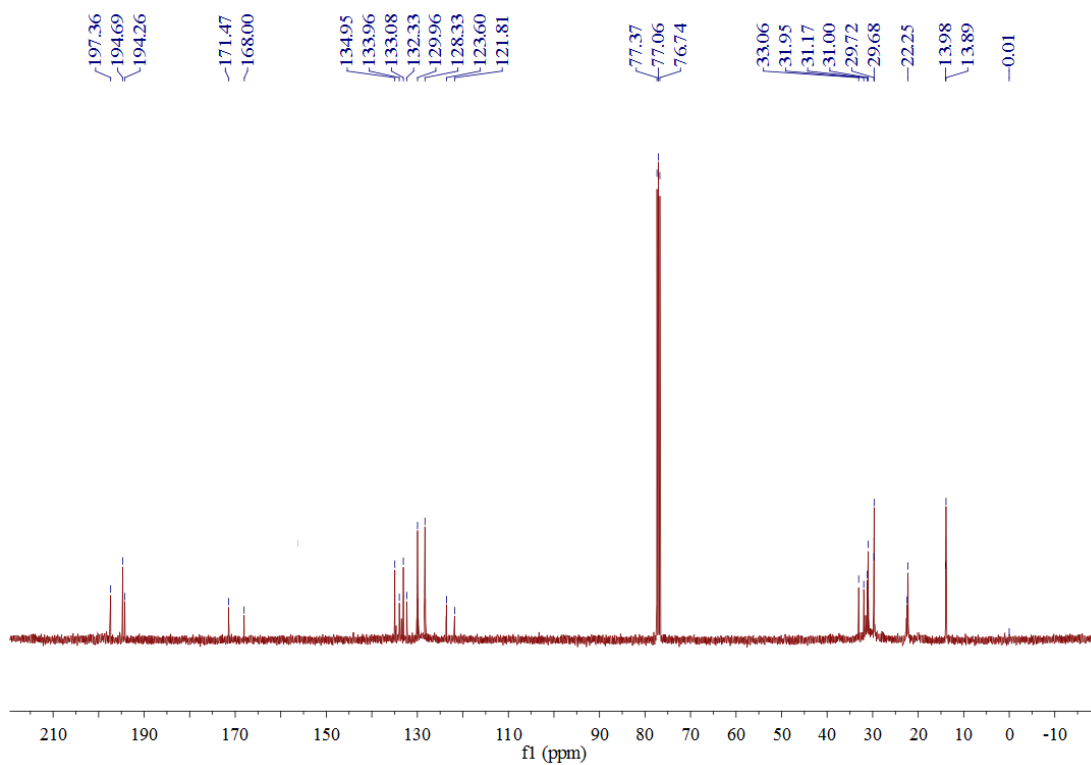
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **1c**.



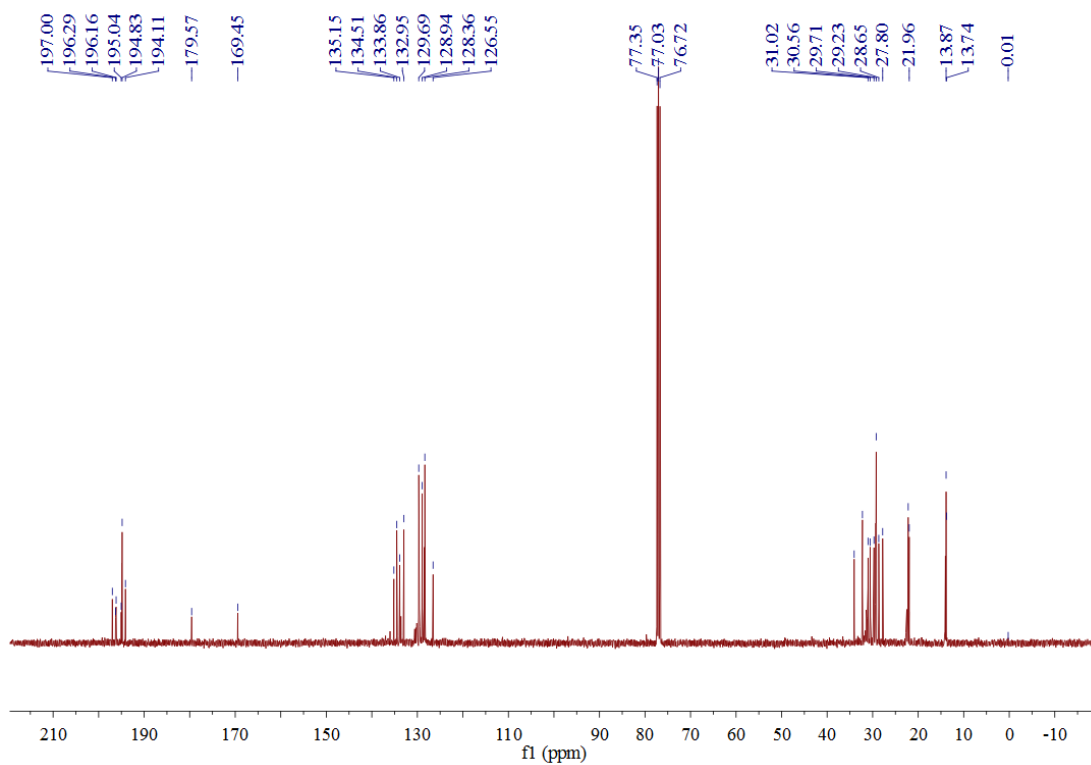
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2a**.



