



Supplementary 3 FigureS1 Heat treated sample group; **(A)** Venn analysis built by intersecting compounds of inoculated samples incubated at 24 (blue) and 144 (yellow), using up accumulated metabolites ($FC > 2$) compared to non-inoculated samples incubated 24 and 144 h. **(B)** Volcano Plot analysis ($p\text{-value} < 0.05$ and $FC > 2$) on 570 common VIP marker compounds identified at both 24 h and 144 h time points. **(C)** Chemical Enrichment analysis generated from the significant compounds: T1 = significant chemical class for inoculated samples at 24 h; T6= significant chemical class for inoculated samples at 144 h

Supplementary 3 Table 1 Biomarker compounds from the Volcano analysis ($p\text{-value} < 0.05$; FC value > 2) conducted using the abundance of the compounds relative to the two incubation times, results from UP-accumulated compared to the control (non-inoculated samples), common between the two incubation times (corresponding to the two levels of *P. fluorescens* 39 contamination); **(A)** Biomarker compounds Non-heat treated sample group - *P. fluorescens* 39 growth after 24 h 6 °C, **(B)** Biomarker compounds Non-heat treated sample group - *P. fluorescens* 39 growth after 144 h 6 °C, **(C)** Biomarker compounds Heat treated sample group - *P. fluorescens* 39 growth after 24 h 6 °C, **(D)** Biomarker compounds Non-heat treated sample group - *P. fluorescens* 39 growth after 144 h 6 °C.

Score description:

p-value Volcano: Volcano analysis applied to UP accumulated compounds common between T1 and T6 produced as output a pValue expressing a statistical difference between the abundance of compounds in the T1 vs T6 group

VIP score (T6vsT1): Variable importance in projection (VIP) was extracted by conducting an OPLS-DA analysis between UP-accumulated against control(CN) T1 and UP-accumulated against control(CN) T6 compounds.

VIP Standard error: VIP standard error is the standard error of the VIP Score model.

LOG2(FC)(T1PFvsT1CN): This value refers to the FC value for the final compounds and the uninoculated control sample (CN).

A

| Non-heat treated sample group -----Pseudomonas growth after 24 h 6 °C | | | | | | |
|--|--------------------------------------|----------------------|------------------------|---------------------------|---------------------------|------------------------------|
| <i>Database Code</i> | <i>Class</i> | <i>Compound Name</i> | <i>p-value Volcano</i> | <i>VIP score (T6vsT1)</i> | <i>VIP Standard error</i> | <i>LOG2(FC)(TIPFvsT1 CN)</i> |
| PAMDB0005 | Alcohols and polyols | 3-Dehydroquinate | 4.28E-05 | 1.27246 | 0.140161 | 20.33422 |
| 82 | | | | | | |
| BMDB62240 | Amino acids, peptides, and analogues | Histidinyl-Proline | 6.18E-08 | 1.27761 | 0.0594045 | 12.27888 |
| BMDB62257 | Amino acids, peptides, and analogues | Prolyl-Histidine | 6.18E-08 | 1.27761 | 0.0594045 | 12.27888 |
| BMDB63626 | Amino acids, peptides, and analogues | Glycyl-Isoleucine | 9.88E-06 | 1.27551 | 0.0925752 | 15.70902 |
| BMDB00759 | Amino acids, peptides, and analogues | Glycyl-L-leucine | 9.88E-06 | 1.27551 | 0.0925752 | 15.70902 |
| BMDB00206 | Amino acids, peptides, and analogues | N6-Acetyl-L-lysine | 9.88E-06 | 1.27551 | 0.0925752 | 15.70902 |
| BMDB00446 | Amino acids, peptides, and analogues | N-Alpha-ccetyllysine | 9.88E-06 | 1.27551 | 0.0925752 | 15.70902 |
| BMDB00670 | Amino acids, peptides, and analogues | Homo-L-arginine | 0.000804 | 1.25087 | 0.289548 | 0.33309 |
| BMDB01890 | Amino acids, peptides, and analogues | Acetylcysteine | 0.003296 | 1.23151 | 0.419201 | 1.9797 |
| BMDB62246 | Amino acids, peptides, and analogues | Leucyl-Serine | 0.003293 | 1.2306 | 0.418402 | 7.345736 |

