Supplementary Information for

# Molecular Formula Prediction for Chemical Filtering of 3D OrbiSIMS Datasets

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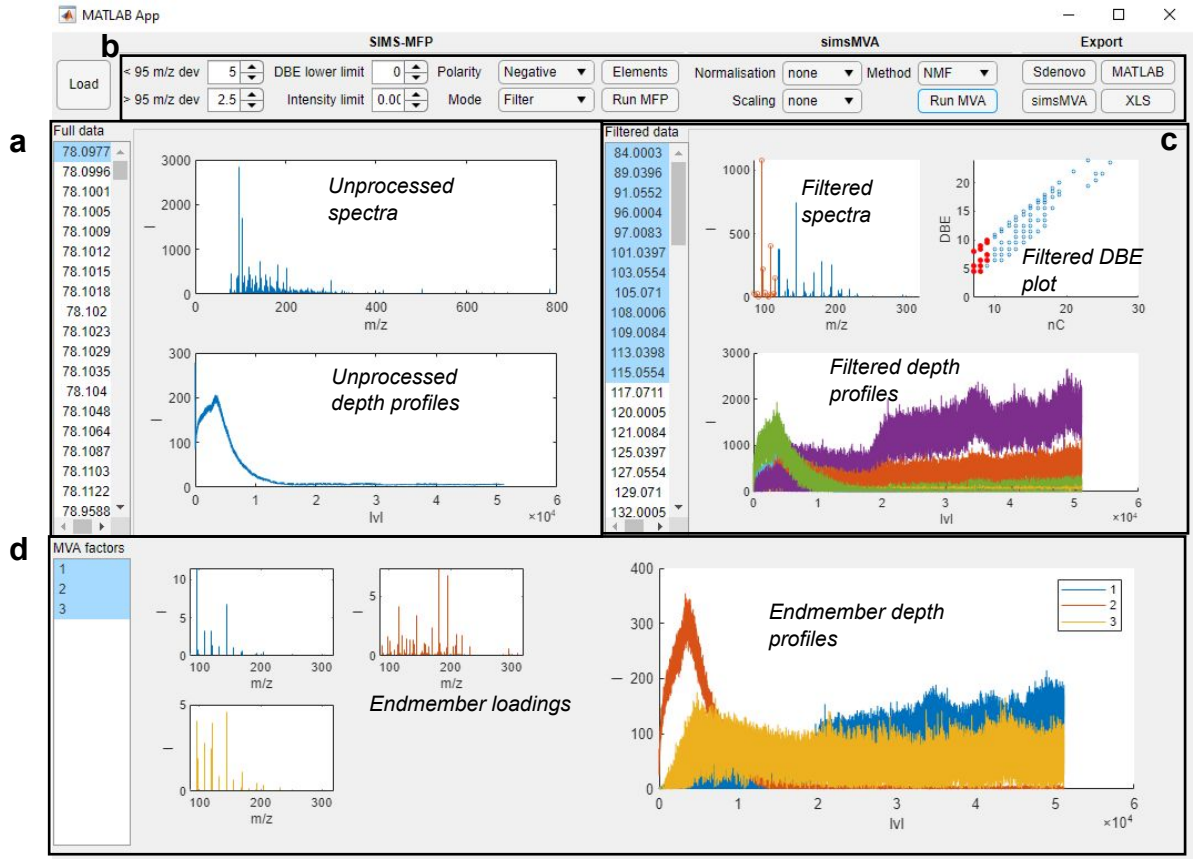
## Supplementary note 1 - SIMS-MFP software graphical user interface

The need to simplify high-resolution 3D SIMS datasets is ever-growing in the field, SIMS-MFP software combines tools for MFP, categorization of species by double bond equivalence (DBE) and integrates existing MVA tools which can be linked to existing SIMS-MVA software.[9] A unique feature of this program is its incorporation to SIMS depth profiling data and the graphical user interface (GUI) (**Supplementary Figure 1**) is to display the profiles in both the pre and post filtered list and throughout this work we show its use for validating the grouping of secondary ions and is discussed in this work.



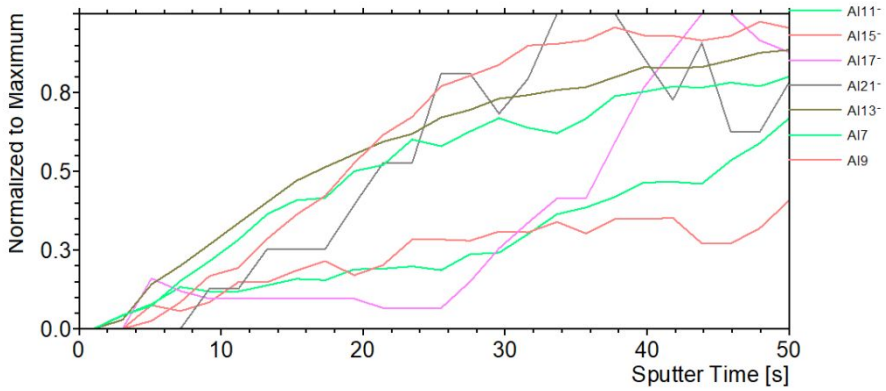

***Supplementary Figure 1****. Interface of the SIMS-MFP software showing key steps for the workflow an example 3D OrbiSIMS dataset. A. Display of the pre-filtered data including raw spectra and profiles of selected species. B. Inputting search criteria, error thresholds, DBE and intensity lower limits, polarity and the elemental compositions ('elements' button must be selected). C, After selecting 'Run MFP' the output data is shown. The filtered spectra of ions identified (left) and DBE versus carbon number of ions found in the search are displayed. Depth profiles for species can be selected also. D. The result of 'Run MVA' on the filtered depth profiling data. Data output is shown after performing MVA on the filtered list.*

Upon loading a selected depth profile matrix by selecting the 'Load' button, the software displays the peak list and profiles for each ion in the list (**Supplementary Figure 1a**). Next, the user enters pre-set criteria for the filter, namely elemental compositions by clicking the 'elements' button (**Supplementary Figure 1b**), which brings up a

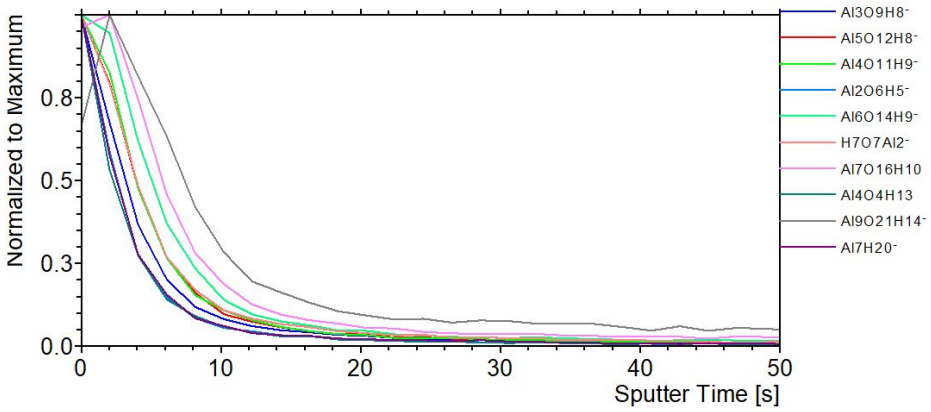
table where maximum and minimum values are chosen, an untargeted approach can be used by selecting '-1' in the maximum value. Other constraints can be determined such as minimum DBE value, maximum error threshold (we recommend < 2 ppm for ions > *m/z* 95) and minimum peak intensity which are selected using the buttons in **Supplementary Figure 1b**. After selecting the 'Run MFP' button the program will run and cycle through each *m/z* value in the list and attempt to calculate its formula based on the preset criteria and will calculate DBE on proposed molecular formula. The program generates several plots (**Supplementary Figure 1c**). Firstly, a mass spectrum containing only ions with formula meeting the preset criteria (termed 'filtered spectra'). Second, a plot of the DBE versus carbon number of all possible assignments in the filtered data ('filtered DBE plot'). The list of ions with possible matching formula are displayed and their profiles can be displayed as well. A file is also produced which is exported to MATLAB and contains the formula predictions of each ion, and DBE value of each candidate for further interrogation by the user. If more than one formula can be assigned to a peak this is also shown. We include code which can match assigned ions to those in the LIPIDMAPS. Another feature in the SIMS-MFP toolkit is a 'mass separator' button which is accessed in the 'mode' drop-down menu (**Supplementary Figure 1a**). This generates a separated spectrum containing all peaks that could not be matched to the preset criteria. A list of non-included ions is generated which can be put back into the formula finder if the user wishes to further interrogate separated species which may be of use when analyzing sample and substrate peaks, for example. The user can perform MVA on filtered datasets by accessing the MVA tab in the GUI (**Supplementary Figure 1b**). We show an example after running non-negative matrix factorization (NMF) on the filtered depth profile data. The number of iterations and endmembers can be chosen and are displayed in the lower portion of the GUI which shows loadings and profiles of each endmember (**Supplementary Figure 1d**). In each case the plots can be exported as png. or svg. files. SIMS-MFP can incorporate datasets from multiple samples, allowing other MVA techniques to be performed such as principal component analysis or K-means clustering. Filtered data can be exported to simsMVA[5] for further interrogation by MVA techniques.

