Electronic Supplementary Information

Biomimetic Design of Protic Lipidic Ionic Liquids with Enhanced Fluidity

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I. Computational Modeling and Simulation

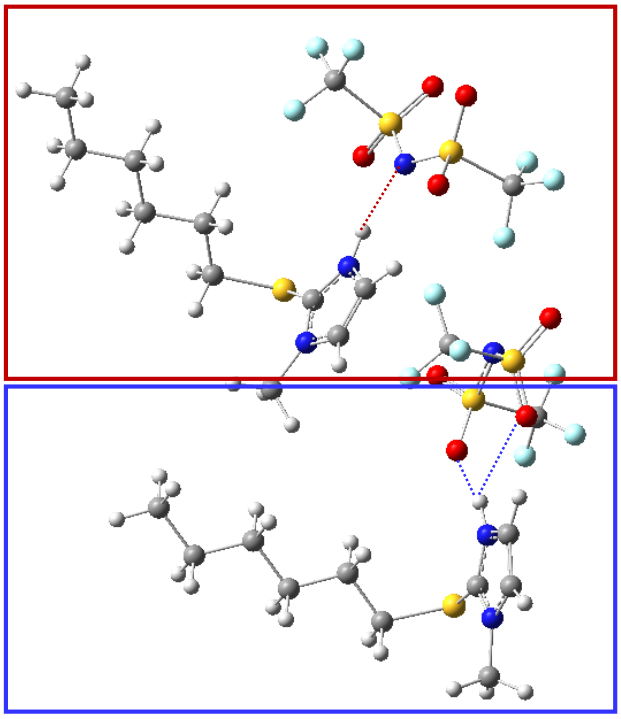


Figure S1. Considering in the x-ray structure, the LIL **2**, [mimSC$_{16}$][NTf$_2$], complexes were packed more tightly, which may favor the formation of both conformers. A large model including two units was used. The solvent effect was considered by CPCM solvation model. In the optimized structure, both conformers (a, in red box) and (b, in blue square box) exist. The N–H···N–anion distance amounts to 2.0059 Å in the conformer (a), while the distances between the imidazolium hydrogen atom with oxygen atoms of the anion are 1.8416 and 2.6581 Å, respectively.

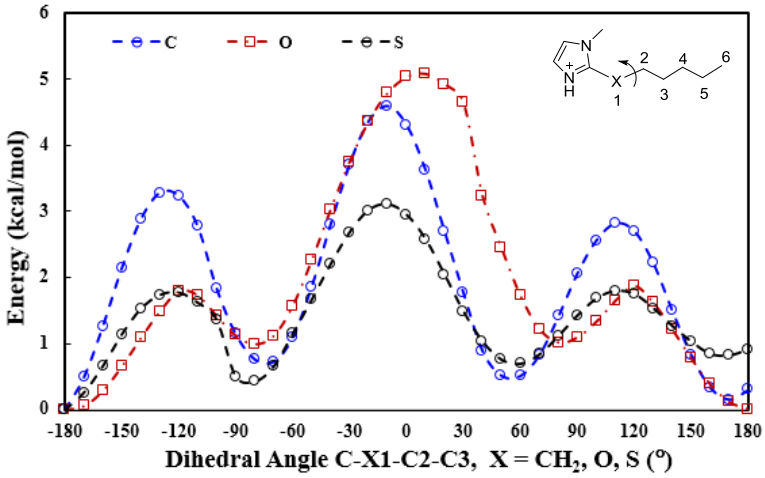
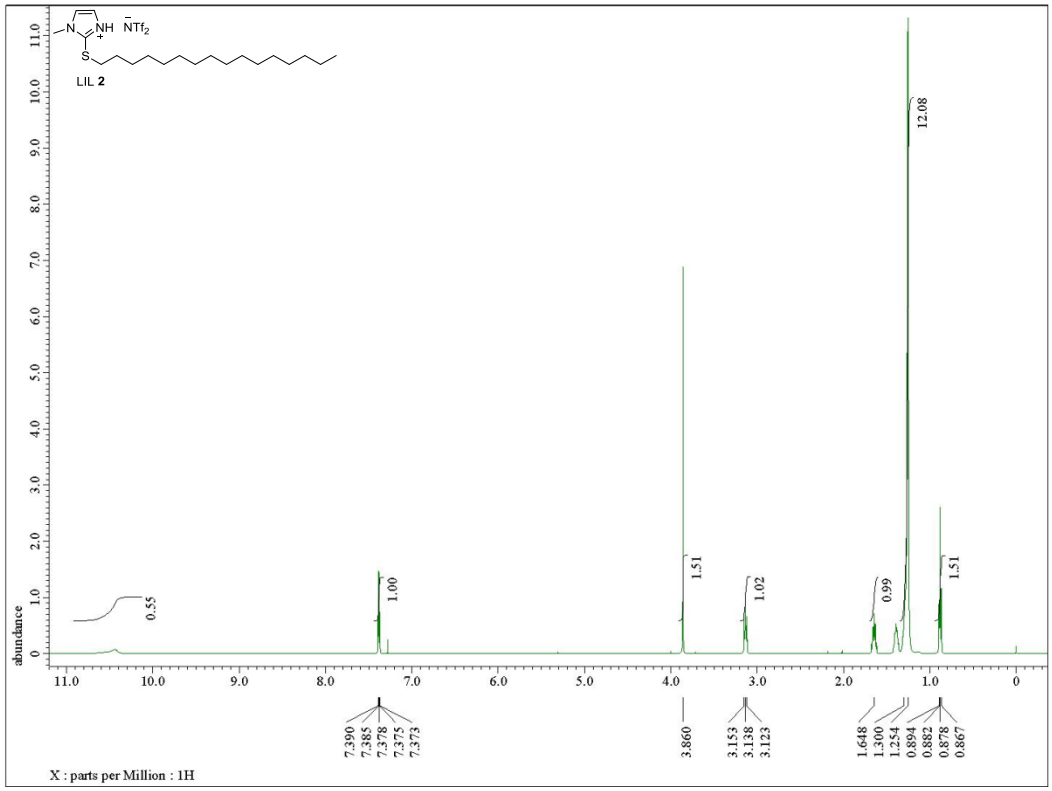
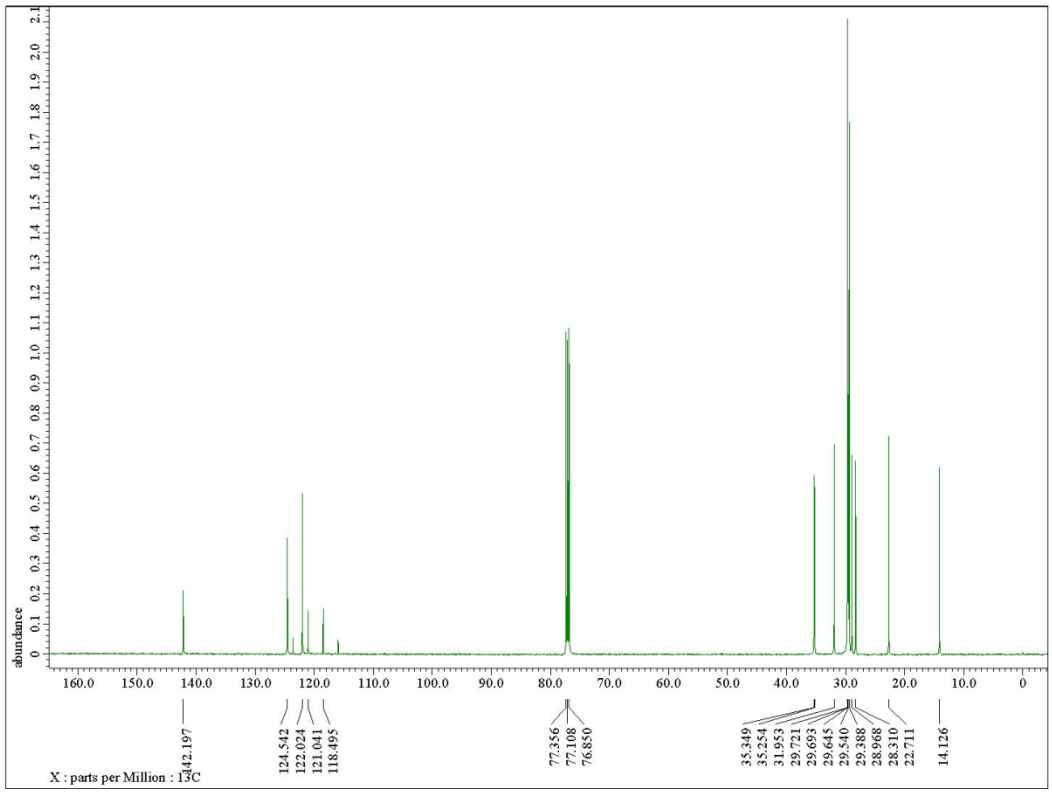
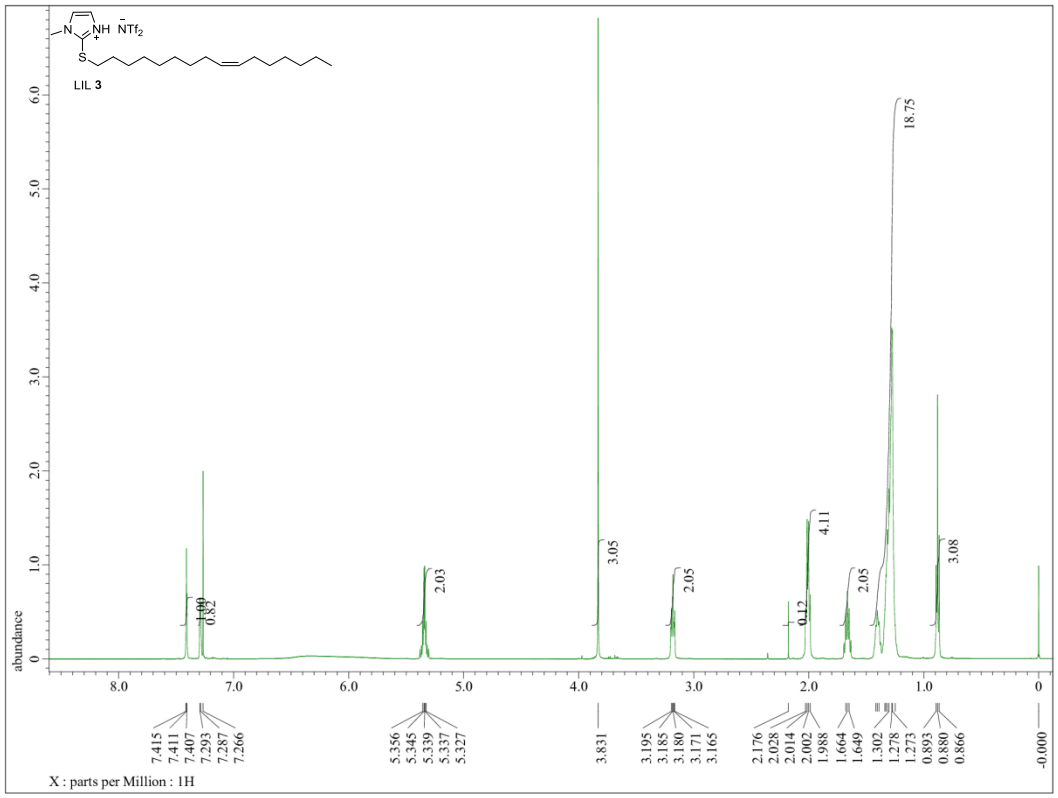