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|-----------|--------------------------------------|-------------------------------------|----------|---------|----------|----------|
| BMDB62262 | Amino acids, peptides, and analogues | Threoninyl-Valine | 0.003293 | 1.2306 | 0.418402 | 7.345736 |
| PAMDB0001 | Amino acids, peptides, and analogues | Ureidosuccinic acid | 0.005891 | 1.22319 | 0.468699 | 0.043821 |
| 89 | | | | | | |
| BMDB00821 | Amino acids, peptides, and analogues | Phenylacetylglycine | 0.006092 | 1.22243 | 0.475567 | 0.010616 |
| BMDB01539 | Amino acids, peptides, and analogues | Dimethyl-L-arginine | 0.009645 | 1.20819 | 0.536462 | 7.656083 |
| BMDB00267 | Amino acids, peptides, and analogues | Pyroglutamic acid | 0.014315 | 1.19781 | 0.602924 | 0.559079 |
| BMDB62223 | Amino acids, peptides, and analogues | Alanyl-Proline | 0.009221 | 1.19464 | 0.580857 | 0.127488 |
| BMDB11175 | Amino acids, peptides, and analogues | L-leucyl-L-proline | 0.010535 | 1.18144 | 0.547645 | 6.729813 |
| BMDB62574 | Amino acids, peptides, and analogues | Pro-Ile | 0.010535 | 1.18144 | 0.547645 | 6.729813 |
| BMDB05960 | Amino acids, peptides, and analogues | D-Pipecolic acid | 0.023623 | 1.17629 | 0.649788 | 6.424854 |
| BMDB00716 | Amino acids, peptides, and analogues | L-Pipecolic acid | 0.023623 | 1.17629 | 0.649788 | 6.424854 |
| BMDB00070 | Amino acids, peptides, and analogues | Pipecolic acid | 0.023623 | 1.17629 | 0.649788 | 6.424854 |
| BMDB63628 | Amino acids, peptides, and analogues | Phenyl-Leucine | 0.039477 | 1.11473 | 0.768373 | 8.06525 |
| PAMDB0003 | Benzene and substituted derivatives | 4-Nitrophenol | 0.00212 | 1.24628 | 0.428985 | 6.846095 |
| 05 | | | | | | |
| PAMDB0009 | Benzene and substituted derivatives | 3-Carbamoyl-2-phenylpropionaldehyde | 0.006092 | 1.22243 | 0.475567 | 0.010616 |
| 14 | | | | | | |

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|-----------------|---|---|----------|---------|----------|----------|
| PAMDB0009 39 | Benzene and substituted derivatives | 4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one | 0.006092 | 1.22243 | 0.475567 | 0.010616 |
| PAMDB0050 09 | Benzene and substituted derivatives | Benzyl alcohol | 0.008693 | 1.20658 | 0.539232 | 1.336482 |
| PAMDB0017 47 | Benzene and substituted derivatives | p-Cresol | 0.008693 | 1.20658 | 0.539232 | 7.150248 |
| PAMDB0001 94 | Carbohydrates and carbohydrate conjugates | Nicotinamide riboside | 9.24E-05 | 1.27042 | 0.145404 | 21.32872 |
| PAMDB0001 60 | Carbohydrates and carbohydrate conjugates | Gluconic acid | 0.004859 | 1.20642 | 0.510627 | 19.2813 |
| PAMDB0000 57 | Carbohydrates and carbohydrate conjugates | Gluconolactone | 0.004859 | 1.20642 | 0.510627 | 19.2813 |
| PAMDB0017 72 | Carbohydrates and carbohydrate conjugates | L-Idonate | 0.004859 | 1.20642 | 0.510627 | 19.2813 |
| PAMDB0002 16 | Carbohydrates and carbohydrate conjugates | S-Adenosylmethioninamine | 0.012316 | 1.19274 | 0.600925 | 0.79528 |
| PAMDB0013 78 | Carboxylic acids and derivatives | L-Ala-gamma-D-Glu-Dap | 2.16E-06 | 1.27678 | 0.100431 | 11.72484 |

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|-----------|----------------------------------|----------------------------------|----------|---------|-----------|----------|
| PAMDB0002 | Carboxylic acids and derivatives | Iminoaspartic acid | 0.008628 | 1.20693 | 0.537915 | 0.074889 |
| 67 | | | | | | |
| PAMDB0001 | Carboxylic acids and derivatives | Pyrrolidonecarboxylic acid | 0.014315 | 1.19781 | 0.602924 | 0.537683 |
| 87 | | | | | | |
| PAMDB0003 | Carboxylic acids and derivatives | Pyrroline hydroxycarboxylic acid | 0.014315 | 1.19781 | 0.602924 | 0.559079 |
| 59 | | | | | | |
| PAMDB0003 | Carboxylic acids and derivatives | Pantetheine 4'-phosphate | 0.035834 | 1.15637 | 0.739801 | 9.584125 |
| 79 | | | | | | |
| PAMDB0036 | Carboxylic acids and derivatives | pantotheine 4'-phosphate | 0.035834 | 1.15637 | 0.739801 | 9.584125 |
| 06 | | | | | | |
| PAMDB1000 | Carboxylic acids and derivatives | N-isopropyl-L-glutamine | 9.88E-06 | 1.27551 | 0.0925752 | 15.70902 |
| 20 | | | | | | |
| PAMDB0036 | Diacylglycerols | DG(12:0/15:0/0:0) | 4.1E-07 | 1.27735 | 0.0581857 | 6.651486 |
| 43 | | | | | | |
| PAMDB0036 | Diacylglycerols | DG(15:0/12:0/0:0) | 4.1E-07 | 1.27735 | 0.0581857 | 6.651486 |
| 59 | | | | | | |
| PAMDB0001 | Fatty Acyls | 2-Isopropylmalic acid | 2.83E-06 | 1.2767 | 0.11142 | 11.4809 |
| 35 | | | | | | |

