Supporting Information

Development of New and Efficient Copper(II) Complexes of Hexyl bis(pyrazolyl)acetate Ligands as Catalyst for Allylic Oxidation

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Table S1. Detailed SR-XPS data analysis results concerning C1s, N1s, O1s, Cl2p and Cu2p core levels (Binding Energy (BE), Full Width Half Maximum (FWHM), and assignments), confirming the proposed molecular structures.

Sample	Signal	BE (eV)	FWHM (eV)	Assignment
1	C1s	284.87	1.56	C-C aromatic + aliphatic
		286.52	1.56	C-N, C-O
		288.03	1.56	C=O (impurities)
		289.37	1.56	COOR
	N1s	400.31	2.85	C-N
		402.49	2.85	C=N
	O1s	532.21	1.61	C=O
		533.52	1.61	C-O, OH
3	C1s	284.59	1.81	C-C aromatic + aliphatic
		286.39	1.81	C-N, C-O
		288.59	1.81	COOR
	N1s	400.58	3.34	C-N
	O1s	532.02	2.04	C=O
		533.59	2.04	C-O, OH
	$Cl2p_{3/2}$	197.10	2.71	Cl-Cu complex
	$Cu2p_{3/2}$	933.50	3.75	Cu(II) in $CuCl_2$ or CuO
		936.03	3.75	Cu(II) in coordination compound
5	C1s	284.50	1.59	C-C aromatic + aliphatic
		286.11	1.59	C-N, C-O
		288.35	1.59	COOR
	N1s	400.60	2.78	C-N
	O1s	532.15	1.65	C=O
		533.50	1.65	C-O, OH
	$Cl2p_{3/2}$	198.30	2.71	Cl-Cu complex
	$Cu2p_{3/2}$	933.24	3.53	Cu(II) in $CuCl_2$ or CuO
		936.00	3.53	Cu(II) in coordination compound

Table S2. Best fit results for Cu K Edge XAFS Data Analysis of **5** and **3**.

	5		**3**	
	R (Å)	$\sigma^2(\times 10^{-2}$ Å$^2)$	R (Å)	$\sigma^2(\times 10^{-2}$ Å$^2)$
Cu-N	1.948(5)	0.48(2)	2.002(5)	0.52(3)
Cu-Cl	2.20(5)	0.29(1)	2.256(5)	0.55(3)
Cu-N(2)	2.95(1)	0.93(5)	2.96(1)	1.10(6)
Cu-N-C(2)	4.22(1)	0.91(5)	4.68(1)	0.55(3)
Cu-N-C(2)-N	4.57(1)	1.20(6)	4.25(1)	0.95(5)

Figure S1. C1s spectra of **1**, **3** and **5**.

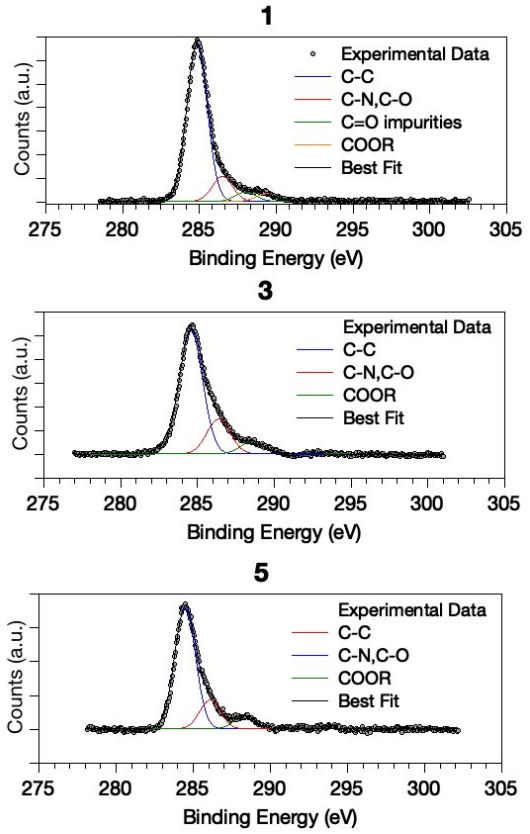


Figure S2. N1s spectra of **1**, **3** and **5**.

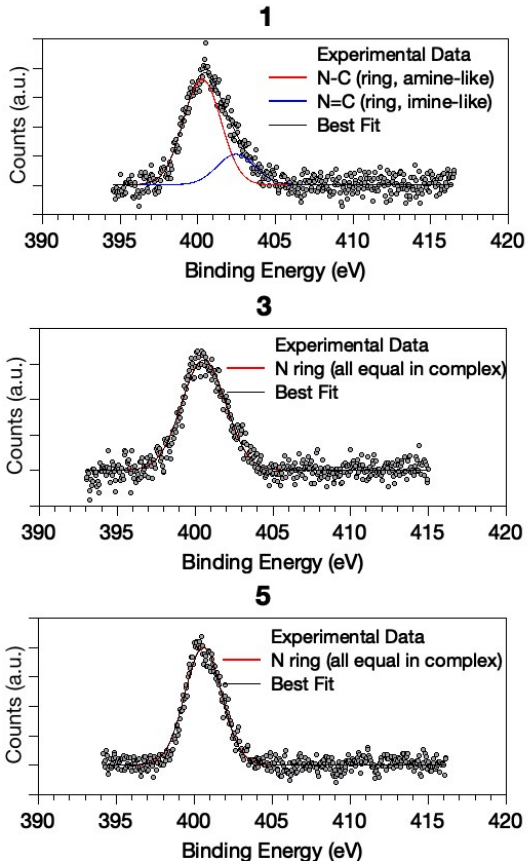


Figure S3. Cl2p spectra of complexes **3** and **5**.

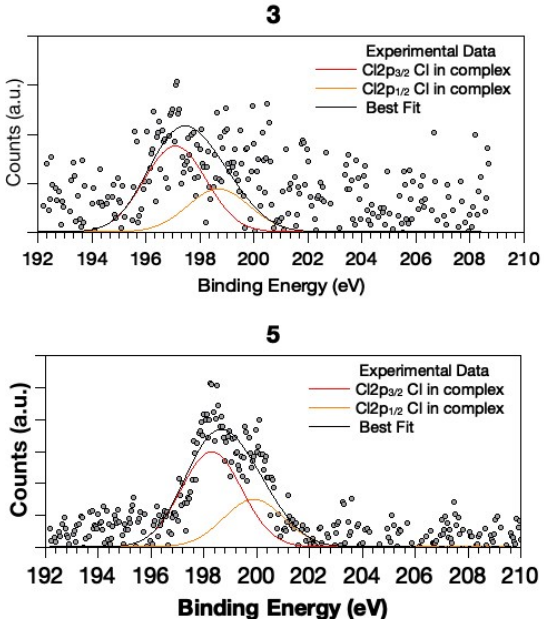


Figure S4. Cu2p spectra of complexes **3** and **5**.

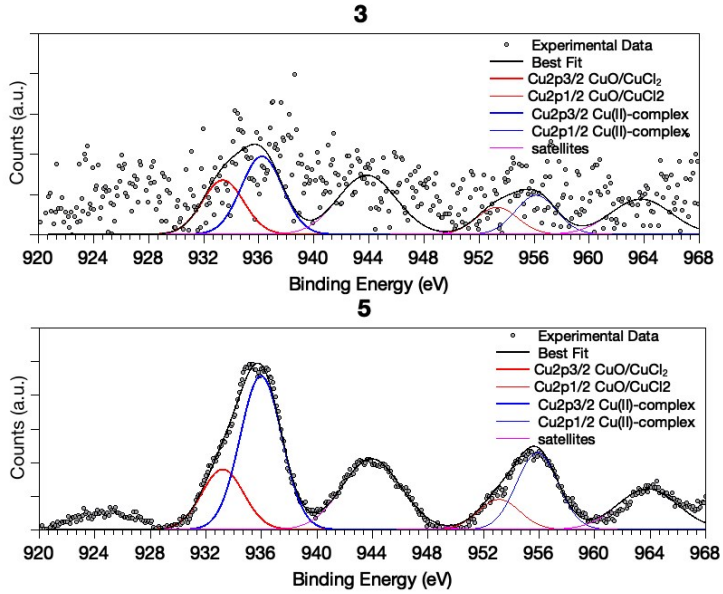
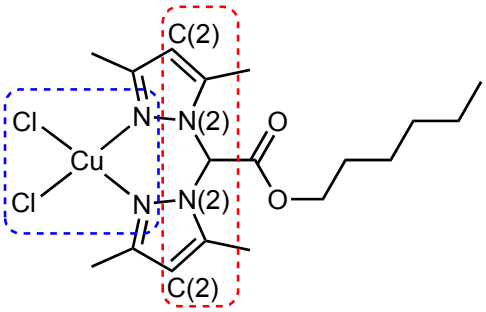
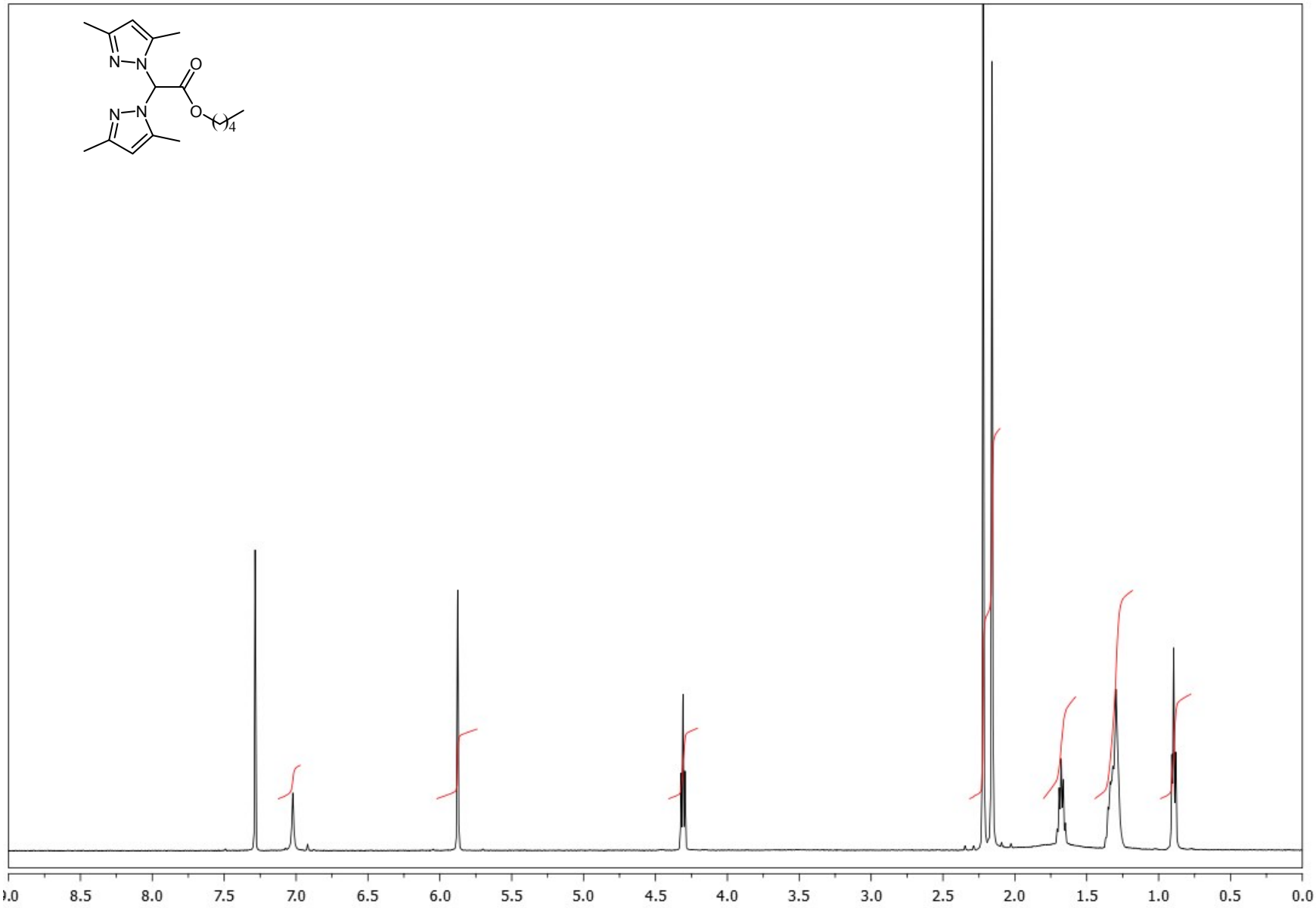


