

Table S1. Assignment of absorption bands in the IR spectra of acetylacetonate complexes of scandium, yttrium and lanthanum, cm^{-1} .

Sc(acac)₃	Y(acac)₃	La(acac)₃
3384	3409	3415, 1681
The absorption bands in this region characterize the hydrated form of the complex and correspond to the symmetric stretching vibrations of the O–H bond in a coordinated or intercrystalline water molecule. For the lanthanum complex, this band is duplicated in the region of 1681 cm^{-1}		
2900-3000		
Weakly intense stretching vibrations of the C–H group.		
1604, 1519	1608, 1521	1593, 1523
Stretching vibrations of conjugated bonds $\nu(\text{C}=\text{O})$ and $\nu(\text{C}=\text{C})$ in the chelate ring.		
1394	1398	1392
Intense absorption band corresponding to the symmetric stretching vibrations of the enolate ion.		
1261	1263	1259
Bending vibrations of the C–H bond in the methyl substituent of the acetylacetonate fragment.		
1018, 920, 763	1018, 920, 763	1016, 920, 777, 758
Out-of-plane bending vibrations of the C–H bond in the chelate ring.		
655	655	653
Bands caused by in-plane bending vibrations of the chelate ring.		
532, 410	534, 414	526, 412
Stretching vibrations of the M–O bond in the chelate ring.		

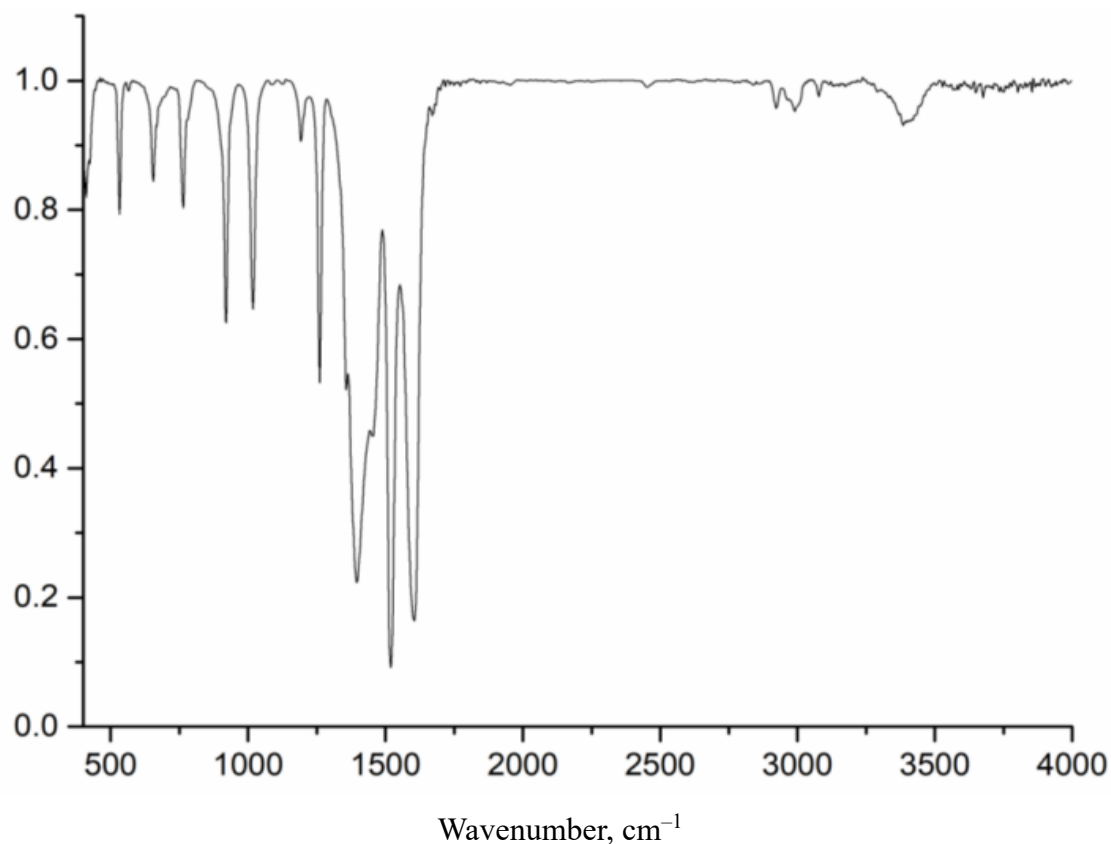


Figure S1. IR spectrum of scandium tris-acetylacetonate.