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|-----------|---------------------------------|-------------------------|----------|---------|-----------|----------|
| PAMDB0006 | Fatty Acyls | 3-Isopropylmalate | 2.83E-06 | 1.2767 | 0.11142 | 11.4809 |
| 41 | | | | | | |
| PAMDB0018 | Fatty Acyls | Palmitoleic acid | 0.000325 | 1.26304 | 0.285528 | 1.099567 |
| 37 | | | | | | |
| PAMDB0009 | Fatty Acyls | D-Galactonate | 0.004859 | 1.20642 | 0.510627 | 19.2813 |
| 88 | | | | | | |
| PAMDB0009 | Fatty Acyls | 7,8-Diaminononanoate | 0.008497 | 1.18366 | 0.594083 | 0.66059 |
| 57 | | | | | | |
| PAMDB0065 | Glycerophosphoglycerophosphates | PGP(12:0(3-OH)/15:0) | 1.75E-05 | 1.27516 | 0.0770524 | 5.595836 |
| 52 | | | | | | |
| PAMDB0065 | Glycerophosphoglycerophosphates | PGP(15:0/12:0(3-OH)) | 1.75E-05 | 1.27516 | 0.0770524 | 5.595836 |
| 86 | | | | | | |
| PAMDB0020 | Glycerophospholipids | PE(12:0/19:1(12Z)) | 2.66E-09 | 1.27774 | 0.0714262 | 7.766574 |
| 02 | | | | | | |
| PAMDB0067 | Glycerophospholipids | CDP-DG(10:0(3-OH)/12:0) | 5.82E-06 | 1.27625 | 0.0861194 | 7.037282 |
| 49 | | | | | | |
| PAMDB0067 | Glycerophospholipids | CDP-DG(10:0/12:0(3-OH)) | 5.82E-06 | 1.27625 | 0.0861194 | 7.037282 |
| 57 | | | | | | |

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|-----------|----------------------|---------------------------|----------|---------|-----------|----------|
| PAMDB0067 | Glycerophospholipids | CDP-DG(12:0(3-OH)/10:0) | 5.82E-06 | 1.27625 | 0.0861194 | 7.037282 |
| 60 | | | | | | |
| PAMDB0067 | Glycerophospholipids | CDP-DG(12:0/10:0(3-OH)) | 5.82E-06 | 1.27625 | 0.0861194 | 7.037282 |
| 71 | | | | | | |
| PAMDB0039 | Glycerophospholipids | PS(10:0(3-OH)/17:0cycw7c) | 0.026957 | 1.15909 | 0.74802 | 2.08493 |
| 35 | | | | | | |
| PAMDB0039 | Glycerophospholipids | PS(12:0(3-OH)/15:0cyclo) | 0.026957 | 1.15909 | 0.74802 | 2.08493 |
| 50 | | | | | | |
| PAMDB0039 | Glycerophospholipids | PS(15:0cyclo/12:0(3-OH)) | 0.026957 | 1.15909 | 0.74802 | 2.08493 |
| 84 | | | | | | |
| PAMDB0039 | Glycerophospholipids | PS(17:0cycw7c/10:0(3-OH)) | 0.026957 | 1.15909 | 0.74802 | 2.08493 |
| 95 | | | | | | |
| PAMDB0000 | Glycerophospholipids | Glycerophosphocholine | 0.037794 | 1.1336 | 0.820864 | 13.57909 |
| 32 | | | | | | |
| PAMDB0067 | Glycerophospholipids | PS(14:0/15:0cyclo) | 0.04157 | 1.13266 | 0.758625 | 0.120545 |
| 10 | | | | | | |
| PAMDB0067 | Glycerophospholipids | PS(15:0cyclo/14:0) | 0.04157 | 1.13266 | 0.758625 | 0.120545 |
| 14 | | | | | | |

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| PAMDB0067 | Glycerophospholipids | PS(17:0cycw7c/12:0) | 0.04157 | 1.13266 | 0.758625 | 0.120545 |
| 27 | | | | | | |
| PAMDB0067 | Glycerophospholipids | PS(19:0cycw8c/10:0) | 0.04157 | 1.13266 | 0.758625 | 0.120545 |
| 46 | | | | | | |
| BMDB02226 | Lipids and lipid-like molecules | Adrenic acid | 2.71E-09 | 1.27773 | 0.0831744 | 7.293566 |
| BMDB62590 | Lipids and lipid-like molecules | 5Z-hexadecenoic acid | 0.000325 | 1.26304 | 0.285528 | 1.099567 |
| BMDB12328 | Lipids and lipid-like molecules | Palmitelaidic acid | 0.000325 | 1.26304 | 0.285528 | 1.099567 |
| BMDB12971 | Lipids and lipid-like molecules | 1-Hexanol | 0.001821 | 1.23531 | 0.373137 | 0.295552 |
| BMDB00847 | Lipids and lipid-like molecules | Pelargonic acid | 0.036856 | 1.1113 | 0.822183 | 21.24929 |
| BMDB62282 | Lipids and lipid-like molecules | Pentyl butanoate | 0.036856 | 1.1113 | 0.822183 | 21.24929 |
| PAMDB0008 | Naphthalenes | (1R,2S)-Naphthalene 1,2-oxide | 0.004458 | 1.22659 | 0.447207 | 17.56378 |
| 50 | | | | | | |
| PAMDB0063 | Not Available | N2-succinylglutamate | 0.007569 | 1.2022 | 0.529412 | 8.040167 |
| 08 | | | | | | |
| PAMDB0035 | Organic phosphoric acids and derivatives | 1-Deoxy-L-glycero-tetrulose 4-phosphate | 0.017373 | 1.15201 | 0.65812 | 22.97467 |
| 12 | | | | | | |
| PAMDB1000 | Organooxygen compounds | 2-aminobenzoylacetate | 0.004859 | 1.20642 | 0.510627 | 19.2813 |
| 92 | | | | | | |

