SUPPORTING INFORMATION

Lithium C_1-C_{12} *n*-alkanoates: Thermal behavior from –30 to 600 °C

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The primary aim of the investigation was to study thermal behaviour. The spectroscopic data was employed to support the thermal investigation. The reasoning behind the collection of the spectroscopic data was as follows:

(a) Infrared (IR) spectroscopy is sensitive for the detection of carbonyl and carboxylate compounds. It could therefore be used to confirm synthesis of the lithium carboxylates, as well as provide an indication of purity. Synthesis was performed with a 2 % molar excess of carboxylic acid and if the acid was not completely removed during purification, it would be visible on the infrared spectrum.

(b) IR spectroscopy was also employed to determine whether chemical changes took place during calorimetry. Once a thermal event was observed, a sample was run to a temperature just above the temperature of the observed thermal event and the IR spectrum of the sample thus treated was collected and compared with the starting material.

(c) IR, Raman and Ultraviolet-Visible (UV-Vis) spectra were collected in the hope of finding explanations for differences in thermal behaviour, and in the hope that additional information about the nature of the lithium carboxylates can be deduced.

The thermal behaviour was studied by differential scanning calorimetry (DSC) and by thermogravimetric analysis (TGA). Phase behaviour and thermal decomposition measurements are reported.

1. Infrared (IR) Spectra

1.1 Lithium methanoate (formate)

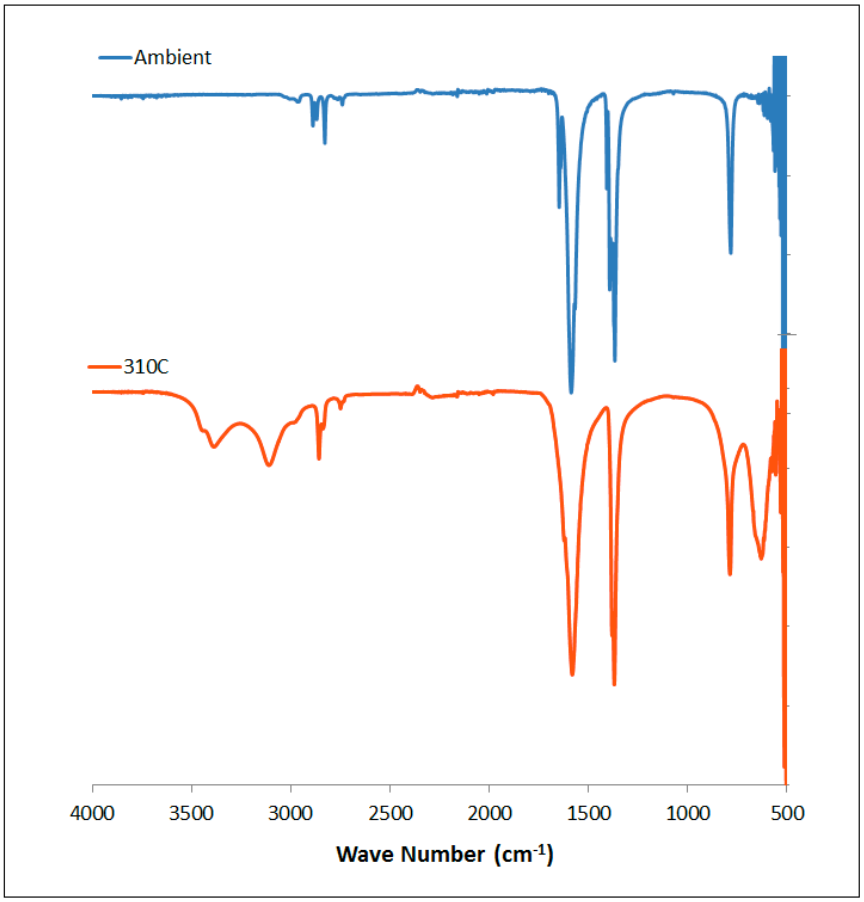

Figure S 1. IR spectrum of lithium methanoate before and after melting.

1.2 Lithium ethanoate (acetate)

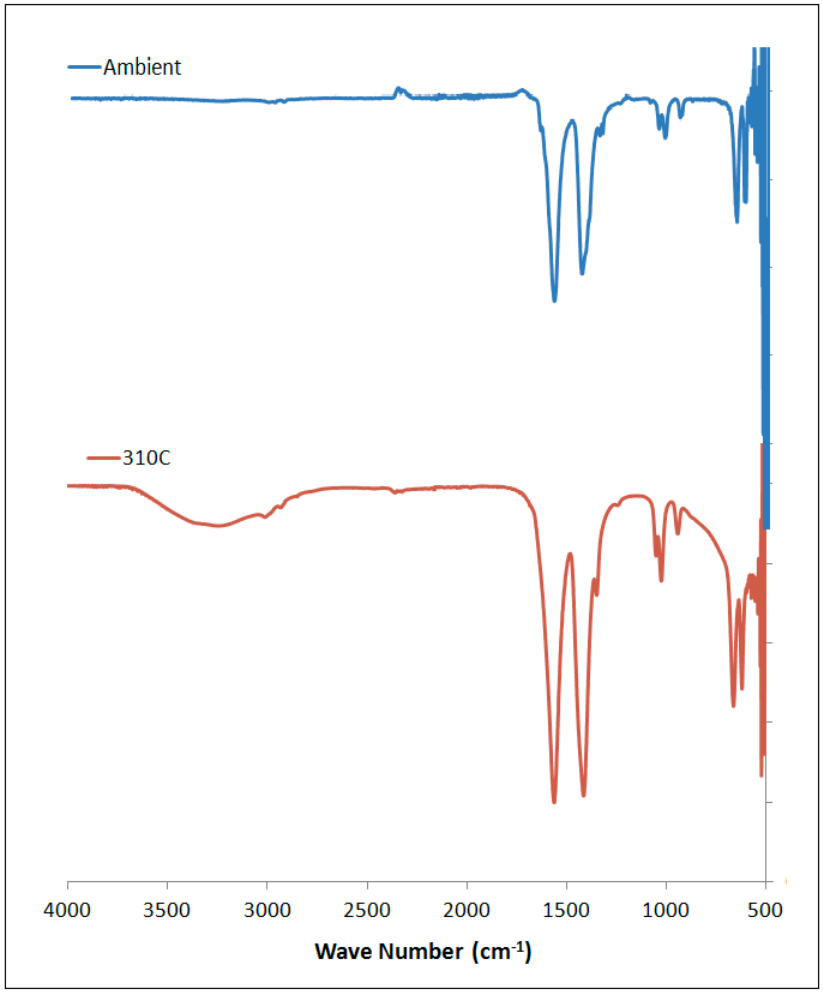

Figure S 2. IR spectrum of lithium ethanoate before and after melting.

1.3 Lithium propanoate

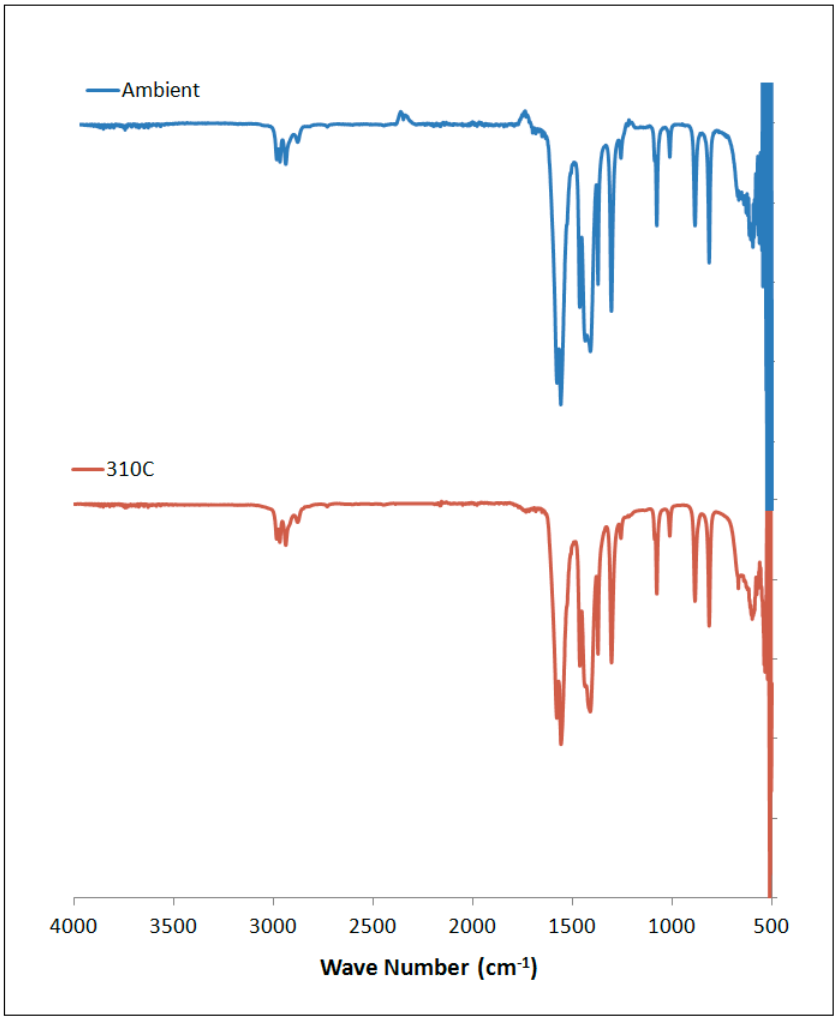

Figure S 3. IR spectrum of lithium propanoate before and after melting.

1.4 Lithium butanoate (butyrate)

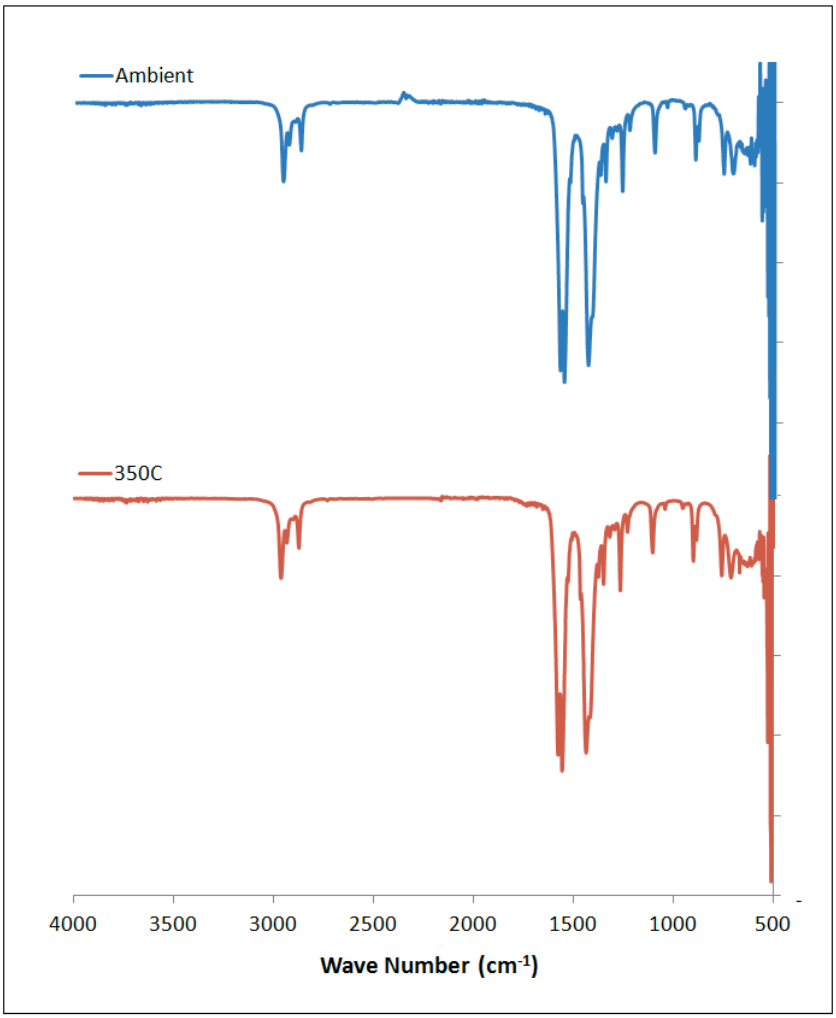

Figure S 4. IR spectrum of lithium butanoate before and after melting.

1.5 Lithium pentanoate (valerate)

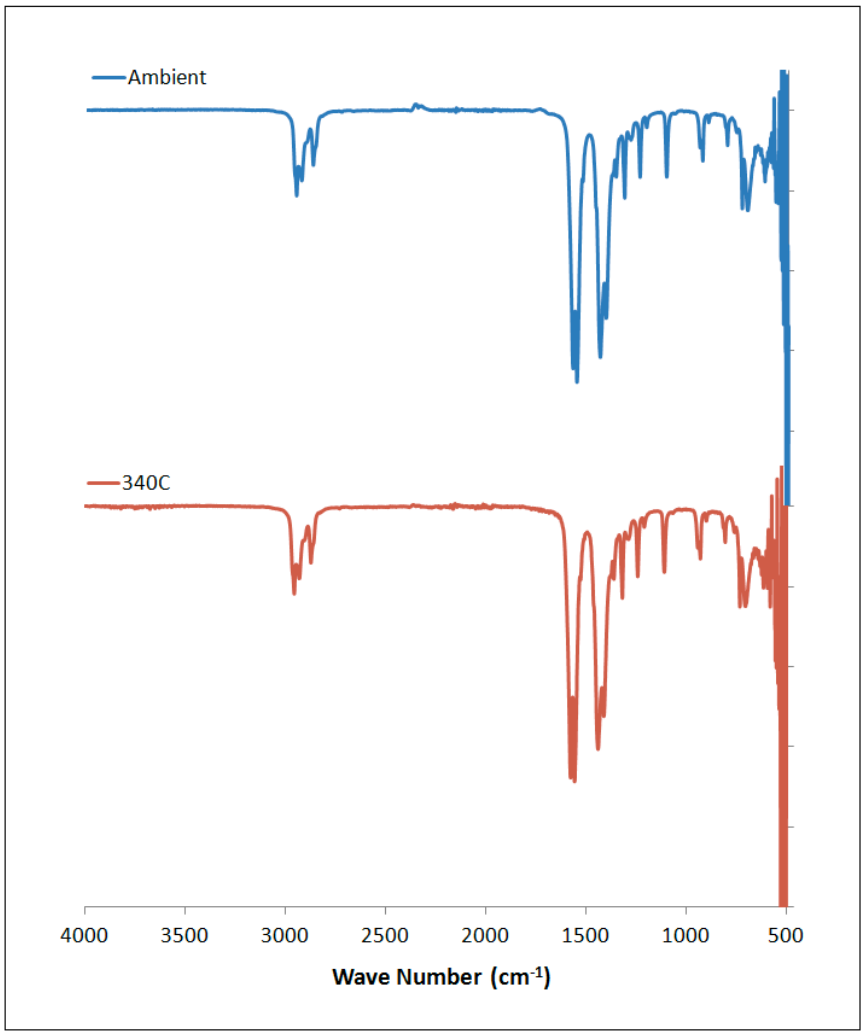

Figure S 5. IR spectrum of lithium pentanoate before and after melting.

1.6 Lithium hexanoate (caproate)

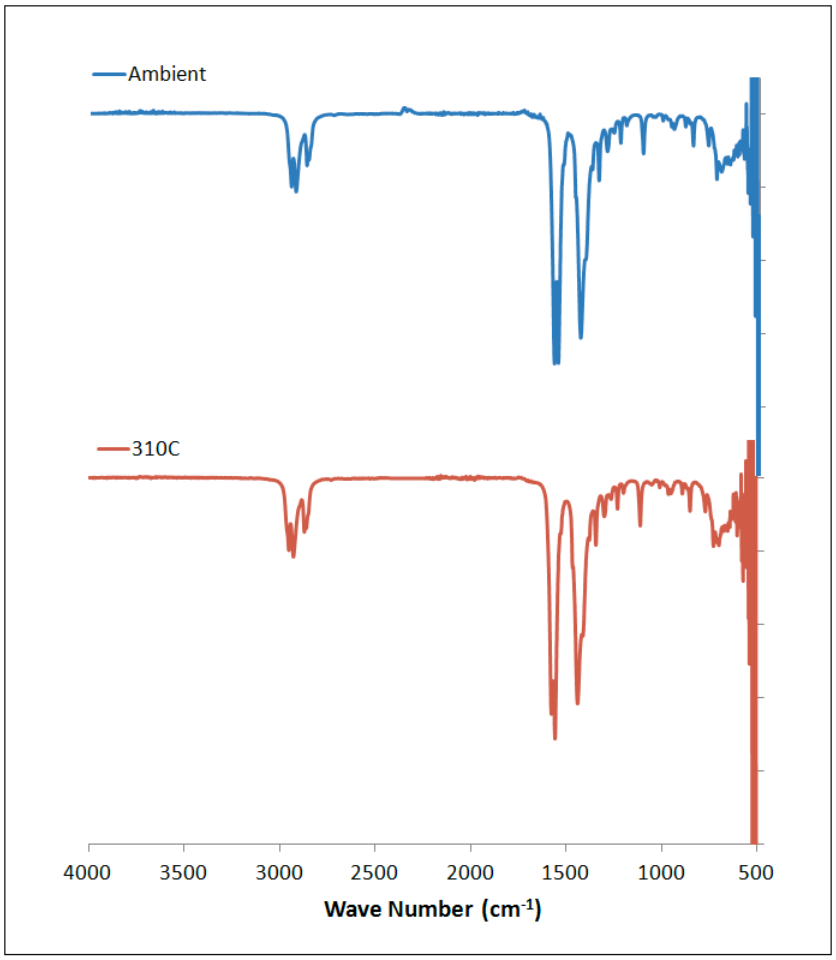

Figure S 6. IR spectrum of lithium hexanoate before and after melting.