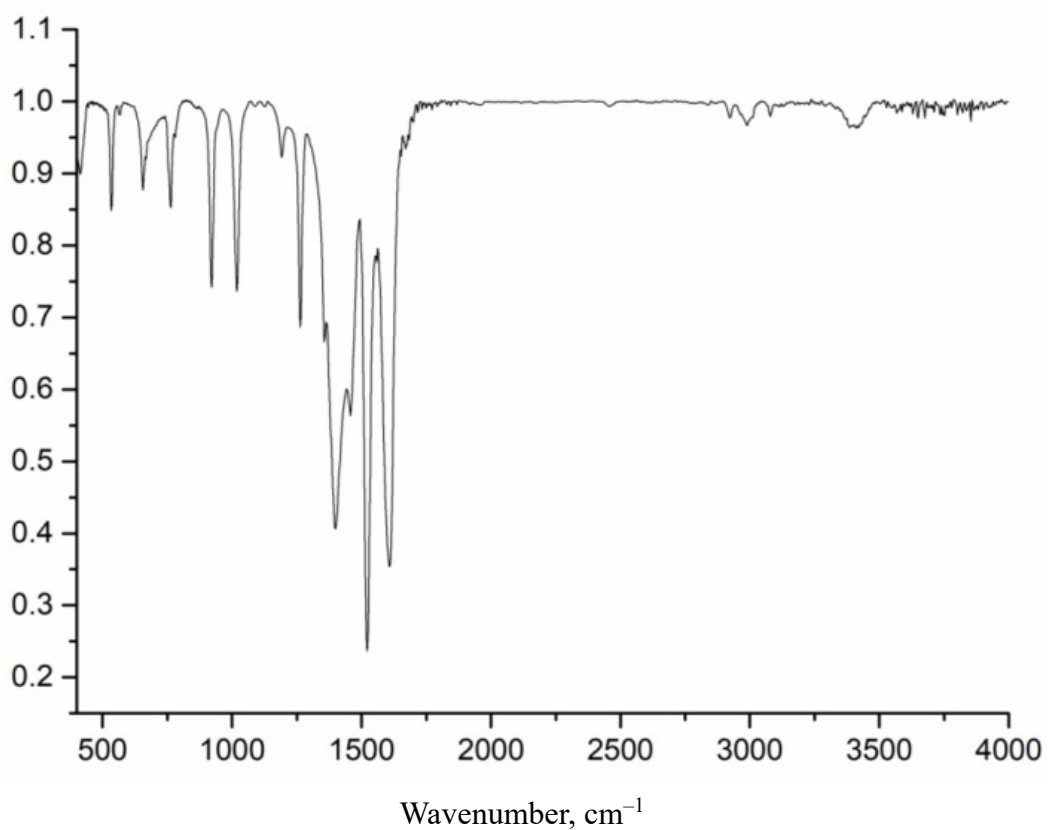


Figure S2. IR spectrum of yttrium tris-acetylacetonate.

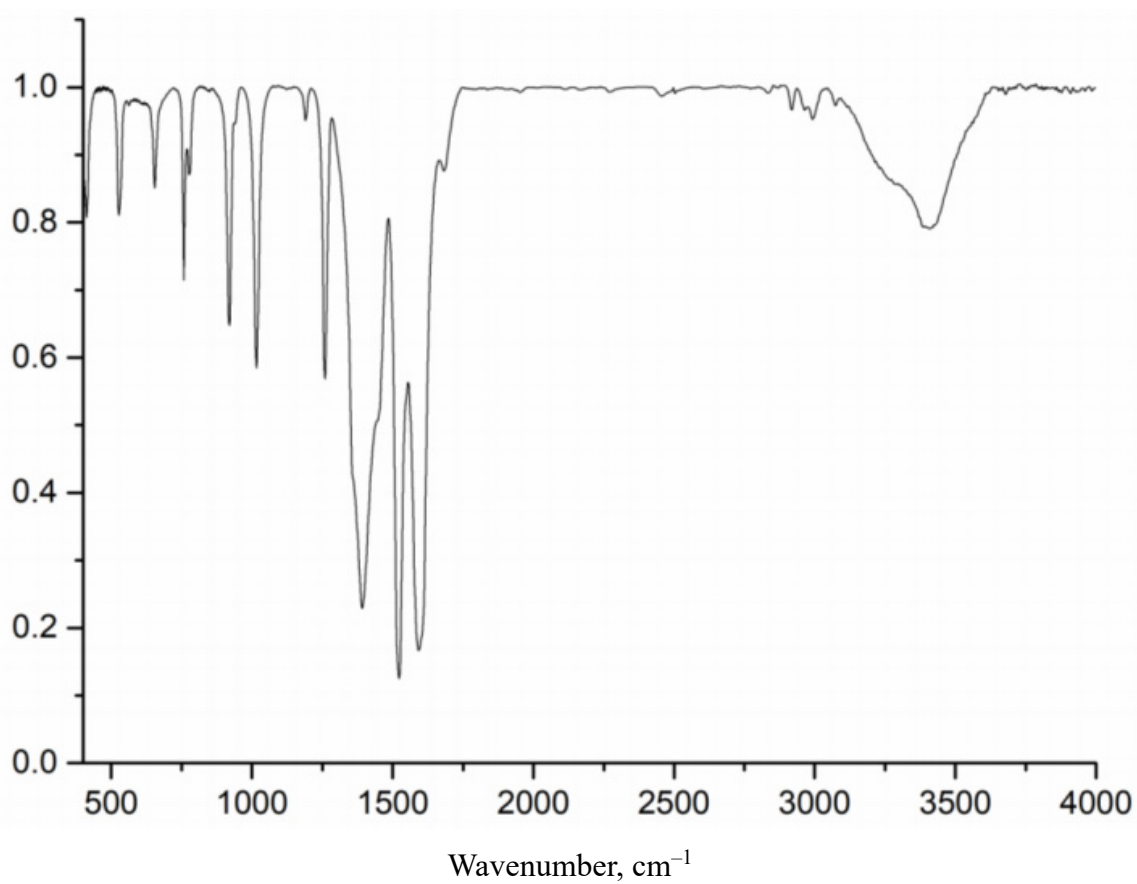


Figure S3. IR spectrum of lanthanum tris-acetylacetonate.