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|-----------|-------------------------------------|----------------------------------|----------|---------|----------|----------|
| PAMDB0035 | Prenol lipids 27 | Geranyl diphosphate | 0.002413 | 1.23904 | 0.37 | 0.316446 |
| PAMDB0002 | Prenol lipids 51 | Octaprenyl diphosphate | 0.002413 | 1.23904 | 0.37 | 0.316446 |
| PAMDB0005 | Purine nucleotides 09 | DIDP | 0.00217 | 1.23875 | 0.37844 | 21.88411 |
| PAMDB0004 | Pyrrolopyrimidines 03 | Queuine | 0.000714 | 1.2604 | 0.254861 | 0.847293 |
| PAMDB1000 | Signaling molecule 77 | N-Butanoyl-D-homoserine lactone | 0.005801 | 1.22356 | 0.467017 | 14.65361 |
| PAMDB1000 | Signaling molecule 73 | 2-nonyl-4-hydroxyquinoline (NHQ) | 0.03253 | 1.15514 | 0.79634 | 0.200451 |
| PAMDB0054 | Tetralins 78 | tRNA(Tyr) | 0.005888 | 1.22333 | 0.468036 | 15.49892 |
| PAMDB0001 | Tetrapyrroles and derivatives 51 | Coproporphyrin III | 0.00034 | 1.25966 | 0.256728 | 5.76322 |

B

| Non-heat treated sample group -----Pseudomonas growth after 144 h 6 °C | | | | | | |
|--|---|--|-----------------|--------------------|--------------------|----------------------|
| Database Code | Class | Compound Name | p-value Volcano | VIP score (T6vsT1) | VIP Standard error | LOG2(FC)(T1PFvsT1CN) |
| BMDB018 90 | Amino acids, peptides, and analogues_T6 | Acetylcysteine | 0.032862 | 1.23151 | 0.419201 | 1.9797 |
| BMDB625 59 | Amino acids, peptides, and analogues_T6 | Ile-Ile-Ile-Pro | 0.018056 | 1.19352 | 0.688296 | 0.149989 |
| BMDB622 32 | Amino acids, peptides, and analogues_T6 | Glutaminyllysine | 0.012877 | 1.17882 | 0.607882 | 6.379116 |
| BMDB625 72 | Amino acids, peptides, and analogues_T6 | Phe-Pro-Ile | 0.029662 | 1.10502 | 0.724945 | 7.168326 |
| BMDB621 97 | Amino acids, peptides, and analogues_T6 | N-(2-Oxohexanoyl)homoserine lactone | 0.042278 | 1.06648 | 0.833997 | 0.040207 |
| PAMDB00 1585 | Carboxylic acids and derivatives _T6 | 5,10-Methenyltetrahydrofolate | 0.010337 | 1.19848 | 0.642769 | 5.401918 |
| PAMDB00 0094 | Diazines _T6 | Orotic acid | 0.02777 | 1.13715 | 0.626357 | 4.783832 |
| PAMDB00 0968 | Fatty Acyls _T6 | Benzoyl acetyl-CoA | 3.38E-07 | 1.27725 | 0.091134 | 0.276173 |
| PAMDB00 0536 | Fatty Acyls _T6 | (S)-Hydroxyoctanoyl-CoA | 3.84E-07 | 1.27721 | 0.092011 | 0.276173 |
| PAMDB00 1517 | Glycerolipids _T6 | 1,2-Diacyl-sn-glycerol (ditetradec-7-enoyl, n-C14:1) | 0.007938 | 1.18716 | 0.557108 | 0.618484 |
| PAMDB00 1676 | Glycerophosphoglycerophosphates _T6 | PGP(14:0/14:0) | 6.73E-09 | 1.27771 | 0.076302 | 0.276173 |
| PAMDB00 6594 | Glycerophosphoglycerophosphates _T6 | PGP(15:0cyclo/15:0cyclo) | 6.41E-09 | 1.27771 | 0.07629 | 0.276173 |
| PAMDB00 6557 | Glycerophosphoglycerophosphates _T6 | PGP(12:0(3-OH)/18:1(9Z)) | 1.2E-08 | 1.27768 | 0.076512 | 0.276173 |