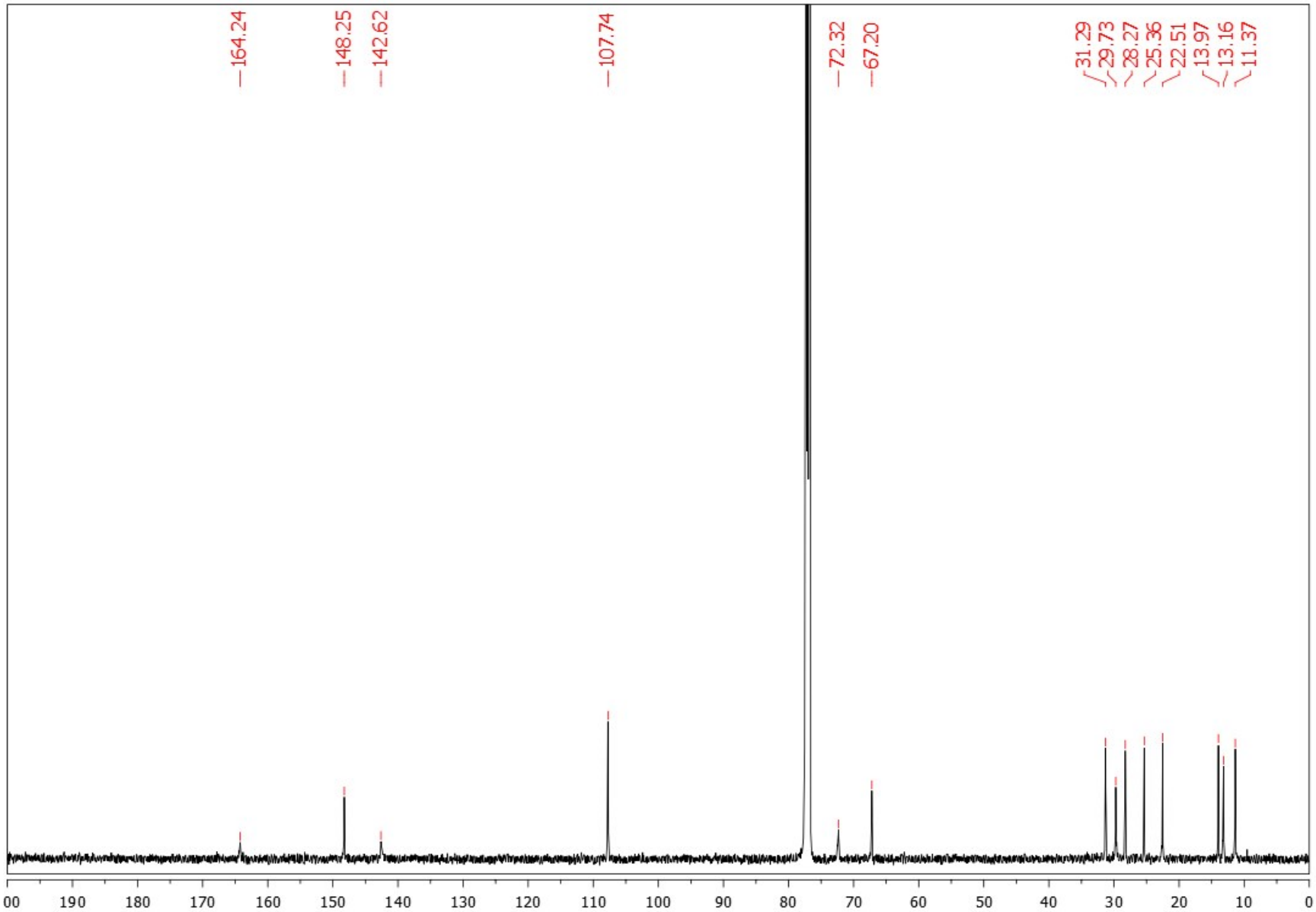
Figure S5. Structure of complex **5.** First and second shell are indicated with dotted lines.



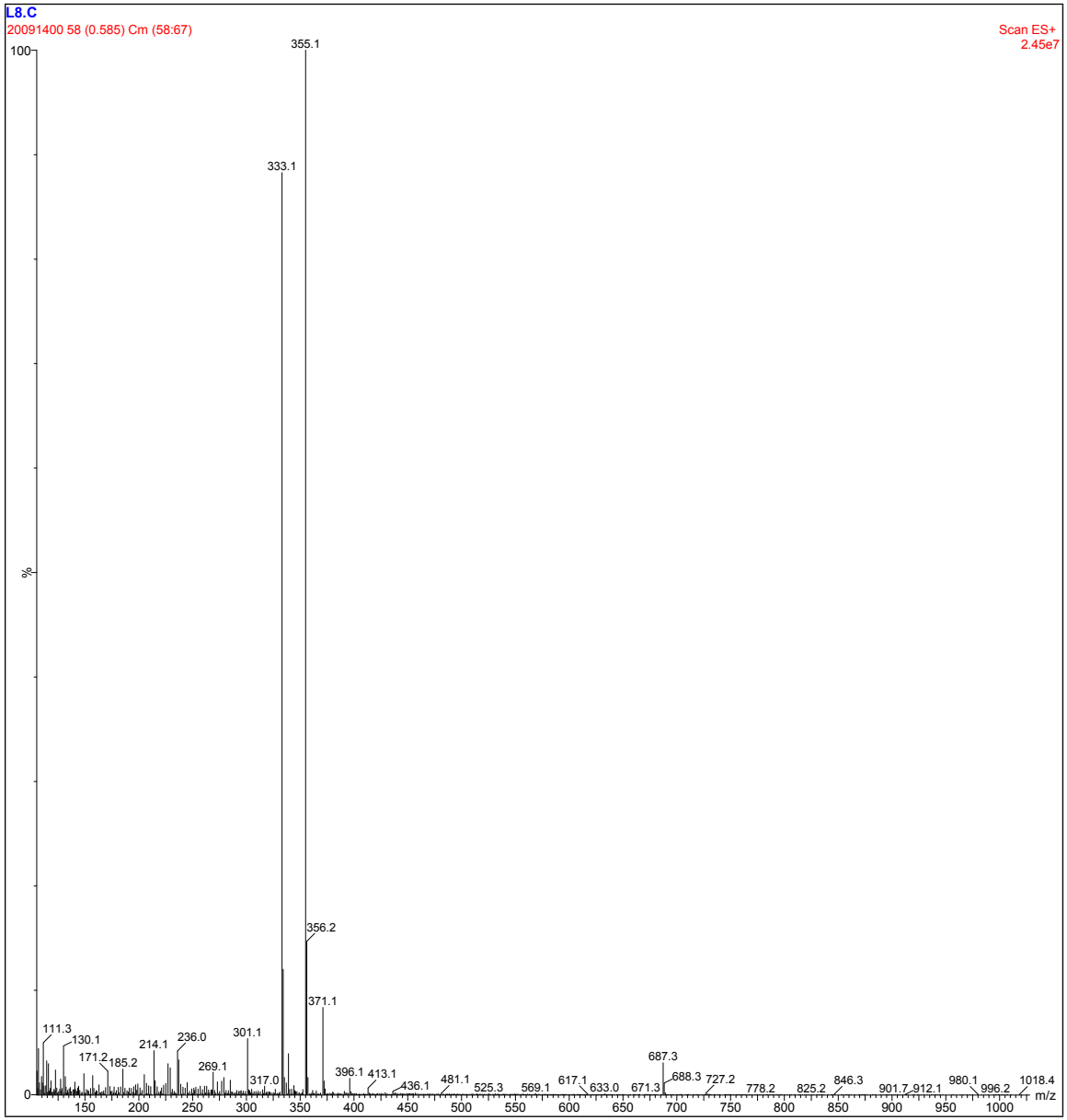
^{1}H-NMR of compound **1** (L^{2OHex}).



