# Supplementary file

## Sustainable Lipid Extraction: Green Solvents and Hydrotalcite as Alternatives to Conventional Methods for Measuring Fatty acids in Fat, oil and grease

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Table S1: Composition of synthetic FOG preparation

| Sources | Components | mg |
|---|---|---|
| Fatty acids | C10:0 | 60.00 |
| | C12:0 | 60.00 |
| | C14:0 | 60.00 |
| | C16:0 | 60.00 |
| | C18:0 | 60.00 |
| | C18:1n9c | 60.00 |
| Glycerides | Mono and diglycerides | 100.0 |
| | Triglycerides | 50.00 |
| Metal salts | NaCl | 100.0 |
| | KOH | 100.0 |
| | $CaCO_3$ | 100.0 |
| | $MgCl_2$ (anhydrous) | 100.0 |
| Cooked oil | C12:0 | 1.86 |
| | C14:0 | 2.34 |
| | C15:0 | 3.50 |
| | C16:0 | 40.0 |
| | C16:1 | 3.00 |
| | C17:0 | 3.16 |
| | C17:1 | 1.76 |
| | C18:0 | 30.0 |
| | C18:1n9t | 3.34 |
| | C18:1n9c | 400.0 |
| | C18:2n6c | 178.71 |
| | C18:3n6 | 1.05 |
| | C18:3n3 | 90.92 |
| | C20:0 | 1.40 |
| | C20:1n9 | 9.09 |
| | C22:0 | 15.25 |
| | C23:0 | 3.12 |
| | C24:0 | 0.65 |
| | C24:1n9 | 1.72 |
| Others | Dishwashing detergent | 50.0 |
| | Water (mL) | 500.0 |

Table S2: Surface charge and mapping calculation of d-limonene from computational modelling

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.00913 | -1.17209 | -0.00016 |
| C | 1.40364 | -1.21464 | -0.0005 |
| C | 2.13769 | -0.02872 | 0.00001 |
| C | 1.47722 | 1.2005 | -0.00033 |
| C | 0.08304 | 1.24296 | -0.00046 |
| C | -0.65108 | 0.05659 | 0.00002 |

| | | | |
|---|---|---|---|
| H | -0.56941 | -2.1072 | -0.00012 |
| H | 1.92385 | -2.18347 | 0.00013 |
| H | 2.0562 | 2.13542 | 0.00002 |
| H | -0.43778 | 2.21158 | -0.00074 |
| C | 3.67698 | -0.07558 | 0.00052 |
| H | 4.0342 | -0.07348 | -1.00809 |
| H | 4.05969 | 0.78027 | 0.51622 |
| H | 4.00654 | -0.96608 | 0.49377 |
| C | -2.19036 | 0.10382 | 0.00015 |
| C | -2.83638 | 1.29513 | 0.00032 |
| H | -2.28044 | 2.20937 | 0.00037 |
| H | -3.90605 | 1.32159 | 0.00041 |
| C | -2.9983 | -1.20723 | 0.00008 |
| H | -2.75605 | -1.77542 | -0.87363 |
| H | -2.75597 | -1.77556 | 0.87367 |
| H | -4.04424 | -0.98161 | 0.00015 |

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.009132 | -1.172088 | -0.000160 |
| 2 | 6 | 0 | 1.403643 | -1.214637 | -0.000505 |
| 3 | 6 | 0 | 2.137691 | -0.028721 | 0.000010 |
| 4 | 6 | 0 | 1.477218 | 1.200503 | -0.000328 |
| 5 | 6 | 0 | 0.083039 | 1.242964 | -0.000462 |
| 6 | 6 | 0 | -0.651085 | 0.056595 | 0.000019 |
| 7 | 1 | 0 | -0.569414 | -2.107196 | -0.000116 |
| 8 | 1 | 0 | 1.923846 | -2.183466 | 0.000132 |
| 9 | 1 | 0 | 2.056200 | 2.135423 | 0.000019 |
| 10 | 1 | 0 | -0.437785 | 2.211580 | -0.000737 |
| 11 | 6 | 0 | 3.676977 | -0.075576 | 0.000517 |
| 12 | 1 | 0 | 4.034205 | -0.073480 | -1.008088 |
| 13 | 1 | 0 | 4.059691 | 0.780273 | 0.516223 |
| 14 | 1 | 0 | 4.006541 | -0.966077 | 0.493768 |
| 15 | 6 | 0 | -2.190361 | 0.103818 | 0.000148 |
| 16 | 6 | 0 | -2.836377 | 1.295132 | 0.000321 |
| 17 | 1 | 0 | -2.280439 | 2.209371 | 0.000369 |
| 18 | 1 | 0 | -3.906050 | 1.321588 | 0.000410 |
| 19 | 6 | 0 | -2.998300 | -1.207226 | 0.000079 |
| 20 | 1 | 0 | -2.756049 | -1.775423 | -0.873629 |
| 21 | 1 | 0 | -2.755967 | -1.775563 | 0.873674 |
| 22 | 1 | 0 | -4.044243 | -0.981610 | 0.000146 |

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Distance matrix (angstroms):

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 2 | C | 1.395160 | 0.000000 | | | |
| 3 | C | 2.416205 | 1.394712 | 0.000000 | | |
| 4 | C | 2.790065 | 2.416260 | 1.395427 | 0.000000 | |
| 5 | C | 2.416183 | 2.789946 | 2.416356 | 1.394825 | 0.000000 |
| 6 | C | 1.394829 | 2.416183 | 2.790080 | 2.416236 | 1.395138 |
| 7 | H | 1.099610 | 2.165553 | 3.412986 | 3.889675 | 3.413102 |
| 8 | H | 2.165414 | 1.099655 | 2.165330 | 3.413316 | 3.889601 |
| 9 | H | 3.889745 | 3.413024 | 2.165678 | 1.099680 | 2.165606 |
| 10 | H | 3.413055 | 3.889707 | 3.413506 | 2.165528 | 1.099761 |
| 11 | C | 3.828241 | 2.542737 | 1.540000 | 2.543093 | 3.828178 |
| 12 | H | 4.292327 | 3.039296 | 2.148263 | 3.029323 | 4.284863 |
| 13 | H | 4.526079 | 3.361735 | 2.148263 | 2.666943 | 4.036682 |
| 14 | H | 4.033073 | 2.661046 | 2.148263 | 3.366849 | 4.529679 |
| 15 | C | 2.542775 | 3.828209 | 4.330080 | 3.828035 | 2.542833 |
| 16 | C | 3.766178 | 4.927141 | 5.147226 | 4.314633 | 2.919882 |
| 17 | H | 4.083675 | 5.029542 | 4.952668 | 3.890732 | 2.553423 |
| 18 | H | 4.641882 | 5.884325 | 6.192749 | 5.384629 | 3.989864 |
| 19 | C | 3.007637 | 4.401949 | 5.269466 | 5.082068 | 3.936760 |
| 20 | H | 2.961957 | 4.287174 | 5.269051 | 5.247793 | 4.234796 |
| 21 | H | 2.962017 | 4.287329 | 5.269026 | 5.247924 | 4.235042 |
| 22 | H | 4.057848 | 5.452868 | 6.254942 | 5.937015 | 4.688623 |

| | | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|
| 6 | C | 0.000000 | | | | |
| 7 | H | 2.165331 | 0.000000 | | | |
| 8 | H | 3.412938 | 2.494427 | 0.000000 | | |
| 9 | H | 3.413344 | 4.989355 | 4.320917 | 0.000000 | |
| 10 | H | 2.165516 | 4.320781 | 4.989362 | 2.495147 | 0.000000 |
| 11 | C | 4.330080 | 4.707369 | 2.741654 | 2.741430 | 4.707691 |
| 12 | H | 4.794282 | 5.132769 | 3.149947 | 3.131778 | 5.122006 |
| 13 | H | 4.793911 | 5.480209 | 3.689435 | 2.473231 | 4.747965 |
| 14 | H | 4.794072 | 4.741882 | 2.462383 | 3.696880 | 5.485806 |
| 15 | C | 1.540000 | 2.741541 | 4.707267 | 4.707515 | 2.741201 |
| 16 | C | 2.511867 | 4.088392 | 5.895793 | 4.964212 | 2.567708 |
| 17 | H | 2.699859 | 4.643312 | 6.080545 | 4.337269 | 1.842656 |
| 18 | H | 3.492135 | 4.784317 | 6.802433 | 6.017537 | 3.580636 |
| 19 | C | 2.665832 | 2.590257 | 5.018024 | 6.059808 | 4.271354 |
| 20 | H | 2.924110 | 2.377913 | 4.778219 | 6.262245 | 4.693877 |
| 21 | H | 2.924142 | 2.377920 | 4.778087 | 6.262271 | 4.694239 |
| 22 | H | 3.548435 | 3.652585 | 6.087902 | 6.850642 | 4.816950 |

| | | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|
| 11 | C | 0.000000 | | | | |
| 12 | H | 1.070000 | 0.000000 | | | |
| 13 | H | 1.070000 | 1.747303 | 0.000000 | | |
| 14 | H | 1.070000 | 1.747303 | 1.747303 | 0.000000 | |
| 15 | C | 5.870080 | 6.308184 | 6.307699 | 6.307925 | 0.000000 |
| 16 | C | 6.656022 | 7.077774 | 6.934478 | 7.223717 | 1.355200 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 17 | H | 6.380579 | 6.789928 | 6.519637 | 7.060667 | 2.107479 |
| 18 | H | 7.710666 | 8.124711 | 8.000757 | 8.251418 | 2.103938 |
| 19 | C | 6.770521 | 7.194297 | 7.350632 | 7.026356 | 1.540000 |
| 20 | H | 6.710994 | 7.001588 | 7.410639 | 6.946757 | 2.148263 |
| 21 | H | 6.710823 | 7.248763 | 7.287885 | 6.821372 | 2.148263 |
| 22 | H | 7.774197 | 8.191615 | 8.309291 | 8.065918 | 2.148263 |

| | | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|
| 16 | C | 0.000000 | | | | |
| 17 | H | 1.070000 | 0.000000 | | | |
| 18 | H | 1.070000 | 1.852234 | 0.000000 | | |
| 19 | C | 2.507591 | 3.491197 | 2.686802 | 0.000000 | |
| 20 | H | 3.193516 | 4.107147 | 3.417297 | 1.070000 | 0.000000 |
| 21 | H | 3.193490 | 4.107127 | 3.417254 | 1.070000 | 1.747303 |
| 22 | H | 2.577304 | 3.646007 | 2.307340 | 1.070000 | 1.747303 |

| | | 21 | 22 |
|---|---|---|---|
| 21 | H | 0.000000 | |
| 22 | H | 1.747303 | 0.000000 |

Stoichiometry C10H12
Framework group C1[X(C10H12)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Table S3: Surface charge and mapping calculation of *n*-hexane from computational modelling

n-hexane
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Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.56308 | -1.85313 | 0. |
| C | 0.21242 | -3.1374 | 0. |
| H | -1.21444 | -1.78494 | 0.90505 |
| H | -1.21444 | -1.78494 | -0.90505 |
| H | 0.86382 | -3.20602 | -0.9049 |
| H | 0.86382 | -3.20602 | 0.9049 |
| H | -0.47794 | -4.01574 | 0. |
| C | 0.38821 | -0.64208 | 0. |
| C | -0.38821 | 0.64208 | 0. |
| H | 1.03971 | -0.71038 | -0.90495 |
| H | 1.03971 | -0.71038 | 0.90495 |
| H | -1.03971 | 0.71038 | -0.90495 |
| H | -1.03971 | 0.71038 | 0.90495 |
| C | 0.56308 | 1.85313 | 0. |
| C | -0.21242 | 3.1374 | 0. |
| H | 1.21444 | 1.78494 | -0.90505 |

| | | | |
|---|---|---|---|
| H | 1.21444 | 1.78494 | 0.90505 |
| H | 0.47794 | 4.01574 | 0. |
| H | -0.86382 | 3.20602 | -0.9049 |
| H | -0.86382 | 3.20602 | 0.9049 |