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|-----------------|--|----------------------------|----------|---------|----------|----------|
| PAMDB00 6568 | Glycerophosphoglycerophosphates _T6 | PGP(14:0(3-OH)/14:0(3-OH)) | 1.27E-08 | 1.27768 | 0.07684 | 0.276173 |
| PAMDB00 6573 | Glycerophosphoglycerophosphates _T6 | PGP(14:0(3-OH)/16:1(9Z)) | 1.2E-08 | 1.27768 | 0.076512 | 0.276173 |
| PAMDB00 6609 | Glycerophosphoglycerophosphates _T6 | PGP(16:1(9Z)/14:0(3-OH)) | 1.2E-08 | 1.27768 | 0.076512 | 0.276173 |
| PAMDB00 6625 | Glycerophosphoglycerophosphates _T6 | PGP(18:1(9Z)/12:0(3-OH)) | 1.2E-08 | 1.27768 | 0.076512 | 0.276173 |
| PAMDB00 6539 | Glycerophosphoglycerophosphates _T6 | PGP(10:0(3-OH)/18:1(9Z)) | 3.07E-08 | 1.27761 | 0.07822 | 0.276173 |
| PAMDB00 6555 | Glycerophosphoglycerophosphates _T6 | PGP(12:0(3-OH)/16:1(9Z)) | 3.07E-08 | 1.27761 | 0.07822 | 0.276173 |
| PAMDB00 6608 | Glycerophosphoglycerophosphates _T6 | PGP(16:1(9Z)/12:0(3-OH)) | 3.07E-08 | 1.27761 | 0.07822 | 0.276173 |
| PAMDB00 6624 | Glycerophosphoglycerophosphates _T6 | PGP(18:1(9Z)/10:0(3-OH)) | 3.07E-08 | 1.27761 | 0.07822 | 0.276173 |
| PAMDB00 6545 | Glycerophosphoglycerophosphates _T6 | PGP(10:0/19:iso) | 3.63E-08 | 1.2776 | 0.074608 | 0.276173 |
| PAMDB00 6650 | Glycerophosphoglycerophosphates _T6 | PGP(19:iso/10:0) | 1.41E-05 | 1.2776 | 0.074608 | 0.276173 |
| PAMDB00 6409 | Glycerophosphoglycerophosphates _T6 | PGP(16:1(9Z)/12:0) | 4.01E-05 | 1.27719 | 0.081166 | 0.276173 |
| PAMDB00 6541 | Glycerophosphoglycerophosphates _T6 | PGP(10:0(3-OH)/19:iso) | 1.21E-05 | 1.27438 | 0.139491 | 0.276173 |
| PAMDB00 6570 | Glycerophosphoglycerophosphates _T6 | PGP(14:0(3-OH)/15:0) | 1.21E-05 | 1.27438 | 0.139491 | 0.276173 |
| PAMDB00 6649 | Glycerophosphoglycerophosphates _T6 | PGP(19:iso/10:0(3-OH)) | 0.007343 | 1.27438 | 0.139491 | 0.276173 |
| PAMDB00 1677 | Glycerophosphoglycerophosphates _T6 | PGP(14:1(7Z)/14:1(7Z)) | 0.003621 | 1.27083 | 0.168696 | 0.276173 |

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|-----------------|--|---|----------|---------|----------|----------|
| PAMDB00 6538 | Glycerophosphoglycerophosphates _T6 | PGP(10:0(3-OH)/17:0cycw7c) | 0.000047 | 1.27062 | 0.163213 | 0.276173 |
| PAMDB00 6553 | Glycerophosphoglycerophosphates _T6 | PGP(12:0(3-OH)/15:0cyclo) | 0.000047 | 1.27062 | 0.163213 | 0.276173 |
| PAMDB00 6591 | Glycerophosphoglycerophosphates _T6 | PGP(15:0cyclo/12:0(3-OH)) | 0.000047 | 1.27062 | 0.163213 | 0.276173 |
| PAMDB00 6613 | Glycerophosphoglycerophosphates _T6 | PGP(17:0cycw7c/10:0(3-OH)) | 0.000047 | 1.27062 | 0.163213 | 0.276173 |
| PAMDB00 6610 | Glycerophosphoglycerophosphates _T6 | PGP(16:1(9Z)/17:0cycw7c) | 0.00852 | 1.21644 | 0.573545 | 0.276173 |
| PAMDB00 6618 | Glycerophosphoglycerophosphates _T6 | PGP(17:0cycw7c/16:1(9Z)) | 0.00852 | 1.21644 | 0.573545 | 0.276173 |
| PAMDB00 6627 | Glycerophosphoglycerophosphates _T6 | PGP(18:1(9Z)/15:0cyclo) | 0.00852 | 1.21644 | 0.573545 | 0.276173 |
| PAMDB00 6955 | Glycerophospholipids _T6 | CL(10:0(3-OH)/12:0/10:0(3-OH)/12:0) | 3.38E-09 | 1.27773 | 0.075253 | 0.276173 |
| PAMDB00 6964 | Glycerophospholipids _T6 | CL(10:0/12:0(3-OH)/10:0/12:0(3-OH)) | 3.38E-09 | 1.27773 | 0.075253 | 0.276173 |
| PAMDB00 6967 | Glycerophospholipids _T6 | CL(12:0(3-OH)/10:0/12:0(3-OH)/10:0) | 3.38E-09 | 1.27773 | 0.075253 | 0.276173 |
| PAMDB00 6979 | Glycerophospholipids _T6 | CL(12:0/10:0(3-OH)/12:0/10:0(3-OH)) | 3.38E-09 | 1.27773 | 0.075253 | 0.276173 |
| PAMDB00 6954 | Glycerophospholipids _T6 | CL(10:0(3-OH)/12:0(3-OH)/10:0(3-OH)/12:0(3-OH)) | 6.33E-09 | 1.27771 | 0.075454 | 0.276173 |
| PAMDB00 6966 | Glycerophospholipids _T6 | CL(12:0(3-OH)/10:0(3-OH)/12:0(3-OH)/10:0(3-OH)) | 6.33E-09 | 1.27771 | 0.075454 | 0.276173 |
| PAMDB00 3954 | Glycerophospholipids _T6 | PS(12:0(3-OH)/18:1(9Z)) | 3.1E-08 | 1.27761 | 0.074397 | 0.276173 |
| PAMDB00 3970 | Glycerophospholipids _T6 | PS(14:0(3-OH)/16:1(9Z)) | 3.1E-08 | 1.27761 | 0.074397 | 0.276173 |