1.7 Lithium heptanoate

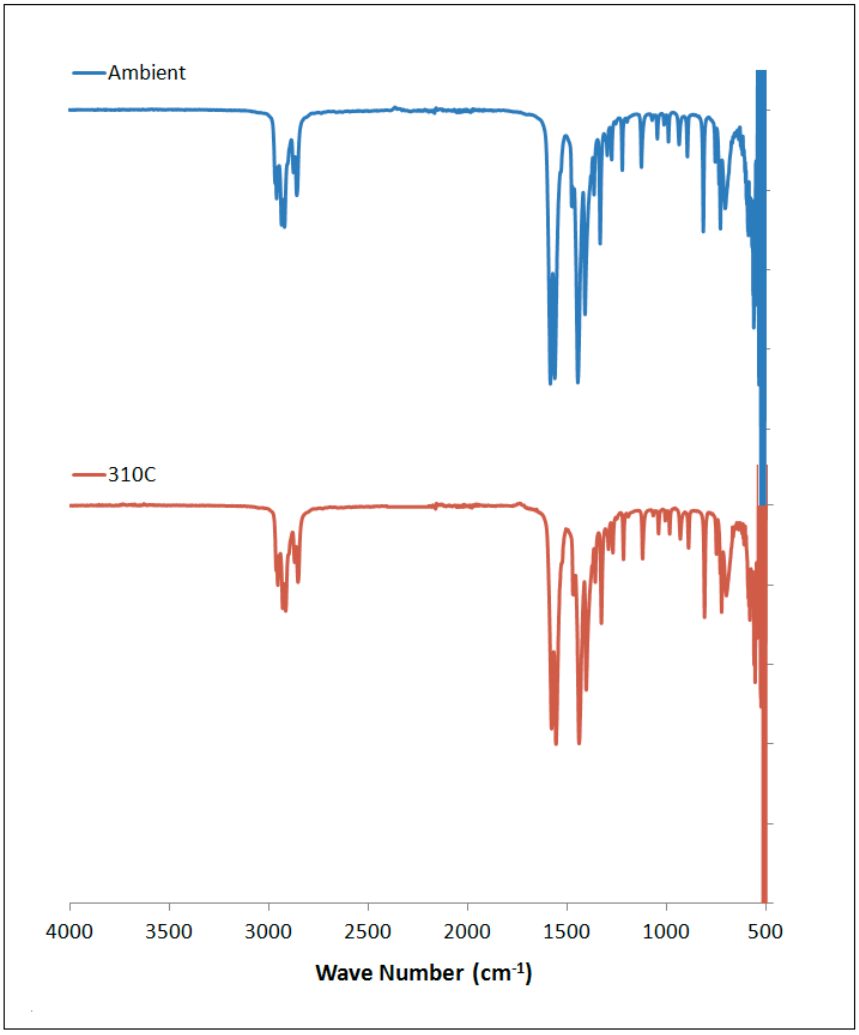

Figure S 7. IR spectrum of lithium heptanoate before and after melting.

1.8 Lithium octanoate (caprylate)

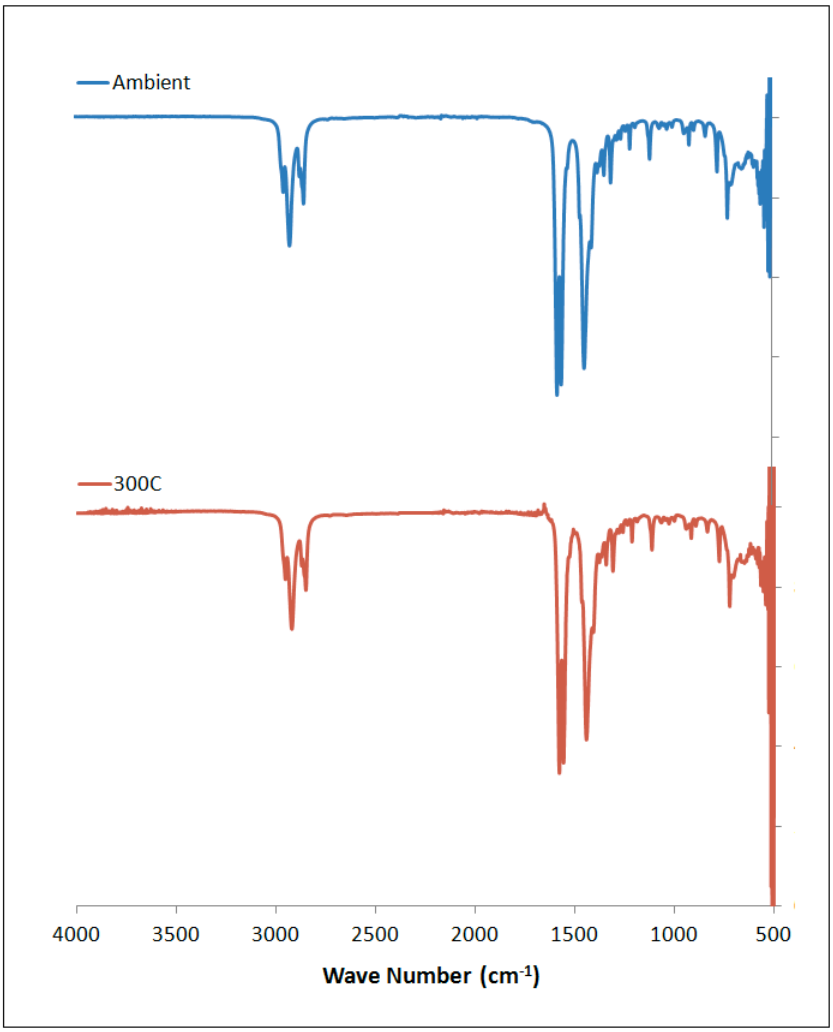

Figure S 8. IR spectrum of lithium octanoate before and after melting.

1.9 Lithium nonanoate (pelargonate)

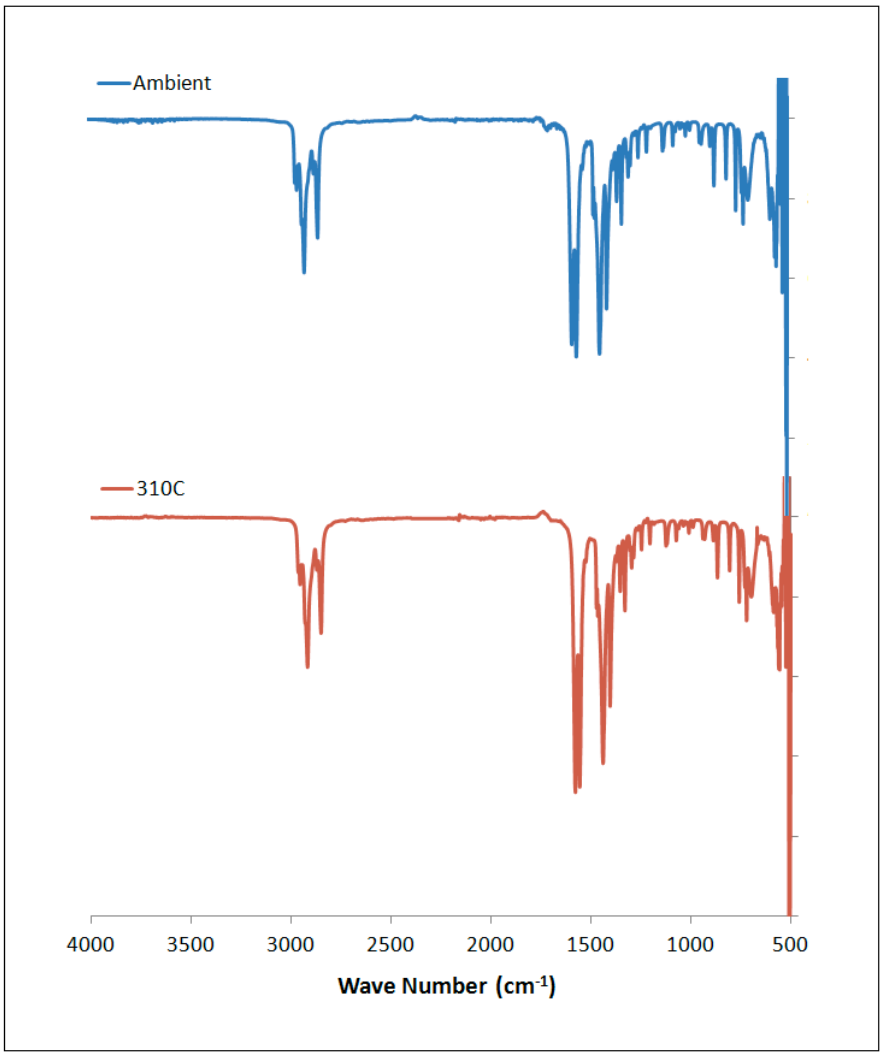

Figure S 9. IR spectrum of lithium nonanoate before and after melting.

1.10 Lithium decanoate (caprate)

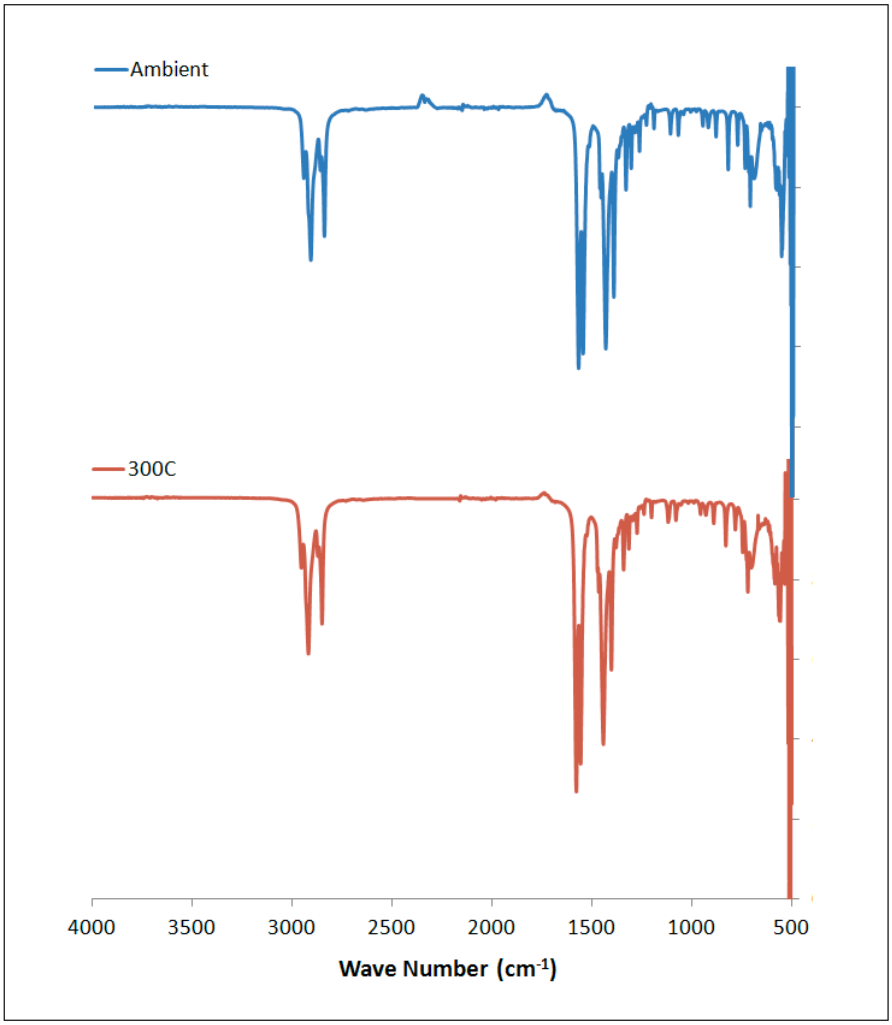

Figure S 10. IR spectrum of lithium decanoate before and after melting.

1.11 Lithium undecanoate

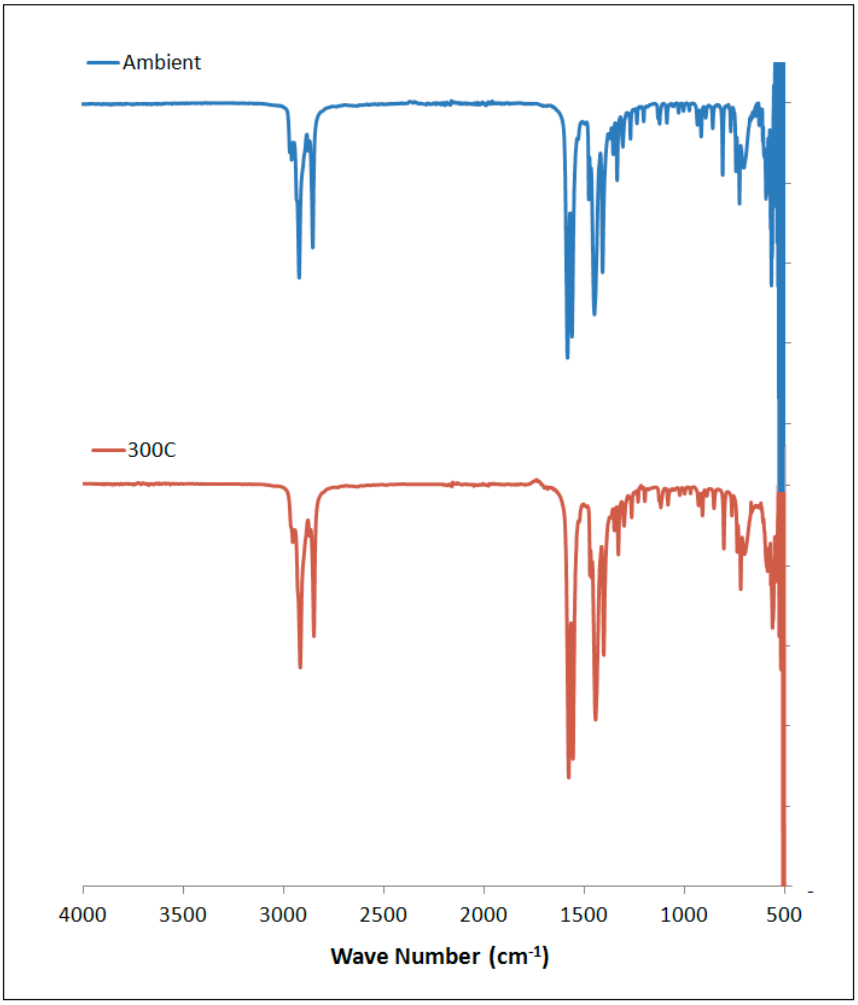

Figure S 11. IR spectrum of lithium undecanoate before and after melting.