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.563078 | -1.853130 | 0.000000 |
| 2 | 6 | 0 | 0.212416 | -3.137404 | 0.000000 |
| 3 | 1 | 0 | -1.214437 | -1.784937 | 0.905047 |
| 4 | 1 | 0 | -1.214437 | -1.784937 | -0.905047 |
| 5 | 1 | 0 | 0.863822 | -3.206020 | -0.904895 |
| 6 | 1 | 0 | 0.863822 | -3.206020 | 0.904895 |
| 7 | 1 | 0 | -0.477943 | -4.015743 | 0.000000 |
| 8 | 6 | 0 | 0.388214 | -0.642080 | 0.000000 |
| 9 | 6 | 0 | -0.388214 | 0.642080 | 0.000000 |
| 10 | 1 | 0 | 1.039708 | -0.710376 | -0.904953 |
| 11 | 1 | 0 | 1.039708 | -0.710376 | 0.904953 |
| 12 | 1 | 0 | -1.039708 | 0.710376 | -0.904953 |
| 13 | 1 | 0 | -1.039708 | 0.710376 | 0.904953 |
| 14 | 6 | 0 | 0.563078 | 1.853130 | 0.000000 |
| 15 | 6 | 0 | -0.212416 | 3.137404 | 0.000000 |
| 16 | 1 | 0 | 1.214437 | 1.784937 | -0.905047 |
| 17 | 1 | 0 | 1.214437 | 1.784937 | 0.905047 |
| 18 | 1 | 0 | 0.477943 | 4.015743 | 0.000000 |
| 19 | 1 | 0 | -0.863822 | 3.206020 | -0.904895 |
| 20 | 1 | 0 | -0.863822 | 3.206020 | 0.904895 |

Distance matrix (angstroms):

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.500250 | 0.000000 | | | |
| 3 | H | 1.117152 | 2.164298 | 0.000000 | | |
| 4 | H | 1.117152 | 2.164298 | 1.810094 | 0.000000 | |
| 5 | H | 2.164530 | 1.117083 | 3.100730 | 2.517665 | 0.000000 |
| 6 | H | 2.164530 | 1.117083 | 2.517665 | 3.100730 | 1.809791 |
| 7 | H | 2.164288 | 1.117173 | 2.517544 | 2.517544 | 1.809646 |
| 8 | C | 1.540000 | 2.501509 | 2.166500 | 2.166500 | 2.760223 |
| 9 | C | 2.501330 | 3.826912 | 2.718854 | 2.718854 | 4.146601 |
| 10 | H | 2.166507 | 2.719158 | 3.084145 | 2.497169 | 2.501834 |
| 11 | H | 2.166507 | 2.719158 | 2.497169 | 3.084145 | 3.087835 |
| 12 | H | 2.760015 | 4.146344 | 3.087591 | 2.501423 | 4.354490 |
| 13 | H | 2.760015 | 4.146344 | 2.501423 | 3.087591 | 4.715627 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 14 | C | 3.873577 | 5.002839 | 4.149000 | 4.149000 | 5.148231 |
| 15 | C | 5.002839 | 6.289174 | 5.104175 | 5.104175 | 6.497396 |
| 16 | H | 4.149000 | 5.104175 | 4.681866 | 4.317804 | 5.003257 |
| 17 | H | 4.149000 | 5.104175 | 4.317804 | 4.681866 | 5.320571 |
| 18 | H | 5.960487 | 7.158074 | 6.109922 | 6.109922 | 7.288457 |
| 19 | H | 5.148231 | 6.497396 | 5.320571 | 5.003257 | 6.640709 |
| 20 | H | 5.148231 | 6.497396 | 5.003257 | 5.320571 | 6.882903 |

| | | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|
| 6 | H | 0.000000 | | | | |
| 7 | H | 1.809646 | 0.000000 | | | |
| 8 | C | 2.760223 | 3.483078 | 0.000000 | | |
| 9 | C | 4.146601 | 4.658687 | 1.500635 | 0.000000 | |
| 10 | H | 3.087835 | 3.748020 | 1.117162 | 2.164957 | 0.000000 |
| 11 | H | 2.501834 | 3.748020 | 1.117162 | 2.164957 | 1.809907 |
| 12 | H | 4.715627 | 4.844659 | 2.164957 | 1.117162 | 2.518434 |
| 13 | H | 4.354490 | 4.844659 | 2.164957 | 1.117162 | 3.101334 |
| 14 | C | 5.148231 | 5.960487 | 2.501330 | 1.540000 | 2.760015 |
| 15 | C | 6.497396 | 7.158074 | 3.826912 | 2.501509 | 4.146344 |
| 16 | H | 5.320571 | 6.109922 | 2.718854 | 2.166500 | 2.501423 |
| 17 | H | 5.003257 | 6.109922 | 2.718854 | 2.166500 | 3.087591 |
| 18 | H | 7.288457 | 8.088170 | 4.658687 | 3.483078 | 4.844659 |
| 19 | H | 6.882903 | 7.288457 | 4.146601 | 2.760223 | 4.354490 |
| 20 | H | 6.640709 | 7.288457 | 4.146601 | 2.760223 | 4.715627 |

| | | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|
| 11 | H | 0.000000 | | | | |
| 12 | H | 3.101334 | 0.000000 | | | |
| 13 | H | 2.518434 | 1.809907 | 0.000000 | | |
| 14 | C | 2.760015 | 2.166507 | 2.166507 | 0.000000 | |
| 15 | C | 4.146344 | 2.719158 | 2.719158 | 1.500250 | 0.000000 |
| 16 | H | 3.087591 | 2.497169 | 3.084145 | 1.117152 | 2.164298 |
| 17 | H | 2.501423 | 3.084145 | 2.497169 | 1.117152 | 2.164298 |
| 18 | H | 4.844659 | 3.748020 | 3.748020 | 2.164288 | 1.117173 |
| 19 | H | 4.715627 | 2.501834 | 3.087835 | 2.164530 | 1.117083 |
| 20 | H | 4.354490 | 3.087835 | 2.501834 | 2.164530 | 1.117083 |

| | | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|
| 16 | H | 0.000000 | | | | |
| 17 | H | 1.810094 | 0.000000 | | | |
| 18 | H | 2.517544 | 2.517544 | 0.000000 | | |
| 19 | H | 2.517665 | 3.100730 | 1.809646 | 0.000000 | |
| 20 | H | 3.100730 | 2.517665 | 1.809646 | 1.809791 | 0.000000 |

