Supplementary Material – xyz coordinates for

“Understanding the Chemistry of Cationized Triacylglycerols Using Electrospray Ionization Mass Spectrometry and Density Functional Theory Computations”,

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Table 2S. Computed atom coordinates for structures in Figures and Schemes from Figure 2

1A -927.81395 H, 0 kJ mol⁻¹

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1B -927.809786 H, +11 kJ mol⁻¹

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Figure 3

1H -927.755831 H, $E = + 153 \text{ kJ mol}^{-1}$

2A -1869.451701 H
Scheme 1d

1A' -927.811645 H, + 6 kJ mol⁻¹
6 -0.055263000 0.595192000 1.697028000
6 -0.293917000 -0.915165000 1.708206000
1 0.784368000 0.823010000 2.059521000
1 -0.951967000 1.097803000 2.066947000
1 -0.369264000 -1.170502000 2.769014000
3 0.291490000 0.078143000 -1.586522000
8 0.284751000 1.045042000 0.375520000
8 -1.617759000 -1.287237000 1.228810000
6 -0.783210000 -1.821406000 1.053127000
1 0.505152000 -2.080089000 0.304254000
1 0.886293000 -2.734912000 1.641037000
8 2.092000000 2.118887000 1.049543000
6 -0.246488000 2.117077000 -0.275688000
8 -0.157953000 2.054598000 -1.492016000
1 -1.979173000 -1.278687000 -0.896842000
6 -1.264379000 -0.881088000 -0.980430000
6 2.609054000 -0.804282000 -0.126140000
1 1.959706000 -0.764338000 -1.164359000
6 4.062146000 -0.431015000 0.000481000
1 4.183333000 0.139714000 0.928730000

SP13 -927.693772 H, + 316 kJ mol⁻¹
6 -0.000476000 0.332346000 1.889540000
6 -0.202748000 -1.166444000 1.661982000
1 0.818932000 0.470164000 2.598394000
1 -0.914223000 0.772058000 2.298587000
1 -0.257055000 -1.583894000 2.671311000
3 0.271008000 0.241175000 -1.855753000
8 0.381672000 1.020079000 0.682260000
6 -1.526375000 -1.500628000 1.151287000
6 0.888723000 -0.832730000 0.846966000
1 0.581382000 -2.081173000 -0.167365000
1 1.059713000 -2.903382000 1.333070000
6 2.167091000 -1.268355800 0.887724000
6 -0.378407000 1.968929000 0.149909000
-0.198042000 2.104126000 -1.151674000
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6 4.046105000 -0.229731000 -0.103420000
1 4.141905000 0.276264000 0.864841000

1A" -927.774872 H, + 103 kJ mol⁻¹
6 -0.086385000 0.451488000 1.695237000
6 -0.589383000 -0.992030000 1.670528000
1 0.748651000 0.516451000 2.400242000
1 -0.894393000 1.102074000 2.044398000
1 -0.682349000 -1.261516000 2.720911000
3 0.106847000 0.028927000 -1.427299000

Scheme 1d

-927.811645 H, + 6 kJ mol⁻¹

-927.774872 H, + 103 kJ mol⁻¹

-927.693772 H, + 316 kJ mol⁻¹
Cat31 and EtCOOLi separated + 207 kJ mol-1

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Scheme 4b

SP41 -927.666914 H, + 386 kJ mol-1

IN41 -927.7030 H, + 291 kJ mol-1
and EtCOOH separated + 131 kJ mol⁻¹

and $-927.818899$ H, –13 kJ mol⁻¹

and $-927.716991$ H, +255 kJ mol⁻¹

and $-927.188899$ H, –13 kJ mol⁻¹
sn2H Li+ -275.664892 kJ mol⁻¹

3-methyl-5-pentenolactone, -383.759597 kJ mol⁻¹