Supporting information for “Hands-on Inquiry-Based Qualitative Identification of Metals in Coins Utilizing Atmospheric Pressure Chemical Ionization Mass Spectrometry”

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1. MASS SPECTROMETRIC STUDIES

This practical introduces first-year undergraduates to mass spectrometry in a research setting and, consequently, we have made efforts to simplify the fragmentation patterns to make the spectra more accessible. In the practical the low fragmentation setting is used exclusively, again to simplify the procedure; however, work has been carried out showing fine-tuning of the temperature at which the ionization is carried out can further improve the spectra (**Table 1**, **2**).

Table S1. Source parameters for the nine preset fragmentation modes on the Advion mass spectrometer. The current of the corona discharge is 5 µA for all entries.

Entry	Fragmentation setting	Capillary T / °C	Capillary voltage / V	Ion source T / °C	Source voltage offset / V	Source voltage range / V
1	Low T/Low fragmentation	135	120	250	25	0
2	Low T/Med fragmentation	135	160	250	30	5
3	Low T/High fragmentation	135	180	250	55	20
4	Med T/Low fragmentation	200	120	350	25	0
5	Med T/Med fragmentation	200	160	350	30	5
6	Med T/High fragmentation	200	180	350	55	20
7	High T/Low temperature	250	120	400	25	0

8	High T/Med temperature	250	160	400	30	5
9	High T/High temperature	250	180	400	55	20

Table S2. Mass spectrometric data for 10 pure samples of transition metal acetylacetonates including their method of acquisition and the relevant ion formed.

Entry	Complex	Frag. method	Temperature	Mass expected[a]	Mass found[a]	Ion[b]
1	$Co(acac)_2$	Low	Low	258.0	257.9	$[^{59}Co(acac)_2+H]^+$
2	$Ni(acac)_2$	Low	Medium	257.0	257.0	$[^{58}Ni(acac)_2+H]^+$
3	$Cu(acac)_2$	Low	High	262.0	261.9	$[^{63}Cu(acac)_2+H]^+$
4	$Zn(acac)_2$	Low	Medium	263.0	262.9	$[^{64}Zn(acac)_2+H]^+$
5	$V(acac)_3$	Low	Low	348.1	349.0	$[^{51}V(acac)_3+H]^+$
6	$Cr(acac)_3$	Low	Low	350.1	350.0	$[^{52}Cr(acac)_3+H]^+$
7	$Mn(acac)_3$	Low	Low	253.0	252.9	$[^{55}Mn(acac)_2]^+$
8	$Fe(acac)_3$	Low	Medium	254.1	254.0	$[^{56}Fe(acac)_2]^+$
9	$Co(acac)_3$	Low	High	257.0	256.9	$[^{59}Co(acac)_2]^+$
10	$V(O)(acac)_2$	Low	Medium	266.0	265.9	$[^{51}V(O)(acac)_2+H]^+$

[a]Mass for most naturally abundant isotope shown; [b]positive ionization allowed more reliable characterization of the ion peaks than negative ionization.

2. EXAMPLE MASS SPECTROMETRY DATA

Below are instructor generated data for all typical coinage metal acac complexes, for reference.

Table S3. Observed isotopic abundances using ASAP-MS.

Entry	Ion[a]	Expected Mass[c]	Expected abundance[c]	Observed Mass	Observed abundance
1	$[^{x}Ni(acac)_2+H]^+$	257.0	100.0%	257.0	100.0%
		258.0	10.8%	258.0	12.5%
		259.0	38.5%	259.0	34.5%
		260.0	5.9%	260.0	5.2%
		261.0	5.3%	261.0	5.1%
		263.0	1.4%	263.0	1.2%
2	$[^{x}Cu(acac)_2+H]^+$	262.0	100.0%	261.9	100%
		263.0	10.8%	263.0	8.5%
		264.0	44.6%	263.9	47.4%
		265.0	4.8%	265.0	5.1%
3	$[^{x}Zn(acac)_2+H]^+$	263.0	100.0%	262.9	100.0%
		264.0	10.8%	264.0	11.3%
		265.0	57.4%	264.9	64.0%
		266.0	14.6%	265.9	13.6%
		267.0	38.6%	266.9	39.4%
		268.0	4.2%	267.9	3.8%
		269.0	1.3%	-[b]	-[b]
4	$[^{x}Cr(acac)_3+H]^+$	348.1	5.2%	348.0	5.8%
		-[b]	-[b]	349.0	17.8%
		350.1	100.0%	350.0	100.0%
		351.1	27.5%	351.0	32.1%
		352.1	7.0%	352.0	7.8%
5	$[^{x}Fe(acac)_2]^+$	252.0	6.4%	7.1%	7.1%
		254.0	100.0%	100.0%	100.0%
		255.0	10.8%	12.8%	12.8%

[a] Co and V were not included in this analysis due to the very high natural abundance of their major isotopes; [b] peak too faint for accurate relative abundance analysis; [c] obtained from ChemDraw prediction.