## Supplementary Figures

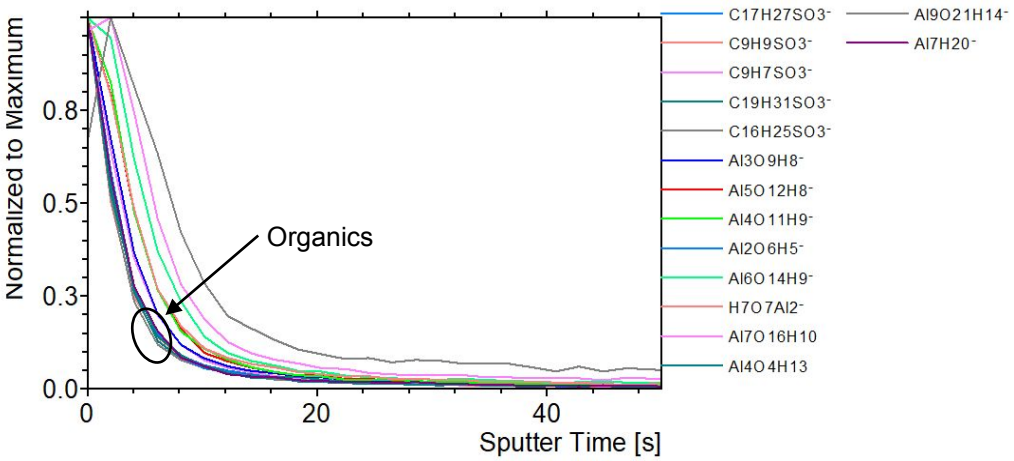
**(a)** Al clusters



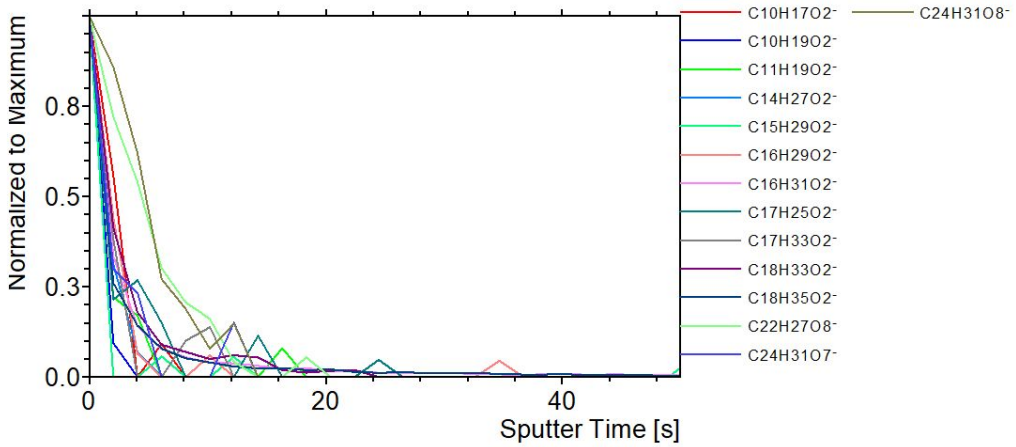

**(b)** Al oxides and hydroxides



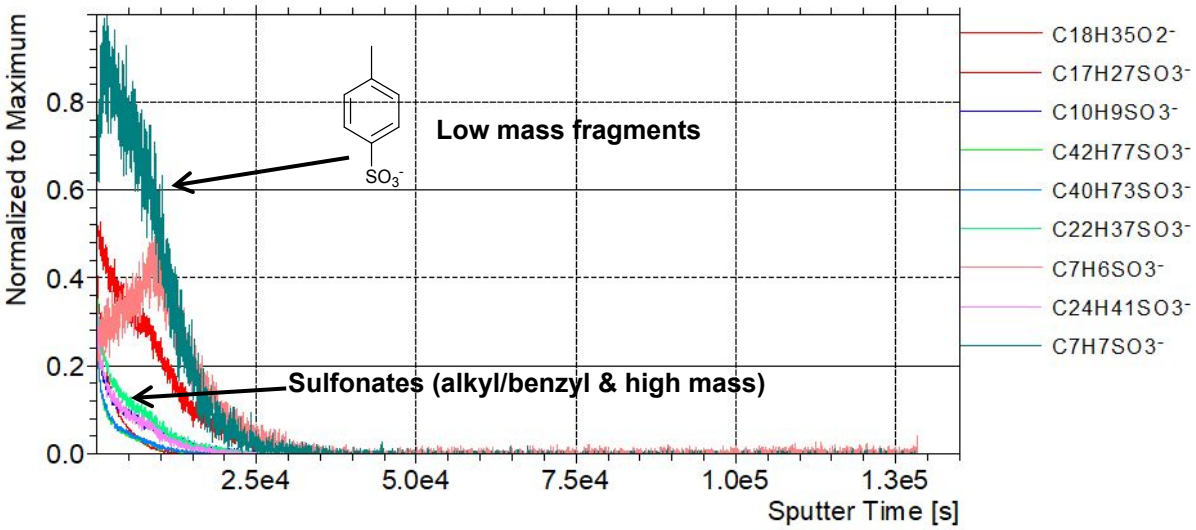

**(c)** Al oxides and hydroxides and intense organics ions



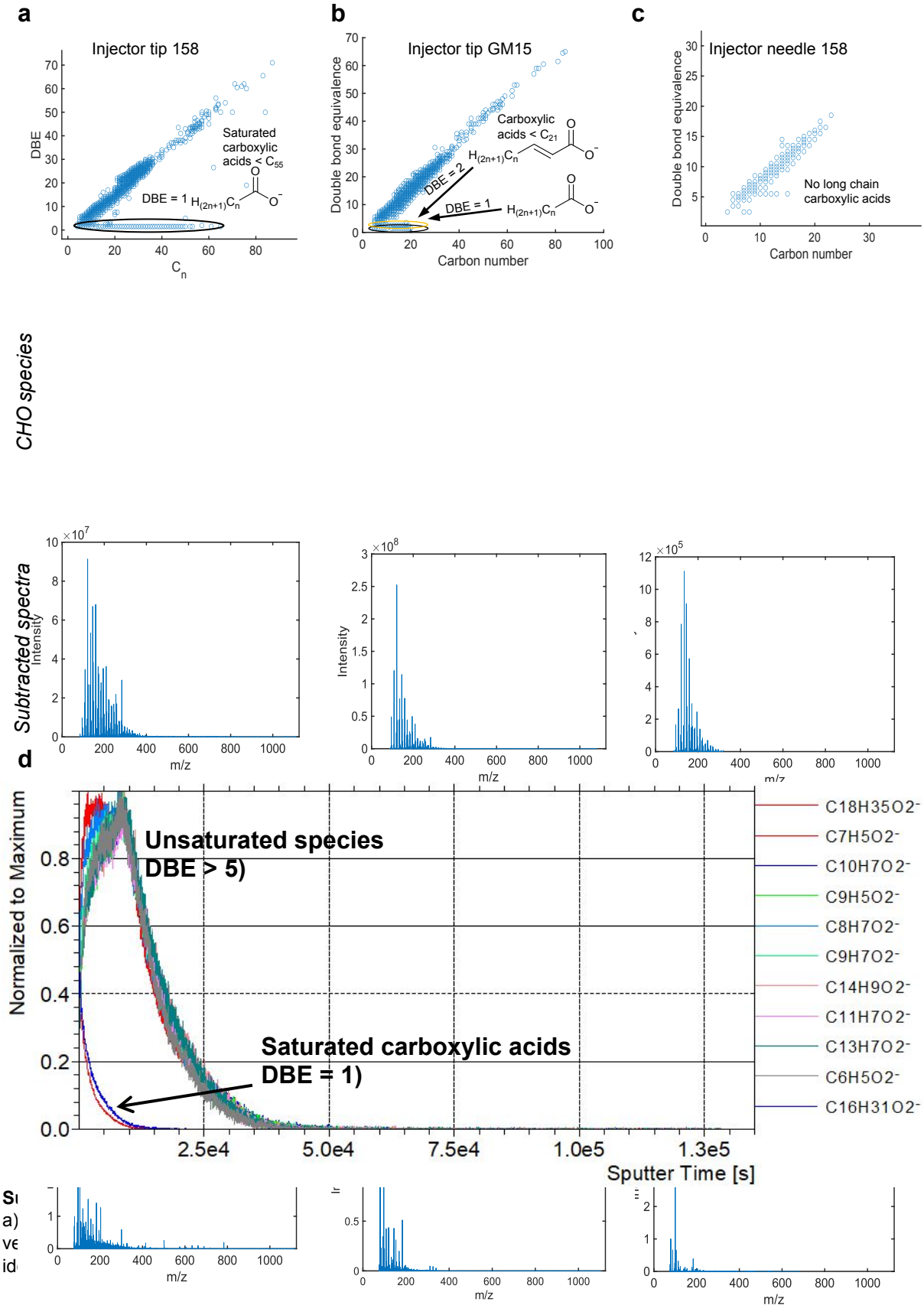
**(d)** Species in LIPIDMAPS

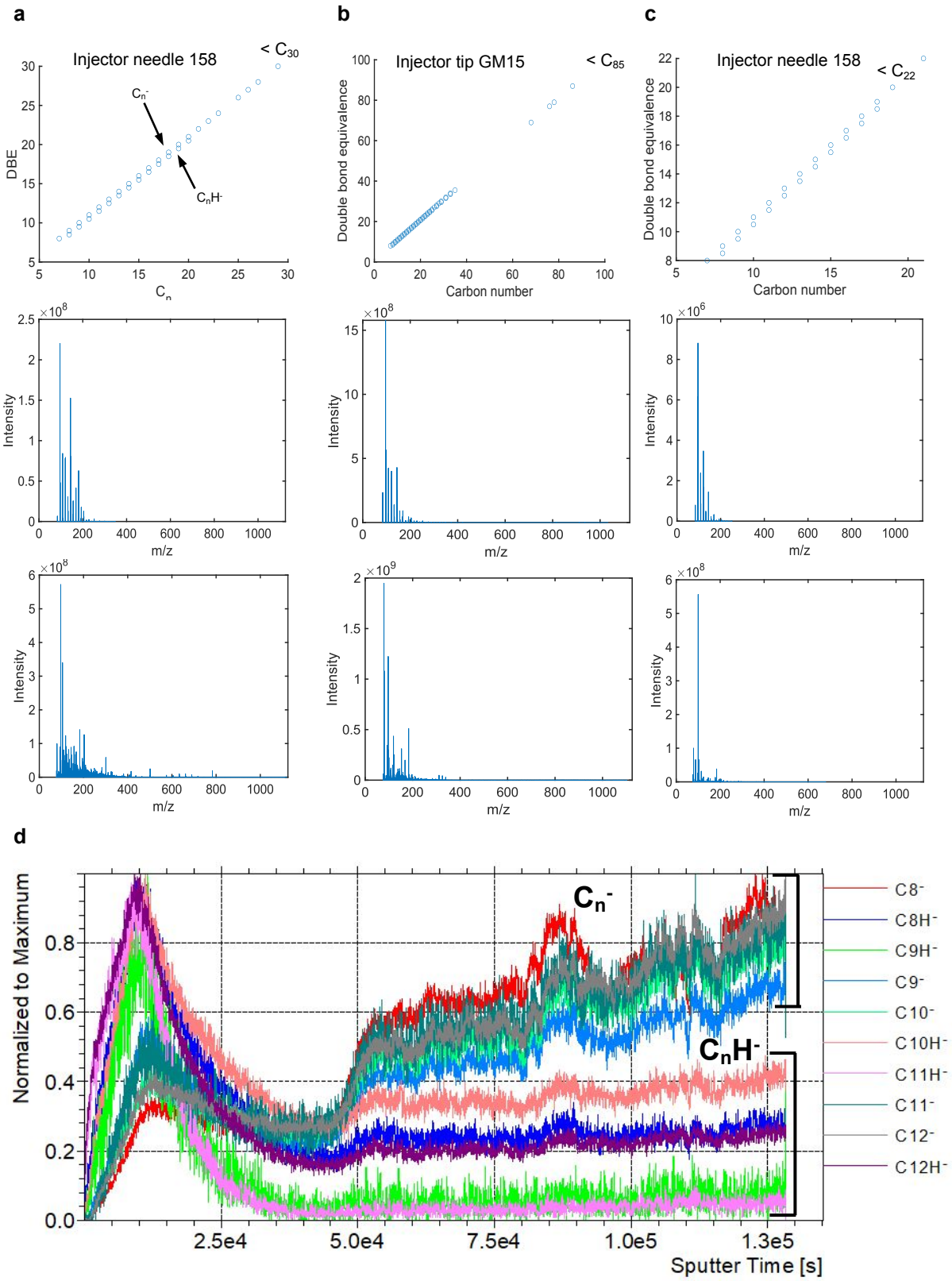



**Supplementary Figure 2**: 3D OrbiSIMS depth profiles of the organic and inorganic species on the dull side of the aluminum foil.

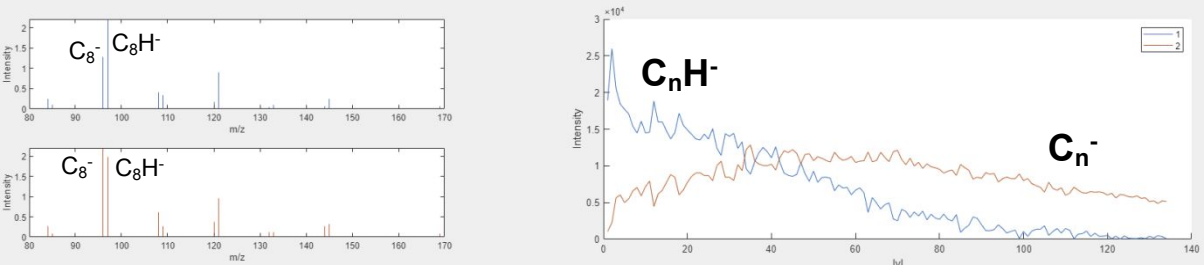



**Supplementary Figure 3**. Application of MFP to identify sulfated species (C & H = any, O = 3, S = 1) in engine deposits. Depth profiles of the 10 most intense species found in the search are shown.


a
Injector tip 158
DBE
Saturated carboxylic acids < C55
DBE = 1
Cn
b
Injector tip GM15
Double bond equivalence
Carboxylic acids < C21
DBE = 2
DBE = 1
Carbon number
c
Injector needle 158
Double bond equivalence
No long chain carboxylic acids
Carbon number
CHO species
Subtracted spectra
Intensity
m/z
d
Normalized to Maximum
Unsaturated species
DBE > 5)
Saturated carboxylic acids
DBE = 1)
C18H35O2-
C7H5O2-
C10H7O2-
C9H5O2-
C8H7O2-
C9H7O2-
C14H9O2-
C11H7O2-
C13H7O2-
C6H5O2-
C16H31O2-
Sputter Time [s]

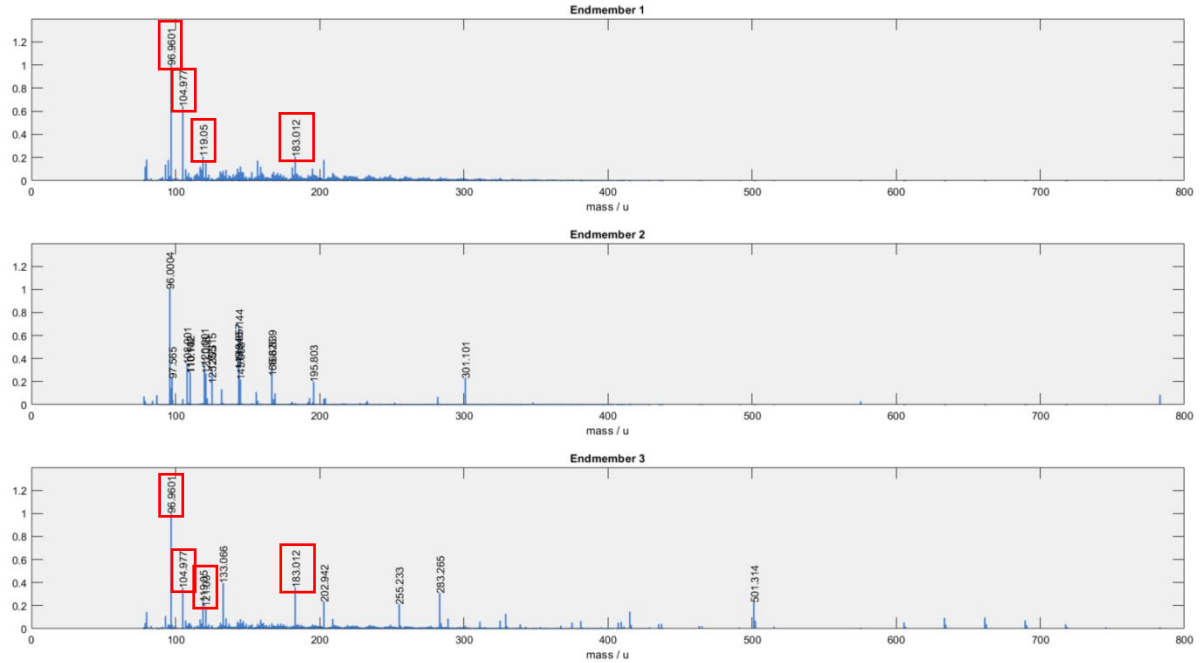

a
b
c
Injector needle 158
< C30
DBE
Cn-
CnH-
Cn
Injector tip GM15
< C85
Double bond equivalence
Carbon number
Injector needle 158
< C22
Intensity
m/z
d
Normalized to Maximum
Cn-
CnH-
Sputter Time [s]
C8-
C8H-
C9H-
C9-
C10-
C10H-
C11H-
C11-
C12-
C12H-

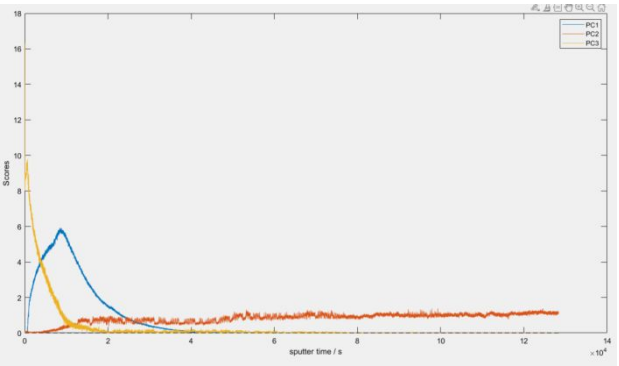
**e**




**Supplementary Figure 5**. Application of the SIMS-MFP software to identify carbonaceous ions (C = any, H ≤ 1) in engine deposits. a) injector tip 1, b) injector tip deposit 2 and c) injector needle 1. In each case the double bond equivalence (DBE) versus carbon number of each ion identified is displayed above, the middle plot shows the spectra of species identified and below are the subtracted spectra of species not found in the search. d) Depth profiles of intense ions in the filtered data set. e) NMF outputs on carbonaceous ions from injector needle 1.

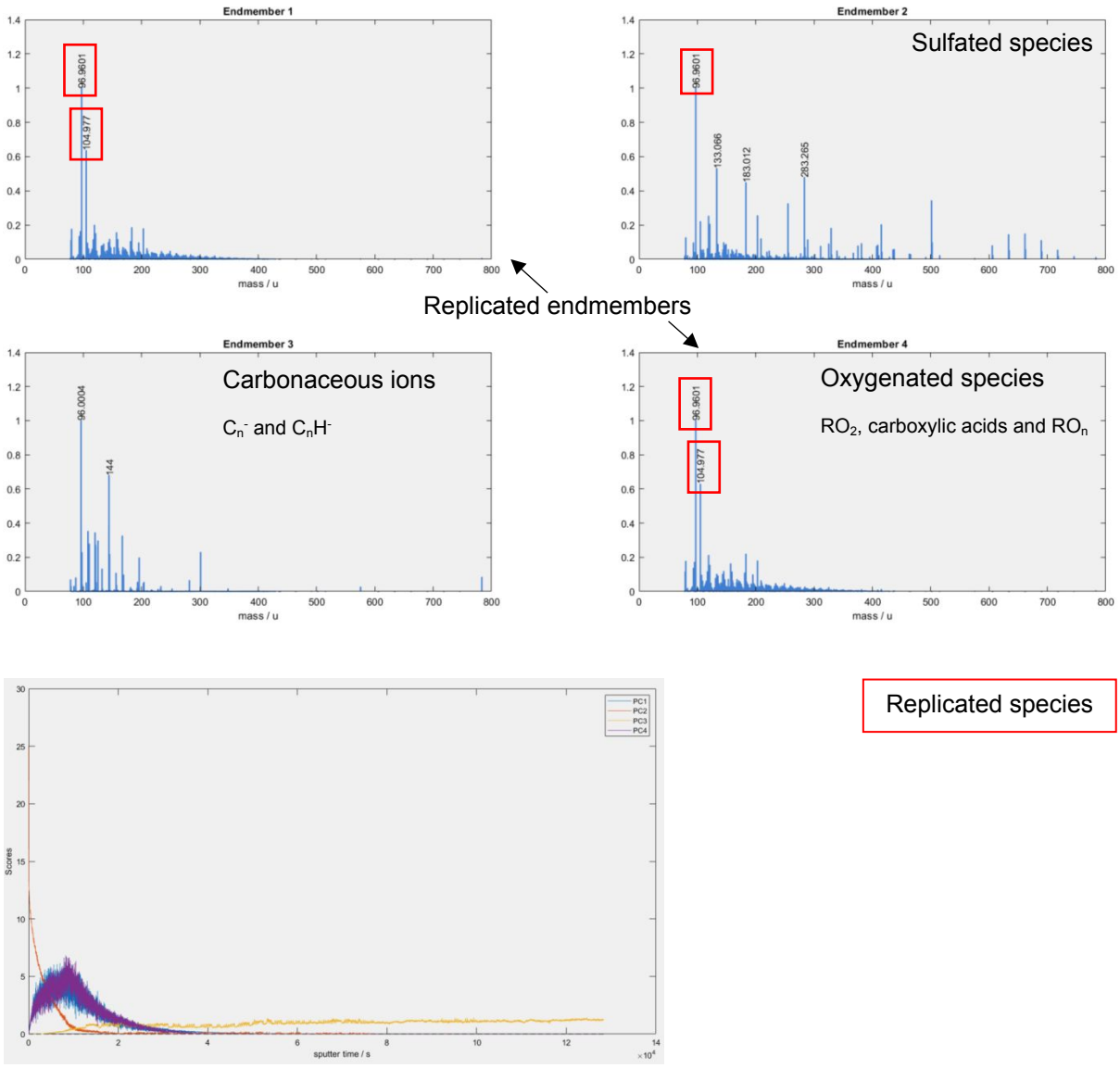
**a)** 3 endmembers (200 iterations)




Replicated species

**b)** 4 endmembers (200 iterations)




**Supplementary Figure 6**. NMF analysis on the raw 3D OrbiSIMS spectra with different conditions, a) with 3 endmembers, b) with 4 endmembers. In each case there was overfitting of data, loadings grouped species together with different elemental compositions and depth profiling behaviors.