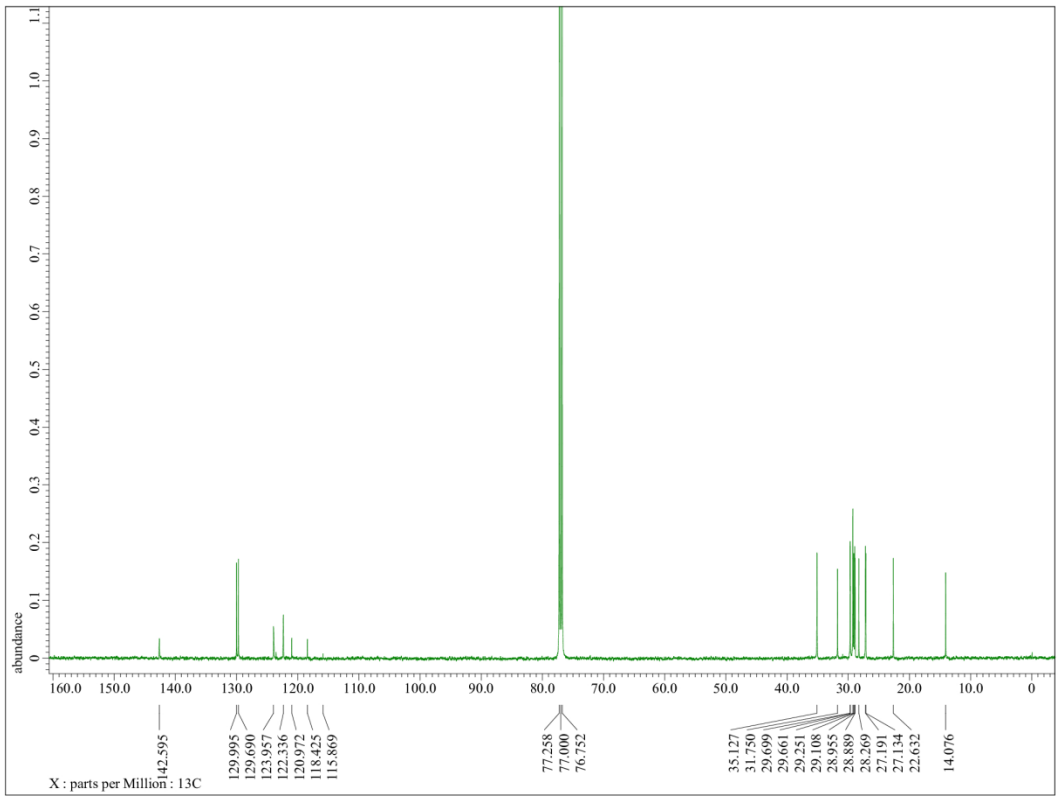
Figure S2. Relative conformational-energy landscape for the rotation along the X1−C2 bond.

