

## Supplements

### **Lipidomics of bacterial strain *Raoultella* sp. KDF8 degrading the nonsteroidal anti-inflammatory drug diclofenac**

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#### **Isolation of lipids**

The extraction procedure was based on the method of Bligh and Dyer (1959). Briefly, the lyophilized cells were suspended in a chloroform-methanol mixture (2:1) for 30 min with stirring, and after that chloroform and water were added and the insoluble material was separated by centrifugation. The aqueous phase was aspirated off and the chloroform phase was washed three times with two parts 1 M KCl each. The resulting chloroform phase was evaporated to dryness under reduced pressure.

Total lipid extracts were applied to a Sep-Pak Vac Silica cartridge 35cc (Waters; with 10 grams of normal-phase silica), and non-polar lipids were subsequently eluted from the cartridge with 40 mL of chloroform-methanol (9:1). Polar lipids were eluted from the cartridge by a mixture of 50 mL of methanol acidified with 0.1% formic acid. The eluate of polar lipids was evaporated, and the oil samples were further hydrolysed.

Fatty acids were released from polar lipids, see above, by acid hydrolysis (2 M HCl, 100 °C, 2.5 h), extracted with hexane and methylated with 10% (w/v) methanolic BF<sub>3</sub>, (80 °C, 10 min). Gas chromatography-mass spectrometry (GC-MS) of the FAME mixture was done on a Finnigan 1020 B in EI mode. Splitless injection was at 100 °C, and a fused silica capillary column (Supelcowax 10; 60 m × 0.25 mm i.d., 0.25 mm film thickness; Supelco, Munich, Germany) was used. The temperature programme was as follows: 100 °C for 1 min, subsequently increasing at 20 °C/min to 180 °C and at 2 °C/min to 280 °C, which was maintained for 1 min. The carrier gas was helium at a linear velocity of 60 cm/s. All spectra were scanned within the range of *m/z* 50–500. The structures of FAME were confirmed by the comparison of retention times and the fragmentation patterns with those of the standard FAME (Sigma-Aldrich; Dembitsky et al. 1992. Vancura et al. 1987).

#### **Shotgun analysis**

An LTQ-Orbitrap Velos mass spectrometer (Thermo Fisher Scientific) equipped with a heated electrospray interface (HESI) was operated in negative ionization mode. The MS scan range

was performed in the FT cell and recorded within a window between 200–2000  $m/z$ . The mass resolution was set to 105 000, and the ion spray voltage was set at  $-2.5$  kV (in the negative ionization mode). The negative ionization mode used the following parameters: sheath gas flow, 18 arbitrary units (AU); auxiliary gas flow, 7 AU; ion source temperature,  $250$  °C; capillary temperature,  $230$  °C; capillary voltage,  $50$  V; and tube lens voltage,  $170$  V. Helium was used as a collision gas for collision-induced dissociation (CID) experiments. The CID normalization energy of 35% was used for the fragmentation of parent ions.

The calibration of the MS spectrometer was conducted with the use of a Pierce LTQ Orbitrap negative ion calibration solution (Thermo Fisher Scientific). The internal lock mass was used in mass spectra acquisition, i.e.,  $255.2330$   $m/z$   $[M-H]^-$  palmitic acid in the negative ESI. The mass accuracy was better than 2 ppm. The chemical structure of the compounds was confirmed with the help of the spectral database LIPtdInsD MAPtdSer<sup>®</sup> Lipidomics Gateway (<http://www.lipidmaps.org/>) and the CycloBranch program (Novak et al., 2017).

### Phosphatidic acid (PtdOH)

In the negative ESI tandem mass spectra, PtdOH molecules with palmitic acid and 9,10-methylene hexadecanoic acid mainly produce precursor ion  $[M-H]^-$  at  $m/z$  657.4503 and further 4 abundant ions at  $m/z$  421.2361, 407.2204, 403.2255, and 389.2099. These result from a loss of *sn*-1 acyl and/or *sn*-2 acyl chains as ketenes ( $R'_{(1 \text{ or } 2)}CH=C=O$ ) and neutral loss of the  $R_{(1 \text{ or } 2)}COOH$  group. In all cases, it is a loss from  $[M-H]^-$ . In addition, two ions of the  $RCOO^-$  *sn*-1 type are present in tandem MS, at  $m/z$  253.2173 and *sn*-1  $RCOO^-$  (267.2330 Da).

The remaining two abundant ions, glycerol-3-phosphate ions at  $m/z$  171.0064 and glycerol-3-phosphate ion with loss of  $H_2O$  at  $m/z$  152.9958 were also present. The individual regioisomers of the molecular PtdOH species were determined based on the above rule of preferential loss of FA from *sn*-1. The  $[M-H-R_2COOH]^-$  ion at  $m/z$  389.2099 was more abundant than the  $[M-H-R_1COOH]^-$  ion at  $m/z$  403.2255. At the same time, the ion  $[M-H-R'_2CH=C=O]^-$  at  $m/z$  407.2204 was more abundant than the ion  $[M-H-R'_1CH=C=O]^-$  at  $m/z$  421.2361. This fully confirmed the 16:1/c17:0-PtdOH structure. Other molecular species of PtdOH were determined in a similar way, which also applies to dozens of other molecular species of other phospholipids.

### Phosphatidylserine (PtdSer)

In the negative ESI tandem MS of PtdSer with palmitic and 9,10-methylene hexadecanoic acid, the acid precursor ion  $[M-H]^-$  at  $m/z$  744.4819 produces ion at  $m/z$  657.4501 resulting from loss of serine from precursor ion  $[M-H]^-$ . The tandem MS spectrum of PtdSer is very similar to the tandem MS of PtdOH. The presence and abundance of two pairs of ions having a structure resulting from loss of acyl chains as ketene ( $R'CH=C=O$ ) and serine from  $[M-H]^-$ , i.e. two ions at  $m/z$  421.2361 (loss of *sn*-1 ketene) and 407.2204 (loss of *sn*-2 ketene), and loss of  $R_1COOH$  group and serine from  $[M-H]^-$  at  $m/z$  403.2255, and loss of  $R_2COOH$  group and serine from  $[M-H]^-$  at  $m/z$  389.2099 fully confirms the above structure. In addition, the *sn*-2  $RCOO^-$  ion at  $m/z$  267.2330, the *sn*-1  $RCOO^-$  ion at  $m/z$  253.2173 and the glycerol-3-phosphate ion with loss of  $H_2O$  at  $m/z$  152.9958 were present. Therefore, the structure of this molecular species was finally determined as 16:1/c17:0-PtdSer.

### Phosphatidylethanolamine (PtdEtn)

PtdEtn was the most abundant phospholipid found in cells of the cultured bacterium regardless of the carbon source used. As noted above, three major types of ions were identified in negative tandem mass spectrometry of PtdEtn. These include primarily ions resulting from neutral loss of ketene ( $[M-H-R'CH=C=O]^-$ ), neutral loss of free fatty acid ( $[M-H-RCOOH]^-$ ) and fatty carboxylic acid anion ( $RCOO^-$ ) from ( $[M-H]^-$  ion at  $m/z$  700.4925). The polar head was identified by the presence of three ions at  $m/z$  152.9958 (glycerol-3-phosphate ion with loss of  $H_2O$ ), at  $m/z$  140.0118 (ethanolamine phosphate ion) and at  $m/z$  122.0013 (ethanolamine phosphate ion with loss of  $H_2O$ ). Based on the above rule that the abundance of fragment ions depends on the position of the acyls on the glycerol backbone, PtdEtn regioisomers can be determined. Tandem MS spectrum of molecular species of PtdEtn containing palmitoleic and 9,10-methylene hexadecanoic acids contained two pairs of ions at  $m/z$  464.2783 (loss of *sn*-1 acyl chain as ketene),  $m/z$  450.2626 (loss of *sn*-2 acyl chain as ketene),  $m/z$  446.2677 (neutral loss of *sn*-1  $RCOOH$ ), and at  $m/z$  432.2521 (neutral loss of *sn*-2  $RCOOH$ ). More abundant were always ions corresponding to loss of groups (ketene or acid) from *sn*-2 position. Furthermore, ions at  $m/z$  267.2330 (*sn*-2  $RCOO^-$  ion) and at  $m/z$  253.2173 (*sn*-1  $RCOO^-$  ion) were present in tandem MS. Therefore, it can be inferred that the resulting structure is 16:1/c17:0-PtdEtn.

### Phosphatidylinositol (PtdIns)

In the negative ESI tandem MS spectrum of PtdIns containing again palmitic and 9,10-methylene hexadecanoic acids there is an abundant precursor ion  $[M-H]^-$  at  $m/z$  819.5027. The tandem MS spectrum again contained the main fragments of the three pairs of ions formed by the loss of acyl chains as  $R'_{(1 \text{ or } 2)}CH=C=O$  and  $R_{(1 \text{ or } 2)}COOH$  from  $[M-H]^-$  and *sn*-1(2)  $RCOO^-$  ions, i.e. six ions at  $m/z$  583.2889, 569.2732, 565.2783, 551.2627, 267.2330, and 253.2173. Present are also further ions due to loss of  $R'_{(1 \text{ or } 2)}CH=C=O$  and  $R_{(1 \text{ or } 2)}COOH$  including inositol from  $[M-H]^-$ . These ions have  $m/z$  values of 421.2361, 407.2204, 403.2255, and 389.2099 Da. Other present ions confirm that the given molecular species is PtdIns. These are ions at  $m/z$  657.4501 (loss of inositol from  $[M-H]^-$ ), and five ions in the lower region of tandem MS spectrum (glycerophosphoinositol- $H_2O$  (315.0487 Da), glycerophosphoinositol-  $2xH_2O$  (297.0381 Da), inositol phosphate ion (259.0225 Da), inositol phosphate ion- $H_2O$  (241.0119 Da), inositol phosphate ion- $2xH_2O$  (223.0013 Da), and glycerol-3-phosphate ion with loss of  $H_2O$  (152.9958 Da). These data point to the structure 16:1/c17:0-PtdIns of the molecular species.

### Phosphatidylcholine (PtdCho)

PtdCho contains a quaternary amino group and acetate buffer is therefore required to measure this phospholipid in a negative ESI.  $[M+CH_3COO]^-$  ion can then be detected. In the tandem MS there is a loss of methyl group and acetate from the precursor ion, i.e.  $[M+acetate]^-$  at  $m/z$  802.5606 if PtdCho contains palmitoleic and 9,10-methylene hexadecanoic acids. Major ions, like in other phospholipids, were three pairs of neutral loss ions - ions at  $m/z$  492.3096 (loss of *sn*-1 acyl chain as ketene) and at  $m/z$  478.2939 (loss of *sn*-2 acyl chain as ketene). Further neutral loss of free fatty acids (at  $m/z$  474.2990), neutral loss of *sn*-1 fatty acid) and ion at  $m/z$  460.2834 (neutral loss of *sn*-2 fatty acid), always from ion at  $m/z$  728.5236, i.e. ( $[M+acetate]^-$ ), and acyl anions of fatty acids (267.2330 Da for *sn*-2  $RCOO^-$  ion and 253.2173 Da for *sn*-1  $RCOO^-$  ion). Other ions present in the spectrum included, e.g. ion at  $m/z$  728.5236 (loss of methyl and acetate), ion at  $m/z$  657.4501 (loss of choline and acetate), in both cases loss from precursor ion. Further, ions at  $m/z$  224.0693 (glycerophosphocholine with loss of methyl and water), at  $m/z$  168.0431 (phosphocholine

with loss of methyl) and, finally, ion at  $m/z$  152.995 (glycerol-3-phosphate ion with loss of water). The ions resulting from the tandem MS loss from the *sn*-2 position are more abundant than those resulting from the *sn*-1 loss. Further, the ionic structure of  $R_2COO^-$  is more abundant than the  $R_1COO^-$  ion. These findings are consistent with the proposed structure, which is 16:1/c17:0-PtdGro.