**Supplementary Table 1:** Output data file from SIMS-MFP of molecular formula which fit the constraints of from the searches of the aluminum foil. a) Al search showing species containing at least one Al atom. b) Categories of organic species by compound class found by using MFP. i. sulfonated species on the dull side, ii. sulfonated species on the shiny side, iii. hydrocarbons, iv. ions with matching formulas in the LIPIDMAPS database. The full table of all possibilities of organic assignments can be found in the data repository.

**a)**

| Mass | Deviation (ppm) | DBE | Area (AU) | H | O | Al |
|---|---|---|---|---|---|---|
| 81.9528 | -2.36599 | 0.5 | 29202.37 | 1 | 0 | 3 |
| 93.9851 | -1.31829 | -0.5 | 6304.99 | 3 | 4 | 1 |
| 94.9929 | -1.56748 | -1 | 215412.1 | 4 | 4 | 1 |
| 120.9667 | -0.52824 | -0.5 | 50637.13 | 3 | 4 | 2 |
| 135.0452 | -2.06523 | -5 | 3058.09 | 12 | 6 | 1 |
| 138.9772 | -0.92749 | -1.5 | 1581.66 | 5 | 5 | 2 |
| 153.9643 | -0.77226 | -1 | 8159.43 | 4 | 6 | 2 |
| 154.9722 | -0.28328 | -1.5 | 1201790 | 5 | 6 | 2 |
| 157.9997 | 2.285453 | -64 | 4875.14 | 130 | 0 | 1 |
| 161.8897 | -0.54914 | 1 | 1529.14 | 0 | 0 | 6 |
| 164.9508 | -1.47862 | -1 | 3050.22 | 4 | 5 | 3 |
| 169.9592 | -0.78784 | -1 | 4463.18 | 4 | 7 | 2 |
| 172.9827 | -0.62954 | -2.5 | 896617.4 | 7 | 7 | 2 |
| 185.0078 | -1.58858 | -5.5 | 668558.8 | 13 | 4 | 4 |
| 186.0155 | -2.25196 | -6 | 6841.45 | 14 | 4 | 4 |
| 188.8712 | -0.68248 | 1 | 17995.48 | 0 | 0 | 7 |
| 188.9395 | -2.34942 | -2 | 1539.45 | 6 | 3 | 5 |
| 196.9406 | -1.39077 | -1 | 7909.87 | 4 | 7 | 3 |
| 198.9563 | -1.12537 | -2 | 28016.37 | 6 | 7 | 3 |
| 203.0869 | -1.84108 | -9.5 | 1875.03 | 21 | 8 | 2 |
| 207.0121 | -0.38114 | -8 | 179955.3 | 18 | 0 | 7 |
| 209.0078 | 1.153547 | -65.5 | 2076.58 | 133 | 3 | 1 |
| 209.0277 | -0.61666 | -9 | 365964.6 | 20 | 0 | 7 |
| 210.0354 | -1.20884 | -9.5 | 10927.99 | 21 | 0 | 7 |
| 211.0191 | -2.31685 | -5.5 | 3120.67 | 13 | 9 | 2 |
| 211.0235 | 1.379469 | -66.5 | 6722.66 | 135 | 3 | 1 |
| 211.0434 | -0.37386 | -10 | 156752 | 22 | 0 | 7 |
| 212.051 | -1.43314 | -10.5 | 4717.13 | 23 | 0 | 7 |
| 212.9392 | -0.98103 | -62 | 6239.8 | 126 | 2 | 2 |
| 213.0349 | -1.59082 | -6.5 | 2032.9 | 15 | 9 | 2 |
| 213.0392 | 1.601116 | -67.5 | 3124.41 | 137 | 3 | 1 |
| 213.0588 | -1.5437 | -11 | 2889.3 | 24 | 0 | 7 |
| 213.9435 | -0.53238 | -1.5 | 10948.61 | 5 | 8 | 3 |
| 214.9513 | -0.64619 | -2 | 12324.95 | 6 | 8 | 3 |
| 219.8909 | -0.97275 | 1 | 2648.68 | 0 | 7 | 4 |
| 222.9145 | -0.39881 | -0.5 | 13956.12 | 3 | 7 | 4 |
| 224.9984 | -2.01734 | -4.5 | 3661.26 | 11 | 10 | 2 |
| 227.014 | -2.21968 | -5.5 | 1604.1 | 13 | 10 | 2 |
| 229.0296 | -2.41846 | -6.5 | 2111.22 | 15 | 10 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 230.9498 | -0.75298 | -63 | 3515.04 | 128 | 3 | 2 |
| 230.9701 | -0.62302 | -6.5 | 15964.91 | 15 | 0 | 8 |
| 231.0453 | -2.18095 | -7.5 | 3092.73 | 17 | 10 | 2 |
| 231.9542 | 0.090966 | -2.5 | 1910.03 | 7 | 9 | 3 |
| 232.897 | -0.03821 | -61 | 1674.67 | 124 | 0 | 4 |
| 232.9619 | -0.446 | -3 | 2453274 | 8 | 9 | 3 |
| 235.8859 | -0.54645 | 1 | 2038.91 | 0 | 8 | 4 |
| 240.0779 | -2.28634 | -11.5 | 12662.63 | 25 | 5 | 5 |
| 242.8341 | -1.27206 | 1 | 16137.36 | 0 | 0 | 9 |
| 244.0408 | -1.36821 | -10.5 | 1646.89 | 23 | 2 | 7 |
| 244.9291 | -0.5671 | -62 | 3319.85 | 126 | 4 | 2 |
| 247.9488 | -1.18532 | -2.5 | 4929 | 7 | 10 | 3 |
| 248.9604 | -0.55792 | -64 | 6450.88 | 130 | 4 | 2 |
| 249.0224 | 0.767401 | -69 | 2295.21 | 140 | 0 | 4 |
| 255.0036 | -1.05449 | -6 | 2315.91 | 14 | 10 | 3 |
| 256.9197 | -1.43586 | -1.5 | 6397.06 | 5 | 9 | 4 |
| 256.9439 | -0.22923 | -6 | 1886 | 14 | 0 | 9 |
| 258.9354 | -1.23158 | -2.5 | 14957.81 | 7 | 9 | 4 |
| 265.1478 | 1.475029 | -77 | 6666.44 | 156 | 0 | 4 |
| 266.9023 | -0.70775 | -62 | 6290.46 | 126 | 2 | 4 |
| 266.9406 | 1.240352 | -62.5 | 2124.37 | 127 | 7 | 1 |
| 268.1092 | -0.05184 | -73.5 | 2645.02 | 149 | 4 | 2 |
| 269.9835 | -1.90345 | -7.5 | 2998 | 17 | 4 | 7 |
| 272.9387 | -0.63714 | -6 | 11529.97 | 14 | 1 | 9 |
| 273.9227 | -0.39756 | -2 | 6549.23 | 6 | 10 | 4 |
| 274.9306 | -0.1233 | -2.5 | 293296.2 | 7 | 10 | 4 |
| 276.0415 | -0.10469 | -69.5 | 2922.1 | 141 | 5 | 2 |
| 276.946 | -1.02511 | -3.5 | 6642.39 | 9 | 10 | 4 |
| 277.9468 | -1.30924 | -6 | 1631.78 | 14 | 3 | 8 |
| 281.0767 | -1.18793 | -11 | 3047.29 | 24 | 11 | 3 |
| 282.8972 | -0.72076 | -62 | 4146.27 | 126 | 3 | 4 |
| 282.9355 | 1.117217 | -62.5 | 5475.78 | 127 | 8 | 1 |
| 283.9424 | -2.14444 | -63 | 1676.86 | 128 | 8 | 1 |
| 284.9396 | -2.34751 | -4.5 | 1825.86 | 11 | 7 | 6 |
| 284.9777 | -1.2243 | -5 | 3069.42 | 12 | 12 | 3 |
| 291.0496 | 2.443232 | -12.5 | 6319.25 | 27 | 3 | 8 |
| 292.9412 | 0.003755 | -3.5 | 1304009 | 9 | 11 | 4 |
| 296.7971 | -1.31032 | 1 | 9700.74 | 0 | 0 | 11 |
| 298.8881 | -2.00376 | -1 | 1746.54 | 4 | 10 | 5 |
| 298.9123 | -0.9665 | -5.5 | 1528.59 | 13 | 1 | 10 |
| 300.9041 | -0.82717 | -2 | 8798.71 | 6 | 10 | 5 |
| 300.946 | 0.83437 | -63.5 | 21292.28 | 129 | 9 | 1 |
| 301.1269 | -0.79335 | -17.5 | 19725.67 | 37 | 3 | 8 |
| 302.9618 | 1.323931 | -64.5 | 5982.54 | 131 | 9 | 1 |
| 310.9071 | 0.196522 | -6 | 23629.31 | 14 | 0 | 11 |
| 312.9399 | -0.95513 | -64 | 4938.33 | 130 | 8 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 314.1677 | 1.610926 | -19 | 3247.27 | 40 | 7 | 6 |
| 314.9075 | -0.01238 | -5.5 | 4991.72 | 13 | 2 | 10 |
| 316.8989 | -1.14831 | -2 | 86121.06 | 6 | 11 | 5 |
| 316.9409 | 0.744934 | -63.5 | 10638.62 | 129 | 10 | 1 |
| 318.9146 | -0.98428 | -3 | 49841.9 | 8 | 11 | 5 |
| 318.9773 | 2.244992 | -8 | 18616.73 | 18 | 7 | 7 |
| 321.153 | -1.10197 | -19.5 | 2471.43 | 41 | 4 | 8 |
| 323.1684 | -1.86868 | -20.5 | 29233.22 | 43 | 4 | 8 |
| 323.7786 | -1.32467 | 1 | 2130.99 | 0 | 0 | 12 |
| 324.9041 | 0.880568 | -62 | 3430.59 | 126 | 9 | 2 |
| 326.9199 | 1.333968 | -63 | 5664.87 | 128 | 9 | 2 |
| 327.1798 | -0.7149 | -79 | 25940.16 | 160 | 7 | 2 |
| 329.0854 | -0.81711 | -15.5 | 1705.15 | 33 | 5 | 8 |
| 331.8862 | -0.46371 | -1.5 | 2805.83 | 5 | 12 | 5 |
| 332.9358 | 0.664092 | -63.5 | 1850.93 | 129 | 11 | 1 |
| 333.9018 | -0.61066 | -2.5 | 1722.55 | 7 | 12 | 5 |
| 334.8652 | 0.286981 | -4.5 | 2857.95 | 11 | 0 | 12 |
| 334.9098 | -0.08629 | -3 | 1340626 | 8 | 12 | 5 |
| 338.1877 | 2.2801 | -22.5 | 2243.7 | 47 | 3 | 9 |
| 340.203 | 1.237792 | -23.5 | 91269.14 | 49 | 3 | 9 |
| 342.9146 | 0.644767 | -63 | 49945.41 | 128 | 10 | 2 |
| 344.9303 | 0.785957 | -64 | 5542.95 | 130 | 10 | 2 |
| 344.9567 | -1.57672 | -5.5 | 1709.57 | 13 | 14 | 4 |
| 346.898 | 1.920165 | -5.5 | 1713.31 | 13 | 4 | 10 |
| 348.8861 | 0.949021 | -65 | 3429.6 | 132 | 0 | 8 |
| 349.8966 | -0.91141 | -2.5 | 27254.5 | 7 | 13 | 5 |
| 350.7602 | -1.05171 | 1 | 51917.75 | 0 | 0 | 13 |
| 352.8757 | 0.088133 | -5.5 | 35307.89 | 13 | 1 | 12 |
| 352.9201 | -0.83277 | -4 | 40186.92 | 10 | 13 | 5 |
| 353.2155 | 0.229605 | -83.5 | 2991.85 | 169 | 3 | 5 |
| 358.9097 | 1.131484 | -63 | 7517.81 | 128 | 11 | 2 |
| 360.9253 | 0.986632 | -64 | 2416.75 | 130 | 11 | 2 |
| 361.0065 | -1.06341 | -12.5 | 4500.14 | 27 | 4 | 10 |
| 364.854 | 2.264198 | 0.5 | 2284.31 | 1 | 16 | 4 |
| 367.9073 | -0.49985 | -3.5 | 5101.49 | 9 | 14 | 5 |
| 376.878 | -1.21763 | -2.5 | 62255.23 | 7 | 13 | 6 |
| 376.9201 | 0.639659 | -64 | 2396.32 | 130 | 12 | 2 |
| 376.977 | -2.41102 | -8 | 4376.94 | 18 | 14 | 5 |
| 378.8938 | -0.81527 | -3.5 | 6509.01 | 9 | 13 | 6 |
| 380.8102 | -0.28597 | 1 | 13134.39 | 0 | 12 | 7 |
| 390.9117 | -1.91577 | -8.5 | 3025.44 | 19 | 3 | 12 |
| 390.9926 | 2.483685 | -70.5 | 37688.26 | 143 | 7 | 5 |
| 391.9959 | 0.168624 | -10 | 2669.14 | 22 | 13 | 6 |
| 392.9421 | 0.282739 | -5.5 | 1797.47 | 13 | 17 | 4 |
| 393.8808 | -1.01274 | -3 | 5938.65 | 8 | 14 | 6 |
| 394.8888 | -0.56699 | -3.5 | 1087778 | 9 | 14 | 6 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 395.8929 | -1.57593 | -67 | 1890.61 | 136 | 1 | 9 |
| 397.2269 | -0.03499 | -25.5 | 3301.21 | 53 | 8 | 8 |
| 399.2426 | 0.090421 | -26.5 | 5782.89 | 55 | 8 | 8 |
| 400.8368 | 0.688809 | -1 | 2540.34 | 4 | 13 | 7 |
| 402.8938 | 0.56119 | -63.5 | 46224.41 | 129 | 12 | 3 |
| 404.7232 | -1.10915 | 1 | 3493.63 | 0 | 0 | 15 |
| 404.7783 | -1.57839 | -56.5 | 3641.25 | 115 | 13 | 3 |
| 404.9099 | 1.669757 | -64.5 | 2043.09 | 131 | 12 | 3 |
| 410.9107 | -1.82253 | -69 | 4008.89 | 140 | 0 | 10 |
| 412.8549 | 0.08744 | -6 | 23628.63 | 14 | 3 | 13 |
| 412.8994 | -0.4575 | -4.5 | 33010.23 | 11 | 15 | 6 |
| 418.8888 | 0.74268 | -63.5 | 3135.5 | 129 | 13 | 3 |
| 420.1835 | -1.42533 | -21.5 | 1561.28 | 45 | 15 | 5 |
| 420.9254 | 2.35458 | -8 | 2205.53 | 18 | 10 | 9 |
| 420.9734 | 1.534779 | -67.5 | 2314.24 | 137 | 16 | 1 |
| 422.878 | -0.91965 | -4 | 2567.98 | 10 | 14 | 7 |
| 434.8689 | -1.41169 | -67.5 | 2382.1 | 137 | 0 | 11 |
| 436.7681 | -1.53147 | -56.5 | 2913.45 | 115 | 15 | 3 |
| 436.8571 | -1.26792 | -3 | 24950.08 | 8 | 15 | 7 |
| 436.8993 | 0.563288 | -64.5 | 3586.29 | 131 | 14 | 3 |
| 438.8729 | -0.92031 | -4 | 24098.95 | 10 | 15 | 7 |
| 438.936 | 2.337704 | -9 | 2606.05 | 20 | 11 | 9 |
| 444.8628 | 1.339965 | -63 | 3079.37 | 128 | 13 | 4 |
| 446.8784 | 1.222034 | -64 | 2728.54 | 130 | 13 | 4 |
| 450.8465 | -2.18233 | -61 | 7394.06 | 124 | 17 | 2 |
| 452.8795 | -1.27826 | -68.5 | 23665.13 | 139 | 1 | 11 |
| 454.868 | -0.48124 | -4 | 733576.5 | 10 | 16 | 7 |
| 456.8836 | -0.58855 | -5 | 5443.52 | 12 | 16 | 7 |
| 458.6863 | -0.93506 | 1 | 1977.8 | 0 | 0 | 17 |
| 462.8731 | 0.715315 | -64 | 29426.72 | 130 | 14 | 4 |
| 464.8464 | -1.33141 | -3.5 | 2200.82 | 9 | 15 | 8 |
| 464.8885 | 0.17445 | -65 | 1585.85 | 132 | 14 | 4 |
| 472.8341 | 0.086923 | -6.5 | 5342.63 | 15 | 5 | 14 |
| 472.8784 | -0.81184 | -5 | 314998.5 | 12 | 17 | 7 |
| 476.8374 | -1.56007 | -67 | 3615.09 | 136 | 1 | 12 |
| 478.8255 | -1.63713 | -2.5 | 12168.34 | 7 | 16 | 8 |
| 478.8682 | 1.077751 | -64 | 2992.68 | 130 | 15 | 4 |
| 480.8415 | -0.90238 | -3.5 | 16318.35 | 9 | 16 | 8 |
| 480.8835 | 0.345406 | -65 | 16139.15 | 132 | 15 | 4 |
| 486.8231 | -1.6205 | -64.5 | 2477.15 | 131 | 7 | 9 |
| 490.8446 | -0.04869 | -7.5 | 4459.35 | 17 | 6 | 14 |
| 494.8477 | -2.0388 | -68 | 1556.51 | 138 | 2 | 12 |
| 494.8784 | -2.31147 | -70.5 | 1621.41 | 143 | 0 | 13 |
| 495.8287 | -0.65325 | -3 | 12089.7 | 8 | 17 | 8 |
| 496.8366 | -0.50097 | -3.5 | 341243.3 | 9 | 17 | 8 |
| 496.8785 | 0.505355 | -65 | 2344.72 | 132 | 16 | 4 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 498.8523 | -0.39872 | -4.5 | 4357.32 | 11 | 17 | 8 |
| 503.1381 | 1.343768 | -24.5 | 3592.69 | 51 | 8 | 12 |
| 504.8417 | 0.596425 | -63.5 | 19519.03 | 129 | 15 | 5 |
| 511.8235 | -0.85752 | -3 | 8127.86 | 8 | 18 | 8 |
| 512.6489 | -1.77295 | 1 | 1867.35 | 0 | 0 | 19 |
| 512.8584 | -1.70398 | -69 | 26787.39 | 140 | 3 | 12 |
| 514.8026 | -0.17269 | -6 | 6929.98 | 14 | 6 | 15 |
| 514.8346 | 2.09019 | -8.5 | 41063.77 | 19 | 4 | 16 |
| 514.847 | -0.80393 | -4.5 | 143334.2 | 11 | 18 | 8 |
| 519.1491 | -1.44255 | -81.5 | 7266.41 | 165 | 17 | 3 |
| 520.1519 | 2.251463 | -84 | 2472.89 | 170 | 10 | 7 |
| 520.8364 | 0.165311 | -63.5 | 2349.5 | 129 | 16 | 5 |
| 522.852 | 0.069044 | -64.5 | 7139.5 | 131 | 16 | 5 |
| 532.8451 | 1.897553 | -9.5 | 4832.82 | 21 | 5 | 16 |
| 532.8575 | -0.89874 | -5.5 | 49580.92 | 13 | 19 | 8 |
| 538.8044 | -2.00239 | -3 | 4106.47 | 8 | 18 | 9 |
| 540.8205 | -1.16286 | -4 | 4869.56 | 10 | 18 | 9 |
| 550.868 | -0.98735 | -6.5 | 1618.11 | 15 | 20 | 8 |
| 554.8116 | 1.155529 | -62 | 3299.58 | 126 | 20 | 4 |
| 554.827 | -1.62915 | -68.5 | 16224.14 | 139 | 4 | 13 |
| 556.8035 | 2.417555 | -8 | 7175.95 | 18 | 5 | 17 |
| 556.8155 | -0.9768 | -4 | 67832.97 | 10 | 19 | 9 |
| 558.8311 | -1.06275 | -5 | 1945.4 | 12 | 19 | 9 |
| 564.821 | 0.718989 | -64 | 2596.35 | 130 | 17 | 6 |