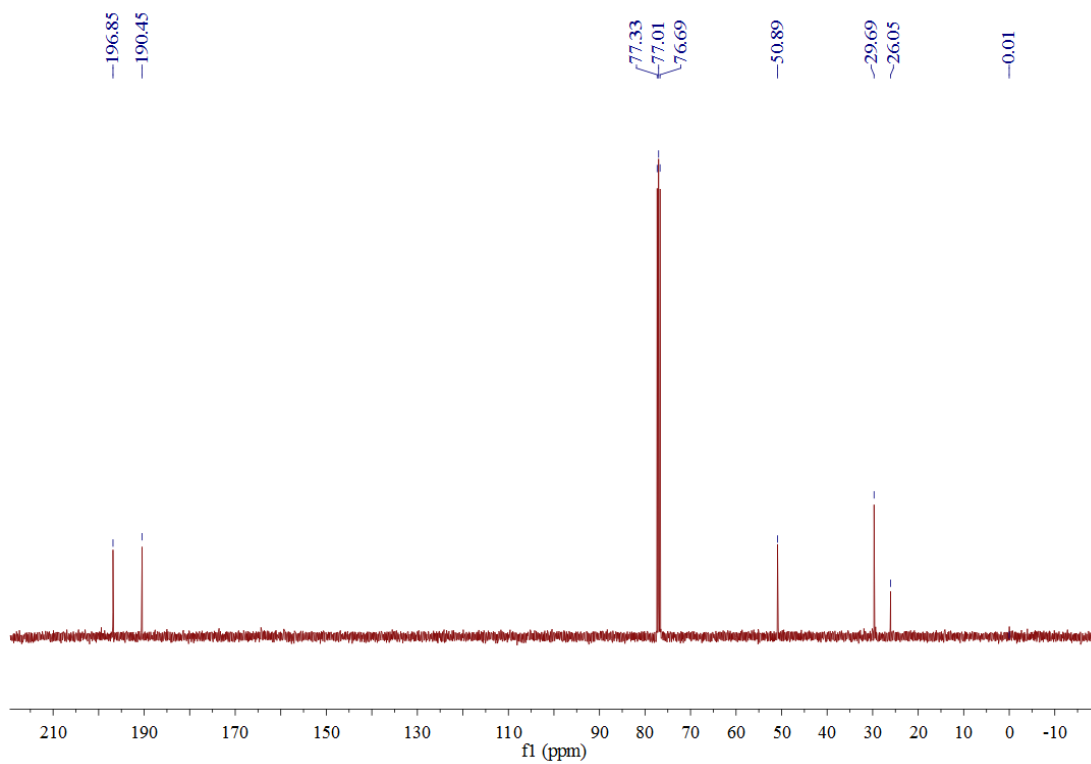
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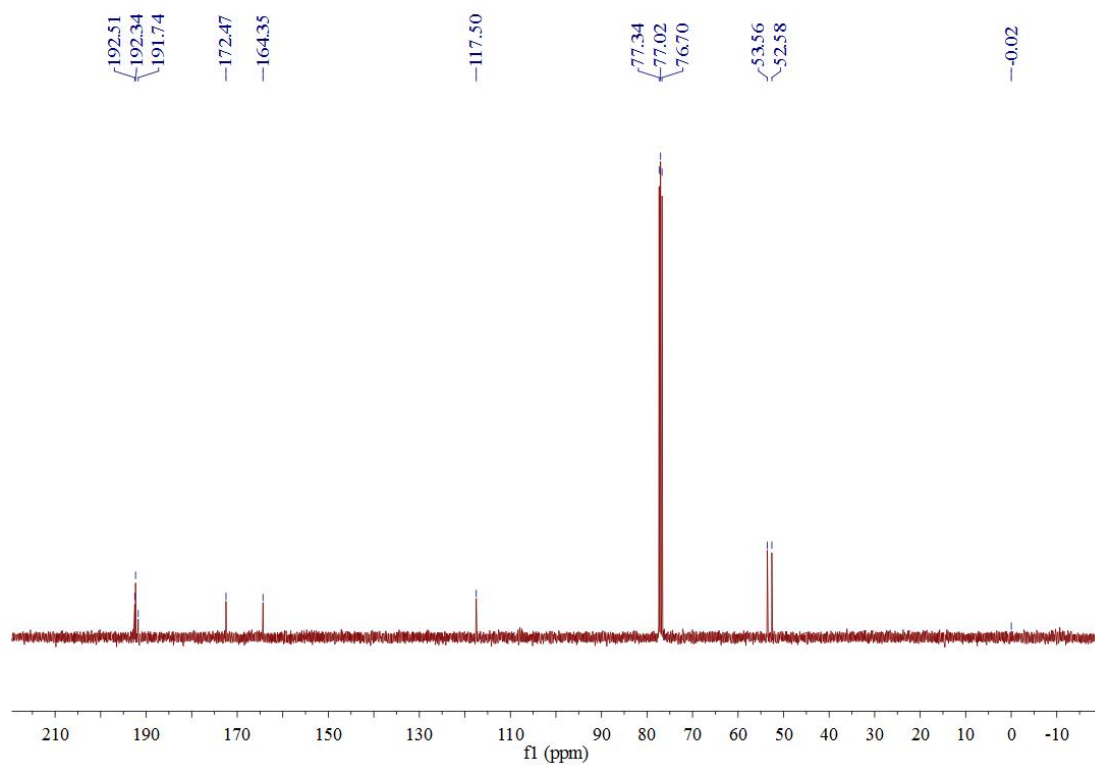