### Phosphatidylglycerol (PtdGro)

The negative ESI tandem MS spectra of PtdGro containing palmitic and 9,10-methylene hexadecanoic acids contained in particular the ions determining the polar heads of the phospholipid. These are ions at  $m/z$  657.4501 (loss of glycerol from the precursor ion  $[M-H]^-$  having a value of 731.4871 Da), ions at  $m/z$  245.0432 (glycerophosphoglycerol ion) and its two dehydration products at  $m/z$  of 227.0326 (minus one molecule of water) and at  $m/z$  209.0221 ( $-2 \times H_2O$ ) and also ion at  $m/z$  152.9958 (glycerol-3-phosphate ion with loss of one water). Important for the complete structure of the given PtdGro, including the determination of the regioisomers, is the presence of two groups of four ions resulting from loss of ketenes (at  $m/z$  495.2729, i.e. loss of *sn*-1 ketene, at  $m/z$  481.2572, i.e. loss of *sn*-2 ketene, both from  $[M-H]^-$ ). Further, the ions at  $m/z$  421.2361 (loss of *sn*-1 ketene and glycerol), at  $m/z$  407.2204, (loss of *sn*-2 ketene and glycerol from  $[M-H]^-$ ) and similar ions produced by the loss of fatty acids, or FA plus glycerol from  $[M-H]^-$  at  $m/z$  477.2623, at  $m/z$  463.2466, at  $m/z$  403.2255, at  $m/z$  389.2099, were identified. Of course, as with other phospholipids, two acyls are abundant, i.e. ion at  $m/z$  267.2330 (*sn*-2  $RCOO^-$  ion) and ion at  $m/z$  253.2173 (*sn*-1  $RCOO^-$  ion). Again the ions  $[M-H-R_2COOH]^-$  and  $[M-H-R'_2CH=C=O]^-$  are more abundant than the  $[M-H-R_1COOH]^-$  and  $[M-H-R'_1CH=C=O]^-$ . These facts, described also in the literature (Hsu and Turk 2009) point to the 16:1/c17:0-PtdGro structure.

### Cardiolipin (Ptd<sub>2</sub>Gro)

The last and most complex phospholipid to be analyzed was Ptd<sub>2</sub>Gro. In tandem MS spectra are primarily abundant ions of four acyls, i.e.  $R_1-R_4COO^-$  groups. The following acid moieties (acyls) at  $m/z$  281.2486 (oleic acid), 253.2173 (palmitoleic acid), 255.2330 (palmitic acid), and 267.2330 (c17:0, i.e., 9,10-methylene hexadecanoic acid) have been identified. The  $MS^2$  spectrum is dominated by  $[M-H]^-$  ion at  $m/z$  1387.9655; the ion corresponding to the double

charged  $[M-2H]^{2-}$  ion at  $m/z$  693.9825 was minor under the conditions used. The spectrum is further dominated by six ions, designated by Hsu et al. (2005) as **a**, **b**, **a**+56, **b**+56, **a**+136 and **b**+136 having the  $m/z$  values 671.4657, 659.4657, 727.4919, 715.4919, 807.4583, and 795.4583 Da. Based on the  $m/z$  values of these ions, two C34:2 and C33:1 phosphatidyl moieties can be considered to be present in the Ptd2Gro molecule. Furthermore, it was found that the ion at  $m/z$  417.2411 and the ion at  $m/z$  389.2098 respectively resulted from the loss of palmitoleic acid at *sn*-2 and oleic acid at *sn*-1. Similarly, the structure of the ions **a(b)**+56 and **a(b)**+136 and their fragmentation products have been proved. The final step was to find the connection of the two diacylglycerol moieties to central glycerol, which was done on the basis of the finding that the ion **a** at  $m/z$  727.4919 had a higher abundance than the ion **b** at  $m/z$  715.4919 in tandem MS of  $[M-H]^-$  as previously described (Hsu et al. 2005). Based on the above, the structure (18:1/16:1)(16:0/c17:0)-Ptd<sub>2</sub>Gro can be assigned to Ptd<sub>2</sub>Gro containing 4 different FA, as described above.

Fig. 1S. Quantification of lipids separated by TLC and calculated using Statistica 9 software.

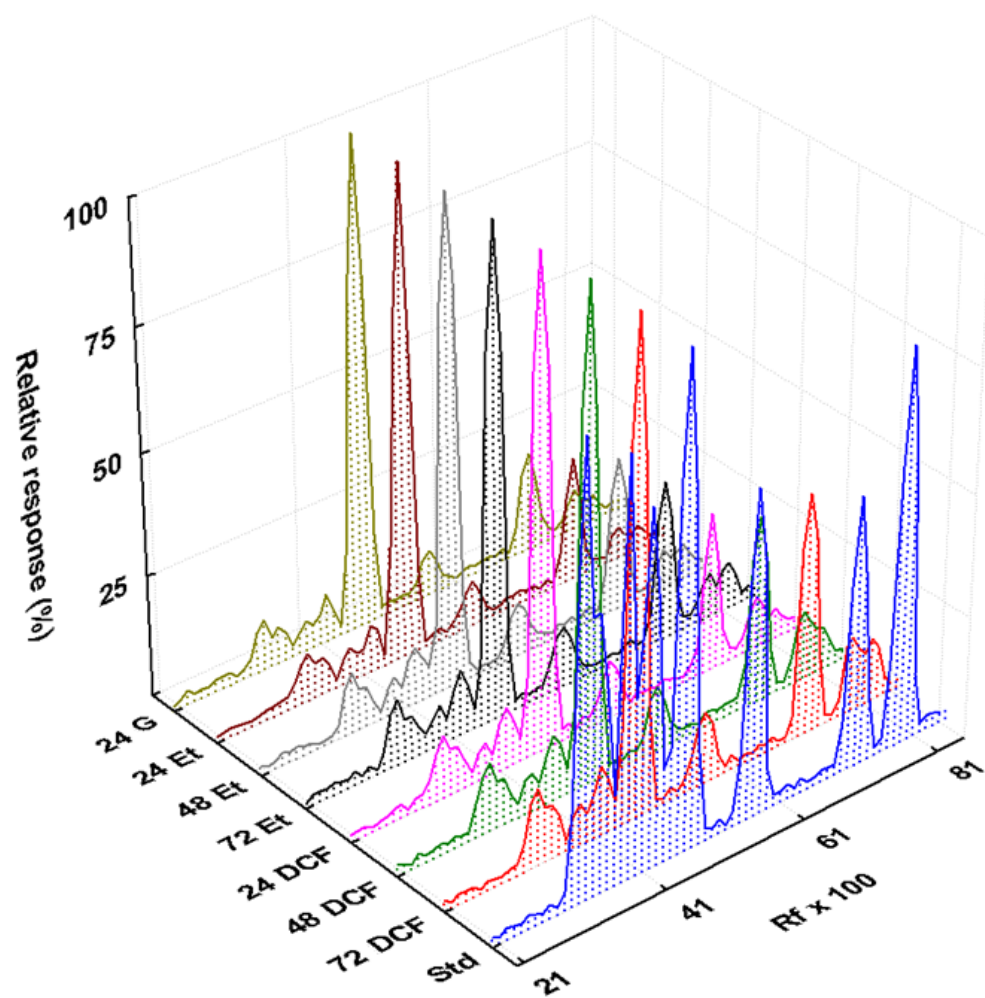


Fig. 2S. Model of 16:1/16:1-PE

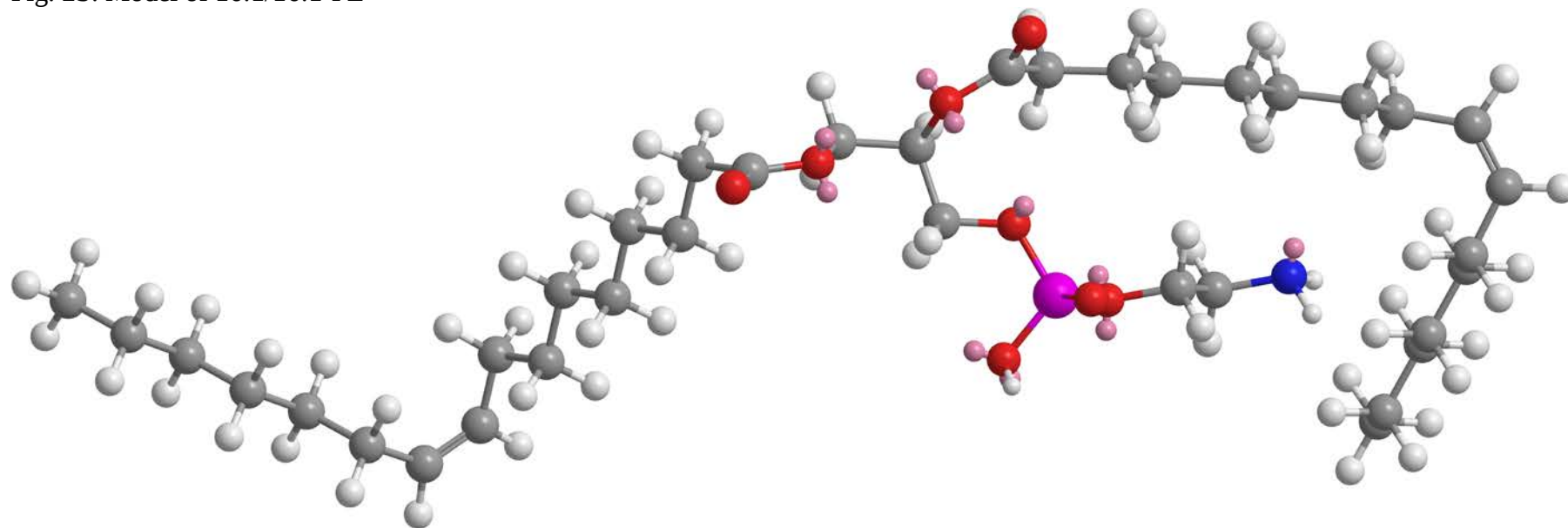


Fig. 3S. Model of c17:0/c17:0-PE

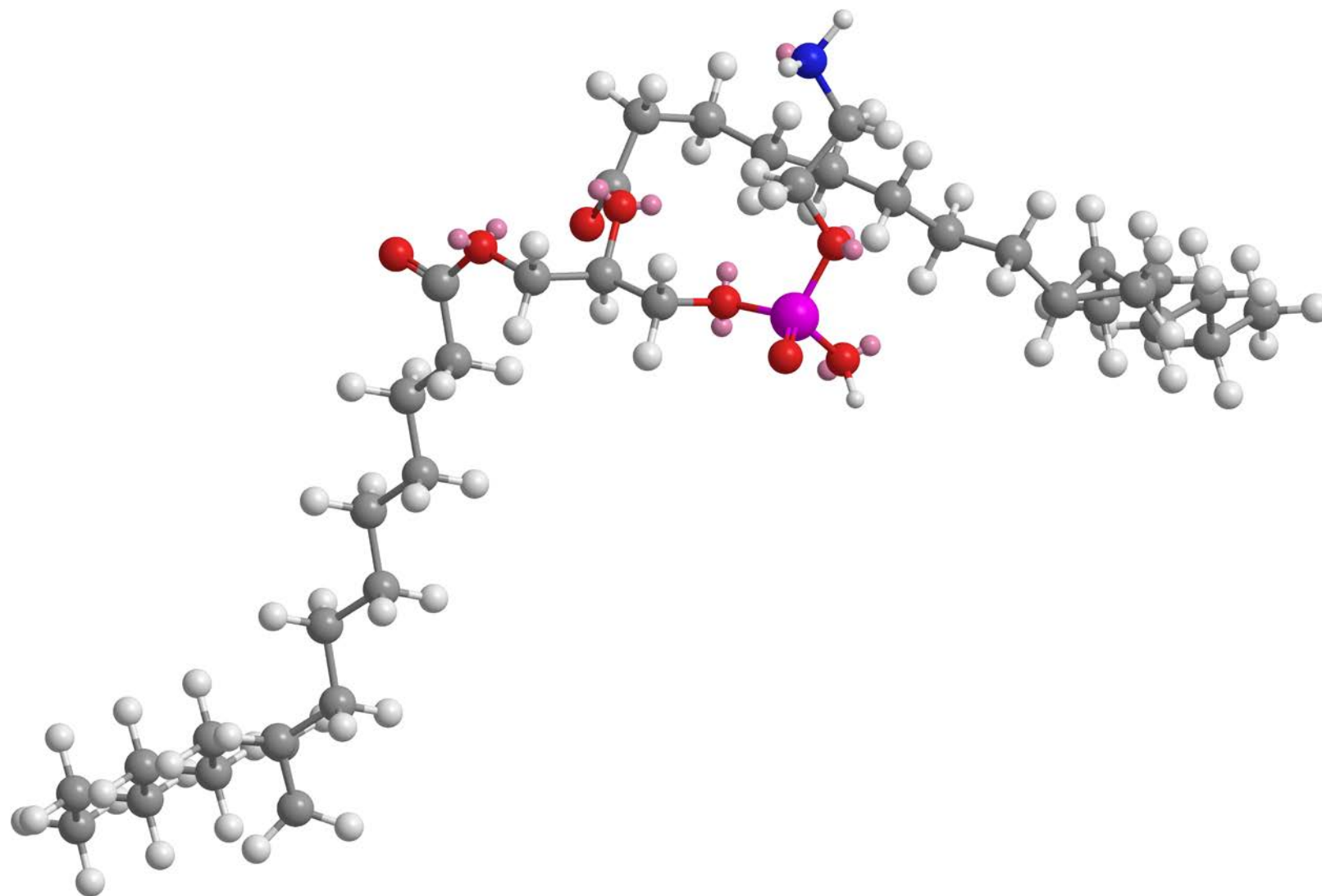


Table 1S. Selected data from two cultivations of *Raoultella* - cultivation on glycerol for 24 hours and cultivation on DCF for 72 hours.