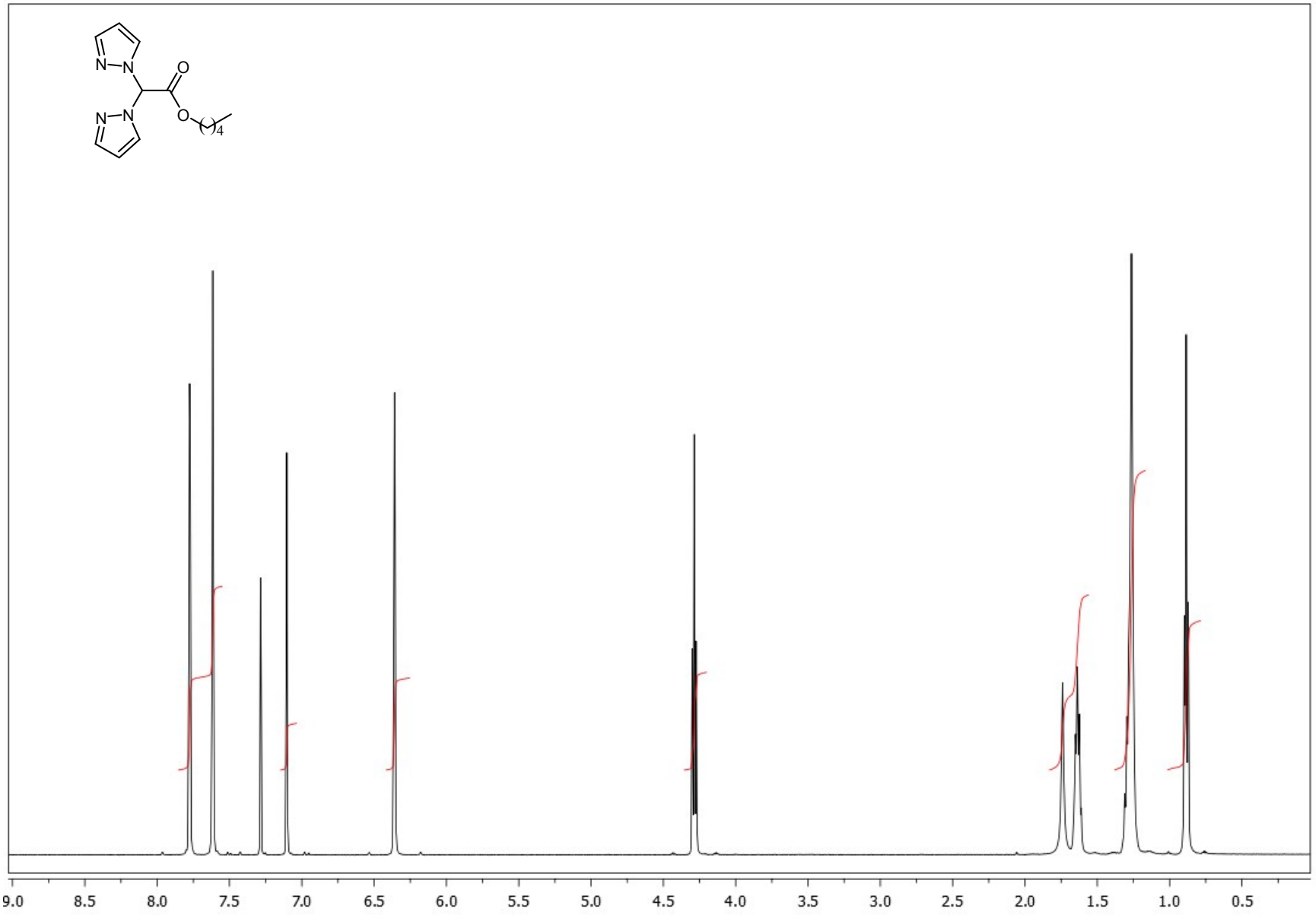
^{13}C-NMR of compound **1** (L^{2OHex}).



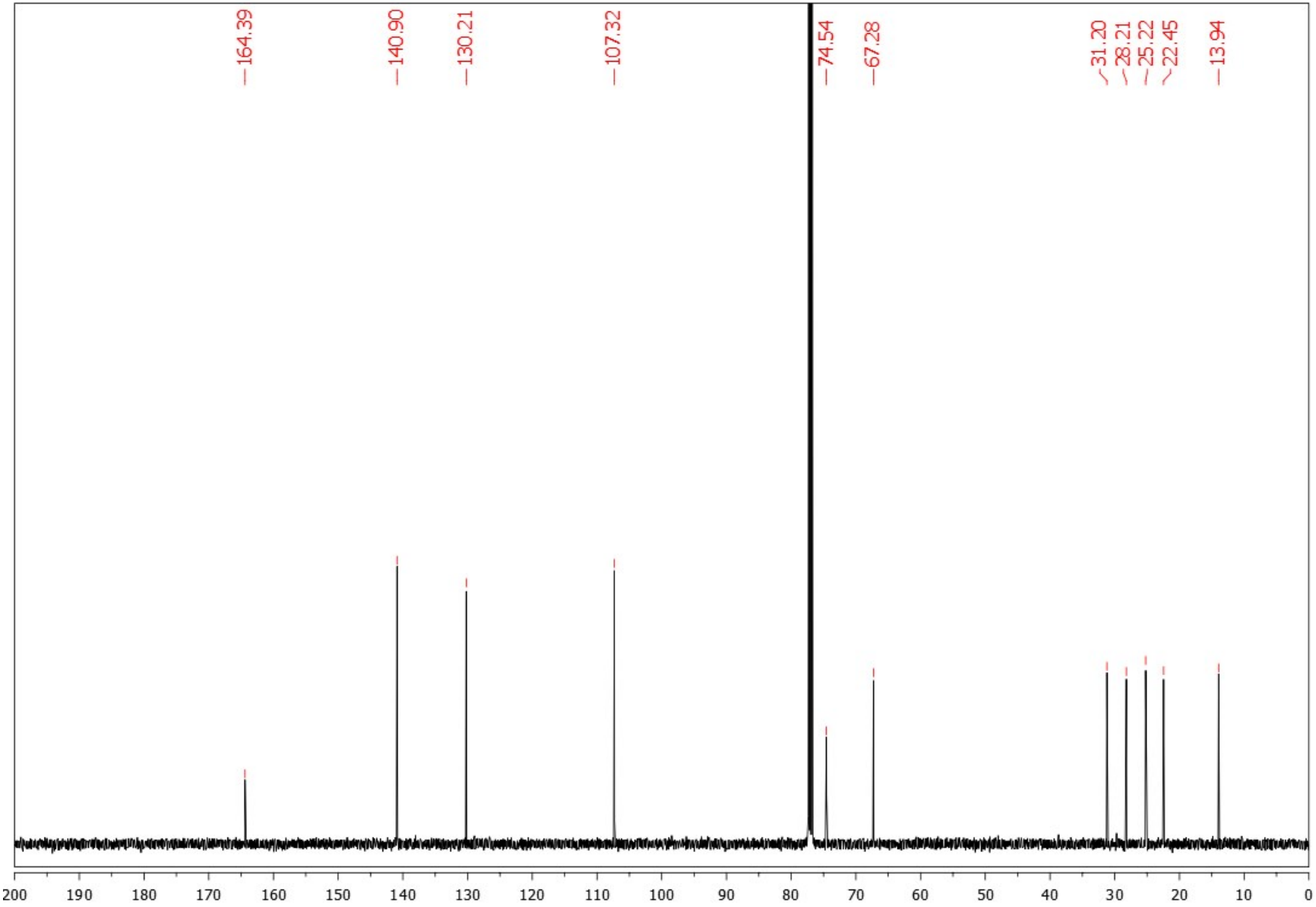
ESI-MS(+) of compound **1** (L^{2OHex}) in CH_3CN.



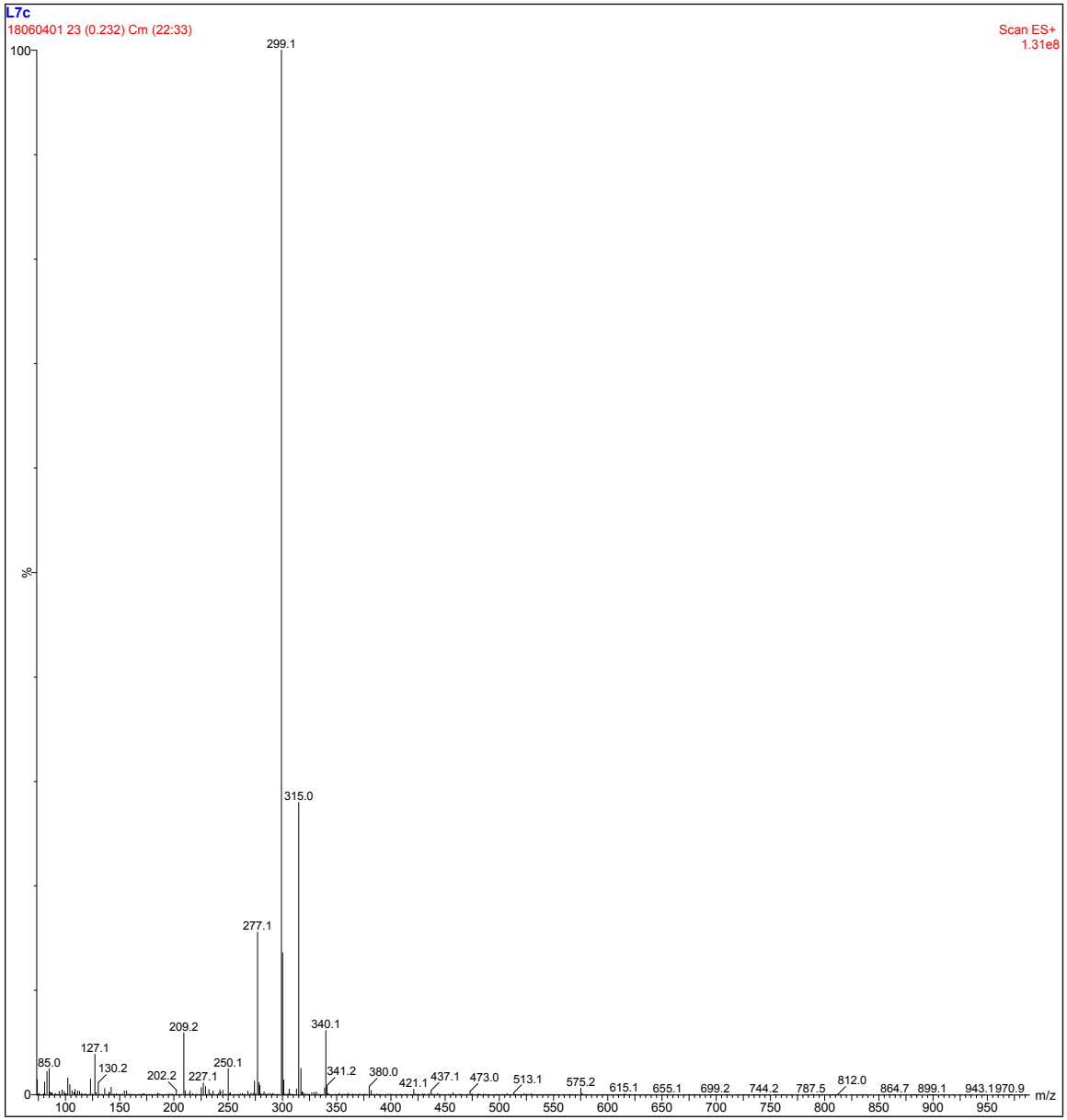
^{1}H-NMR of compound **2** (L^{OHex}).



