Table of chemical shifts.

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| **№** | **Metabolite** | **Chemical shift and multiplicity [proton(s)]** | **NMR spectra** |
|  | TSP | 0.000 s [-Si(CH3)3] | 1D |
| 1 | TA | 2.1236 s [2'CH3];  2.1379 s [2''CH3];  4.3045 dd [1b,3bCH2];  4.3603 dd [1a,3aCH2];  5.3145 m [2CH] | 1D+2D(COSY) |
| 2 | 1,2-DA | 3.775 m [3CH2];  4.245 dd [1bCH2];  4.341 dd [1aCH2];  5.134 m [2CH] | 1D+2D(COSY) |
| 3 | 2-MA | 3.740 m [1,3CH2];  4.971 m [2CH] | 1D+2D(COSY) |
| 4 | 1-MA | 3.616 dd [3bCH2];  3.665 dd [3aCH2];  3.972 m [2CH];  4.105 dd [1bCH2];  4.205 dd [1aCH2] | 1D+2D(COSY) |
| 5 | Caprylic/capric triglyceride | 0.8828 t [n'CH3];  1.295 m [4'-n'CH2];  1.584 t [3'CH2];  2.252 t [2'CH2];  4.0995 dd [1b,3bCH2];  4.2842 dd [1a,3aCH2];  5.2159 m [2CH] | 1D+2D(COSY) |
| 6 | Caprylic/capric acids | 0.8828 t [n'CH3];  1.295 m [4'-n'CH2];  1.584 t [3'CH2];  2.1754 t [2'CH2] | 1D+2D(COSY) |
| Abbreviations: t - triplet; m – multiplet, s –singlet, d – doublet of doublets. TSP - Sodium trimethylsilyl propionate; TA –triacetin; 1,2-DA – 1,2-diacetin; 2-MA – 2-monoacetin; 1-MA – 1-monoacetin | | | |