| 566.6124 | -1.86 | -49.5 | 1597.33 | 101 | 24 | 3 |
| 566.6124 | -0.86285 | 1 | 1597.33 | 0 | 0 | 21 |
| 570.7927 | 1.254573 | -66 | 2023.35 | 134 | 7 | 12 |
| 570.8046 | -2.23176 | -62 | 52757.65 | 126 | 21 | 4 |
| 574.8141 | 2.402696 | -9 | 3334.66 | 20 | 6 | 17 |
| 574.8262 | -0.71134 | -5 | 152035.5 | 12 | 20 | 9 |
| 576.8307 | -2.23445 | -71 | 2347.48 | 144 | 0 | 16 |
| 576.8418 | -0.79554 | -6 | 1859.49 | 14 | 20 | 9 |
| 582.8313 | 0.242094 | -65 | 10533.82 | 132 | 18 | 6 |
| 592.8369 | -0.46202 | -6 | 473484.2 | 14 | 21 | 9 |
| 594.8411 | -2.44418 | -72 | 11451.41 | 146 | 1 | 16 |
| 598.11 | 0.578656 | -83 | 7906.48 | 168 | 15 | 7 |
| 598.7719 | 1.863985 | -7.5 | 8138.63 | 17 | 6 | 18 |
| 598.7835 | -1.96047 | -3.5 | 2486.63 | 9 | 20 | 10 |
| 600.7994 | -1.53778 | -4.5 | 1715.84 | 11 | 20 | 10 |
| 600.8419 | 0.293089 | -66 | 24342.64 | 134 | 19 | 6 |
| 602.8042 | -2.49483 | -70.5 | 8650.9 | 143 | 0 | 17 |
| 614.8061 | -1.62474 | -69 | 23534.69 | 140 | 6 | 14 |
| 616.7825 | 1.866302 | -8.5 | 7165.81 | 19 | 7 | 18 |
| 616.7948 | -0.71158 | -4.5 | 94714.97 | 11 | 21 | 10 |
| 618.8101 | -1.27486 | -5.5 | 1972.34 | 13 | 21 | 10 |
| 624.7995 | -0.46239 | -64.5 | 2272.9 | 131 | 19 | 7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 630.7837 | -2.17015 | -62.5 | 56721.14 | 127 | 23 | 5 |
| 631.7817 | -0.99544 | -4 | 1743.03 | 10 | 22 | 10 |
| 634.8055 | -0.47873 | -5.5 | 121932.7 | 13 | 22 | 10 |
| 636.81 | -1.85911 | -71.5 | 2847.78 | 145 | 2 | 17 |
| 640.7522 | -1.72282 | -3 | 3742.27 | 8 | 21 | 11 |
| 642.8105 | 0.227283 | -65.5 | 4737.88 | 133 | 20 | 7 |
| 644.7726 | 2.048944 | -59.5 | 4441.15 | 121 | 31 | 1 |
| 648.7942 | -2.2101 | -63.5 | 7499.56 | 129 | 24 | 5 |
| 648.7942 | -1.33925 | -13 | 7499.56 | 28 | 0 | 23 |
| 649.7926 | -0.4523 | -5 | 4745.4 | 12 | 23 | 10 |
| 652.7714 | -0.37364 | -8 | 2414.52 | 18 | 11 | 17 |
| 652.8161 | -0.41191 | -6.5 | 57372.26 | 15 | 23 | 10 |
| 656.7729 | 1.204527 | -7.5 | 1733.43 | 17 | 13 | 16 |
| 658.7513 | 1.147779 | -58.5 | 4929.29 | 119 | 32 | 1 |
| 658.7513 | 2.005465 | -8 | 4929.29 | 18 | 8 | 19 |
| 658.7634 | -0.71179 | -4 | 82697.02 | 10 | 22 | 11 |
| 660.7787 | -1.23929 | -5 | 2804.9 | 12 | 22 | 11 |
| 663.1981 | 2.27851 | -89 | 2994.34 | 180 | 20 | 6 |
| 666.7684 | -0.02835 | -64 | 2049.16 | 130 | 20 | 8 |
| 672.7525 | -1.78208 | -62 | 2325.56 | 126 | 24 | 6 |
| 672.7525 | -0.94225 | -11.5 | 2325.56 | 25 | 0 | 24 |
| 674.7855 | -1.17652 | -69.5 | 7444.77 | 141 | 8 | 15 |
| 676.7739 | -0.78889 | -5 | 158328.5 | 12 | 23 | 11 |
| 678.7784 | 2.417732 | -60.5 | 1787.86 | 123 | 33 | 1 |
| 678.7784 | -2.083 | -71 | 1787.86 | 144 | 3 | 18 |
| 684.779 | 0.023511 | -65 | 3938.77 | 132 | 21 | 8 |
| 690.763 | -1.82971 | -63 | 25286.2 | 128 | 25 | 6 |
| 690.763 | -1.01178 | -12.5 | 25286.2 | 27 | 1 | 24 |
| 691.2296 | -0.74346 | -37.5 | 2550.31 | 77 | 8 | 18 |
| 692.7955 | -1.96147 | -70.5 | 1554.2 | 143 | 9 | 15 |
| 694.7845 | -0.71806 | -6 | 199984 | 14 | 24 | 11 |
| 696.7887 | 1.974921 | -61.5 | 5090.96 | 125 | 34 | 1 |
| 696.7887 | -2.40948 | -72 | 5090.96 | 146 | 4 | 18 |
| 702.7896 | 0.07271 | -66 | 6189.19 | 134 | 22 | 8 |
| 708.7735 | -1.87493 | -64 | 2127.22 | 130 | 26 | 6 |
| 708.7735 | -1.07778 | -13.5 | 2127.22 | 29 | 2 | 24 |
| 712.795 | -0.79111 | -7 | 73770.21 | 16 | 25 | 11 |
| 716.7534 | -2.12611 | -69 | 2005.94 | 140 | 9 | 16 |
| 718.7426 | -0.64543 | -4.5 | 16000.37 | 11 | 24 | 12 |
| 722.7618 | 1.053045 | -61 | 1607.32 | 124 | 34 | 2 |
| 722.7618 | 1.834771 | -10.5 | 1607.32 | 23 | 10 | 20 |
| 732.7311 | -2.44823 | -62.5 | 8359.36 | 127 | 26 | 7 |
| 732.7311 | 2.492189 | -1.5 | 8359.36 | 5 | 32 | 8 |
| 732.7311 | -1.67715 | -12 | 8359.36 | 26 | 2 | 25 |
| 734.7645 | -1.34587 | -70 | 5654.86 | 142 | 10 | 16 |
| 736.741 | 0.944838 | -60 | 3632.61 | 122 | 35 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 736.741 | 1.711731 | -9.5 | 3632.61 | 21 | 11 | 20 |
| 736.7532 | -0.58215 | -5.5 | 48166.19 | 13 | 25 | 12 |
| 750.7421 | -1.81007 | -63.5 | 21860.15 | 129 | 27 | 7 |
| 750.7421 | -1.05749 | -13 | 21860.15 | 28 | 3 | 25 |
| 752.7744 | -2.19707 | -71 | 2090.45 | 144 | 11 | 16 |
| 754.7515 | 0.83617 | -61 | 1615.77 | 124 | 36 | 2 |
| 754.7515 | 1.584763 | -10.5 | 1615.77 | 23 | 12 | 20 |
| 754.7636 | -0.78687 | -6.5 | 48259.7 | 15 | 26 | 12 |
| 760.7093 | 1.223991 | -67 | 5436.34 | 136 | 12 | 16 |
| 764.7312 | 2.002145 | -60.5 | 1520.84 | 123 | 35 | 3 |
| 764.7312 | -1.99272 | -71 | 1520.84 | 144 | 5 | 20 |
| 768.7524 | -2.11238 | -64.5 | 9037.25 | 131 | 28 | 7 |
| 768.7524 | -1.37742 | -14 | 9037.25 | 30 | 4 | 25 |
| 772.7741 | -0.85264 | -7.5 | 16513.84 | 17 | 27 | 12 |
| 778.7214 | -1.10296 | -5 | 43712.09 | 12 | 26 | 13 |
| 782.9308 | -1.77397 | -74.5 | 2395.38 | 151 | 31 | 5 |
| 782.9308 | -1.05233 | -24 | 2395.38 | 50 | 7 | 23 |
| 792.7105 | -2.00438 | -63 | 7411.53 | 128 | 28 | 8 |
| 792.7105 | -1.29164 | -12.5 | 7411.53 | 27 | 4 | 26 |
| 796.7319 | -1.15961 | -6 | 166162.3 | 14 | 27 | 13 |
| 798.736 | 1.06556 | -61.5 | 3684.13 | 125 | 37 | 3 |
| 798.736 | 1.772929 | -11 | 3684.13 | 24 | 13 | 21 |
| 804.7375 | 0.156697 | -66 | 3545.97 | 134 | 25 | 10 |
| 804.7375 | 0.85879 | -15.5 | 3545.97 | 33 | 1 | 28 |
| 805.6601 | 0.572326 | -57 | 6704.97 | 116 | 38 | 3 |
| 805.6601 | 1.273616 | -6.5 | 6704.97 | 15 | 14 | 21 |
| 806.6627 | -1.08335 | -70 | 1712.3 | 142 | 1 | 24 |
| 810.7213 | -1.66999 | -64 | 8319.18 | 130 | 29 | 8 |
| 810.7213 | -0.97308 | -13.5 | 8319.18 | 29 | 5 | 26 |
| 814.7425 | -1.09102 | -7 | 85343.27 | 16 | 28 | 13 |
| 820.6886 | 1.262478 | -67.5 | 1622.74 | 137 | 14 | 17 |
| 822.7475 | -0.53346 | -67 | 3739.08 | 136 | 26 | 10 |
| 822.7475 | 0.153267 | -16.5 | 3739.08 | 35 | 2 | 28 |
| 828.7317 | -1.8328 | -65 | 2281.57 | 132 | 30 | 8 |
| 828.7317 | -1.15103 | -14.5 | 2281.57 | 31 | 6 | 26 |
| 832.753 | -1.14548 | -8 | 47756.77 | 18 | 29 | 13 |
| 833.6908 | 1.152827 | -68.5 | 19895.85 | 139 | 13 | 18 |
| 834.6943 | -0.37008 | -58.5 | 9660.89 | 119 | 43 | 1 |
| 834.6943 | 0.306819 | -8 | 9660.89 | 18 | 19 | 19 |
| 836.7122 | 2.319919 | -59.5 | 2451.36 | 121 | 43 | 1 |
| 836.7122 | -1.33128 | -70 | 2451.36 | 142 | 13 | 18 |
| 838.7012 | -0.30273 | -5.5 | 18205.62 | 13 | 28 | 14 |
| 852.6897 | -1.85753 | -63.5 | 12964.92 | 129 | 30 | 9 |
| 852.6897 | 2.387861 | -2.5 | 12964.92 | 7 | 36 | 10 |
| 852.6897 | -1.19492 | -13 | 12964.92 | 28 | 6 | 27 |
| 854.7226 | 2.077988 | -60.5 | 2193.17 | 123 | 44 | 1 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 854.7226 | -1.49627 | -71 | 2193.17 | 144 | 14 | 18 |
| 856.6984 | -0.34306 | -61 | 1835.08 | 124 | 39 | 4 |
| 856.6984 | 0.316448 | -10.5 | 1835.08 | 23 | 15 | 22 |
| 856.7115 | -0.60569 | -6.5 | 29082.96 | 15 | 29 | 14 |
| 861.7225 | -1.65819 | -67.5 | 16151.86 | 137 | 25 | 12 |
| 861.7225 | -1.00253 | -17 | 16151.86 | 36 | 1 | 30 |
| 862.7265 | -1.89388 | -7 | 10341.58 | 16 | 31 | 13 |
| 862.7265 | 1.960185 | -70 | 10341.58 | 142 | 18 | 16 |
| 870.6999 | -2.23831 | -64.5 | 10686.7 | 131 | 31 | 9 |
| 870.6999 | 1.919264 | -3.5 | 10686.7 | 9 | 37 | 10 |
| 870.6999 | -1.58941 | -14 | 10686.7 | 30 | 7 | 27 |
| 874.7219 | -0.78185 | -7.5 | 21714.19 | 17 | 30 | 14 |
| 880.6688 | -1.45787 | -5 | 13205.71 | 12 | 29 | 15 |
| 880.6688 | 2.317676 | -68 | 13205.71 | 138 | 16 | 18 |
| 888.7111 | -1.47843 | -65.5 | 2627.37 | 133 | 32 | 9 |
| 888.7111 | -0.84268 | -15 | 2627.37 | 32 | 8 | 27 |
| 889.7542 | -0.22354 | -5.5 | 3427.01 | 13 | 43 | 7 |
| 889.7542 | 0.07991 | -79 | 3427.01 | 160 | 0 | 27 |
| 890.7576 | -1.45819 | -69 | 2136.35 | 140 | 30 | 10 |
| 890.7576 | -0.8239 | -18.5 | 2136.35 | 39 | 6 | 28 |
| 892.7327 | -0.50284 | -8.5 | 4653.6 | 19 | 31 | 14 |
| 898.6795 | -1.27843 | -6 | 46504.7 | 14 | 30 | 15 |
| 898.6795 | 2.421448 | -69 | 46504.7 | 140 | 17 | 18 |
| 912.6681 | 1.359861 | -3 | 4785.81 | 8 | 38 | 11 |
| 912.6681 | -1.98747 | -13.5 | 4785.81 | 29 | 8 | 28 |
| 916.6901 | -1.21513 | -7 | 92431.71 | 16 | 31 | 15 |
| 916.6901 | 2.412053 | -70 | 92431.71 | 142 | 18 | 18 |
| 918.6945 | 1.04616 | -62.5 | 1933.54 | 127 | 41 | 5 |
| 918.6945 | -2.27921 | -73 | 1933.54 | 148 | 11 | 22 |
| 918.6945 | 1.661164 | -12 | 1933.54 | 26 | 17 | 23 |
| 930.6793 | -1.87379 | -65 | 4280.68 | 132 | 33 | 10 |
| 930.6793 | 2.015843 | -4 | 4280.68 | 10 | 39 | 11 |
| 930.6793 | -1.26671 | -14.5 | 4280.68 | 31 | 9 | 28 |
| 934.7007 | -1.15427 | -8 | 54620.55 | 18 | 32 | 15 |
| 934.7007 | 2.403021 | -71 | 54620.55 | 144 | 19 | 18 |
| 940.6472 | -2.21007 | -5.5 | 2528.65 | 13 | 31 | 16 |
| 940.6472 | 1.324728 | -68.5 | 2528.65 | 139 | 18 | 19 |
| 952.7115 | -0.88579 | -9 | 13503.7 | 20 | 33 | 15 |
| 954.6363 | 0.849644 | -2.5 | 1932.2 | 7 | 39 | 12 |
| 954.6363 | -2.35052 | -13 | 1932.2 | 28 | 9 | 29 |
| 958.6593 | -0.56735 | -6.5 | 11926.17 | 15 | 32 | 16 |
| 972.6473 | -2.44065 | -64.5 | 6835.33 | 131 | 34 | 11 |
| 972.6473 | 1.281144 | -3.5 | 6835.33 | 9 | 40 | 12 |
| 972.6473 | -1.85977 | -14 | 6835.33 | 30 | 10 | 29 |
| 976.6697 | -0.72583 | -7.5 | 14488.9 | 17 | 33 | 16 |
| 982.6166 | -1.33205 | -5 | 2994.6 | 12 | 32 | 17 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 982.6166 | 2.051771 | -68 | 2994.6 | 138 | 19 | 20 |
| 990.6581 | -2.15907 | -65.5 | 6748.9 | 133 | 35 | 11 |
| 990.6581 | 1.495069 | -4.5 | 6748.9 | 11 | 41 | 12 |
| 990.6581 | -1.58874 | -15 | 6748.9 | 32 | 11 | 29 |
| 994.6799 | -1.07964 | -8.5 | 4559.81 | 19 | 34 | 16 |
| 994.6799 | 2.263145 | -71.5 | 4559.81 | 145 | 21 | 19 |
| 1000.627 | -1.77279 | -6 | 20101.58 | 14 | 33 | 17 |
| 1000.627 | 1.550131 | -69 | 20101.58 | 140 | 20 | 20 |
| 1008.668 | 0.908228 | -5.5 | 1855.88 | 13 | 42 | 12 |
| 1008.668 | -2.12051 | -16 | 1855.88 | 34 | 12 | 29 |
| 1018.638 | -1.3144 | -7 | 56745.63 | 16 | 34 | 17 |
| 1018.638 | 1.949765 | -70 | 56745.63 | 142 | 21 | 20 |
| 1032.627 | -2.10037 | -65 | 2121.67 | 132 | 36 | 12 |
| 1032.627 | 1.405253 | -4 | 2121.67 | 10 | 42 | 13 |
| 1032.627 | -1.55322 | -14.5 | 2121.67 | 31 | 12 | 30 |
| 1036.648 | -1.35427 | -8 | 51168.79 | 18 | 35 | 17 |
| 1036.648 | 1.853188 | -71 | 51168.79 | 144 | 22 | 20 |
| 1038.573 | 0.241774 | -1.5 | 1823.71 | 5 | 41 | 14 |
| 1040.607 | 1.240719 | -59.5 | 1916.97 | 121 | 49 | 5 |
| 1040.607 | -1.69507 | -70 | 1916.97 | 142 | 19 | 22 |
| 1040.607 | 1.783673 | -9 | 1916.97 | 20 | 25 | 23 |
| 1054.658 | -1.86686 | -9 | 10774.39 | 20 | 36 | 17 |
| 1054.658 | 1.285821 | -72 | 10774.39 | 146 | 23 | 20 |
| 1056.584 | 0.744002 | -2.5 | 3066.42 | 7 | 42 | 14 |
| 1056.584 | -2.14739 | -13 | 3066.42 | 28 | 12 | 31 |
| 1060.606 | -1.85639 | -6.5 | 4709.2 | 15 | 35 | 18 |
| 1060.606 | 1.278611 | -69.5 | 4709.2 | 141 | 22 | 21 |
| 1074.597 | -0.92956 | -64.5 | 4204.08 | 131 | 37 | 13 |
| 1074.597 | 2.439154 | -3.5 | 4204.08 | 9 | 43 | 14 |
| 1074.597 | -0.40378 | -14 | 4204.08 | 30 | 13 | 31 |
| 1078.618 | 0.061282 | -7.5 | 16474.9 | 17 | 36 | 18 |
| 1080.545 | 0.001018 | -62 | 1775.88 | 126 | 36 | 14 |
| 1080.545 | 0.523903 | -11.5 | 1775.88 | 25 | 12 | 32 |
| 1084.566 | -0.64441 | -55.5 | 80878.64 | 113 | 59 | 1 |
| 1084.566 | -0.12346 | -5 | 80878.64 | 12 | 35 | 19 |
| 1086.571 | -0.10483 | -71 | 1535.24 | 144 | 15 | 26 |
| 1092.607 | -1.2483 | -65.5 | 1648.47 | 133 | 38 | 13 |
| 1092.607 | 2.064883 | -4.5 | 1648.47 | 11 | 44 | 14 |
| 1092.607 | -0.73119 | -15 | 1648.47 | 32 | 14 | 31 |
| 1092.607 | 2.311999 | -78 | 1648.47 | 158 | 1 | 34 |
| 1102.575 | -1.32771 | -56.5 | 21976.82 | 115 | 60 | 1 |
| 1102.575 | -0.81527 | -6 | 21976.82 | 14 | 36 | 19 |
| 1102.575 | 2.200399 | -69 | 21976.82 | 140 | 23 | 22 |
| 1120.586 | -1.00742 | -57.5 | 36511.15 | 117 | 61 | 1 |
| 1120.586 | -0.50322 | -7 | 36511.15 | 16 | 37 | 19 |
| 1120.586 | 2.463984 | -70 | 36511.15 | 142 | 24 | 22 |