| m/z       | CN/DB | class                | mol spec           | 24G   | 72DCF | DCF/G   | mol spec        | 24G  | 72DCF | DCF/G  | mol spec        | 24G  | 72DCF | DCF/G  | mol spec        | 24G  | 72DCF | DCF/G | 24G total | 72DCF total | 72DCF/24G |
|-----------|-------|----------------------|--------------------|-------|-------|---------|-----------------|------|-------|--------|-----------------|------|-------|--------|-----------------|------|-------|-------|-----------|-------------|-----------|
| 901.6539  | 44:1  | APtdGro <sup>a</sup> | 13:0/14:0/c17:0    | 0.01  | 1.98  | 198.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.01      | 1.98        | 198.00    |
| 915.6696  | 45:1  | APtdGro              | 14:0/14:0/c17:0    | 0.01  | 2.10  | 210.00  | 13:0/15:0/c17:0 | 0.00 | 0.36  | 360.00 |                 |      |       |        |                 |      |       |       | 0.01      | 2.46        | 223.64    |
| 927.6696  | 46:2  | APtdGro              | 13:0/16:1/c17:0    | 0.09  | 3.18  | 35.33   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.09      | 3.18        | 35.33     |
| 929.6853  | 46:1  | APtdGro              | 13:0/14:0/c19:0    | 0.00  | 0.38  | 380.00  | 14:0/15:0/c17:0 | 0.00 | 0.38  | 380.00 | 13:0/16:0/c17:0 | 0.08 | 0.40  | 5.00   |                 |      |       |       | 0.08      | 1.16        | 14.15     |
| 941.6853  | 47:2  | APtdGro              | 14:0/16:1/c17:0    | 0.19  | 3.30  | 17.37   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.19      | 3.30        | 17.37     |
| 943.7010  | 47:1  | APtdGro              | 14:0/16:0/c17:0    | 0.18  | 2.22  | 12.33   | 14:0/14:0/c19:0 | 0.00 | 0.09  | 90.00  | 13:0/15:0/c19:0 | 0.00 | 0.05  | 50.00  |                 |      |       |       | 0.18      | 2.36        | 12.97     |
| 953.6852  | 48:3  | APtdGro              | 16:1/16:1/16:1     | 3.58  | 1.46  | 0.41    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 3.58      | 1.46        | 0.41      |
| 955.7010  | 48:2  | APtdGro              | 13:0/16:1/c19:0    | 0.01  | 1.58  | 158.00  | 15:0/16:1/c17:0 | 0.04 | 0.60  | 15.00  | 13:0/18:1/c17:0 | 0.08 | 0.69  | 8.63   |                 |      |       |       | 0.13      | 2.87        | 22.08     |
| 957.7167  | 48:1  | APtdGro              | 14:0/15:0/c19:0    | 0.00  | 0.39  | 390.00  | 13:0/16:0/c19:0 | 0.01 | 0.09  | 9.00   | 15:0/16:0/c17:0 | 0.04 | 0.40  | 10.00  |                 |      |       |       | 0.05      | 0.88        | 17.25     |
| 967.7010  | 49:3  | APtdGro              | 16:1/16:1/c17:0    | 1.32  | 2.50  | 1.89    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 1.32      | 2.50        | 1.89      |
| 971.7324  | 49:1  | APtdGro              | 16:0/16:0/c17:0    | 1.43  | 2.82  | 1.97    | 14:0/16:0/c19:0 | 0.01 | 0.12  | 12.00  | 14:0/18:0/c17:0 | 0.01 | 0.38  | 38.00  |                 |      |       |       | 1.45      | 3.32        | 2.29      |
| 981.7165  | 50:3  | APtdGro              | 16:1/c17:0/c17:0   | 0.81  | 3.19  | 3.94    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.81      | 3.19        | 3.94      |
| 983.7324  | 50:2  | APtdGro              | 16:1/17:0/c17:0    | 0.33  | 3.16  | 9.58    | 13:0/18:1/c19:0 | 0.01 | 0.38  | 38.00  | 15:0/18:1/c17:0 | 0.04 | 0.69  | 17.25  |                 |      |       |       | 0.38      | 4.23        | 11.13     |
| 985.7481  | 50:1  | APtdGro              | 15:0/16:0/c19:0    | 0.00  | 0.50  | 500.00  | 14:0/17:0/c19:0 | 0.00 | 0.07  | 70.00  | 13:0/18:0/c19:0 | 0.00 | 0.05  | 50.00  |                 |      |       |       | 0.00      | 0.62        | 206.67    |
| 995.7324  | 51:3  | APtdGro              | c17:0/c17:0/c17:0  | 0.26  | 3.90  | 15.00   | 16:1/16:1/c19:0 | 0.36 | 0.57  | 1.58   |                 |      |       |        |                 |      |       |       | 0.62      | 4.47        | 7.21      |
| 997.7481  | 51:2  | APtdGro              | 16:0/18:1/c17:0    | 0.68  | 2.74  | 4.03    | 16:0/16:1/c19:0 | 0.24 | 1.82  | 7.58   |                 |      |       |        |                 |      |       |       | 0.92      | 4.56        | 4.96      |
| 999.7638  | 51:1  | APtdGro              | 16:0/16:0/c19:0    | 0.22  | 0.72  | 3.27    | 15:0/17:0/c19:0 | 0.00 | 0.05  | 50.00  | 17:0/17:0/c17:0 | 0.00 | 0.34  | 340.00 | 16:0/18:0/c17:0 | 0.08 | 0.10  | 1.25  | 0.30      | 1.21        | 4.01      |
| 1011.7638 | 52:2  | APtdGro              | 17:0/18:1/c17:0    | 0.03  | 3.61  | 120.33  | 16:1/17:0/c19:0 | 0.00 | 0.29  | 290.00 | 15:0/18:1/c19:0 | 0.00 | 0.38  | 380.00 |                 |      |       |       | 0.03      | 4.28        | 133.75    |
| 1013.7795 | 52:1  | APtdGro              | 15:0/18:0/c19:0    | 0.00  | 0.31  | 310.00  | 17:0/18:0/c17:0 | 0.00 | 0.36  | 360.00 |                 |      |       |        |                 |      |       |       | 0.00      | 0.67        | 335.00    |
| 1023.7638 | 53:3  | APtdGro              | 16:1/18:1/c19:0    | 0.22  | 3.35  | 15.23   | 18:1/18:1/c17:0 | 2.54 | 1.03  | 0.41   |                 |      |       |        |                 |      |       |       | 2.76      | 4.38        | 1.59      |
| 1025.7795 | 53:2  | APtdGro              | 18:1/18:0/c17:0    | 0.08  | 3.68  | 46.00   | 16:0/18:1/c19:0 | 0.21 | 0.43  | 2.05   |                 |      |       |        |                 |      |       |       | 0.29      | 4.11        | 14.17     |
| 1027.7952 | 53:1  | APtdGro              | 16:0/18:0/c19:0    | 0.01  | 0.53  | 53.00   | 18:0/18:0/c17:0 | 0.00 | 0.38  | 380.00 | 17:0/17:0/c19:0 | 0.00 | 0.05  | 50.00  |                 |      |       |       | 0.01      | 0.96        | 80.00     |
| 1039.7952 | 54:2  | APtdGro              | 17:0/18:1/c19:0    | 0.00  | 2.01  | 2010.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 2.01        | 2010.00   |
| 1041.8109 | 54:1  | APtdGro              | 17:0/18:0/c19:0    | 0.00  | 0.29  | 290.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.29        | 290.00    |
| 1051.7952 | 55:3  | APtdGro              | 18:1/18:1/c19:0    | 0.20  | 3.80  | 19.00   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.20      | 3.80        | 19.00     |
| 1053.8109 | 55:2  | APtdGro              | 18:1/18:0/c19:0    | 0.01  | 2.06  | 206.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.01      | 2.06        | 206.00    |
| 1055.8266 | 55:1  | APtdGro              | 18:0/18:0/c19:0    | 0.00  | 0.34  | 340.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.34        | 340.00    |
| 1183.7771 | 52:0  | Ptd2Gro              | 13:0/13:0/13:0/13: | 0.00  | 0.40  | 400.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.40        | 400.00    |
| 1197.7928 | 53:0  | Ptd2Gro              | 13:0/13:0/13:0/14: | 0.00  | 0.07  | 70.00   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.07        | 70.00     |
| 1211.8084 | 54:0  | Ptd2Gro              | 13:0/13:0/14:0/14: | 0.00  | 0.24  | 240.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.24        | 240.00    |
| 1225.8241 | 55:0  | Ptd2Gro              | 13:0/14:0/14:0/14: | 0.00  | 0.43  | 430.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.43        | 430.00    |
| 1239.8398 | 56:0  | Ptd2Gro              | 14:0/14:0/14:0/14: | 0.00  | 0.62  | 620.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.62        | 620.00    |
| 1251.8398 | 57:1  | Ptd2Gro              | 14:0/14:0/14:0/16: | 0.00  | 0.81  | 810.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.81        | 810.00    |
| 1253.8554 | 57:0  | Ptd2Gro              | 15:0/14:0/14:0/14: | 0.00  | 1.00  | 1000.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 1.00        | 1000.00   |
| 1263.8397 | 58:2  | Ptd2Gro              | 13:0/13:0/16:0/16: | 0.01  | 2.85  | 285.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.01      | 2.85        | 285.00    |
| 1265.8555 | 58:1  | Ptd2Gro              | 14:0/14:0/15:0/16: | 0.00  | 0.81  | 810.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.81        | 810.00    |
| 1267.8710 | 58:0  | Ptd2Gro              | 15:0/15:0/14:0/14: | 0.00  | 0.98  | 980.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.98        | 980.00    |
| 1277.8553 | 59:2  | Ptd2Gro              | 13:0/14:0/16:0/16: | 0.02  | 2.66  | 133.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.02      | 2.66        | 133.00    |
| 1279.8712 | 59:1  | Ptd2Gro              | 14:0/15:0/15:0/16: | 0.00  | 0.64  | 640.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.64        | 640.00    |
| 1281.8866 | 59:0  | Ptd2Gro              | 15:0/15:0/15:0/14: | 0.00  | 1.17  | 1170.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 1.17        | 1170.00   |
| 1291.8709 | 60:2  | Ptd2Gro              | 14:0/14:0/16:0/16: | 0.03  | 2.49  | 83.00   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.03      | 2.49        | 83.00     |
| 1295.9022 | 60:0  | Ptd2Gro              | 15:0/15:0/15:0/15: | 0.00  | 0.46  | 460.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.46        | 460.00    |
| 1303.8713 | 61:3  | Ptd2Gro              | 13:0/16:1/16:1/16: | 0.33  | 1.34  | 4.06    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.33      | 1.34        | 4.06      |
| 1305.8865 | 61:2  | Ptd2Gro              | 14:0/15:0/16:0/16: | 0.01  | 0.29  | 29.00   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.01      | 0.29        | 29.00     |
| 1307.9026 | 61:1  | Ptd2Gro              | 15:0/15:0/15:0/16: | 0.00  | 6.37  | 6370.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 6.37        | 6370.00   |
| 1309.9178 | 61:0  | Ptd2Gro              | 16:0/15:0/15:0/15: | 0.00  | 1.17  | 1170.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 1.17        | 1170.00   |
| 1317.8870 | 62:3  | Ptd2Gro              | 14:0/16:1/16:1/16: | 0.70  | 2.32  | 3.31    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.70      | 2.32        | 3.31      |
| 1319.9021 | 62:2  | Ptd2Gro              | 15:0/15:0/16:0/16: | 0.00  | 0.64  | 640.00  |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 0.64        | 640.00    |
| 1321.9183 | 62:1  | Ptd2Gro              | 15:0/15:0/16:0/16: | 0.00  | 6.56  | 6560.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 6.56        | 6560.00   |
| 1323.9334 | 62:0  | Ptd2Gro              | 16:0/16:0/15:0/15: | 0.00  | 1.00  | 1000.00 |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.00      | 1.00        | 1000.00   |
| 1331.9027 | 63:3  | Ptd2Gro              | 15:0/16:1/16:1/16: | 0.15  | 2.66  | 17.73   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.15      | 2.66        | 17.73     |
| 1333.9177 | 63:2  | Ptd2Gro              | 15:0/16:1/16:0/16: | 0.12  | 1.00  | 8.33    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.12      | 1.00        | 8.33      |
| 1335.9340 | 63:1  | Ptd2Gro              | 15:0/16:0/16:0/16: | 0.12  | 6.37  | 53.08   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.12      | 6.37        | 53.08     |
| 1337.9490 | 63:0  | Ptd2Gro              | 16:0/16:0/16:0/15: | 0.11  | 2.89  | 26.27   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.11      | 2.89        | 26.27     |
| 1343.9020 | 64:4  | Ptd2Gro              | 16:1/16:1/16:1/16: | 12.14 | 3.02  | 0.25    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 12.14     | 3.02        | 0.25      |
| 1345.9184 | 64:3  | Ptd2Gro              | 16:0/16:1/16:1/16: | 11.05 | 1.34  | 0.12    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 11.05     | 1.34        | 0.12      |
| 1347.9333 | 64:2  | Ptd2Gro              | 16:1/16:1/16:0/16: | 10.17 | 8.40  | 0.83    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 10.17     | 8.40        | 0.83      |
| 1349.9497 | 64:1  | Ptd2Gro              | 16:0/16:0/16:0/16: | 9.36  | 6.73  | 0.72    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 9.36      | 6.73        | 0.72      |
| 1351.9646 | 64:0  | Ptd2Gro              | 16:0/16:0/16:0/16: | 8.62  | 5.05  | 0.59    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 8.62      | 5.05        | 0.59      |
| 1357.9176 | 65:4  | Ptd2Gro              | 16:1/16:1/16:1/c17 | 1.43  | 3.38  | 2.36    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 1.43      | 3.38        | 2.36      |
| 1359.9341 | 65:3  | Ptd2Gro              | 16:0/16:1/16:1/c17 | 1.32  | 1.70  | 1.29    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 1.32      | 1.70        | 1.29      |
| 1361.9489 | 65:2  | Ptd2Gro              | 16:0/16:0/16:1/c17 | 1.21  | 9.04  | 7.47    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 1.21      | 9.04        | 7.47      |
| 1363.9654 | 65:1  | Ptd2Gro              | 16:0/16:0/16:0/c17 | 1.12  | 7.37  | 6.58    |                 |      |       |        |                 |      |       |        |                 |      |       |       | 1.12      | 7.37        | 6.58      |
| 1365.9802 | 65:0  | Ptd2Gro              | 16:0/16:0/16:0/17: | 0.09  | 5.69  | 63.22   |                 |      |       |        |                 |      |       |        |                 |      |       |       | 0.09      | 5.69        | 63.22     |

