Supporting Information

Structural elucidation of triacylglycerol using online acetone Paternò–Büchi reaction paired with reversed-phase liquid chromatography mass spectrometry

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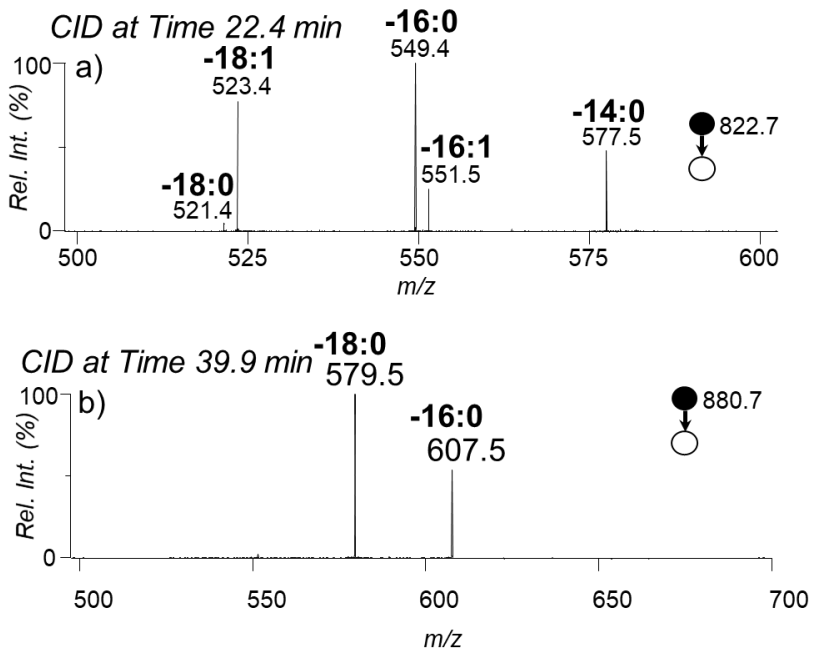
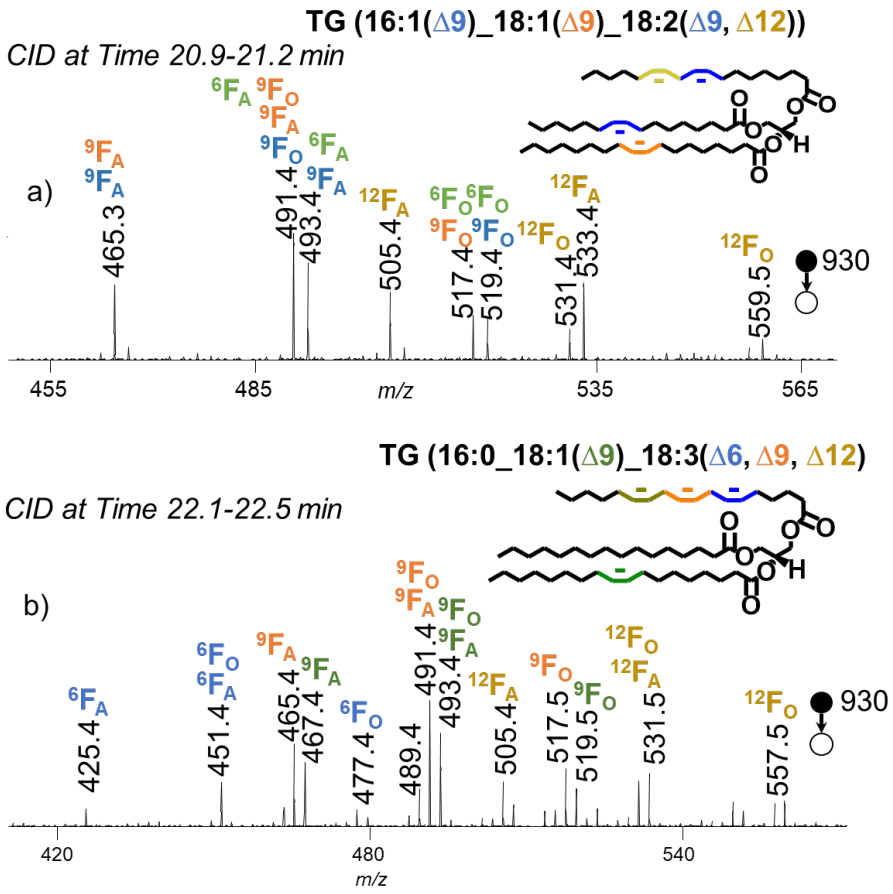


Supplementary Figure S1. a) The CID spectrum of the ions at *m/z* 880.7 eluted at 22.4 minutes from panel a). b) The CID spectrum of the ions at *m/z* 880.7 eluted at 39.9 minutes.



Supplementary Figure S2. a) The CID spectrum of the ions at *m/z* 930.8 eluted from time 20.9-21.2 minutes, b) The CID spectrum of the ions at *m/z* 930.8 eluted from time 22.1-22.5 minutes.

