# Metabolite-related dietary patterns and the development of islet autoimmunity

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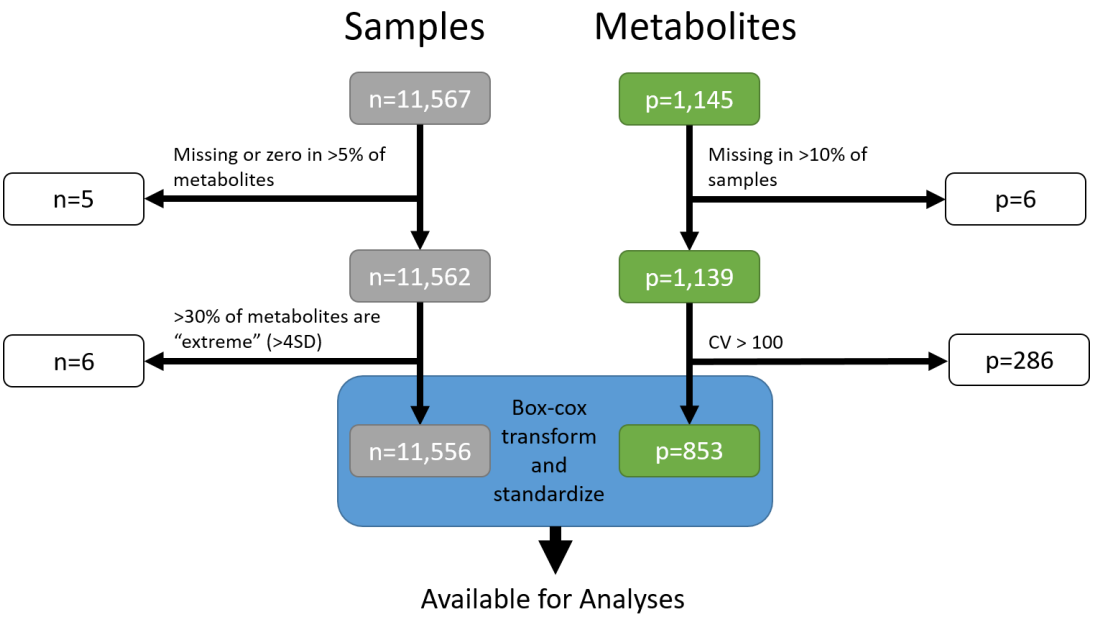
**Supplemental Figure 1—Summary of metabolomics data pre-processing pipeline in all TEDDY metabolomics samples.**




*n=number of samples, p=number of metablites/features, CV=coefficient of variation, SD=standard deviation*

**Supplemental Table 1: Chemically identified metabolites used in ChemRICH metabolomics set enrichment analysis**

| Variable | Compound Name | InChiKeys | Pubchem ID | SMILES |
|---|---|---|---|---|
| t74 | 3-aminoisobutyric acid | QCHPKSFMDHPSNR-UHFFFAOYSA-N | 25201103 | CC(C[NH3+])C(=O)[O-] |
| t147 | Acylcarnitine (C10:1) | GOOOCIIXFLVRAG-UHFFFAOYSA-N | 53481651 | C[N+](C)(C)CC(CC(=O)[O-])OC(=O)CCCCCCCCC=C |
| t148 | Acylcarnitine (C14:2) | HXOGMKPCIDSSKJ-NKBLVAAJSA-N | 53481681 | CCCCCCCC/C=C/C=C/CC(=O)O[C@@H](CCC(=O)[O-])[N+](C)(C)C |
| t149 | Acylcarnitine (C18:3) | DFVGGGHKDAHYIU-UHMZJXMFSA-N | 53477821 | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O[C@@H](CCC(=O)[O-])[N+](C)(C)C |
| t150 | Acylcarnitine (C8:0) | CXTATJFJDMJMIY-CYBMUJFWSA-N | 11953814 | CCCCCCCC(=O)O[C@H](CC(=O)[O-])C[N+](C)(C)C |
| t151 | Acylcarnitine (C8:1) | YMIVWYONPRZBEJ-LXKVQUBZSA-N | 53481667 | CCCCC/C=C/C(=O)O[C@@H](CCC(=O)[O-])[N+](C)(C)C |
| t141 | Acylcarnitine C10:0 | LZOSYCMHQXPBFU-UHFFFAOYSA-N | 10245190 | CCCCCCCCCC(=O)OC(CC(=O)[O-])C[N+](C)(C)C |
| t142 | Acylcarnitine C12:0 | FUJLYHJROOYKRA-QGZVFWFLSA-N | 168381 | CCCCCCCCCCCC(=O)O[C@H](CC(=O)[O-])C[N+](C)(C)C |
| t144 | Acylcarnitine C18:0 | FNPHNLNTJNMAEE-UHFFFAOYSA-N | 6426855 | CCCCCCCCCCCCCCCCCC(=O)OC(CC(=O)[O-])C[N+](C)(C)C |
| t145 | Acylcarnitine C18:1 | HITOYGLMAFIRNI-YSESTWPTSA-N | 53477830 | CCCCCC/C=C/CCCCCCCCCC(=O)O[C@@H](CCC(=O)[O-])[N+](C)(C)C |
| t146 | Acylcarnitine C18:2 | MJLXQSQYKZWZCB-DQFWFXSYSA-N | 6450015 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O[C@H](CC(=O)[O-])C[N+](C)(C)C |
| t73 | adipic acid | WNLRTRBMVRJNCN-UHFFFAOYSA-N | 196 | C(CCC(=O)O)CC(=O)O |
| t72 | alanine | QNAYBMKLOCPYGJ-REOHCLBHSA-N | 5950 | C[C@@H](C(=O)O)N |
| t70 | asparagine | DCXYFEDJOCDNAF-REOHCLBHSA-N | 6267 | C([C@@H](C(=O)O)N)C(=O)N |
| t69 | aspartic acid | CKLJMWTZIZZHCS-REOHCLBHSA-N | 44367445 | C([C@@H](C(=O)O)[NH3+])C(=O)[O-] |
| t68 | benzoic acid | WPYMKLBDIGXBTP-UHFFFAOYSA-N | 20144841 | [H+].C1=CC=C(C=C1)C(=O)[O-] |
| t67 | capric acid | GHVNFZFCNZKVNT-UHFFFAOYSA-N | 2969 | CCCCCCCCCC(=O)O |

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| t66 | caprylic acid | WWZKQHOCKIZLMA-UHFFFAOYSA-N | 379 | CCCCCCCC(=O)O |
| t433 | CE (16:1) | HODJWNWCVNUPAQ-FSAOOAOSSA-N | 22833543 | CCCCCC/C=C\CCCCCCCC(=O)OC1CC[C@@]2(C3CC[C@@]4([C@H](CCC4C3CC=C2C1)[C@H](C)CCCC(C)C)C)C |
| t434 | CE (18:1) | RJECHNNFRHZQKU-RMUVNZEASA-N | 5283632 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@H]([C@@H]3CC=C2C1)CC[C@@H]4[C@H](C)CCCC(C)C)C)C |
| t435 | CE (18:2) | NAACPBBQTFFYQB-LJAITQKLSA-N | 5287939 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@H]([C@@H]3CC=C2C1)CC[C@@H]4[C@H](C)CCCC(C)C)C)C |
| t436 | CE (18:3) | FYMCIBHUFSIWCE-WVXFKAQASA-N | 6436907 | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@H]([C@@H]3CC=C2C1)CC[C@@H]4[C@H](C)CCCC(C)C)C)C |
| t152 | CE (20:3) | MLPRJPSMAFZPLA-PJSAOELNSA-N | 53477892 | CCCCC/C=C\C/C=C\C/C=C\CCCCCCC(=O)O[C@H]1CC[C@@]2(C3CC[C@]4(C(C3CC=C2C1)CCC4[C@H](C)CCCC(C)C)C)C |
| t437 | CE (20:4) | IMXSFYNMSOULQS-BEDFLICRSA-N | 6479222 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@H]([C@@H]3CC=C2C1)CC[C@@H]4[C@H](C)CCCC(C)C)C)C |
| t438 | CE (20:5) | XZFUGMCJZFRBKF-JIKDAPOUSA-N | 53477889 | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O[C@H]1CC[C@@]2(C3CC[C@]4(C(C3CC=C2C1)CCC4[C@H](C)CCCC(C)C)C)C |
| t439 | CE (22:6) | VOEVEGPMRIYYKC-HNJOWPRISA-N | 14274978 | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@H]([C@@H]3CC=C2C1)CC[C@@H]4[C@H](C)CCCC(C)C)C)C |
| t848 | Ceramide (d33:1) | QBFXCLDNTKBAPQ-STSAHMJASA-N | 52931112 | CCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCC)O |
| t849 | Ceramide (d34:0) | GCGTXOVNNFGTPQ-JHOUSYSJSA-N | 5283572 | CCCCCCCCCCCCCCCC[C@H]([C@H](CO)NC(=O)CCCCCCCCCCCCCCC)O |
| t850 | Ceramide (d34:1) | YDNKGFDKKRUKPY-TURZORIXSA-N | 5283564 | CCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t851 | Ceramide (d34:2) | XXWRZIYYFPIQHE-XPAOSYCESA-N | 52931118 | CCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t852 | Ceramide (d36:1) | MJQIARGPQMNBGT-WWUCIAQXSA-N | 6442676 | CCCCCCCCCCCCCCC[C@H]([C@H](CO)NC(=O)CCCCCCC/C=C\CCCCCCCC)O |
| t853 | Ceramide (d38:1) | XWBWIAOWSABHFI-NUKVNZTCSA-N | 5283566 | CCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t854 | Ceramide (d39:1) | WYSRACVJQVNCRW-PQPBPFPMSA-N | 11273482 | CCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCC)O |
| t855 | Ceramide (d40:0) | SXPRAKSDHOEHIG-ZESVVUHVSA-N | 5283575 | CCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](CCCCCCCCCCCCCC)O |
| t856 | Ceramide (d40:1) | KEPQASGDXIEOIL-GLQCRSEXSA-N | 5283567 | CCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCCC)O |