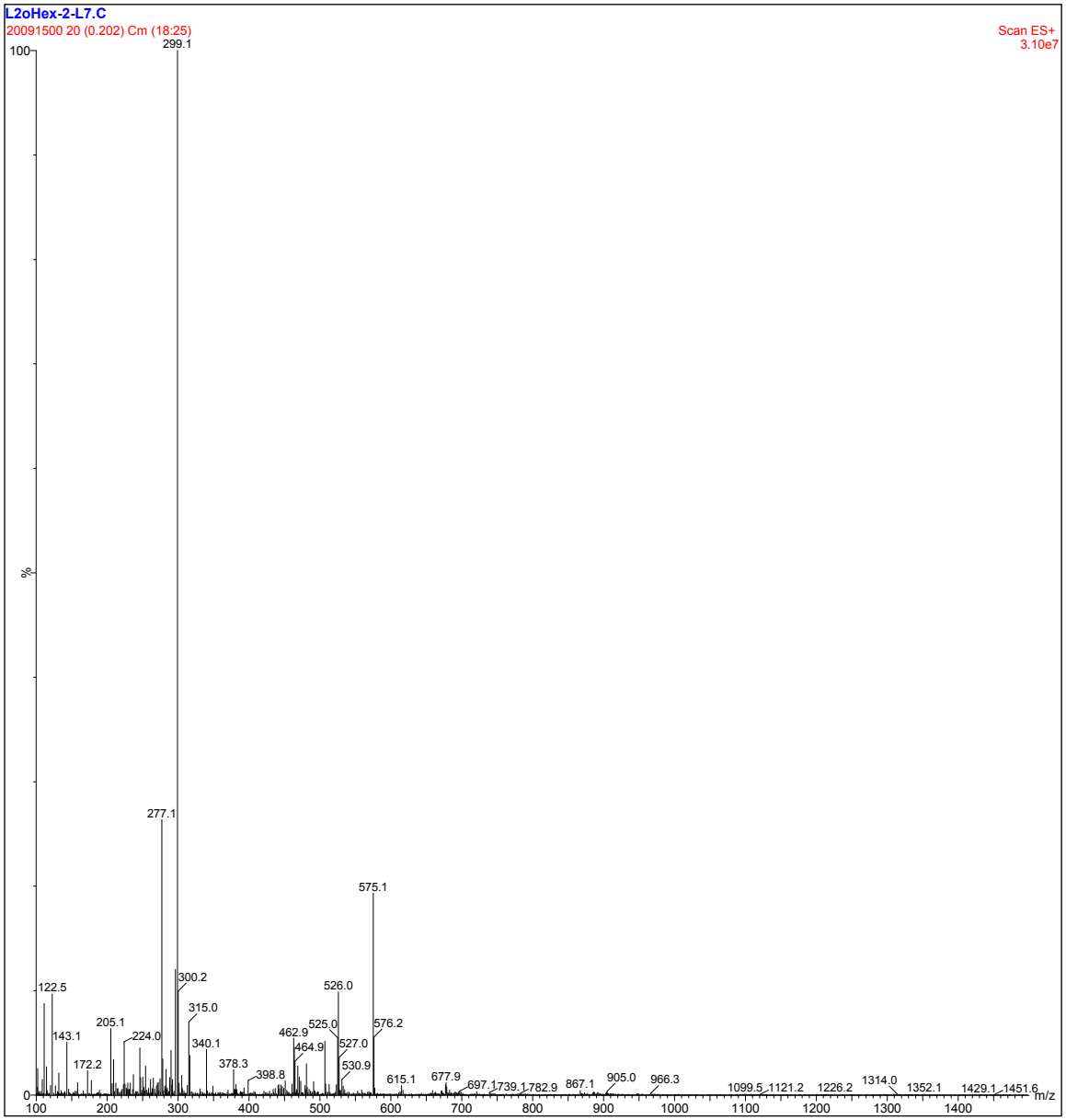
^{13}C-NMR of compound **2** (L^{OHex}).



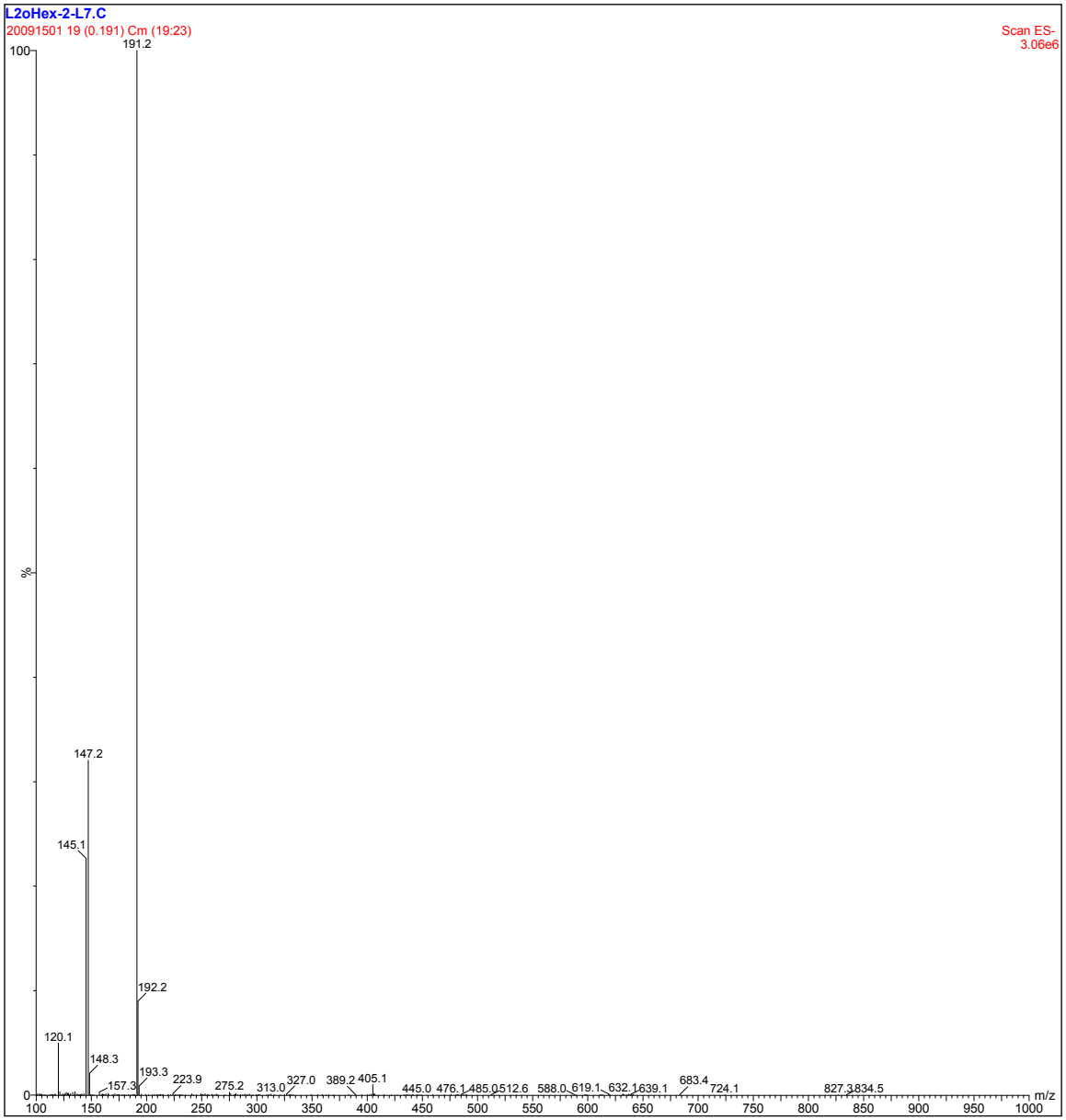
ESI-MS(+) of compound **2** (L^{2OHex}) in CH_3CN.