Table S2. Composition of the ethanol-extracted reaction mixture.

Peak #	R.T., min	First scan	Max scan	Last scan	Peak height	corr. area	corr. % max.	% of total	Compound name
1	1.61	226	235	250	26273795	130155818	27.23	6.643	Carbon dioxide
2	1.74	250	256	261	3343581	57908134	12.11	2.956	Ethanol
3	1.81	261	266	278	14301483	258795022	54.14	13.209	Acetone
4	2.1	292	311	321	14451709	296066865	61.94	15.112	2,3-Butanedione
5	2.23	321	331	339	8840664	216895172	45.37	11.071	Ethyl Acetate
6	2.35	339	350	367	2729967	118174458	24.72	6.032	Acetic acid
7	4.05	601	613	651	9118834	240670702	50.35	12.284	Toluene
8	4.43	651	671	726	82888162	47801719	100.00	24.399	2,4-Pentanedione
9	5.03	756	765	799	882588	23757112	4.97	1.213	Propanoic acid, 2-oxo-, ethyl ester
10	6.43	971	980	1016	896140	17623508	3.69	0.900	2-Propanone, 1-(acetyloxy)-
11	8.58	1303	1313	1318	5572103	97607603	20.42	4.982	Ethyl 2-acetoxy-2-methylacetoacetate

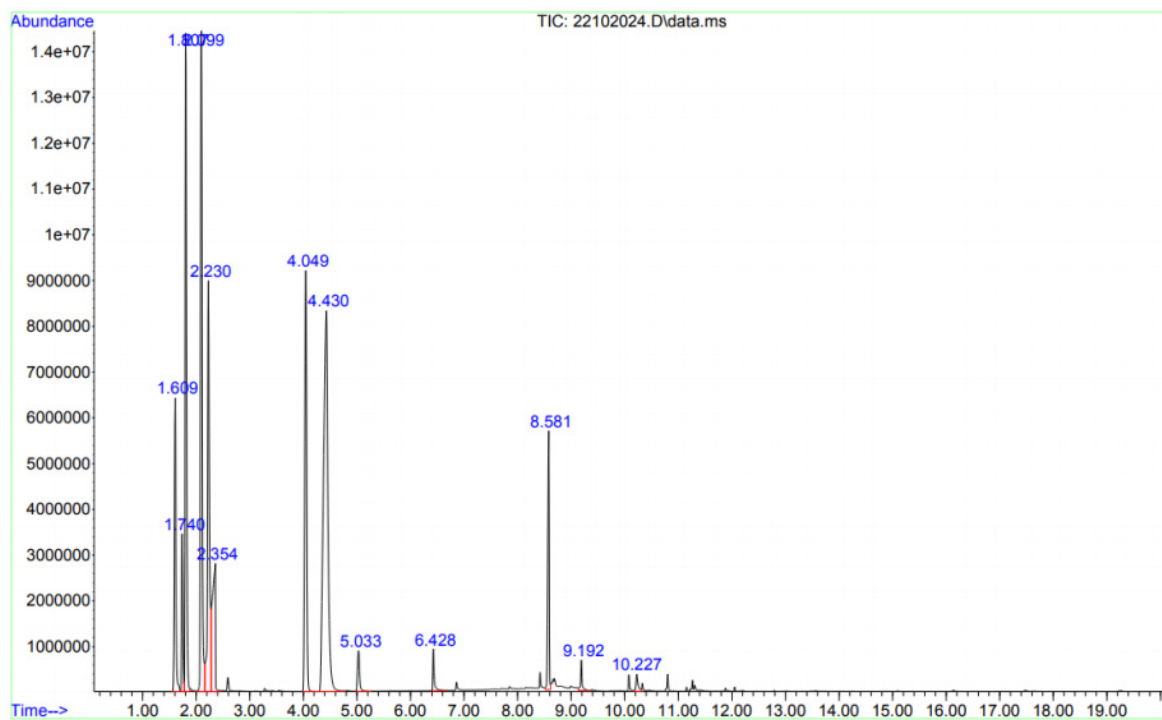
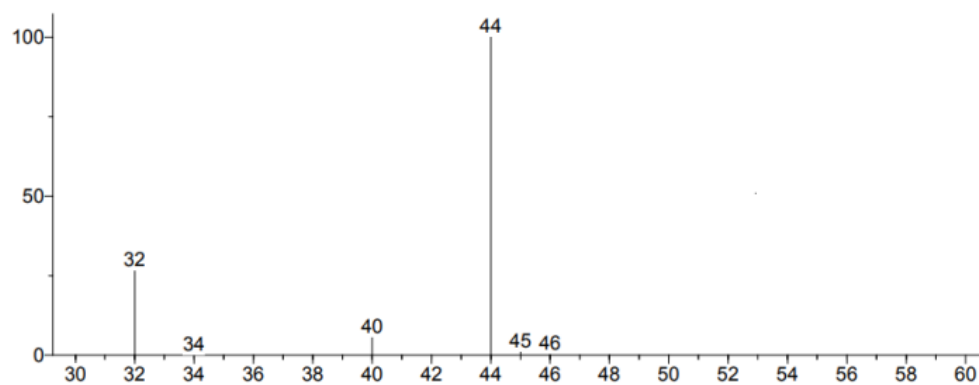


Figure S4. Gas chromatogram of the ethanol-extracted reaction mixture.