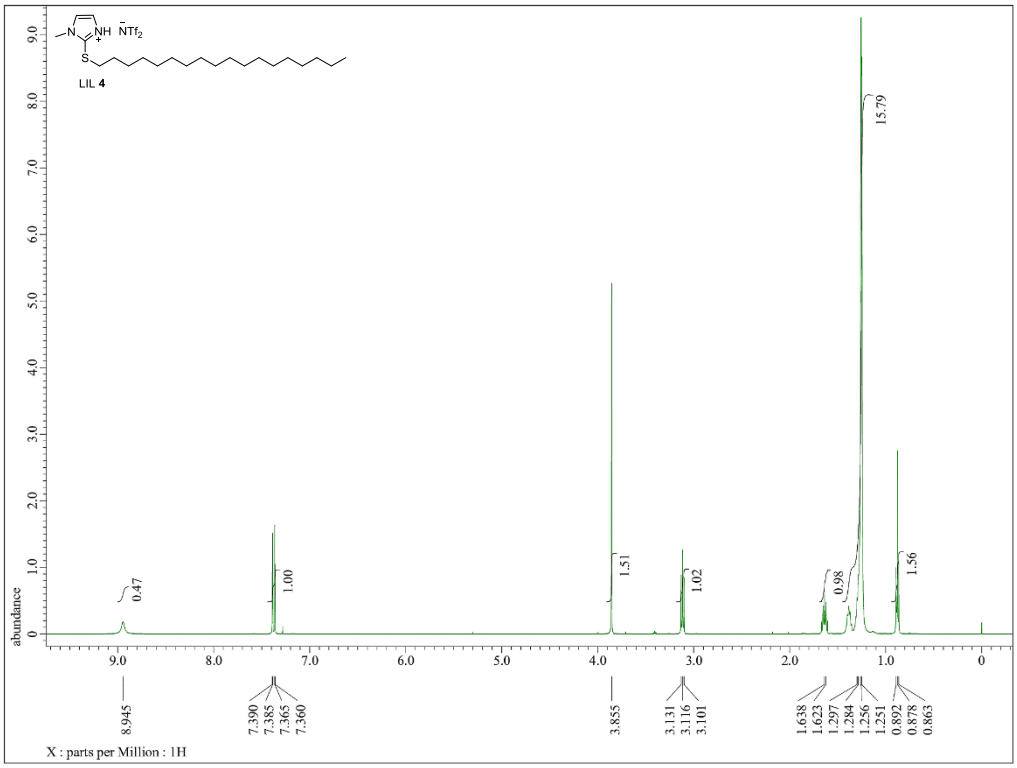
II. ^{1}H and ^{13}C NMR Spectra

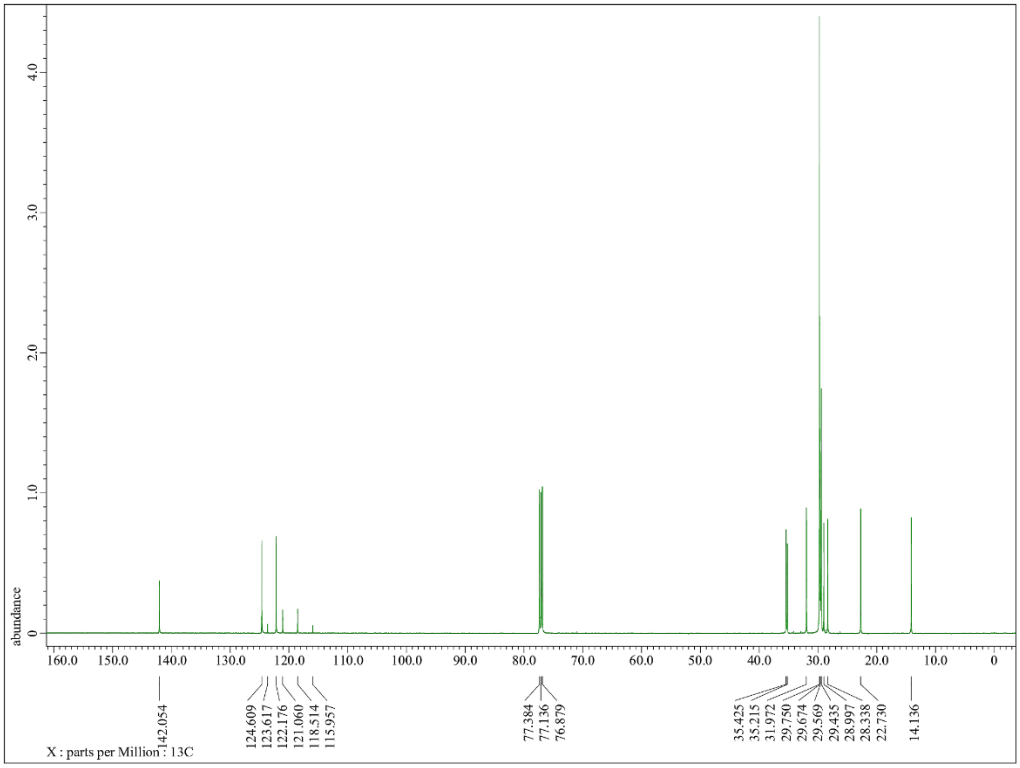


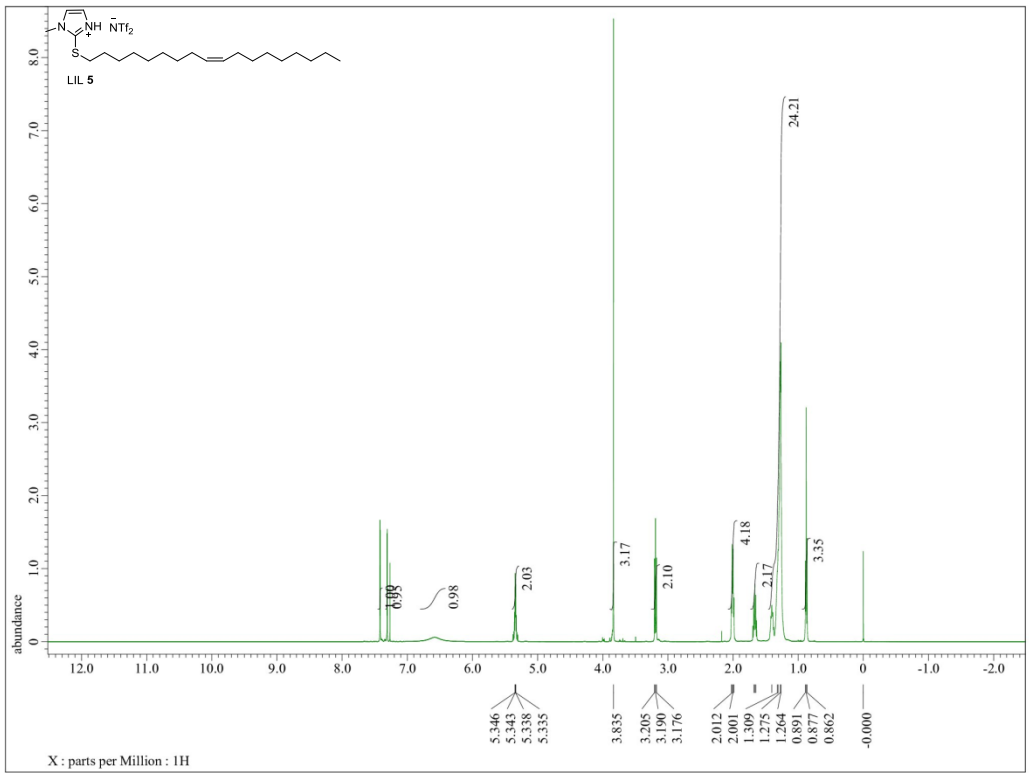


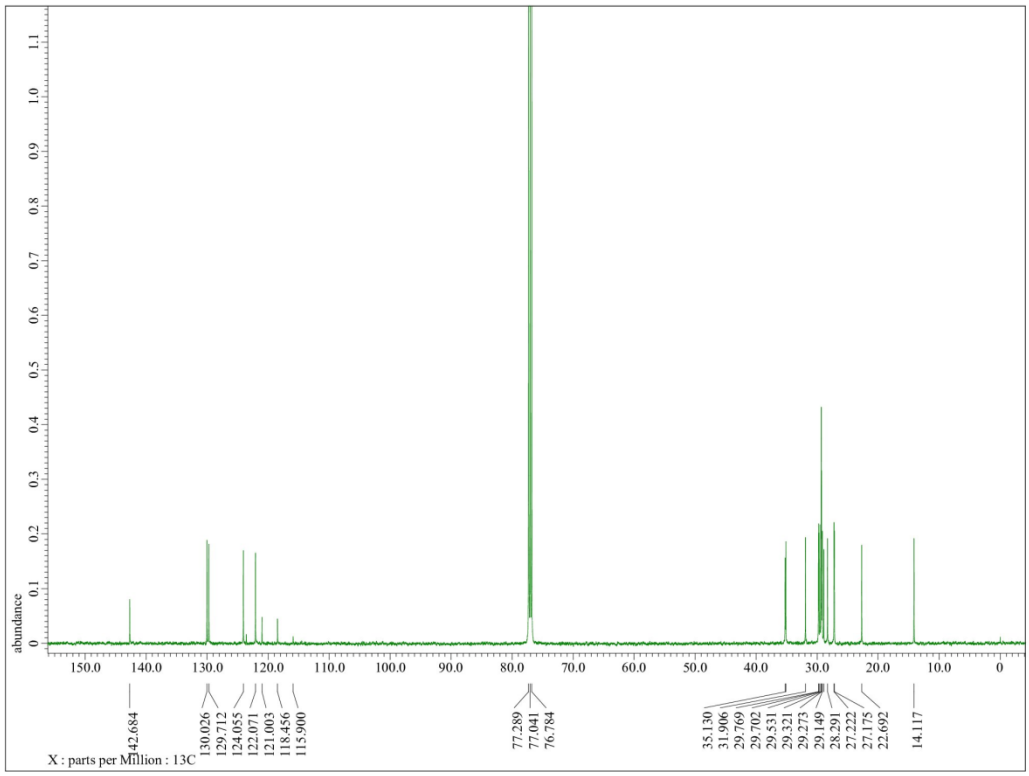

LIL 3
abundance
X : parts per Million : 1H
7.415
7.411
7.407
7.293
7.287
7.266
5.356
5.345
5.339
5.337
5.327
3.831
3.195
3.185
3.180
3.171
3.165
2.176
2.028
2.014
2.002
1.988
1.664
1.649
1.302
1.278
1.273
0.893
0.880
0.866
-0.000

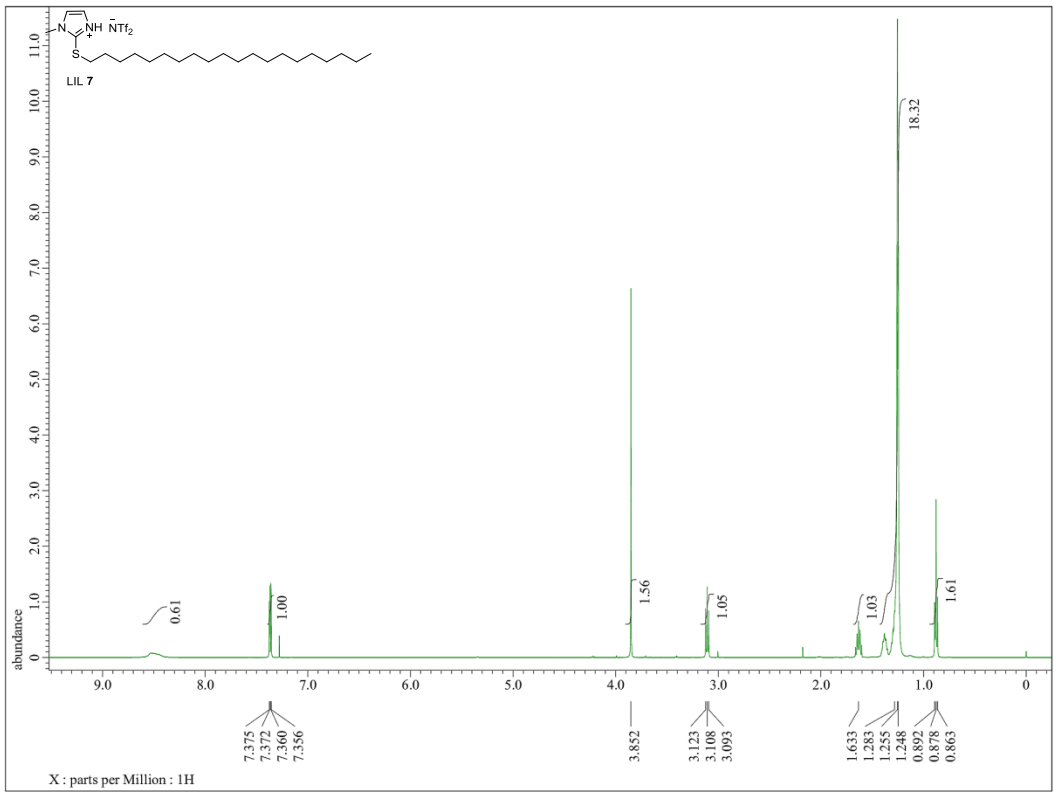