Figure S1. Mass spectrum of $Co(acac)_2$.

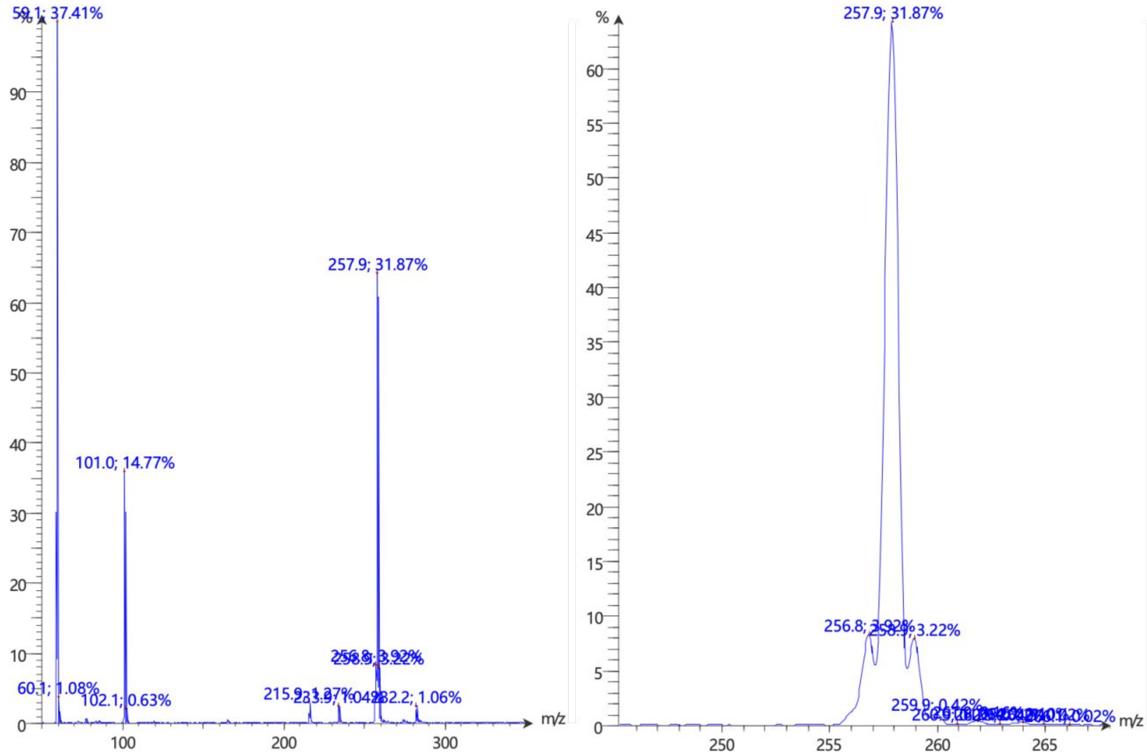

Figure S2. Mass spectrum of $Ni(acac)_2$.