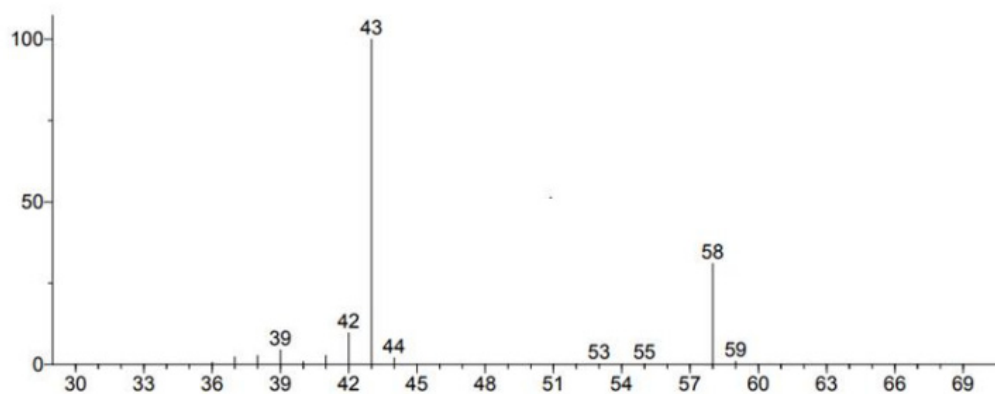
Unknown: Average of 1.607 to 1.607 min.: 22102024.D\data.ms
Compound in Library Factor = -135



Hit 1 : Carbon dioxide
CO₂; MF: 856; RMF: 972; Prob 68.2%; CAS: 124-38-9; Lib: mainlib; ID: 13226.

Figure S5. Mass spectrum of Carbon dioxide.

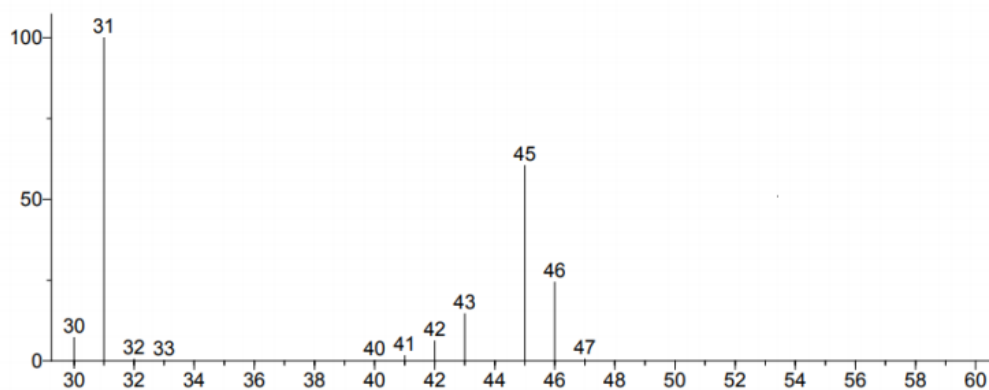
Unknown: Scan 266 (1.808 min): 22102024.D\data.ms (-261)
Compound in Library Factor = 210



Hit 1 : Acetone
C₃H₆O; MF: 974; RMF: 977; Prob 83.8%; CAS: 67-64-1; Lib: replib; ID: 2169.

Figure S6. Mass spectrum of Acetone.

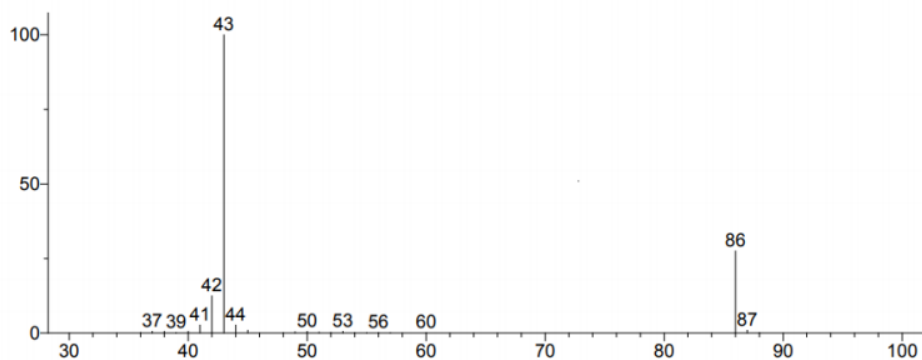
Unknown: Scan 255 (1.737 min): 22102024.D\data.ms (-250)
Compound in Library Factor = 603



Hit 1 : Ethanol
C₂H₆O; MF: 980; RMF: 983; Prob 98.0%; CAS: 64-17-5; Lib: mainlib; ID: 1334.

Figure S7. Mass spectrum of Ethanol.