Stoichiometry C6H14
Framework group C2H[SGH(C6H2),X(H12)]
Deg. of freedom 16
Full point group C2H NOp 4
Largest Abelian subgroup C2H NOp 4
Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.432151 | 1.887961 | 0.000000 |
| 2 | 6 | 0 | -0.431228 | 3.114879 | 0.000000 |
| 3 | 1 | 0 | 1.086683 | 1.865470 | 0.905047 |
| 4 | 1 | 0 | 1.086683 | 1.865470 | -0.905047 |
| 5 | 1 | 0 | -1.085837 | 3.137788 | -0.904895 |
| 6 | 1 | 0 | -1.085837 | 3.137788 | 0.904895 |
| 7 | 1 | 0 | 0.196038 | 4.039331 | 0.000000 |
| 8 | 6 | 0 | -0.432151 | 0.613369 | 0.000000 |
| 9 | 6 | 0 | 0.432151 | -0.613369 | 0.000000 |
| 10 | 1 | 0 | -1.086826 | 0.635954 | -0.904953 |
| 11 | 1 | 0 | -1.086826 | 0.635954 | 0.904953 |
| 12 | 1 | 0 | 1.086826 | -0.635954 | -0.904953 |
| 13 | 1 | 0 | 1.086826 | -0.635954 | 0.904953 |
| 14 | 6 | 0 | -0.432151 | -1.887961 | 0.000000 |
| 15 | 6 | 0 | 0.431228 | -3.114879 | 0.000000 |
| 16 | 1 | 0 | -1.086683 | -1.865470 | -0.905047 |
| 17 | 1 | 0 | -1.086683 | -1.865470 | 0.905047 |
| 18 | 1 | 0 | -0.196038 | -4.039331 | 0.000000 |
| 19 | 1 | 0 | 1.085837 | -3.137788 | -0.904895 |
| 20 | 1 | 0 | 1.085837 | -3.137788 | 0.904895 |

Rotational constants (GHZ): 14.0462312 1.1827785 1.1396477

Table S4: Surface charge and mapping calculation of MeTHF from computational modelling MeTHF

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Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.46122 | 0.27254 | 0. |
| C | 0.91837 | 0.27254 | 0. |
| C | 1.3331 | 1.6599 | 0. |
| C | 0.17903 | 2.416 | -0.00009 |
| O | -0.94047 | 1.58321 | -0.00022 |
| H | -1.23486 | -0.48867 | -0.00001 |
| H | 1.58288 | -0.58616 | 0.00011 |
| H | 2.35969 | 2.0134 | 0. |
| C | -0.14653 | 3.9212 | -0.00016 |
| H | -0.71479 | 4.16316 | -0.87391 |
| H | -0.71507 | 4.16318 | 0.8734 |
| H | 0.76408 | 4.48307 | -0.00002 |

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.461216 | 0.272537 | 0.000000 |
| 2 | 6 | 0 | 0.918366 | 0.272537 | 0.000000 |
| 3 | 6 | 0 | 1.333100 | 1.659904 | 0.000000 |
| 4 | 6 | 0 | 0.179034 | 2.416003 | -0.000089 |
| 5 | 8 | 0 | -0.940468 | 1.583214 | -0.000222 |
| 6 | 1 | 0 | -1.234862 | -0.488668 | -0.000011 |
| 7 | 1 | 0 | 1.582884 | -0.586159 | 0.000105 |
| 8 | 1 | 0 | 2.359687 | 2.013402 | -0.000004 |
| 9 | 6 | 0 | -0.146527 | 3.921197 | -0.000160 |
| 10 | 1 | 0 | -0.714787 | 4.163160 | -0.873908 |
| 11 | 1 | 0 | -0.715074 | 4.163180 | 0.873395 |
| 12 | 1 | 0 | 0.764077 | 4.483068 | -0.000017 |

Distance matrix (angstroms):

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.379582 | 0.000000 | | | |
| 3 | C | 2.268118 | 1.448030 | 0.000000 | | |
| 4 | C | 2.237044 | 2.267390 | 1.379693 | 0.000000 | |
| 5 | O | 1.395549 | 2.274453 | 2.274861 | 1.395286 | 0.000000 |
| 6 | H | 1.085339 | 2.283818 | 3.348252 | 3.230513 | 2.092693 |
| 7 | H | 2.217139 | 1.085791 | 2.259910 | 3.314177 | 3.327685 |
| 8 | H | 3.314831 | 2.260092 | 1.085745 | 2.217507 | 3.328075 |
| 9 | C | 3.662206 | 3.800884 | 2.702359 | 1.540000 | 2.469111 |
| 10 | H | 3.995617 | 4.309043 | 3.350201 | 2.148263 | 2.733199 |
| 11 | H | 3.995543 | 4.309066 | 3.350258 | 2.148263 | 2.733173 |
| 12 | H | 4.385193 | 4.213357 | 2.879938 | 2.148263 | 3.363722 |

| | | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|
| 6 | H | 0.000000 | | | | |
| 7 | H | 2.819432 | 0.000000 | | | |
| 8 | H | 4.379627 | 2.713142 | 0.000000 | | |
| 9 | C | 4.542178 | 4.827745 | 3.149729 | 0.000000 | |
| 10 | H | 4.761688 | 5.347824 | 3.851955 | 1.070000 | 0.000000 |
| 11 | H | 4.761587 | 5.347847 | 3.852081 | 1.070000 | 1.747303 |
| 12 | H | 5.358537 | 5.134930 | 2.940276 | 1.070000 | 1.747303 |

| | | 11 | 12 |
|---|---|---|---|
| 11 | H | 0.000000 | |
| 12 | H | 1.747303 | 0.000000 |

Stoichiometry C5H6O
Framework group C1[X(C5H6O)]
Deg. of freedom 30

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.410594 | -0.761953 | -0.000084 |
| 2 | 6 | 0 | -1.577969 | 0.607439 | -0.000084 |
| 3 | 6 | 0 | -0.251167 | 1.187428 | -0.000084 |
| 4 | 6 | 0 | 0.639361 | 0.133619 | 0.000005 |
| 5 | 8 | 0 | -0.051455 | -1.078649 | 0.000138 |
| 6 | 1 | 0 | -2.072316 | -1.622235 | -0.000073 |
| 7 | 1 | 0 | -2.510943 | 1.162868 | -0.000189 |
| 8 | 1 | 0 | -0.024829 | 2.249319 | -0.000080 |
| 9 | 6 | 0 | 2.172935 | -0.006923 | 0.000076 |
| 10 | 1 | 0 | 2.482053 | -0.541629 | 0.873823 |
| 11 | 1 | 0 | 2.482108 | -0.541912 | -0.873480 |
| 12 | 1 | 0 | 2.620178 | 0.965123 | -0.000068 |