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| t857 | Ceramide (d40:2) | HILTUFAERVOALR-MQXYEJFFSA-N | 52931123 | CCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t859 | Ceramide (d42:0) | BPLYVSYSBPLDOA-WVILEFPPSA-N | 5283577 | CCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](CCCCCCCCCCCCCCCC)O |
| t860 | Ceramide (d42:1) | ZJVVOYPTFQEGPH-AUTSUKAISA-N | 5283571 | CCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCC)O |
| t861 | Ceramide (d42:2) | VJSBNBBOSZJDKB-KPEYJIHVSA-N | 5283568 | CCCCCCCCCCCCC/C=C/[C@H]([C@H](CO)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |
| t863 | Ceramide (d43:1) | QHPYSHVSWAOLHS-PVNBSDFKSA-N | 9547202 | CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCC)O |
| t864 | Ceramide (d44:1) | CJROVRTUSFQVMR-GVOPMEMSSA-N | 5283570 | CCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCCCCCCC)O |
| t64 | citramalic acid | XFTRTWQBIOMVPK-UHFFFAOYSA-N | 1081 | CC(CC(=O)O)(C(=O)O)O |
| t63 | creatinine | DDRJAANPRJIHGJ-UHFFFAOYSA-N | 588 | CN1CC(=O)N=C1N |
| t62 | cystine | LEVWYRKDKASIDU-UHFFFAOYSA-N | 24798687 | C(C(C(=O)[O-])[NH3+])SSCC(C(=O)[O-])[NH3+] |
| t61 | deoxypentitol | FJGNTEKSQVNVTJ-UHFFFAOYSA-N | 270738 | CC(C(C(CO)O)O)O |
| t444 | DG (32:1) | XEQQGHISHUGMIP-ASUORMEESA-N | 14275341 | CCCCCCCCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t445 | DG (34:1) | YEJYLHKQOBOSCP-OZKTZCCCSA-N | 5282283 | CCCCCCCCCCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t156 | DG (36:1) | SAEPUUXWQQNLGN-LVVMQYBKSA-N | 6443547 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t447 | DG (36:2) | AFSHUZFNMVJNKX-LLWMBOQKSA-N | 9543716 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\CCCCCCC |
| t448 | DG (36:3) | BLZVZPYMHLXLHG-JOBMVARSSA-N | 9543722 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t157 | DG (36:4) | MQGBAQLIFKSMEM-ZHARMHCNSA-N | 9543729 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t159 | DG (36:5) | PGXBELQFNRPKBC-WBVIKXMWSA-N | 9543737 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC |
| t160 | DG (38:0) | IQNYOCFHHRCMKY-KDXMTYKHSA-N | 53478362 | CCCCCCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCCCCCCCCCCCC |
| t161 | DG (38:3) | ADXAWIIUCSQOAS-SMJOZILHSA-N | 9543766 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](CO)OC(=O)CCCCCCCCC/C=C\C/C=C\CCCCC |

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| t449 | DG (38:5) | GRGDLDNREYVILP-CNWVQWJYSA-N | 9543784 | CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)O[C@@H](CO)COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC |
| t450 | DG (38:6) | YDVDXUYJFQLPEG-CTHJWPIASA-N | 9543795 | CCCCC/C=C\C/C=C\C/C=C\CCCCCCC(=O)O[C@@H](CO)COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC |
| t60 | erythronic acid lactone | SGMJBNSHAZVGMC-PWNYCUMCSA-N | 5325915 | C1[C@H]([C@H](C(=O)O1)O)O |
| t514 | FA (16:0) | IPCSVZSSVZVIGE-UHFFFAOYSA-N | 985 | CCCCCCCCCCCCCCCC(=O)O |
| t515 | FA (16:1) | SECPZKHBENQXJG-FPLPWBNLSA-N | 445638 | CCCCCC/C=C\CCCCCCCC(=O)O |
| t516 | FA (18:0) | QIQXTHQIDYTFRH-UHFFFAOYSA-N | 5281 | CCCCCCCCCCCCCCCCCC(=O)O |
| t517 | FA (18:1) | ZQPPMHVWECSIRJ-KTKRTIGZSA-N | 445639 | CCCCCCCC/C=C\CCCCCCCC(=O)O |
| t518 | FA (18:2) | JBYXPOFIGCOSSB-XBLVEGMJSA-N | 5282796 | CCCCCC/C=C/C=C/CCCCCCCC(=O)O |
| t519 | FA (20:4) | YZXBAPSDXZZRGB-DOFZRALJSA-N | 444899 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O |
| t520 | FA (22:4) | TWSWSIQAPQLDBP-DOFZRALJSA-N | 5497181 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCCC(=O)O |
| t59 | fucose | SHZGCJCMOBCMKK-FPRJBGLDSA-N | 439650 | C[C@@H]1[C@@H]([C@@H]([C@@H]([C@H]([C@@H](O1)O)O)O)O)O |
| t58 | galactonic acid | RGHNJXZEOKUKBD-MGCNEYSASA-N | 128869 | C([C@H]([C@@H]([C@@H]([C@H](C(=O)O)O)O)O)O)O)O |
| t451 | Gal-Gal-Cer(d18:1/16:0) or Lactosylceramide(d18:1/16:0) | HLIJNIKSBCIDGO-QKLMXXKVSA-N | 53477895 | CCCCCCCCCCCCCCCC(=O)N[C@@H](CO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O[C@H]2[C@@H]([C@H]([C@H]([C@H](O2)CO)O)O)O)O)O)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t865 | GlcCer (d38:1) | DFELABABMXOKTD-IYFIADHGSA-N | 20057356 | CCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t452 | GlcCer (d40:1) | QMYGQSYNQBLKGY-YAEABVQUSA-N | 70699232 | CCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO[C@H]1C(C([C@@H]([C@H](O1)CO)O)O)O)[C@@H](/C=C/CCCCCCCCCCC)O |
| t867 | GlcCer (d41:1) | SJGWLQDELUWRDA-MUYAOIFFSA-N | 52931253 | CCCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](CO[C@H]1C(C([C@@H]([C@H](O1)CO)O)O)O)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t453 | GlcCer (d42:1) | SNVYJLGKALMFOP-MOLROICHSA-N | 6321367 | CCCCCCCCCCCCCCC[C@H]([C@H](CO[C@H]1C(C([C@@H]([C@H](O1)CO)O)O)O)O)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |
| t454 | GlcCer (d42:2) | WBOZIXHPUPAOIA-RBELZSLISA-N | 6321360 | CCCCCCCCCCCCC/C=C/[C@H]([C@H](CO[C@H]1C(C([C@@H]([C@H](O1)CO)O)O)O)O)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |

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| t870 | GlcCer(d14:1(4E)/20:0(2OH)) | YYILQTLJZBSOCA-IMJQGFQJSA-N | 70699246 | CCCCCCCCCCCCCCCCCCC(C(=O)N[C@@H](CO[C@H]1C(C([C@@H]([C@H](O1)CO)O)O)O)[C@@H](/C=C/CCCCCCCCC)O)O |
| t57 | gluconic acid | RGHNJXZEOKUKBD-QTBDOELSSA-N | 6857417 | C([C@@H]([C@H]([C@@H]([C@@H](C(=O)O)O)O)O)O)O |
| t56 | glucose | WQZGKKKJIJFFOK-VFUOTHLCSA-N | 64689 | C([C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)O)O)O)O)O |
| t55 | glutamine | ZDXPYRJPNDTMRX-VKHMYHEASA-N | 5961 | C(CC(=O)N)[C@@H](C(=O)O)N |
| t54 | glutaric acid | JFCQEDHGNNZCLN-UHFFFAOYSA-N | 23322899 | [H+].[H+].C(CC(=O)[O-])CC(=O)[O-] |
| t53 | glycerol | PEDCQBHIVMGVHV-UHFFFAOYSA-N | 753 | C(C(CO)O)O |
| t52 | glycine | DHMQDGOQFOQNFH-UHFFFAOYSA-N | 5257127 | C(C(=O)[O-])[NH3+] |
| t51 | heptadecanoic acid | KEMQGTRYUADPNZ-UHFFFAOYSA-N | 10465 | CCCCCCCCCCCCCCCCC(=O)O |
| t50 | hexitol | FBPFZTCFMRRESA-UHFFFAOYSA-N | 453 | C(C(C(C(C(CO)O)O)O)O)O |
| t49 | histidine | HNDVDQJCIGZPNO-YFKPBYRVSA-N | 6274 | C1=C(NC=N1)C[C@@H](C(=O)O)N |
| t47 | hydroxylamine | AVXURJPOCDRRFD-UHFFFAOYSA-N | 787 | NO |
| t46 | indole-3-acetate | SEOVTRFCIGRIMH-UHFFFAOYSA-N | 802 | C1=CC=C2C(=C1)C(=CN2)CC(=O)O |
| t45 | indoxyl sulfate | BXFFHSIDQOFMLE-UHFFFAOYSA-N | 10258 | C1=CC=C2C(=C1)C(=CN2)OS(=O)(=O)O |
| t44 | isoleucine | AGPKZVBTJJNPAG-WHFBIAKZSA-N | 6306 | CC[C@H](C)[C@@H](C(=O)O)N |
| t43 | isothreonic acid | JPIJQSOTBSSVTP-GBXIJSLDSA-N | 151152 | C([C@H]([C@@H](C(=O)O)O)O)O |
| t42 | lactic acid | JVTAAEKCZFNVCJ-UHFFFAOYSA-N | 19789253 | [H+].CC(C(=O)[O-])O |
| t455 | Lactosylceramide (d18:1/24:1(15Z)) | MKOKWBRPIBQYJJ-LWQSSKHKSA-N | 20057309 | CCCCCCCCCCCCCC/C=C/[C@H]([C@H](CO[C@H]1C([C@H]([C@@H]([C@H](O1)CO)O)O[C@H]2[C@@H]([C@H]([C@H]([C@H](O2)CO)O)O)O)O)O)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |
| t41 | lauric acid | POULHZVOKOAJMA-UHFFFAOYSA-N | 3893 | CCCCCCCCCCCC(=O)O |
| t40 | leucine | ROHFNLRQFUQHCH-YFKPBYRVSA-N | 6106 | CC(C)C[C@@H](C(=O)O)N |