abundance
X : parts per Million : 13C
142.595
129.995
129.690
123.957
122.336
120.972
118.425
115.869
77.258
77.000
76.752
35.127
31.750
29.699
29.661
29.251
29.108
28.955
28.889
28.269
27.191
27.134
22.632
14.076

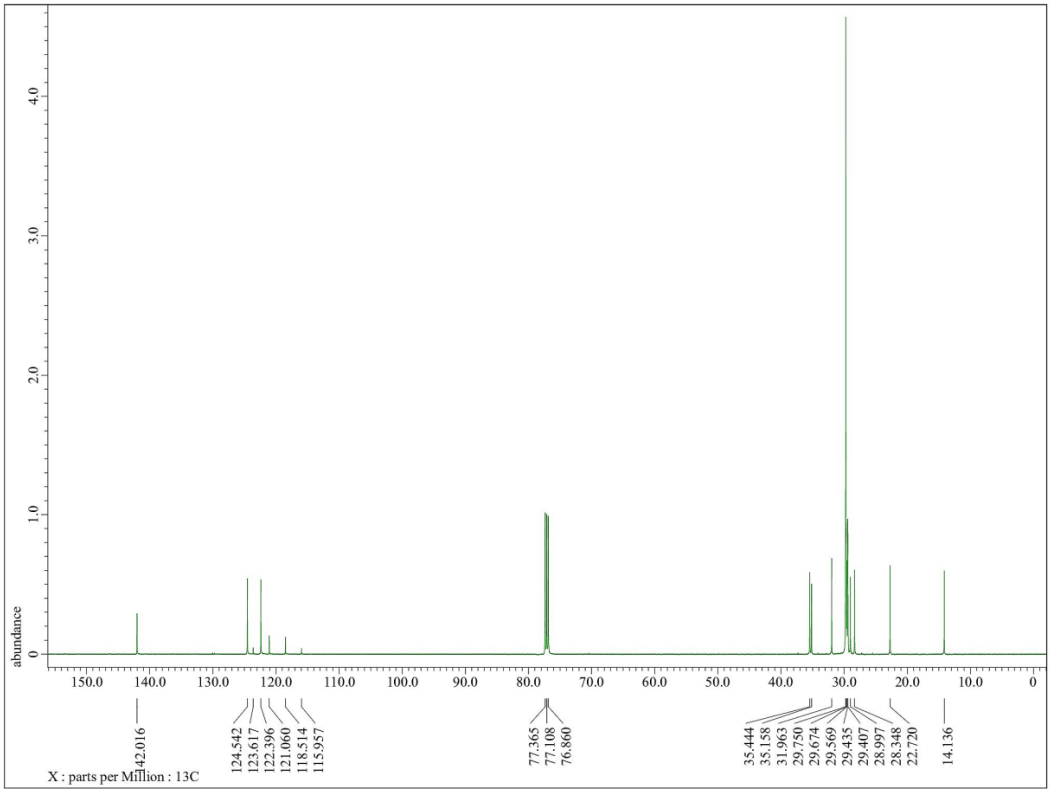

LIL 4
abundance
0.47
1.00
1.51
1.02
0.98
15.79
1.56
8.945
7.390
7.385
7.365
7.360
3.855
3.131
3.116
3.101
1.638
1.623
1.297
1.284
1.256
1.251
0.892
0.878
0.863
X : parts per Million : 1H