|           |      |          |                        |      |       |          |                 |      |      |      |                 |      |      |      |                 |      |      |      |      |      |       |          |
|-----------|------|----------|------------------------|------|-------|----------|-----------------|------|------|------|-----------------|------|------|------|-----------------|------|------|------|------|------|-------|----------|
| 1371.9332 | 66:4 | Ptd2Gro  | 16:1/16:1/c17:0/c17:0  | 0.17 | 4.00  | 23.53    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.17 | 4.00  | 23.53    |
| 1373.9498 | 66:3 | Ptd2Gro  | 16:0/16:1/c17:0/c17:0  | 0.16 | 1.32  | 8.25     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.16 | 1.32  | 8.25     |
| 1375.9645 | 66:2 | Ptd2Gro  | 16:0/16:0/16:1/18:1    | 8.89 | 9.67  | 1.09     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 8.89 | 9.67  | 1.09     |
| 1377.9811 | 66:1 | Ptd2Gro  | 16:0/16:0/16:0/18:1    | 8.19 | 7.99  | 0.98     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 8.19 | 7.99  | 0.98     |
| 1379.9958 | 66:0 | Ptd2Gro  | 16:0/16:0/17:0/17:0    | 0.00 | 5.74  | 5740.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 5.74  | 5740.00  |
| 1385.9488 | 67:4 | Ptd2Gro  | 16:1/c17:0/c17:0/c17:0 | 0.15 | 4.05  | 27.00    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.15 | 4.05  | 27.00    |
| 1387.9655 | 67:3 | Ptd2Gro  | 16:0/16:1/c17:0/18:1   | 1.15 | 13.94 | 12.12    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 1.15 | 13.94 | 12.12    |
| 1389.9801 | 67:2 | Ptd2Gro  | 16:0/16:0/c17:0/18:1   | 1.06 | 10.29 | 9.71     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 1.06 | 10.29 | 9.71     |
| 1389.9801 | 67:2 | Ptd2Gro  | 16:0/16:0/16:1/c19:0   | 0.09 | 8.04  | 89.33    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.09 | 8.04  | 89.33    |
| 1391.9968 | 67:1 | Ptd2Gro  | 16:0/16:0/c17:0/18:1   | 1.06 | 6.37  | 6.01     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 1.06 | 6.37  | 6.01     |
| 1394.0114 | 67:0 | Ptd2Gro  | 16:0/17:0/17:0/17:0    | 0.00 | 3.21  | 3210.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 3.21  | 3210.00  |
| 1399.9644 | 68:4 | Ptd2Gro  | c17:0/c17:0/c17:0/c17: | 0.03 | 6.37  | 212.33   |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.03 | 6.37  | 212.33   |
| 1401.9812 | 68:3 | Ptd2Gro  | 16:0/c17:0/c17:0/c17:0 | 0.02 | 0.57  | 28.50    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.02 | 0.57  | 28.50    |
| 1403.9957 | 68:2 | Ptd2Gro  | 16:0/16:0/18:1/18:1    | 7.78 | 10.93 | 1.40     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 7.78 | 10.93 | 1.40     |
| 1406.0125 | 68:1 | Ptd2Gro  | 16:0/17:0/17:0/18:1    | 0.00 | 8.62  | 8620.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 8.62  | 8620.00  |
| 1408.0270 | 68:0 | Ptd2Gro  | 17:0/17:0/17:0/17:0    | 0.00 | 6.42  | 6420.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 6.42  | 6420.00  |
| 1413.9800 | 69:4 | Ptd2Gro  | 18:1/c17:0/c17:0/c17:0 | 0.02 | 3.30  | 165.00   |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.02 | 3.30  | 165.00   |
| 1415.9969 | 69:3 | Ptd2Gro  | 16:0/c17:0/18:1/18:1   | 1.01 | 0.17  | 0.17     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 1.01 | 0.17  | 0.17     |
| 1418.0113 | 69:2 | Ptd2Gro  | 16:0/16:0/18:1/c19:0   | 0.08 | 10.98 | 137.25   |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.08 | 10.98 | 137.25   |
| 1420.0282 | 69:1 | Ptd2Gro  | 18:0/17:0/17:0/18:1    | 0.00 | 8.73  | 8730.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 8.73  | 8730.00  |
| 1422.0426 | 69:0 | Ptd2Gro  | 18:0/17:0/17:0/17:0    | 0.00 | 3.90  | 3900.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 3.90  | 3900.00  |
| 1427.9956 | 70:4 | Ptd2Gro  | 18:1/18:1/c17:0/c17:0  | 0.13 | 3.01  | 23.15    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.13 | 3.01  | 23.15    |
| 1430.0126 | 70:3 | Ptd2Gro  | 16:0/18:1/18:1/18:1    | 7.39 | 0.26  | 0.04     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 7.39 | 0.26  | 0.04     |
| 1432.0269 | 70:2 | Ptd2Gro  | 16:0/16:0/c19:0/c19:0  | 0.00 | 11.03 | 11030.00 |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 11.03 | 11030.00 |
| 1434.0439 | 70:1 | Ptd2Gro  | 18:0/18:0/17:0/18:1    | 0.00 | 8.78  | 8780.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 8.78  | 8780.00  |
| 1436.0582 | 70:0 | Ptd2Gro  | 18:0/18:0/17:0/17:0    | 0.00 | 1.39  | 1390.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 1.39  | 1390.00  |
| 1442.0112 | 71:4 | Ptd2Gro  | 18:1/18:1/18:1/c17:0   | 0.96 | 3.09  | 3.22     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.96 | 3.09  | 3.22     |
| 1444.0283 | 71:3 | Ptd2Gro  | 16:0/18:1/18:1/c19:0   | 0.08 | 0.36  | 4.50     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.08 | 0.36  | 4.50     |
| 1448.0596 | 71:1 | Ptd2Gro  | 18:0/18:0/18:0/18:1    | 0.00 | 11.08 | 11080.00 |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 11.08 | 11080.00 |
| 1450.0738 | 71:0 | Ptd2Gro  | 18:0/18:0/18:0/17:0    | 0.00 | 6.25  | 6250.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 6.25  | 6250.00  |
| 1456.0268 | 72:4 | Ptd2Gro  | 18:1/18:1/18:1/18:1    | 7.02 | 3.18  | 0.45     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 7.02 | 3.18  | 0.45     |
| 1458.0440 | 72:3 | Ptd2Gro  | 16:0/18:1/c19:0/c19:0  | 0.00 | 0.45  | 450.00   |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 0.45  | 450.00   |
| 1464.0894 | 72:0 | Ptd2Gro  | 18:0/18:0/18:0/18:0    | 0.01 | 11.13 | 1113.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.01 | 11.13 | 1113.00  |
| 1470.0424 | 73:4 | Ptd2Gro  | 18:1/18:1/18:1/c19:0   | 0.07 | 3.75  | 53.57    |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.07 | 3.75  | 53.57    |
| 1472.0597 | 73:3 | Ptd2Gro  | 16:0/c19:0/c19:0/c19:0 | 0.00 | 0.53  | 530.00   |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 0.53  | 530.00   |
| 1484.0580 | 74:4 | Ptd2Gro  | 18:1/18:1/c19:0/c19:0  | 0.00 | 8.62  | 8620.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 8.62  | 8620.00  |
| 1498.0736 | 75:4 | Ptd2Gro  | 18:1/c19:0/c19:0/c19:0 | 0.00 | 1.22  | 1220.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 1.22  | 1220.00  |
| 1512.0892 | 76:4 | Ptd2Gro  | c19:0/c19:0/c19:0/c19: | 0.00 | 6.10  | 6100.00  |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.00 | 6.10  | 6100.00  |
| 870.6593  | 44:1 | NAPtdEtn | 13:0/14:0/c17:0        | 0.13 | 0.53  | 4.08     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.13 | 0.53  | 4.08     |
| 884.6750  | 45:1 | NAPtdEtn | 14:0/14:0/c17:0        | 0.13 | 0.19  | 1.46     | 13:0/15:0/c17:0 | 0.12 | 0.67 | 5.58 |                 |      |      |      |                 |      |      |      |      | 0.25 | 0.86  | 3.44     |
| 896.6750  | 46:2 | NAPtdEtn | 13:0/16:1/c17:0        | 0.20 | 0.72  | 3.60     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.20 | 0.72  | 3.60     |
| 898.6907  | 46:1 | NAPtdEtn | 13:0/14:0/c19:0        | 0.12 | 0.33  | 2.75     | 14:0/15:0/c17:0 | 0.12 | 0.80 | 6.67 | 13:0/16:0/c17:0 | 0.20 | 0.89 | 4.45 |                 |      |      |      |      | 0.44 | 2.02  | 4.59     |
| 910.6907  | 47:2 | NAPtdEtn | 14:0/16:1/c17:0        | 0.30 | 0.46  | 1.53     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.30 | 0.46  | 1.53     |
| 912.7064  | 47:1 | NAPtdEtn | 14:0/16:0/c17:0        | 0.29 | 0.85  | 2.93     | 14:0/14:0/c19:0 | 0.12 | 0.52 | 4.33 | 13:0/15:0/c19:0 | 0.12 | 0.49 | 4.08 |                 |      |      |      |      | 0.53 | 1.86  | 3.51     |
| 922.6906  | 48:3 | NAPtdEtn | 16:1/16:1/16:1         | 4.24 | 1.79  | 0.42     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 4.24 | 1.79  | 0.42     |
| 924.7064  | 48:2 | NAPtdEtn | 13:0/16:1/c19:0        | 0.13 | 0.35  | 2.69     | 15:0/16:1/c17:0 | 0.16 | 0.99 | 6.19 | 13:0/18:1/c17:0 | 0.20 | 0.88 | 4.40 |                 |      |      |      |      | 0.49 | 2.22  | 4.53     |
| 926.7221  | 48:1 | NAPtdEtn | 14:0/15:0/c19:0        | 0.12 | 0.38  | 3.17     | 13:0/16:0/c19:0 | 0.13 | 0.45 | 3.46 | 15:0/16:0/c17:0 | 0.16 | 0.68 | 4.25 |                 |      |      |      |      | 0.41 | 1.51  | 3.68     |
| 936.7064  | 49:3 | NAPtdEtn | 16:1/16:1/c17:0        | 3.21 | 4.37  | 1.36     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 3.21 | 4.37  | 1.36     |
| 938.7221  | 49:2 | NAPtdEtn | 16:0/16:1/c17:0        | 2.97 | 8.26  | 2.78     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 2.97 | 8.26  | 2.78     |
| 940.7378  | 49:1 | NAPtdEtn | 16:0/16:0/c17:0        | 2.28 | 6.13  | 2.69     | 14:0/16:0/c19:0 | 0.13 | 0.36 | 2.77 | 14:0/18:0/c17:0 | 0.13 | 0.67 | 5.15 | 14:0/18:0/c17:0 | 0.13 | 0.58 | 4.46 | 2.67 | 7.74 | 2.90  |          |
| 950.7219  | 50:3 | NAPtdEtn | 16:1/c17:0/c17:0       | 2.67 | 8.14  | 3.05     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 2.67 | 8.14  | 3.05     |
| 952.7378  | 50:2 | NAPtdEtn | 16:1/17:0/c17:0        | 0.15 | 0.29  | 1.93     | 13:0/18:1/c19:0 | 0.13 | 0.78 | 6.00 | 15:0/18:1/c17:0 | 0.16 | 0.25 | 1.56 |                 |      |      |      |      | 0.44 | 1.32  | 3.00     |
| 954.7535  | 50:1 | NAPtdEtn | 15:0/16:0/c19:0        | 0.12 | 0.34  | 2.83     | 14:0/17:0/c19:0 | 0.12 | 0.50 | 4.17 | 13:0/18:0/c19:0 | 0.12 | 0.49 | 4.08 |                 |      |      |      |      | 0.36 | 1.33  | 3.69     |
| 964.7378  | 51:3 | NAPtdEtn | c17:0/c17:0/c17:0      | 1.83 | 9.85  | 5.38     | 16:1/18:1/c17:0 | 0.91 | 2.94 | 3.23 |                 |      |      |      |                 |      |      |      |      | 2.74 | 12.79 | 4.67     |
| 966.7535  | 51:2 | NAPtdEtn | 16:0/16:1/c19:0        | 0.34 | 0.46  | 1.35     | 16:0/18:1/c17:0 | 2.61 | 8.51 | 3.26 |                 |      |      |      |                 |      |      |      |      | 2.95 | 8.97  | 3.04     |
| 968.7692  | 51:1 | NAPtdEtn | 16:0/16:0/c19:0        | 0.33 | 0.64  | 1.94     | 15:0/17:0/c19:0 | 0.12 | 0.49 | 4.08 | 17:0/17:0/c17:0 | 0.12 | 0.56 | 4.67 | 16:0/18:0/c17:0 | 0.20 | 1.71 | 8.55 | 0.77 | 3.40 | 4.42  |          |
| 980.7692  | 52:2 | NAPtdEtn | 17:0/18:1/c17:0        | 0.15 | 0.44  | 2.93     | 16:1/17:0/c19:0 | 0.12 | 0.29 | 2.42 | 15:0/18:1/c19:0 | 0.12 | 0.17 | 1.42 |                 |      |      |      |      | 0.39 | 0.90  | 2.31     |
| 982.7849  | 52:1 | NAPtdEtn | 15:0/18:0/c19:0        | 0.12 | 0.40  | 3.33     | 17:0/18:0/c17:0 | 0.12 | 0.37 | 3.08 |                 |      |      |      |                 |      |      |      |      | 0.24 | 0.77  | 3.21     |
| 992.7692  | 53:3 | NAPtdEtn | 16:1/18:1/c19:0        | 0.33 | 0.53  | 1.61     | 18:1/18:1/c17:0 | 2.48 | 9.34 | 3.77 |                 |      |      |      |                 |      |      |      |      | 2.81 | 9.87  | 3.51     |
| 994.7849  | 53:2 | NAPtdEtn | 18:1/18:0/c17:0        | 0.20 | 0.28  | 1.40     | 16:0/18:1/c19:0 | 0.32 | 0.70 | 2.19 |                 |      |      |      |                 |      |      |      |      | 0.52 | 0.98  | 1.88     |
| 996.8006  | 53:1 | NAPtdEtn | 16:0/18:0/c19:0        | 0.13 | 0.41  | 3.15     | 18:0/18:0/c17:0 | 0.12 | 0.22 | 1.83 | 17:0/17:0/c19:0 | 0.12 | 0.24 | 2.00 |                 |      |      |      |      | 0.37 | 0.87  | 2.35     |
| 1008.8006 | 54:2 | NAPtdEtn | 17:0/18:1/c19:0        | 0.12 | 0.57  | 4.75     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.12 | 0.57  | 4.75     |
| 1010.8163 | 54:1 | NAPtdEtn | 17:0/18:0/c19:0        | 0.12 | 0.25  | 2.08     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.12 | 0.25  | 2.08     |
| 1020.8006 | 55:3 | NAPtdEtn | 18:1/18:1/c19:0        | 0.31 | 0.88  | 2.84     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.31 | 0.88  | 2.84     |
| 1022.8163 | 55:2 | NAPtdEtn | 18:1/18:0/c19:0        | 0.13 | 0.77  | 5.92     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.13 | 0.77  | 5.92     |
| 1024.8320 | 55:1 | NAPtdEtn | 18:0/18:0/c19:0        | 0.12 | 0.69  | 5.75     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.12 | 0.69  | 5.75     |
| 577.3875  | 27:0 | PtdOH    | 13:0/14:0              | 0.01 | 0.03  | 3.00     |                 |      |      |      |                 |      |      |      |                 |      |      |      |      | 0.01 | 0.03  | 3.00     |