1.12 Lithium dodecanoate (laurate)

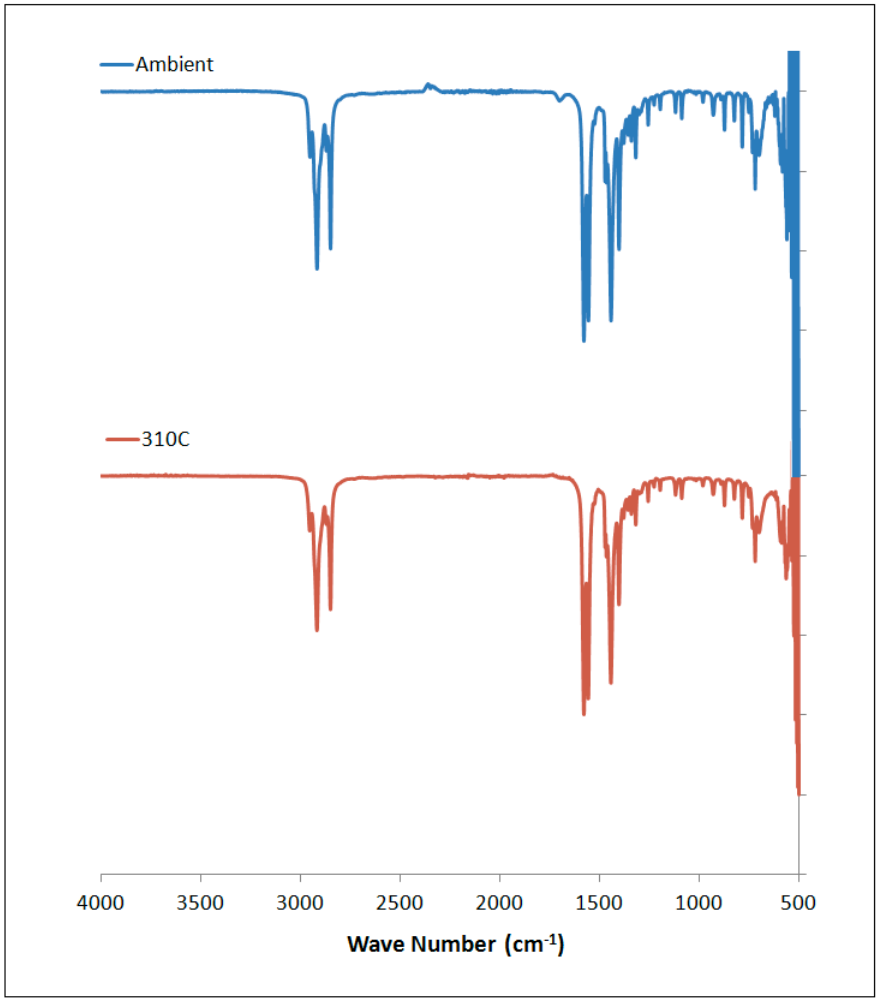

Figure S 12. IR spectrum of lithium dodecanoate before and after melting.

2. Raman Spectra

2.1 Lithium methanoate (formate)

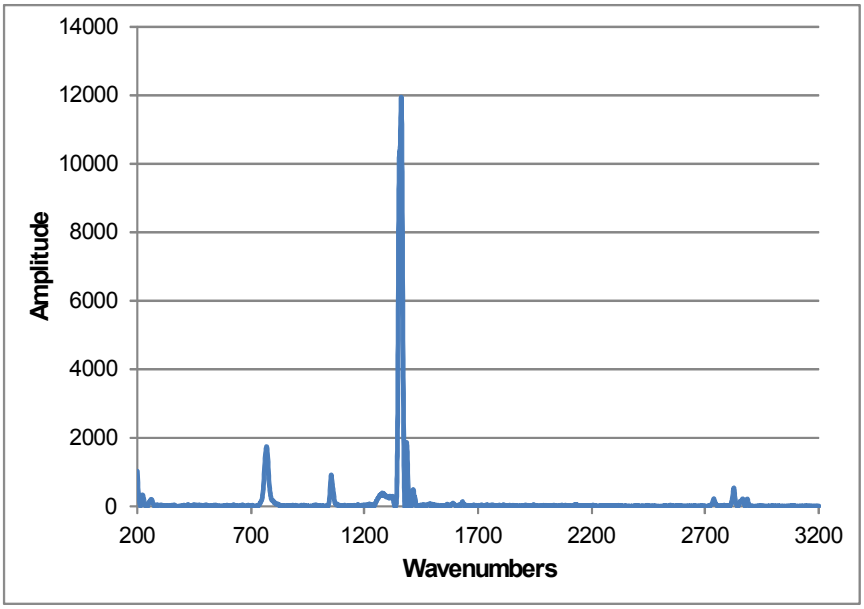

Figure S 13. Raman spectrum of lithium methanoate.

2.2 Lithium Ethanoate (acetate)

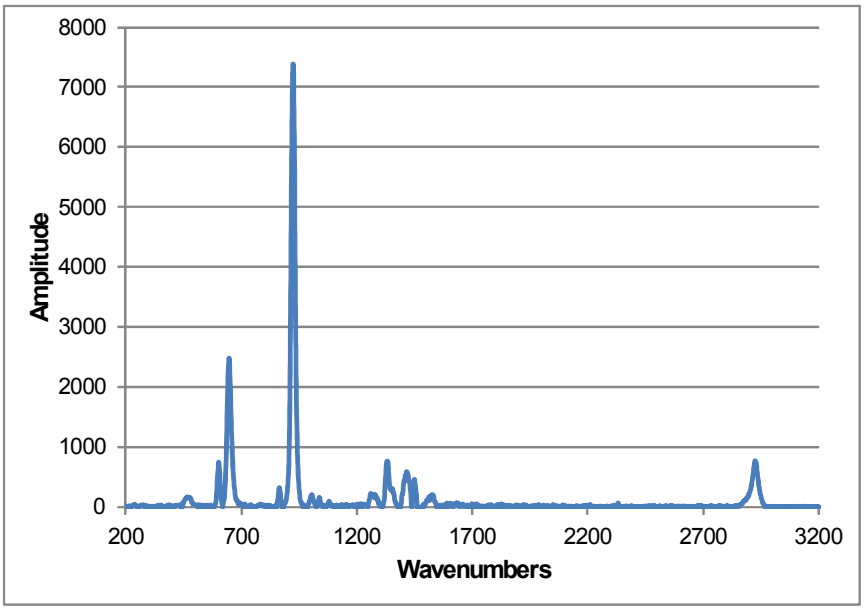

Figure S 14. Raman spectrum of lithium ethanoate.

2.3 Lithium Propanoate

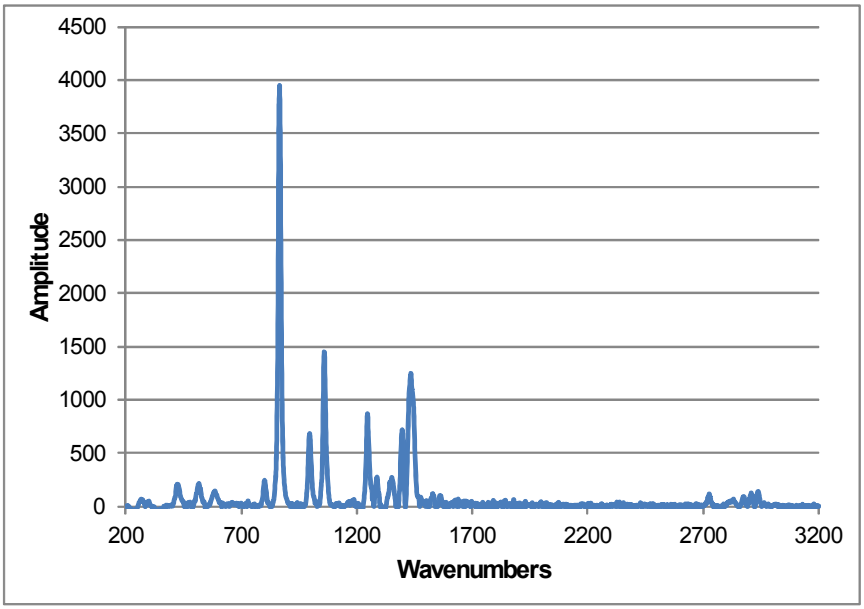

Figure S 15. Raman spectrum of lithium propanoate.

2.4 Lithium Butanoate (butyrate)

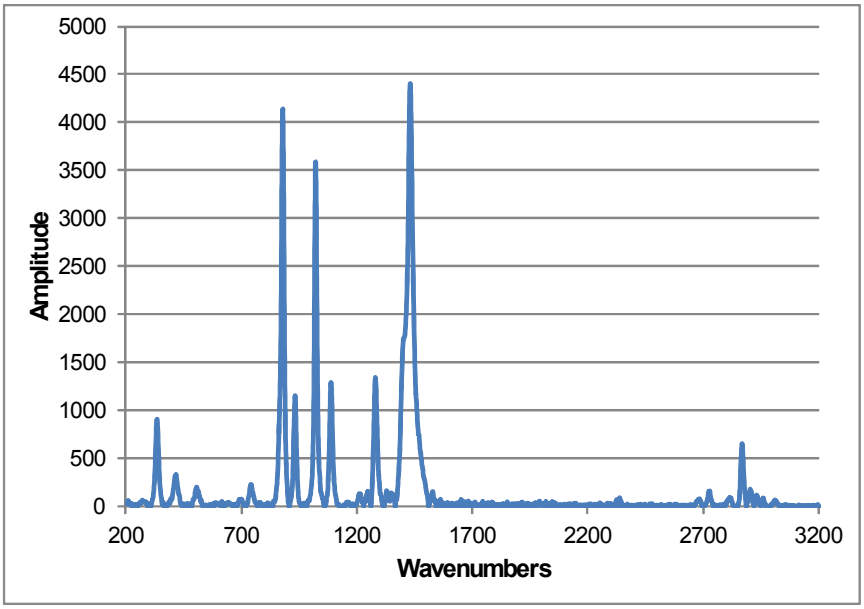

Figure S 16. Raman spectrum of lithium butanoate.

2.5 Lithium Pentanoate (valerate)

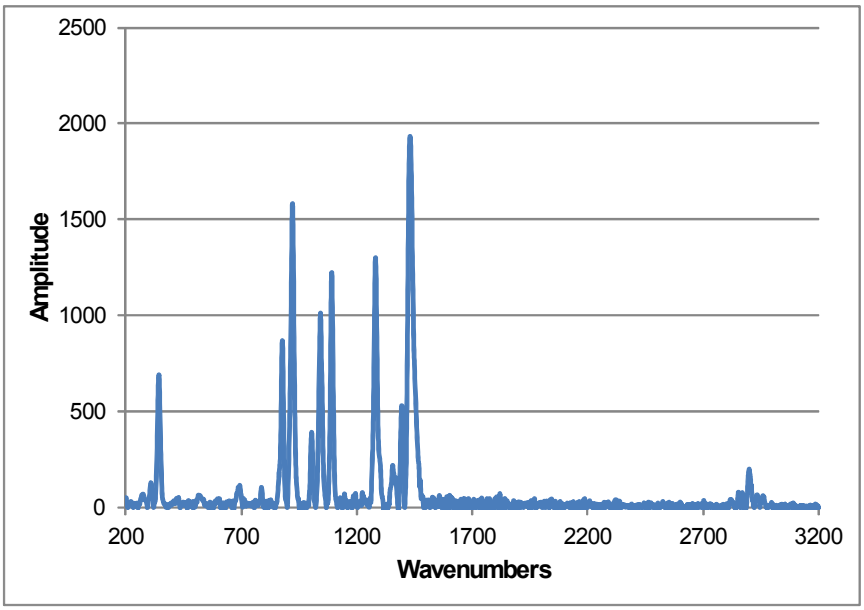

Figure S 17. Raman spectrum of lithium pentanoate.

2.6 Lithium Hexanoate (caproate)

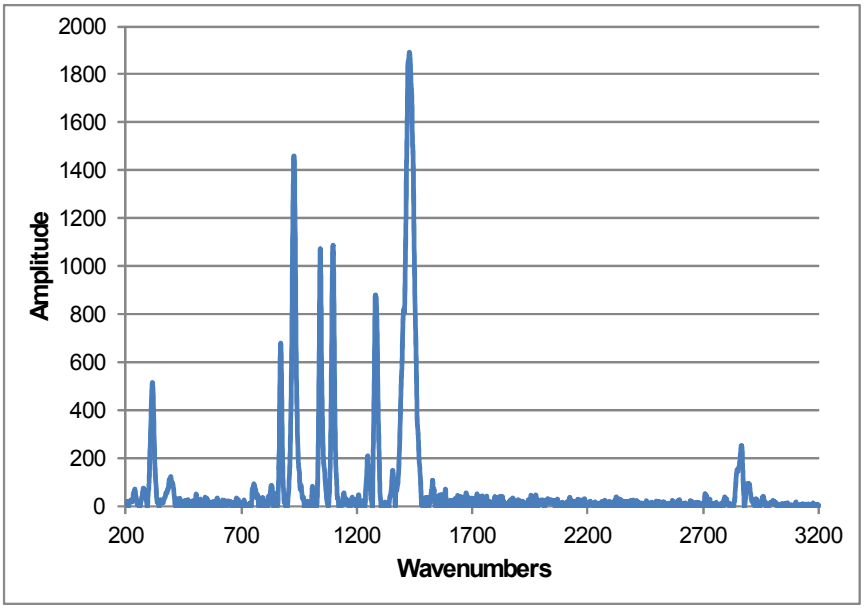

Figure S 18. Raman spectrum of lithium hexanoate.

2.7 Lithium Heptanoate

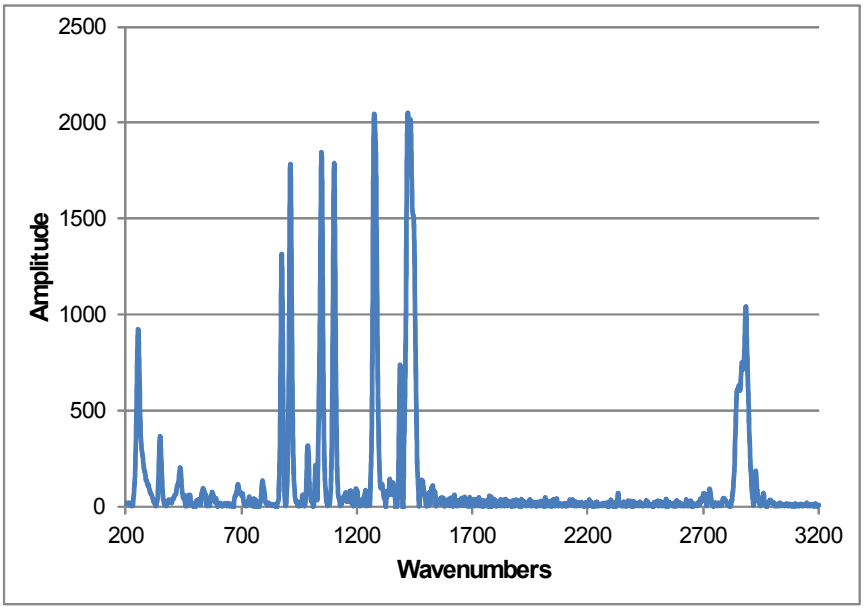

Figure S 19. Raman spectrum of lithium heptanoate.

2.8 Lithium Octanoate (caprylate)

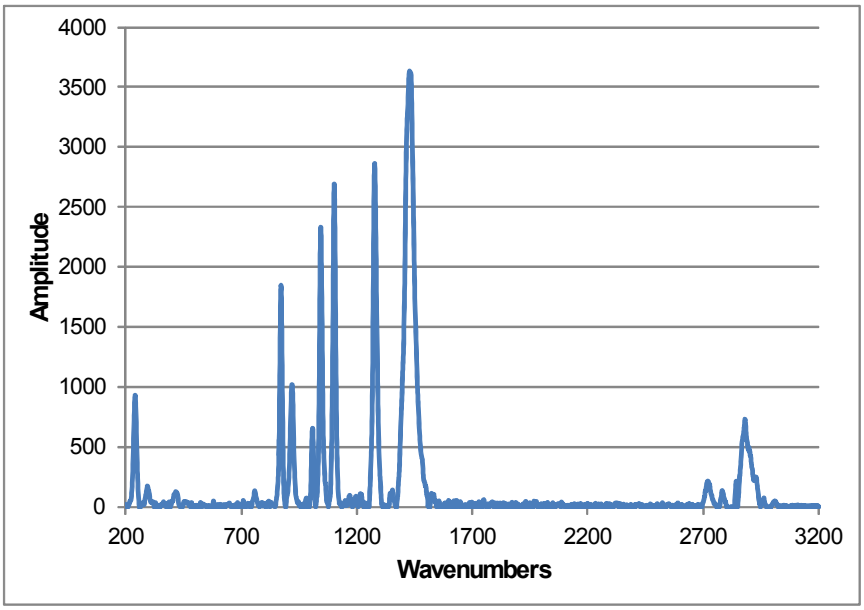

Figure S 20. Raman spectrum of lithium octanoate.

