

# Supplemental Figure

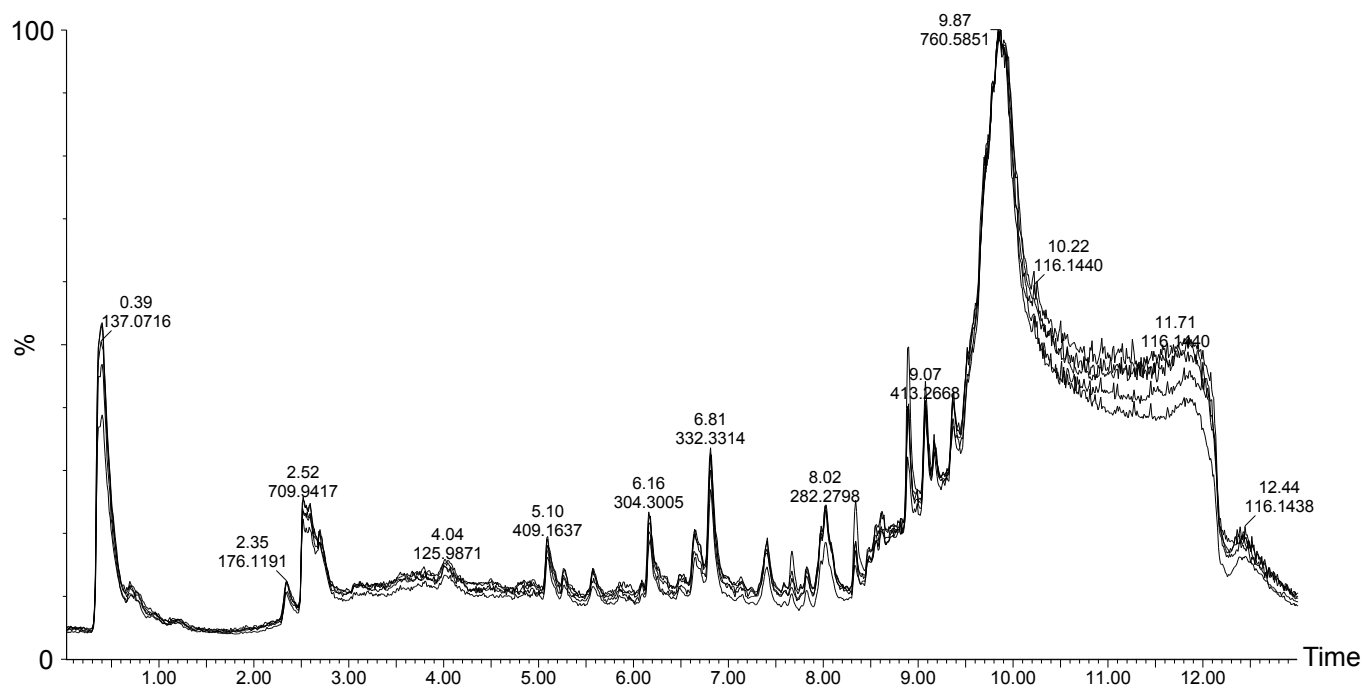
## Metabolomics studies to assess biological functions of vitamin E nicotinate