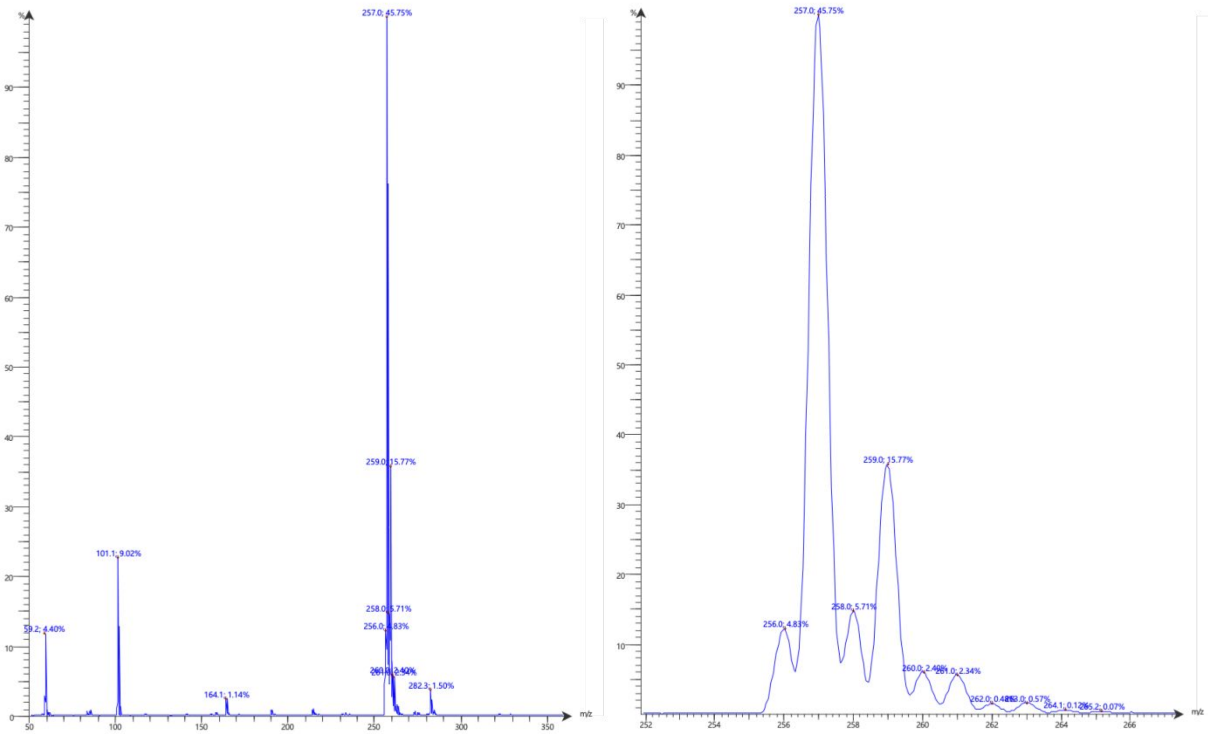

Figure S3. Mass spectrum of $Cu(acac)_2$.