2.9 Lithium Nonanoate (pelargonate)

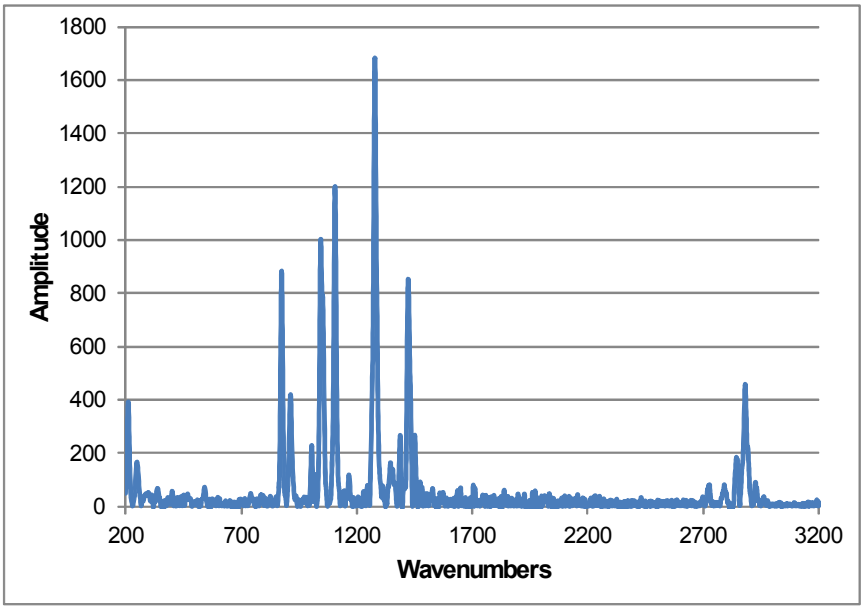

Figure S 21. Raman spectrum of lithium nonanoate.

2.10 Lithium Decanoate (caprate)

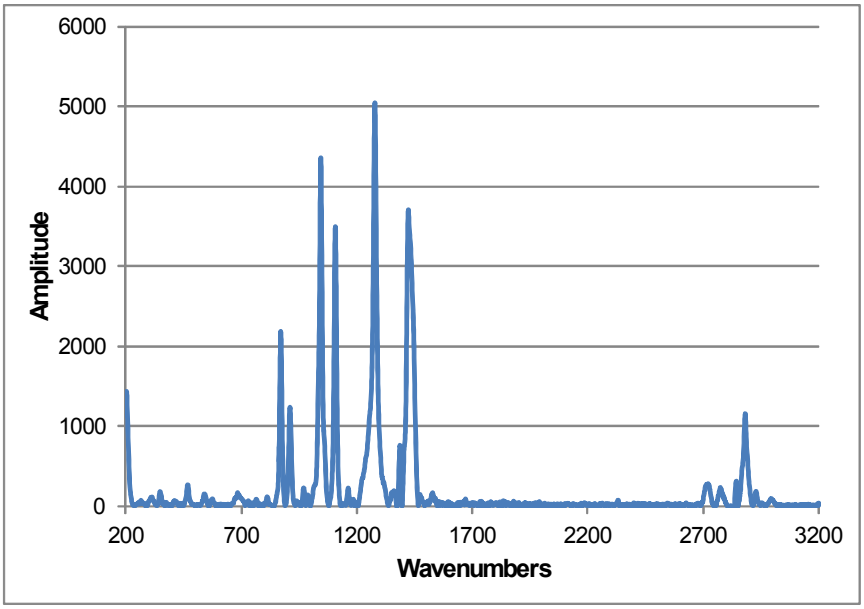

Figure S 22. Raman spectrum of lithium decanoate.

2.11 Lithium Undecanoate

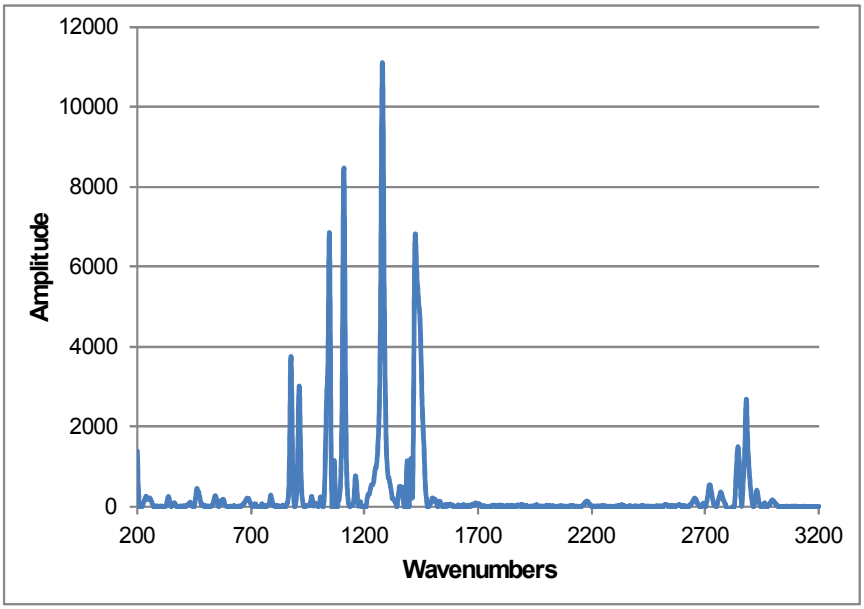

Figure S 23. Raman spectrum of lithium undecanoate.

2.12 Lithium Dodecanoate (laurate)

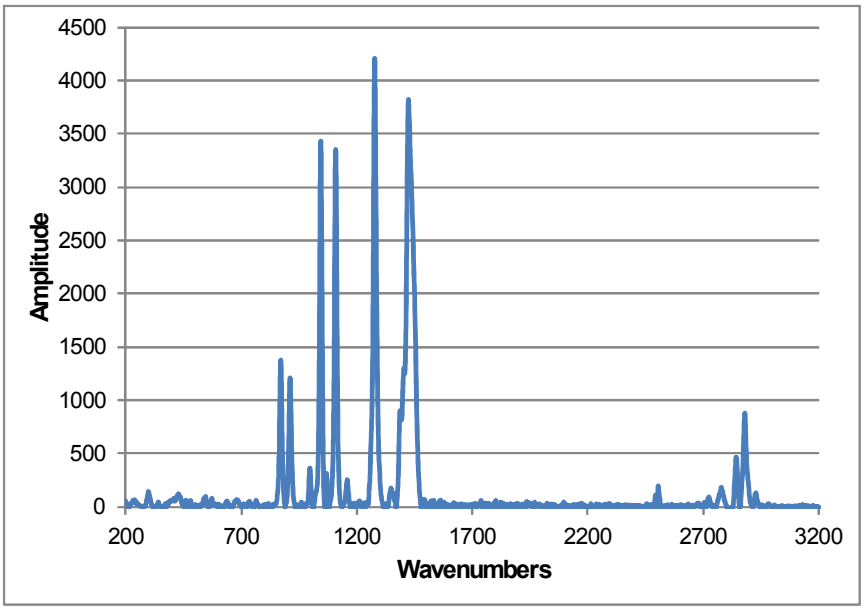

Figure S 24. Raman spectra of lithium dodecanoate.

3. UV-Vis Spectra

3.1 Lithium Methanoate

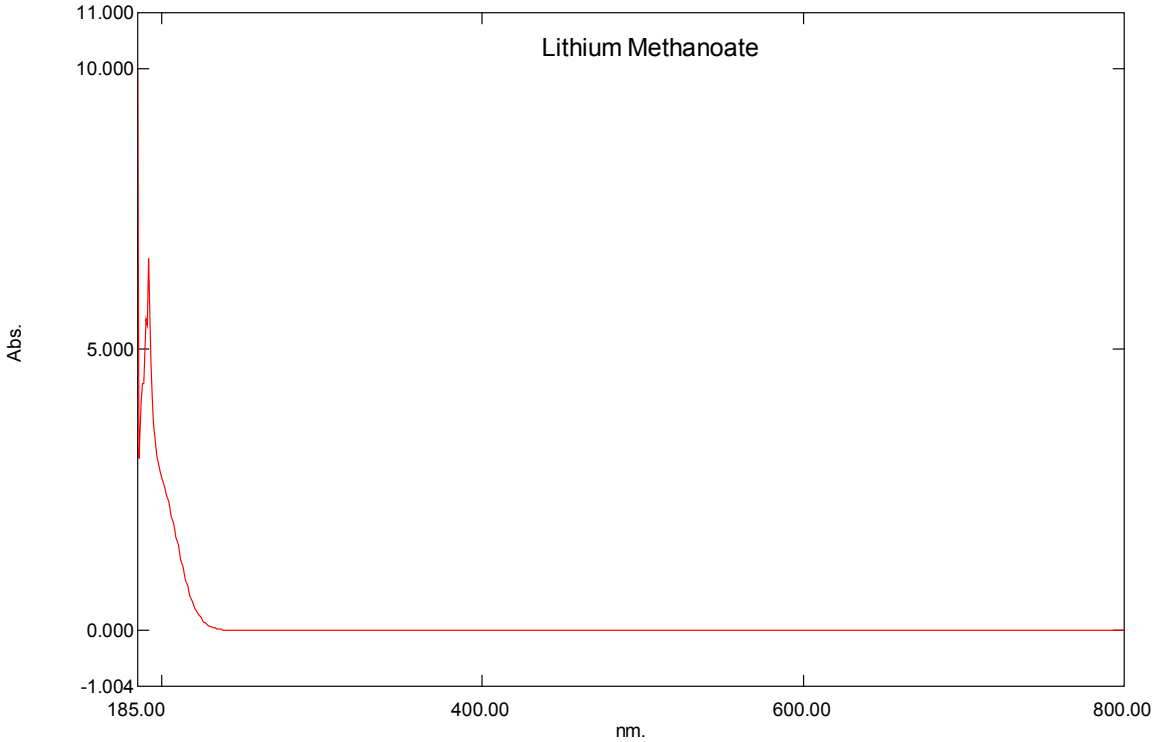

Figure S 25. UV-Vis spectrum of lithium methanoate.

3.2 Lithium Ethanoate

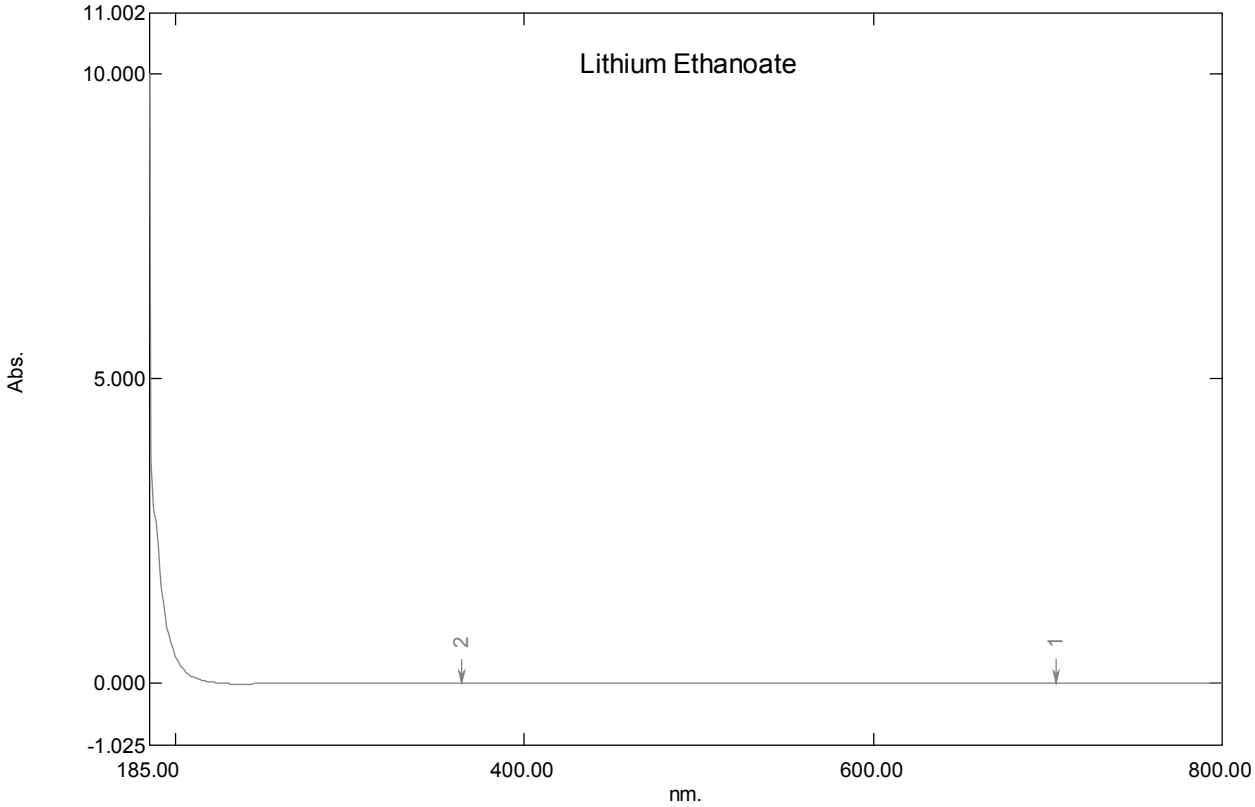

Figure S 26. UV-Vis spectrum of lithium ethanoate.

3.3 Lithium Propanoate

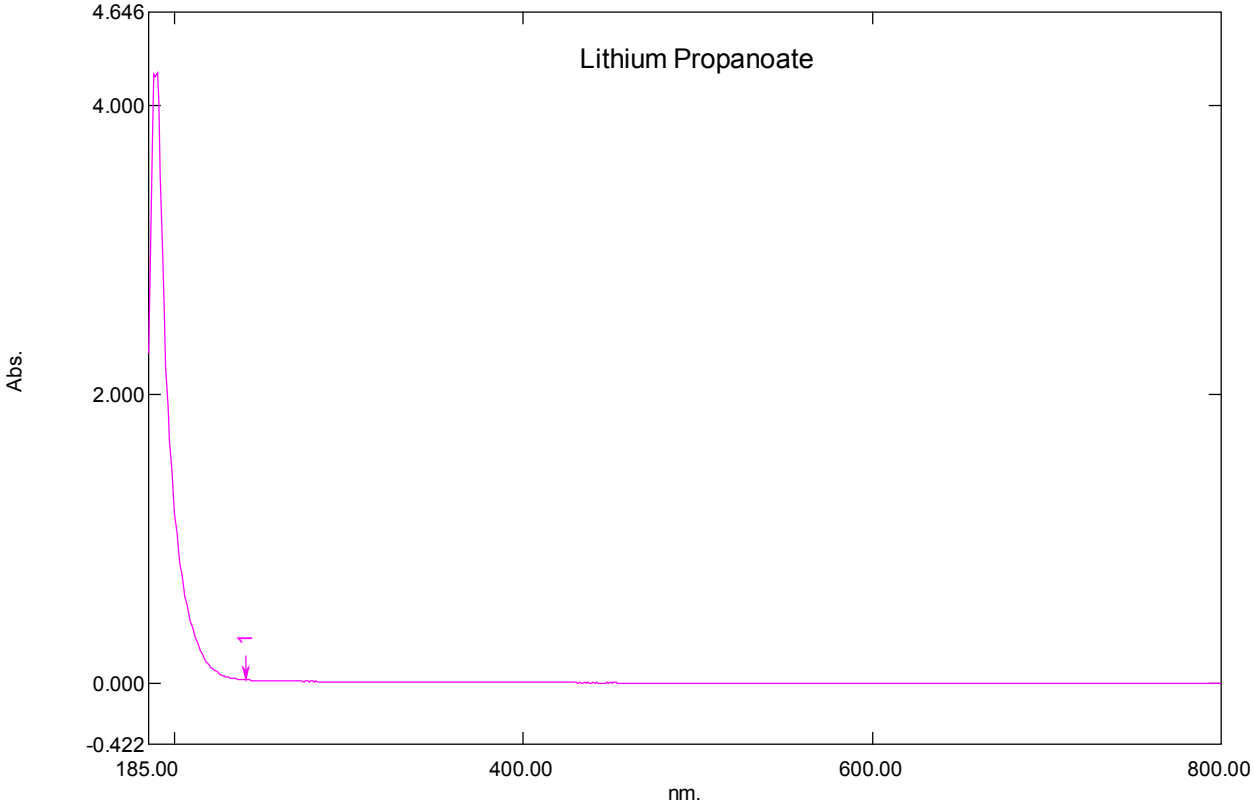

Figure S 27. UV-Vis spectrum of lithium propanoate.