Lucia Marcocci<sup>a</sup> and Yuichiro J. Suzuki<sup>b</sup>

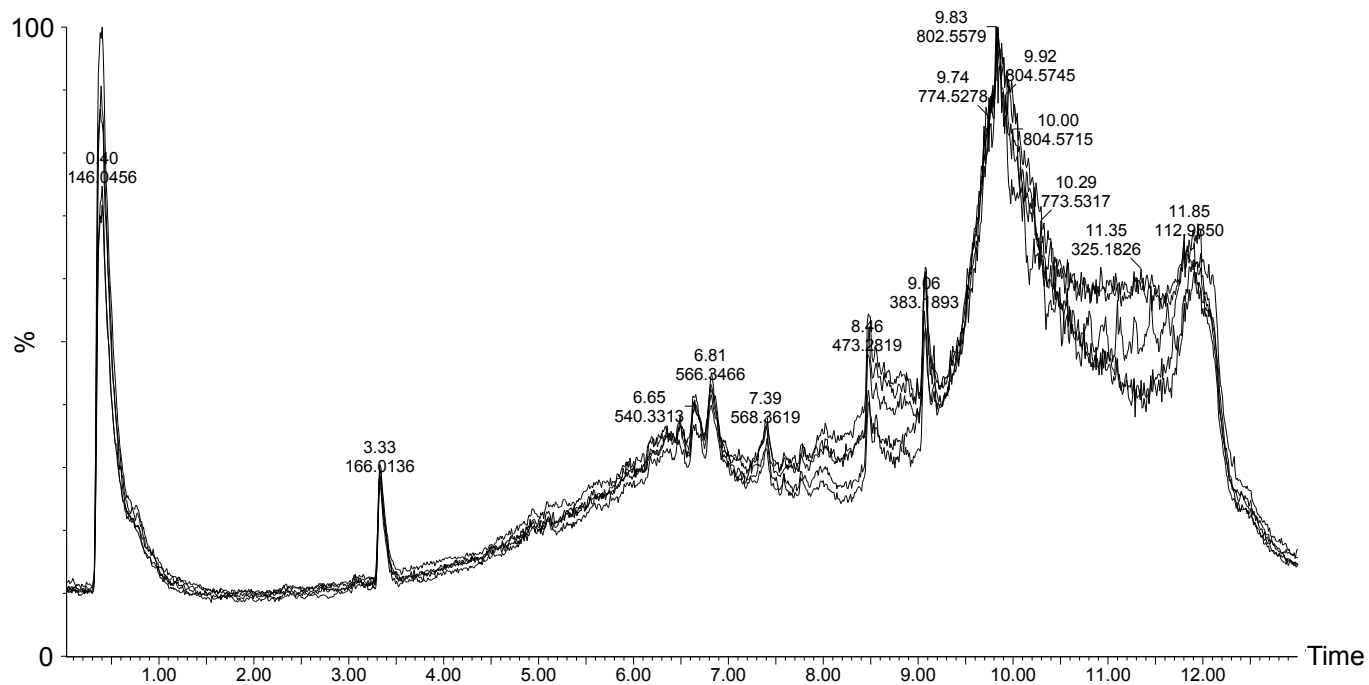
<sup>a</sup>Department of Biochemical Sciences “A. Rossi Fanelli”, Sapienza University of Rome,  
00185 Rome, Italy

<sup>b</sup>Department of Pharmacology and Physiology, Georgetown University Medical Center,  
Washington, DC 20057 USA

Total ion chromatogram for ESI+



Total ion chromatogram for ESI-



# Supplemental Files

**Metabolomics studies to assess biological functions of vitamin E nicotinate**

Lucia Marcocci<sup>a</sup> and Yuichiro J. Suzuki<sup>b</sup>

<sup>a</sup>Department of Biochemical Sciences “A. Rossi Fanelli”, Sapienza University of Rome, 00185

Rome, Italy

<sup>b</sup>Department of Pharmacology and Physiology, Georgetown University Medical Center,

Washington, DC 20057 USA

**Supplemental File S1: List of masses identified to be differentially affected by TN vs. TA+N that correspond to lipids**

Positive mode

Experimental mass: 536.4102  
 Fold change (TA+N / TN): 0.0010047  
 P value: 0.000000000000000749  
 dl-alpha-Tocopherol nicotinate

Experimental mass: 354.3348  
 Fold change (TA+N / TN): 0.2839  
 P value: 0.0000152  
 Anandamide (20:1, n-9)

Experimental mass: 376.3189  
 Fold change (TA+N / TN): 0.28947  
 P value: 0.0000396  
 N-(5Z,8Z,11Z,14Z-docosatetraenoyl)-ethanolamine  
 Adrenoyl-EA  
 alpha,alpha-dimethyl anandamide  
 N-(5Z,8Z,11Z,14Z-docosatetraenoyl)-ethanolamine  
 N-(1,1-dimethyl-2-hydroxy-ethyl) arachidonoyl amine  
 N-ethyl N-(2-hydroxy-ethyl) arachidonoyl amine  
 Anandamide (20:1, n-9)

Experimental mass: 256.2639  
 Fold change (TA+N / TN): 0.37363  
 P value: 0.00010254  
 Palmitamide

Experimental mass: 378.331  
 Fold change (TA+N / TN): 0.31426  
 P value: 0.00011665  
 Eicosanoyl-EA  
 Guazatine

Experimental mass: 320.2558  
 Fold change (TA+N / TN): 0.27002  
 P value: 0.00012562  
 Anandamide (18:4, n-3)  
 N-hydroxy arachidonoyl amine  
 (Z)-N-(2-hydroxyethyl)hexadec-7-enamide  
 Cassine  
 Spiroxamine  
 3-ketosphingosine

Palmitoleoyl-EA  
 2S-amino-octadeca-4E,6E-diene-1,3R-diol  
 3-ketosphingosine  
 4E,14Z-Sphingadiene  
 (4E,8E,d18:2) sphingosine  
 (4E,8Z,d18:2) sphingosine  
 Lepadine D

Experimental mass: 348.2867

Fold change (TA+N / TN): 0.33043

P value: 0.00036519

O-Arachidonoyl Ethanolamine  
 N-(7Z,10Z,13Z,16Z-docosatetraenoyl)-ethanolamide  
 Anandamide (20:4, n-6)  
 Virodhamine  
 N-oleoyl ethanolamine