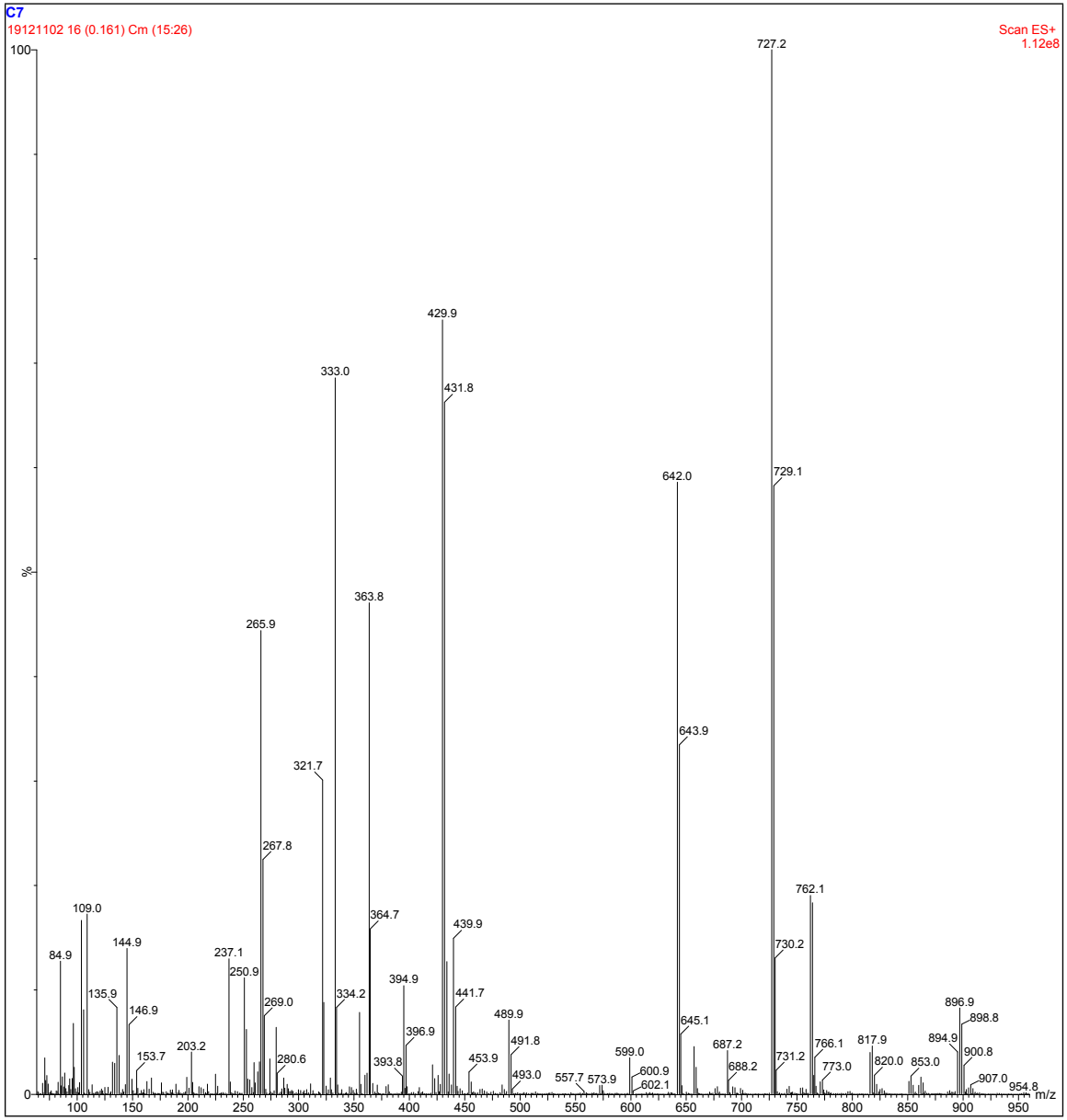
ESI-MS(+) of compound **2** (L^{2OHex}) in H_2O.



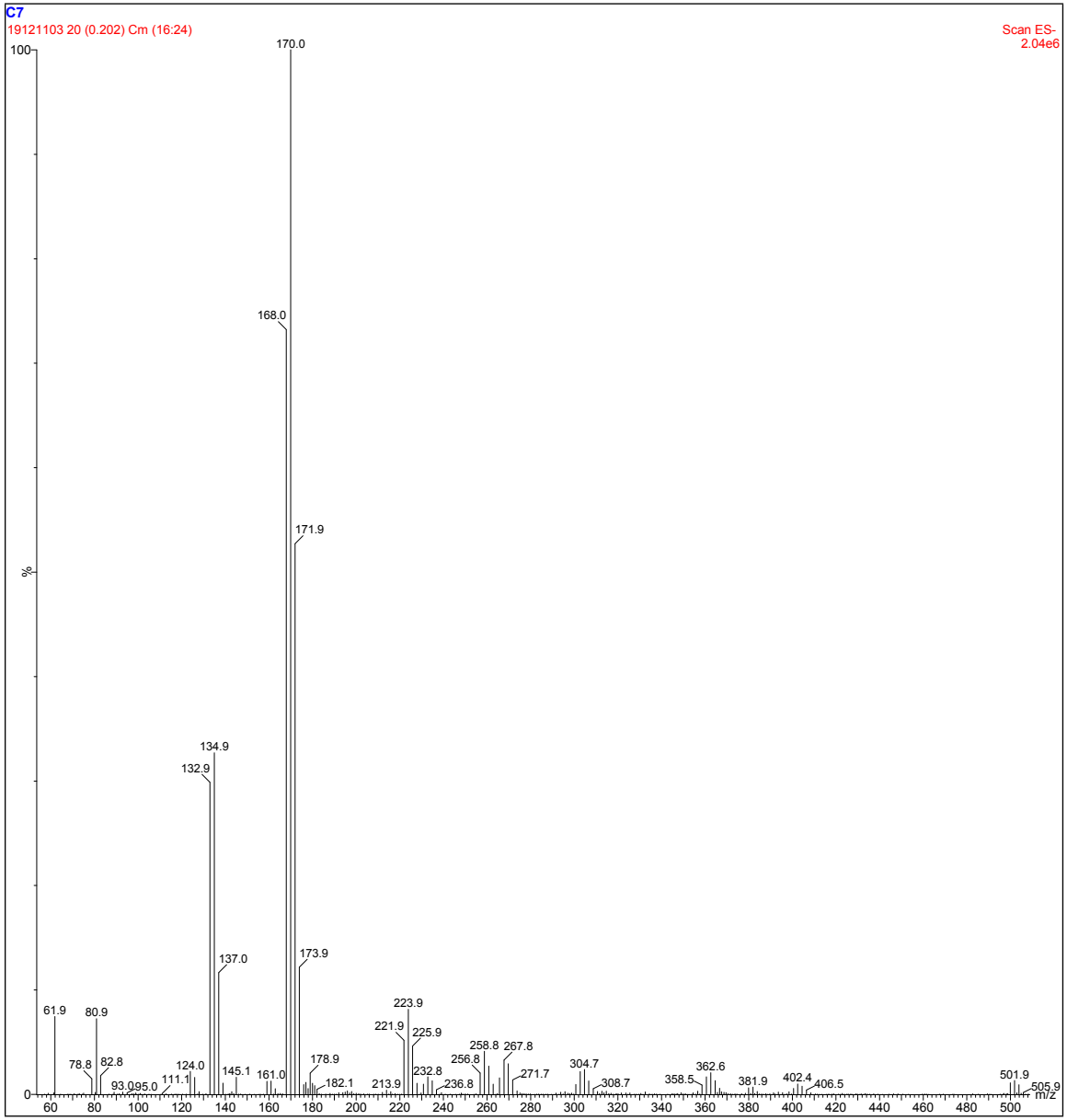
ESI-MS(-) of compound **2** (L^{2OHex}) in H_2O.



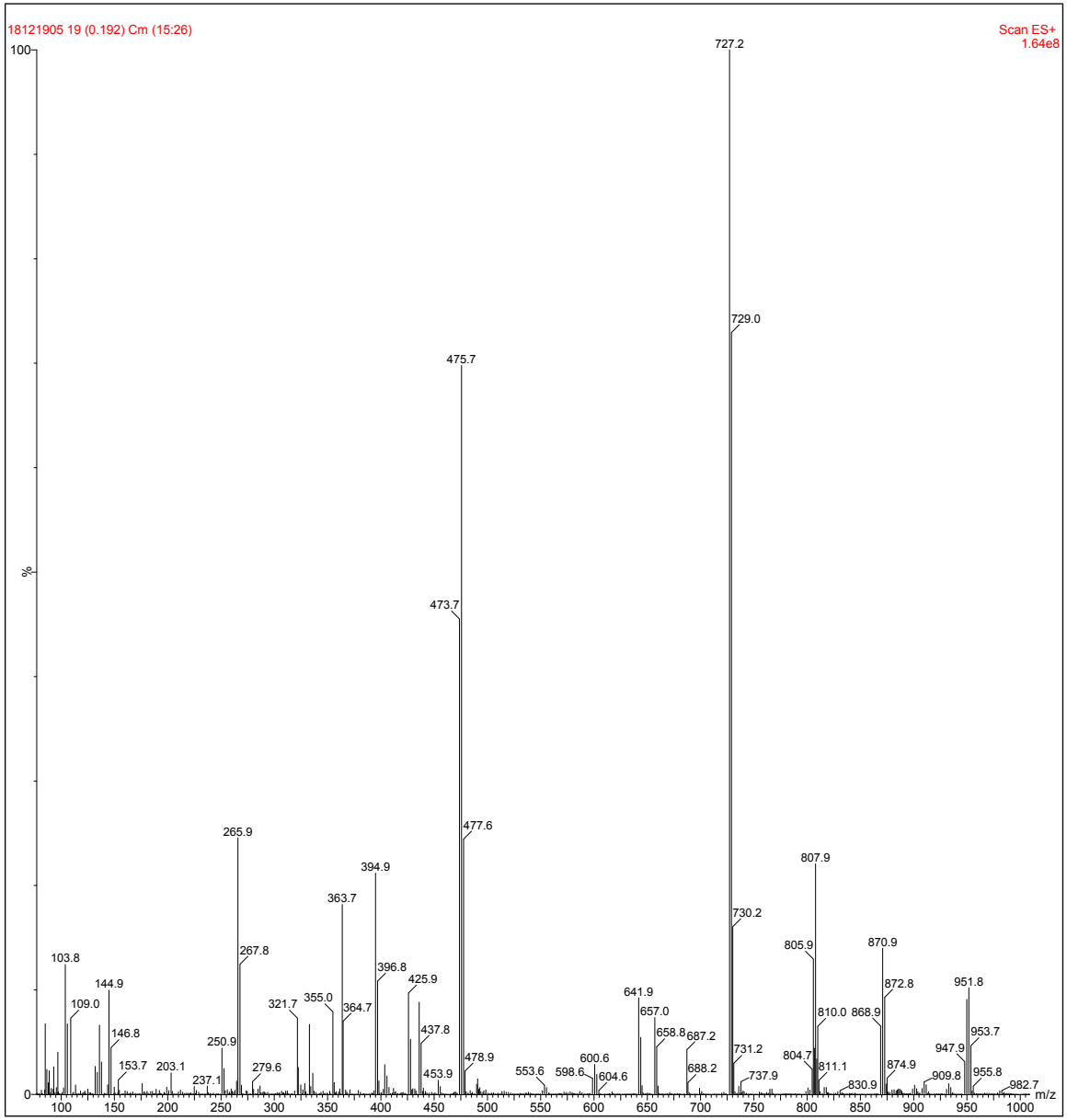
ESI-MS(+) of compound **3**, $[(L^{2OHex})CuCl_2]$ in CH_3CN.