|          |      |        |             |      |       |        |             |      |       |        |            |      |      |       |            |      |      |      |       |        |      |
|----------|------|--------|-------------|------|-------|--------|-------------|------|-------|--------|------------|------|------|-------|------------|------|------|------|-------|--------|------|
| 591.4031 | 28:0 | PtdOH  | 14:0/14:0   | 0.03 | 0.12  | 4.00   | 13:0/15:0   | 0.00 | 0.02  | 20.00  |            |      |      |       |            |      |      | 0.03 | 0.14  | 4.52   |      |
| 603.4031 | 29:1 | PtdOH  | 13:0/16:1   | 0.22 | 0.27  | 1.23   |             |      |       |        |            |      |      |       |            |      |      | 0.22 | 0.27  | 1.23   |      |
| 605.4188 | 29:0 | PtdOH  | 13:0/16:0   | 0.20 | 0.05  | 0.25   | 14:0/15:0   | 0.01 | 0.03  | 3.00   |            |      |      |       |            |      |      | 0.21 | 0.08  | 0.38   |      |
| 617.4187 | 30:1 | PtdOH  | 14:0/16:1   | 0.44 | 1.00  | 2.27   | 13:0/c17:0  | 0.03 | 0.36  | 12.00  |            |      |      |       |            |      |      | 0.47 | 1.36  | 2.89   |      |
| 619.4345 | 30:0 | PtdOH  | 14:0/16:0   | 0.40 | 0.21  | 0.53   | 15:0/15:0   | 0.00 | 0.02  | 20.00  |            |      |      |       |            |      |      | 0.40 | 0.23  | 0.57   |      |
| 631.4343 | 31:1 | PtdOH  | 14:0/c17:0  | 0.05 | 1.29  | 25.80  | 13:0/18:1   | 0.19 | 0.36  | 1.89   | 15:0/16:1  | 0.11 | 0.31 | 2.82  |            |      |      | 0.35 | 1.96  | 5.60   |      |
| 633.4502 | 31:0 | PtdOH  | 14:0/17:0   | 0.01 | 0.02  | 2.00   | 13:0/18:0   | 0.01 | 0.02  | 2.00   | 15:0/16:0  | 0.10 | 0.07 | 0.70  |            |      |      | 0.12 | 0.11  | 0.92   |      |
| 643.4346 | 32:2 | PtdOH  | 16:1/16:1   | 8.14 | 8.16  | 1.00   |             |      |       |        |            |      |      |       |            |      |      | 8.14 | 8.16  | 1.00   |      |
| 645.4499 | 32:1 | PtdOH  | 16:0/16:1   | 6.58 | 1.68  | 0.26   | 15:0/c17:0  | 0.01 | 0.40  | 40.00  | 14:0/18:0  | 0.38 | 0.07 | 0.18  |            |      |      | 6.97 | 2.15  | 0.31   |      |
| 647.4659 | 32:0 | PtdOH  | 16:0/16:0   | 6.06 | 0.34  | 0.06   |             |      |       |        |            |      |      |       |            |      |      | 6.06 | 0.34  | 0.06   |      |
| 657.4503 | 33:2 | PtdOH  | 16:1/c17:0  | 0.87 | 10.58 | 12.16  |             |      |       |        |            |      |      |       |            |      |      | 0.87 | 10.58 | 12.16  |      |
| 659.4655 | 33:1 | PtdOH  | 15:0/18:1   | 0.10 | 0.41  | 4.10   | 16:1/17:0   | 0.09 | 0.21  | 2.33   | 16:0/c17:0 | 0.80 | 2.18 | 2.73  | 14:0/c19:0 | 0.00 | 0.01 | 0.10 | 0.99  | 2.81   | 2.84 |
| 661.4816 | 33:0 | PtdOH  | 15:0/18:0   | 0.00 | 0.02  | 20.00  |             |      |       |        |            |      |      |       |            |      |      | 0.00 | 0.02  | 20.00  |      |
| 671.4660 | 34:2 | PtdOH  | c17:0/c17:0 | 0.11 | 13.74 | 124.91 | 16:1/18:1   | 5.62 | 8.64  | 1.54   |            |      |      |       |            |      |      | 5.73 | 22.38 | 3.91   |      |
| 673.4811 | 34:1 | PtdOH  | c17:0/17:0  | 0.01 | 0.27  | 27.00  | 16:0/18:1   | 5.75 | 2.22  | 0.39   | 15:0/c19:0 | 0.00 | 0.03 | 30.00 |            |      |      | 5.76 | 2.52  | 0.44   |      |
| 675.4973 | 34:0 | PtdOH  | 17:0/17:0   | 0.00 | 0.00  | 1.00   | 16:0/18:0   | 0.20 | 0.12  | 0.60   |            |      |      |       |            |      |      | 0.20 | 0.12  | 0.60   |      |
| 685.4817 | 35:2 | PtdOH  | c17:0/18:1  | 0.76 | 14.02 | 18.45  | 16:1/c19:0  | 0.09 | 1.07  | 11.89  |            |      |      |       |            |      |      | 0.85 | 15.09 | 17.75  |      |
| 687.4967 | 35:1 | PtdOH  | c17:0/18:0  | 0.03 | 0.70  | 23.33  | 16:0/c19:0  | 0.08 | 0.22  | 2.75   | 17:0/18:1  | 0.08 | 0.27 | 3.38  |            |      |      | 0.19 | 1.19  | 6.26   |      |
| 689.5130 | 35:0 | PtdOH  | 17:0/18:0   | 0.00 | 0.02  | 20.00  | 16:0/c19:0  | 0.08 | 0.22  | 2.75   |            |      |      |       |            |      |      | 0.08 | 0.24  | 2.96   |      |
| 699.4974 | 36:2 | PtdOH  | 18:1/18:1   | 5.47 | 14.29 | 2.61   | c17:0/c19:0 | 0.01 | 1.37  | 137.00 |            |      |      |       |            |      |      | 5.48 | 15.66 | 2.86   |      |
| 701.5123 | 36:1 | PtdOH  | 18:1/18:0   | 0.19 | 0.72  | 3.79   | 17:0/c19:0  | 0.00 | 0.03  | 30.00  |            |      |      |       |            |      |      | 0.19 | 0.75  | 3.93   |      |
| 703.5287 | 36:0 | PtdOH  | 18:0/18:0   | 0.01 | 0.03  | 3.00   |             |      |       |        |            |      |      |       |            |      |      | 0.01 | 0.03  | 3.00   |      |
| 713.5131 | 37:2 | PtdOH  | 18:1/c19:0  | 0.08 | 1.41  | 17.63  |             |      |       |        |            |      |      |       |            |      |      | 0.08 | 1.41  | 17.63  |      |
| 715.5279 | 37:1 | PtdOH  | 18:0/c19:0  | 0.00 | 0.07  | 70.00  |             |      |       |        |            |      |      |       |            |      |      | 0.00 | 0.07  | 70.00  |      |
| 727.5288 | 38:2 | PtdOH  | c19:0/c19:0 | 0.00 | 0.14  | 140.00 |             |      |       |        |            |      |      |       |            |      |      | 0.00 | 0.14  | 140.00 |      |
| 708.4821 | 26:0 | PtdCho | 13:0/13:0   | 0.01 | 0.00  | 0.10   |             |      |       |        |            |      |      |       |            |      |      | 0.01 | 0.00  | 0.10   |      |
| 722.4978 | 27:0 | PtdCho | 13:0/14:0   | 0.01 | 0.03  | 3.00   |             |      |       |        |            |      |      |       |            |      |      | 0.01 | 0.03  | 3.00   |      |
| 736.5134 | 28:0 | PtdCho | 14:0/14:0   | 0.02 | 0.10  | 5.00   |             |      |       |        |            |      |      |       |            |      |      | 0.02 | 0.10  | 5.00   |      |
| 748.5134 | 29:1 | PtdCho | 13:0/16:1   | 0.20 | 0.22  | 1.10   |             |      |       |        |            |      |      |       |            |      |      | 0.20 | 0.22  | 1.10   |      |
| 750.5291 | 29:0 | PtdCho | 13:0/16:0   | 0.18 | 0.05  | 0.28   | 14:0/15:0   | 0.01 | 0.03  | 3.00   |            |      |      |       |            |      |      | 0.19 | 0.08  | 0.42   |      |
| 762.5290 | 30:1 | PtdCho | 14:0/16:1   | 0.39 | 0.79  | 2.03   | 13:0/c17:0  | 0.02 | 0.29  | 14.50  |            |      |      |       |            |      |      | 0.41 | 1.08  | 2.63   |      |
| 764.5448 | 30:0 | PtdCho | 14:0/16:0   | 0.36 | 0.17  | 0.47   | 15:0/15:0   | 0.00 | 0.02  | 20.00  |            |      |      |       |            |      |      | 0.36 | 0.19  | 0.53   |      |
| 776.5446 | 31:1 | PtdCho | 14:0/c17:0  | 0.05 | 1.03  | 20.60  | 13:0/18:1   | 0.17 | 0.29  | 1.71   | 15:0/16:1  | 0.10 | 0.24 | 2.40  |            |      |      | 0.32 | 1.56  | 4.88   |      |
| 778.5605 | 31:0 | PtdCho | 14:0/17:0   | 0.00 | 0.02  | 20.00  | 13:0/18:0   | 0.01 | 0.02  | 2.00   | 15:0/16:0  | 0.09 | 0.05 | 0.56  |            |      |      | 0.10 | 0.09  | 0.89   |      |
| 788.5449 | 32:2 | PtdCho | 16:1/16:1   | 6.43 | 6.53  | 1.02   |             |      |       |        |            |      |      |       |            |      |      | 6.43 | 6.53  | 1.02   |      |
| 790.5602 | 32:1 | PtdCho | 16:0/16:1   | 5.92 | 1.34  | 0.23   | 15:0/c17:0  | 0.01 | 0.33  | 33.00  | 14:0/18:0  | 0.34 | 0.05 | 0.15  |            |      |      | 6.27 | 1.72  | 0.27   |      |
| 792.5762 | 32:0 | PtdCho | 16:0/16:0   | 5.45 | 0.27  | 0.05   | 14:0/18:0   | 0.01 | 0.05  | 5.00   |            |      |      |       |            |      |      | 5.46 | 0.32  | 0.06   |      |
| 802.5606 | 33:2 | PtdCho | 16:1/c17:0  | 2.78 | 8.47  | 3.05   |             |      |       |        |            |      |      |       |            |      |      | 2.78 | 8.47  | 3.05   |      |
| 804.5758 | 33:1 | PtdCho | 15:0/18:1   | 0.09 | 0.33  | 3.67   | 16:0/c17:0  | 0.72 | 1.75  | 2.43   | 16:1/17:0  | 0.08 | 0.17 | 2.13  |            |      |      | 0.89 | 2.25  | 2.53   |      |
| 806.5919 | 33:0 | PtdCho | 15:0/18:0   | 0.00 | 0.02  | 20.00  |             |      |       |        |            |      |      |       |            |      |      | 0.00 | 0.02  | 20.00  |      |
| 816.5763 | 34:2 | PtdCho | c17:0/c17:0 | 0.10 | 10.99 | 109.90 | 16:1/18:1   | 6.25 | 10.79 | 1.73   |            |      |      |       |            |      |      | 6.35 | 21.78 | 3.43   |      |
| 818.5914 | 34:1 | PtdCho | c17:0/17:0  | 0.01 | 0.21  | 21.00  | 16:0/18:1   | 5.18 | 1.77  | 0.34   | 15:0/c19:0 | 0.00 | 0.03 | 30.00 |            |      |      | 5.19 | 2.01  | 0.39   |      |
| 820.6076 | 34:0 | PtdCho | 17:0/17:0   | 0.00 | 0.00  | 1.00   | 16:0/18:0   | 0.18 | 0.09  | 0.50   |            |      |      |       |            |      |      | 0.18 | 0.09  | 0.50   |      |
| 830.5920 | 35:2 | PtdCho | c17:0/18:1  | 0.69 | 11.22 | 16.26  | 16:1/c19:0  | 0.08 | 0.84  | 10.50  |            |      |      |       |            |      |      | 0.77 | 12.06 | 15.66  |      |
| 832.6070 | 35:1 | PtdCho | c17:0/18:0  | 0.02 | 0.57  | 28.50  | 16:0/c19:0  | 0.07 | 0.17  | 2.43   | 17:0/18:1  | 0.07 | 0.22 | 3.14  |            |      |      | 0.16 | 0.96  | 6.00   |      |
| 834.6233 | 35:0 | PtdCho | 17:0/18:0   | 0.00 | 0.02  | 20.00  | 16:0/c19:0  | 0.07 | 0.17  | 2.4    |            |      |      |       |            |      |      |      |       |        |      |