**(b)**

## i. Sulfonated species 'dull side'

| Total ion counts | 65318098 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Mass** | **Deviation (ppm)** | **DBE** | **Area (AU)** | **Area (normalised to total)** | **H** | **C** | **O** | **S** |
| 79.9571 | -3.313015634 | 1 | 1410502 | 0.021594359 | 0 | 0 | 3 | 1 |
| 80.9649 | -3.580551103 | 0.5 | 60736.96 | 0.000929864 | 1 | 0 | 3 | 1 |
| 93.0012 | -4.031114531 | 0.5 | 4341.78 | 6.64713E-05 | 5 | 2 | 2 | 1 |
| 94.9806 | -2.525772569 | 0.5 | 1823.17 | 2.79122E-05 | 3 | 1 | 3 | 1 |
| 106.9809 | 0.561782839 | 1.5 | 4474.98 | 6.85106E-05 | 3 | 2 | 3 | 1 |
| 154.9807 | -0.90269223 | 5.5 | 7529.78 | 0.000115279 | 3 | 6 | 3 | 1 |
| 155.9885 | -1.057128094 | 5 | 21774.88 | 0.000333367 | 4 | 6 | 3 | 1 |
| 156.9964 | -0.572624268 | 4.5 | 184933.2 | 0.002831271 | 5 | 6 | 3 | 1 |
| 170.0043 | -0.087644834 | 5 | 457859.3 | 0.007009685 | 6 | 7 | 3 | 1 |
| 171.0121 | -0.233316769 | 4.5 | 3294.94 | 5.04445E-05 | 7 | 7 | 3 | 1 |
| 180.9966 | 0.608299089 | 6.5 | 186107.8 | 0.002849253 | 5 | 8 | 3 | 1 |
| 182.0042 | -0.631303714 | 6 | 3418.3 | 5.23331E-05 | 6 | 8 | 3 | 1 |
| 183.012 | -0.764430163 | 5.5 | 16487489 | 0.252418393 | 7 | 8 | 3 | 1 |
| 185.0274 | -2.107251026 | 4.5 | 10200.43 | 0.000156165 | 9 | 8 | 3 | 1 |
| 194.0041 | -1.107707322 | 7 | 9953 | 0.000152377 | 6 | 9 | 3 | 1 |
| 195.0121 | -0.204602647 | 6.5 | 1046453 | 0.016020872 | 7 | 9 | 3 | 1 |
| 196.0199 | -0.331088724 | 6 | 216077.5 | 0.00330808 | 8 | 9 | 3 | 1 |
| 197.0277 | -0.456280812 | 5.5 | 1179238 | 0.018053764 | 9 | 9 | 3 | 1 |
| 198.0354 | -1.085158344 | 5 | 21783.01 | 0.000333491 | 10 | 9 | 3 | 1 |
| 199.0433 | -0.702861647 | 4.5 | 5890.7 | 9.01848E-05 | 11 | 9 | 3 | 1 |
| 220.0198 | -0.74947744 | 8 | 6971.02 | 0.000106724 | 8 | 11 | 3 | 1 |
| 221.0276 | -0.859167981 | 7.5 | 56598.33 | 0.000866503 | 9 | 11 | 3 | 1 |
| 223.0433 | -0.627232077 | 6.5 | 63655.04 | 0.000974539 | 11 | 11 | 3 | 1 |
| 225.0591 | 0.044877103 | 5.5 | 161277.1 | 0.002469103 | 13 | 11 | 3 | 1 |
| 227.0746 | -0.616096709 | 4.5 | 5045.03 | 7.72379E-05 | 15 | 11 | 3 | 1 |
| 233.0276 | -0.814924263 | 8.5 | 8708.8 | 0.000133329 | 9 | 12 | 3 | 1 |
| 235.0432 | -1.020662394 | 7.5 | 12561.1 | 0.000192307 | 11 | 12 | 3 | 1 |
| 237.059 | -0.379230343 | 6.5 | 19805.2 | 0.000303212 | 13 | 12 | 3 | 1 |
| 239.0747 | -0.166893416 | 5.5 | 169418.7 | 0.002593749 | 15 | 12 | 3 | 1 |
| 241.0902 | -0.78767138 | 4.5 | 2222.52 | 3.40261E-05 | 17 | 12 | 3 | 1 |
| 247.0432 | -0.971084276 | 8.5 | 3510.43 | 5.37436E-05 | 11 | 13 | 3 | 1 |
| 249.0589 | -0.762469662 | 7.5 | 2523.48 | 3.86337E-05 | 13 | 13 | 3 | 1 |
| 250.9813 | 1.833207667 | 13.5 | 2284.82 | 3.49799E-05 | 3 | 14 | 3 | 1 |
| 251.0745 | -0.955492377 | 6.5 | 6193.21 | 9.48161E-05 | 15 | 13 | 3 | 1 |
| 253.0902 | -0.750324815 | 5.5 | 63732.73 | 0.000975729 | 17 | 13 | 3 | 1 |
| 255.106 | -0.156405548 | 4.5 | 4814.29 | 7.37053E-05 | 19 | 13 | 3 | 1 |
| 265.0902 | -0.716359428 | 6.5 | 3934.13 | 6.02303E-05 | 17 | 14 | 3 | 1 |
| 267.1058 | -0.898145172 | 5.5 | 35113.34 | 0.000537574 | 19 | 14 | 3 | 1 |
| 269.1215 | -0.705628744 | 4.5 | 4592.12 | 7.03039E-05 | 21 | 14 | 3 | 1 |
| 273.0016 | 0.091940861 | 15.5 | 1713.35 | 2.62309E-05 | 5 | 17 | 2 | 1 |
| 279.1057 | -1.217816713 | 6.5 | 2035.94 | 3.11696E-05 | 19 | 15 | 3 | 1 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 281.0281 | 1.103449592 | 12.5 | 11803.52 | 0.000180708 | 9 | 16 | 3 | 1 |
| 281.1215 | -0.675508176 | 5.5 | 26750 | 0.000409534 | 21 | 15 | 3 | 1 |
| 283.1371 | -0.84729199 | 4.5 | 9159.3 | 0.000140226 | 23 | 15 | 3 | 1 |
| 293.1216 | -0.306698559 | 6.5 | 2488.22 | 3.80939E-05 | 21 | 16 | 3 | 1 |
| 295.137 | -1.151667221 | 5.5 | 30857.55 | 0.00047242 | 23 | 16 | 3 | 1 |
| 297.1528 | -0.639064746 | 4.5 | 492311.7 | 0.007537141 | 25 | 16 | 3 | 1 |
| 307.1371 | -0.781083798 | 6.5 | 1980.87 | 3.03265E-05 | 23 | 17 | 3 | 1 |
| 309.1528 | -0.614258979 | 5.5 | 41137.21 | 0.000629798 | 25 | 17 | 3 | 1 |
| 311.1686 | -0.128226289 | 4.5 | 1402522 | 0.021472181 | 27 | 17 | 3 | 1 |
| 335.1687 | 0.179312719 | 6.5 | 1569.71 | 2.40318E-05 | 27 | 19 | 3 | 1 |
| 337.1842 | -0.266619777 | 5.5 | 16850.5 | 0.000257976 | 29 | 19 | 3 | 1 |
| 339.1998 | -0.412441111 | 4.5 | 630590.6 | 0.009654148 | 31 | 19 | 3 | 1 |