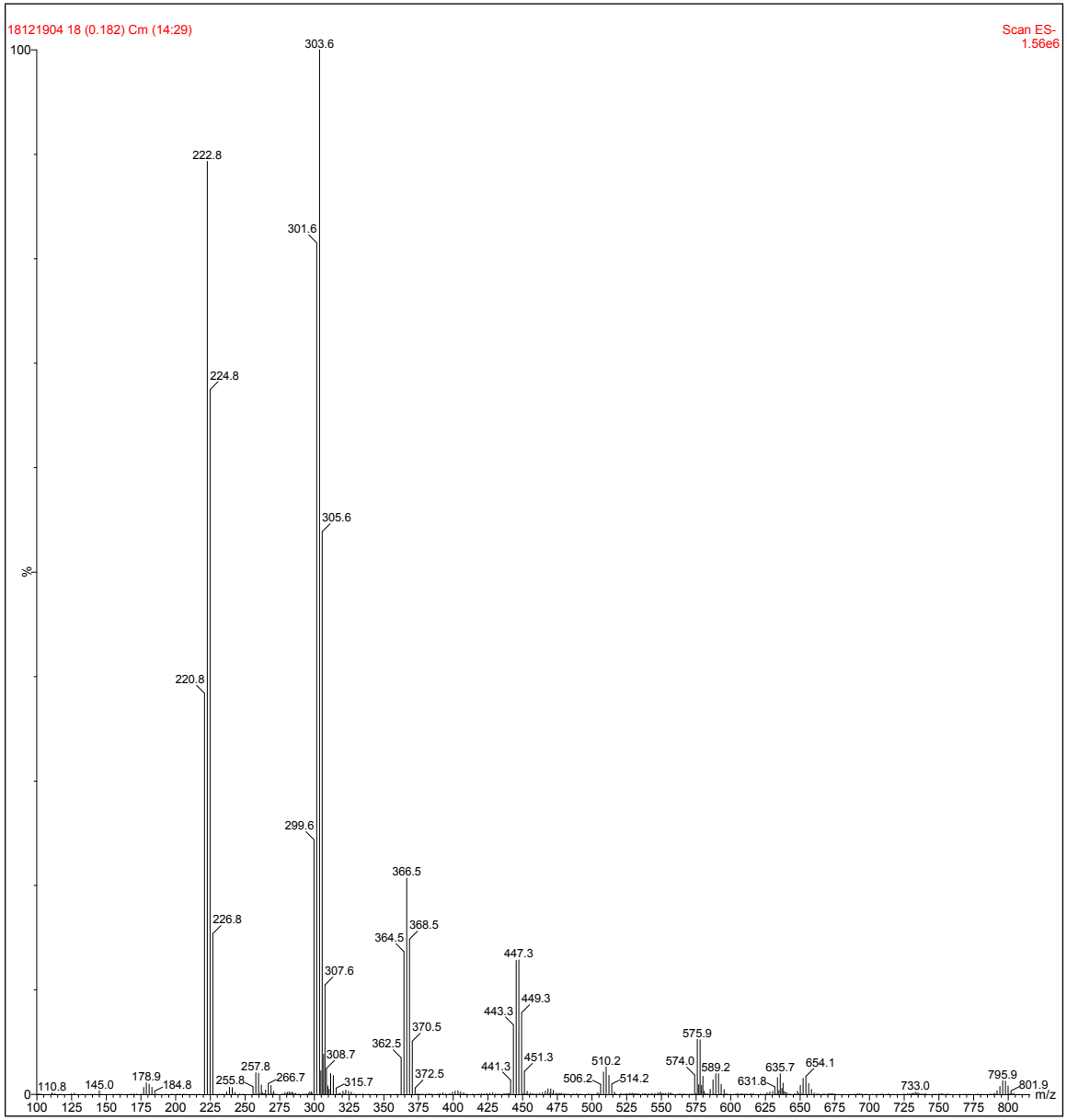
ESI-MS(-) of compound **3**, $[(L^{2OHex})CuCl_2]$ in CH_3CN.



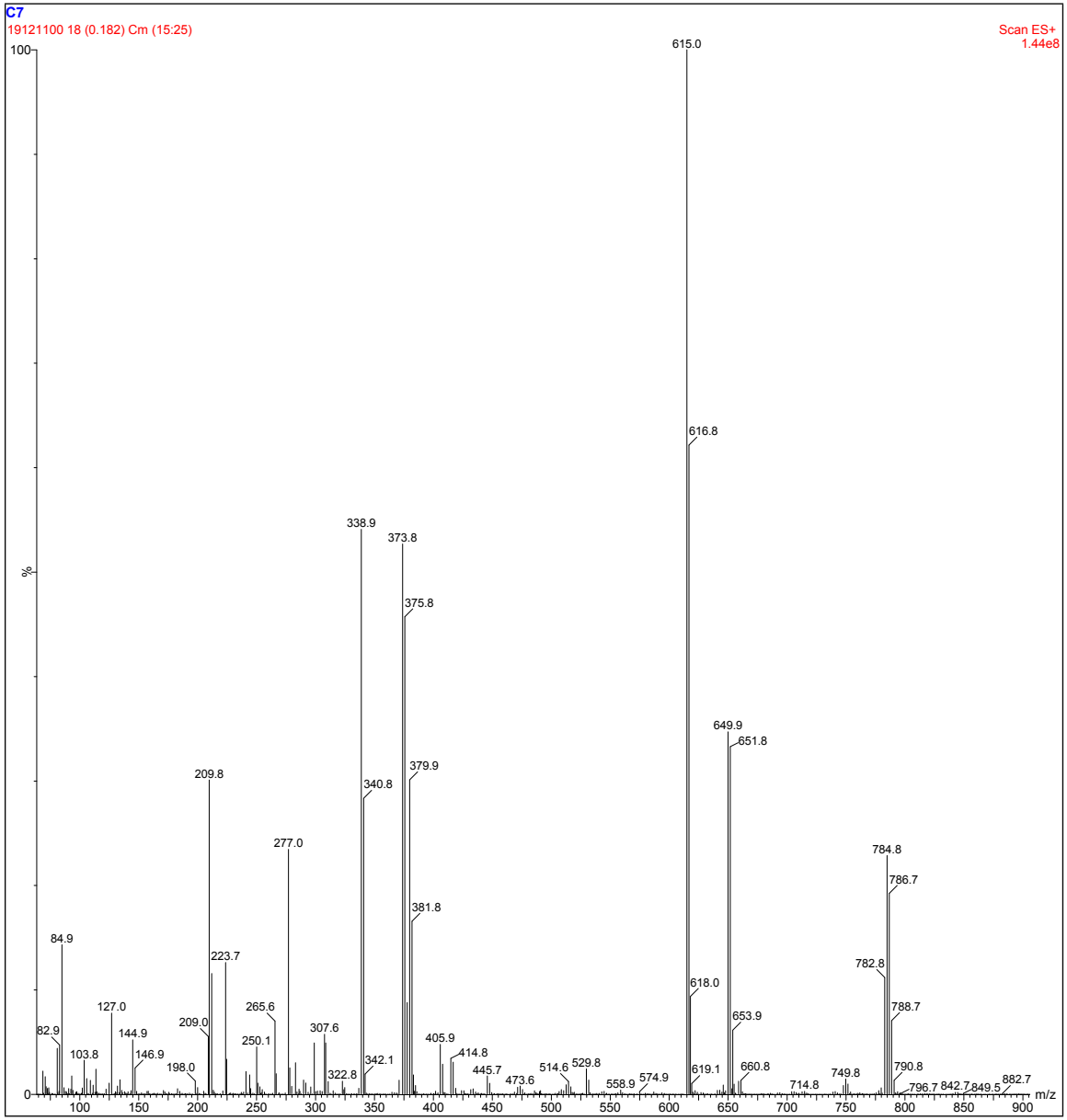
ESI-MS(+) of compound **4**, $[(L^{2OHex})CuBr_2]$ in CH_3CN.



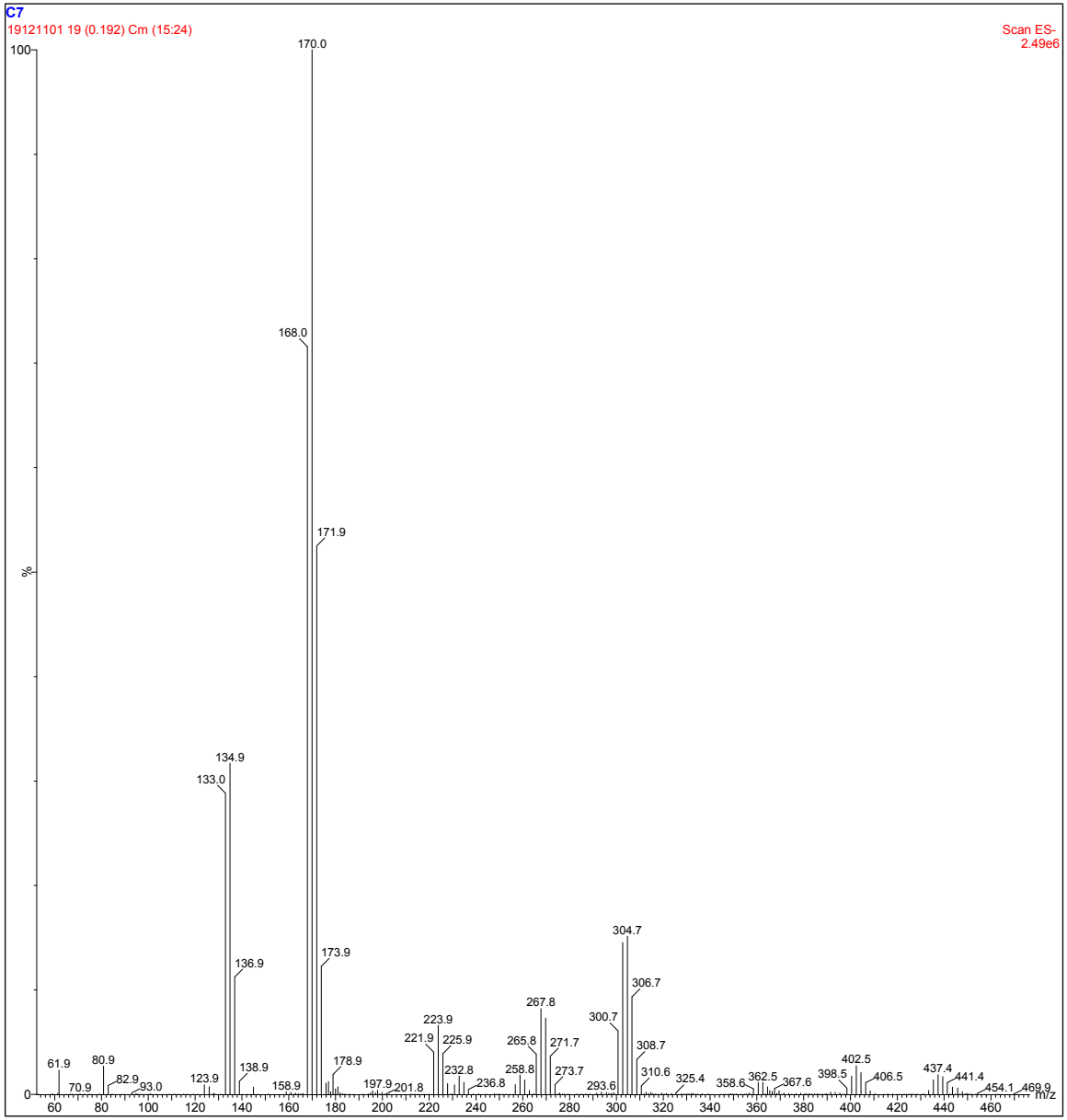
ESI-MS(-) of compound **4**, $[(L^{2OHex})CuBr_2]$ in CH_3CN.