Supplementary Table S1. TG molecular species identified at fatty acyl compositional level in pooled human plasma using RPLC-MS/MS.

m/z	Subclass	Species
708.6	40:2	TG (18:2_16:0_6:0)
710.6	40:1	TG (18:1_16:0_6:0)
712.6	40:0	TG (12:0_12:0_16:0)
724.6	41:1	TG (12:0_18:1_11:0)
734.6	42:3	TG (12:0_18:3_12:0)
734.6	42:3	TG (8:1_16:0_18:2)
736.7	42:2	TG (8:1_16:0_18:1)
736.7	42:2	TG (18:2_12:0_12:0)
738.7	42:1	TG (12:0_18:1_12:0)
740.7	42:0	TG (16:0_14:0_12:0)
750.7	43:3	TG (9:0_16:0_18:2)
760.6	44:4	TG (18:2_18:2_8:0)
762.6	44:3	TG (10:1_18:2_16:0)
764.7	44:2	TG (18:2_16:0_10:0)
766.7	44:1	TG (18:1_16:0_10:0)
768.7	44:0	TG (14:0_14:0_16:0)
780.7	44:1	TG (16:1_14:0_15:0)
782.7	45:0	TG (16:0_15:0_14:0)
786.7	46:5	TG (18:2_10:0_18:3)
788.7	46:4	TG (18:2_10:0_18:2)
794.7	46:1	TG (16:0_14:0_16:1)
796.7	46:0	TG (16:0_14:0_16:0)
806.7	47:2	TG (18:2_15:0_14:0)
808.7	47:1	TG (16:0_15:0_16:1)
810.7	47:0	TG (16:0_15:0_16:0)
814.7	48:5	TG (12:0_18:2_18:3)
816.7	48:4	TG (12:0_18:2_18:2)
818.7	48:3	TG (12:0_18:1_18:2)
820.7	48:2	TG (16:0_16:1_16:1)
822.7	48:1	TG (14:0_16:0_18:1)
822.7	48:1	TG (14:0_16:1_18:0)
824.8	48:0	TG (16:0/16:0/16:0)
824.8	48:0	TG (14:0_16:0_18:0)
834.7	49:2	TG (16:0_18:2_15:0)

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Supplementary Table S1. (continued)

m/z	Subclass	Species
836.8	49:1	TG (16:0_18:1_15:0)
838.8	49:0	TG (16:0_16:0_17:0)
842.7	50:5	TG (18:2_18:3_14:0)
844.7	50:4	TG (14:0_18:2_18:2)
846.7	50:3	TG (14:0_18:1_18:2)
846.7	50:3	TG (16:0_16:1_18:2)
846.7	50:3	TG (16:0_16:0_18:3)
848.8	50:2	TG (14:0_18:1_18:1)
848.8	50:2	TG (16:0_16:1_18:1)
848.8	50:2	TG (16:0_16:0_18:2)
850.8	50:1	TG 16:0_16:0_18:1
852.8	50:0	TG (16:0_18:0_16:0)
856.7	51:5	TG (18:2_18:3_15:0)
856.7	51:5	TG (15:1_18:2_18:2)
858.8	51:4	TG (18:2_18:2_15:0)
860.8	51:3	TG (18:2_18:1_15:0)
862.8	51:2	TG (18:1_18:1_15:0)
864.8	51:1	TG (18:1_16:0_17:0)
866.8	51:0	TG (16:0_18:0_17:0)
866.8	51:0	TG (19:0_16:0_16:0)
870.7	52:5	TG (16:1_18:2_18:2)
870.7	52:5	TG (16:0_18:2_18:3)
872.8	52:4	TG (16:0_18:2_18:2)
872.8	52:4	TG (16:0_18:1_18:3)
872.8	52:4	TG (16:0_16:0_20:4)
872.8	52:4	TG (16:1_18:1_18:2)
874.8	52:3	TG (16:1_18:1_18:1)
874.8	52:3	TG (16:0_18:1_18:2)
876.8	52:2	TG (16:0_18:1_18:1)
876.8	52:2	TG (16:0_18:0_18:2)
878.8	52:1	TG (16:0_18:0_18:1)
880.8	52:0	TG (18:0_18:0_16:0)
884.8	53:5	TG (18:2_17:1_18:2)
888.8	53:3	TG (18:1_18:2_17:0)
888.8	53:3	TG (18:1_17:1_18:1)
890.8	53:2	TG (18:1_17:0_18:1)
892.8	53:1	TG (16:0_19:0_18:1)
892.8	54:8	TG (18:3_18:3_18:2)

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Supplementary Table S1. (continued)

m/z	Subclass	Species
894.8	54:7	TG (18:3_18:2_18:2)
896.8	54:6	TG (18:2_18:2_18:2)
896.8	54:6	TG (16:0_18:2_20:4)
898.8	54:5	TG (18:1_18:2_18:2
898.8	54:5	TG (16:0_18:1_20:4)
900.8	54:4	TG (18:1_18:1_18:2)
900.8	54:4	TG (16:0_18:0_20:3)
902.8	54:3	TG (18:1_18:1_18:1)
902.8	54:3	TG (18:0_18:1_18:2)
902.8	54:3	TG (18:0_18:1_18:2)
904.8	54:2	TG (18:0_18:1_18:1)