|          |      |        |             |       |        |        |             |       |       |        |            |      |      |       |       |        |        |
|----------|------|--------|-------------|-------|--------|--------|-------------|-------|-------|--------|------------|------|------|-------|-------|--------|--------|
| 714.5082 | 34:2 | PtdEtn | c17:0/c17:0 | 1.49  | 26.24  | 17.61  | 16:1/18:1   | 75.55 | 87.50 | 0.86   |            |      |      |       | 77.04 | 113.74 | 1.48   |
| 716.5233 | 34:1 | PtdEtn | c17:0/17:0  | 0.15  | 1.87   | 12.47  | 16:0/18:1   | 80.56 | 15.55 | 0.19   | 15:0/c19:0 | 0.02 | 0.27 | 13.50 | 80.73 | 17.69  | 0.22   |
| 718.5395 | 34:0 | PtdEtn | 17:0/17:0   | 0.01  | 0.03   | 3.00   | 16:0/18:0   | 2.81  | 0.79  | 0.28   |            |      |      |       | 2.82  | 0.82   | 0.29   |
| 728.5239 | 35:2 | PtdEtn | c17:0/18:1  | 10.67 | 98.09  | 9.19   | 16:1/c19:0  | 1.22  | 7.44  | 6.10   |            |      |      |       | 11.89 | 105.53 | 8.88   |
| 730.5389 | 35:1 | PtdEtn | c17:0/18:0  | 0.37  | 4.98   | 13.46  | 16:0/c19:0  | 1.12  | 1.53  | 1.37   | 17:0/18:1  | 1.07 | 1.91 | 1.79  | 2.56  | 8.42   | 3.29   |
| 732.5552 | 35:0 | PtdEtn | 17:0/18:0   | 0.04  | 0.10   | 2.50   | 16:0/c19:0  | 1.12  | 1.53  | 1.37   |            | 0.00 | 0.00 |       | 1.16  | 1.63   | 1.41   |
| 742.5396 | 36:2 | PtdEtn | 18:1/18:1   | 76.56 | 100.00 | 1.31   | c17:0/c19:0 | 0.15  | 9.65  | 64.33  |            |      |      |       | 76.71 | 109.65 | 1.43   |
| 744.5545 | 36:1 | PtdEtn | 18:1/18:0   | 2.67  | 5.08   | 1.90   | 17:0/c19:0  | 0.01  | 0.19  | 19.00  |            |      |      |       | 2.68  | 5.27   | 1.97   |
| 746.5709 | 36:0 | PtdEtn | 18:0/18:0   | 0.09  | 0.26   | 2.89   |             |       |       |        |            |      |      |       | 0.09  | 0.26   | 2.89   |
| 756.5553 | 37:2 | PtdEtn | 18:1/c19:0  | 1.07  | 9.84   | 9.20   |             |       |       |        |            |      |      |       | 1.07  | 9.84   | 9.20   |
| 758.5701 | 37:1 | PtdEtn | 18:0/c19:0  | 0.04  | 0.50   | 12.50  |             |       |       |        |            |      |      |       | 0.04  | 0.50   | 12.50  |
| 770.5710 | 38:2 | PtdEtn | c19:0/c19:0 | 0.01  | 0.96   | 96.00  |             |       |       |        |            |      |      |       | 0.01  | 0.96   | 96.00  |
| 637.4086 | 26:0 | PtdGro | 13:0/13:0   | 0.01  | 0.00   | 0.10   |             |       |       |        |            |      |      |       | 0.01  | 0.00   | 0.10   |
| 651.4243 | 27:0 | PtdGro | 13:0/14:0   | 0.01  | 0.03   | 3.00   |             |       |       |        |            |      |      |       | 0.01  | 0.03   | 3.00   |
| 665.4399 | 28:0 | PtdGro | 14:0/14:0   | 0.02  | 0.10   | 5.00   | 13:0/15:0   | 0.00  | 0.02  | 20.00  |            |      |      |       | 0.02  | 0.12   | 5.71   |
| 677.4399 | 29:1 | PtdGro | 13:0/16:1   | 0.17  | 0.24   | 1.41   |             |       |       |        |            |      |      |       | 0.17  | 0.24   | 1.41   |
| 679.4556 | 29:0 | PtdGro | 13:0/16:0   | 0.16  | 0.05   | 0.31   | 14:0/15:0   | 0.01  | 0.03  | 3.00   |            |      |      |       | 0.17  | 0.08   | 0.47   |
| 691.4555 | 30:1 | PtdGro | 14:0/16:1   | 0.35  | 0.88   | 2.51   | 13:0/c17:0  | 0.02  | 0.31  | 15.50  |            |      |      |       | 0.37  | 1.19   | 3.22   |
| 693.4713 | 30:0 | PtdGro | 14:0/16:0   | 0.32  | 0.17   | 0.53   | 15:0/15:0   | 0.00  | 0.02  | 20.00  |            |      |      |       | 0.32  | 0.19   | 0.59   |
| 705.4711 | 31:1 | PtdGro | 14:0/c17:0  | 0.04  | 1.13   | 28.25  | 13:0/18:1   | 0.15  | 0.33  | 2.20   | 15:0/16:1  | 0.09 | 0.27 | 3.00  | 0.28  | 1.73   | 6.18   |
| 707.4870 | 31:0 | PtdGro | 14:0/17:0   | 0.00  | 0.02   | 20.00  | 13:0/18:0   | 0.01  | 0.02  | 2.00   | 15:0/16:0  | 0.08 | 0.05 | 0.63  | 0.09  | 0.09   | 0.99   |
| 717.4714 | 32:2 | PtdGro | 16:1/16:1   | 5.71  | 7.18   | 1.26   |             |       |       |        |            |      |      |       | 5.71  | 7.18   | 1.26   |
| 719.4867 | 32:1 | PtdGro | 16:0/16:1   | 5.26  | 1.48   | 0.28   | 15:0/c17:0  | 0.01  | 0.36  | 36.00  | 14:0/18:0  | 0.30 | 0.05 | 0.17  | 5.57  | 1.89   | 0.34   |
| 721.5027 | 32:0 | PtdGro | 16:0/16:0   | 4.84  | 0.31   | 0.06   | 14:0/18:0   | 0.01  | 0.05  | 5.00   |            |      |      |       | 4.85  | 0.36   | 0.07   |
| 731.4871 | 33:2 | PtdGro | 16:1/c17:0  | 2.75  | 9.31   | 3.39   |             |       |       |        |            |      |      |       | 2.75  | 9.31   | 3.39   |
| 733.5023 | 33:1 | PtdGro | 15:0/18:1   | 0.08  | 0.36   | 4.50   | 16:1/17:0   | 0.07  | 0.19  | 2.71   | 16:0/c17:0 | 0.64 | 1.92 | 3.00  | 0.79  | 2.47   | 3.13   |
| 735.5184 | 33:0 | PtdGro | 15:0/18:0   | 0.00  | 0.02   | 20.00  |             |       |       |        |            |      |      |       | 0.00  | 0.02   | 20.00  |
| 745.5028 | 34:2 | PtdGro | c17:0/c17:0 | 0.08  | 12.09  | 151.13 | 16:1/18:1   | 5.00  | 9.50  | 1.90   |            |      |      |       | 5.08  | 21.59  | 4.25   |
| 747.5179 | 34:1 | PtdGro | c17:0/17:0  | 0.01  | 0.24   | 24.00  | 16:0/18:1   | 4.60  | 1.96  | 0.43   | 15:0/c19:0 | 0.00 | 0.03 | 30.00 | 4.61  | 2.23   | 0.48   |
| 749.5341 | 34:0 | PtdGro | 17:0/17:0   | 0.00  | 0.00   | 1.00   | 16:0/18:0   | 0.16  | 0.10  | 0.63   |            |      |      |       | 0.16  | 0.10   | 0.63   |
| 759.5185 | 35:2 | PtdGro | c17:0/18:1  | 0.61  | 12.33  | 20.21  | 16:1/c19:0  | 0.07  | 0.93  | 13.29  |            |      |      |       | 0.68  | 13.26  | 19.50  |
| 761.5335 | 35:1 | PtdGro | c17:0/18:0  | 0.02  | 0.62   | 31.00  | 16:0/c19:0  | 0.06  | 0.19  | 3.17   | 17:0/18:1  | 0.06 | 0.24 | 4.00  | 0.14  | 1.05   | 7.50   |
| 763.5498 | 35:0 | PtdGro | 17:0/18:0   | 0.00  | 0.02   | 20.00  | 16:0/c19:0  | 0.06  | 0.19  | 3.17   |            |      |      |       | 0.06  | 0.21   | 3.44   |
| 773.5342 | 36:2 | PtdGro | 18:1/18:1   | 4.37  | 12.58  | 2.88   | c17:0/c19:0 | 0.01  | 1.22  | 122.00 |            |      |      |       | 4.38  | 13.80  | 3.15   |
| 775.5491 | 36:1 | PtdGro | 18:1/18:0   | 0.15  | 0.64   | 4.27   | 17:0/c19:0  | 0.00  | 0.02  | 20.00  |            |      |      |       | 0.15  | 0.66   | 4.37   |
| 777.5655 | 36:0 | PtdGro | 18:0/18:0   | 0.01  | 0.03   | 3.00   |             |       |       |        |            |      |      |       | 0.01  | 0.03   | 3.00   |
| 787.5499 | 37:2 | PtdGro | 18:1/c19:0  | 0.06  | 1.24   | 20.67  |             |       |       |        |            |      |      |       | 0.06  | 1.24   | 20.67  |
| 789.5647 | 37:1 | PtdGro | 18:0/c19:0  | 0.00  | 0.07   | 70.00  |             |       |       |        |            |      |      |       | 0.00  | 0.07   | 70.00  |
| 801.5656 | 38:2 | PtdGro | c19:0/c19:0 | 0.00  | 0.12   | 120.00 |             |       |       |        |            |      |      |       | 0.00  | 0.12   | 120.00 |
| 725.4247 | 26:0 | PtdIns | 13:0/13:0   | 0.00  | 0.00   | 1.00   |             |       |       |        |            |      |      |       | 0.00  | 0.00   | 1.00   |
| 739.4403 | 27:0 | PtdIns | 13:0/14:0   | 0.01  | 0.02   | 2.00   |             |       |       |        |            |      |      |       | 0.01  | 0.02   | 2.00   |
| 753.4560 | 28:0 | PtdIns | 14:0/14:0   | 0.02  | 0.07   | 3.50   |             |       |       |        |            |      |      |       | 0.02  | 0.07   | 3.50   |
| 765.4560 | 29:1 | PtdIns | 13:0/16:1   | 0.13  | 0.17   | 1.31   |             |       |       |        |            |      |      |       | 0.13  | 0.17   | 1.31   |
| 767.4716 | 29:0 | PtdIns | 13:0/16:0   | 0.12  | 0.03   | 0.25   | 14:0/15:0   | 0.00  | 0.02  | 20.00  |            |      |      |       | 0.12  | 0.05   | 0.41   |
| 779.4717 | 30:1 | PtdIns | 14:0/16:1   | 0.26  | 0.60   | 2.31   | 13:0/c17:0  | 0.02  | 0.21  | 10.50  |            |      |      |       | 0.28  | 0.81   | 2.89   |
| 781.4872 | 30:0 | PtdIns | 14:0/16:0   | 0.24  | 0.12   | 0.50   | 15:0/15:0   | 0.00  | 0.00  | 1.00   |            |      |      |       | 0.24  | 0.12   | 0.50   |
| 793.4874 | 31:1 | PtdIns | 14:0/c17:0  | 0.03  | 0.77   | 25.67  | 13:0/18:1   | 0.11  | 0.22  | 2.00   | 15:0/16:1  | 0.11 | 0.19 | 1.73  | 0.25  | 1.18   | 4.72   |
| 795.5028 | 31:0 | PtdIns | 14:0/17:0   | 0.00  | 0.02   | 20.00  | 13:0/18:0   | 0.00  | 0.02  | 20.00  | 15:0/16:0  | 0.10 | 0.03 | 0.30  | 0.10  | 0.07   | 0.69   |
| 805.4871 | 32:2 | PtdIns | 16:1/16:1   | 4.29  | 4.90   | 1.14   |             |       |       |        |            |      |      |       | 4.29  | 4.90   | 1.14   |
| 807.5031 | 32:1 | PtdIns | 16:0/16:1   | 3.95  | 1.01   | 0.26   | 15:0/c17:0  | 0.01  | 0.24  | 24.00  | 14:0/18:0  | 0.38 | 0.03 | 0.08  | 4.34  | 1.28   | 0.29   |
| 809.5184 | 32:0 | PtdIns | 16:0/16:0   | 3.63  | 0.21   | 0.06   | 15:0/17:0   | 0.00  | 0.00  | 1.00   | 14:0/18:0  | 0.01 | 0.03 | 3.00  | 3.64  | 0.24   | 0.07   |
| 819.5027 | 33:2 | PtdIns | 16:1/c17:0  | 1.52  | 6.36   | 4.18   |             |       |       |        |            |      |      |       | 1.52  | 6.36   | 4.18   |
| 821.5188 | 33:1 | PtdIns | 15:0/18:1   | 0.06  | 0.24   | 4.00   | 16:1/17:0   | 0.05  | 0.12  | 2.40   | 16:0/c17:0 | 0.80 | 1.31 | 1.64  | 0.91  | 1.67   | 1.84   |
| 823.5340 | 33:0 | PtdIns | 15:0/18:0   | 0.00  | 0.02   | 20.00  |             |       |       |        |            |      |      |       | 0.00  | 0.02   | 20.00  |
| 833.5183 | 34:2 | PtdIns | c17:0/c17:0 | 0.06  | 8.25   | 137.50 | 16:1/18:1   | 3.75  | 6.48  | 1.73   |            |      |      |       | 3.81  | 14.73  | 3.87   |
| 835.5345 | 34:1 | PtdIns | c17:0/17:0  | 0.01  | 0.15   | 15.00  | 16:0/18:1   | 3.45  | 1.34  | 0.39   | 15:0/c19:0 | 0.00 | 0.02 | 20.00 | 3.46  | 1.51   | 0.44   |
| 837.5496 | 34:0 | PtdIns | 16:0/18:0   | 0.12  | 0.07   | 0.58   |             |       |       |        |            |      |      |       | 0.12  | 0.07   | 0.58   |
| 847.5339 | 35:2 | PtdIns | c17:0/18:1  | 0.46  | 8.40   | 18.26  | 16:1/c19:0  | 0.05  | 0.64  | 12.80  |            |      |      |       | 0.51  | 9.04   | 17.73  |
| 849.5502 | 35:1 | PtdIns | c17:0/18:0  | 0.02  | 0.43   | 21.50  | 16:0/c19:0  | 0.05  | 0.14  | 2.80   | 17:0/18:1  | 0.08 | 0.15 | 1.88  | 0.15  | 0.72   | 4.80   |
| 851.5652 | 35:0 | PtdIns | 16:0/c19:0  | 0.05  | 0.14   | 2.80   |             |       |       |        |            |      |      |       | 0.05  | 0.14   | 2.80   |
| 861.5495 | 36:2 | PtdIns | 18:1/18:1   | 3.28  | 8.57   | 2.61   | c17:0/c19:0 | 0.01  | 0.82  | 82.00  |            |      |      |       | 3.29  | 9.39   | 2.85   |
| 863.5659 | 36:1 | PtdIns | 18:1/18:0   | 0.11  | 0.43   | 3.91   | 17:0/c19:0  | 0.00  | 0.02  | 20.00  |            |      |      |       | 0.11  | 0.45   | 4.05   |
| 865.5808 | 36:0 | PtdIns | 18:0/18:0   | 0.00  | 0.02   | 20.00  |             |       |       |        |            |      |      |       | 0.00  | 0.02   | 20.00  |
| 875.5651 | 37:2 | PtdIns | 18:1/c19:0  | 0.05  | 0.84   | 16.80  |             |       |       |        |            |      |      |       | 0.05  | 0.84   | 16.80  |
| 877.5816 | 37:1 | PtdIns | 18:0/c19:0  | 0.00  | 0.03   | 30.00  |             |       |       |        |            |      |      |       | 0.00  | 0.03   | 30.00  |
| 889.5807 | 38:2 | PtdIns | c19:0/c19:0 | 0.00  | 0.09   | 90.00  |             |       |       |        |            |      |      |       | 0.00  | 0.09   | 90.00  |
| 650.4039 | 26:0 | PtdSer | 13:0/13:0   | 0.00  | 0.00   | 1.00   |             |       |       |        |            |      |      |       | 0.00  | 0.00   | 1.00   |