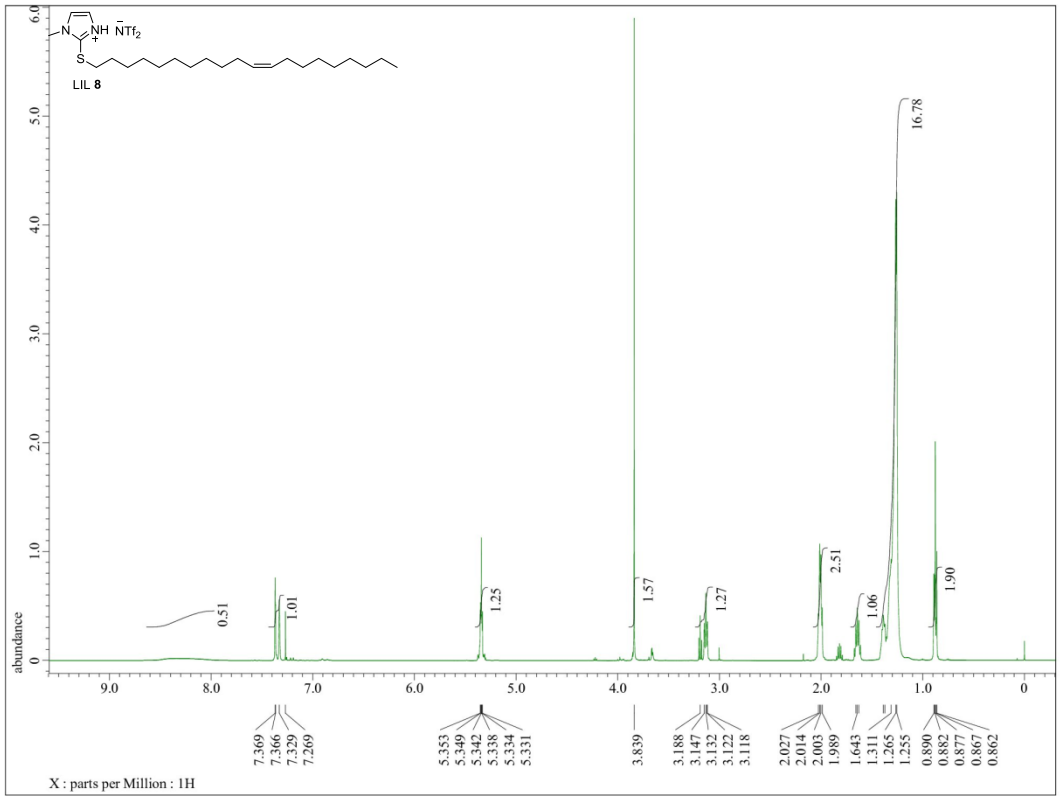

abundance
142.054
124.609
123.617
122.176
121.060
118.514
115.957
77.384
77.136
76.879
35.425
35.215
31.972
29.750
29.674
29.569
29.435
28.997
28.338
22.730
14.136
X : parts per Million : 13C