### ii. Sulfonates on ‘shiny’ side

| Total ion counts | 13252804 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Mass** | **Deviation (ppm)** | **DBE** | **Area (AU)** | **Area (normalised to total)** | **H** | **C** | **O** | **S** |
| 79.957 | -4.56368 | 1 | 405941.7 | 0.03063063 | 0 | 0 | 3 | 1 |
| 80.9648 | -4.81565 | 0.5 | 8469.62 | 0.000639081 | 1 | 0 | 3 | 1 |
| 155.9885 | -1.05713 | 5 | 1193.58 | 9.00625E-05 | 4 | 6 | 3 | 1 |
| 156.9963 | -1.20958 | 4.5 | 9213.94 | 0.000695245 | 5 | 6 | 3 | 1 |
| 170.0042 | -0.67587 | 5 | 35700.8 | 0.00269383 | 6 | 7 | 3 | 1 |
| 180.9963 | -1.04919 | 6.5 | 11106.82 | 0.000838073 | 5 | 8 | 3 | 1 |
| 183.012 | -0.76443 | 5.5 | 2163489 | 0.163247657 | 7 | 8 | 3 | 1 |
| 184.0197 | -1.43952 | 5 | 34155.49 | 0.002577227 | 8 | 8 | 3 | 1 |
| 195.012 | -0.71739 | 6.5 | 102706.8 | 0.007749815 | 7 | 9 | 3 | 1 |
| 196.0198 | -0.84124 | 6 | 14610.44 | 0.001102441 | 8 | 9 | 3 | 1 |
| 197.0277 | -0.45628 | 5.5 | 119683.7 | 0.009030824 | 9 | 9 | 3 | 1 |
| 198.0354 | -1.08516 | 5 | 1338.89 | 0.000101027 | 10 | 9 | 3 | 1 |
| 207.012 | -0.67581 | 7.5 | 8764.75 | 0.000661351 | 7 | 10 | 3 | 1 |
| 209.0276 | -0.90849 | 6.5 | 23687.29 | 0.001787342 | 9 | 10 | 3 | 1 |
| 211.0433 | -0.6629 | 5.5 | 9903.8 | 0.000747298 | 11 | 10 | 3 | 1 |
| 221.0277 | -0.40674 | 7.5 | 2308.33 | 0.000174177 | 9 | 11 | 3 | 1 |
| 223.0434 | -0.17889 | 6.5 | 2038.84 | 0.000153842 | 11 | 11 | 3 | 1 |
| 225.0589 | -0.84378 | 5.5 | 13135.47 | 0.000991146 | 13 | 11 | 3 | 1 |
| 239.0746 | -0.58517 | 5.5 | 12771.19 | 0.000963659 | 15 | 12 | 3 | 1 |
| 253.0903 | -0.35521 | 5.5 | 3729.99 | 0.000281449 | 17 | 13 | 3 | 1 |
| 267.1058 | -0.89815 | 5.5 | 1633.07 | 0.000123224 | 19 | 14 | 3 | 1 |
| 281.0282 | 1.459286 | 12.5 | 3408.93 | 0.000257223 | 9 | 16 | 3 | 1 |
| 281.1216 | -0.31979 | 5.5 | 1821.95 | 0.000137477 | 21 | 15 | 3 | 1 |
| 295.137 | -1.15167 | 5.5 | 1895.88 | 0.000143055 | 23 | 16 | 3 | 1 |
| 297.1527 | -0.97559 | 4.5 | 59676.37 | 0.004502924 | 25 | 16 | 3 | 1 |
| 301.1269 | 0.41544 | 8.5 | 4028.46 | 0.00030397 | 21 | 18 | 2 | 1 |
| 309.1529 | -0.29079 | 5.5 | 2388.25 | 0.000180207 | 25 | 17 | 3 | 1 |
| 311.1684 | -0.77096 | 4.5 | 198286 | 0.014961814 | 27 | 17 | 3 | 1 |
| 323.1684 | -0.74234 | 5.5 | 1451.48 | 0.000109522 | 27 | 18 | 3 | 1 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 325.184 | -0.89149 | 4.5 | 161031 | 0.012150711 | 29 | 18 | 3 | 1 |
| 339.1996 | -1.00206 | 4.5 | 96113.36 | 0.007252304 | 31 | 19 | 3 | 1 |

### iii. Hydrocarbons

| Mass | Deviation (ppm) | DBE | Area (AU) | H | C |
|---|---|---|---|---|---|
| 133.0086 | 1.699892972 | 11.5 | 62811.9 | 1 | 11 |
| 181.0087 | 1.801574109 | 15.5 | 56127.39 | 1 | 15 |
| 145.0086 | 1.559220298 | 12.5 | 45572.59 | 1 | 12 |
| 115.0553 | -0.207726155 | 6.5 | 27339.38 | 7 | 9 |
| 175.0555 | 1.005967691 | 11.5 | 14052.58 | 7 | 14 |
| 169.0086 | 1.337803535 | 14.5 | 11746.09 | 1 | 14 |
| 159.0242 | 1.107379852 | 12.5 | 11695.77 | 3 | 13 |
| 121.0085 | 1.042076643 | 10.5 | 8921.82 | 1 | 10 |
| 97.0083 | -0.761789906 | 8.5 | 7849.16 | 1 | 8 |
| 157.0085 | 0.803141876 | 13.5 | 7737.51 | 1 | 13 |
| 195.0241 | 0.390208337 | 15.5 | 7076.74 | 3 | 16 |
| 91.0551 | -2.458944633 | 4.5 | 6976.75 | 7 | 7 |
| 147.0242 | 1.197763436 | 11.5 | 6476.88 | 3 | 12 |
| 173.0398 | 0.728734614 | 12.5 | 5951.68 | 5 | 14 |
| 171.0243 | 1.614393076 | 13.5 | 5697.24 | 3 | 14 |
| 89.0394 | -3.076156819 | 5.5 | 5170.44 | 5 | 7 |
| 207.0242 | 0.850625916 | 16.5 | 3869.71 | 3 | 17 |
| 185.0395 | -0.939798457 | 13.5 | 2676.91 | 5 | 15 |
| 101.0397 | 0.258314373 | 6.5 | 2386.55 | 5 | 8 |
| 221.0399 | 1.022893293 | 16.5 | 2043.35 | 5 | 18 |
| 193.0085 | 0.653339528 | 16.5 | 1939.62 | 1 | 16 |
| 110.1101 | 0.009990001 | 2 | 1846.99 | 14 | 8 |
| 265.009 | 2.362566853 | 22.5 | 1787.15 | 1 | 22 |
| 219.024 | -0.10912045 | 17.5 | 1741.7 | 3 | 18 |
| 189.0708 | -0.919760429 | 11.5 | 1720.39 | 9 | 15 |
| 141.0709 | -0.52384979 | 7.5 | 1658.86 | 9 | 11 |

### iv. Species in LIPIDMAPS

| Mass | Intensity | H | C | O | Lipid assignments |
|---|---|---|---|---|---|
| 169.1233 | 2491.73 | 17 | 10 | 2 | 'FA 10:1' |
| 171.1391 | 2313.68 | 19 | 10 | 2 | 'FA 10:0' |
| 183.1388 | 1659.13 | 19 | 11 | 2 | 'FA 11:1' |
| 227.2016 | 3222.71 | 27 | 14 | 2 | 'FA 14:0' |
| 241.2172 | 3010.97 | 29 | 15 | 2 | 'FA 15:0' |
| 253.2171 | 4602.82 | 29 | 16 | 2 | 'FA 16:1' |
| 255.2329 | 311343.4 | 31 | 16 | 2 | 'FA 16:0' |
| 261.2221 | 5096.02 | 29 | 18 | 1 | 'ST 18:0;O' |
| 269.2487 | 2213.19 | 33 | 17 | 2 | 'FA 17:0' |
| 281.2484 | 21013.3 | 33 | 18 | 2 | 'FA 18:1' |
| 283.2642 | 261965.6 | 35 | 18 | 2 | 'FA 18:0' |

| | | | | | |
|---|---|---|---|---|---|
| 419.1711 | 19105.95 | 27 | 22 | 8 | 'ST 22:5;O8' |
| 431.2072 | 1619.65 | 31 | 24 | 7 | 'ST 18:3;O;GlCA/ST 18:4;O2;Hex/ST 24:5;O7' |
| 447.2023 | 16996.62 | 31 | 24 | 8 | 'ST 18:3;O2;GlCA/ST 18:4;O3;Hex/ST 24:5;O8' |

**Supplementary Table 2**. Lipid group assignments made automatically in the human serum sample, using SIMS-MFP with LIPID MAPS® database of "bulk" lipid species.

| Mass (m/z) | Intensity | Assignment | Deviation (ppm) | DBE | Lipid groups |
|---|---|---|---|---|---|
| 597.4852 | 1547942 | $C_{37}H_{66}O_4Na^+$ | -0.2178 | 4.5 | DG O-34:4/MG 34:4/MG O-34:5;O |
| 459.2481 | 1515874 | $C_{21}H_{41}O_7PNa^+$ | -0.2419 | 1.5 | LPA 18:1/LPA O-18:2;O |
| 780.5511 | 1151521 | $C_{42}H_{80}NO_8PNa^+$ | -0.3524 | 3.5 | CerP 42:3;O4/LPC 34:3;O/PC 34:2/PC O-34:3;O/PE 37:2/PE O-37:3;O |
| 671.5737 | 872161.2 | $C_{45}H_{76}O_2Na^+$ | -0.0746 | 7.5 | CE 18:2 |
| 599.5009 | 869365.6 | $C_{37}H_{68}O_4Na^+$ | -0.1336 | 3.5 | DG O-34:3/MG 34:3/MG O-34:4;O |
| 625.5163 | 834726.9 | $C_{39}H_{70}O_4Na^+$ | -0.5277 | 4.5 | DG O-36:4 |
| 879.7408 | 782883.4 | $C_{55}H_{100}O_6Na^+$ | -0.4662 | 5.5 | CE 28:0;O4/DG 52:4;O/DG O-52:5;O2/TG 52:3/TG O-52:4;O |
| 782.5669 | 643310.7 | $C_{42}H_{82}NO_8PNa^+$ | -0.1599 | 2.5 | CerP 42:2;O4/LPC 34:2;O/PC 34:1/PC O-34:2;O/PE 37:1/PE O-37:2;O |
| 881.7565 | 635687.6 | $C_{55}H_{102}O_6Na^+$ | -0.4084 | 4.5 | DG 52:3;O/DG O-52:4;O2/TG 52:2/TG O-52:3;O |
| 542.4906 | 590690.2 | $C_{34}H_{65}NO_2Na^+$ | -0.2748 | 2.5 | Cer 34:2;O/NAE 32:2 |
| 808.5826 | 582898 | $C_{44}H_{84}NO_8PNa^+$ | -0.0929 | 3.5 | CerP 44:3;O4/PC 36:2/PC O-36:3;O/PE 39:2/PE O-39:3;O |
| 621.4850 | 501055.7 | $C_{39}H_{66}O_4Na^+$ | -0.5312 | 6.5 | CE 12:1;O2/DG O-36:6 |
| 721.4777 | 469499 | $C_{39}H_{71}N_0O_8PNa^+$ | -0.2441 | 4.5 | LPG O-33:5/PA 36:3/PA O-36:4;O |
| 666.4832 | 376432.7 | $C_{36}H_{70}NO_6PNa^+$ | -0.1427 | 2.5 | CerP 36:2;O2/LPC O-28:3/LPE O-31:3 |
| 623.5007 | 374497.3 | $C_{39}H_{68}O_4Na^+$ | -0.4492 | 5.5 | CE 12:0;O2/DG O-36:5 |
| 487.2793 | 362594 | $C_{23}H_{45}O_7PNa^+$ | -0.4332 | 1.5 | LPA 20:1/LPA O-20:2;O/PA O-20:1 |
| 478.3290 | 256273.9 | $C_{29}H_{45}NO_3Na^+$ | -0.3431 | 7.5 | NAE 27:7;O |
| 804.5517 | 215617.9 | $C_{44}H_{80}NO_8PNa^+$ | 0.4038 | 5.5 | CerP 44:5;O4/PC 36:4/PC O-36:5;O/PE 39:4/PE O-39:5;O |
| 877.7251 | 191341.8 | $C_{55}H_{98}O_6Na^+$ | -0.5242 | 6.5 | CE 28:1;O4/DG 52:5;O/DG O-52:6;O2/TG 52:4/TG O-52:5;O |
| 518.3214 | 188496.7 | $C_{24}H_{50}NO_7PNa^+$ | -0.5983 | 0.5 | LPC 16:0/LPC O-16:1;O/LPE 19:0/LPE O-19:1;O |
| 723.4933 | 176029.2 | $C_{39}H_{73}O_8PNa^+$ | -0.3125 | 3.5 | LPG O-33:4/PA 36:2/PA O-36:3;O |
| 853.7250 | 175051.1 | $C_{53}H_{98}O_6Na^+$ | -0.6561 | 4.5 | DG 50:3;O/DG O-50:4;O2/TG 50:2/TG O-50:3;O |
| 749.5087 | 163238.5 | $C_{41}H_{75}O_8PNa^+$ | -0.6352 | 4.5 | PA 38:3/PA O-38:4;O |
| 725.5567 | 155429 | $C_{39}H_{79}N_2O_6PNa^+$ | -0.1297 | 1.5 | PE-Cer 37:1;O2/SM 34:1;O2 |
| 649.5164 | 151706.7 | $C_{41}H_{70}O_4Na^+$ | -0.3543 | 6.5 | CE 14:1;O2/DG O-38:6 |
| 855.7407 | 121068.6 | $C_{53}H_{100}O_6Na^+$ | -0.5961 | 3.5 | DG 50:2;O/DG O-50:3;O2/TG 50:1/TG O-50:2;O |

| | | | | | |
|---|---|---|---|---|---|
| 806.5670 | 112865.7 | $C_{44}H_{82}NO_8PNa^+$ | -0.0311 | 4.5 | CerP 44:4;O4/PC 36:3/PC O-36:4;O/PE 39:3/PE O-39:4;O |
| 722.4811 | 80283.96 | $C_{38}H_{69}NO_{10}Na^+$ | -0.3725 | 4.5 | HexCer 32:3;O4 |
| 652.6001 | 68362.82 | $C_{42}H_{79}NO_2Na^+$ | -0.3051 | 3.5 | Cer 42:3;O |
| 303.2294 | 66453.01 | $C_{18}H_{32}O_2Na^+$ | -0.1652 | 2.5 | FA 18:2 |
| 905.7565 | 58932.6 | $C_{57}H_{102}O_6Na^+$ | -0.3976 | 6.5 | CE 30:1;O4/DG 54:5;O/DG O-54:6;O2/TG 54:4/TG O-54:5;O |
| 907.7722 | 55999.47 | $C_{57}H_{104}O_6Na^+$ | -0.3416 | 5.5 | CE 30:0;O4/DG 54:4;O/DG O-54:5;O2/TG 54:3/TG O-54:4;O |
| 673.5889 | 53426.17 | $C_{45}H_{78}O_2Na^+$ | -0.7424 | 6.5 | CE 18:1 |
| 510.2683 | 52896.44 | $C_{24}H_{41}NO_9Na^+$ | 1.8537 | 4.5 | ST 22:0;O8;G |
| 832.5827 | 51443.43 | $C_{46}H_{84}NO_8PNa^+$ | 0.0299 | 5.5 | CerP 46:5;O4/PC 38:4/PC O-38:5;O/PE 41:4/PE O-41:5;O |
| 468.2577 | 45102.01 | $C_{22}H_{39}NO_8Na^+$ | 1.9453 | 3.5 | CAR 15:2;O4 |
| 745.4776 | 42706.51 | $C_{41}H_{71}O_8PNa^+$ | -0.3704 | 6.5 | PA 38:5/PA O-38:6;O |
| 506.3602 | 40323.07 | $C_{31}H_{49}NO_3Na^+$ | -0.5216 | 7.5 | NAE 29:7;O |
| 523.2636 | 36065.95 | $C_{22}H_{45}O_{10}PNa^+$ | -1.2539 | 0.5 | LPG 16:0;O |
| 509.2478 | 35391.98 | $C_{21}H_{43}O_{10}PNa^+$ | -1.5829 | 0.5 | LPG 15:0;O |
| 485.2636 | 35124.92 | $C_{23}H_{43}O_7PNa^+$ | -0.5381 | 2.5 | LPA 20:2/LPA O-20:3;O/PA O-20:2 |
| 466.2055 | 34824.63 | $C_{21}H_{33}NO_9Na^+$ | 1.5999 | 5.5 | ST 19:1;O8;G |
| 508.2523 | 32734.41 | $C_{24}H_{39}NO_9Na^+$ | 1.1725 | 5.5 | ST 22:1;O8;G |
| 776.5928 | 32402.18 | $C_{44}H_{84}NO_6PNa^+$ | -0.0581 | 3.5 | CerP 44:3;O2 |
| 495.2323 | 28166.2 | $C_{20}H_{41}O_{10}PNa^+$ | -1.3248 | 0.5 | LPG 14:0;O |
| 443.2531 | 28076.86 | $C_{21}H_{41}O_6PNa^+$ | -0.4424 | 1.5 | LPA O-18:2 |
| 810.5984 | 27569.85 | $C_{44}H_{86}NO_8PNa^+$ | 0.0924 | 2.5 | CerP 44:2;O4/PC 36:1/PC O-36:2;O/PE 39:1/PE O-39:2;O |
| 522.2677 | 27082.08 | $C_{25}H_{41}NO_9Na^+$ | 0.6623 | 5.5 | ST 23:1;O8;G |
| 470.2733 | 26738.39 | $C_{22}H_{41}NO_8Na^+$ | 1.8306 | 2.5 | CAR 15:1;O4 |
| 521.2479 | 25951.87 | $C_{22}H_{43}O_{10}PNa^+$ | -1.3546 | 1.5 | BMP 16:0/LPG 16:1;O |
| 627.5322 | 25947.93 | $C_{39}H_{72}O_4Na^+$ | -0.1276 | 3.5 | DG O-36:3 |
| 747.4935 | 25694.17 | $C_{41}H_{73}O_8PNa^+$ | -0.0349 | 5.5 | PA 38:4/PA O-38:5;O |
| 750.5122 | 25413.56 | $C_{40}H_{73}NO_{10}Na^+$ | -0.6250 | 4.5 | HexCer 34:3;O4 |
| 851.7092 | 24492.81 | $C_{53}H_{96}O_6Na^+$ | -0.8337 | 5.5 | CE 26:0;O4/DG 50:4;O/DG O-50:5;O2/TG 50:3/TG O-50:4;O |
| 626.5843 | 23724.68 | $C_{40}H_{77}NO_2Na^+$ | -0.5572 | 2.5 | Cer 40:2;O |
| 536.2829 | 23127.3 | $C_{26}H_{43}NO_9Na^+$ | -0.1941 | 5.5 | ST 18:0;O4;HexNAC/ST 24:1;O8;G |
| 724.4968 | 21669.66 | $C_{38}H_{71}NO_{10}Na^+$ | -0.3024 | 3.5 | HexCer 32:2;O4 |
| 507.2321 | 21401.27 | $C_{21}H_{41}O_{10}PNa^+$ | -1.6878 | 1.5 | BMP 15:0/LPG 15:1;O |
| 524.2839 | 21249.69 | $C_{25}H_{43}NO_9Na^+$ | 1.7088 | 4.5 | ST 23:0;O8;G |
| 480.2575 | 21193.84 | $C_{23}H_{39}NO_8Na^+$ | 1.4803 | 4.5 | CAR 16:3;O4/ST 21:0;O7;G |
| 537.2793 | 21045.04 | $C_{23}H_{47}O_{10}PNa^+$ | -1.1281 | 0.5 | LPG 17:0;O |
| 835.6663 | 20630.22 | $C_{47}H_{93}N_2O_6PNa^+$ | -0.0528 | 2.5 | PE-Cer 45:2;O2/SM 42:2;O2 |
| 546.3528 | 19623.92 | $C_{26}H_{54}NO_7PNa^+$ | -0.3846 | 0.5 | LPC 18:0/LPC O-18:1;O/LPE 21:0/LPE O-21:1;O/PE O-21:0 |
| 494.2732 | 18997.13 | $C_{24}H_{41}NO_8Na^+$ | 1.5394 | 4.5 | CAR 17:3;O4/ST 22:0;O7;G |
| 551.2946 | 18521.88 | $C_{24}H_{49}O_{10}PNa^+$ | -1.7343 | 0.5 | LPG 18:0;O |