Experimental mass: 310.3108

Fold change (TA+N / TN): 0.41919

P value: 0.00053591

Oleoyl Ethyl Amide  
 N-Hexadecanoylpyrrolidine

Experimental mass: 460.2464

Fold change (TA+N / TN): 0.42446

P value: 0.00080586

Cerivastatin  
 13-Desoxyterpendole I  
 beta-Paxitriol  
 PC(O-10:1(9E)/2:0)  
 PE(15:1(9Z)/0:0)

Experimental mass: 282.2795

Fold change (TA+N / TN): 0.39156

P value: 0.0011243

Dodemorph  
 Oleamide  
 Elaidamide

Experimental mass: 752.5217

Fold change (TA+N / TN): 0.49992

P value: 0.0011482

PE(18:4(6Z,9Z,12Z,15Z)/19:1(9Z))  
 PE(18:4(6Z,9Z,12Z,15Z)/19:1(9Z))  
 PE(19:1(9Z)/18:4(6Z,9Z,12Z,15Z))  
*(Partial listing)*

Experimental mass: 322.2717

Fold change (TA+N / TN): 0.30181

P value: 0.0012571

Anandamide (18:3, n-3)

Anandamide (18:3, n-6)

L-threo-Sphingosine C-18

2R-aminooctadec-4Z-ene-1,3S-diol

Sphingosine

Palmitoyl-EA

3-ketosphinganine

Sphingosine

12-amino-octadecanoic acid

2-amino-octadecanoic acid

Sphingosine

5-hydroxy,3E-sphingosine

(8Z,d18:1) sphingosine

Experimental mass: 421.3126

Fold change (TA+N / TN): 0.44451

P value: 0.0013067

1alpha-hydroxy-22-(3-methylphenyl)-23,24,25,26,27-pentanorvitamin D3

Experimental mass: 525.4709

Fold change (TA+N / TN): 0.4845

P value: 0.0014075

all-trans-retinyl Palmitate

11-cis-retinyl palmitate

Linolenyl linolenate

Experimental mass: 426.3538

Fold change (TA+N / TN): 0.44338

P value: 0.0023548

Elaidic carnitine

O-oleoylcarnitine

11Z-Octadecenylcarnitine

Oleoylcarnitine

Octadecenoylcarnitine

Vaccenyl carnitine

Experimental mass: 545.397

Fold change (TA+N / TN): 0.44229

P value: 0.0025414

Panaxydol linoleate

Experimental mass: 619.4357

Fold change (TA+N / TN): 0.49666

P value: 0.0032261

3,6-Epoxy-5,5',6,6'-tetrahydro-b,b-carotene-3',5,5',6'-tetrol

PA(17:1(9Z)/13:0)

PA(18:1(9Z)/12:0)

PA(13:0/17:1(9Z))

PA(14:1(9Z)/16:0)

PA(15:0/15:1(9Z))

PA(15:1(9Z)/15:0)

PA(14:0/16:1(9Z))

PA(12:0/18:1(9Z))

PA(16:0/14:1(9Z))

PA(16:1(9Z)/14:0)

Experimental mass: 843.524

Fold change (TA+N / TN): 0.45725

P value: 0.003386

Spiramycin 1

PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z))

PG(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Experimental mass: 608.602

Fold change (TA+N / TN): 0.39738

P value: 0.0037891

Cer(d16:1/23:0)

Cer(d15:1/24:0)

Experimental mass: 650.4363

Fold change (TA+N / TN): 0.48641

P value: 0.0040958

PC(16:0/9:0(CHO))

Experimental mass: 254.2472

Fold change (TA+N / TN): 0.40412

P value: 0.0049162

Palmitoleamide

Experimental mass: 819.5243

Fold change (TA+N / TN): 0.48035

P value: 0.0050407

PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z))

PG(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))

PG(20:3(8Z,11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z))

PG(20:5(5Z,8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z))

LBPA(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))

PG(18:4(6Z,9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z))  
 PG(22:4(7Z,10Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))  
 PG(18:3(6Z,9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 PG(18:3(9Z,12Z,15Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 PG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,10Z,13Z,16Z))  
 PG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))  
 PG(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Experimental mass: 829.5704  
 Fold change (TA+N / TN): 0.48177  
 P value: 0.0052563  
 PA(22:1(11Z)/22:4(7Z,10Z,13Z,16Z))  
 PA(22:4(7Z,10Z,13Z,16Z)/22:1(11Z))

Experimental mass: 356.2745  
 Fold change (TA+N / TN): 0.46424  
 P value: 0.0055133  
 6,9,12,15,18,21-Tetracosahexaenoic acid

Experimental mass: 300.2901  
 Fold change (TA+N / TN): 0.49945  
 P value: 0.006185  
 L-threo-Sphingosine C-18  
 2R-aminooctadec-4Z-ene-1,3S-diol  
 Sphingosine  
 Palmitoyl-EA  
 3-ketosphinganine  
 Sphingosine  
 12-amino-octadecanoic acid  
 2-amino-octadecanoic acid  
 Sphingosine  
 5-hydroxy,3E-sphingosine  
 (8Z,d18:1) sphingosine