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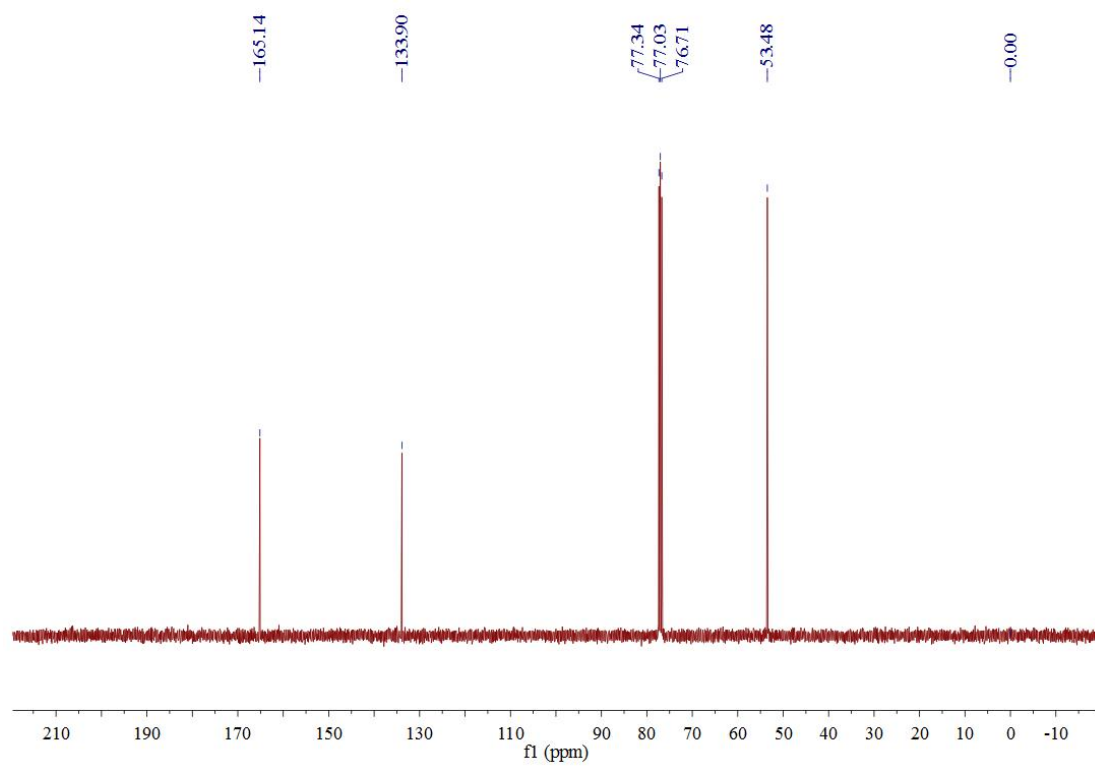
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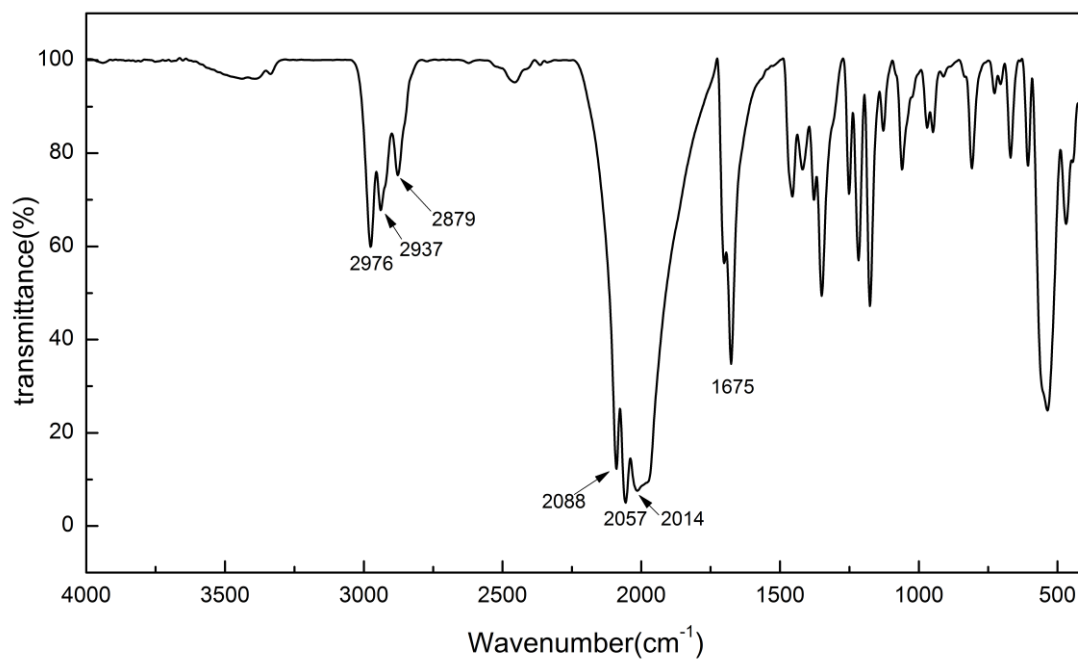