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|-----------------|--------------------------|-------------------------------------|----------|---------|----------|----------|
| PAMDB00 3993 | Glycerophospholipids _T6 | PS(16:1(9Z)/14:0(3-OH)) | 3.1E-08 | 1.27761 | 0.074397 | 0.276173 |
| PAMDB00 4000 | Glycerophospholipids _T6 | PS(18:1(9Z)/12:0(3-OH)) | 3.1E-08 | 1.27761 | 0.074397 | 0.276173 |
| PAMDB00 2026 | Glycerophospholipids _T6 | PE(19:0cycw8c/12:0) | 8.48E-08 | 1.27747 | 0.079929 | 0.276173 |
| PAMDB00 6675 | Glycerophospholipids _T6 | PE(16:0/19:0cycv8c) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 3898 | Glycerophospholipids _T6 | PE(16:1(9Z)/19:iso) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 2020 | Glycerophospholipids _T6 | PE(18:0/17:0cycw7c) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 1474 | Glycerophospholipids _T6 | PE(18:1(11Z)/17:0) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 6695 | Glycerophospholipids _T6 | PE(19:0cycv8c/16:0) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 3920 | Glycerophospholipids _T6 | PE(19:iso/16:1(9Z)) | 1.43E-07 | 1.27742 | 0.080868 | 0.276173 |
| PAMDB00 6853 | Glycerophospholipids _T6 | CDP-DG(19:iso/19:0cycv8c) | 4.66E-07 | 1.27711 | 0.083882 | 0.276173 |
| PAMDB00 6953 | Glycerophospholipids _T6 | CL(10:0(3-OH)/10:0/10:0(3-OH)/10:0) | 4.66E-07 | 1.27711 | 0.083882 | 0.276173 |
| PAMDB00 6963 | Glycerophospholipids _T6 | CL(10:0/10:0(3-OH)/10:0/10:0(3-OH)) | 4.66E-07 | 1.27711 | 0.083882 | 0.276173 |
| PAMDB00 1500 | Glycerophospholipids _T6 | PG(16:0/19:0) | 4.16E-07 | 1.27709 | 0.084081 | 0.276173 |
| PAMDB00 4086 | Glycerophospholipids _T6 | PG(16:0/19:iso) | 4.16E-07 | 1.27709 | 0.084081 | 0.276173 |
| PAMDB00 1448 | Glycerophospholipids _T6 | PG(19:0/16:0) | 4.16E-07 | 1.27709 | 0.084081 | 0.276173 |

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| PAMDB00 4111 | Glycerophospholipids _T6 | PG(19:iso/16:0) | 4.16E-07 | 1.27709 | 0.084081 | 0.276173 |
| PAMDB00 0798 | Glycerophospholipids _T6 | PG(18:1(11Z)/16:1(9Z)) | 4.52E-07 | 1.27706 | 0.084458 | 0.276173 |
| PAMDB00 6501 | Glycerophospholipids _T6 | PG(16:0/19:1(9Z)) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 1491 | Glycerophospholipids _T6 | PG(16:1(9Z)/19:0) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 4090 | Glycerophospholipids _T6 | PG(16:1(9Z)/19:iso) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 1485 | Glycerophospholipids _T6 | PG(17:0/18:1(11Z)) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 1483 | Glycerophospholipids _T6 | PG(18:1(11Z)/17:0) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 1488 | Glycerophospholipids _T6 | PG(19:0/16:1(9Z)) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 6517 | Glycerophospholipids _T6 | PG(19:0cycv8c/16:0) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 6525 | Glycerophospholipids _T6 | PG(19:1(9Z)/16:0) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 4112 | Glycerophospholipids _T6 | PG(19:iso/16:1(9Z)) | 6.04E-06 | 1.27516 | 0.113525 | 0.276173 |
| PAMDB00 3934 | Glycerophospholipids _T6 | PS(10:0(3-OH)/16:1(9Z)) | 3.19E-05 | 1.27378 | 0.202015 | 18.07214 |
| PAMDB00 3991 | Glycerophospholipids _T6 | PS(16:1(9Z)/10:0(3-OH)) | 3.19E-05 | 1.27378 | 0.202015 | 18.07214 |
| PAMDB00 4102 | Glycerophospholipids _T6 | PG(19:0cycv8c/19:iso) | 0.00005 | 1.27083 | 0.180677 | 0.276173 |
| PAMDB00 4115 | Glycerophospholipids _T6 | PG(19:iso/19:0cycv8c) | 0.00005 | 1.27083 | 0.180677 | 0.276173 |