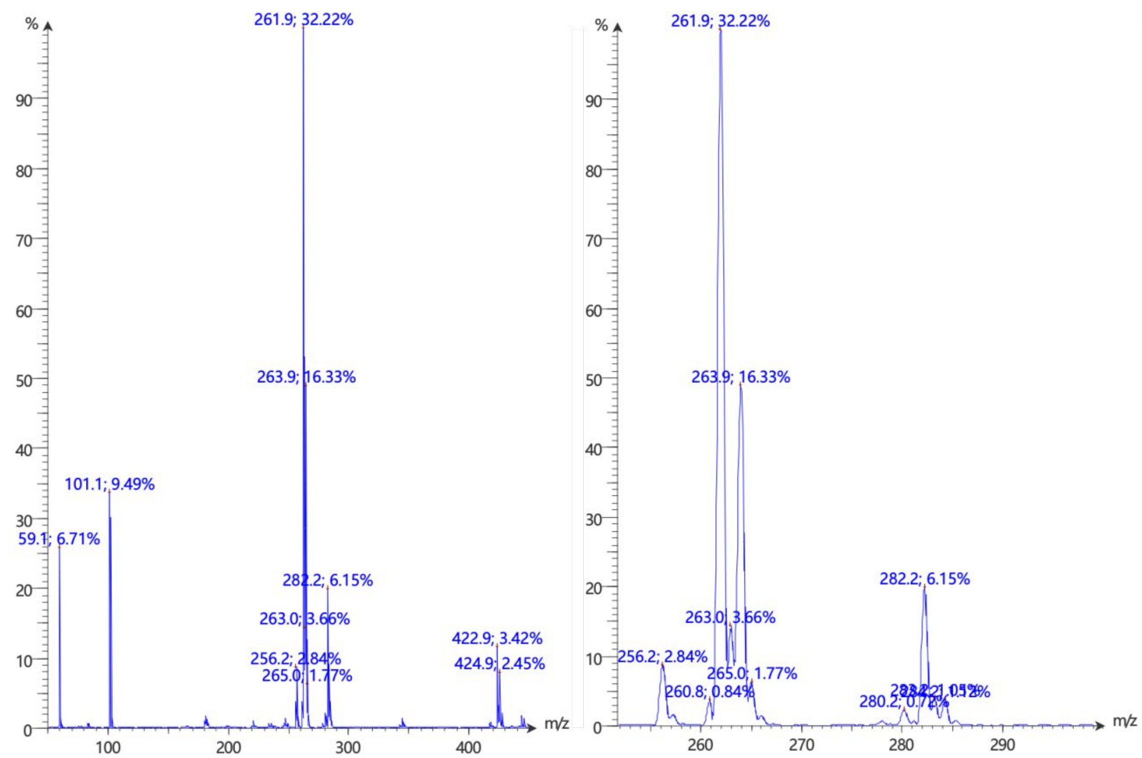

Figure S4. Mass spectrum of $Zn(acac)_2$.

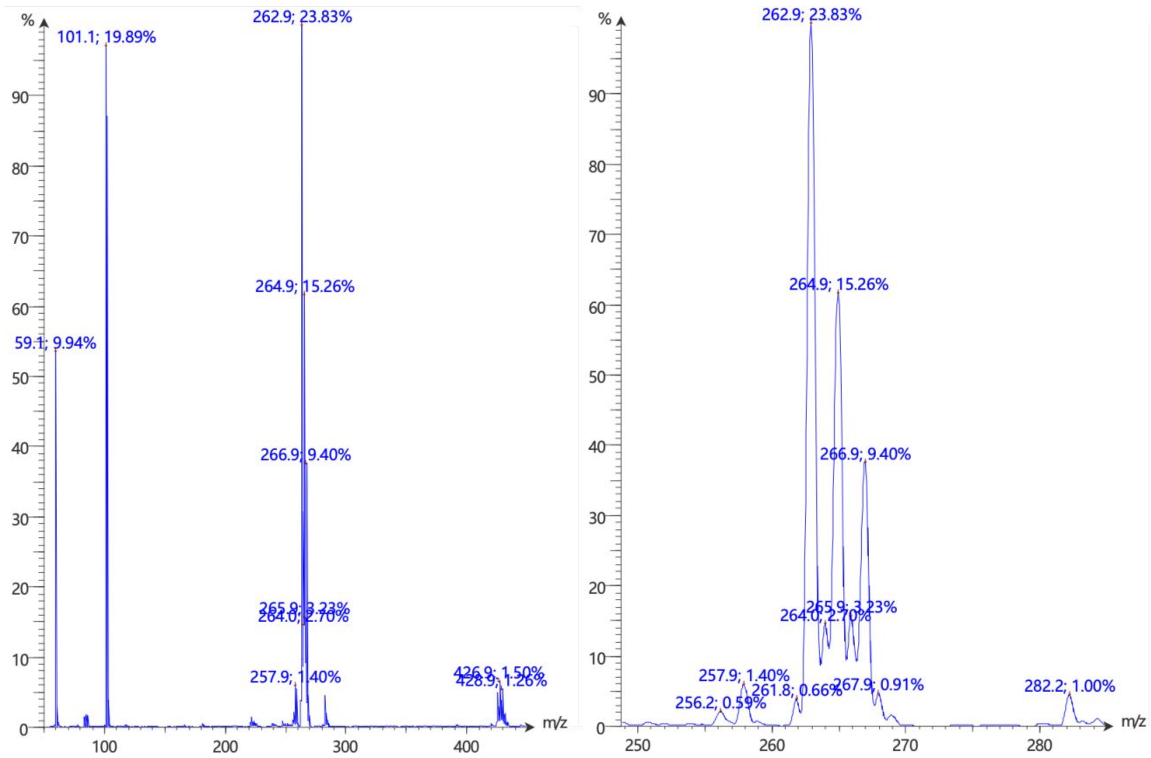

Figure S5. Mass spectrum of $V(acac)_3$.