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4a**.



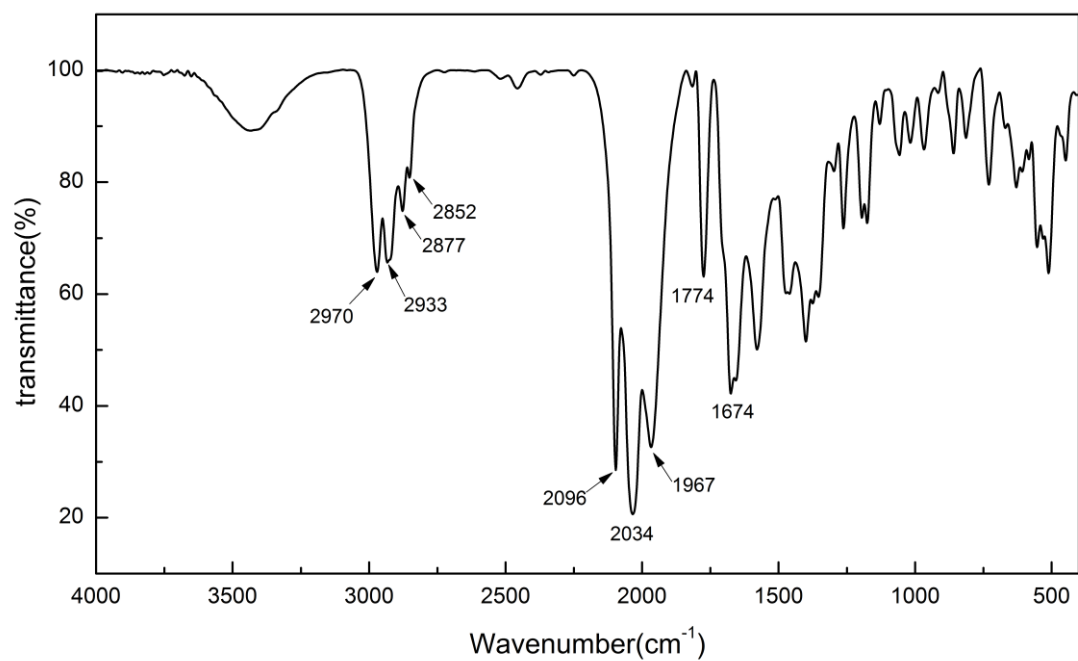
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5a**.