3.4 Lithium Butanoate (butyrate)

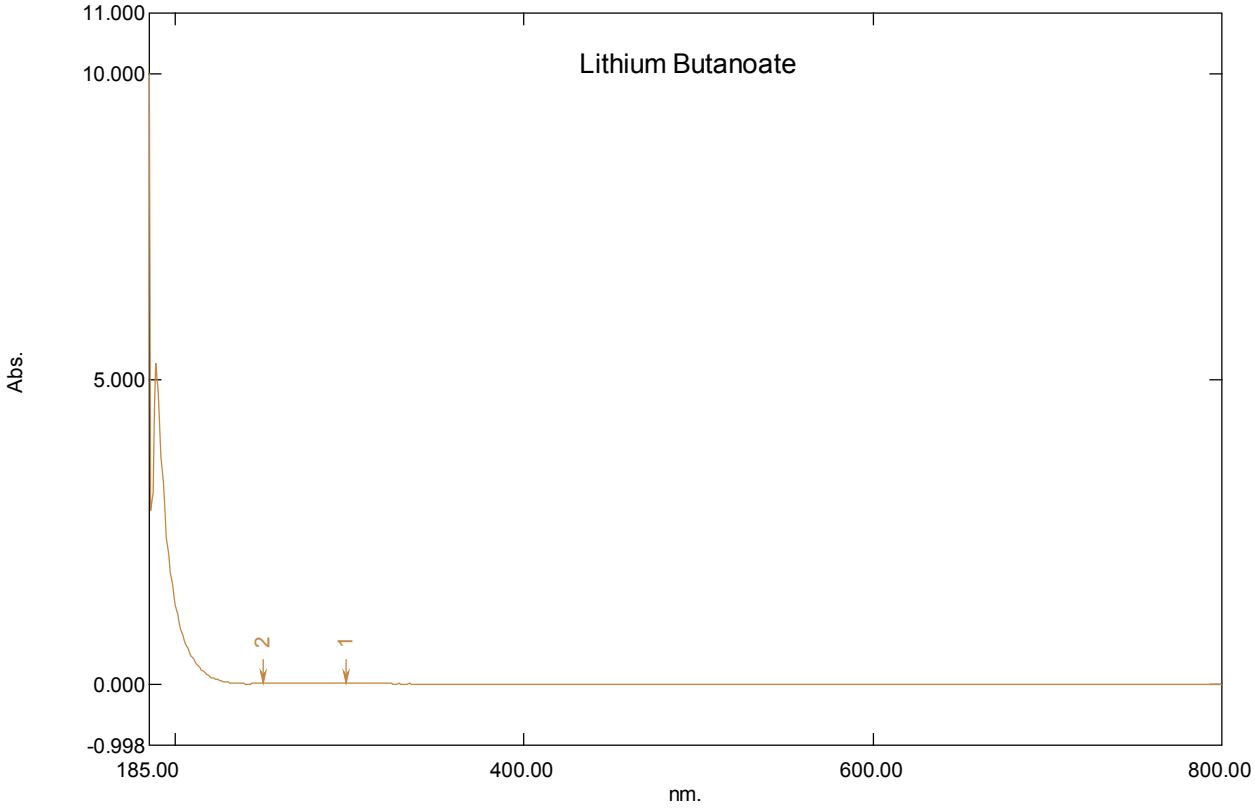

Figure S 28. UV-Vis spectrum of lithium butanoate.

3.5 Lithium Pentanoate (valerate)

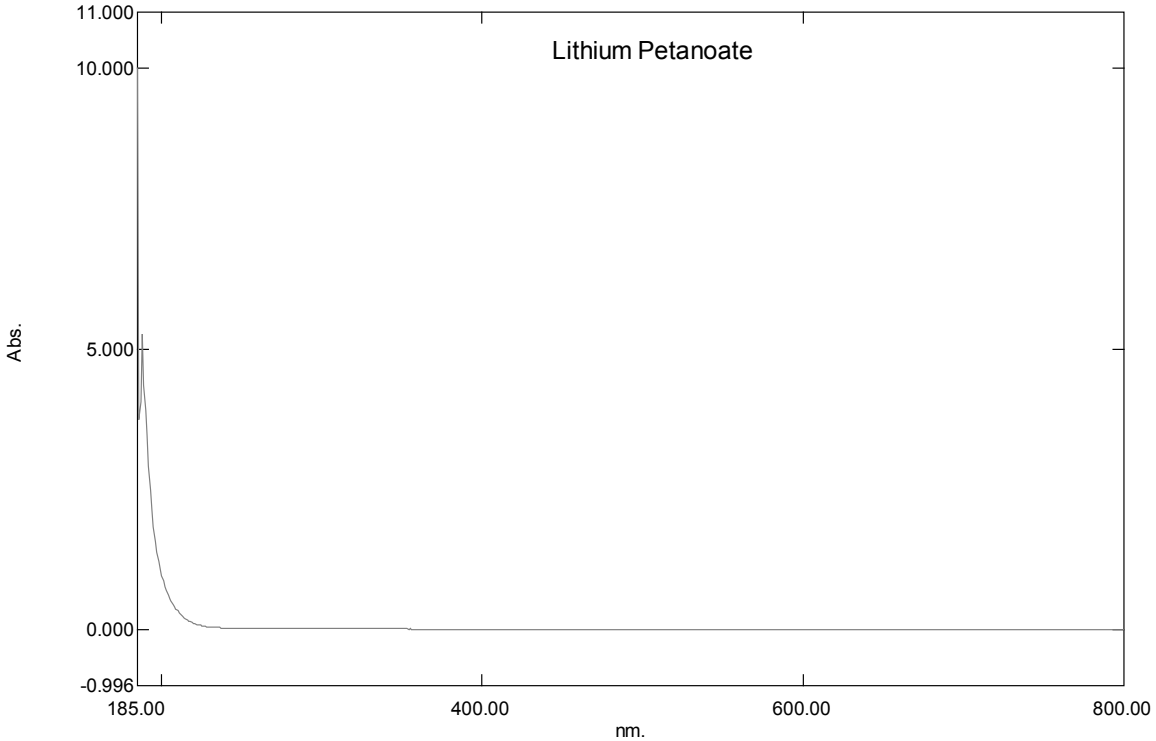

Figure S 29. UV-Vis spectrum of lithium pentanoate.

3.6 Lithium Hexanoate (caproate)

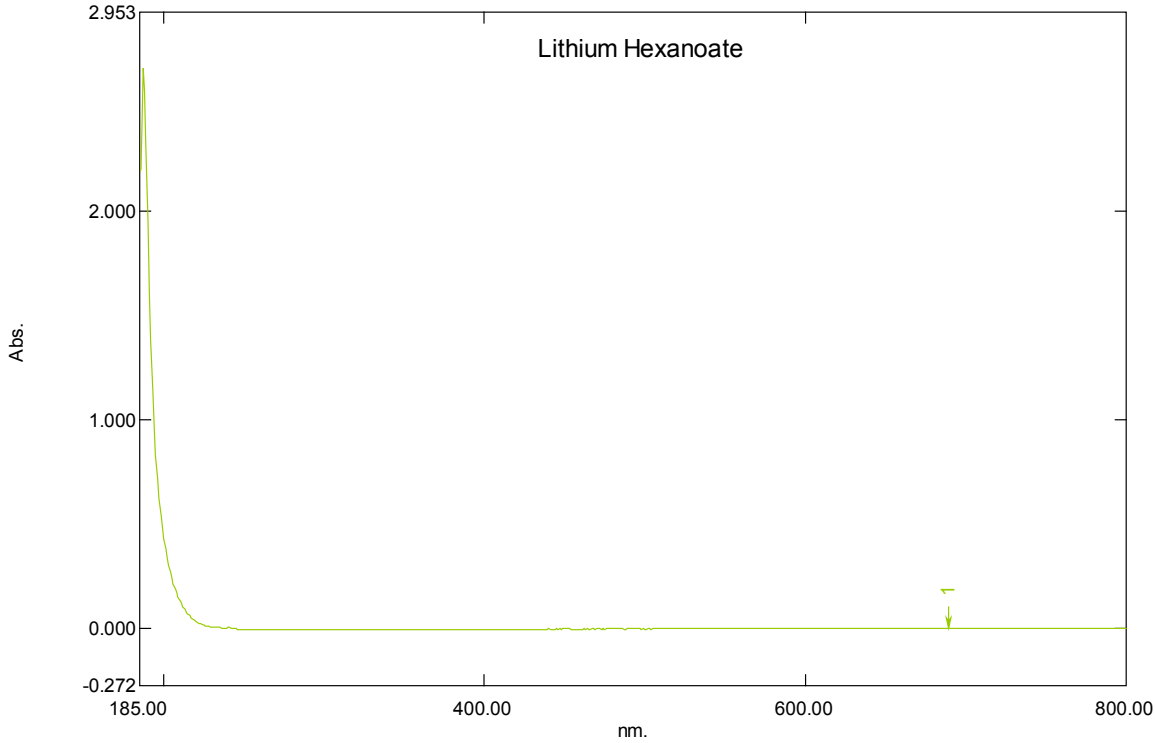

Figure S 30. UV-Vis spectrum of lithium hexanoate.

3.7 Lithium Heptanoate

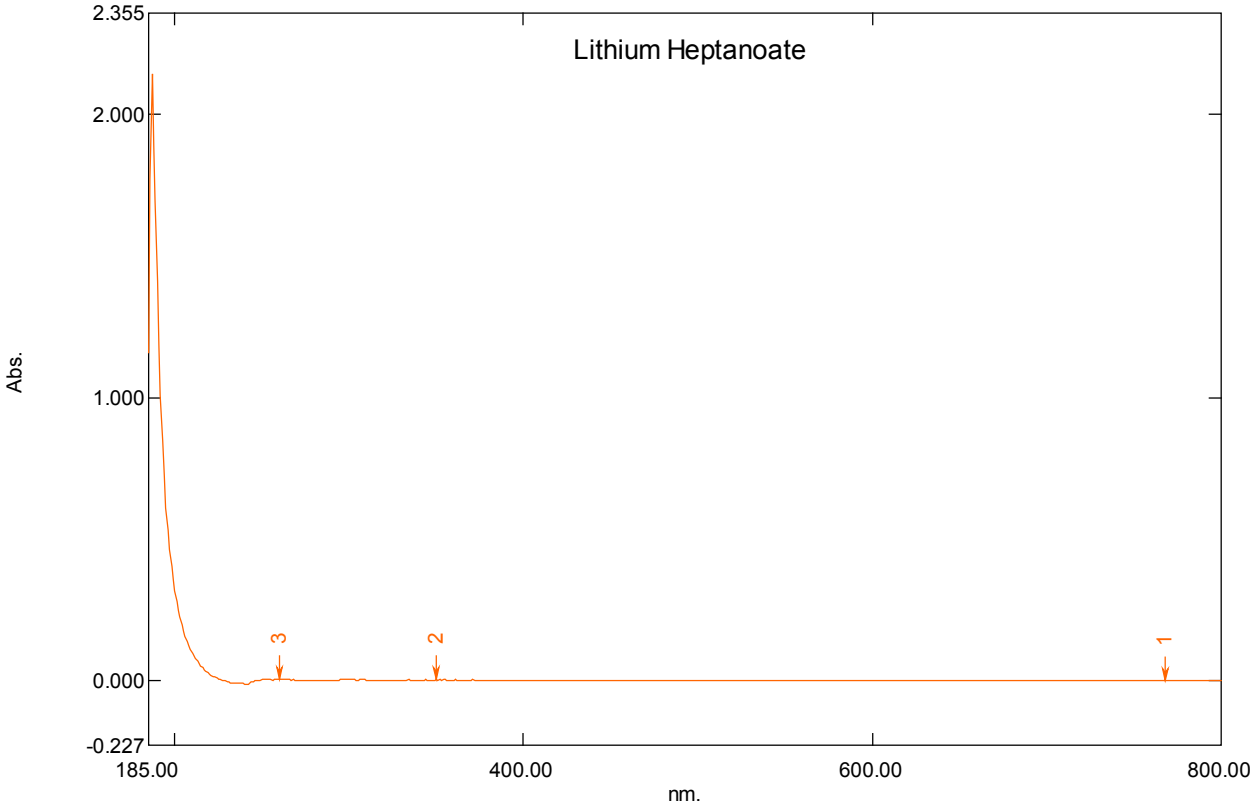

Figure S 31. UV-Vis spectrum of lithium heptanoate.

3.8 Lithium Octanoate (caprylate)

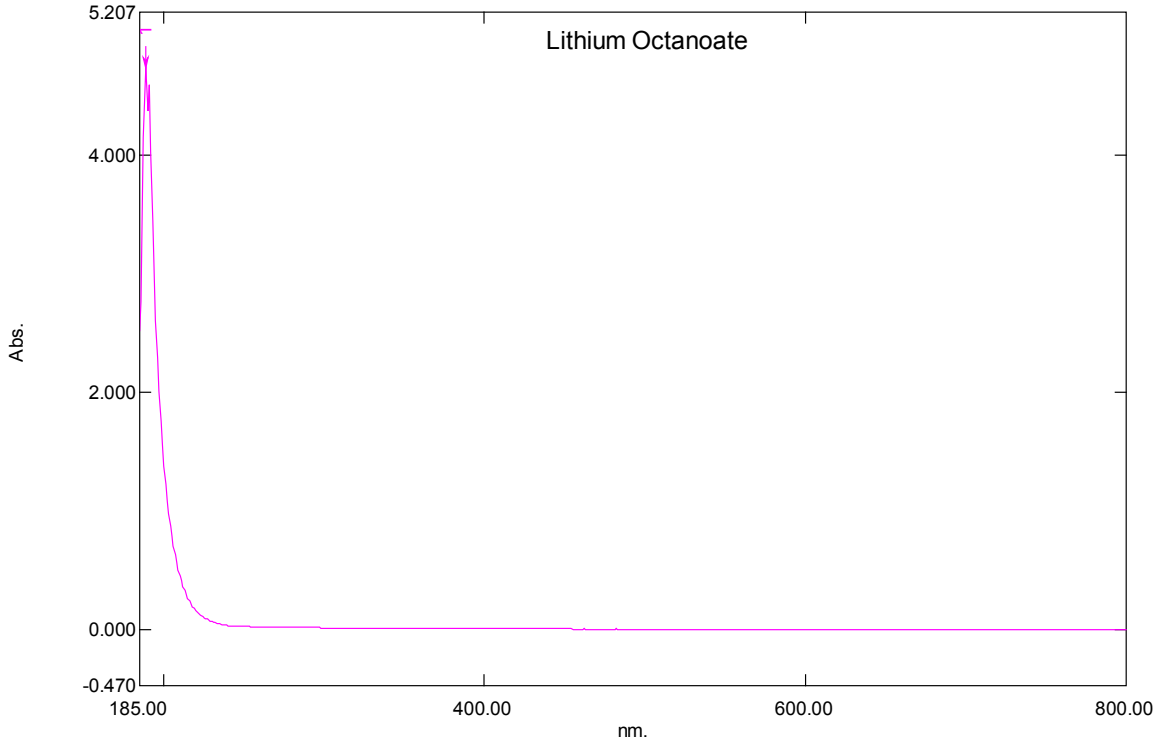

Figure S 32. UV-Vis spectrum of lithium octanoate.

3.9 Lithium Nonanoate (pelargonate)

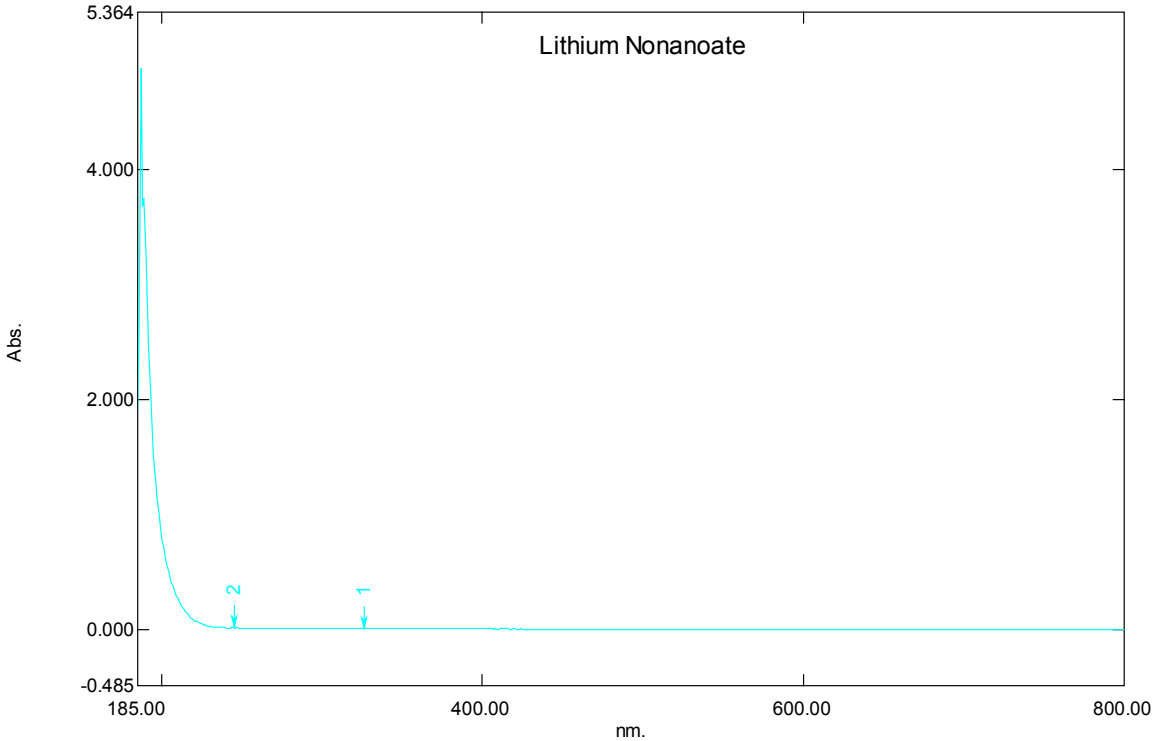

Figure S 33. UV-Vis spectrum of lithium nonanoate.