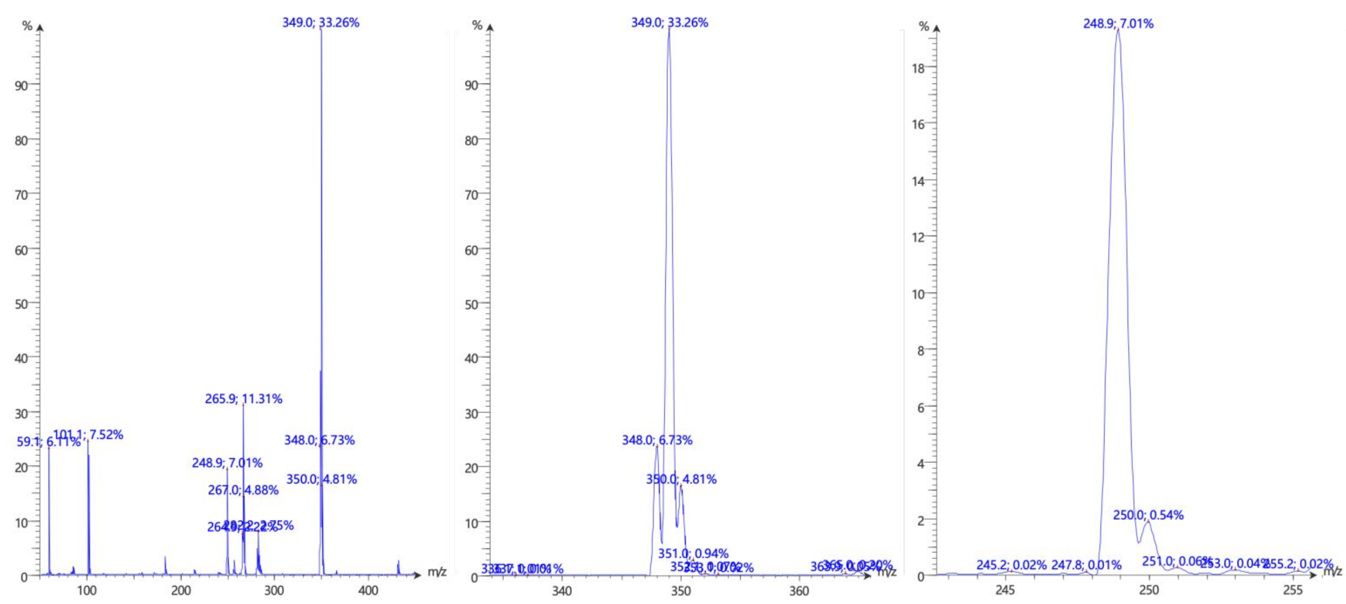

Figure S6. Mass spectrum of $Cr(acac)_3$.

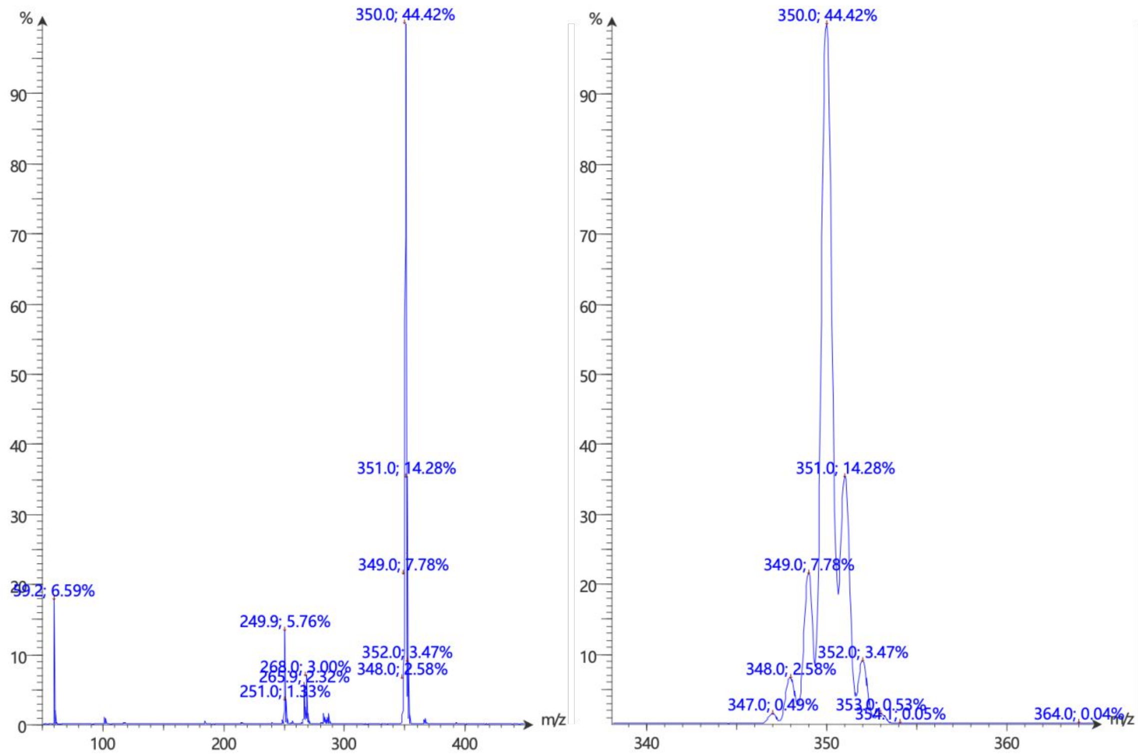

Figure S7. Mass spectrum of $Mn(acac)_3$.