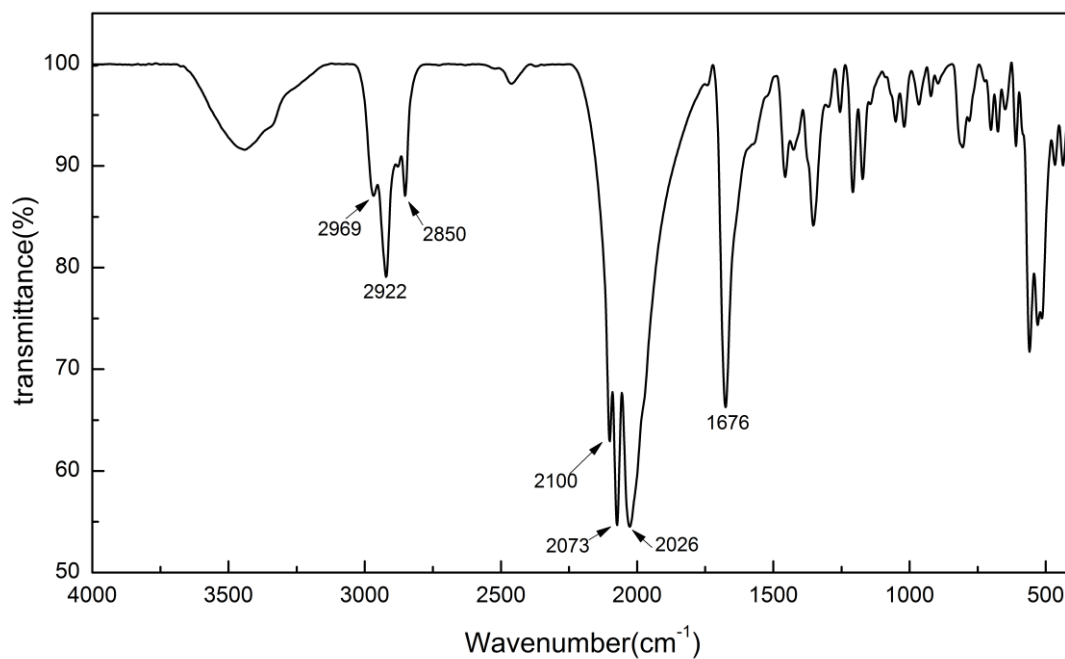
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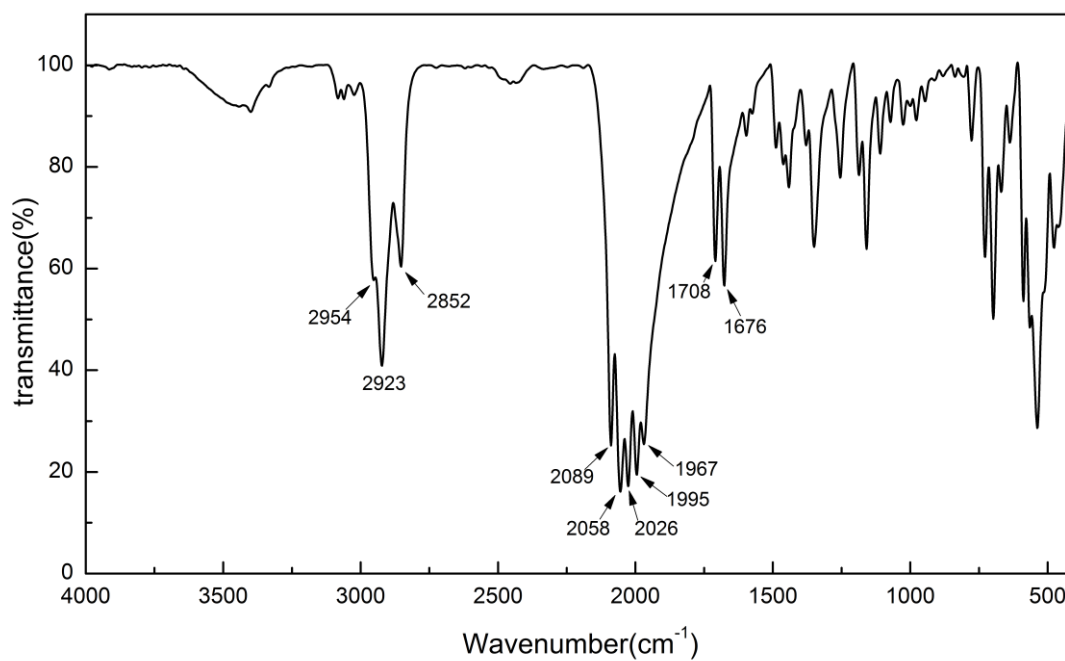
IR spectrum of compound **1a**.