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| t39 | linoleic acid | OYHQOLUKZRVURQ-HZJYTTRNSA-N | 5280450 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O |
| t521 | LPC (14:0) | VXUOFDJKYGDUJI-OAQYLSRUSA-N | 460604 | CCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t163 | LPC (15:0) | RJZVWDTYEWCUAR-JOCHJYFZSA-N | 24779458 | CCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t871 | LPC (16:0) | ASWBNKHCZGQVJV-HSZRJFAPSA-N | 460602 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t522 | LPC (16:1) | LFUDDCMNKWEORN-ZXEGGCGDSA-N | 24779461 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t166 | LPC (17:1) | LPMGFNAQZPADDZ-FJIRUFBNSA-N | 24779451 | CCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t523 | LPC (18:0) | IHNKQIMGVNPMTC-RUZDIDTESA-N | 497299 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t525 | LPC (18:1) | YAMUFBLWGFFICM-PTGWMXDISA-N | 16081932 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t872 | LPC (18:2) | SPJFYYJXNPEZDW-FTJOPAKQSA-N | 11005824 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t170 | LPC (18:3) | WKQNRCYKYCKESD-YVHLTTHBSA-N | 24779469 | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t171 | LPC (20:0) | UATOAILWGVYRQS-HHHXNRCGSA-N | 24779473 | CCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t526 | LPC (20:1) | GJTDRNFWIDPARY-GTPZACKGSA-N | 24779475 | CCCCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t527 | LPC (20:2) | YYQVCMMXPIJVHY-ZOIJLGJPSA-N | 52924053 | CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t528 | LPC (20:3) | BBNHCUBQEQJHIG-FZZJNMCHSA-N | 52924055 | CCCCC/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t175 | LPC (20:4) | GOMVPVRDBLLHQC-VEJNOCSESA-N | 53480469 | CC/C=C\C/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t176 | LPC (20:5) | PDIGSOAOQOXRDU-WJPZTBRDSA-N | 11757087 | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t177 | LPC (22:4) | ZOJBSSVHFSBHMP-JJJSWPRASA-N | 52924039 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t529 | LPC (22:5) | YBUXFQUGNPBZPS-YNBHEIDWSA-N | 53480473 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t179 | LPC (22:6) | LSOWKZULVQWMLY-APPDJCNMSA-N | 10415542 | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |

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| t180 | LPC (o-16:0) | VLBPIWYTPAXCFJ-DEOSSOPVSA-N | 10480367 | CCCCCCCCCCCCCCCCOC[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t181 | LPC (p-16:0) or LPC (o-16:1) | HTZINLFNXLXRBC-CQLBIITFSA-N | 10917802 | CCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)O |
| t530 | LPE (16:0) | CKPBBEOJHAPPBT-HXUWFJFHSA-N | 53480922 | CCCCCCCCCCCCCCCC(=O)O[C@H](CO)COP(=O)(O)OCCN |
| t531 | LPE (18:2) | DBHKHNGBVGWQJE-USWSLJGRSA-N | 52925130 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)(O)OCCN)O |
| t532 | LPE (20:4) | JPNPIRVRGLGTRE-YSKCIPFOSA-N | 53480952 | CC/C=C\C/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@H](COP(=O)(O)OCCN)O |
| t533 | LPE (22:6) | XEVRBOQZSXWGQO-PAUXXPOVSA-N | 52925132 | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC(=O)OC[C@H](COP(=O)(O)OCCN)O |
| t38 | lysine | KDXKERNSBIXSRK-YFKPBYRVSA-N | 5962 | C(CCN)C[C@@H](C(=O)O)N |
| t37 | lyxitol | HEBKCHPVOIAQTA-IMJSIDKUSA-N | 439255 | C([C@@H](C([C@H](CO)O)O)O)O |
| t36 | malic acid | BJEPYKJPYRNKOW-UHFFFAOYSA-N | 20130941 | [H+].[H+].C(C(C(=O)[O-])O)C(=O)[O-] |
| t35 | methanolphosphate | CAAULPUQFIIOTL-UHFFFAOYSA-N | 13130 | COP(=O)(O)O |
| t34 | methionine | FFEARJCKVFRZRR-BYPYZUCNSA-N | 6137 | CSCC[C@@H](C(=O)O)N |
| t32 | myo-inositol | CDAISMWEOUEBRE-UHFFFAOYSA-N | 892 | C1(C(C(C(C(C1O)O)O)O)O)O |
| t31 | N-methylalanine | GDFAOVXKHJXLEI-VKHMYHEASA-N | 5288725 | C[C@@H](C(=O)O)NC |
| t30 | nornicotine | MYKUKUCHPMASKF-UHFFFAOYSA-N | 412 | C1CC(NC1)C2=CN=CC=C2 |
| t28 | ornithine | AHLPHDHHMVZTML-BYPYZUCNSA-N | 6262 | C(C[C@@H](C(=O)O)N)CN |
| t27 | oxoproline | ODHCTXKNWHHXJC-VKHMYHEASA-N | 7405 | C1CC(=O)N[C@@H]1C(=O)O |
| t184 | PC (16:0/9:0(CHO)) | PPTNNIINSOQWCE-WJOKGBTCSA-N | 46907874 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCC=O |
| t185 | PC (28:0) | CITHEXJVPOWHKC-UUWRZZSWSA-N | 5459377 | CCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCC |
| t186 | PC (30:0) | RFVFQQWKPSOBED-PSXMRANNSA-N | 129657 | CCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |

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| t187 | PC (30:1) | ANKCYRKQDLQXGL-MRDDHZETSA-N | 52922250 | CCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\CCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t188 | PC (31:0) | NPGWXTIWUUFYAB-DIPNUNPCSA-N | 24778680 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC |
| t189 | PC (31:1) | QFVHCMLUKNHDSH-WTWBAFHPSA-N | 24778657 | CCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCC |
| t873 | PC (32:0) | KILNVBDSWZSGLL-KXQOOQHDSA-N | 452110 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC |
| t534 | PC (32:1) | QIBZFHLFHCIUOT-NPBIGWJUSA-N | 6443788 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCC |
| t192 | PC (32:2) | GPWHCUUIQMGELX-VHQDNGOZSA-N | 24778764 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCC |
| t193 | PC (32:3) | UXEFXNOSLOCOLX-ZCHSEWAGSA-N | 52922763 | CCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCC/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t194 | PC (33:0) | FHENRYRLCPXONH-LDLOPFEMSA-N | 52922645 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCC |
| t196 | PC (33:2) | SBNDHGBVMZMSNL-UESLNCBNSA-N | 52922715 | CCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t197 | PC (34:0) | PZNPLUBHRSSFHT-RRHRGVEJSA-N | 24778686 | CCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCCCCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t874 | PC (34:1) | WTJKGGKOPKCXLL-VYOBOKEXSA-N | 5497103 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t875 | PC (34:2) | JLPULHDHAOZNQI-ZTIMHPMXSA-N | 5287971 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t539 | PC (34:3) | CNNSEHUKQJCGTE-UPPWDXJYSA-N | 24778699 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCC/C=C\C/C=C\C/C=C\CCCCC |
| t200 | PC (34:4) | YWDDIWXKFJEMKF-JTZVLWBESA-N | 52922891 | CCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCC/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t201 | PC (35:1) | MFHIZGSSDZJFKD-IYEJTHTFSA-N | 52922679 | CCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t541 | PC (35:2) | ZSKWZJYUVZYDQU-WESJWMGVSA-N | 52922491 | CCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t203 | PC (35:2) B | LNGBVAOHJZCRIL-GPDPEMMZSA-N | 52923157 | CCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCCCC/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t204 | PC (35:3) | AYXGHIQPMDYMJC-AHMBLZLYSA-N | 52924614 | CCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC)COP(=O)(O)OCCN |
| t205 | PC (35:4) | OROZWUJCDDCYAU-IPUAOQJZSA-N | 52922204 | CCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |

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| t543 | PC (36:1) | ATHVAWFAEPLPPQ-VRDBWYNSSA-N | 24778825 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t876 | PC (36:2) | SNKAWJBJQDLSFF-NVKMUCNASA-N | 10350317 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t545 | PC (36:3) | YPAZQMWFRMHBBM-CLKMJQEKSA-N | 53478785 | CCCCCC/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t208 | PC (36:3) A | BXRLDROZWDUSGM-ZRYFCQOPSA-N | 24778937 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCC/C=C\C/C=C\CCCCCCCC |
| t211 | PC (36:4) A | NKQPOVROGSWLTO-NVPMBMBWSA-N | 52922783 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCCC/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t212 | PC (36:4) C | IIZPXYDJLKNOIY-JXPKJXOSSA-N | 10747814 | CCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t548 | PC (36:5) | DYDDZDMJSQYFGN-OIVUZXIWSA-N | 24778771 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t214 | PC (36:5) B | SUZYROYNFNQALJ-MHEIZRSESA-N | 52923341 | CCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t215 | PC (36:6) | SPWBDEZMKCRQSX-NGPPOSSDSA-N | 52922847 | CCCCC/C=C\C/C=C\C/C=C\CCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t550 | PC (37:2) | MCZUABDVGPPWPM-HJTCUGKVSA-N | 52922735 | CCCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t217 | PC (37:3) | OOYQEEUUQRMQKL-JUUDQZDJSA-N | 52922851 | CCCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t218 | PC (37:4) | QRPUCJXFPYFTMB-FBFLODOBSA-N | 52922853 | CCCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t219 | PC (37:5) | URYYGMVXBWUJFP-LQYSTYLLSA-N | 53478655 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC |
| t220 | PC (37:6) | GEINPYKZLFHHIL-HEXXMCQTSA-N | 52922342 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC |
| t552 | PC (38:2) | KXXLFCAPKGRXBT-FMJYHZMHSA-N | 24779263 | CCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t877 | PC (38:3) | OJHJKEBRZSDTTL-VHWCKNCUSA-N | 52922741 | CCCCCCCC/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t223 | PC (38:4) A | PSVRFUPOQYJOOZ-QNPWAGBNSA-N | 16219824 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t224 | PC (38:4) B | DNYKSJQVBCVGOF-LCKGXUDJSA-N | 52923291 | CCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t553 | PC (38:5) | YLWBKBDNHWQEFU-YJXJLLHLSA-N | 53479033 | CCCCCC/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |

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| t225 | PC (38:5) A | SUACBSWYGWBPFC-GPUJSUHJSA-N | 52923235 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t555 | PC (38:6) | PLZBTDKJYHXIEW-DZUXOTHRSA-N | 52923295 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t229 | PC (38:7) | BNNUJTATKJXKJP-XCDHYEIISA-N | 53479075 | CCCCC/C=C\C/C=C\C/C=C\CCCCC(=O)O[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t230 | PC (39:6) | QMCWOGICYCFNBF-BWHZRABLSA-N | 52922637 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t556 | PC (40:4) | QQIYXJBHMDYXHH-NMUBDWGHSA-N | 52923573 | CCCCC/C=C\C/C=C\CCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t558 | PC (40:5) | LJFKFKIYUJNFPZ-ZLFSCUDPSA-N | 52923133 | CCCCCCCC/C=C\CCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t232 | PC (40:5) A | IJTJDJOOHZVSAC-NDRUHXFFSA-N | 53479083 | CCCCCCCC/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t233 | PC (40:5) B | SFESOYFQZQJCOY-FXYWPAEZSA-N | 52923365 | CCCCCCCCCCCCCCCCCCCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t879 | PC (40:6) | FYVNIFOYDIIODX-KNKJIUSSSA-N | 24778900 | CCCCCC/C=C\CCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC |
| t234 | PC (40:6) B | TYRTWVKQVGNGSZ-RGBTVBCDSA-N | 52923195 | CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t560 | PC (40:7) | BPUROMFCPFGBOT-ZEGPSQTJSA-N | 24778982 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t561 | PC (40:8) | BFCSBEFTXQRIOJ-IMYLGOOQSA-N | 53479093 | CC/C=C\C/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC |
| t237 | PC (42:10) | GILJCAGAMFVHNE-QEOOLSSISA-N | 53479133 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC(=O)O[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t238 | PC (42:5) | APYSSUSAYQRESE-VZWUYPTESA-N | 52923591 | CCCCC/C=C\C/C=C\CCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC |
| t239 | PC (42:6) | DSVRMAGYENFTLY-GDDYDVMSSA-N | 52923651 | CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t562 | PC (o-32:0) | SVWBXNAUENUONE-LDLOPFEMSA-N | 173570 | CCCCCCCCCCCCCCCCCO[C@H](COC(=O)CCCCCCCCCCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t241 | PC (o-34:0) | ZKTXOJMFIAILJG-VQJSHJPSSA-N | 24779361 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OCCCCCCCCCCCCCCCCC |
| t563 | PC (p-32:0) or PC (o-32:1) | KEVGQWGZKKFGDC-JCUPVDEDSA-N | 53478671 | CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O/C=C\CCCCCCCCCCCCCC |
| t243 | PC (p-32:1) or PC (o-32:2) | FZMYLOBGNYZPQO-QLSONYGBSA-N | 52923882 | CCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCC |

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| t564 | PC (p-34:0) or PC (o-34:1) | QCGUXAIDEOWPBV-SNKLRXETSA-N | 53481719 | CCCCCCCCCCCCCCCC(=O)O[C@H](COCCCCCCCCCC/C=C\CCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t566 | PC (p-34:1) or PC (o-34:2) | MBRHHFWRXQYYAN-RTVLTNFHSA-N | 53480735 | CCCCCCCCCCCCCCCC(=O)OC(CO/C=C\CCCCCCCC/C=C\CCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t245 | PC (p-34:1) or PC (o-34:2) A | MBRHHFWRXQYYAN-JEPFLRBFSA-N | 70698781 | CCCCCCCCCCCCCCCC(=O)O[C@H](CO/C=C\CCCCCCCC/C=C\CCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t246 | PC (p-34:1) or PC (o-34:2) B | KMNVIRCHUMQGHD-RCINKDPXSA-N | 52923934 | CCCCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\CCCCCC |
| t567 | PC (p-34:2) or PC (o-34:3) | QLEHHUPUHJPURI-PWYDUFMYSA-N | 24779386 | CCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t568 | PC (p-36:1) or PC (o-36:2) | ZOTYCHIFTCFAHC-KOUVQCMKSA-N | 53480797 | CCCCCCCCCCCCCCCCCC(=O)O[C@H](CO/C=C\CCCCCC/C=C\CCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t249 | PC (p-36:1) or PC (o-36:2) B | ZYLPVUZBZNMVMR-ZBBHDILGSA-N | 52923754 | CCCCCCCCCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCC/C=C\C/C=C\CCCCC |
| t250 | PC (p-36:2) or PC (o-36:3) | DIHWZUCEXWUHOD-IIVNATNGSA-N | 53480801 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](CO/C=C\CCCCCC/C=C\CCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t570 | PC (p-36:3) or PC (o-36:4) | SOUZQPFUXRVDGK-KCTKZSJBSA-N | 53481701 | CCCCCCCCCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC |
| t880 | PC (p-36:4) or PC (o-36:5) | IOYKZPNDXIIXLN-LOQSCQKMSA-N | 24779388 | CCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t571 | PC (p-38:3) or PC (o-38:4) | GWBOVQHRCURSPU-QMFAPAEZSA-N | 53480815 | CCCCCCCC/C=C\CCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCC/C=C\C/C=C\CCCCC |
| t572 | PC (p-38:4) or PC (o-38:5) | DBQMOXDLWKVKKG-REWQMPQJSA-N | 53480761 | CCCCCC/C=C\CCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC |
| t255 | PC (p-38:4) or PC (o-38:5) A | YPAPIRJFGNBODV-AMFPDOHCSA-N | 53480715 | CCCCCCCCCCCCCCCC/C=C\OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC |
| t256 | PC (p-38:4) or PC (o-38:5) B | DYFGXBAIDOATAE-DSLLYOFSSA-N | 53480759 | CCCCCCCC/C=C\C/C=C\C/C=C\CCCC(=O)OC(CO/C=C\CCCCCCCC/C=C\CCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t573 | PC (p-38:5) or PC (o-38:6) | ATTCDOPAYPGSLE-LQULQHAGSA-N | 53479121 | CCCCCCCC/C=C\CCCCCC/C=C\OC(COC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t257 | PC (p-38:5) or PC (o-38:6) A | FAKYQMLQEAQOLK-LHZZQLRFSA-N | 53480695 | CCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t574 | PC (p-40:1) or PC (o-40:2) | KYEGAYPFBCAHDL-SPACVREBSA-N | 53480827 | CCCCCCCCCCCCCCCCCCCCCCC(=O)O[C@H](CO/C=C\CCCCCC/C=C\CCCCCCCC)COP(=O)([O-])OCC[N+](C)(C)C |
| t261 | PC (p-40:3) or PC (o-40:4) | RDNHPNJCALITSY-MBZSPAKGSA-N | 52923852 | CCCCCCCCCCCCCCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t262 | PC (p-40:4) or PC (o-40:5) | UWNFEVACEPZILS-RNNLSGHUSA-N | 52924022 | CCCCCCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |

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| t263 | PC (p-40:5) or PC (o-40:6) | KUHMJRMPHBRAMY-DDURNVNNSA-N | 53480775 | CCCCCC/C=C\CCCCCCCC/C=C\OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t264 | PC (p-40:6) or PC (o-40:7) A | XUVCLJCZWPTAIO-OAKHYACESA-N | 53479405 | CCCCCCCC/C=C\CCCCCC/C=C\OC(COC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t265 | PC (p-40:6) or PC (o-40:7) B | FMBYBTSZVHUJMV-DIVFMYBRSA-N | 53479425 | CCCCCCCCCCCCCCCC/C=C\OC(COC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)([O-])OCC[N+](C)(C)C |
| t267 | PC (p-42:2) or PC (o-42:3) | ZLQCRABYIDJNLT-AZPQEANBSA-N | 53479549 | CCCCCCCC/C=C\CCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O/C=C\CCCCCC/C=C\CCCCCCCC |
| t269 | PC (p-42:4) or PC (o-42:5) | NLEDXBSUDVLSEN-UFFJXODHSA-N | 52924034 | CCCCCCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t270 | PC (p-42:5) or PC (o-42:6) A | QZMFOSCFDWPISC-KQHSIIGPSA-N | 53481769 | CCCCC/C=C\C/C=C\C/C=C\CCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCC/C=C\C/C=C\C/C=C\CCCCC |
| t271 | PC (p-42:5) or PC (o-42:6) B | CMUBJJYJAQLOOD-XSOFIKLRSA-N | 52923864 | CCCCCCCCCCCCCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC |
| t272 | PC (p-44:4) or PC (o-44:5) | CEZAZXUWDFPTTE-FHIJIHMSSA-N | 53481767 | CCCCC/C=C\C/C=C\CCCCCCCCCCCCOC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCC/C=C\C/C=C\C/C=C\CCCCC |
| t274 | PE (34:2) | HBZNVZIRJWODIB-NHCUFCNUSA-N | 46891780 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[NH3+])OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t275 | PE (36:1) | JQKOHRZNEOQNJE-ZZEZOPTASA-N | 25244969 | CCCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[NH3+])OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t276 | PE (36:4) | KZLUVTCXBFEIFJ-XGLJQOENSA-N | 52924904 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)(O)OCCN)OC(=O)CCCC/C=C\C/C=C\C/C=C\C/C=C\CC |
| t277 | PE (38:4) | ANRKEHNWXKCXDB-BHFWLYLHSA-N | 46891781 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[NH3+])OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t278 | PE (38:6) | LFGBKOUQHCWBQI-BZGLIJSBSA-N | 52924893 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)(O)OCCN)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t279 | PE (p-34:1) or PE (o-34:2) | SMPXBIVJXNXOAL-PRWZWGSOSA-N | 53479657 | CCCCCCCCCCCCCC/C=C\O[C@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)COP(=O)(O)OCCN |
| t281 | PE (p-36:2) or PE (o-36:3) | CFANDHZPOSNKNO-UDHSZFGOSA-N | 53480897 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](CO/C=C\CCCCCC/C=C\CCCCCCCC)COP(=O)(O)OCCN |
| t282 | PE (p-36:4) or PE (o-36:5) | ADWDFBQPQIEGRZ-XBICFDGKSA-N | 53480870 | CCCCCC/C=C\CCCCCCCC/C=C\OC[C@H](COP(=O)(O)OCCN)OC(=O)CCCC/C=C\C/C=C\C/C=C\CCCCC |
| t283 | PE (p-38:4) or PE (o-38:5) | ZTZQZGHJLWFLFQ-VZBWJDOASA-N | 53480855 | CCCCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)(O)OCCN)OC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC |
| t284 | PE (p-38:5) or PE (o-38:6) | IQSPCSIULMCRPM-ZAJUHDLGSA-N | 53479831 | CCCCCCCC/C=C\CCCCCC/C=C\O[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\C/C=C\CC)COP(=O)(O)OCCN |
| t286 | PE (p-40:5) or PE (o-40:6) | HHQFKPJXVYWLLJ-ABYSKWQHSA-N | 53480857 | CCCCCCCCCCCCCCCC/C=C\OC[C@H](COP(=O)(O)OCCN)OC(=O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC |

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| t25 | pelargonic acid | FBUKVWPVBMHYJY-UHFFFAOYSA-N | 8158 | CCCCCCCCC(=O)O |
| t24 | phenylalanine | COLNVLDHVKWLRT-QMMMGPOBSA-N | 6140 | C1=CC=C(C=C1)C[C@@H](C(=O)O)N |
| t23 | phosphate | NBIIXXVUZAFLBC-UHFFFAOYSA-N | 1004 | OP(=O)(O)O |
| t22 | proline | ONIBWKKTOPOVIA-BYPYZUCNSA-N | 145742 | C1C[C@H](NC1)C(=O)O |
| t21 | pseudo-uridine | PTJWIQPHWPFNBW-GBNDHIKLSA-N | 15047 | C1=C(C(=O)NC(=O)N1)[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O |
| t19 | salicylaldehyde | SMQUZDBALVYZAC-UHFFFAOYSA-N | 6998 | C1=CC=C(C(=C1)C=O)O |
| t18 | serine | MTCFGRXMJLQNBG-REOHCLBHSA-N | 5951 | C([C@@H](C(=O)O)N)O |
| t287 | SM (d30:1) | HZCLJRFPXMKWHR-FEBLJDHQSA-N | 44260123 | CCCCCCCCCCCCCC/C=C/[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCC)O |
| t288 | SM (d32:0) | MJAFYELZQYPMQG-MPQUPPDSSA-N | 44260138 | CCCCCCCCCCCCCCCC[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCCCCC)O |
| t289 | SM (d32:1) | KYICBZWZQPCUMO-PSALXKTOSA-N | 11433862 | CCCCCCCCCCCCCC/C=C/[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCCCC)O |
| t291 | SM (d33:1) | LQINJRUGTUOHGS-YPDYIYJKSA-N | 52931139 | CCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t292 | SM (d34:0) | QHZIGNLCLJPLCU-QPPIDDCLSA-N | 9939965 | CCCCCCCCCCCCCCCC[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCCCCCC)O |
| t293 | SM (d34:1) | RWKUXQNLWDTSLO-GWQJGLRPSA-N | 9939941 | CCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t294 | SM (d34:2) | YLWSJLLZUHSIEA-CKSUKHGVSA-N | 52931235 | CCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t295 | SM (d36:0) | JCELSEVNSMXGKA-IOLBBIBUSA-N | 44260130 | CCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](CCCCCCCCCCCCCCC)O |
| t296 | SM (d36:1) | LKQLRGMMMAHREN-YJFXYUILSA-N | 6453725 | CCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t297 | SM (d36:2) | NBEADXWAAWCCDG-QDDWGVBQSA-N | 6443882 | CCCCCCCCCCCCC/C=C/[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCC/C=C\CCCCCCCC)O |
| t298 | SM (d36:3) | YMTVMVYOUDDTQJ-UOMMIRHQSA-N | 52931155 | CCCCCCCC/C=C\CCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t301 | SM (d38:1) | AADLTHQNYQJHQV-SVLGDMRNSA-N | 44260124 | CCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |

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| t302 | SM (d38:2) | MDRFMTLYKHBJTF-NQYLGBTJSA-N | 52931179 | CCCCCCCCCCCCC/C=C/[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCC/C=C\CCCCCCCC)O |
| t305 | SM (d40:0) | FONAXCRWZQFJHY-JCGOJSMZSA-N | 44260132 | CCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](CCCCCCCCCCCCCCCC)O |
| t307 | SM (d40:2) | FOULCGVQZYQEQM-DNXGLLHMSA-N | 52931201 | CCCCCCCCCCC/C=C/[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |
| t309 | SM (d41:1) | SXZWBNWTCVLZJN-NMIJJABPSA-N | 46891684 | CCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t310 | SM (d41:2) A | JBDGKEXQKCCQFK-JWQIMADESA-N | 52931209 | CCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t312 | SM (d42:1) | QEDPUVGSSDPBMD-XTAIVQBESA-N | 44260127 | CCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCCCCCCC)O |
| t314 | SM (d42:2) | DACOGJMBYLZYDH-GXJPFUDISA-N | 52931217 | CCCCCCCCCCCCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t315 | SM (d42:3) | TXFLWJQVQCDUDZ-BRUGZULGSA-N | 52931215 | CCCCCCCC/C=C\CCCCCCCCCCCCCC(=O)N[C@@H](COP(=O)([O-])OCC[N+](C)(C)C)[C@@H](/C=C/CCCCCCCC/C=C\CCC)O |
| t316 | SM (d43:1) | LXMARZYBSFYVSY-KUQVZNNZSA-N | 52931225 | CCCCCCCCCCCCCCCC[C@H]([C@H](COP(=O)([O-])OCC[N+](C)(C)C)NC(=O)CCCCCCCCCCCCC/C=C\CCCCCCCC)O |
| t16 | succinic acid | KDYFGRWQOYBRFD-UHFFFAOYSA-N | 1110 | C(CC(=O)O)C(=O)O |
| t15 | taurine | XOAAWQZATWQOTB-UHFFFAOYSA-N | 1123 | C(CS(=O)(=O)O)N |
| t457 | TG (48:0) | PVNIQBQSYATKKL-UHFFFAOYSA-N | 11147 | CCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCC |
| t458 | TG (48:1) | FEKLSEFRUGWUOS-DLOIZKPKSA-N | 9543986 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCCCCCCCCCC |
| t459 | TG (48:2) | RUOVJPPUXXFZPC-YZEIBMOJSA-N | 9543987 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCC/C=C\CCCCC |
| t320 | TG (49:0) | TTWJTJMWHOYBPQ-ANFMRNGASA-N | 9543988 | CCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCC |
| t460 | TG (49:1) | VYYGQDOPVVYUKW-UKFBYESTSA-N | 9543991 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCCCCCCCCC |
| t322 | TG (49:2) | QZYSUBAQYSVFNX-PSMULLBHSA-N | 9543993 | CCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCC/C=C\CCCCC |
| t461 | TG (49:3) | DIGMYZZFQSIQBD-PNLKURBTSA-N | 56938088 | CCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCC/C=C\CCCCCC |
| t462 | TG (50:0) | MARPCPMDFOPPJX-UHFFFAOYSA-N | 545588 | CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCC |

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| t463 | TG (50:1) | YHMDGPZOSGBQRH-YYSBDVFPSA-N | 25240460 | CCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)OC(=O)CCCCCCCCCCCCCCC |
| t464 | TG (50:2) | QEZWFCZNHWUARW-XQCAQTCHSA-N | 9544010 | CCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCCC/C=C\CCCCCC |
| t465 | TG (50:3) | UFHNZOACKFBCOM-YXKNDSBASA-N | 25240357 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCCC/C=C\CCCCCC |
| t466 | TG (50:4) | PVMBAGXWHHZKFP-JMPJWMFJSA-N | 25240359 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\CCCCCC |
| t467 | TG (50:5) | AFTBPUXZTDLRSP-UDQIKIEDSA-N | 9544045 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)OC(=O)CCCCCCC/C=C\CCCCCC |
| t468 | TG (51:1) | OZAXLAGNPZMZAD-BOEMPQCLSA-N | 9544006 | CCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCCC)OC(=O)CCCCCCCCCCCCCCCC |
| t469 | TG (51:2) | NSNSZGBCOIKUBU-SZOKBDNISA-N | 9544013 | CCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCCC)OC(=O)CCCCCCC/C=C\CCCCCCC |
| t470 | TG (51:3) | ISSGPXMQOMAFMJ-DMGKHJLRSA-N | 9544023 | CCCCCCC/C=C\CCCCCCCC(=O)OCC(OC(=O)CCCCCCC/C=C\CCCCCCC)COC(=O)CCCCCCC/C=C\CCCCCCC |
| t471 | TG (51:4) | IIRQXNVLAXQEKB-KBEZCZBDSA-N | 9544052 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCC |
| t472 | TG (52:0) | SDNYRTVJOFMYIW-OIVUAWODSA-N | 545690 | CCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCCCCC |
| t473 | TG (52:1) | NPCZZYKITFKRQZ-RFBIWTDZSA-N | 5365005 | CCCCCCCCCCCCCCCCCC(=O)OC(COC(=O)CCCCCCCCCCCCCCCC)COC(=O)CCCCCCC/C=C\CCCCCCCC |
| t474 | TG (52:2) | TXMWKTABZBAJCW-QLHBUVOUSA-N | 56938176 | CCCCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCCCCCCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t475 | TG (52:3) | DQXQIWIQYYEGLG-MMWLGPPDSA-N | 56938177 | CCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCCCC/C=C\CCCCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t476 | TG (52:4) | WHSWXEYWNPTUPW-HNJDVRDNSA-N | 25240364 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\CCCCCC)COC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t477 | TG (52:5) | CQZAAIKPSLHIBC-KDJOUNIJSA-N | 25240366 | CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t478 | TG (52:6) | SSOSFUDNINFYLJ-KIYGNKBKSA-N | 56938180 | CCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t479 | TG (53:2) | RSINITWKVQRWSZ-RFVLVDBCSA-N | 9544102 | CCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCC)OC(=O)CCCCCCCCCCCCCCCCC |
| t480 | TG (53:3) | ZNQBEJJYVJSZLM-LEDQTTRKSA-N | 9544126 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCC)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t324 | TG (53:4) | BMSDHYZLQWTKSQ-LSJAAEOESA-N | 9544152 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCC)OC(=O)CCCCCCC/C=C\CCCCCCCC |

| | | | | |
|---|---|---|---|---|
| t481 | TG (53:5) | QHYAATSKYBYSLG-BXDFBOBBSA-N | 9544183 | CCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t483 | TG (54:1) | YFFIQXNTTVSKJC-NZEOUKRFSA-N | 16058371 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)OC(=O)CCCCCCCCCCCCCCCCC |
| t484 | TG (54:2) | WUUWGORPQFKFQN-XDVOZUNOSA-N | 56938183 | CCCCCCCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t326 | TG (54:3) | PHYFQTYBJUILEZ-IUPFWZBJSA-N | 5497163 | CCCCCCCC/C=C\CCCCCCCC(=O)OCC(OC(=O)CCCCCCC/C=C\CCCCCCCC)COC(=O)CCCCCCC/C=C\CCCCCCCC |
| t329 | TG (54:4) | BRLGHZXETDWABO-NOFIOOQLSA-N | 9544255 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t486 | TG (54:5) | OEJXMJPFOHYSIU-GRLFFVHSSA-N | 9544294 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t488 | TG (54:6) | CDNDFDKFZBPPFW-AXJGXPKFSA-N | 9544363 | CCCCCCCC/C=C\CCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\CCCCCC)COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t489 | TG (54:8) | BMPVTDWOWBNPJU-NYRSPQLFSA-N | 9544413 | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCC |
| t490 | TG (56:2) | PDEQUPGHMOMBFC-FYEHETCMSA-N | 9544390 | CCCCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t491 | TG (56:3) | QXMHHXQBBKDSSL-BAQZNRHJSA-N | 9544447 | CCCCCCCC/C=C\CCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)OC(=O)CCCCCCC/C=C\CCCCCCCC |
| t330 | TG (56:4) | YONCDTJKIZDSKQ-IYASBODOSA-N | 25240379 | CCCCCCCC/C=C\CCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t493 | TG (56:5) A | UHEJWASONFIROS-YPSHDQQVSA-N | 25240380 | CCCCCCCC/C=C\CCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t494 | TG (56:6) | ZTNDRFCABXFVMY-WJTCTALZSA-N | 9544625 | CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t332 | TG (56:7) B | DODZUDCYRVWEOJ-GKZBLMSTSA-N | 9544695 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC |
| t496 | TG (56:8) | UBGUHMDKBGQUND-VPFWBQFRSA-N | 9544762 | CCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t498 | TG (58:1) | OWZMHFAFGQCCNI-FBXRAONGSA-N | 25240381 | CCCCCCCCCCCCCCCCCCCCC(=O)OC[C@@H](COC(=O)CCCCCCC/C=C\CCCCCCC)OC(=O)CCCCCCCCCCCCCCCCCCCCC |
| t497 | TG (58:10) | GXWBCAVCOMAOHT-VMCJOIRWSA-N | 9545277 | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t499 | TG (58:6) | GSNFRUMSEHHPSY-LCXCSEBNSA-N | 9544977 | CCCCCCCC/C=C\CCCCCCCCCC(=O)O[C@H](COC(=O)CCCCCCC/C=C\CCCCCCC)COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t336 | TG (58:8) | KWIGMCRWEINBIR-HUPVKWKYSA-N | 9545124 | CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC |

| | | | | |
|---|---|---|---|---|
| t500 | TG (58:9) | RVXFSLZMZOFGEQ-SWIIBWKZSA-N | 9545200 | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC |
| t14 | threitol | UNXHWFMMPAWVPI-QWWZWVQMSA-N | 169019 | C([C@H]([C@@H](CO)O)O)O |
| t13 | threonic acid | JPIJQSOTBSSVTP-STHAYSLISA-N | 5460407 | C([C@@H]([C@H](C(=O)O)O)O)O |
| t12 | threonine | AYFVYJQAPQTCCC-GBXIJSLDSA-N | 6288 | C[C@H]([C@@H](C(=O)O)N)O |
| t11 | tocopherol alpha- | NCYCYZXNIZJOKI-OVSJKPMPSA-N | 638015 | CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C=O)/C)/C |
| t10 | tocopherol gamma- | QUEDXNHFTDJVIY-DQCZWYHMSA-N | 92729 | CC1=C(C=C2CC[C@@](OC2=C1C)(C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C)O |
| t9 | trans-4-hydroxyproline | PMMYEEVYMWASQN-DMTCNVIQSA-N | 5810 | C1[C@H](CN[C@@H]1C(=O)O)O |
| t8 | tryptophan | QIVBCDIJIAJPQS-VIFPVBQESA-N | 6305 | C1=CC=C2C(=C1)C(=CN2)C[C@@H](C(=O)O)N |
| t7 | tyrosine | OUYCCCASQSFEME-QMMMGPOBSA-N | 6057 | C1=CC(=CC=C1C[C@@H](C(=O)O)N)O |
| t6 | urea | XSQUKJJJFZCRTK-UHFFFAOYSA-N | 1176 | C(=O)(N)N |
| t5 | uric acid | LEHOTFFKMJEONL-UHFFFAOYSA-N | 1175 | C12=C(NC(=O)N1)NC(=O)NC2=O |
| t4 | uridine | DRTQHJPVMGBUCF-XVFCMESISA-N | 6029 | C1=CN(C(=O)NC1=O)[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O |
| t3 | valine | KZSNJWFQEVHDMF-BYPYZUCNSA-N | 6287 | CC(C)[C@@H](C(=O)O)N |
| t2 | xanthine | LRFVTYWOQMYALW-UHFFFAOYSA-N | 1188 | C1=NC2=C(N1)C(=O)NC(=O)N2 |
| t1 | xylulose | LQXVFWRQNMEDEE-PYHARJCCSA-N | 439205 | C1[C@@H]([C@H](C(O1)(CO)O)O)O |