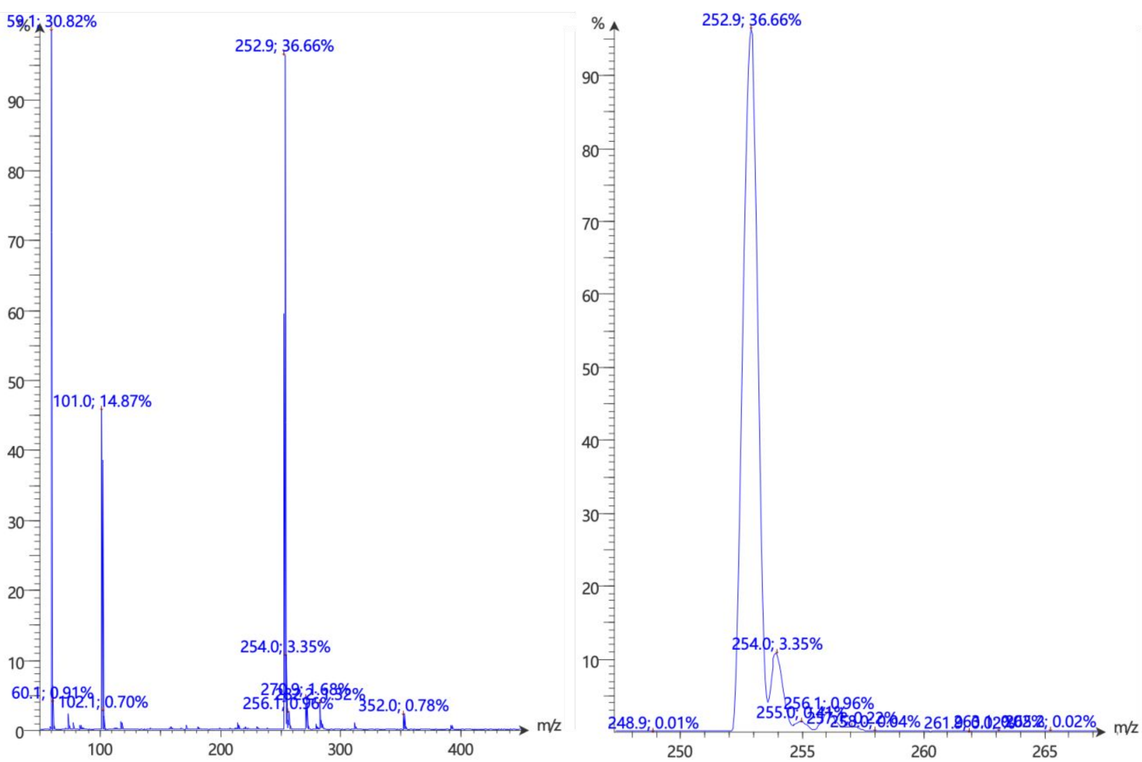

Figure S8. Mass spectrum of $Fe(acac)_3$.