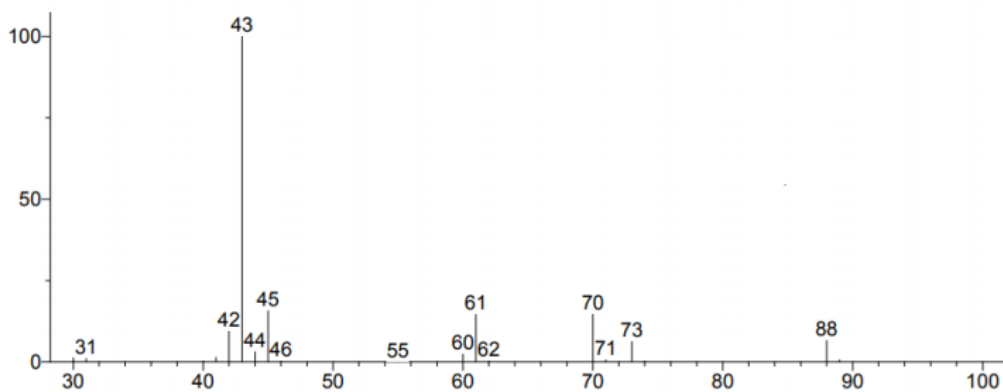
Unknown: Scan 311 (2.099 min): 22102024.D\data.ms (-300)
Compound in Library Factor = 320



Hit 1 : 2,3-Butanedione
C₄H₆O₂; MF: 941; RMF: 942; Prob 80.5%; CAS: 431-03-8; Lib: mainlib; ID: 8875.

Figure S8. Mass spectrum of 2,3-Butanedione.

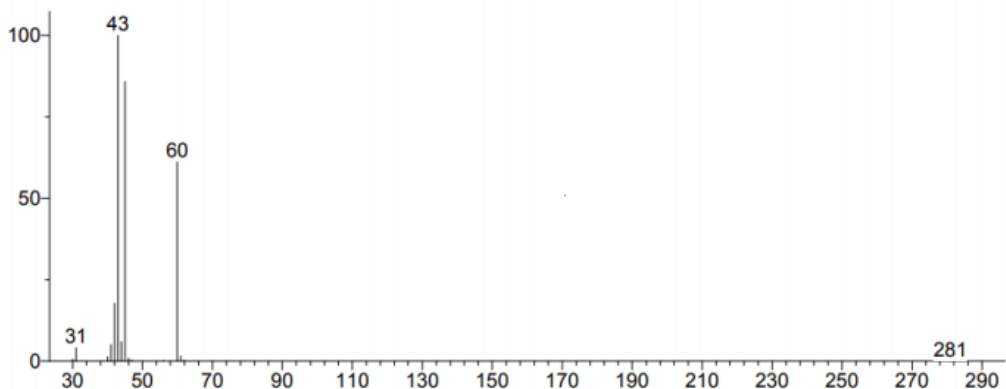
Unknown: Scan 331 (2.228 min): 22102024.D\data.ms (-321)
Compound in Library Factor = 374



Hit 1 : Ethyl Acetate
C₄H₈O₂; MF: 924; RMF: 924; Prob 94.8%; CAS: 141-78-6; Lib: mainlib; ID: 7435.

Figure S9. Mass spectrum of Ethyl Acetate.

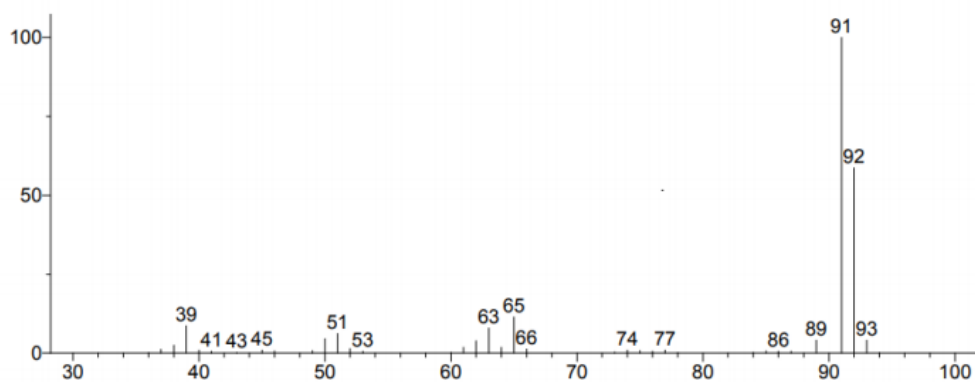
Unknown: Scan 348 (2.338 min): 22102024.D\data.ms (-296)
Compound in Library Factor = 522



Hit 1 : Acetic acid
C₂H₄O₂; MF: 965; RMF: 965; Prob 73.6%; CAS: 64-19-7; Lib: replib; ID: 1852.

Figure S10. Mass spectrum of Acetic acid.

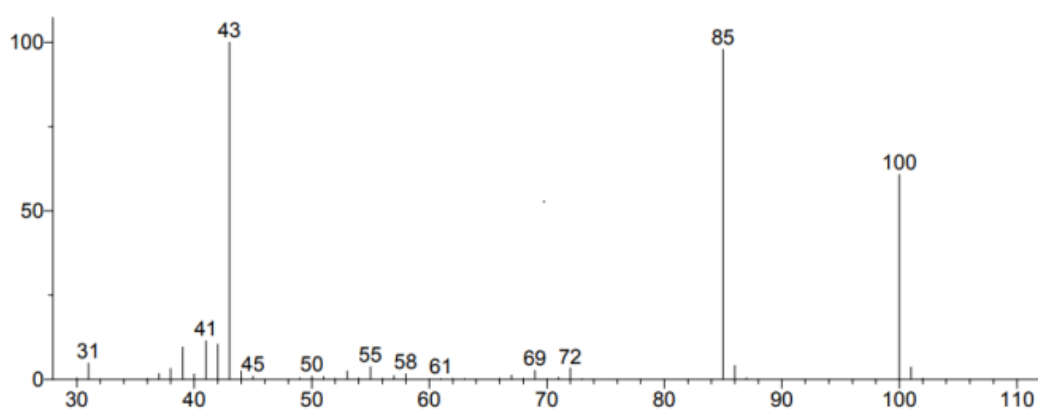
Unknown: Scan 612 (4.046 min): 22102024.D\data.ms (-593)
Compound in Library Factor = 120



Hit 1 : Toluene
C7H8; MF: 962; RMF: 962; Prob 64.2%; CAS: 108-88-3; Lib: replib; ID: 11301.