|          |      |        |             |      |      |        |             |      |      |        |            |      |      |       |  |  |      |      |       |
|----------|------|--------|-------------|------|------|--------|-------------|------|------|--------|------------|------|------|-------|--|--|------|------|-------|
| 664.4195 | 27:0 | PtdSer | 13:0/14:0   | 0.01 | 0.02 | 2.00   |             |      |      |        |            |      |      |       |  |  | 0.01 | 0.02 | 2.00  |
| 678.4352 | 28:0 | PtdSer | 14:0/14:0   | 0.01 | 0.05 | 5.00   | 13:0/15:0   | 0.00 | 0.00 | 1.00   |            |      |      |       |  |  | 0.01 | 0.05 | 4.64  |
| 690.4352 | 29:1 | PtdSer | 13:0/16:1   | 0.09 | 0.10 | 1.11   |             |      |      |        |            |      |      |       |  |  | 0.09 | 0.10 | 1.11  |
| 692.4508 | 29:0 | PtdSer | 13:0/16:0   | 0.08 | 0.02 | 0.25   | 14:0/15:0   | 0.00 | 0.02 | 20.00  |            |      |      |       |  |  | 0.08 | 0.04 | 0.49  |
| 704.4509 | 30:1 | PtdSer | 14:0/16:1   | 0.17 | 0.40 | 2.35   | 13:0/c17:0  | 0.01 | 0.14 | 14.00  |            |      |      |       |  |  | 0.18 | 0.54 | 3.00  |
| 706.4664 | 30:0 | PtdSer | 14:0/16:0   | 0.16 | 0.09 | 0.56   | 15:0/15:0   | 0.00 | 0.00 | 1.00   |            |      |      |       |  |  | 0.16 | 0.09 | 0.57  |
| 718.4666 | 31:1 | PtdSer | 14:0/c17:0  | 0.02 | 0.52 | 26.00  | 13:0/18:1   | 0.08 | 0.14 | 1.75   | 15:0/16:1  | 0.04 | 0.12 | 3.00  |  |  | 0.14 | 0.78 | 5.57  |
| 720.4820 | 31:0 | PtdSer | 14:0/17:0   | 0.00 | 0.02 | 20.00  | 15:0/16:0   | 0.04 | 0.02 | 0.50   |            |      |      |       |  |  | 0.04 | 0.04 | 0.98  |
| 730.4663 | 32:2 | PtdSer | 16:1/16:1   | 3.86 | 3.26 | 0.84   |             |      |      |        |            |      |      |       |  |  | 3.86 | 3.26 | 0.84  |
| 732.4823 | 32:1 | PtdSer | 16:0/16:1   | 2.63 | 0.67 | 0.25   | 15:0/c17:0  | 0.01 | 0.15 | 15.00  | 14:0/18:0  | 0.15 | 0.03 | 0.20  |  |  | 2.79 | 0.85 | 0.30  |
| 734.4976 | 32:0 | PtdSer | 16:0/16:0   | 2.42 | 0.14 | 0.06   | 15:0/17:0   | 0.00 | 0.00 | 1.00   | 14:0/18:0  | 0.01 | 0.03 | 3.00  |  |  | 2.43 | 0.17 | 0.07  |
| 744.4819 | 33:2 | PtdSer | 16:1/c17:0  | 1.35 | 4.24 | 3.14   |             |      |      |        |            |      |      |       |  |  | 1.35 | 4.24 | 3.14  |
| 746.4980 | 33:1 | PtdSer | 15:0/18:1   | 0.04 | 0.17 | 4.25   | 16:1/17:0   | 0.03 | 0.09 | 3.00   | 16:0/c17:0 | 0.32 | 0.88 | 2.75  |  |  | 0.39 | 1.14 | 2.92  |
| 758.4975 | 34:2 | PtdSer | c17:0/c17:0 | 0.14 | 5.50 | 39.29  | 16:1/18:1   | 2.50 | 4.31 | 1.72   |            |      |      |       |  |  | 2.64 | 9.81 | 3.72  |
| 760.5137 | 34:1 | PtdSer | c17:0/17:0  | 0.00 | 0.10 | 100.00 | 16:0/18:1   | 2.30 | 0.89 | 0.39   | 15:0/c19:0 | 0.00 | 0.02 | 20.00 |  |  | 2.30 | 1.01 | 0.44  |
| 762.5288 | 34:0 | PtdSer | 16:0/18:0   | 0.08 | 0.05 | 0.63   |             |      |      |        |            |      |      |       |  |  | 0.08 | 0.05 | 0.63  |
| 772.5131 | 35:2 | PtdSer | c17:0/18:1  | 0.30 | 5.60 | 18.67  | 16:1/c19:0  | 0.03 | 0.43 | 14.33  |            |      |      |       |  |  | 0.33 | 6.03 | 18.27 |
| 774.5294 | 35:1 | PtdSer | c17:0/18:0  | 0.01 | 0.29 | 29.00  | 16:0/c19:0  | 0.03 | 0.09 | 3.00   | 17:0/18:1  | 0.03 | 0.10 | 3.33  |  |  | 0.07 | 0.48 | 6.86  |
| 776.5444 | 35:0 | PtdSer | 16:0/c19:0  | 0.03 | 0.09 | 3.00   |             |      |      |        |            |      |      |       |  |  | 0.03 | 0.09 | 3.00  |
| 786.5287 | 36:2 | PtdSer | 18:1/18:1   | 2.19 | 5.72 | 2.61   | c17:0/c19:0 | 0.00 | 0.55 | 550.00 |            |      |      |       |  |  | 2.19 | 6.27 | 2.86  |
| 788.5451 | 36:1 | PtdSer | 18:1/18:0   | 0.08 | 0.29 | 3.63   | 17:0/c19:0  | 0.00 | 0.02 | 20.00  |            |      |      |       |  |  | 0.08 | 0.31 | 3.83  |
| 790.5600 | 36:0 | PtdSer | 18:0/18:0   | 0.00 | 0.02 | 20.00  |             |      |      |        |            |      |      |       |  |  | 0.00 | 0.02 | 20.00 |
| 800.5443 | 37:2 | PtdSer | 18:1/c19:0  | 0.03 | 0.57 | 19.00  |             |      |      |        |            |      |      |       |  |  | 0.03 | 0.57 | 19.00 |
| 802.5608 | 37:1 | PtdSer | 18:0/c19:0  | 0.00 | 0.03 | 30.00  |             |      |      |        |            |      |      |       |  |  | 0.00 | 0.03 | 30.00 |
| 814.5599 | 38:2 | PtdSer | c19:0/c19:0 | 0.00 | 0.05 | 50.00  |             |      |      |        |            |      |      |       |  |  | 0.00 | 0.05 | 50.00 |