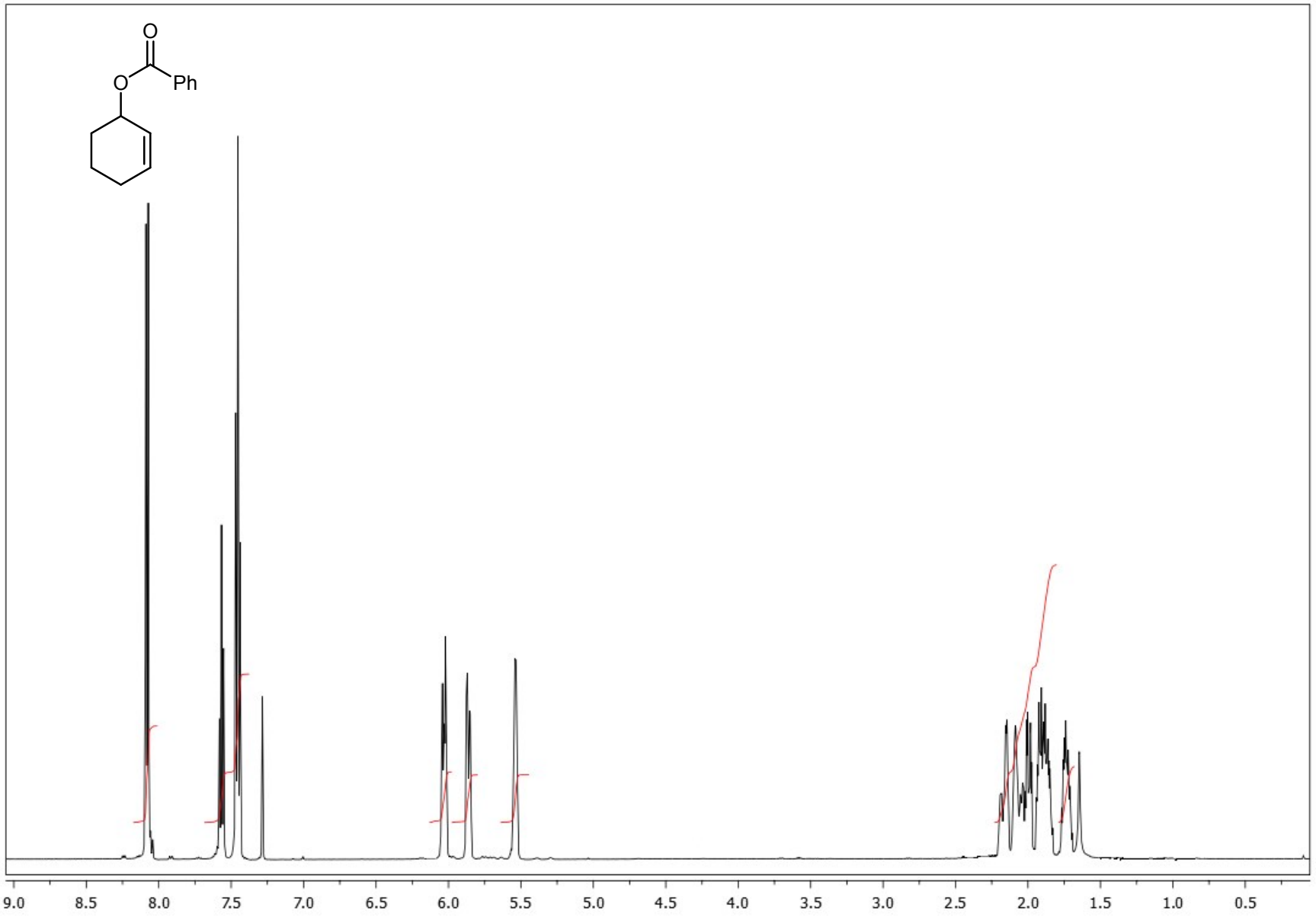
ESI-MS(+) of compound **5**, $[(L^{OHex})CuCl_2]$ in CH_3CN.



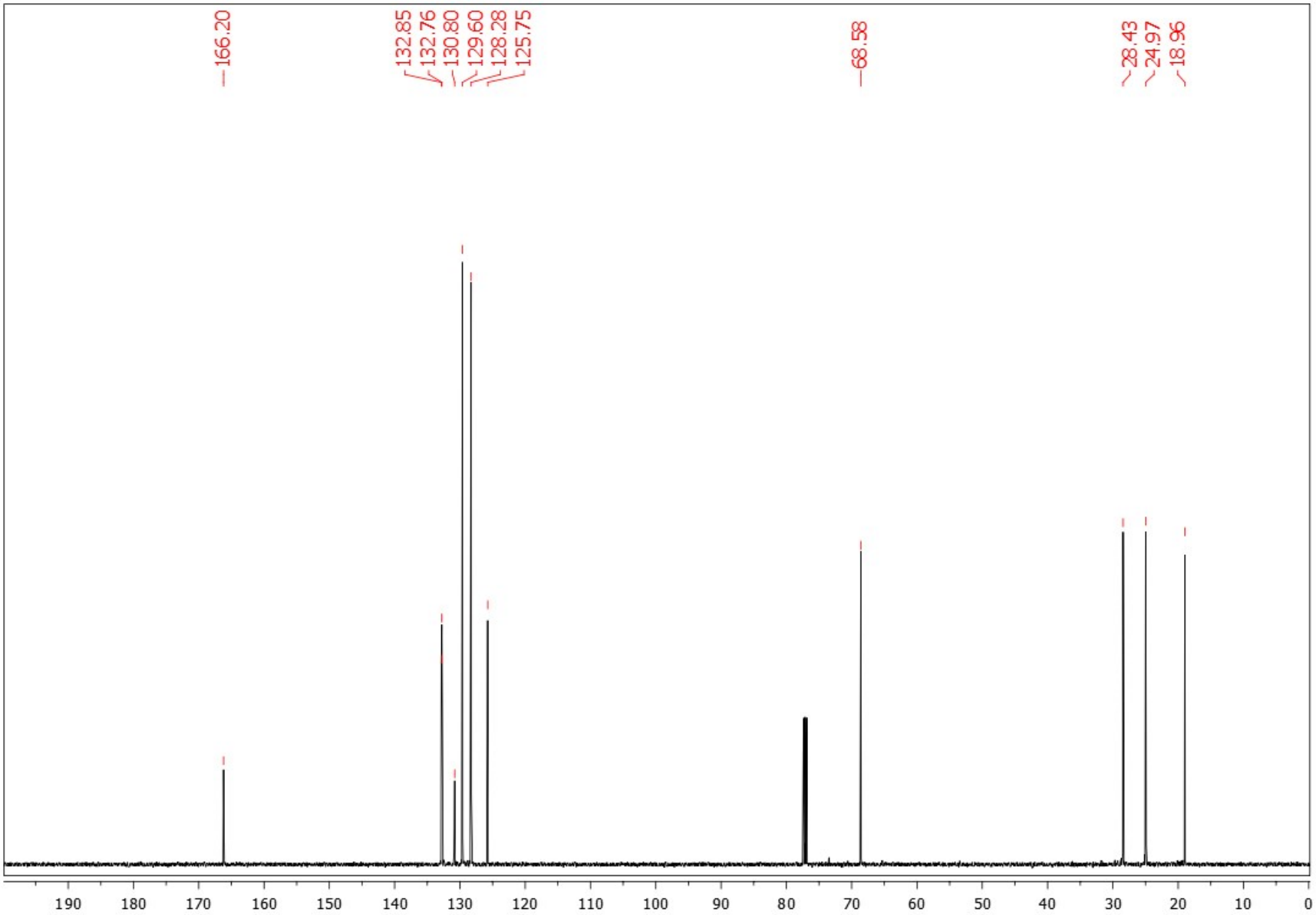
ESI-MS(-) of compound **5**, $[(L^{OHex})CuCl_2]$ in CH_3CN.