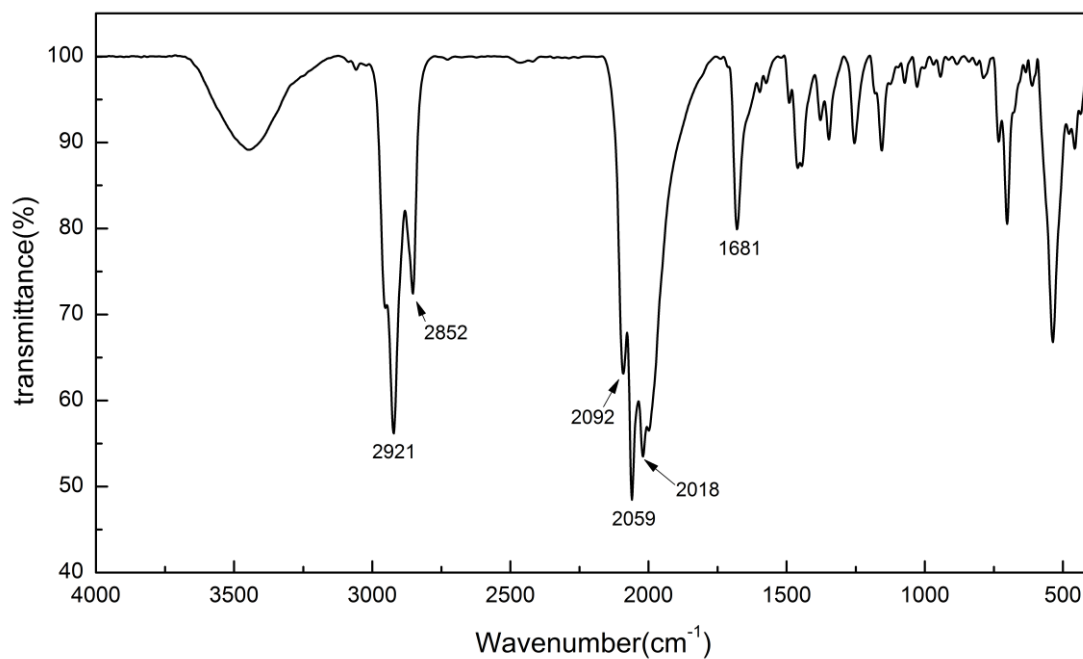
IR spectrum of compound **1b**.



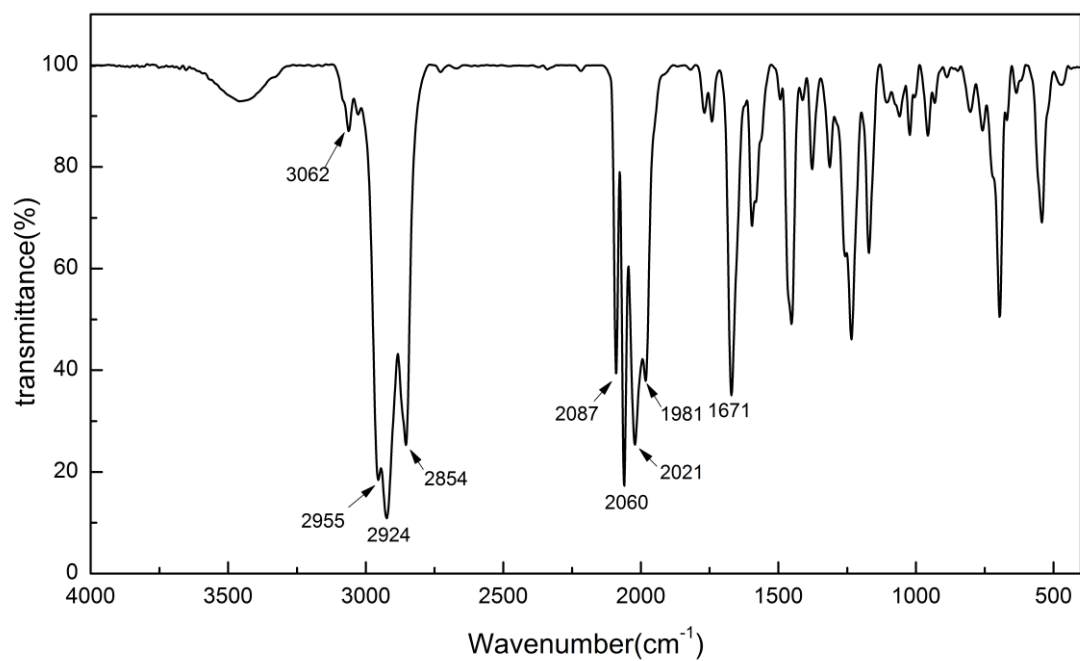
IR spectrum of compound **1c**.