3.10 Lithium Decanoate (caprate)

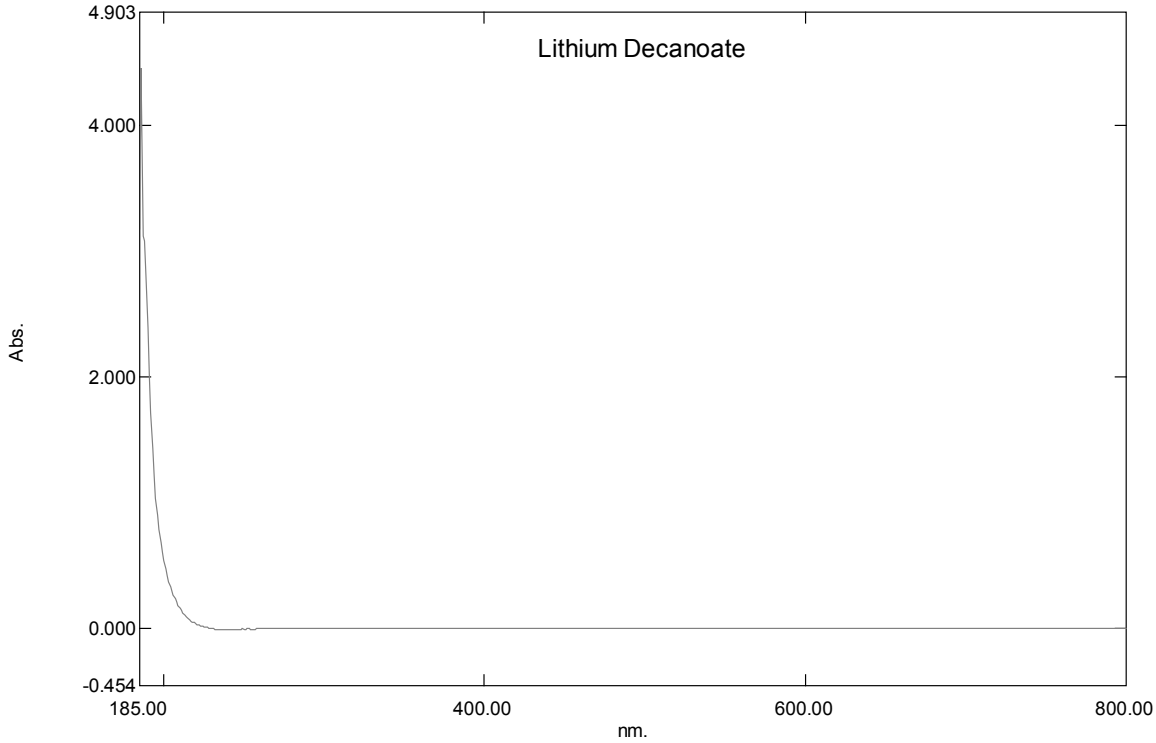

Figure S 34. UV-Vis spectrum of lithium decanoate.

3.11 Lithium Undecanoate

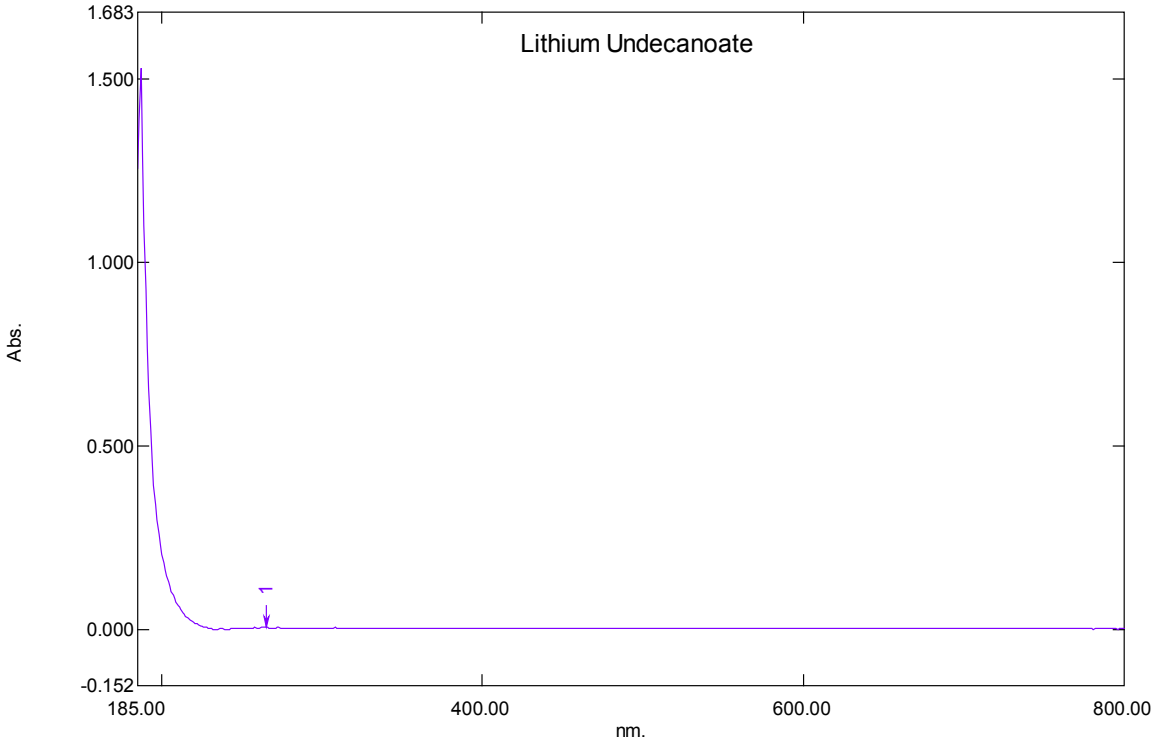

Figure S 35. UV-Vis spectrum of lithium undecanoate.

3.12 Lithium Dodecanoate (laurate)

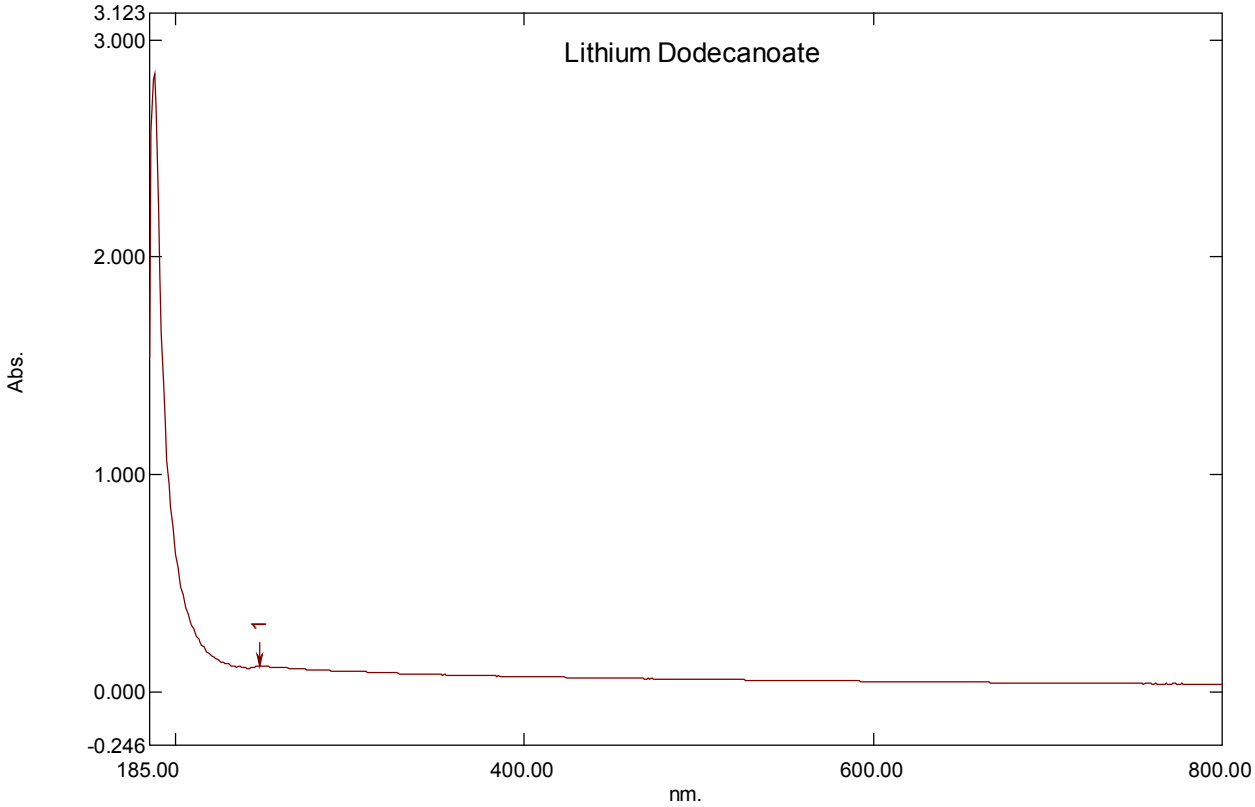

Figure S 36. UV-Vis spectrum of lithium dodecanoate.

4. Termogravimetric Analysis (TGA) Results

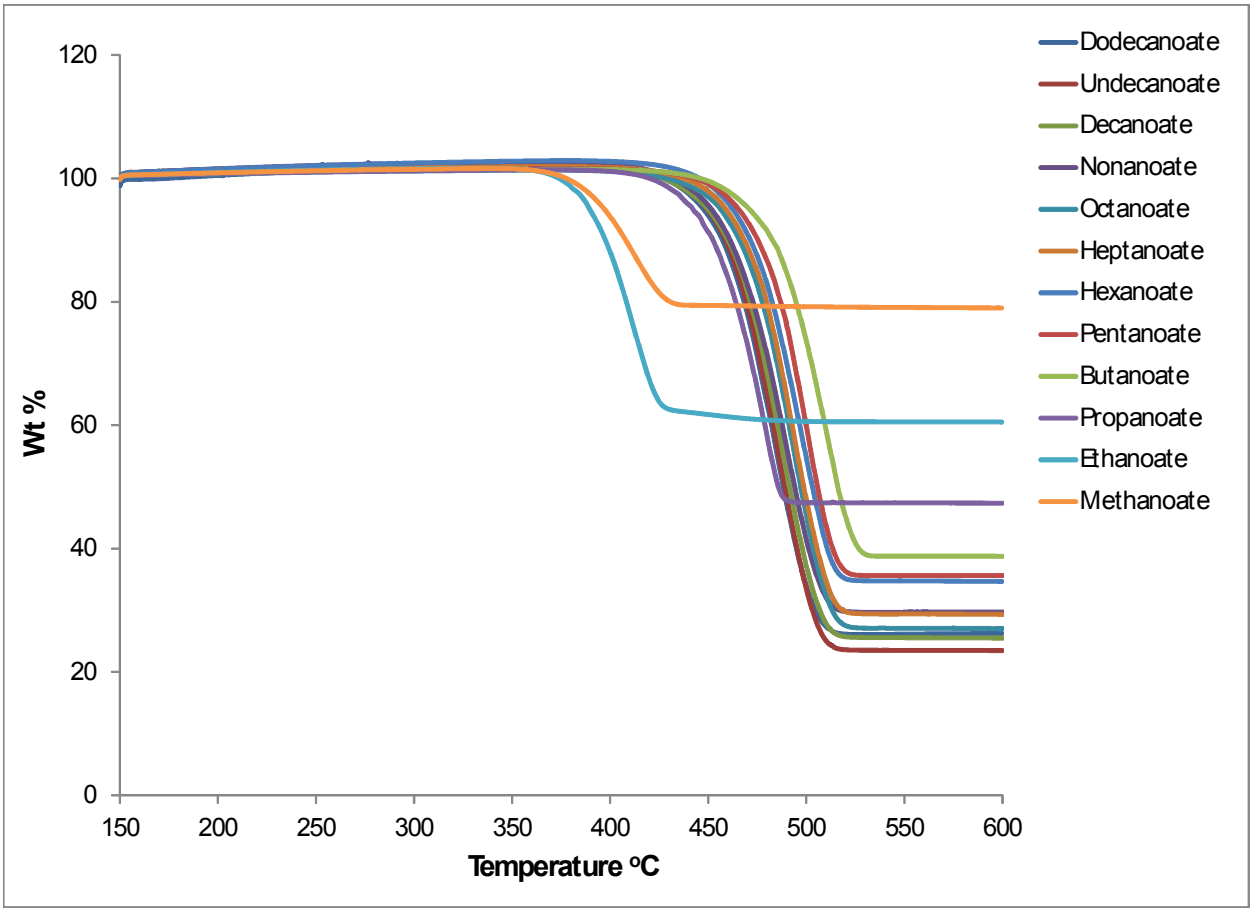

Figure S 37. TGA mass loss with temperature of the C_1-C_{12} Li-carboxylates over the range T/°C = (150 to 600) at a heating rate of β/°C·s^{-1} (0.167) and conducted under inert atmosphere (N_2).

Table S1. Single point measurements to verify temperature and calorific calibration of TGA.

Material	Experimental		Literature values	
	T_m (°C)	ΔH_m ($J \cdot g^{-1}$)	T_m (°C)	ΔH_m ($J \cdot g^{-1}$)
In	156.44	30.42	156.60	28.58 ± 0.07
Al	661.55	394.07	660.32	399.9 ± 1.3
Au	1064.03	62.30	1064.18	64.6 ± 1.5

[a] Literature values taken from: Höhne, G. W. H.; Hemminger, W. F.; Flammersheim, H.-J. *Differential scanning calorimetry*, 2ed; Springer: Berlin, 2003, p. 108.