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| PAMDB00 3948 | Glycerophospholipids _T6 | PS(12:0(3-OH)/14:0(3-OH)) | 0.000573 | 1.2599 | 0.334872 | 0.276173 |
| PAMDB00 3964 | Glycerophospholipids _T6 | PS(14:0(3-OH)/12:0(3-OH)) | 0.000573 | 1.2599 | 0.334872 | 0.276173 |
| PAMDB00 1572 | Glycerophospholipids _T6 | 2-octadecanoyl-sn-glycerol 3-phosphate | 0.000569 | 1.25989 | 0.282614 | 14.85499 |
| PAMDB00 6218 | Glycerophospholipids _T6 | LPA(18:0/0:0) | 0.000569 | 1.25989 | 0.282614 | 14.85499 |
| PAMDB00 3860 | Glycerophospholipids _T6 | PE(12:0(3-OH)/19:iso) | 0.00042 | 1.25974 | 0.308052 | 0.114885 |
| PAMDB00 3914 | Glycerophospholipids _T6 | PE(19:iso/12:0(3-OH)) | 0.00042 | 1.25974 | 0.308052 | 0.114885 |
| PAMDB00 6365 | Glycerophospholipids _T6 | sn-glycero-3-phosphocholine | 0.001227 | 1.25535 | 0.406735 | 12.19687 |
| PAMDB00 3745 | Glycerophospholipids _T6 | CDP-DG(15:0/19:1(9Z)) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 0711 | Glycerophospholipids _T6 | CDP-DG(16:0/18:1(9Z)) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 3757 | Glycerophospholipids _T6 | CDP-DG(16:1(9Z)/18:0) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 3764 | Glycerophospholipids _T6 | CDP-DG(18:0/16:1(9Z)) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 0726 | Glycerophospholipids _T6 | CDP-DG(18:1(11Z)/16:0) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 0735 | Glycerophospholipids _T6 | CDP-DG(18:1(9Z)/16:0) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 3776 | Glycerophospholipids _T6 | CDP-DG(19:1(9Z)/15:0) | 0.001275 | 1.25312 | 0.406637 | 0.019423 |
| PAMDB00 6805 | Glycerophospholipids _T6 | CDP-DG(16:0/19:0cycw8c) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |

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| PAMDB00 3751 | Glycerophospholipids _T6 | CDP-DG(16:0/19:1(9Z)) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 6809 | Glycerophospholipids _T6 | CDP-DG(16:1(9Z)/19:0) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 6827 | Glycerophospholipids _T6 | CDP-DG(18:1(11Z)/17:0) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 6834 | Glycerophospholipids _T6 | CDP-DG(19:0/16:1(9Z)) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 6840 | Glycerophospholipids _T6 | CDP-DG(19:0cycv8c/16:0) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 3777 | Glycerophospholipids _T6 | CDP-DG(19:1(9Z)/16:0) | 0.001495 | 1.25245 | 0.416628 | 0.276173 |
| PAMDB00 4050 | Glycerophospholipids _T6 | PG(12:0(3-OH)/18:1(9Z)) | 0.001725 | 1.24974 | 0.417768 | 7.727007 |
| PAMDB00 4066 | Glycerophospholipids _T6 | PG(14:0(3-OH)/16:1(9Z)) | 0.001725 | 1.24974 | 0.417768 | 7.727007 |
| PAMDB00 4089 | Glycerophospholipids _T6 | PG(16:1(9Z)/14:0(3-OH)) | 0.001725 | 1.24974 | 0.417768 | 7.727007 |
| PAMDB00 4096 | Glycerophospholipids _T6 | PG(18:1(9Z)/12:0(3-OH)) | 0.001725 | 1.24974 | 0.417768 | 7.727007 |
| PAMDB00 3966 | Glycerophospholipids _T6 | PS(14:0(3-OH)/14:0(3-OH)) | 0.009303 | 1.21365 | 0.596249 | 5.351209 |
| PAMDB00 3951 | Glycerophospholipids _T6 | PS(12:0(3-OH)/16:0) | 0.006808 | 1.1907 | 0.519693 | 1.665435 |
| PAMDB00 3965 | Glycerophospholipids _T6 | PS(14:0(3-OH)/14:0) | 0.006808 | 1.1907 | 0.519693 | 1.665435 |
| PAMDB00 3977 | Glycerophospholipids _T6 | PS(14:0/14:0(3-OH)) | 0.006808 | 1.1907 | 0.519693 | 1.665435 |
| PAMDB00 3988 | Glycerophospholipids _T6 | PS(16:0/12:0(3-OH)) | 0.006808 | 1.1907 | 0.519693 | 1.665435 |