Figure S11. Mass spectrum of Toluene.

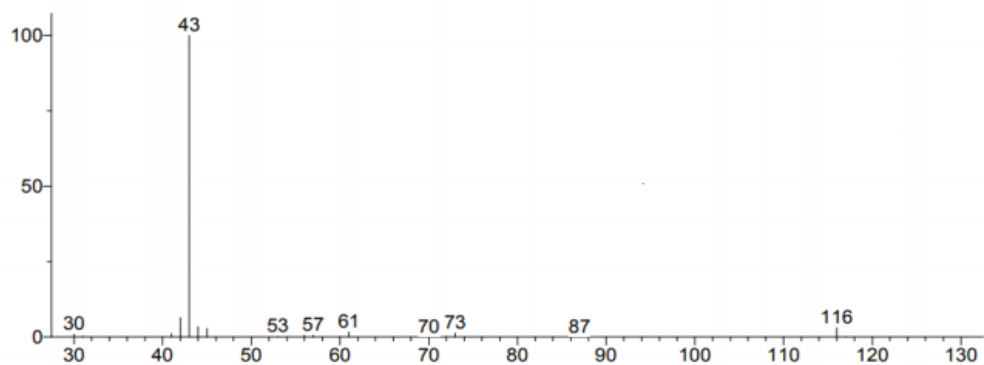
Unknown: Scan 671 (4.428 min): 22102024.D\data.ms (-642)
Compound in Library Factor = 103



Hit 1 : 2,4-Pentanedione
C5H8O2; MF: 894; RMF: 896; Prob 66.8%; CAS: 123-54-6; Lib: replib; ID: 2646.

Figure S12. Mass spectrum of 2,4-Pentanedione.

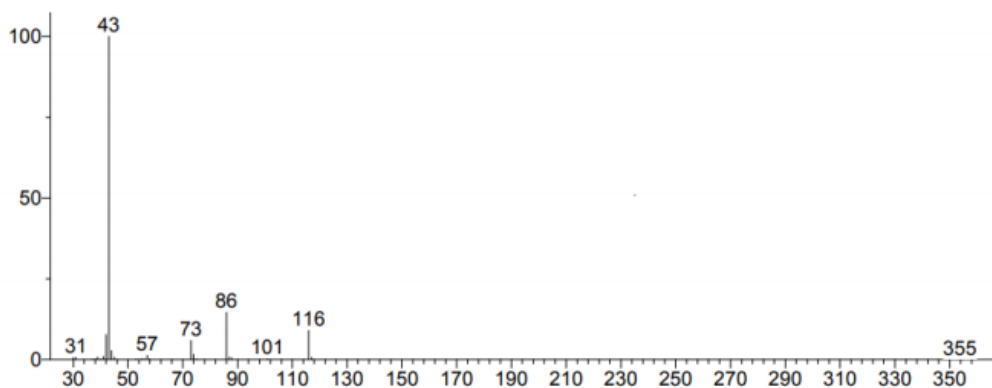
Unknown: Scan 763 (5.023 min): 22102024.D\data.ms (-747)
Compound in Library Factor = 326



Hit 1 : Propanoic acid, 2-oxo-, ethyl ester
C5H8O3; MF: 954; RMF: 980; Prob 90.2%; CAS: 617-35-6; Lib: mainlib; ID: 4981.

Figure S13. Mass spectrum of 2-oxo-ethyl ester of Propanoic acid.

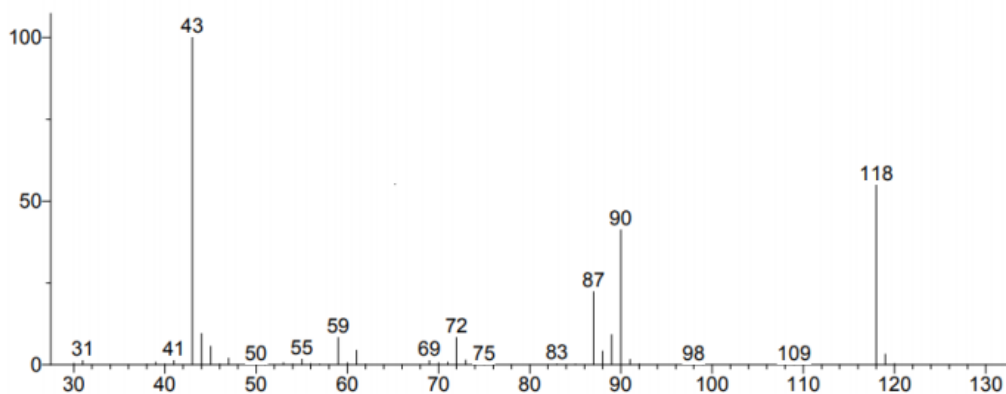
Unknown: Scan 979 (6.420 min): 22102024.D\data.ms (-960)
Compound in Library Factor = 301



Hit 1 : 2-Propanone, 1-(acetyloxy)-
C₅H₈O₃; MF: 924; RMF: 933; Prob 75.7%; CAS: 592-20-1; Lib: replib; ID: 2661.