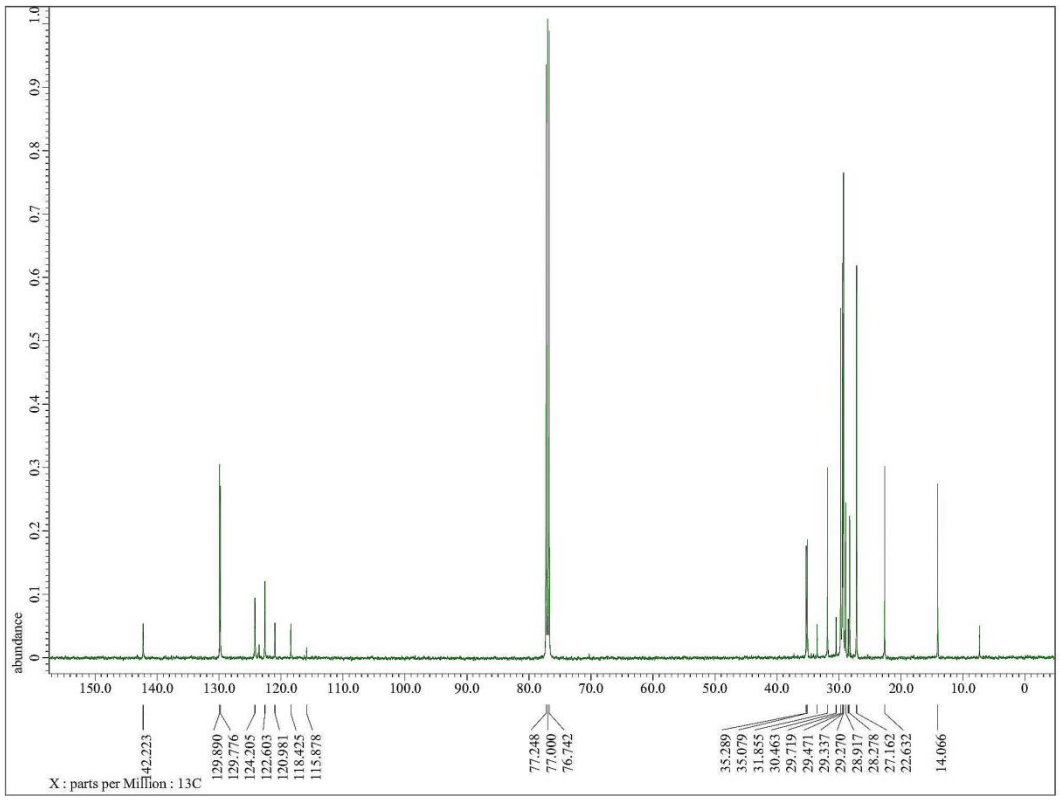

LIL 5
abundance
X : parts per Million : 1H


abundance
X : parts per Million : 13C


LIL 7
abundance
X : parts per Million : 1H

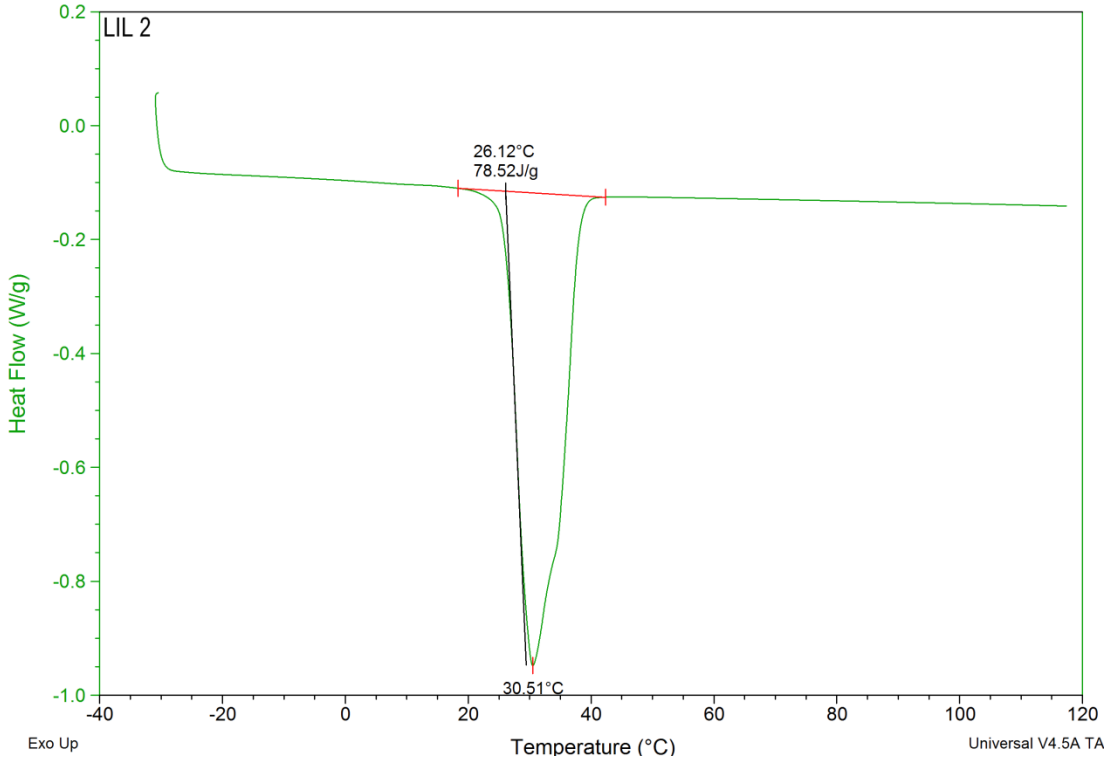

abundance
X : parts per Million : 13C

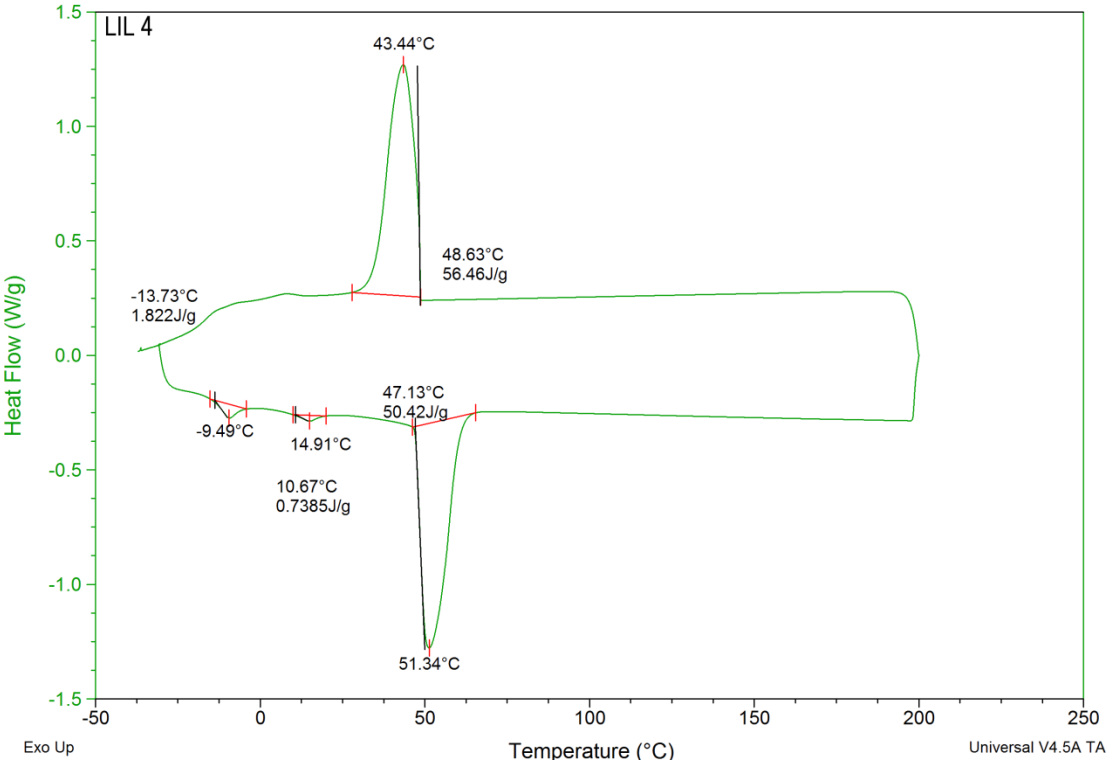

LIL 8
abundance
X : parts per Million : 1H
0.51
1.01
1.25
1.57
1.27
2.51
1.06
16.78
1.90
7.369
7.366
7.329
7.269
5.353
5.349
5.342
5.338
5.334
5.331
3.839
3.188
3.147
3.132
3.122
3.118
2.027
2.014
2.003
1.989
1.643
1.311
1.265
1.255
0.890
0.882
0.877
0.867
0.862

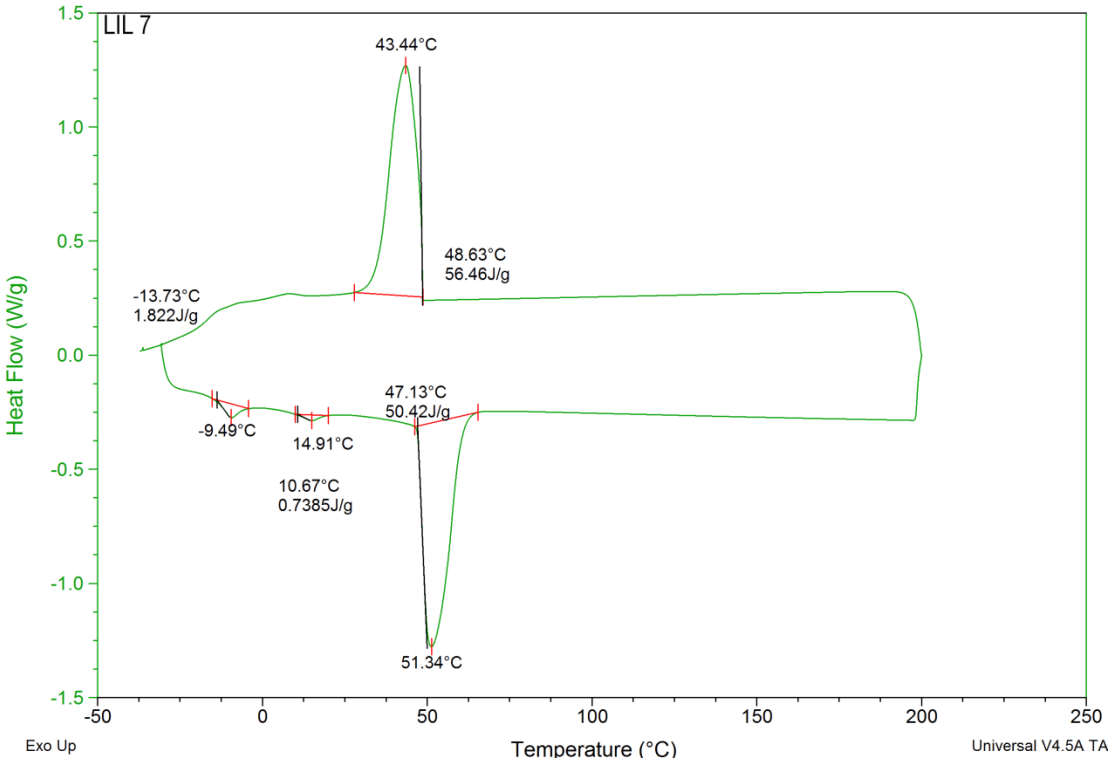

abundance
X : parts per Million : 13C
142.223
129.890
129.776
124.205
122.603
120.981
118.425
115.878
77.248
77.000
76.742
35.289
35.079
31.855
30.463
29.719
29.471
29.337
29.270
28.917
28.278
27.162
22.632
14.066

III. Differential Scanning Calorimetry (DSC) thermograms

DSC curves were obtained using a TA Instruments Q20 DSC with cooling/heating rates of 5°C/min. Sample sizes ranged from 5-20 mg. As is routine in DSC experiments on lipids, thermal pre-treatment of the samples were helpful in obtaining clean phase transitions.