| | | | | | |
|---|---|---|---|---|---|
| 483.2480 | 18465.82 | $C_{23}H_{41}O_7PNa^+$ | -0.4368 | 3.5 | LPA 20:3/LPA O-20:4;O/PA O-20:3 |
| 481.2166 | 18290.46 | $C_{19}H_{39}O_{10}PNa^+$ | -1.4673 | 0.5 | LPG 13:0;O |
| 447.2406 | 18160.77 | $C_{23}H_{38}NO_4SNa^+$ | -1.7331 | 5 | ST 23:1;O;S |
| 419.2093 | 17245.78 | $C_{21}H_{34}NO_4SNa^+$ | -1.8490 | 5 | ST 21:1;O;S |
| 903.7407 | 17062.67 | $C_{57}H_{100}O_6Na^+$ | -0.5644 | 7.5 | CE 30:2;O4/DG 54:6;O/DG O-54:7;O2/TG 54:5/TG O-54:6;O |
| 595.4695 | 16856.68 | $C_{37}H_{64}O_4Na^+$ | -0.3025 | 5.5 | CE 10:0;O2/DG O-34:5/MG 34:5/MG O-34:6;O |
| 493.2167 | 16832 | $C_{20}H_{39}O_{10}PNa^+$ | -1.2289 | 1.5 | BMP 14:0/LPG 14:1;O |
| 695.5732 | 16706.24 | $C_{47}H_{76}O_2Na^+$ | -0.7909 | 9.5 | CE 20:4 |
| 773.5087 | 16264.88 | $C_{43}H_{75}O_8PNa^+$ | -0.6155 | 6.5 | PA 40:5/PA O-40:6;O |
| 482.2733 | 16199.64 | $C_{23}H_{41}NO_8Na^+$ | 1.7851 | 3.5 | CAR 16:2;O4 |
| 578.2908 | 15851.31 | $C_{32}H_{45}NO_5SNa^+$ | -0.4584 | 10.5 | ST 30:7;O3;T |
| 478.2054 | 15515.45 | $C_{22}H_{33}NO_9Na^+$ | 1.3507 | 6.5 | ST 20:2;O8;G |
| 550.2606 | 15338.36 | $C_{30}H_{41}NO_5SNa^+$ | 1.5173 | 10.5 | ST 28:7;O3;T |
| 647.5009 | 15282.13 | $C_{41}H_{68}O_4Na^+$ | -0.1237 | 7.5 | CE 14:2;O2/DG O-38:7 |
| 464.1900 | 15094.65 | $C_{21}H_{31}NO_9Na^+$ | 1.9300 | 6.5 | ST 19:2;O8;G |
| 535.2634 | 14897.59 | $C_{23}H_{45}O_{10}PNa^+$ | -1.5994 | 1.5 | BMP 17:0/LPG 17:1;O |
| 441.2373 | 14757.14 | $C_{21}H_{39}O_6PNa^+$ | -0.7844 | 2.5 | LPA O-18:3 |
| 540.4750 | 14520.16 | $C_{34}H_{63}NO_2Na^+$ | -0.1834 | 3.5 | Cer 34:3;O/NAE 32:3 |
| 505.2532 | 14424.05 | $C_{22}H_{43}O_9PNa^+$ | -0.9720 | 1.5 | LPG 16:1/LPG O-16:2;O |
| 479.2373 | 14186.65 | $C_{20}H_{41}O_9PNa^+$ | -1.5464 | 0.5 | LPG 14:0/LPG O-14:1;O |
| 565.3102 | 14103.68 | $C_{25}H_{51}O_{10}PNa^+$ | -1.7797 | 0.5 | LPG 19:0;O |
| 750.5768 | 14044.44 | $C_{42}H_{82}NO_6PNa^+$ | -0.5264 | 2.5 | CerP 42:2;O2/LPC O-34:3 |
| 437.1905 | 13352.08 | $C_{17}H_{35}O_9PNa^+$ | -1.3520 | 0.5 | LPG 11:0/LPG O-11:1;O |
| 463.2061 | 13298.84 | $C_{19}H_{37}O_9PNa^+$ | -1.3841 | 1.5 | LPG 13:1/LPG O-13:2;O |
| 493.2530 | 13021.22 | $C_{21}H_{43}O_9PNa^+$ | -1.4011 | 0.5 | LPG 15:0/LPG O-15:1;O |
| 477.2218 | 12746.17 | $C_{20}H_{39}O_9PNa^+$ | -1.2386 | 1.5 | LPG 14:1/LPG O-14:2;O |
| 564.2756 | 12467.62 | $C_{31}H_{43}NO_5SNa^+$ | 0.3277 | 10.5 | ST 29:7;O3;T |
| 570.5216 | 12278.62 | $C_{36}H_{69}NO_2Na^+$ | -0.7872 | 2.5 | Cer 36:2;O/NAE 34:2 |
| 519.2321 | 12137.09 | $C_{22}H_{41}O_{10}PNa^+$ | -1.6488 | 2.5 | BMP 16:1/LPG 16:2;O |
| 433.2250 | 11942.48 | $C_{22}H_{36}NO_4SNa^+$ | -1.6737 | 5 | ST 22:1;O;S |
| 538.2997 | 11208.52 | $C_{26}H_{45}NO_9Na^+$ | 1.9430 | 4.5 | ST 24:0;O8;G |
| 451.2060 | 11129.2 | $C_{18}H_{37}O_9PNa^+$ | -1.6425 | 0.5 | LPG 12:0/LPG O-12:1;O |
| 536.2589 | 10937.92 | $C_{22}H_{44}NO_{10}PNa^+$ | -1.1284 | 1.5 | LPS 16:0;O |
| 550.2746 | 10900.72 | $C_{23}H_{46}NO_{10}PNa^+$ | -1.0088 | 1.5 | LPS 17:0;O |
| 651.5323 | 10810.01 | $C_{41}H_{72}O_4Na^+$ | 0.0305 | 5.5 | CE 14:0;O2/DG O-38:5 |
| 552.2788 | 10792.4 | $C_{26}H_{43}NO_{10}Na^+$ | 1.5950 | 5.5 | ST 18:0;O5;HexNAC |
| 573.4857 | 10731.81 | $C_{35}H_{66}O_4Na^+$ | 0.6450 | 2.5 | DG O-32:2/MG 32:2/MG O-32:3;O |
| 465.2217 | 10424.28 | $C_{19}H_{39}O_9PNa^+$ | -1.4855 | 0.5 | LPG 13:0/LPG O-13:1;O |
| 654.6158 | 10274.94 | $C_{42}H_{81}NO_2Na^+$ | -0.2278 | 2.5 | Cer 42:2;O |

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|---|---|---|---|---|---|
| 494.2485 | 10097.97 | $C_{20}H_{42}NO_9PNa^+$ | -0.8904 | 0.5 | LPS O-14:0;O |
| 445.2251 | 9910.76 | $C_{23}H_{36}NO_4SNa^+$ | -1.4040 | 6 | ST 23:2;O;S |
| 484.2890 | 9651.26 | $C_{23}H_{43}NO_8Na^+$ | 1.8809 | 2.5 | CAR 16:1;O4 |
| 507.2684 | 9429.59 | $C_{22}H_{45}O_9PNa^+$ | -1.8552 | 0.5 | LPG 16:0/LPG O-16:1;O |
| 650.5845 | 9362.01 | $C_{42}H_{77}NO_2Na^+$ | -0.2292 | 4.5 | Cer 42:4;O |
| 566.2933 | 9230.5 | $C_{27}H_{45}NO_{10}Na^+$ | -0.4752 | 5.5 | ST 19:0;O5;HexNAC |
| 778.6083 | 9221.58 | $C_{44}H_{86}NO_6PNa^+$ | -0.2506 | 2.5 | CerP 44:2;O2 |
| 552.3141 | 8985.71 | $C_{27}H_{47}NO_9Na^+$ | -0.3695 | 4.5 | ST 25:0;O8;G |
| 443.2092 | 8952.98 | $C_{23}H_{34}NO_4SNa^+$ | -1.9745 | 7 | ST 23:3;O;S |
| 578.3057 | 8931.26 | $C_{25}H_{50}NO_{10}PNa^+$ | -1.3057 | 1.5 | LPS 19:0;O |
| 548.2590 | 8909.32 | $C_{23}H_{44}NO_{10}PNa^+$ | -0.9213 | 2.5 | LPS 17:1;O |
| 564.2901 | 8663.6 | $C_{24}H_{48}NO_{10}PNa^+$ | -1.2495 | 1.5 | LPS 18:0;O |
| 687.5682 | 8627.48 | $C_{45}H_{76}O_3Na^+$ | -0.6764 | 7.5 | CE 18:2;O |
| 453.1851 | 8404.84 | $C_{17}H_{35}O_{10}PNa^+$ | -1.9994 | 0.5 | LPG 11:0;O |
| 503.2373 | 8399.46 | $C_{22}H_{41}O_9PNa^+$ | -1.4727 | 2.5 | LPG 16:2/LPG O-16:3;O |
| 576.2897 | 8376.85 | $C_{25}H_{48}NO_{10}PNa^+$ | -1.9176 | 2.5 | LPS 19:1;O |
| 496.2889 | 8320.76 | $C_{24}H_{43}NO_8Na^+$ | 1.6339 | 3.5 | CAR 17:2;O4 |
| 421.2249 | 8223.45 | $C_{21}H_{36}NO_4SNa^+$ | -1.9588 | 4 | ST 21:0;O;S |
| 436.2314 | 8090.24 | $C_{21}H_{35}NO_7Na^+$ | 1.8933 | 4.5 | CAR 14:3;O3/ST 19:0;O6;G |
| 479.2007 | 7693.71 | $C_{19}H_{37}O_{10}PNa^+$ | -1.9952 | 1.5 | BMP 13:0/LPG 13:1;O |
| 467.2011 | 7659.52 | $C_{18}H_{37}O_{10}PNa^+$ | -1.1903 | 0.5 | LPG 12:0;O |
| 606.3383 | 7640.3 | $C_{27}H_{54}NO_{10}PNa^+$ | 0.8987 | 1.5 | LPS 21:0;O/PS O-21:0;O |
| 491.2010 | 7612.48 | $C_{20}H_{37}O_{10}PNa^+$ | -1.3357 | 2.5 | BMP 14:1/LPG 14:2;O |
| 497.2209 | 7556.49 | $C_{26}H_{36}NO_5SNa^+$ | 0.5227 | 9 | ST 26:5;O2;S |
| 431.2094 | 7454.9 | $C_{22}H_{34}NO_4SNa^+$ | -1.5656 | 6 | ST 22:2;O;S |
| 510.3043 | 7389.54 | $C_{25}H_{45}NO_8Na^+$ | 1.0991 | 3.5 | CAR 18:2;O4 |
| 424.2312 | 7377.99 | $C_{20}H_{35}NO_7Na^+$ | 1.4754 | 3.5 | CAR 13:2;O3 |
| 604.3213 | 7299.58 | $C_{27}H_{52}NO_{10}PNa^+$ | -1.3322 | 2.5 | LPS 21:1;O/PS 21:0/PS O-21:1;O |
| 562.2743 | 7245.42 | $C_{24}H_{46}NO_{10}PNa^+$ | -1.5208 | 2.5 | LPS 18:1;O |
| 457.2325 | 7147.71 | $C_{21}H_{39}O_7PNa^+$ | -0.1336 | 2.5 | LPA 18:2/LPA O-18:3;O |
| 827.7097 | 7011.44 | $C_{51}H_{96}O_6Na^+$ | -0.2538 | 3.5 | DG 48:2;O/DG O-48:3;O2/TG 48:1/TG O-48:2;O |
| 407.2093 | 6951.17 | $C_{20}H_{34}NO_4SNa^+$ | -1.9034 | 4 | ST 20:0;O;S |
| 481.2260 | 6912.66 | $C_{26}H_{36}NO_4SNa^+$ | 0.5713 | 9 | ST 26:5;O;S |
| 475.2723 | 6866.01 | $C_{25}H_{42}NO_4SNa^+$ | -0.7892 | 5 | ST 25:1;O;S |
| 613.4796 | 6861.35 | $C_{37}H_{66}O_5Na^+$ | -1.0515 | 4.5 | DG 34:3/DG O-34:4;O/MG 34:4;O/TG O-34:3 |
| 522.2437 | 6633.85 | $C_{21}H_{42}NO_{10}PNa^+$ | -0.2970 | 1.5 | LPS 15:0;O |
| 457.2254 | 6541.46 | $C_{24}H_{36}NO_4SNa^+$ | -0.7110 | 7 | ST 24:3;O;S |
| 534.2435 | 6525.23 | $C_{22}H_{42}NO_{10}PNa^+$ | -0.6647 | 2.5 | LPS 16:1;O |
| 459.2406 | 6494.27 | $C_{24}H_{38}NO_4SNa^+$ | -1.6878 | 6 | ST 24:2;O;S |