Figure S14. Mass spectrum of 1-(acetyloxy)-2-Propanone.

Unknown: Scan 1312 (8.574 min): 22102024.D\data.ms (-1302)
Compound in Library Factor = -471



Hit 1 : Ethyl 2-acetoxy-2-methylacetoacetate
C₉H₁₄O₅; MF: 709; RMF: 709; Prob 57.9%; CAS: 25409-39-6; Lib: mainlib; ID: 10163.

Figure S15. Mass spectrum of Ethyl 2-acetoxy-2methylacetoacetate.

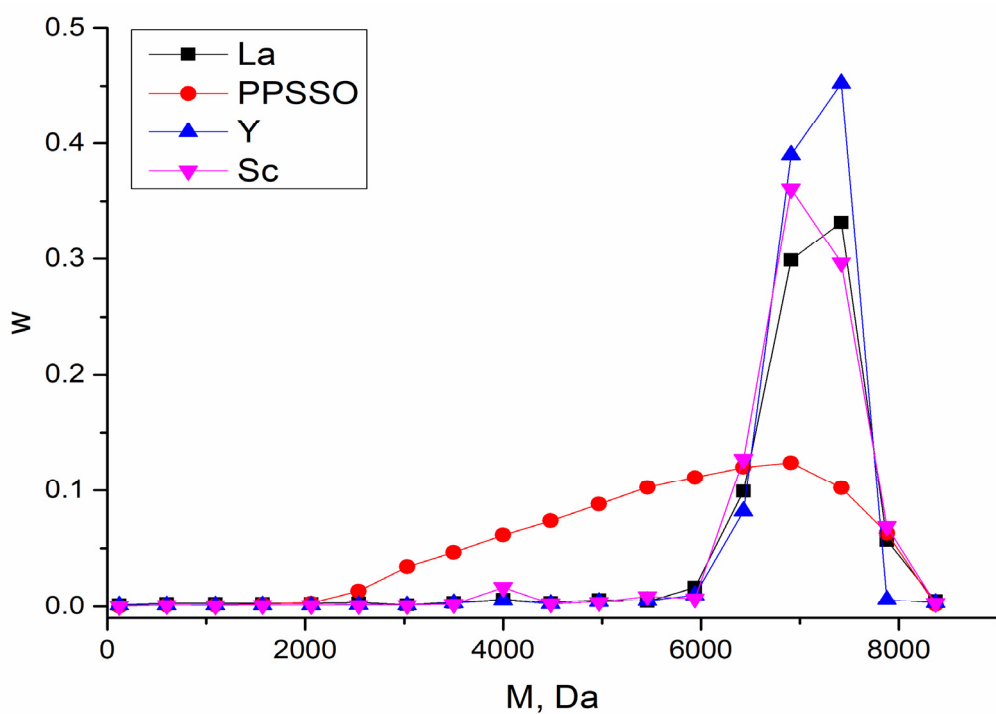


Figure S16. Chromatograms of the initial PPSSO and the products of syntheses 1–3.

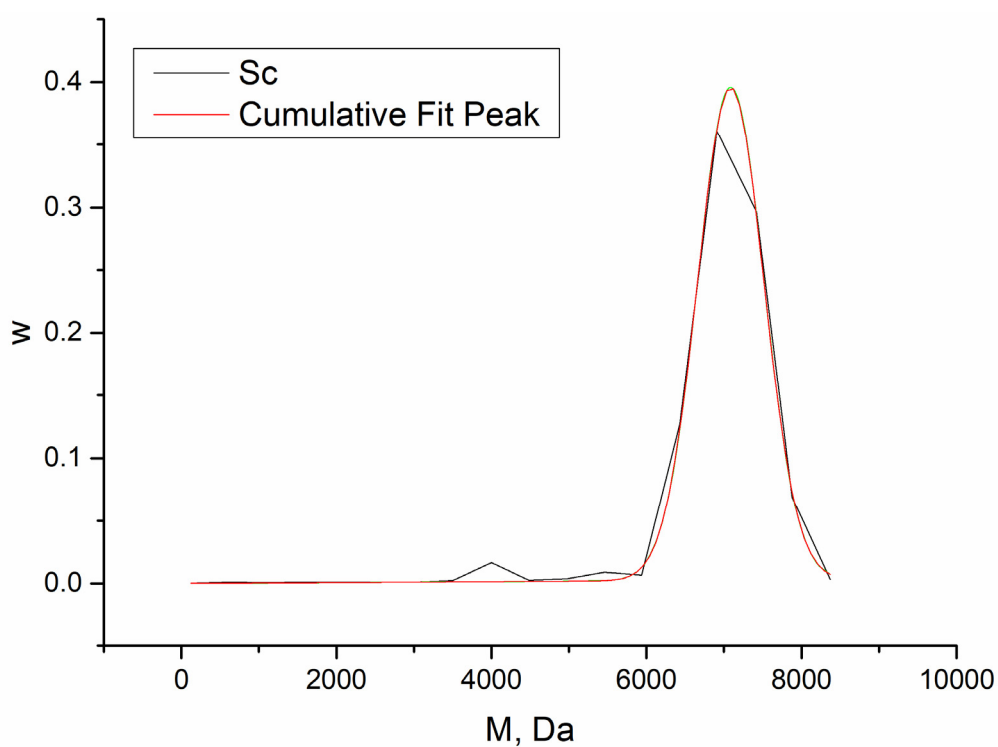


Figure S17. Chromatogram of the products from synthesis 1 based on scandium acetylacetonate.