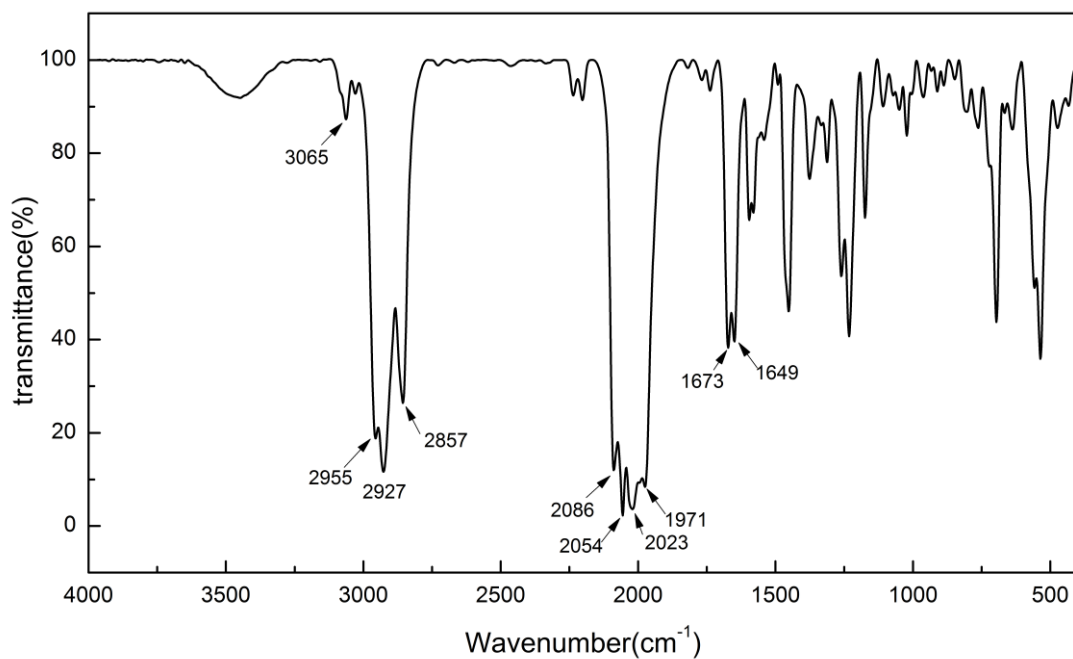
IR spectrum of compound **2a**.



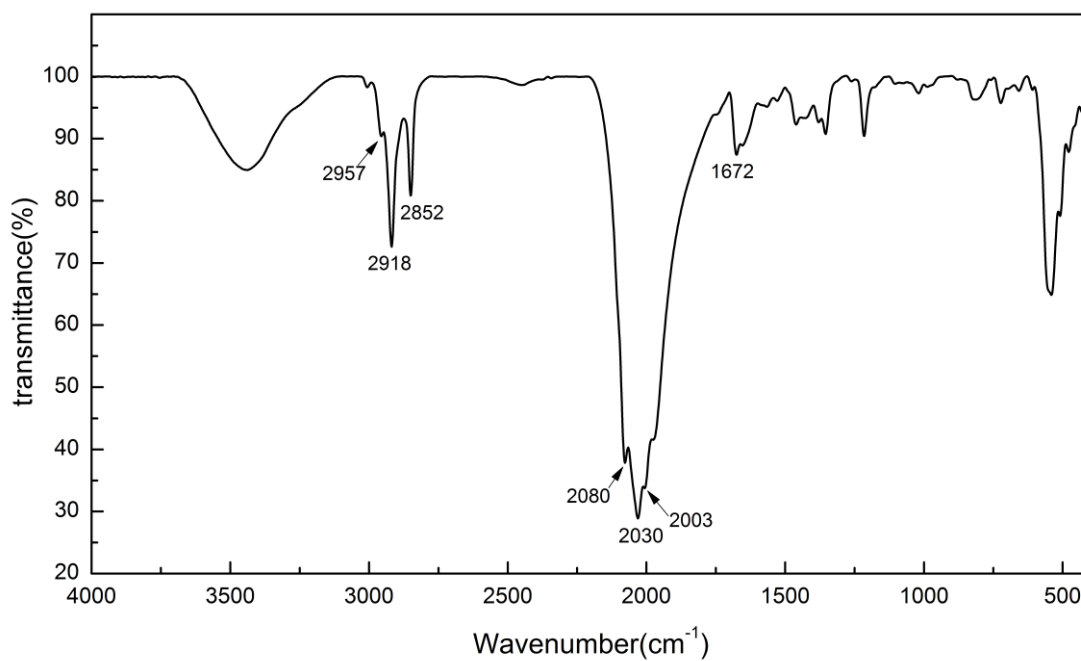
IR spectrum of compound **2b**.