Experimental mass: 572.4878  
 Fold change (TA+N / TN): 0.47355  
 P value: 0.0085978  
 Arachidonic acid leelamide

Experimental mass: 591.4036  
 Fold change (TA+N / TN): 0.32054  
 P value: 0.010837  
 PA(12:0/16:1(9Z))  
 PA(13:0/15:1(9Z))  
 PA(14:0/14:1(9Z))  
 PA(14:1(9Z)/14:0)



PA(15:1(9Z)/13:0)

PA(16:1(9Z)/12:0)

Experimental mass: 605.4216

Fold change (TA+N / TN): 0.42609

P value: 0.01156

PA(17:1(9Z)/12:0)

PA(12:0/17:1(9Z))

PA(13:0/16:1(9Z))

PA(14:0/15:1(9Z))

PA(14:1(9Z)/15:0)

PA(15:0/14:1(9Z))

PA(15:1(9Z)/14:0)

PA(16:1(9Z)/13:0)

Experimental mass: 933.5437

Fold change (TA+N / TN): 0.49111

P value: 0.012819

PI(20:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,10Z,13Z,16Z))

PI(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z))

PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:3(8Z,11Z,14Z))

*(Partial listing)*

Experimental mass: 530.3286

Fold change (TA+N / TN): 0.49079

P value: 0.023337

LysoPE(0:0/22:4(7Z,10Z,13Z,16Z))

PE(22:4(7Z,10Z,13Z,16Z)/0:0)

Gymnodimine

Experimental mass: 644.4963

Fold change (TA+N / TN): 0.36271

P value: 0.026068

PE-NMe(O-14:0/O-14:0)

Experimental mass: 801.5914

Fold change (TA+N / TN): 0.4453

P value: 0.031291

PG(O-16:0/21:0)

PG(O-18:0/19:0)

PG(O-20:0/17:0)

all-trans decaprenyl phosphate

Decaprenyl phosphate

Experimental mass: 700.4934  
 Fold change (TA+N / TN): 0.48083  
 P value: 0.034981

PE(15:1(9Z)/18:2(9Z,12Z))  
 PC(18:3(6Z,9Z,12Z)/12:0)  
 PE(16:1(9Z)/17:2(9Z,12Z))  
 (*Partial listing*)

Experimental mass: 390.2368  
 Fold change (TA+N / TN): 0.48305  
 P value: 0.039787

C17 Sphinganine-1-phosphate

Experimental mass: 424.3039  
 Fold change (TA+N / TN): 0.31603  
 P value: 0.046954

thio-Miltefosine  
 3-hydroxypentadecanoyl carnitine

### Negative mode

Experimental mass: 1063.7471  
 Fold change (TA+N / TN): 0.47802  
 P value: 0.0008945

TG(22:4(7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6]  
 TG(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 TG(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z))  
 TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z))  
 TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 TG(22:4(7Z,10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
 TG(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
 TG(22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z))  
 TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
 TG(22:5(7Z,10Z,13Z,16Z,19Z)/22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
 TG(22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z))

Experimental mass: 630.6242  
 Fold change (TA+N / TN): 0.44392  
 P value: 0.0010138

Cer(m18:1(4E)/24:1(15Z))

Experimental mass: 714.6509  
Fold change (TA+N / TN): 0.49265  
P value: 0.0011828  
Cer(d18:0/26:0)  
Cer(d20:0/24:0)

Experimental mass: 666.5904  
Fold change (TA+N / TN): 0.38035  
P value: 0.0013212  
Cer(m18:1(4E)/24:1(15Z))

Experimental mass: 374.2438  
Fold change (TA+N / TN): 0.47867  
P value: 0.0013433  
N-oleoyl glycine

Experimental mass: 712.6372  
Fold change (TA+N / TN): 0.48793  
P value: 0.0015323  
Ceramide (d18:1/26:0)  
Cer(d18:1/26:0)  
Cer(d18:0/26:1(17Z))

Experimental mass: 672.6115  
Fold change (TA+N / TN): 0.45032  
P value: 0.0015373  
Cer(d18:0/23:0)

Experimental mass: 1016.7482  
Fold change (TA+N / TN): 0.49017  
P value: 0.0015601  
NAPE(18:1(9Z)/16:1(9Z)/18:0)

Experimental mass: 656.6285  
Fold change (TA+N / TN): 0.47662  
P value: 0.0018678  
DG(19:0/0:0/19:0) (d5)

Experimental mass: 846.5826  
Fold change (TA+N / TN): 0.49887  
P value: 0.0018927  
PE(21:0/20:3(8Z,11Z,14Z))  
PC(18:2(9Z,12Z)/20:1(13Z))  
PE(19:1(9Z)/22:2(13Z,16Z))  
PE(22:2(13Z,16Z)/19:1(9Z))  
PE(20:3(8Z,11Z,14Z)/21:0)