Rotational constants (GHZ): 8.5241532 3.4245667 2.4799556

Table S5: Surface charge and mapping calculation of p-cymene from computational modelling

p-cymene
---
Symbolic Z-matrix:
Charge = 0 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.05571 | 1.05571 | 0. |
| C | 0.33945 | 1.05571 | 0. |
| C | 1.03699 | 2.26346 | 0. |
| C | 0.33933 | 3.47197 | -0.0012 |
| C | -1.05549 | 3.47189 | -0.00168 |
| C | -1.75309 | 2.26369 | -0.00068 |
| H | 0.88896 | 0.1032 | 0.00132 |
| H | 2.13667 | 2.26354 | 0.00063 |
| H | -1.60561 | 4.42417 | -0.00263 |
| H | -2.8527 | 2.26387 | -0.00086 |
| C | 1.10984 | 4.80536 | -0.00128 |
| H | 1.30881 | 5.10238 | 1.00723 |
| H | 2.03426 | 4.68308 | -0.52606 |
| H | 0.5218 | 5.55706 | -0.48507 |
| C | -1.82565 | -0.278 | 0.00063 |
| C | -3.22704 | -0.2753 | 0.00063 |
| H | -3.58176 | 0.7342 | 0.0005 |

| | | | |
|---|---|---|---|
| H | -3.58468 | -0.77912 | -0.87296 |
| H | -3.58469 | -0.7789 | 0.87434 |
| C | -1.12249 | -1.49023 | 0.0012 |
| H | -0.50713 | -1.54603 | -0.87237 |
| H | -0.50729 | -1.54529 | 0.87493 |
| H | -1.81615 | -2.30492 | 0.00148 |

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.055711 | 1.055711 | 0.000000 |
| 2 | 6 | 0 | 0.339449 | 1.055711 | 0.000000 |
| 3 | 6 | 0 | 1.036987 | 2.263462 | 0.000000 |
| 4 | 6 | 0 | 0.339333 | 3.471971 | -0.001199 |
| 5 | 6 | 0 | -1.055492 | 3.471893 | -0.001678 |
| 6 | 6 | 0 | -1.753093 | 2.263687 | -0.000682 |
| 7 | 1 | 0 | 0.888957 | 0.103198 | 0.001315 |
| 8 | 1 | 0 | 2.136667 | 2.263542 | 0.000634 |
| 9 | 1 | 0 | -1.605614 | 4.424174 | -0.002631 |
| 10 | 1 | 0 | -2.852697 | 2.263870 | -0.000862 |
| 11 | 6 | 0 | 1.109837 | 4.805359 | -0.001282 |
| 12 | 1 | 0 | 1.308808 | 5.102378 | 1.007227 |
| 13 | 1 | 0 | 2.034256 | 4.683080 | -0.526064 |
| 14 | 1 | 0 | 0.521796 | 5.557065 | -0.485066 |
| 15 | 6 | 0 | -1.825647 | -0.278005 | 0.000630 |
| 16 | 6 | 0 | -3.227044 | -0.275297 | 0.000629 |
| 17 | 1 | 0 | -3.581761 | 0.734196 | 0.000501 |
| 18 | 1 | 0 | -3.584684 | -0.779121 | -0.872959 |
| 19 | 1 | 0 | -3.584685 | -0.778900 | 0.874344 |
| 20 | 6 | 0 | -1.122486 | -1.490229 | 0.001203 |
| 21 | 1 | 0 | -0.507133 | -1.546028 | -0.872369 |
| 22 | 1 | 0 | -0.507293 | -1.545295 | 0.874934 |
| 23 | 1 | 0 | -1.816152 | -2.304923 | 0.001482 |

Distance matrix (angstroms):

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.395160 | 0.000000 | | | |
| 3 | C | 2.416205 | 1.394712 | 0.000000 | | |
| 4 | C | 2.790065 | 2.416260 | 1.395427 | 0.000000 | |
| 5 | C | 2.416183 | 2.789946 | 2.416356 | 1.394825 | 0.000000 |
| 6 | C | 1.394829 | 2.416183 | 2.790080 | 2.416236 | 1.395138 |
| 7 | H | 2.165414 | 1.099655 | 2.165330 | 3.413316 | 3.889601 |
| 8 | H | 3.413229 | 2.165375 | 1.099680 | 2.165806 | 3.413209 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9 | H | 3.413055 | 3.889707 | 3.413506 | 2.165528 | 1.099761 |
| 10 | H | 2.165365 | 3.413128 | 3.889684 | 3.412999 | 2.165471 |
| 11 | C | 4.330065 | 3.827971 | 2.542941 | 1.540000 | 2.542987 |
| 12 | H | 4.793847 | 4.281317 | 3.024539 | 2.148263 | 3.044058 |
| 13 | H | 4.794001 | 4.038182 | 2.669426 | 2.148263 | 3.359836 |
| 14 | H | 4.794372 | 4.531084 | 3.368757 | 2.148263 | 2.658842 |
| 15 | C | 1.540000 | 2.542919 | 3.828019 | 4.330065 | 3.828169 |
| 16 | C | 2.546816 | 3.806764 | 4.962586 | 5.173110 | 4.330945 |
| 17 | H | 2.546429 | 3.934369 | 4.865335 | 4.782300 | 3.725188 |
| 18 | H | 3.244128 | 4.418991 | 5.601715 | 5.850611 | 5.022655 |
| 19 | H | 3.244377 | 4.419174 | 5.601812 | 5.851017 | 5.023293 |
| 20 | C | 2.546816 | 2.935824 | 4.330533 | 5.173040 | 4.962575 |
| 21 | H | 2.798394 | 2.871720 | 4.202089 | 5.162921 | 5.122337 |
| 22 | H | 2.798482 | 2.871883 | 4.202016 | 5.163075 | 5.122611 |
| 23 | H | 3.445597 | 3.992553 | 5.386144 | 6.165925 | 5.826682 |

| | | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|
| 6 | C | 0.000000 | | | | |
| 7 | H | 3.412938 | 0.000000 | | | |
| 8 | H | 3.889760 | 2.494768 | 0.000000 | | |
| 9 | H | 2.165516 | 4.989362 | 4.321228 | 0.000000 | |
| 10 | H | 1.099604 | 4.320704 | 4.989364 | 2.494420 | 0.000000 |
| 11 | C | 3.828376 | 4.707347 | 2.741390 | 2.742076 | 4.707530 |
| 12 | H | 4.295263 | 5.116633 | 3.123711 | 3.158106 | 5.137266 |
| 13 | H | 4.524765 | 4.750279 | 2.478318 | 3.686417 | 5.478205 |
| 14 | H | 4.031883 | 5.487807 | 3.700135 | 2.458060 | 4.739914 |
| 15 | C | 2.542728 | 2.741238 | 4.707376 | 4.707326 | 2.741526 |
| 16 | C | 2.935809 | 4.133367 | 5.934231 | 4.971326 | 2.566615 |
| 17 | H | 2.383982 | 4.515027 | 5.919401 | 4.185822 | 1.694532 |
| 18 | H | 3.657085 | 4.642876 | 6.538717 | 5.634578 | 3.249023 |
| 19 | H | 3.657559 | 4.642602 | 6.538631 | 5.635405 | 3.249653 |
| 20 | C | 3.806515 | 2.566108 | 4.971204 | 5.934104 | 4.133630 |
| 21 | H | 4.101973 | 2.330738 | 4.718542 | 6.132407 | 4.558127 |
| 22 | H | 4.102081 | 2.330290 | 4.718279 | 6.132780 | 4.558254 |
| 23 | H | 4.569046 | 3.621693 | 6.041163 | 6.732391 | 4.684902 |

| | | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|
| 11 | C | 0.000000 | | | | |
| 12 | H | 1.070000 | 0.000000 | | | |
| 13 | H | 1.070000 | 1.747303 | 0.000000 | | |
| 14 | H | 1.070000 | 1.747303 | 1.747303 | 0.000000 | |
| 15 | C | 5.870065 | 6.307659 | 6.307822 | 6.308282 | 0.000000 |
| 16 | C | 6.679941 | 7.106799 | 7.248737 | 6.950262 | 1.401400 |
| 17 | H | 6.211720 | 6.634168 | 6.885536 | 6.350986 | 2.026940 |
| 18 | H | 7.347432 | 7.878667 | 7.844008 | 7.560482 | 2.026940 |
| 19 | H | 7.347735 | 7.652017 | 7.960331 | 7.671742 | 2.026941 |
| 20 | C | 6.679648 | 7.098291 | 6.953615 | 7.252893 | 1.401400 |
| 21 | H | 6.611619 | 7.143656 | 6.736495 | 7.187671 | 2.026940 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 22 | H | 6.611631 | 6.892552 | 6.871311 | 7.304254 | 2.026940 |
| 23 | H | 7.688793 | 8.102161 | 7.996007 | 8.216665 | 2.026941 |

| | | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|
| 16 | C | 0.000000 | | | | |
| 17 | H | 1.070000 | 0.000000 | | | |
| 18 | H | 1.070000 | 1.747303 | 0.000000 | | |
| 19 | H | 1.070000 | 1.747303 | 1.747303 | 0.000000 | |
| 20 | C | 2.430067 | 3.316036 | 2.707813 | 2.707543 | 0.000000 |
| 21 | H | 3.126467 | 3.926150 | 3.171666 | 3.620886 | 1.070000 |
| 22 | H | 3.126395 | 3.925947 | 3.621117 | 3.171389 | 1.070000 |
| 23 | H | 2.471841 | 3.514771 | 2.494078 | 2.493661 | 1.070000 |

| | | 21 | 22 | 23 |
|---|---|---|---|---|
| 21 | H | 0.000000 | | |
| 22 | H | 1.747303 | 0.000000 | |
| 23 | H | 1.747303 | 1.747303 | 0.000000 |

Stoichiometry C10H13(2)
Framework group C1[X(C10H13)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.619787 | 0.000147 | -0.000036 |
| 2 | 6 | 0 | 0.077876 | -1.208049 | -0.000304 |
| 3 | 6 | 0 | 1.472588 | -1.208165 | 0.000202 |
| 4 | 6 | 0 | 2.170278 | 0.000324 | -0.000223 |
| 5 | 6 | 0 | 1.472716 | 1.208191 | -0.000434 |
| 6 | 6 | 0 | 0.077578 | 1.208133 | 0.000056 |
| 7 | 1 | 0 | -0.472206 | -2.160232 | 0.000401 |
| 8 | 1 | 0 | 2.022562 | -2.160438 | 0.000625 |
| 9 | 1 | 0 | 2.022290 | 2.160789 | -0.000777 |
| 10 | 1 | 0 | -0.472130 | 2.160472 | 0.000087 |
| 11 | 6 | 0 | 3.710278 | -0.000153 | 0.000253 |
| 12 | 1 | 0 | 4.066625 | -0.024369 | 1.008881 |
| 13 | 1 | 0 | 4.066840 | -0.861613 | -0.524771 |
| 14 | 1 | 0 | 4.067369 | 0.885190 | -0.483020 |
| 15 | 6 | 0 | -2.159787 | -0.000032 | 0.000035 |
| 16 | 6 | 0 | -2.858223 | 1.214919 | 0.000304 |
| 17 | 1 | 0 | -2.161390 | 2.026907 | 0.000780 |
| 18 | 1 | 0 | -3.473054 | 1.273067 | -0.873482 |
| 19 | 1 | 0 | -3.473497 | 1.272426 | 0.873821 |
| 20 | 6 | 0 | -2.857940 | -1.215147 | -0.000169 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 1 | 0 | -2.598232 | -1.775563 | -0.873888 |
| 22 | 1 | 0 | -2.598311 | -1.775812 | 0.873415 |
| 23 | 1 | 0 | -3.910332 | -1.021834 | -0.000189 |