5. Calorigrams of the C_1-C_{12} Li-Carboxylates as Determined by Differential Scanning Calorimetry (DSC)

5.1 Lithium Methanoate

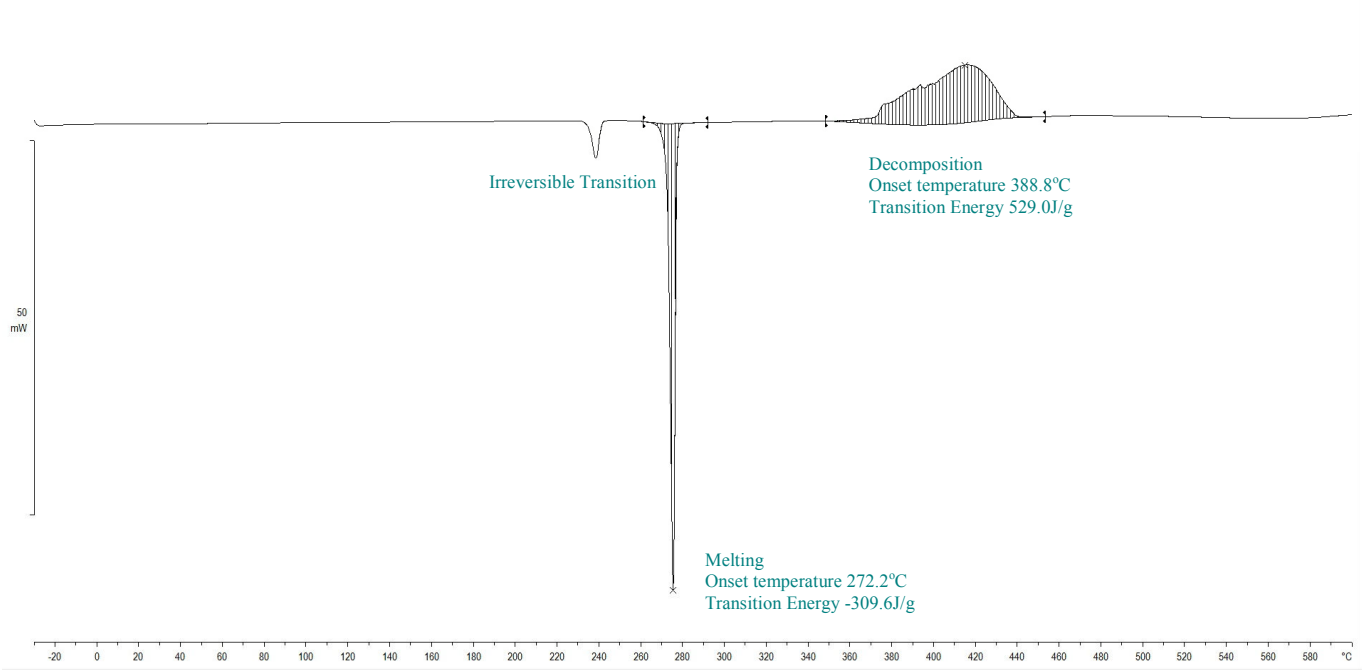

Figure S 38. Calorigram of lithium methanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.2 Lithium Ethanoate

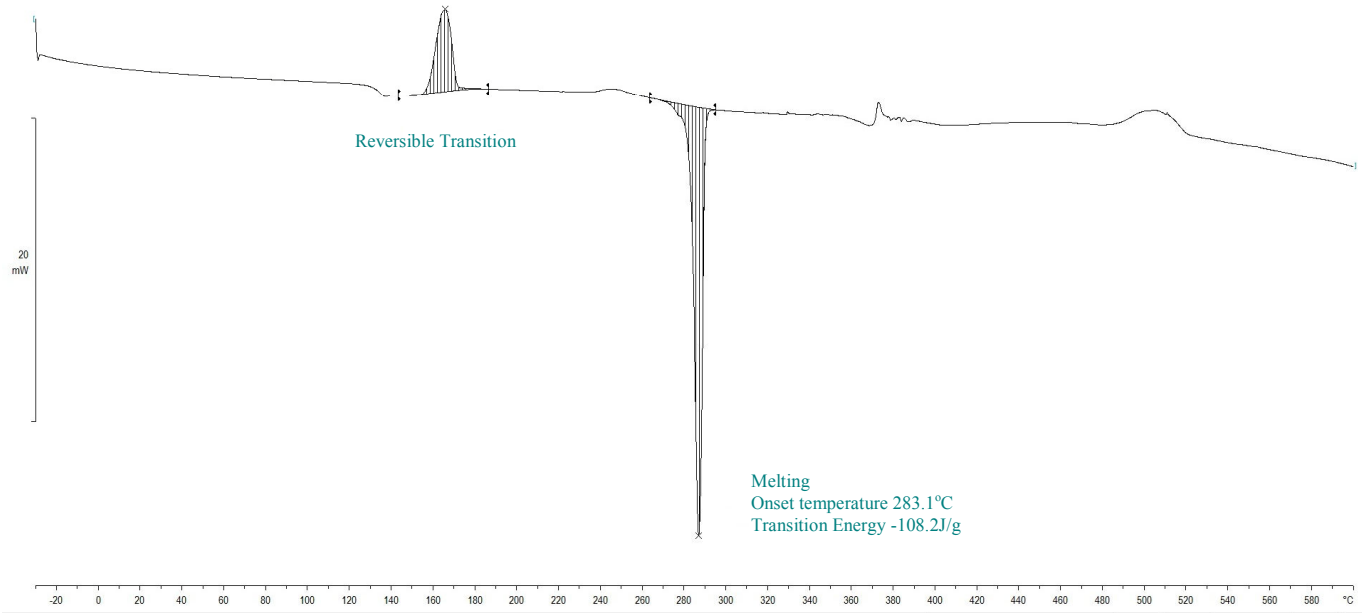

Figure S 39. Calorigram of lithium ethanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.3 Lithium Propanoate

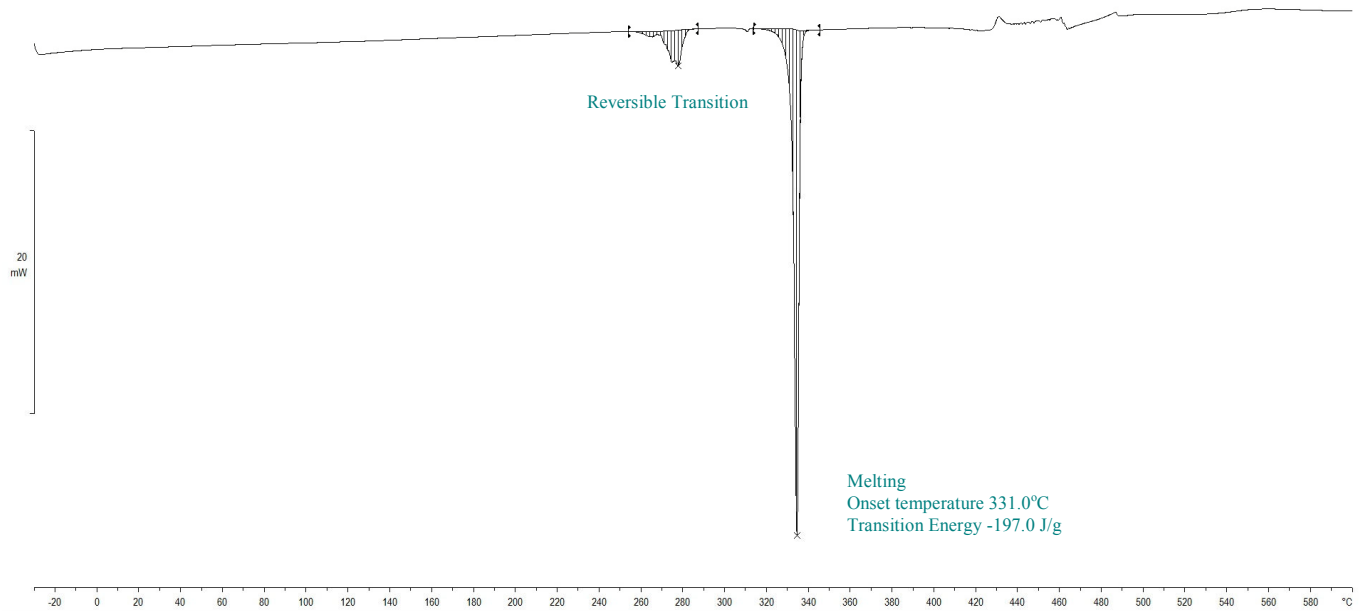

Figure S 40. Calorigram of lithium propanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.4 Lithium Butanoate (butyrate)

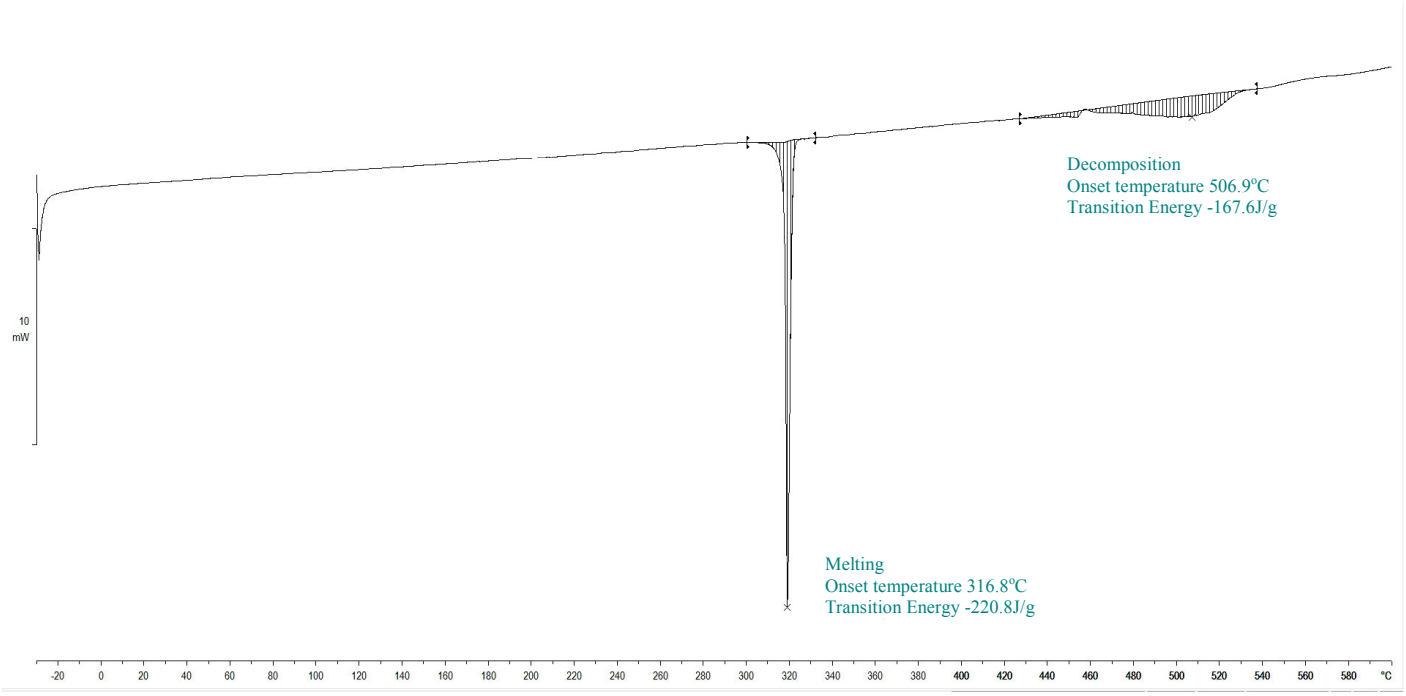

Figure S 41. Calorigram of lithium butanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.5 Lithium Pentanoate (valerate)

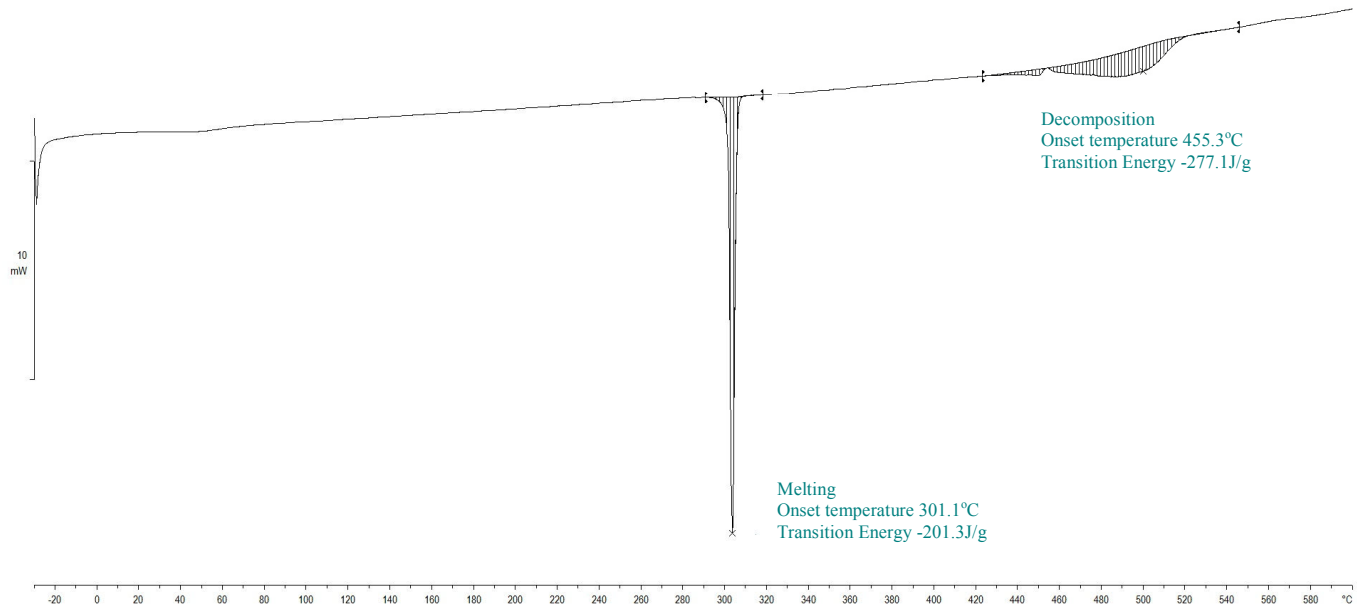

Figure S 42. Calorigram of lithium pentanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.6 Lithium Hexanoate (caproate)

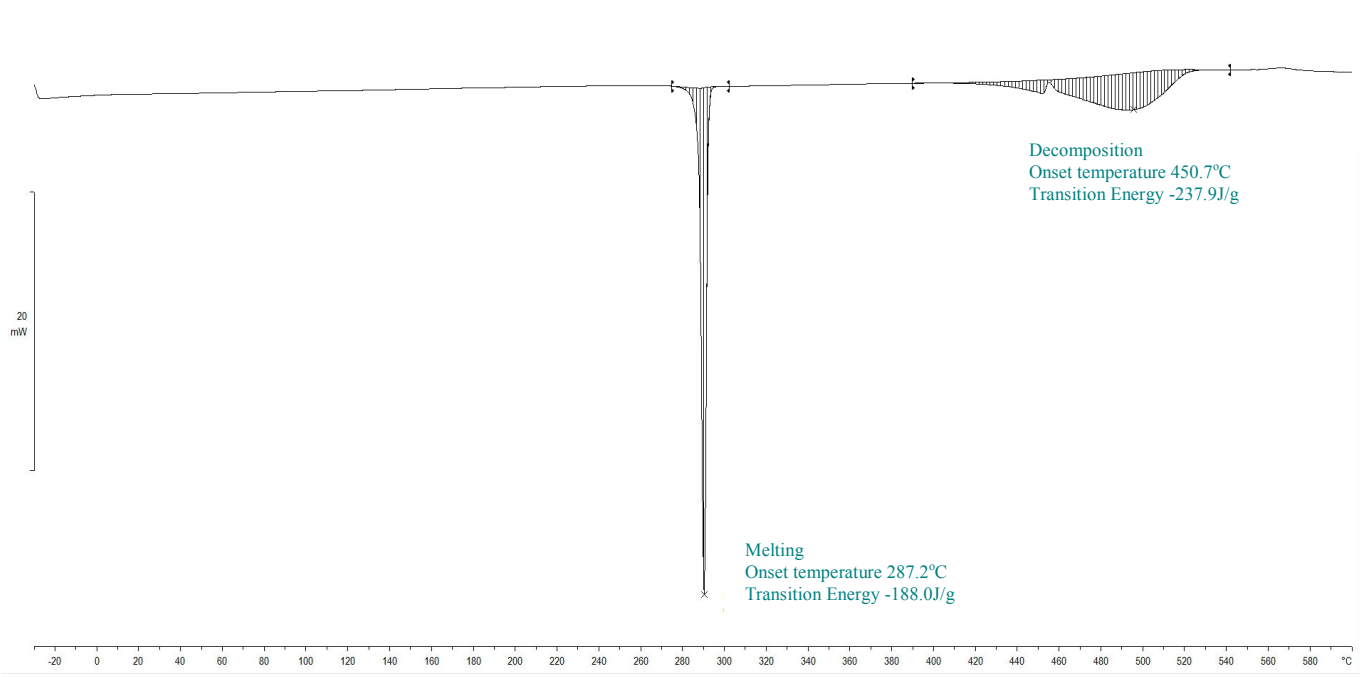

Figure S 43. Calorigram of lithium hexanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.7 Lithium Heptanoate