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| PAMDB00 3870 | Glycerophospholipids _T6 | PE(14:0(3-OH)/14:0(3-OH)) | 0.016662 | 1.15771 | 0.683334 | 0.025551 |
| PAMDB00 6379 | Glycerophospholipids _T6 | PG(10:0/10:0) | 0.038197 | 1.15654 | 0.621711 | 0.276173 |
| PAMDB00 1983 | Glycerophospholipids _T6 | PE(10:0/12:0) | 0.016891 | 1.14799 | 0.656985 | 0.069496 |
| PAMDB00 1993 | Glycerophospholipids _T6 | PE(12:0/10:0) | 0.016891 | 1.14799 | 0.656985 | 0.069496 |
| PAMDB00 4034 | Glycerophospholipids _T6 | PG(10:0(3-OH)/19:iso) | 0.024397 | 1.13334 | 0.78275 | 13.72789 |
| PAMDB00 4063 | Glycerophospholipids _T6 | PG(14:0(3-OH)/15:0) | 0.024397 | 1.13334 | 0.78275 | 13.72789 |
| PAMDB00 4077 | Glycerophospholipids _T6 | PG(15:0/14:0(3-OH)) | 0.024397 | 1.13334 | 0.78275 | 13.72789 |
| PAMDB00 4104 | Glycerophospholipids _T6 | PG(19:iso/10:0(3-OH)) | 0.024397 | 1.13334 | 0.78275 | 13.72789 |
| PAMDB00 3585 | Imidazole ribonucleosides and ribonucleotides _T6 | 1-(5-phosphoribosyl)-5-((5-phosphoribosylamino)methylideneamino)imidazole-4-carboxamide | 2.34E-08 | 1.27765 | 0.07855 | 0.276173 |
| PAMDB00 1692 | Organic phosphoric acids and derivatives _T6 | Tetradecanoyl-phosphate (n-C14:0) | 0.045303 | 1.08899 | 0.844302 | 5.852115 |
| PAMDB00 1054 | Prenol lipids _T6 | Undecaprenyl phosphate | 1.35E-06 | 1.27659 | 0.098523 | 0.276173 |
| PAMDB00 1971 | Prenol lipids _T6 | Ubiquinol-4 | 5.74E-05 | 1.27002 | 0.175978 | 0.276173 |
| PAMDB00 1300 | Pyrimidine nucleotides _T6 | UDP-N-Acetyl muramyl-L-Ala | 7.01E-09 | 1.27771 | 0.076441 | 0.276173 |

C

| <i>Heat treated sample group -----Pseudomonas growth after 24 h 6 °C</i> | | | | | | |
|--|------------------------------------|----------------------|------------------------|---------------------------|---------------------------|-----------------------------|
| <i>Database Code</i> | <i>Class</i> | <i>Compound Name</i> | <i>p-value Volcano</i> | <i>VIP score (T6vsT1)</i> | <i>VIP Standard error</i> | <i>LOG2(FC)(T1PFvsT1CN)</i> |
| PAMDB006398 | Glycerophosphoglycerophosphates_T1 | PGP(10:0/10:0) | 0.021678 | 1.25838 | 0.635046 | 5.1064 |

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| <i>Heat treated sample group -----Pseudomonas growth after 24 h 6 °C</i> | | | | | | |
|---|---|-------------------------------|------------------------|---------------------------|---------------------------|-----------------------------|
| <i>Database Code</i> | <i>Class</i> | <i>Compound Name</i> | <i>p-value Volcano</i> | <i>VIP score (T6vsT1)</i> | <i>VIP Standard error</i> | <i>LOG2(FC)(T6PFvsT6CN)</i> |
| PAMDB006650 | Glycerophosphoglycerophosphates_T6 | PGP(19:iso/10:0) | 0.021678 | 1.30776 | 0.345948 | 10.151 |
| PAMDB006545 | Glycerophosphoglycerophosphates_T6 | PGP(10:0/19:iso) | 0.021678 | 1.30776 | 0.345948 | 10.151 |
| BMDB11175 | Amino acids, peptides, and analogues_T6 | L-leucyl-L-proline | 0.021678 | 1.31501 | 0.319884 | 9.7346 |
| BMDB62574 | Amino acids, peptides, and analogues_T6 | Pro-Ile | 0.021678 | 1.31501 | 0.319884 | 9.7346 |
| PAMDB001600 | Glycerophospholipids _T6 | CDP-12-Dioctadecanoylglycerol | 0.03727 | 1.28676 | 0.316725 | 11.046 |
| PAMDB000736 | Glycerophospholipids _T6 | CDP-DG(18:1(9Z)/18:0) | 0.03727 | 1.28676 | 0.316725 | 11.046 |
| PAMDB000727 | Glycerophospholipids _T6 | CDP-DG(18:1(11Z)/18:0) | 0.03727 | 1.28676 | 0.316725 | 11.046 |
| PAMDB006852 | Glycerophospholipids _T6 | CDP-DG(19:iso/17:0cycw7c) | 0.03727 | 1.28676 | 0.316725 | 11.046 |
| PAMDB000720 | Glycerophospholipids _T6 | CDP-DG(18:0/18:1(9Z)) | 0.03727 | 1.28676 | 0.316725 | 11.046 |
| PAMDB006824 | Glycerophospholipids _T6 | CDP-DG(17:0cycw7c/19:iso) | 0.03727 | 1.28676 | 0.316725 | 11.046 |