---

Rotational constants (GHZ): 3.4787554 0.7753124 0.6414383

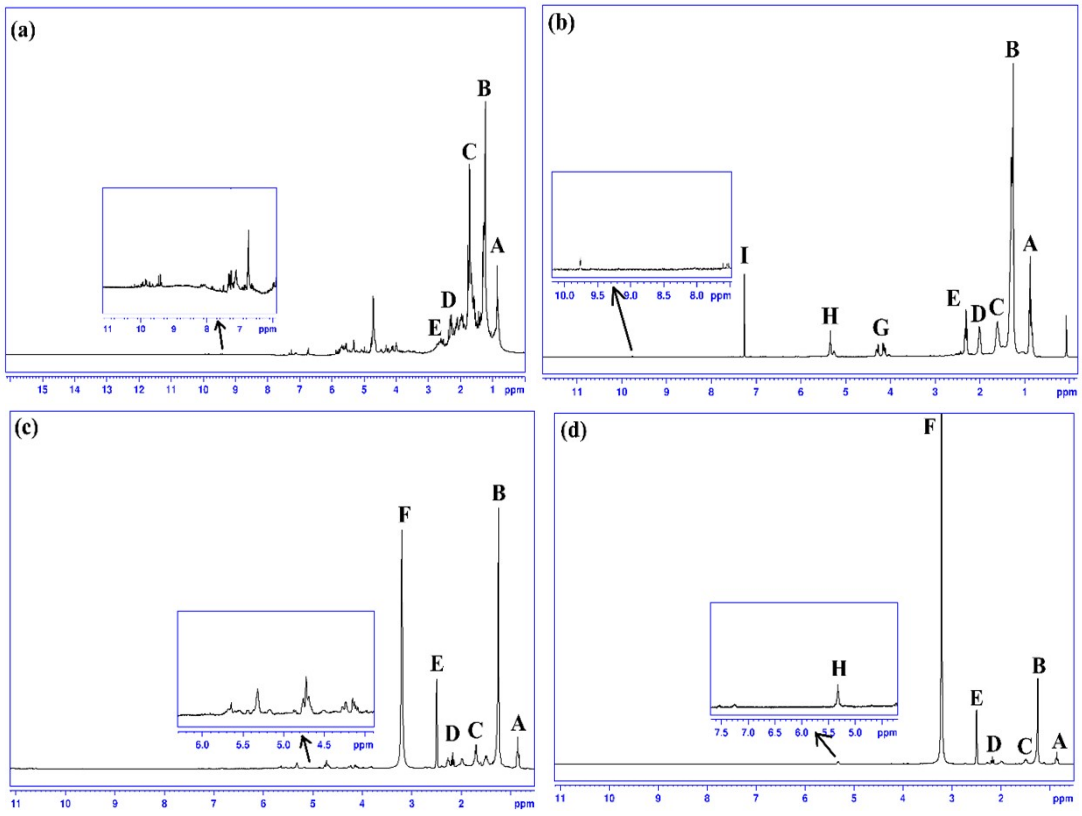


Figure S1: $^{1}$H NMR of lipid fraction of FOG deposit by (a) d-Limonene, showed the absence of spectrum assigned with triglyceride proton (b) p-Cymene, (c) MeTHF and (d) *n*-Hexane with hydrotalcite.

Table S6: Concentration of total lipid in mg/g after first extraction process using d-limonene, p-cymene, MeTHF and *n*-hexane.

| Name of FAs | Limonene | Cymene | MeTHF | *n*-Hexane |
|---|---|---|---|---|
| C8 | 14.79±1.34 | 12.04±1.26 | 10.54±1.31 | 14.02±1.99 |
| C10 | 55.07±0.52 | 47.05±0.62 | 46.25±0.51 | 50.87±1.2 |
| C11 | 10.28±2.01 | 10.03±1.89 | 1.23±2.06 | 10.23±1.67 |
| C12 | 40.52±3.25 | 39.33±2.85 | 35.86±3.12 | 40.37±2.01 |
| C14 | 37.71±1.0 | 31.36±3.5 | 30.34±2.6 | 39.95±3.1 |
| C15 | 8.37±2.14 | 6.24±1.2 | 4.35±1.6 | 8.12±2.01 |
| C16 | 106.41±4.02 | 80.44±5.14 | 95.44±4.37 | 101.2±3.09 |
| C16:1 | 7.5±0.14 | 5.65±0.25 | 2.22±0.21 | 5.0±0.17 |
| C17 | 2.54±2.4 | 3.5±2.1 | 3.16±1.9 | 2.24±1.65 |

| | | | | |
|---|---|---|---|---|
| C17:1 | 1.98±0.2 | 1.32±0.5 | 1.76±0.6 | 1.27±1.2 |
| C18 | 65.31±2.14 | 60.08±2.11 | 58.77±1.77 | 60.76±2.2 |
| C18:1n9t | 2.17±1.1 | 1.7±0.9 | 3.34±1.4 | 2.55±0.8 |
| C18:1n9c | 310.05±5.07 | 275.79±4.98 | 296.61±6.1 | 300.44±4.6 |
| C18:2n6c | 187.86±3.52 | 222.91±6.01 | 217.11±3.8 | 178.25±4.2 |
| C18:3n6 | 1.02±0.6 | 1.04±0.58 | 1.05±0.1 | 1.2±0.23 |
| C18:3n3 | 88.32±1.58 | 85.99±1.51 | 90.92±2.7 | 78±1.7 |
| C20:0 | 8.02±2.3 | 8.24±2.51 | 6.4±2.1 | 8.13±1.9 |
| C20:1n9 | 16.11±1.1 | 15.49±1.23 | 16.09±1.2 | 15.63±1.1 |
| C20:2 | 4.23±0.11 | 3.5±0.87 | 2.58±0.9 | 3.45±1.2 |
| C22:0 | 4.58±0.42 | 4.1±0.14 | 2.24±0.2 | 4.65±2.1 |
| C24 | 2.2±1.0 | 2.1±0.95 | 1.02±0.6 | 2.9±0.9 |
| C24:1n9 | 3.33±0.47 | 2.47±0.13 | 2.03±0.12 | 2.44±0.2 |
| Total (mg/g) | 978.37±3.25 | 920.37±2.26 | 929.31±2.1 | 931.67±4.02 |
| % of recovery | 97.9 | 92.1 | 92.9 | 93.1 |

Table S7: Concentration of FA in mg/g after double extraction process with hydrotalcite using d-limonene, p-cymene, MeTHF and *n*-hexane.