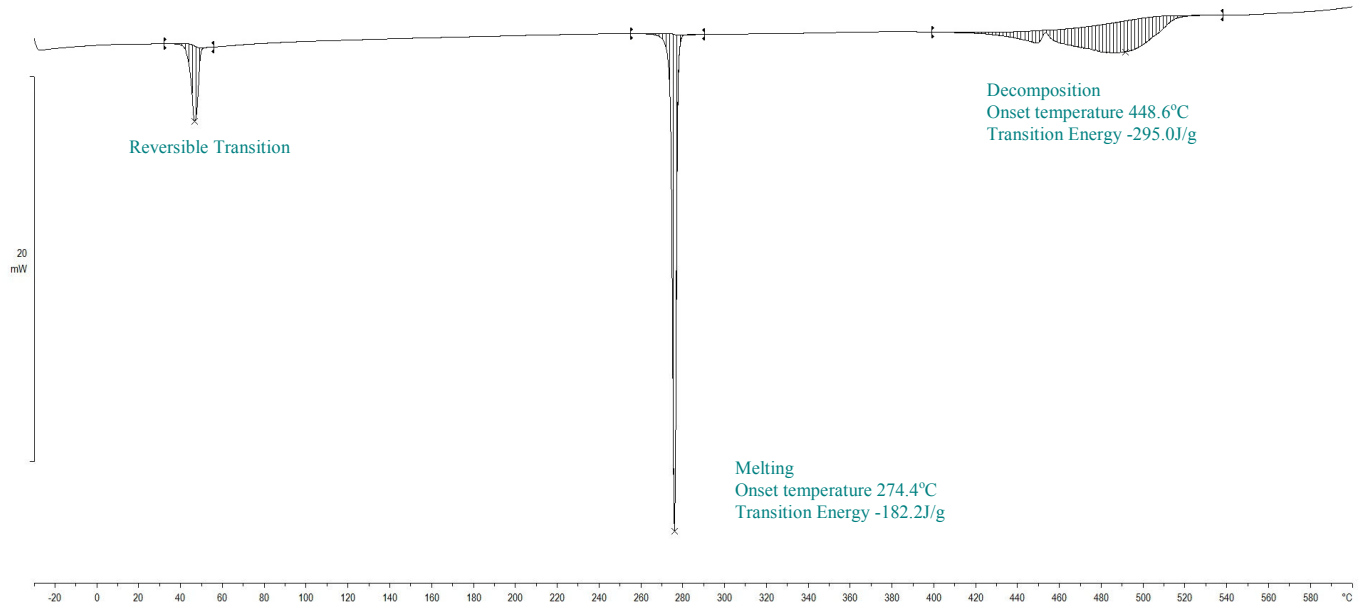

Figure S 44. Calorigram of lithium heptanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.8 Lithium Octanoate (caprylate)

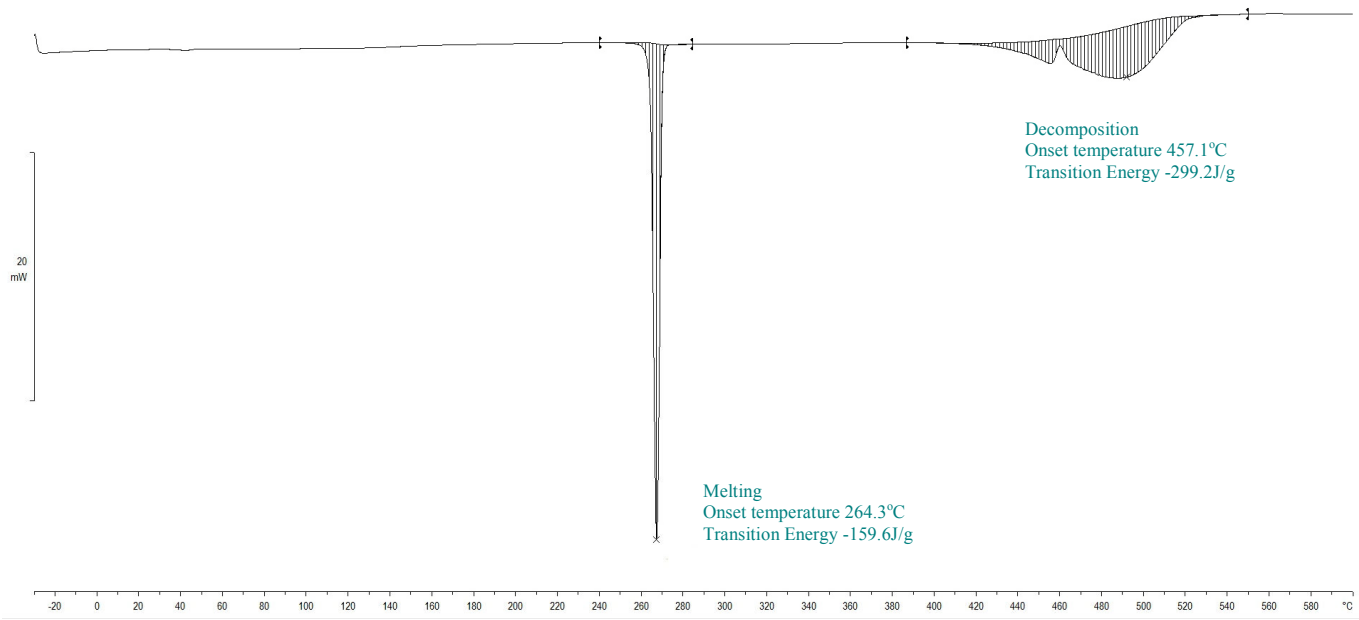

Figure S 45. Calorigram of lithium octanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.9 Lithium Nonanoate (pelargonate)

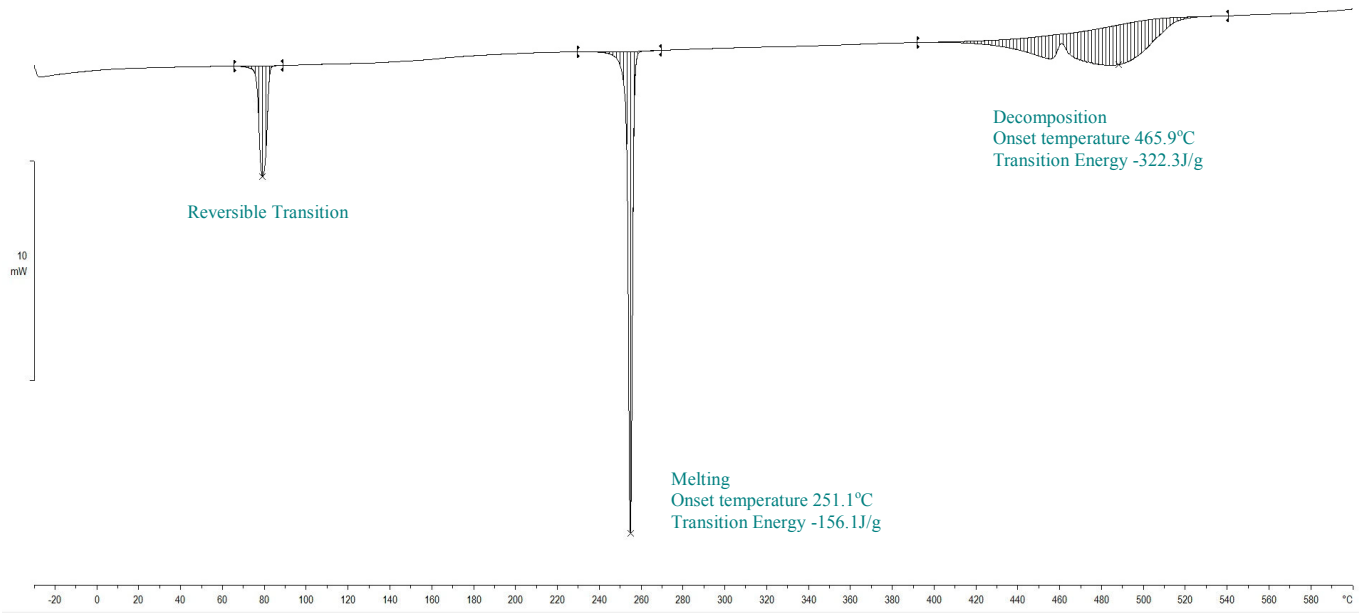

Figure S 46. Calorigram of lithium nonanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.10 Lithium Decanoate (caprate)

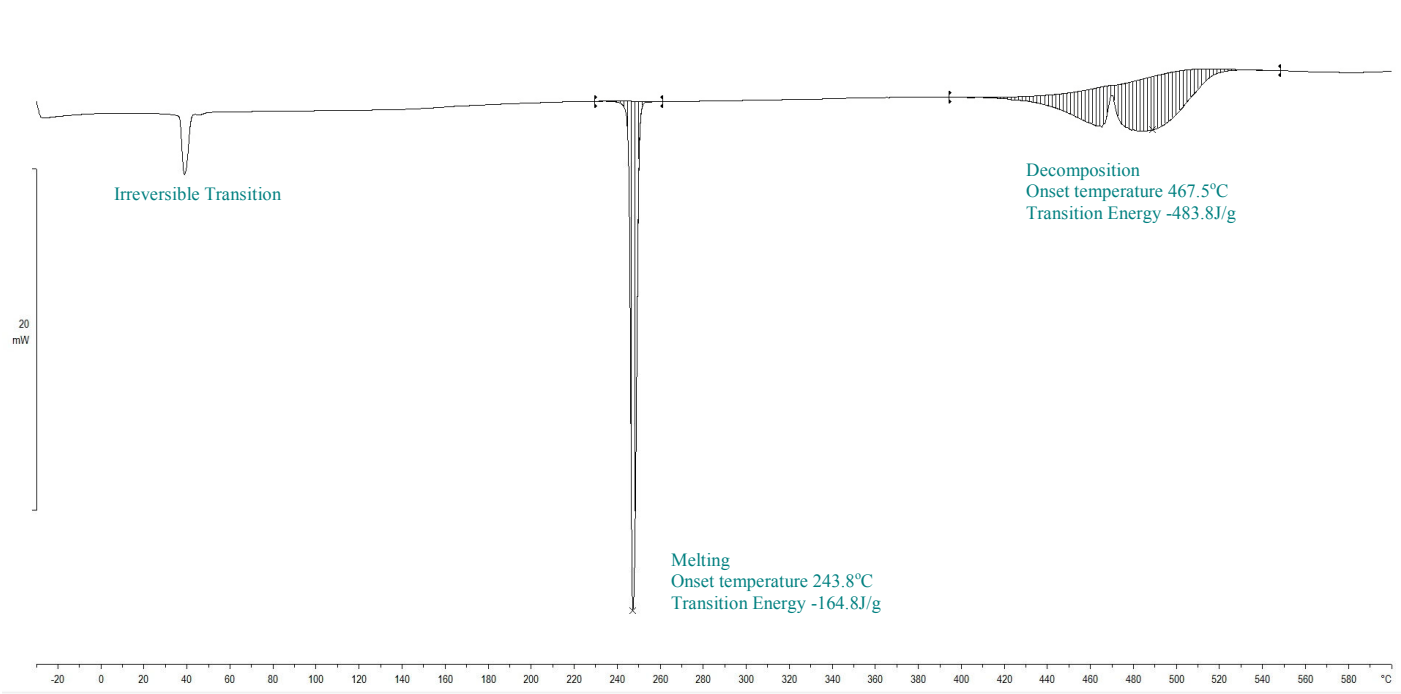

Figure S 47. Calorigram of lithium decanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.11 Lithium Undecanoate

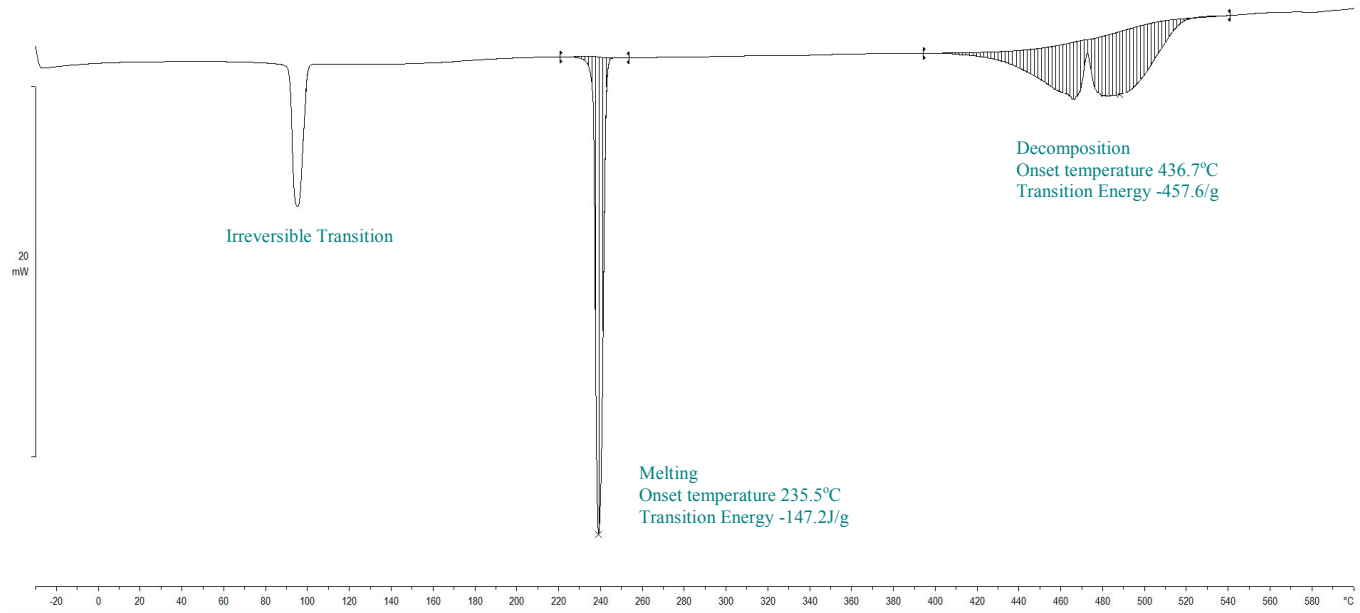

Figure S 48. Calorigram of lithium undecanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.

5.12 Lithium Dodecanoate (laurate)

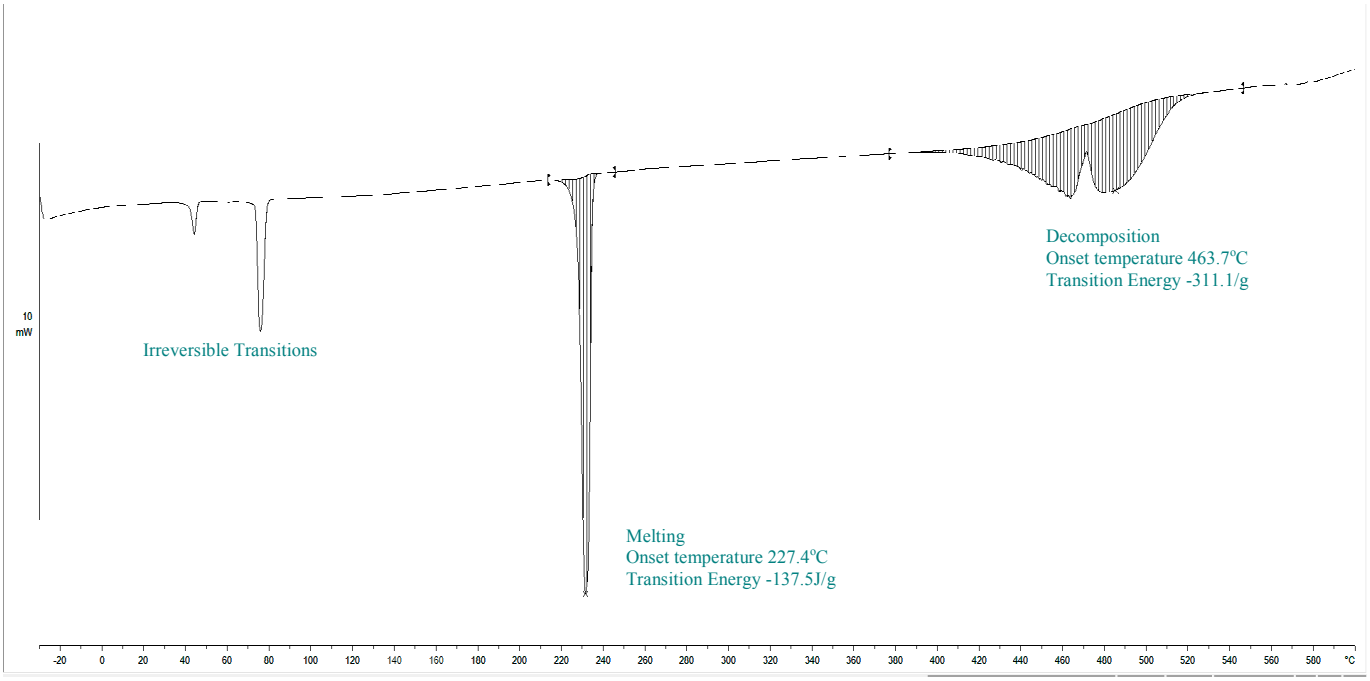

Figure S 49. Calorigram of lithium dodecanoate determined by DSC over the range of T/°C = (–30 to 600) at a heating rate of β/°C·s^{-1} (0.167) and 1.7 mL·s^{-1} nitrogen flow.