PC(18:0/20:3(5Z,11Z,14Z))  
 PC(18:0/20:3(5Z,8Z,14Z))  
 PC(20:3(8Z,11Z,14Z)/18:0)  
 PC(18:2(9Z,12Z)/20:1(11Z))  
 PC(18:1(11Z)/20:2(11Z,14Z))  
 PC(18:3(6Z,9Z,12Z)/20:0)  
 PC(20:2(11Z,14Z)/18:1(11Z))  
 PC(20:3(5Z,8Z,11Z)/18:0)  
 PC(18:3(9Z,12Z,15Z)/20:0)  
 PC(16:0/22:3(13Z,16Z,19Z))[U]  
 PC(18:0/20:3(5E,8E,11E))[U]  
 PC(18:0/20:3(5Z,8Z,11Z))[U]  
 PC(18:0/20:3(8Z,11Z,14Z))[U]  
 PC(16:1(9Z)/22:2(13Z,16Z))  
 PC(22:2(13Z,16Z)/16:1(9Z))  
 PC(20:0/18:3(6Z,9Z,12Z))  
 PC(20:0/18:3(9Z,12Z,15Z))  
 PC(20:1(11Z)/18:2(9Z,12Z))  
 PC(20:2(11Z,14Z)/18:1(9Z))  
 PC(18:0/20:3(5Z,8Z,11Z))  
 PC(18:0/20:3(8Z,11Z,14Z))  
 PC(18:1(9Z)/20:2(11Z,14Z))

Experimental mass: 724.5271

Fold change (TA+N / TN): 0.37514

P value: 0.0022509

PE(20:3(5Z,8Z,11Z)/P-16:0)  
 PE(P-18:1(11Z)/18:2(9Z,12Z))  
 PE(18:2(9Z,12Z)/P-18:1(11Z))  
 PE(P-18:1(9Z)/18:2(9Z,12Z))  
 PE(P-16:0/20:3(5Z,8Z,11Z))  
 PE(P-16:0/20:3(8Z,11Z,14Z))  
 PE(P-18:0/18:3(6Z,9Z,12Z))  
 PE(P-18:0/18:3(9Z,12Z,15Z))  
 PE(18:2(9Z,12Z)/P-18:1(9Z))  
 PE(20:3(8Z,11Z,14Z)/P-16:0)  
 PE(18:3(6Z,9Z,12Z)/P-18:0)  
 PE(18:3(9Z,12Z,15Z)/P-18:0)  
 PE(O-16:0/20:4(5Z,8Z,11Z,14Z))  
 PE(O-18:0/18:4(6Z,9Z,12Z,15Z))

Experimental mass: 730.5394

Fold change (TA+N / TN): 0.44441

P value: 0.0025185

PC(18:1(11Z)/14:0)  
 PC(14:1(9Z)/18:0)

PC(18:1(9Z)/14:0)  
 PC(14:0/18:1(9E))[U]  
 PC(14:0/18:1(9Z))[U]  
 PC(16:0/16:1(9Z))[U]  
 PC(18:1(9Z)/14:0)[U]  
 PC(14:0/18:1(11Z))  
 PC(14:0/18:1(9Z))  
 PE(20:1(11Z)/15:0)  
 PC(16:1(9Z)/16:0)  
 PE-NMe(16:0/18:1(9Z))  
 PC(16:0/16:1(9Z))  
 PC(18:0/14:1(9Z))  
 PE(15:0/20:1(11Z))  
 PE(15:1(9Z)/20:0)  
 PE(16:0/19:1(9Z))  
 PE(19:0/16:1(9Z))  
 PE(16:1(9Z)/19:0)  
 PC(15:0/17:1(9Z))  
 PE(22:1(11Z)/13:0)  
 PE(19:1(9Z)/16:0)  
 PC(15:1(9Z)/17:0)  
 PE(20:0/15:1(9Z))  
 PE(17:1(9Z)/18:0)  
 PE-NMe(18:1(9Z)/16:0)  
 PC(17:0/15:1(9Z))  
 PC(19:1(9Z)/13:0)  
 PC(19:1(9Z)/13:0)  
 PE(18:1(9Z)/17:0)  
 PC(17:1(9Z)/15:0)  
 PE(13:0/22:1(11Z))  
 PC(20:1(11Z)/12:0)  
 PE(17:0/18:1(9Z))  
 PC(12:0/20:1(11Z))  
 PE(14:1(9Z)/21:0)  
 PC(13:0/19:1(9Z))  
 PE(21:0/14:1(9Z))  
 PE-NMe(16:0/18:1(9Z))[U]  
 1,2-Dierucoyl-SN-Glycero-3-Phosphoethanolamine