| Name of FAs | Limonene | Cymene | MeTHF | *n*-hexane |
|---|---|---|---|---|
| C6 | 14.13±1.34 | 10.31±1.06 | 15.22±0.53 | 12.34±1.5 |
| C8 | 13.56±1.6 | 3.44±1.01 | 7.56±2.21 | 9.32±2.1 |
| C10 | 56.83±2.3 | 57.33±1.76 | 35.06±1.5 | 30.87±1.37 |
| C12 | 40.52±2.06 | 39.33±1.94 | 35.86±2.02 | 40.37±2.59 |
| C14 | 40.02±1.51 | 31.36±2.71 | 25.34±3.06 | 35.23±1.22 |
| C15 | 5.94±0.17 | 2.67±0.32 | 4.35±0.41 | 4.22±1.48 |
| C16 | 170.33±0.91 | 180.44±1.36 | 165.39±1.81 | 144.38±0.57 |
| C16:1 | 3.64±0.88 | 1.15±0.52 | 2.04±0.48 | 2.46±0.67 |
| C17 | 2.47±0.66 | 3.1±0.17 | 2.08±0.57 | 2.13±1.75 |
| C17:1 | 0.93±0.21 | 1.32±0.83 | 0.76±0.11 | 0.81±0.1 |
| C18 | 65.31±1.70 | 60.08±1.54 | 42.14±2.11 | 52.43±3.65 |
| C18:1n9t | 2.17±0.56 | 1.7±0.21 | 1.8±0.52 | 2.1±0.61 |
| C18:1n9c | 226.59±0.43 | 200.55±1.04 | 246.61±1.48 | 212.44±1.22 |
| C18:2n6c | 140.86±2.91 | 112.91±1.73 | 127.11±2.1 | 128.25±1.34 |
| C18:3n6 | 1.02±0.34 | 1.04±0.16 | 1.05±0.06 | 1.2±0.61 |
| C18:3n3 | 1.68±1.91 | 1.16±0.23 | 3.16±1.29 | 2.12±0.52 |
| C20:0 | 6.05±0.31 | 3.93±1.32 | 4.44±1.1 | 5.93±0.45 |
| C20:1n9 | 7.08±0.17 | 3.7±1.28 | 5.73±0.73 | 7.09±0.11 |
| C20:2 | 16.33±0.76 | 13.5±1.34 | 12.58±2.07 | 13.45±1.21 |
| C22:0 | 3.12±0.86 | 1.44±0.55 | 2.24±0.14 | 2.7±1.49 |
| C23 | 0.55±0.17 | 0.57±0.07 | 0.54±0.12 | 0.45±0.15 |
| C24 | 1.57±0.26 | 2.09±0.18 | 1.73±0.16 | 1.5±0.34 |
| C24:1n9 | 1.45±1.16 | 1.93±0.5 | 1.23±0.7 | 1.27±1.4 |
| Total (mg/g) | 822.15±4.19 | 735.05±3.98 | 744.02±4.06 | 713.06±9.06 |
| % of extraction | 96.72 | 86.47 | 87.53 | 83.90 |
| %SFAs | 51.13 | 53.89 | 45.96 | 47.94 |
| %MUFAs | 29.42 | 28.62 | 34.7 | 31.72 |

| | | | | |
|---|---|---|---|---|
| %PUFAs | 19.45 | 17.50 | 19.34 | 20.34 |

Table S8: Comparison between the concentration of FA in mg/g obtained by double extraction method and other conventional methods:

| Name of FA | Double extraction methods | | Conventional methods | | |
|---|---|---|---|---|---|
| | Limonene | *n*-hexane | AOAC 996.06 | Transesterification | HEM |
| C6 | 14.13±1.34 | 12.34±1.5 | 15.22±2.43 | - | - |
| C8 | 13.56±1.6 | 9.32±2.1 | 7.56±1.34 | 16.43±4.32 | 14.02±3.02 |
| C10 | 56.83±2.3 | 30.87±1.37 | 35.06±3.54 | 76.7±7.61 | 50.87±5.69 |
| C11 | - | - | 71.09±10.5 | - | 10.23±2.63 |
| C12 | 40.52±2.06 | 40.37±2.59 | 14.56±5.09 | 75.2±3.94 | 40.37±1.74 |
| C14 | 40.02±1.51 | 35.23±1.22 | 10.83±8.69 | 19.04±2.71 | 39.95±4.01 |
| C15 | 5.94±0.17 | 4.22±1.48 | 8.15±2.88 | 1.01±0.19 | 8.12±0.69 |
| C16 | 170.33±0.91 | 144.38±0.57 | 70.5±4.36 | 49.94±3.41 | 101.2±5.16 |
| C16:1 | 3.64±0.88 | 2.46±0.67 | 2.04±1.25 | 6.64±1.06 | 5±1.43 |
| C17 | 2.47±0.66 | 2.13±1.75 | 2.08±2.1 | 1.42±0.17 | 2.24±1.2 |
| C17:1 | 0.93±0.21 | 0.81±0.1 | - | 1.15±0.06 | 1.27±0.38 |
| C18 | 65.31±1.70 | 52.43±3.65 | 42.14±10.56 | 103.27±12.04 | 60.76±1.65 |
| C18:1n9t | 2.17±0.56 | 2.1±0.61 | 2.06±0.19 | - | 2.55±0.19 |
| C18:1n9c | 226.59±0.43 | 212.44±1.22 | 534.15±7.66 | 403.68±5.39 | 300.44±8.09 |
| C18:2n6c | 140.86±2.91 | 128.25±1.34 | 96.62±0.89 | 235.77±2.09 | 178.25±5.45 |
| C18:3n6 | 1.02±0.34 | 1.2±0.61 | - | 1.63±1.48 | 1.2±0.15 |
| C18:3n3 | 1.68±1.91 | 2.12±0.52 | 4.16±6.87 | 79.83±15.76 | 78±1.36 |
| C20:0 | 6.05±0.31 | 5.93±0.45 | 4.44±2.1 | 7.8±1.43 | 8.13±2.11 |
| C20:1n9 | 7.08±0.17 | 7.09±0.11 | 5.73±2.3 | 3.22±4.22 | 15.63±1.05 |
| C20:2 | 16.33±0.76 | 13.45±1.21 | 4.26±3.23 | 1.03±0.11 | 3.45±1.1 |
| C21 | - | - | 0.57±0.14 | 0.8±0.3 | - |
| C22:0 | 3.12±0.86 | 2.7±1.49 | 2.0±0.78 | - | 4.65±1.08 |
| C23 | 0.55±0.17 | 0.45±0.55 | - | - | - |
| C24 | 1.57±0.26 | 1.5±0.34 | 1.73±3.84 | 1.8±0.96 | 2.9±0.74 |
| C24:1n9 | 1.45±1.16 | 1.27±1.4 | 1.23±1.69 | 1.90±0.32 | 2.44±0.37 |
| Total (mg/g) | 822.15±4.19 | 713.06±9.06 | 944.06±5.02 | 1088.26±7.56 | 931.67±6.04 |
| % of extraction | 96.73 | 83.89 | 111.06 | 128.0 | 109.6 |

Table S9: Comparison between the saturated and unsaturated FA in mg/g and wt% obtained by double extraction method and other conventional methods:

| Name of the methods | | SFAs | | MUFAs | | PUFAs | |
|---|---|---|---|---|---|---|---|
| | | mg/g | wt% | mg/g | wt% | mg/g | wt% |
| Double extraction methods | d-Limonene | 420.4 | 51.13 | 241.86 | 29.42 | 159.89 | 19.45 |
| | *n*-hexane | 341.87 | 47.94 | 226.17 | 31.72 | 145.02 | 20.34 |
| Conventional methods | AOAC 996.06 | 285.93 | 30.54 | 545.21 | 58.24 | 105.04 | 11.22 |
| | Transesterification | 353.41 | 32.47 | 416.59 | 38.28 | 318.26 | 29.24 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | HEM | 343.44 | 36.86 | 327.33 | 35.13 | 260.9 | 28.00 |