<sup>a</sup> APtdGro is acyl-PtdGro

<sup>b</sup> NAPtdEtn is acyl-PtdEtn

Fig. 1S. Quantification of rhamnolipids separated by TLC scanner and calculated using Statistica 9 software.

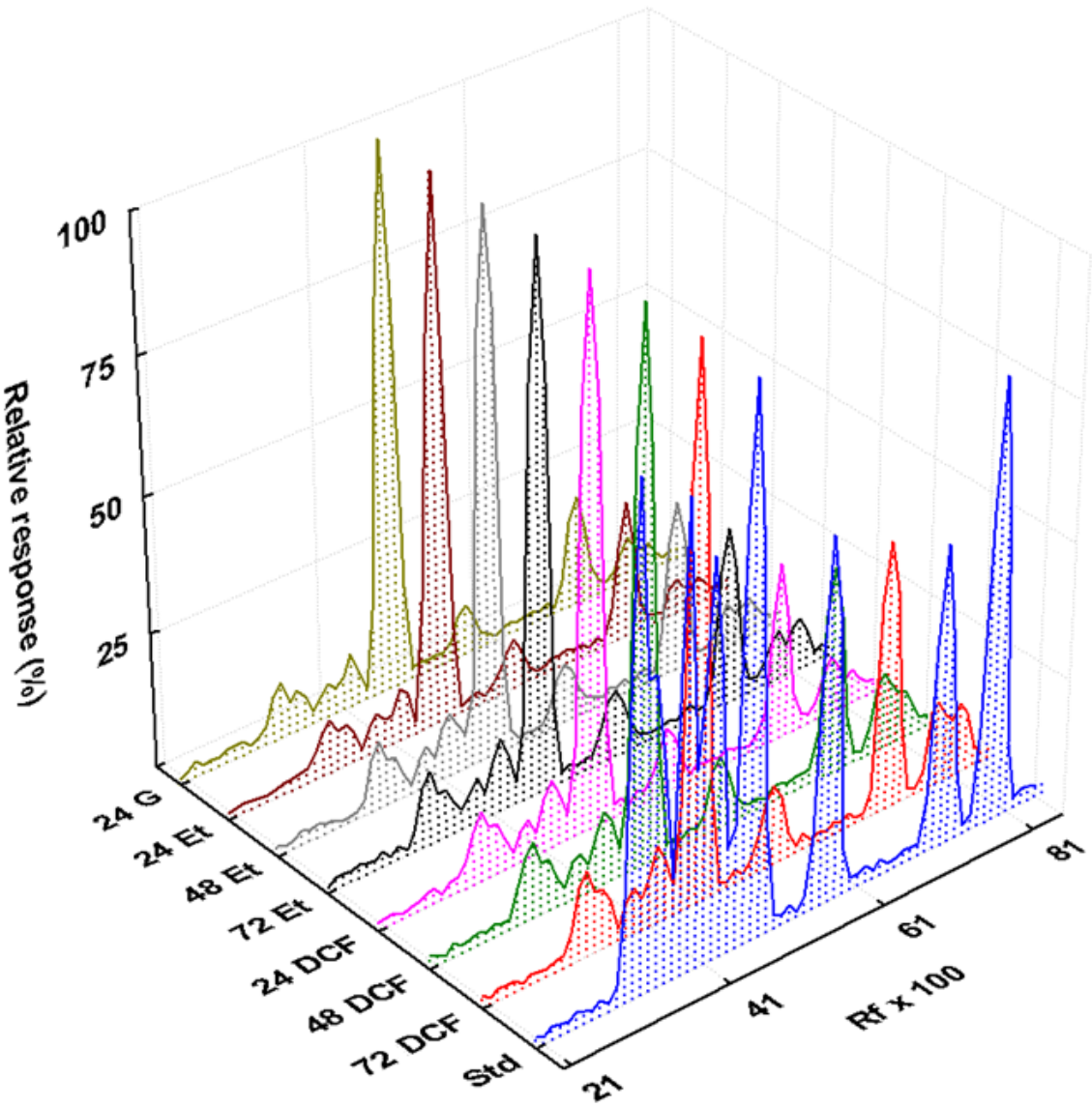


Fig. 2S. Model of 16:1/16:1-PtdEtn

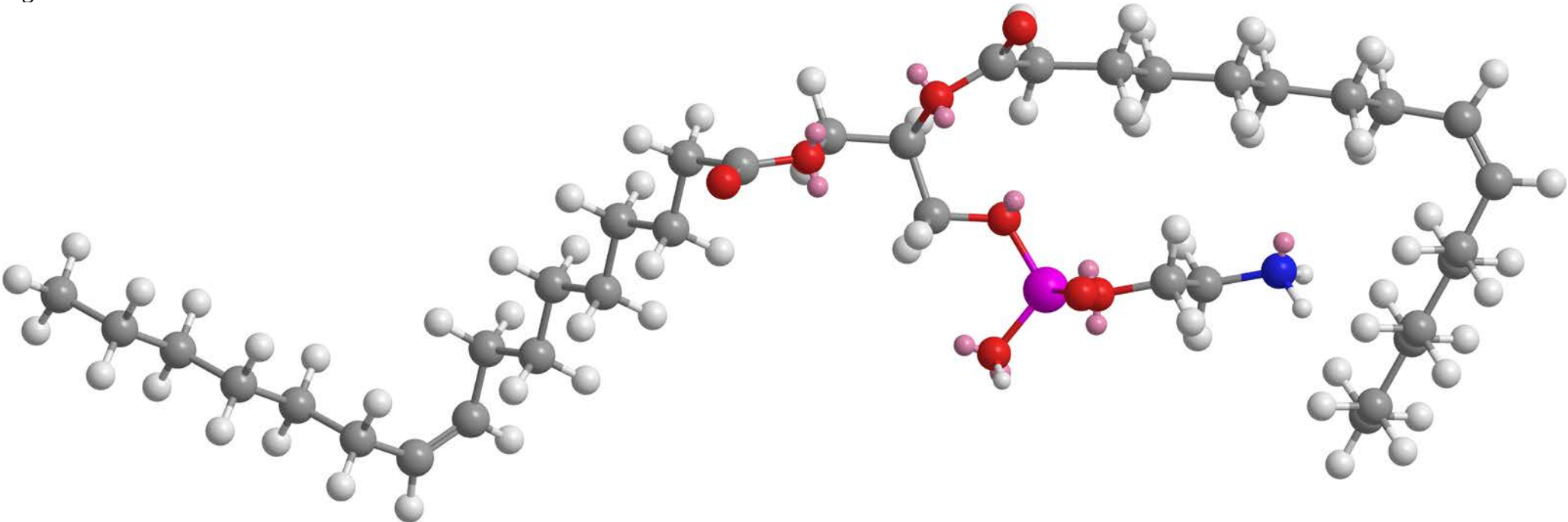


Fig. 3S. Model of c17:0/c17:0-PtdEtn