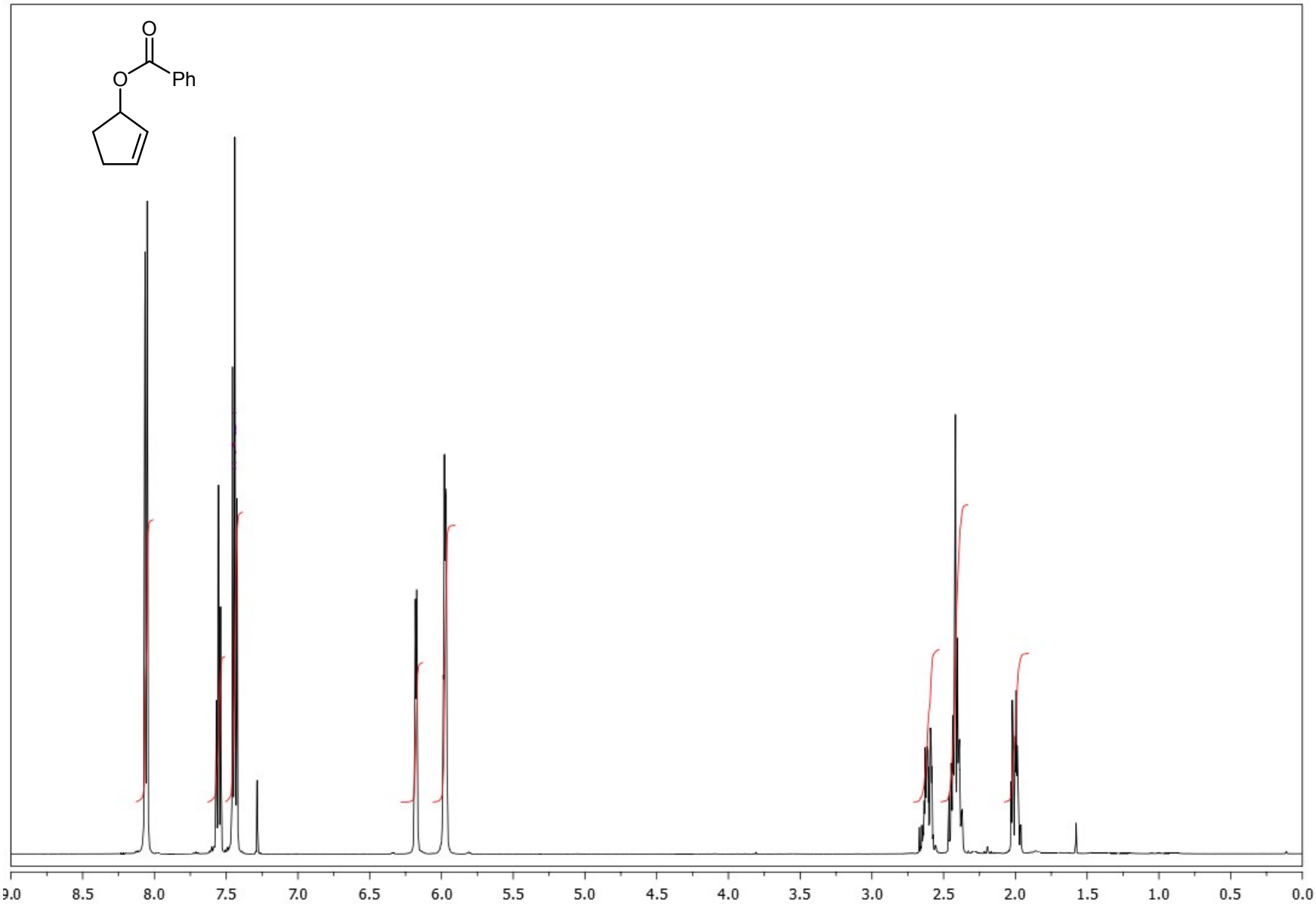
^{1}H-NMR of compound **8**.



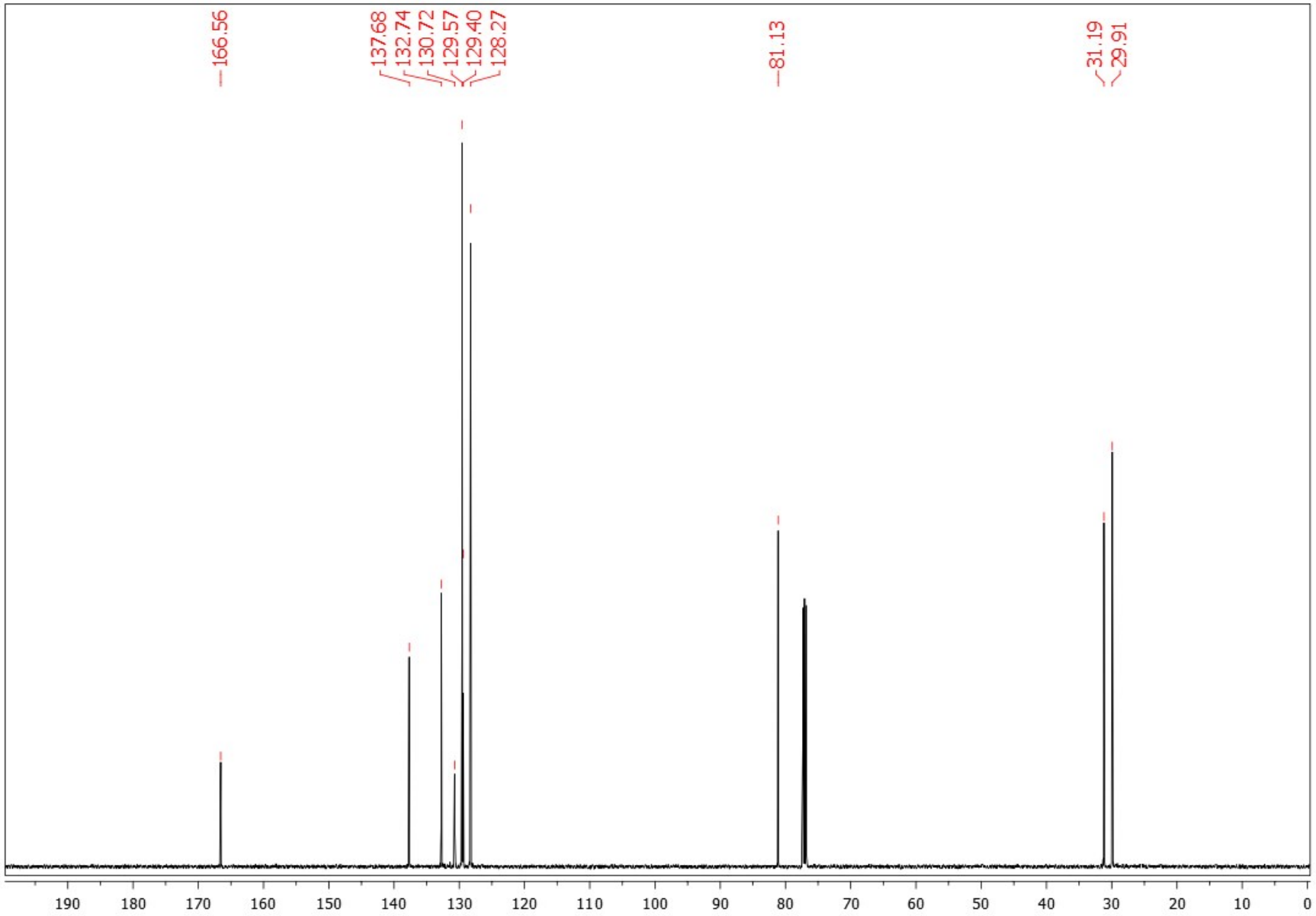
^{13}C-NMR of compound **8**.



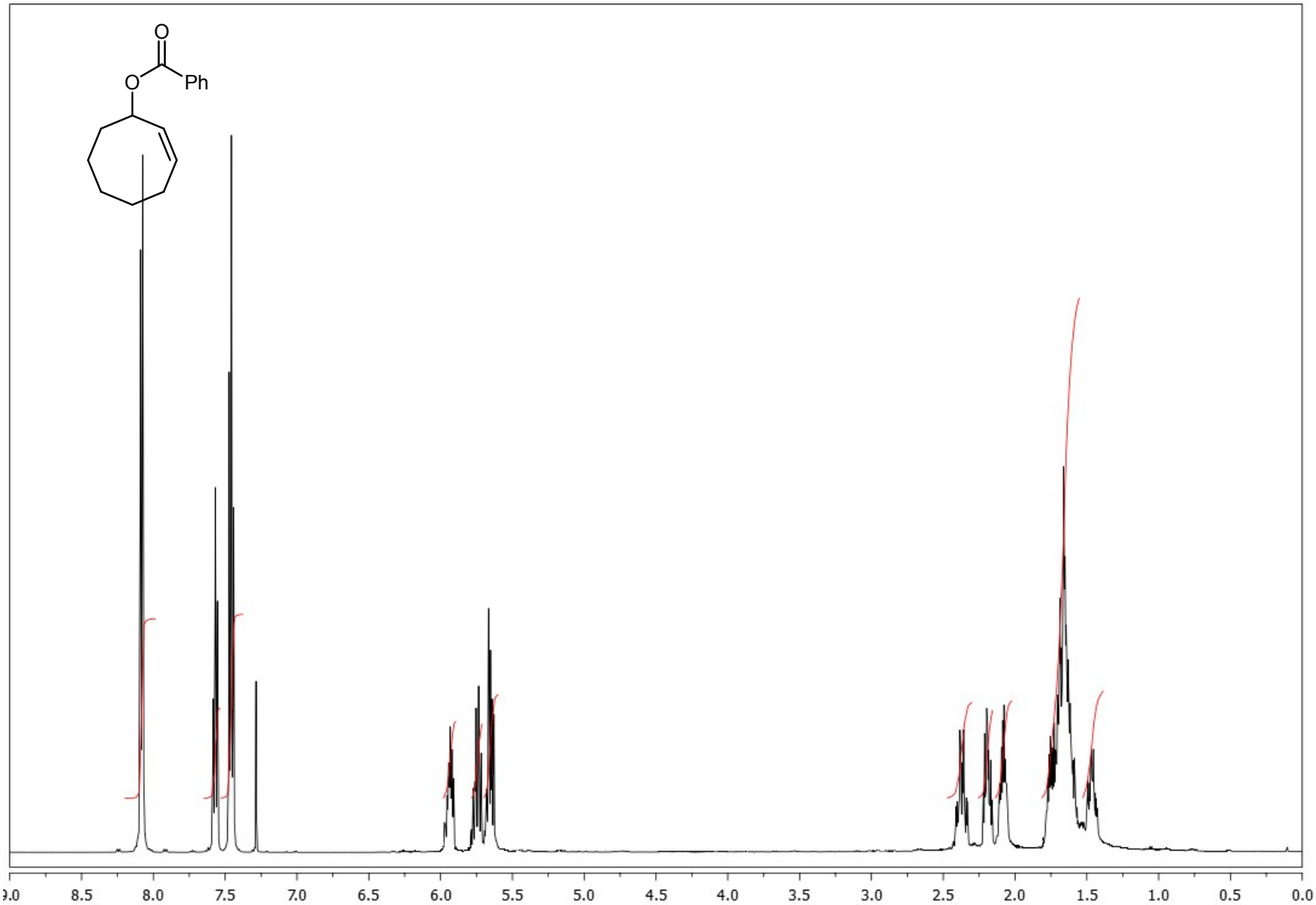
^{1}H-NMR of compound **9**.



^{13}C-NMR of compound **9**.



^{1}H-NMR of compound **10**.



^{13}C-NMR of compound **10**.