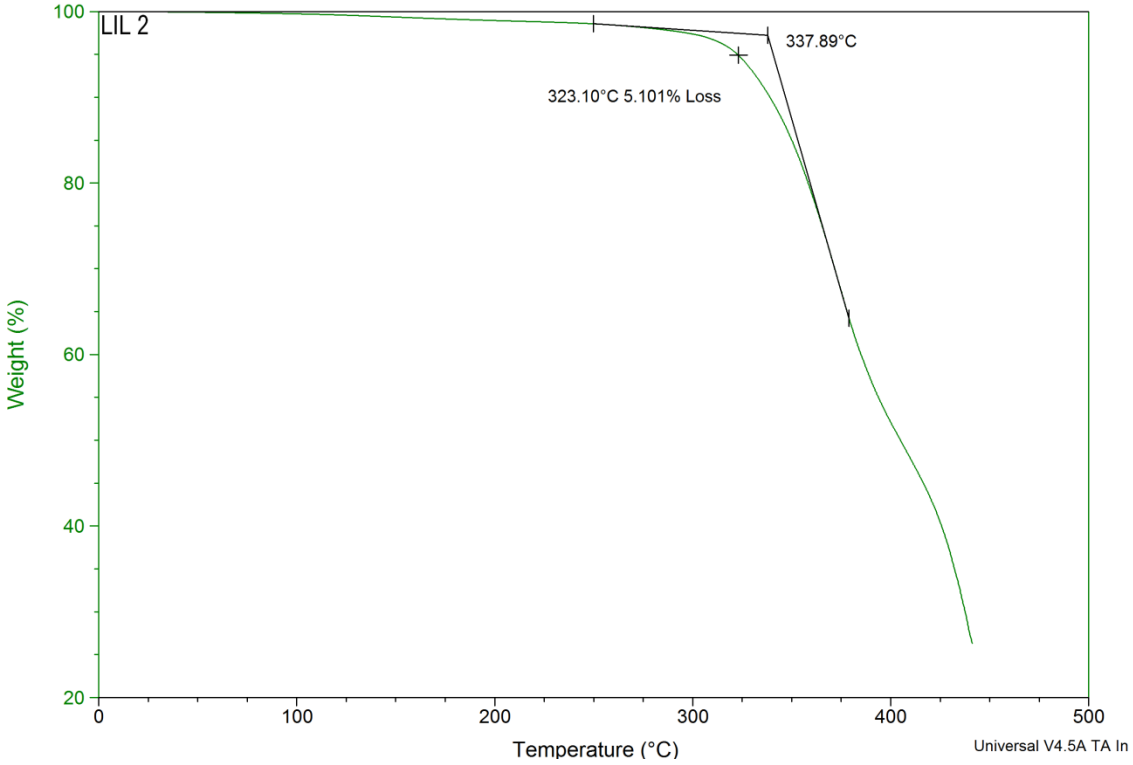


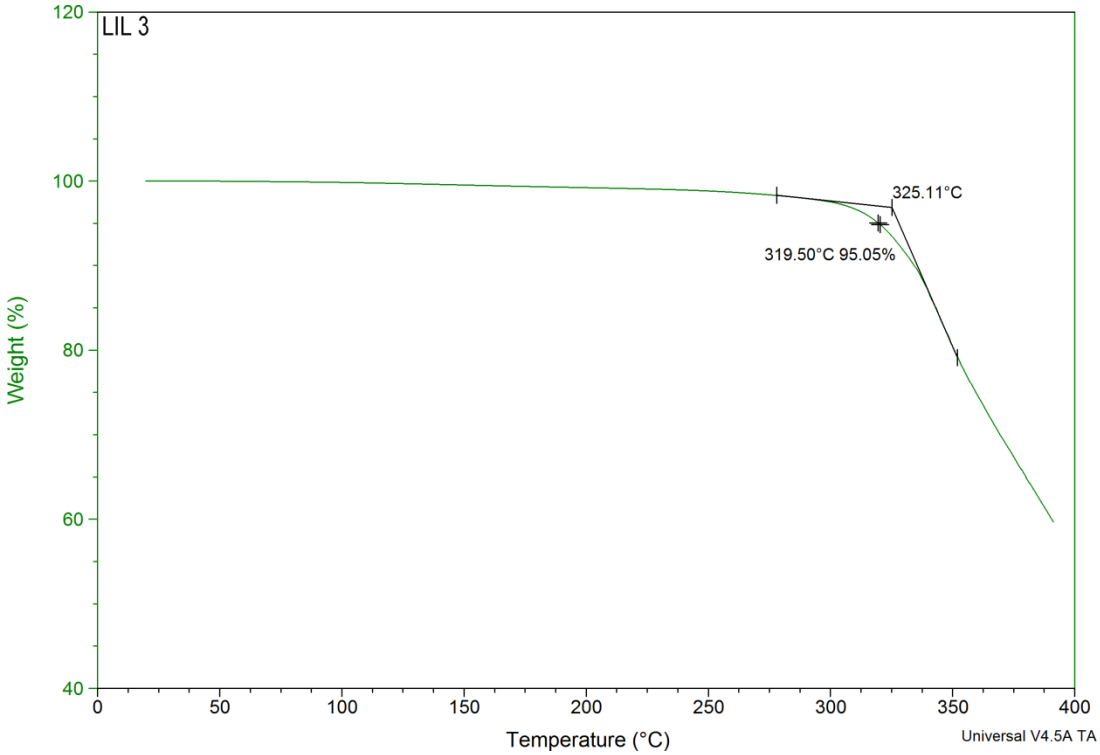


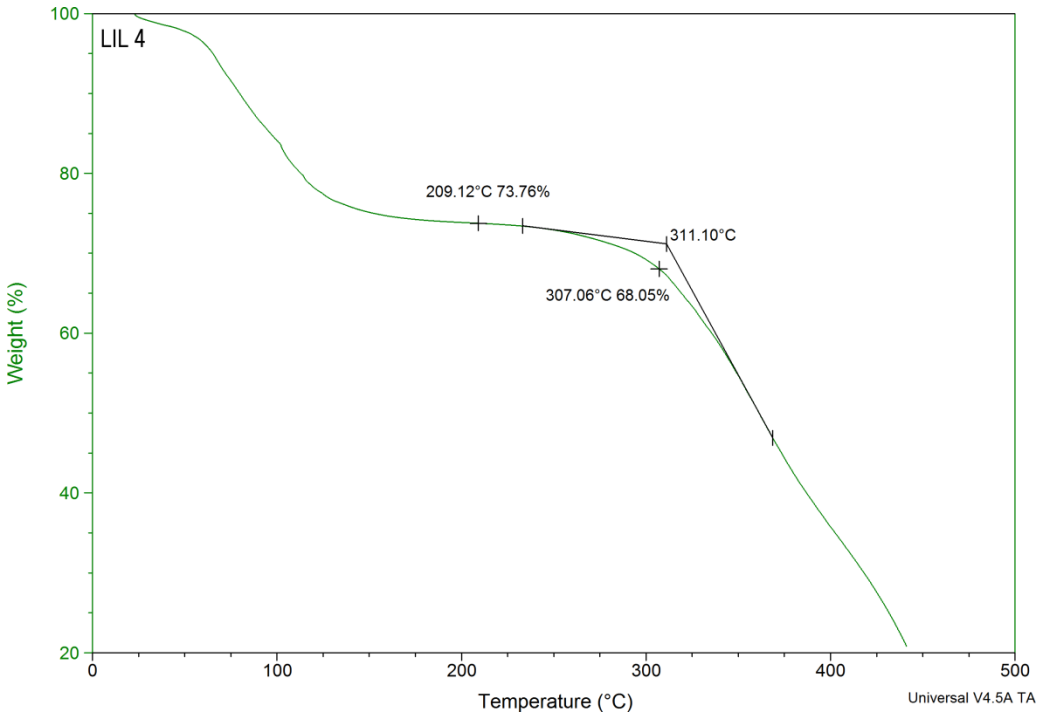

LIL 7
43.44°C
48.63°C
56.46J/g
-13.73°C
1.822J/g
47.13°C
50.42J/g
-9.49°C
14.91°C
10.67°C
0.7385J/g
51.34°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-50
0
50
100
150
200
250