Experimental mass: 1106.7628

Fold change (TA+N / TN): 0.49041

P value: 0.0028715

Trihexosylceramide (d18:1/22:0)  
 Manalpha1-3Manbeta1-4Glcbeta-Cer(d18:1/22:0)  
 Galalpha1-4Galbeta1-4Glcbeta-Cer(d18:1/22:0)  
 Galalpha1-3Galbeta1-4Glcbeta-Cer(d18:1/22:0)

Experimental mass: 726.5384

Fold change (TA+N / TN): 0.39339

P value: 0.0029261

PE(18:1(9Z)/P-18:1(11Z))  
 PE(20:2(11Z,14Z)/P-16:0)  
 PE(18:1(9Z)/P-18:1(9Z))  
 PE(18:1(11Z)/P-18:1(11Z))  
 PE(P-18:1(11Z)/18:1(11Z))  
 PE(18:1(11Z)/P-18:1(9Z))  
 PE(P-18:1(9Z)/18:1(9Z))  
 PE(18:2(9Z,12Z)/P-18:0)  
 PE(P-16:0/20:2(11Z,14Z))  
 PE(P-18:1(9Z)/18:1(11Z))  
 PE(P-18:0/18:2(9Z,12Z))  
 PE(P-18:1(11Z)/18:1(9Z))  
 PC(P-16:0/17:2(9Z,12Z))  
 PE(O-18:0/18:3(6Z,9Z,12Z))  
 PE(O-18:0/18:3(9Z,12Z,15Z))  
 PE(O-16:0/20:3(8Z,11Z,14Z))

Experimental mass: 977.7645

Fold change (TA+N / TN): 0.49521

P value: 0.0033399

TG(20:3n6/22:5(4Z,7Z,10Z,13Z,16Z)/20:4(5Z,8Z,11Z,14Z))  
 TG(20:2n6/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z))  
 TG(20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))[iso3]  
*(Partial listing)*

Experimental mass: 802.464

Fold change (TA+N / TN): 0.40117

P value: 0.0037708

PS(20:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))  
 PS(18:3(6Z,9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z))  
 PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))  
 PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))  
 PS(18:3(9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z))  
 PS(18:4(6Z,9Z,12Z,15Z)/20:4(5Z,8Z,11Z,14Z))

Experimental mass: 1132.783

Fold change (TA+N / TN): 0.48535

P value: 0.0042804

Trihexosylceramide (d18:1/24:1(15Z))  
 Manalpha1-3Manbeta1-4Glcbeta-Cer(d18:1/24:1(15Z))  
 Galalpha1-4Galbeta1-4Glcbeta-Cer(d18:1/24:1(15Z))  
 Galalpha1-3Galbeta1-4Glcbeta-Cer(d18:1/24:1(15Z))

Experimental mass: 706.5428  
 Fold change (TA+N / TN): 0.45163  
 P value: 0.0043004  
 PS(O-16:0/O-16:0)[U]

Experimental mass: 744.5124  
 Fold change (TA+N / TN): 0.38721  
 P value: 0.0043082  
 PS(O-16:0/18:2(9Z,12Z))  
 PS(P-18:0/16:1(9Z))  
 PS(P-20:0/14:1(9Z))  
 PS(P-16:0/18:1(9Z))

Experimental mass: 978.7663  
 Fold change (TA+N / TN): 0.48458  
 P value: 0.0043119  
 PE(24:0/26:0)[U]  
 PE(25:0/25:0)[U]  
 PE(26:0/24:0)[U]  
 PC(21:0/26:0)[U]  
 PC(22:0/25:0)[U]  
 PC(23:0/24:0)[U]  
 PC(24:0/23:0)[U]  
 PC(25:0/22:0)[U]  
 PC(26:0/21:0)[U]

Experimental mass: 919.8131  
 Fold change (TA+N / TN): 0.49921  
 P value: 0.0043614  
 TG(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(9Z)/o-18:0)  
 TG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z)/o-18:0)  
 TG(18:2(9Z,12Z)/o-18:0/22:4(7Z,10Z,13Z,16Z))  
*(Partial listing)*

Experimental mass: 690.5503  
 Fold change (TA+N / TN): 0.46887  
 P value: 0.0048147  
 PC(O-14:0/16:0)[U]  
 PC(O-14:0/16:0)  
 PE(O-18:0/15:0)  
 PE(O-20:0/13:0)  
 PE(O-16:0/17:0)  
 PC(O-16:0/14:0)  
 PC(O-18:0/12:0)