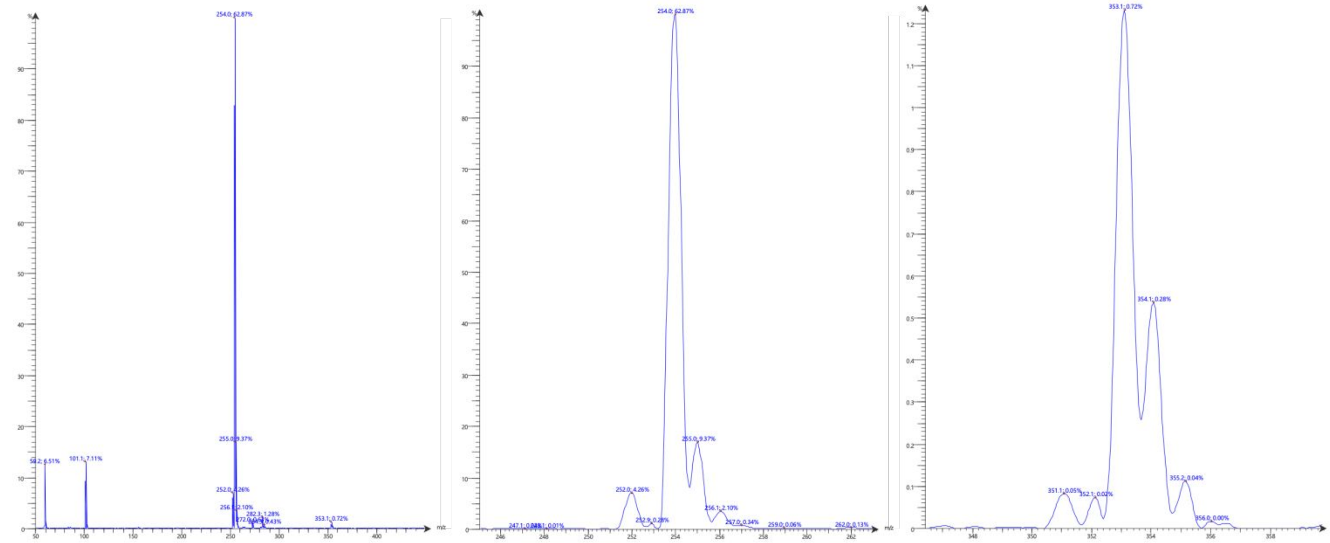

Figure S9. Mass spectrum of $Co(acac)_3$.

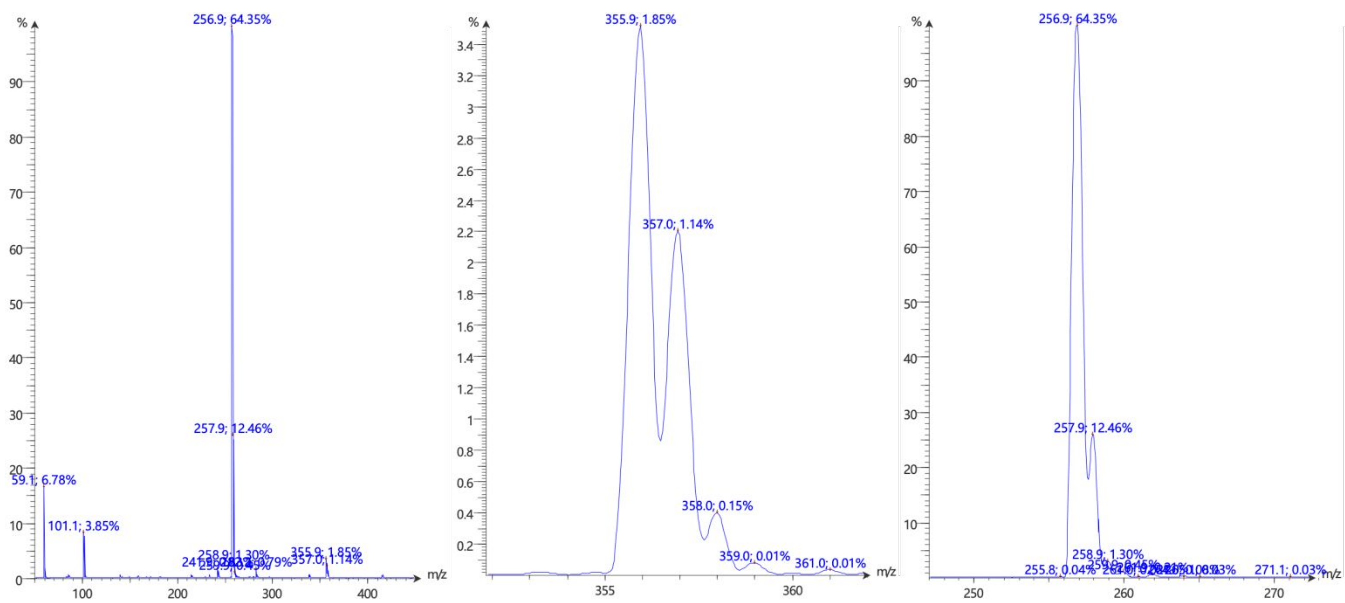

Figure S10. Mass spectrum of $V(O)(acac)_2$.