**Supplemental Table 2: Proportion and amount of subjects eating any amount of food subgroups among TEDDY mAb+ cases and matched controls with metabolomics at 9 months and seroconversion**

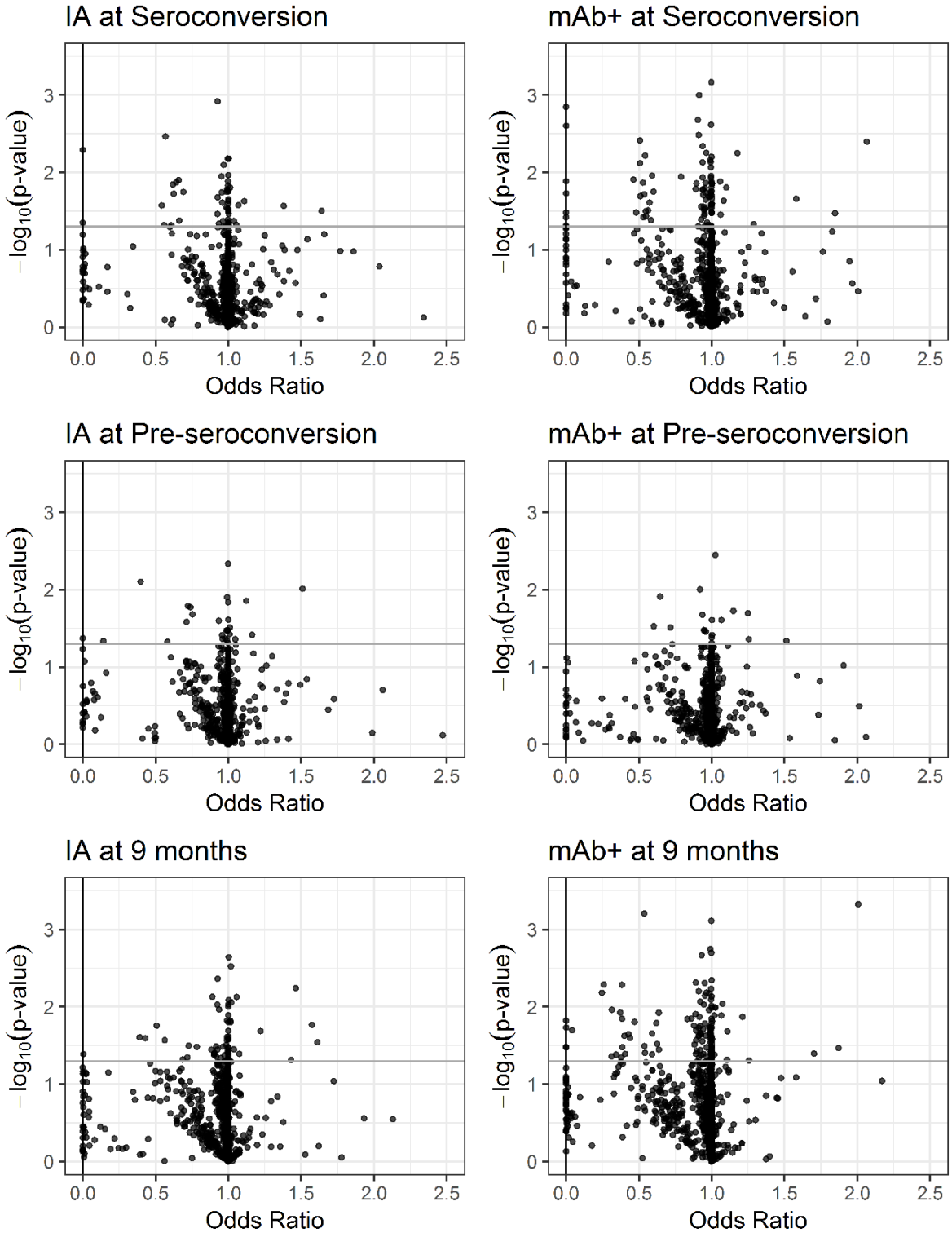
| | Infancy 9-months (n=530) | | |
|---|---|---|---|
| **Food groups (bold) and subgroups** | **n Consumers** | **Mean g/day** | **% Consumers** |
| **BREAST MILK** | 229 | 345.19 | 43.2 |
| **CEREALS** | | | |
| Gluten-containing cereals (wheat, rye, barley) | 469 | 15.56 | 88.5 |
| Gluten-free cereals (rice, oats, corn, other GF flours and starches) | 524 | 30.81 | 98.9 |
| **FRUIT AND BERRIES** | | | |
| Apple | 364 | 44.02 | 68.7 |
| Berries | 253 | 20.63 | 47.7 |
| Citrus | 20 | 17.59 | 3.8 |
| Other fresh fruits | 484 | 59.48 | 91.3 |
| Processed fruits (canned and dried) | 268 | 31.70 | 50.6 |
| **FRUIT, BERRY, VEGETABLE JUICES** | | | |
| Apple Juice | 183 | 22.14 | 34.5 |
| Berry Juice | 8 | 16.89 | 1.5 |
| Citrus Juice | 149 | 7.43 | 28.1 |
| Other fruit juices | 205 | 15.27 | 38.7 |
| Mixed Fruit, Fruit/Vegetables, Vegetables Juices | 74 | 34.64 | 14.0 |
| **VEGETABLES** | | | |
| Potatoes | 416 | 54.60 | 78.5 |
| Roots, Sweet Potatoes | 488 | 39.26 | 92.1 |
| Leafy Vegetables (and Cabbage) | 266 | 19.05 | 50.2 |
| Fruit Vegetables | 391 | 30.38 | 73.8 |
| Onions | 296 | 8.17 | 55.9 |
| Legumes | 241 | 24.85 | 45.5 |
| Processed Vegetables | 237 | 15.68 | 44.7 |
| Soy | 29 | 15.15 | 5.5 |
| **NUTS, SEEDS** | 43 | 0.89 | 8.1 |
| **FATS AND OILS** | | | |
| Vegetables Oils | 432 | 7.99 | 81.5 |
| Saturated Fats (solid vegetable, animal fats) | 251 | 2.13 | 47.4 |
| Low-Fat Butter/Margarine | 42 | 4.83 | 7.9 |
| High-Fat Butter/Margarine | 163 | 3.62 | 30.8 |
| **MILK AND MILK PRODUCTS** | | | |

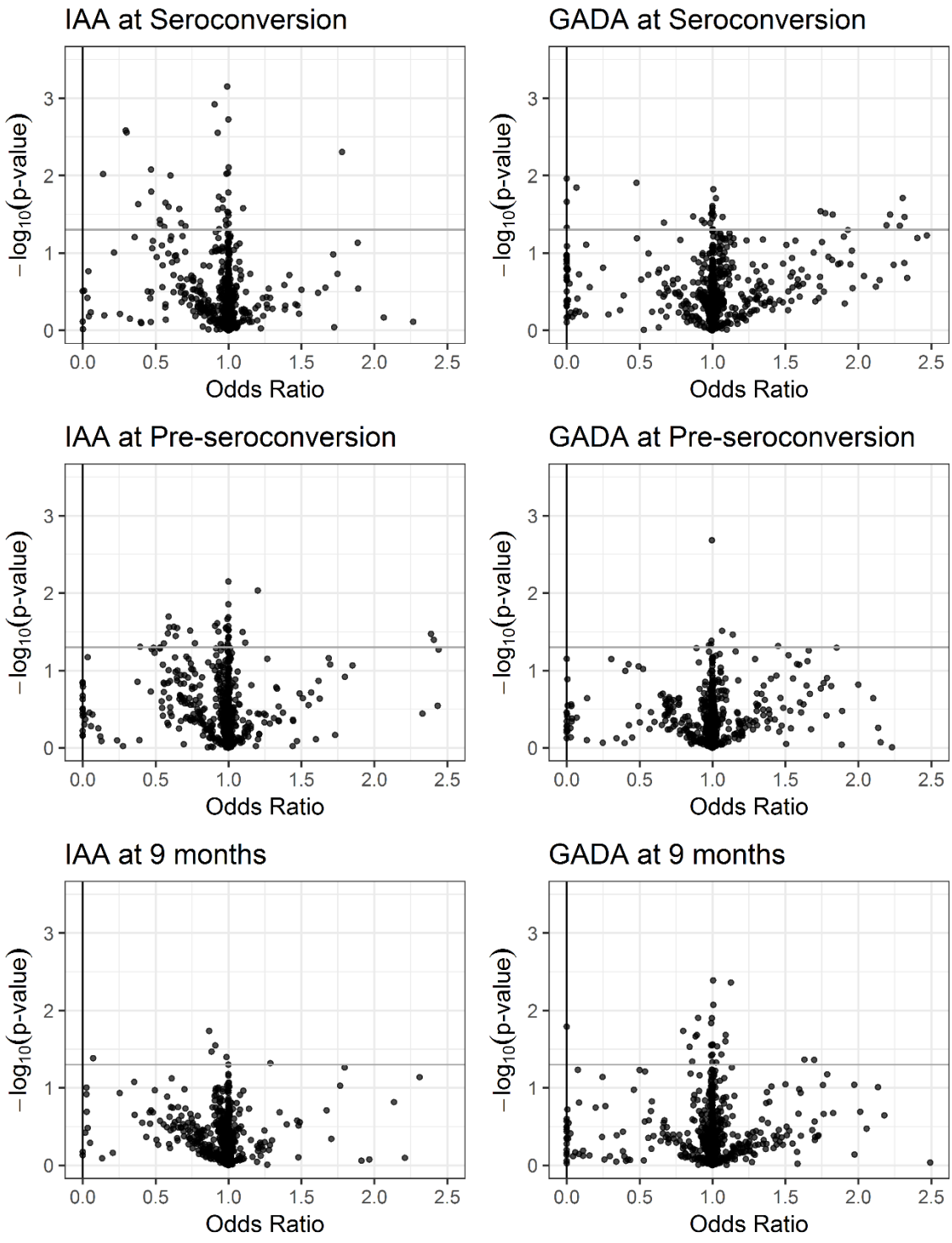
| | | | |
|---|---|---|---|
| Fat-free milk | 252 | 58.40 | 47.6 |
| Milk | 195 | 224.12 | 36.8 |
| Creams | 124 | 7.25 | 23.4 |
| Ice cream | 15 | 10.73 | 2.8 |
| Sour Milk | 193 | 50.47 | 36.4 |
| Cheese | 178 | 9.42 | 33.6 |
| **NON-DAIRY PRODUCTS** | 2 | 13.00 | 0.4 |
| **MEAT AND MEAT PRODUCTS** | | | |
| Red Meat | 368 | 26.39 | 69.4 |
| Poultry | 300 | 19.50 | 56.6 |
| Processed Meats | 67 | 22.10 | 12.6 |
| **FISH AND FISH PRODUCTS** | 134 | 18.67 | 25.3 |
| **EGGS** | 102 | 8.08 | 19.3 |
| **BEVERAGES** | | | |
| Other Beverages | 32 | 75.84 | 6.0 |
| Sugar-Sweetened Beverages | 90 | 39.77 | 17.0 |
| Alcohol | 0 | . | 0.0 |
| **CONFECTIONARY** | 10 | 11.27 | 1.9 |
| **INFANT FORMULAS** | 259 | 523.18 | 48.9 |
| **MISCELLANEOUS** | 10 | 6.45 | 1.9 |