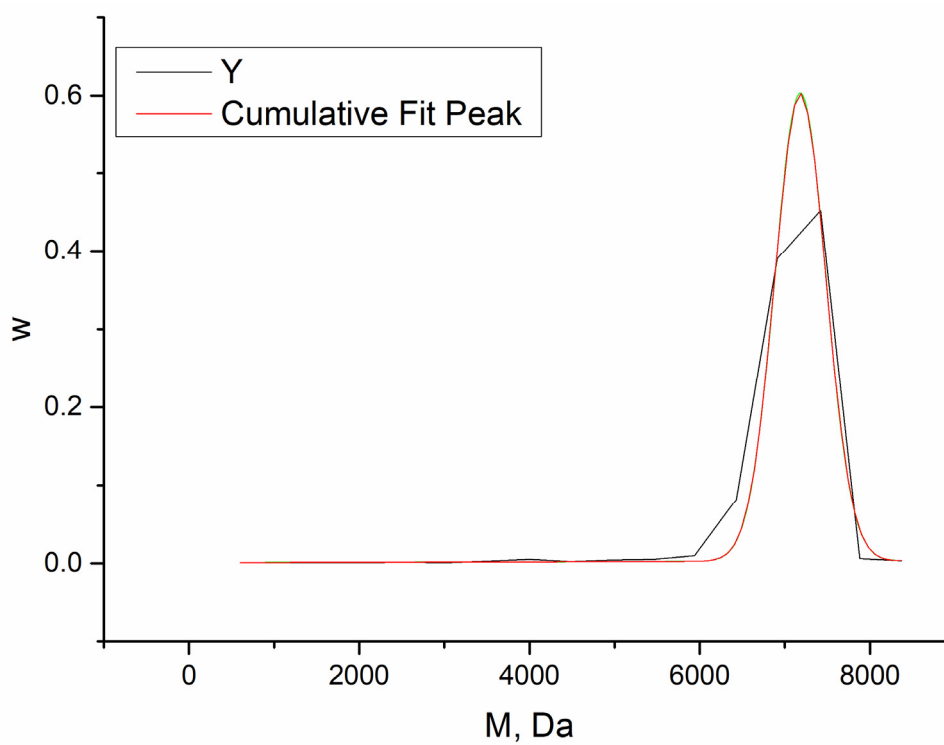


Figure S18. Chromatogram of the products from synthesis 1 based on yttrium acetylacetonate.

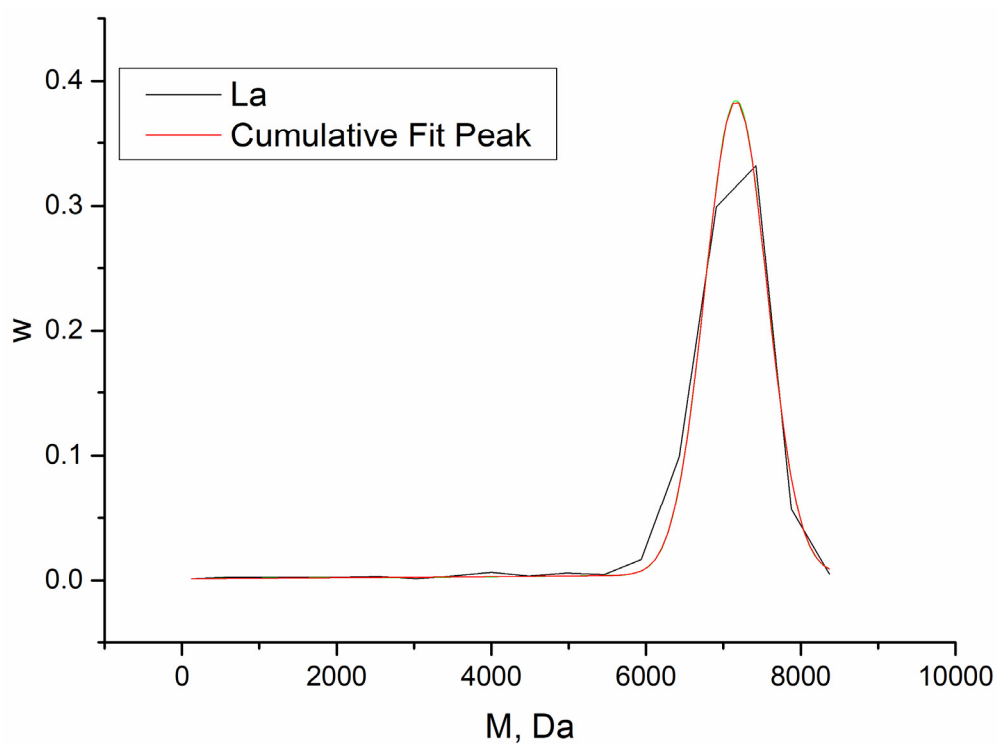


Figure S19. Chromatogram of the products from synthesis 1 based on lanthanum acetylacetonate.