Experimental mass: 790.4361

Fold change (TA+N / TN): 0.398

P value: 0.0048494

PS(22:4(7Z,10Z,13Z,16Z)/12:0)  
 PS(12:0/22:4(7Z,10Z,13Z,16Z))  
 PS(18:3(6Z,9Z,12Z)/16:1(9Z))  
 PS(17:2(9Z,12Z)/17:2(9Z,12Z))  
 PS(16:0/18:4(6Z,9Z,12Z,15Z))  
 PS(18:4(6Z,9Z,12Z,15Z)/16:0)  
 PS(16:1(9Z)/18:3(6Z,9Z,12Z))  
 PS(20:3(8Z,11Z,14Z)/14:1(9Z))  
 PS(20:4(5Z,8Z,11Z,14Z)/14:0)  
 PS(14:1(9Z)/20:3(8Z,11Z,14Z))  
 PS(18:3(9Z,12Z,15Z)/16:1(9Z))  
 PS(14:0/20:4(5Z,8Z,11Z,14Z))  
 PS(16:1(9Z)/18:3(9Z,12Z,15Z))

Experimental mass: 829.4936

Fold change (TA+N / TN): 0.49223

P value: 0.005139

PI(18:3(9Z,12Z,15Z)/16:1(9Z))  
 PI(14:0/20:4(5Z,8Z,11Z,14Z))  
 PI(18:4(6Z,9Z,12Z,15Z)/16:0)  
 PI(16:1(9Z)/18:3(6Z,9Z,12Z))  
 PI(16:1(9Z)/18:3(9Z,12Z,15Z))  
 PI(22:4(7Z,10Z,13Z,16Z)/12:0)  
 PI(12:0/22:4(7Z,10Z,13Z,16Z))  
 PI(20:3(8Z,11Z,14Z)/14:1(9Z))  
 PI(20:4(5Z,8Z,11Z,14Z)/14:0)  
 PI(18:3(6Z,9Z,12Z)/16:1(9Z))  
 PI(17:2(9Z,12Z)/17:2(9Z,12Z))  
 PI(14:1(9Z)/20:3(8Z,11Z,14Z))  
 PI(16:0/18:4(6Z,9Z,12Z,15Z))  
 PGP(16:0/18:0)  
 PGP(18:0/16:0)  
 PI(O-16:0/16:1(9Z))  
 PI(O-18:0/14:1(9Z))  
 PI(P-16:0/16:0)  
 PI(P-18:0/14:0)  
 PI(P-20:0/12:0)  
 SQDG(16:0/16:0)  
 1,2-Di-O-palmitoyl-3-O-(6-sulfoquinovopyranosyl)glycerol



Experimental mass: 1036.734  
 Fold change (TA+N / TN): 0.49118  
 P value: 0.0051402  
 FMC-6(d18:1/24:0(2-OH))  
 LacCer(d18:1/26:0)  
 LacCer(d18:0/26:1)  
 Galalpha1-4Galbeta-Cer(d18:1/26:0)  
 Manbeta1-4Glcbeta-Cer(d18:1/26:0)  
 Galabiosylceramide (d18:1/26:0)  
 Lactosylceramide (d18:1/26:0)

Experimental mass: 756.5168  
 Fold change (TA+N / TN): 0.48914  
 P value: 0.0052972  
 PS(P-18:0/17:2(9Z,12Z))

Experimental mass: 662.5535  
 Fold change (TA+N / TN): 0.45082  
 P value: 0.0059028  
 PE(O-16:0/O-16:0)[U]  
 PE(O-16:0/O-16:0)  
 Cer(t18:0/20:0(2OH))  
 Cer(t20:0/18:0(2OH))

Experimental mass: 804.4608  
 Fold change (TA+N / TN): 0.43847  
 P value: 0.0060608  
 PS(17:0/18:4(6Z,9Z,12Z,15Z))  
 PS(17:1(9Z)/18:3(6Z,9Z,12Z))  
 PS(17:1(9Z)/18:3(9Z,12Z,15Z))  
 PS(22:4(7Z,10Z,13Z,16Z)/13:0)  
 PS(17:2(9Z,12Z)/18:2(9Z,12Z))  
 PS(20:3(8Z,11Z,14Z)/15:1(9Z))  
 PS(13:0/22:4(7Z,10Z,13Z,16Z))  
 PS(18:2(9Z,12Z)/17:2(9Z,12Z))  
 PS(20:4(5Z,8Z,11Z,14Z)/15:0)  
 PS(18:3(6Z,9Z,12Z)/17:1(9Z))  
 PS(18:3(9Z,12Z,15Z)/17:1(9Z))  
 PS(15:0/20:4(5Z,8Z,11Z,14Z))  
 PS(18:4(6Z,9Z,12Z,15Z)/17:0)  
 PS(15:1(9Z)/20:3(8Z,11Z,14Z))

Experimental mass: 778.4682  
 Fold change (TA+N / TN): 0.45468  
 P value: 0.0076298  
 PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/14:0)

PS(14:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
 PS(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))  
 PS(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))  
 PS(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))  
 PS(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))  
 PS(20:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))  
 PS(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))  
 PS(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))  
 PS(16:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))