**Supplemental Table 3: Characteristics and outcomes of TEDDY nested case-control 1:3 matched study at seroconversion**

| | Outcomes | | | |
|---|---|---|---|---|
| | **IA** | **IAA** | **GADA** | **mAb+** |
| **Matching Characteristic** | **n (%)** | **n (%)** | **n (%)** | **n (%)** |
| **Clinical Center** | | | | |
| Colorado | 51 (14.5) | 22 (12.9) | 17 (15.0) | 30 (14.2) |
| Georgia | 28 (8.0) | 8 (4.7) | 12 (10.6) | 18 (8.5) |
| Washington | 32 (9.1) | 16 (9.4) | 14 (12.4) | 15 (7.1) |
| Finland | 100 (28.4) | 59 (34.5) | 23 (20.4) | 72 (34.1) |
| Germany | 28 (8.0) | 11 (6.4) | 9 (8.0) | 16 (7.6) |
| Sweden | 113 (32.1) | 55 (32.2) | 38 (33.6) | 60 (28.4) |
| **Sex** | | | | |
| Female | 158 (44.9) | 71 (41.5) | 56 (49.6) | 91 (43.1) |
| Male | 194 (55.1) | 100 (58.5) | 57 (50.4) | 120 (56.9) |
| **FDR/GP Status** | | | | |
| First Degree Relative | 79 (22.4) | 37 (21.6) | 27 (23.9) | 53 (25.1) |
| General Population | 273 (77.6) | 134 (78.4) | 86 (76.1) | 158 (74.9) |
| **Long Distance Protocol** | | | | |
| Yes | 43 (12.2) | 17 (9.9) | 16 (14.2) | 24 (11.4) |
| No | 309 (87.8) | 154 (90.1) | 97 (85.8) | 187 (88.6) |

**Supplemental Figure 2**: **Volcano plots of the association between 853 metabolites measured at seroconversion, pre-seroconversion, and 9-months and development of islet autoimmunity (IA), multiple autoantibody positivity (mAb+), IAA, and GADA in the TEDDY study.**




IAA at Seroconversion
GADA at Seroconversion
IAA at Pre-seroconversion
GADA at Pre-seroconversion
IAA at 9 months
GADA at 9 months
−log10(p-value)
Odds Ratio
0
1
2
3
0.0
0.5
1.0
1.5
2.0
2.5

**Supplemental Table 4: ChemRICH summary of chemically similar metabolite groups significantly associated with mAb+ (nominal p-value for group<0.05)**

| | | Seroconversion | | | | Pre-seroconversion | | | | Infancy | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Metabolite Groups | | Metabolite | | Group | | Metabolite | | Group | | Metabolite | | Group | |
| Name | Total p | p, p<0.05 | p, OR<1 | p-value | q-value | p, p<0.05 | p, OR<1 | p-value | q-value | p, p<0.05 | p, OR<1 | p-value | q-value |
| Unsaturated Phosphatidylcholines | 76 | 5 | 3 | 2.1E-05 | 0.0003 | 2 | 1 | 0.013 | 0.35 | 29 | 28 | 2.2E-20 | 6.6E-19 |
| Sphingomyelins | 16 | | | | | | | | | 10 | 10 | 1.1E-08 | 1.6E-07 |
| Phosphatidylethanolamines | 10 | 3 | 3 | 0.0047 | 0.042 | | | | | 3 | 3 | 2.9E-06 | 2.9E-05 |
| Galactosylceramides | 4 | | | | | | | | | 2 | 2 | 4.4E-05 | 0.00033 |
| Dicarboxylic Acids | 5 | | | | | | | | | 3 | 0 | 0.0019 | 0.012 |
| Phospholipid Ethers | 6 | | | | | | | | | 2 | 2 | 0.0032 | 0.016 |
| Unsaturated Triglycerides | 43 | 17 | 15 | 3.1E-15 | 9E-14 | | | | | | | | |
| Amino Acids | 6 | 2 | 2 | 0.0074 | 0.042 | | | | | | | | |
| Saturated FA | 7 | 3 | 0 | 0.0074 | 0.042 | | | | | | | | |
| Diglycerides | 11 | 3 | 3 | 0.014 | 0.064 | | | | | | | | |
| Amino Acids, Aromatic | 4 | 2 | 2 | 0.03 | 0.12 | | | | | | | | |

*ChemRICH inputs: p-value and OR=Odds Ratio from conditional logistic regression models adjusted for HLA (DR3/4) and age at blood draw date*
*p=number of metabolites*

**Supplemental Table 5: Correlation between key metabolites and dietary pattern scores in infancy.**

| | Metabolite-related dietary patterns | | | | | |
|---|---|---|---|---|---|---|
| | 1 | | 2 | | 3 | |
| | r | p-value | r | p-value | r | p-value |
| PC (34:3) | 0.1275 | 0.0033 | 0.07447 | 0.0871 | 0.30464 | <.0001 |
| SM (d41:2) A | 0.0415 | 0.3408 | 0.17774 | <.0001 | -0.07351 | 0.0912 |
| PE (34:2) | 0.38408 | <.0001 | 0.10781 | 0.0131 | -0.02897 | 0.5062 |
| GlcCer (d41:1) | -0.12619 | 0.0036 | 0.25199 | <.0001 | -0.06429 | 0.1397 |
| Adipic acid | 0.00103 | 0.9812 | -0.01747 | 0.6884 | 0.00241 | 0.9559 |
| PC (p-32:0) or PC (o-32:1) | -0.12968 | 0.0028 | 0.22418 | <.0001 | 0.16656 | 0.0001 |

*r=Pearson correlation coefficient*

**Supplemental Table 6: Cohort characteristics of TEDDY children with food records at age 9-months**

| | mAb+ by age 6 yr | | mAb- at age 6 yr | | |
|---|---|---|---|---|---|
| | **n** | **%** | **n** | **%** | **p-value** |
| Total Subjects | 300 | | 6237 | | |
| Clinical Center | | | | | 0.196 |
| Colorado | 52 | 17.33 | 987 | 15.82 | |
| Georgia | 25 | 8.33 | 638 | 10.23 | |
| Washington | 29 | 9.67 | 837 | 13.42 | |
| Finland | 77 | 25.67 | 1406 | 22.54 | |
| Germany | 23 | 7.67 | 365 | 5.85 | |
| Sweden | 94 | 31.33 | 2004 | 32.13 | |
| Female | 139 | 46.33 | 3075 | 49.3 | 0.315 |
| First degree relative | 71 | 23.67 | 613 | 9.83 | <0.001 |
| HLA-DR3/4 | 169 | 56.33 | 2354 | 37.74 | <0.001 |
| | **Mean** | **SD** | **Mean** | **SD** | **p-value** |
| Age at first Ab (days) | 990.1 | 517.3 | -- | | |
| Dietary Pattern Scores | | | | | |
| 1 | -0.055 | 1.07 | 0.004 | 0.98 | 0.349 |
| 2 | -0.076 | 0.88 | 0.005 | 0.93 | 0.120 |
| 3 | 0.082 | 1.06 | 0.008 | 1.04 | 0.238 |