Supplementary Table S2. TG molecular species identified at C=C level in pooled human plasma using RPLC-PB-MS/MS

m/z	Subclass	Molecular Species
794.7	46:1	TG (16:0_14:0_16:1(Δ9))
816.7	48:4	TG (12:0_18:2(Δ9, Δ12)_18:2(Δ9, Δ12))
818.7	48:3	TG (12:0_18:1(Δ9)_18:2(Δ9, Δ12))
820.7	48:2	TG (16:0_16:1(Δ9)_16:1(Δ9))
822.7	48:1	TG (14:0_16:0_18:1(Δ9))
822.7	48:1	TG (14:0_16:0_18:1(Δ11))
844.7	50:4	TG (14:0_18:2(Δ9, Δ12)_18:2(Δ9, Δ12))
846.7	50:3	TG (14:0_18:1(Δ9)_18:2(Δ9, Δ12))
846.7	50:3	TG (16:0_16:1(Δ9)_18:2(Δ9, Δ12))
846.7	50:3	TG (16:0_16:0_18:3(Δ6, Δ9, Δ12))
848.8	50:2	TG (14:0_18:1(Δ9)_18:1(Δ9))
848.8	50:2	TG (16:0_16:1(Δ9)_18:1(Δ9))
848.8	50:2	TG (16:0_16:0_18:2(Δ9, Δ12))
850.8	50:1	TG (16:0_16:0_18:1(Δ9))
850.8	50:1	TG (16:0_16:0_18:1(Δ11))
860.8	51:3	TG (18:2(Δ9, Δ12_18:1(Δ9)_15:0)
862.8	51:2	TG (18:1(Δ9)_18:1(Δ9)_15:0)
864.8	51:1	TG (18:1(Δ9)_16:0_17:0)
870.7	52:5	TG (16:1(Δ9)_18:2(Δ9, Δ12)_18:2(Δ9, Δ12))
870.7	52:5	TG (16:0_18:2(Δ9, Δ12)_18:3(Δ6, Δ9, Δ12))
872.8	52:4	TG (16:0_18:2(Δ9, Δ12)_18:2(Δ9, Δ12))
872.8	52:4	TG (16:0_18:1(Δ9)_18:3(Δ6, Δ9, Δ12)
872.8	52:4	TG (16:0_16:0_20:4(Δ5, Δ8, Δ11, Δ14))
872.8	52:4	TG (16:1(Δ9)_18:1(Δ9)_18:2(Δ9, Δ12))
874.8	52:3	TG (16:1(Δ9)_18:1(Δ9)_18:1(Δ9))
874.8	52:3	TG (16:1(Δ9)_18:1(Δ9)_18:1(Δ11))
874.8	52:3	TG (16:0_18:1(Δ9)_18:2(Δ9, Δ12))
874.8	52:3	TG (16:0_18:1(Δ11)_18:2(Δ9, Δ12))
876.8	52:2	TG (16:0_18:1(Δ9)_18:1(Δ9))
876.8	52:2	TG (16:0_18:1(Δ11)_18:1(Δ11))
876.8	52:2	TG (16:0_18:0_18:2(Δ9, Δ12))
878.8	52:1	TG (16:0_18:0_18:1(Δ9))
878.8	52:1	TG (16:0_18:0_18:1(Δ11))
890.8	53:2	TG (18:1(Δ9)_17:0_18:1(Δ9))
896.8	54:6	TG (18:2(Δ9, Δ12)_18:2(Δ9, Δ12)_18:2(Δ9, Δ12)
896.8	54:6	TG (16:0_18:2(Δ9, Δ12)_20:4(Δ5, Δ8, Δ11, Δ15))

Supplementary Table S2. (continued)

m/z	Subclass	Molecular Species
898.8	54:5	TG (18:1(Δ9)_18:2(Δ9, Δ12)_18:2(Δ9, Δ12))
898.8	54:5	TG (16:0_18:1(Δ9)_20:4(Δ5, Δ8, Δ11, Δ14))
900.8	54:4	TG (18:1(Δ9)_18:1(Δ9)_18:2(Δ9, Δ12)
900.8	54:4	TG (18:1(Δ11)_18:1(Δ11)_18:2(Δ9, Δ12)
902.8	54:3	TG (18:1 (Δ9)_18:1(Δ9)_18:1 Δ9))
902.8	54:3	TG (18:1 (Δ11)_18:1(Δ11)_18:1 Δ11))
902.8	54:3	TG (18:0_18:1(Δ9)_18:2(Δ9, Δ12))
902.8	54:3	TG (18:0_18:1(Δ11)_18:2(Δ9, Δ12))
904.8	54:2	TG (18:0_18:1(Δ9) _18:1(Δ9))
904.8	54:2	TG (16:0_20:1(Δ9)_18:1(Δ9))