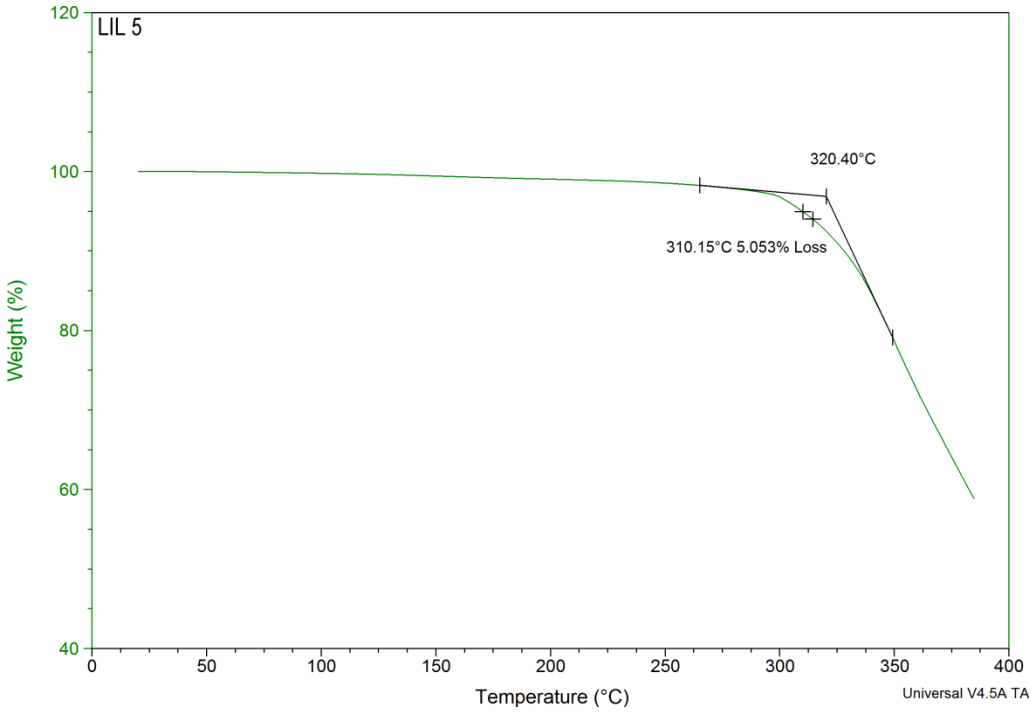
IV. Thermal Gravimetric Analysis (TGA) thermograms

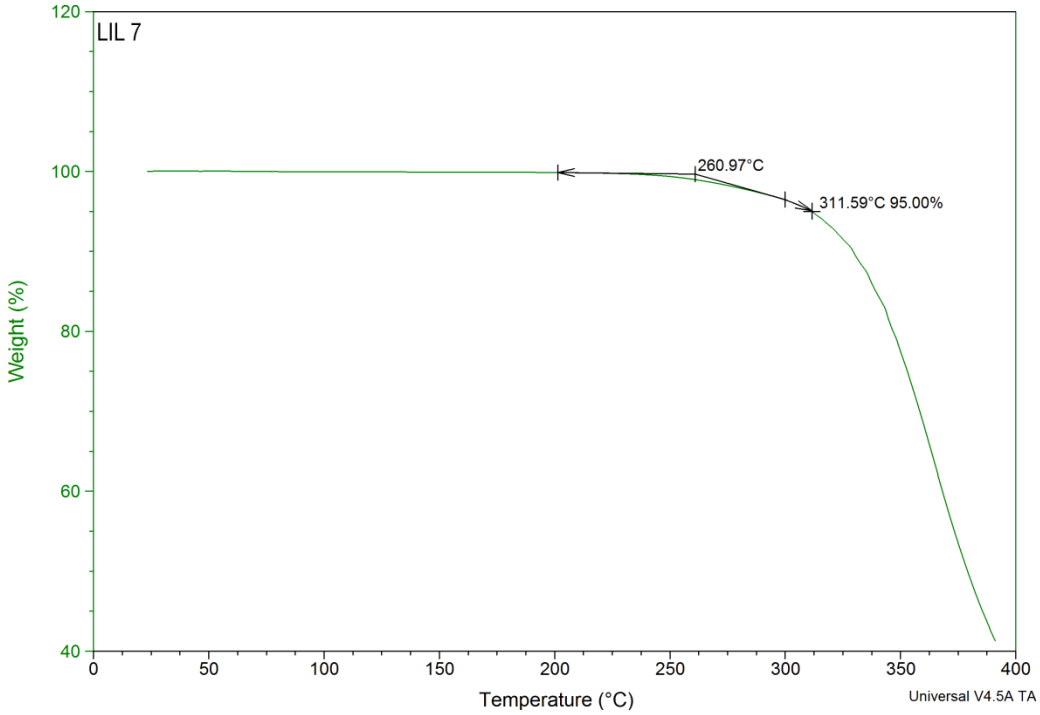
The TGA study was performed, by heating the sample (5 ºC/min) from room temperature to 400 ºC.

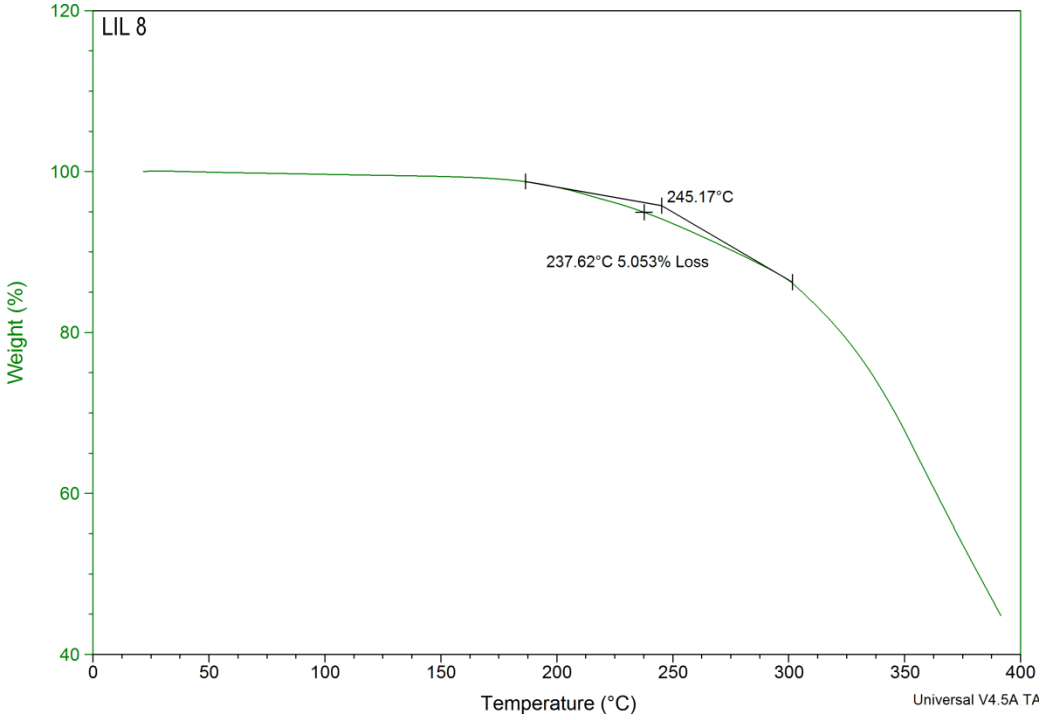





LIL 4
209.12°C 73.76%
311.10°C
307.06°C 68.05%
Weight (%)
Temperature (°C)
Universal V4.5A TA


LIL 5
320.40°C
310.15°C 5.053% Loss
Weight (%)
Temperature (°C)
Universal V4.5A TA


LIL 7
260.97°C
311.59°C 95.00%
Weight (%)
Temperature (°C)
Universal V4.5A TA


LIL 8
245.17°C
237.62°C 5.053% Loss
Weight (%)
Temperature (°C)
Universal V4.5A TA