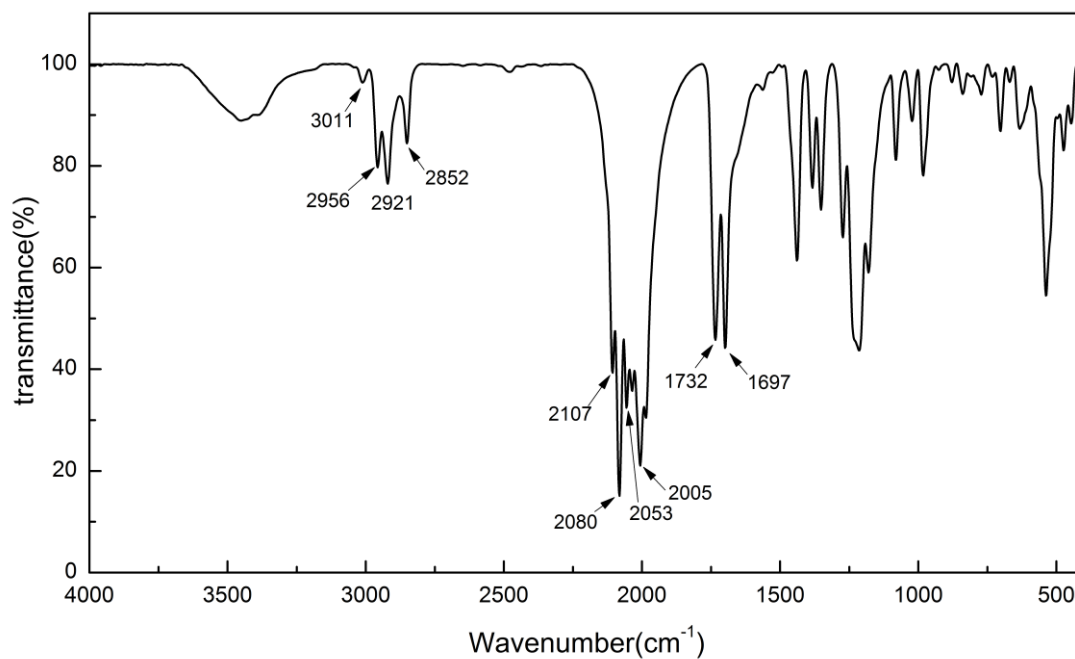
IR spectrum of compound **3a**.



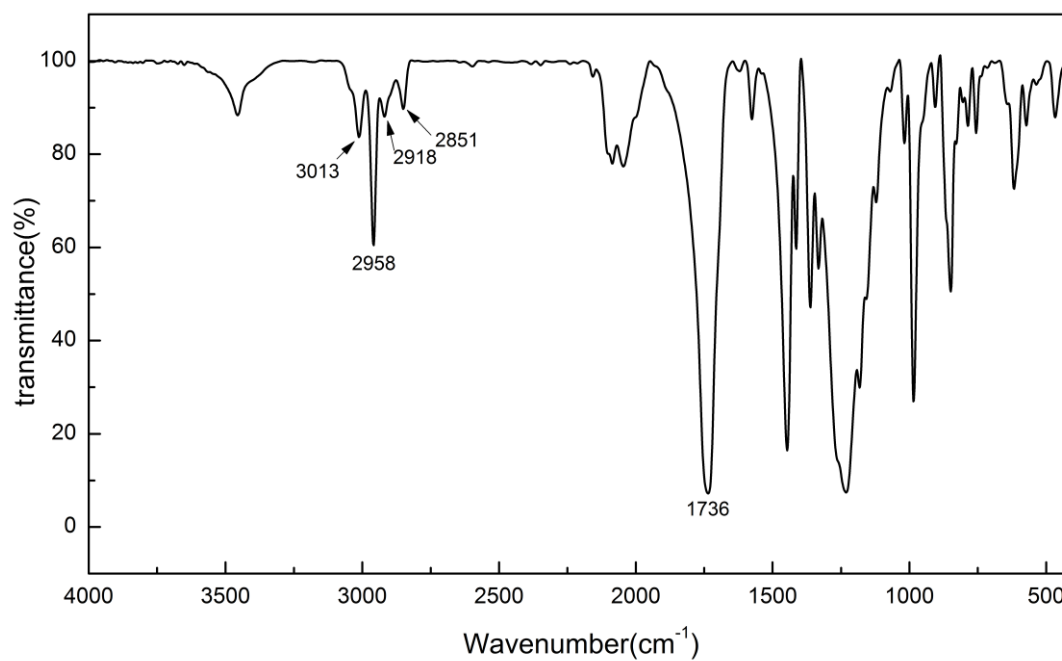
IR spectrum of compound **3c**.



IR spectrum of compound **4a**.



IR spectrum of compound **5a**.



IR spectrum of compound **5b**.