Experimental mass: 780.5185

Fold change (TA+N / TN): 0.44246

P value: 0.007689

PE(18:0/20:4(5Z,8Z,11Z,13E))(15Ke)

Experimental mass: 1003.776

Fold change (TA+N / TN): 0.48768

P value: 0.0079988

TG(22:4(7Z,10Z,13Z,16Z)/20:4(8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z))

TG(22:5(4Z,7Z,10Z,13Z,16Z)/20:3(5Z,8Z,11Z)/22:5(7Z,10Z,13Z,16Z,19Z))

TG(20:3n6/22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

*(Partial listing)*

Experimental mass: 734.5017

Fold change (TA+N / TN): 0.46628

P value: 0.0080514

PS(16:0/16:0)

PS(16:0/16:0)

PS(14:0/18:0)

PS(18:0/14:0)

PS(16:0/16:0)

PS(20:0/12:0)

PS(19:0/13:0)

PS(17:0/15:0)

PS(15:0/17:0)

PS(13:0/19:0)

PS(12:0/20:0)

Experimental mass: 782.5082

Fold change (TA+N / TN): 0.41898

P value: 0.0093905

PS(O-20:0/14:1(9Z))

PS(O-18:0/16:1(9Z))

PS(O-16:0/18:1(9Z))

PS(P-16:0/18:0)

PS(P-18:0/16:0)

PS(P-20:0/14:0)

Experimental mass: 752.4673

Fold change (TA+N / TN): 0.46172

P value: 0.0097428

PS(P-16:0/16:1(9Z))

PS(P-18:0/14:1(9Z))

Experimental mass: 604.6007

Fold change (TA+N / TN): 0.47274

P value: 0.010536

Cer(m18:1(4E)/22:0)

Experimental mass: 810.4087

Fold change (TA+N / TN): 0.43473

P value: 0.013276

PS(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))

Experimental mass: 836.4227

Fold change (TA+N / TN): 0.44307

P value: 0.015383

PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))

PS(18:4(6Z,9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z))

Experimental mass: 676.5301

Fold change (TA+N / TN): 0.4949

P value: 0.016973

PE(O-16:0/16:0)[U]

PE(O-18:0/14:0)

PE(O-20:0/12:0)

PE(O-16:0/16:0)

PC(O-14:0/15:0)

PC(O-16:0/13:0)

Experimental mass: 736.4969

Fold change (TA+N / TN): 0.46899

P value: 0.023788

PE(22:5(7Z,10Z,13Z,16Z,19Z)/14:0)

PE(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))

PE(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))

PE(22:4(7Z,10Z,13Z,16Z)/14:1(9Z))

PE(16:1(9Z)/20:4(8Z,11Z,14Z,17Z))

PE(14:0/22:5(7Z,10Z,13Z,16Z,19Z))

PE(22:5(4Z,7Z,10Z,13Z,16Z)/14:0)

PE(20:4(8Z,11Z,14Z,17Z)/16:1(9Z))

PE(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))

PE(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))  
PE(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))  
PE(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))  
PE(14:0/22:5(4Z,7Z,10Z,13Z,16Z))  
PE(20:4(5Z,8Z,11Z,14Z)/16:1(9Z))  
PE(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))  
PE(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))  
PE(14:1(9Z)/22:4(7Z,10Z,13Z,16Z))  
PE(16:0/20:5(5Z,8Z,11Z,14Z,17Z))  
PE(20:5(5Z,8Z,11Z,14Z,17Z)/16:0)  
PE(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))  
PC(20:5(5Z,8Z,11Z,14Z,17Z)/13:0)  
PC(15:1(9Z)/18:4(6Z,9Z,12Z,15Z))  
PC(18:4(6Z,9Z,12Z,15Z)/15:1(9Z))  
PC(13:0/20:5(5Z,8Z,11Z,14Z,17Z))

**Supplemental File S2: List of masses identified to be differentially affected by TN vs. TA+N that correspond to peptides**Positive mode

Experimental mass: 293.1363

Fold change (TA+N / TN): 0.48969

P value: 0.00021073

Histidiny-Histidine

Coriandrone B

11,12-Dimethoxydihydrokawain

Coriandrone A

Tetrahydrotrimethylhispidin

Negative mode

Experimental mass: 790.4361

Fold change (TA+N / TN): 0.398

P value: 0.0048494

DHOAA(AcO)-Val-Phe(NMe)-Pro-Phe(NMe)-Gly-OMe

Experimental mass: 267.1452

Fold change (TA+N / TN): 0.48336

P value: 0.0074803

Histidylleucine;

Histidiny-Leucine

Leucyl-Histidine

Histidiny-Isoleucine

Experimental mass: 1200.3263

Fold change (TA+N / TN): 0.49912

P value: 0.013454

UDPMurNAc(oyl-L-Ala-gamma-D-Glu-L-Lys-D-Ala-D-Ser)