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| 746.4815 | 6381.01 | $C_{40}H_{69}NO_{10}Na^+$ | 0.1754 | 6.5 | HexCer 34:5;O4 |
| 467.2533 | 5984.55 | $C_{23}H_{41}O_6PNa^+$ | 0.0083 | 3.5 | LPA O-20:4 |
| 558.2305 | 5962.57 | $C_{27}H_{37}NO_{10}Na^+$ | -0.8403 | 9.5 | ST 19:4;O5;HexNAC |
| 809.6504 | 5820.53 | $C_{45}H_{91}N_2O_6PNa^+$ | -0.3632 | 1.5 | PE-Cer 43:1;O2/SM 40:1;O2 |
| 536.2438 | 5745.07 | $C_{29}H_{39}NO_5SNa^+$ | -0.5876 | 10.5 | ST 27:7;O3;T |
| 419.2557 | 5700.08 | $C_{26}H_{36}O_3Na^+$ | 0.0832 | 8.5 | ST 26:5;O3 |
| 624.5689 | 5697.42 | $C_{40}H_{75}NO_2Na^+$ | -0.1587 | 3.5 | Cer 40:3;O |
| 571.4696 | 5446.84 | $C_{35}H_{64}O_4Na^+$ | -0.1402 | 3.5 | DG O-32:3/MG 32:3/MG O-32:4;O |
| 508.2273 | 5391.86 | $C_{20}H_{40}NO_{10}PNa^+$ | -1.7809 | 1.5 | LPS 14:0;O |
| 778.5355 | 5359.71 | $C_{42}H_{78}N_1O_8PNa^+$ | -0.2891 | 4.5 | CerP 42:4;O4/LPC 34:4;O/PC 34:3/PC O-34:4;O/PE 37:3/PE O-37:4;O |
| 774.5770 | 5304.35 | $C_{44}H_{82}NO_6PNa^+$ | -0.2519 | 4.5 | CerP 44:4;O2 |
| 473.2561 | 5298.84 | $C_{25}H_{40}NO_4SNa^+$ | -1.9548 | 6 | ST 25:2;O;S |
| 748.4970 | 5280.62 | $C_{40}H_{71}NO_{10}Na^+$ | -0.0255 | 5.5 | HexCer 34:4;O4 |
| 645.4851 | 5221.8 | $C_{41}H_{66}O_4Na^+$ | -0.3565 | 8.5 | CE 14:3;O2/DG O-38:8 |
| 461.1914 | 5100.13 | $C_{19}H_{35}O_9PNa^+$ | 0.6698 | 2.5 | LPG 13:2/LPG O-13:3;O |
| 469.2250 | 5082.77 | $C_{25}H_{36}NO_4SNa^+$ | -1.5453 | 8 | ST 25:4;O;S |
| 834.5985 | 4980.57 | $C_{46}H_{86}NO_8PNa^+$ | 0.2096 | 4.5 | CerP 46:4;O4/PC 38:3/PC O-38:4;O/PE 41:3/PE O-41:4;O |
| 520.2643 | 4857.49 | $C_{22}H_{44}NO_9PNa^+$ | -0.5576 | 1.5 | LPS 16:0/LPS O-16:1;O |
| 471.2843 | 4853.06 | $C_{23}H_{45}O_6PNa^+$ | -0.6283 | 1.5 | LPA O-20:2 |
| 580.3062 | 4822.21 | $C_{32}H_{47}NO_5SNa^+$ | -0.8876 | 9.5 | ST 30:6;O3;T |
| 545.2879 | 4712.61 | $C_{32}H_{42}O_6Na^+$ | 0.9901 | 11.5 | ST 26:7;O;Hex |
| 449.1902 | 4696.49 | $C_{18}H_{35}O_9PNa^+$ | -1.9838 | 1.5 | LPG 12:1/LPG O-12:2;O |
| 450.1739 | 4633.29 | $C_{20}H_{29}NO_9Na^+$ | 0.9905 | 6.5 | ST 18:2;O8;G |
| 830.5665 | 4516.17 | $C_{46}H_{82}NO_8PNa^+$ | -0.6322 | 6.5 | CerP 46:6;O4/PC 38:5/PC O-38:6;O/PE 41:5/PE O-41:6;O |
| 566.3309 | 4477.09 | $C_{28}H_{49}NO_9Na^+$ | 1.6702 | 4.5 | ST 26:0;O8;G |
| 694.5142 | 4434.42 | $C_{38}H_{74}NO_6PNa^+$ | -0.5689 | 2.5 | CerP 38:2;O2/LPC O-30:3/LPE O-33:3 |
| 439.1696 | 4406.53 | $C_{16}H_{33}O_{10}PNa^+$ | -1.7217 | 0.5 | LPG 10:0;O |
| 449.2270 | 4367.58 | $C_{19}H_{39}O_8PNa^+$ | -1.0598 | 0.5 | LPA 16:0;O/LPG O-13:1 |
| 465.1851 | 4320.91 | $C_{18}H_{35}O_{10}PNa^+$ | -1.9478 | 1.5 | BMP 12:0/LPG 12:1;O |
| 449.2198 | 4289.08 | $C_{22}H_{36}NO_5SNa^+$ | -1.8701 | 5 | ST 22:1;O2;S |
| 455.2098 | 4227 | $C_{24}H_{34}NO_4SNa^+$ | -0.6043 | 8 | ST 24:4;O;S |
| 825.6938 | 4199.59 | $C_{51}H_{94}O_6Na^+$ | -0.5572 | 4.5 | DG 48:3;O/DG O-48:4;O2/TG 48:2/TG O-48:3;O |
| 483.2407 | 4190.32 | $C_{26}H_{38}NO_4SNa^+$ | -1.3970 | 8 | ST 26:4;O;S |
| 637.4802 | 3917.67 | $C_{39}H_{66}O_5Na^+$ | -0.0708 | 6.5 | CE 12:1;O3/DG 36:5/DG O-36:6;O/TG O-36:5 |
| 532.2277 | 3884.2 | $C_{22}H_{40}NO_{10}PNa^+$ | -0.9490 | 3.5 | LPS 16:2;O |
| 537.2886 | 3759.95 | $C_{30}H_{44}NO_4SNa^+$ | 0.5116 | 9 | ST 30:5;O;S |
| 594.2863 | 3682.12 | $C_{32}H_{45}NO_6SNa^+$ | 0.5383 | 10.5 | ST 30:7;O4;T |
| 435.2046 | 3615.16 | $C_{21}H_{34}NO_5SNa^+$ | -0.8964 | 5 | ST 21:1;O2;S |
| 837.6816 | 3613.87 | $C_{47}H_{95}N_2O_6PNa^+$ | -0.4705 | 1.5 | PE-Cer 45:1;O2/SM 42:1;O2 |

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| 421.1886 | 3607.64 | $C_{20}H_{32}NO_5SNa^+$ | -1.7572 | 5 | ST 20:1;O2;S |
| 537.2529 | 3542.27 | $C_{29}H_{40}NO_5SNa^+$ | 1.7867 | 10 | ST 29:6;O2;S |
| 459.1746 | 3474.57 | $C_{19}H_{33}O_9PNa^+$ | -1.8318 | 3.5 | LPG 13:3 |
| 748.5610 | 3469.4 | $C_{42}H_{80}NO_6PNa^+$ | -0.7282 | 3.5 | CerP 42:3;O2/LPC O-34:4 |
| 756.5505 | 3443.01 | $C_{40}H_{80}NO_8PNa^+$ | -1.1567 | 1.5 | CerP 40:1;O4/LPC 32:1;O/LPS O-34:1/PC 32:0/PC O-32:1;O/PE 35:0/PE O-35:1;O |
| 475.2058 | 3402.45 | $C_{20}H_{37}O_9PNa^+$ | -1.9804 | 2.5 | LPG 14:2/LPG O-14:3;O |
| 469.2686 | 3334.18 | $C_{23}H_{43}O_6PNa^+$ | -0.7375 | 2.5 | LPA O-20:3 |
| 647.5732 | 3259.65 | $C_{43}H_{76}O_2Na^+$ | -0.8495 | 5.5 | CE 16:0 |
| 598.5534 | 3227.89 | $C_{38}H_{73}NO_2Na^+$ | 0.0850 | 2.5 | Cer 38:2;O |
| 664.4678 | 3205.49 | $C_{36}H_{68}NO_6PNa^+$ | 0.2331 | 3.5 | CerP 36:3;O2/LPC O-28:4/LPE O-31:4 |
| 498.3047 | 3142.04 | $C_{24}H_{45}NO_8Na^+$ | 1.9283 | 2.5 | CAR 17:1;O4 |
| 478.2168 | 3134.81 | $C_{19}H_{38}NO_9PNa^+$ | -1.7567 | 1.5 | LPS 13:0/LPS O-13:1;O |
| 822.4309 | 3120.31 | $C_{44}H_{66}NO_{10}PNa^+$ | -0.9181 | 12.5 | PS 38:10 |
| 751.5247 | 3097.06 | $C_{41}H_{77}O_8PNa^+$ | -0.1678 | 3.5 | PA 38:2/PA O-38:3;O |
| 901.7249 | 3082.14 | $C_{57}H_{98}O_6Na^+$ | -0.7320 | 8.5 | CE 30:3;O4/DG 54:7;O/DG O-54:8;O2/TG 54:6/TG O-54:7;O |
| 452.2627 | 2998.96 | $C_{22}H_{39}NO_7Na^+$ | 1.8262 | 3.5 | CAR 15:2;O3 |
| 774.5124 | 2979.96 | $C_{42}H_{73}NO_{10}Na^+$ | -0.3474 | 6.5 | HexCer 36:5;O4 |
| 909.7874 | 2963.55 | $C_{57}H_{106}O_6Na^+$ | -0.8355 | 4.5 | DG 54:3;O/DG O-54:4;O2/TG 54:2/TG O-54:3;O |
| 457.1891 | 2915.21 | $C_{23}H_{32}NO_5SNa^+$ | -0.5252 | 8 | ST 23:4;O2;S |
| 561.3197 | 2886.55 | $C_{33}H_{46}O_6Na^+$ | 1.8526 | 10.5 | ST 27:6;O;Hex/TG 30:8 |
| 568.5056 | 2867.78 | $C_{36}H_{67}NO_2Na^+$ | -1.4056 | 3.5 | Cer 36:3;O/NAE 34:3 |
| 833.6506 | 2831.62 | $C_{47}H_{91}N_2O_6PNa^+$ | -0.1129 | 3.5 | PE-Cer 45:3;O2/SM 42:3;O2 |
| 584.2590 | 2806.9 | $C_{26}H_{44}NO_{10}PNa^+$ | -0.8645 | 5.5 | LPS 20:4;O/PS 20:3/PS O-20:4;O |
| 521.2213 | 2800.66 | $C_{28}H_{36}NO_5SNa^+$ | 1.2661 | 11 | ST 28:7;O2;S |
| 771.4922 | 2724.64 | $C_{43}H_{73}O_8PNa^+$ | -1.7189 | 7.5 | PA 40:6/PA O-40:7;O |
| 875.7092 | 2698.43 | $C_{55}H_{96}O_6Na^+$ | -0.8109 | 7.5 | CE 28:2;O4/DG 52:6;O/DG O-52:7;O2/TG 52:5/TG O-52:6;O |
| 538.3360 | 2691.44 | $C_{27}H_{49}NO_8Na^+$ | 1.7849 | 3.5 | CAR 20:2;O4 |
| 640.5999 | 2658.17 | $C_{41}H_{79}NO_2Na^+$ | -0.6230 | 2.5 | Cer 41:2;O |
| 639.4960 | 2534.96 | $C_{39}H_{68}O_5Na^+$ | 0.1640 | 5.5 | CE 12:0;O3/DG 36:4/DG O-36:5;O/TG O-36:4 |
| 723.5408 | 2418.22 | $C_{39}H_{77}N_2O_6PNa^+$ | -0.4756 | 2.5 | PE-Cer 37:2;O2/SM 34:2;O2 |
| 544.3376 | 2394.23 | $C_{26}H_{52}NO_7PNa^+$ | 0.4407 | 1.5 | LPC 18:1/LPC O-18:2;O/LPE 21:1/LPE O-21:2;O/PE O-21:1 |
| 917.5298 | 2375.9 | $C_{52}H_{79}O_{10}PNa^+$ | -0.5516 | 13.5 | PG 46:12 |
| 613.5163 | 2346.66 | $C_{38}H_{70}O_4Na^+$ | -0.5381 | 3.5 | DG O-35:3 |
| 618.3411 | 2326.9 | $C_{35}H_{49}NO_7Na^+$ | 1.5783 | 11.5 | ST 27:6;O2;HexNAC |
| 722.5462 | 2309.97 | $C_{40}H_{78}NO_6PNa^+$ | 0.4220 | 2.5 | CerP 40:2;O2/LPC O-32:3 |
| 753.5873 | 2225.61 | $C_{41}H_{83}N_2O_6PNa^+$ | -1.0538 | 1.5 | PE-Cer 39:1;O2/SM 36:1;O2 |
| 610.2820 | 2187.68 | $C_{32}H_{45}NO_7SNa^+$ | 1.8105 | 10.5 | ST 30:7;O5;T |
| 569.4536 | 2144.58 | $C_{35}H_{62}O_4Na^+$ | -0.7553 | 4.5 | DG O-32:4/MG 32:4/MG O-32:5;O |
| 559.3039 | 2142.82 | $C_{33}H_{44}O_6Na^+$ | 1.5911 | 11.5 | ST 27:7;O;Hex |

| | | | | | |
|---|---|---|---|---|---|
| 731.4985 | 2140.97 | $C_{41}H_{73}O_7PNa^+$ | -0.1519 | 5.5 | PA O-38:5 |
| 514.4590 | 2096.53 | $C_{32}H_{61}NO_2Na^+$ | -0.8730 | 2.5 | Cer 32:2;O/NAE 30:2 |
| 619.4692 | 2086.03 | $C_{39}H_{64}O_4Na^+$ | -0.7750 | 7.5 | CE 12:2;O2/DG O-36:7 |
| 641.5112 | 2054.49 | $C_{39}H_{70}O_5Na^+$ | -0.5380 | 4.5 | DG 36:3/DG O-36:4;O/TG O-36:3 |

**Supplementary Table 3**. First (sorted by m/z) 60 of 3,328 peaks assigned in human serum as potential protein fragments. The assignments were made by matching the elemental composition of peaks assigned by SIMS-MFP with a database of up to 6-membered peptides, calculated using known formulas of each amino acid. Multiple amino acid sequences and ion types (a/b/c) are possible for each assigned peak.

| Mass (m/z) | Deviation (ppm) | DBE | Intensity | H | C | N | O | S | Na | Sequence assignment of the peptide peak |
|---|---|---|---|---|---|---|---|---|---|---|
| 151.0479 | 0.67 | 3 | 64542.42 | 8 | 5 | 2 | 2 | 0 | 1 | AG/GA c |
| 151.0842 | 0.11 | 2 | 33405.07 | 12 | 6 | 2 | 1 | 0 | 1 | VG/GV b |
| 152.0319 | 0.57 | 3 | 13615.05 | 7 | 5 | 1 | 3 | 0 | 1 | SS a |
| 163.0478 | 0.01 | 4 | 64592.73 | 8 | 6 | 2 | 2 | 0 | 1 | QG/NA/AN/GQ/AGG/GAG/GGA a |
| 163.0842 | 0.10 | 3 | 237072.1 | 12 | 7 | 2 | 1 | 0 | 1 | KG/GK a/PA/AP b |
| 165.0635 | 0.31 | 3 | 290507.39 | 10 | 6 | 2 | 2 | 0 | 1 | AA c |
| 165.0999 | 0.41 | 2 | 17348.47 | 14 | 7 | 2 | 1 | 0 | 1 | LG/VA/AV/GL b |
| 166.0587 | 0.02 | 3 | 23661.7 | 9 | 5 | 3 | 2 | 0 | 1 | NG/GN/GGG b |
| 168.0744 | 0.31 | 2 | 81514.22 | 11 | 5 | 3 | 2 | 0 | 1 | AG/GA a-NH3 |
| 177.0635 | 0.29 | 4 | 285218.19 | 10 | 7 | 2 | 2 | 0 | 1 | QA/AQ/AAG/AGA/GAA a /PG/GP c |
| 177.0999 | 0.38 | 3 | 88759.39 | 14 | 8 | 2 | 1 | 0 | 1 | KA/AK a |
| 179.0428 | 0.49 | 4 | 48862.02 | 8 | 6 | 2 | 3 | 0 | 1 | NS/SN/SGG/GSG/GGS a |
| 179.0792 | 0.57 | 3 | 233730.86 | 12 | 7 | 2 | 2 | 0 | 1 | PS/SP b/VG/GV c |
| 180.0744 | 0.29 | 3 | 146285.04 | 11 | 6 | 3 | 2 | 0 | 1 | QG/NA/AN/GQ/AGG/GAG/GGA b |
| 186.0639 | 0.63 | 6 | 101235.05 | 9 | 8 | 3 | 1 | 0 | 1 | HA/AH a |
| 189.0636 | 0.80 | 5 | 28253.7 | 10 | 8 | 2 | 2 | 0 | 1 | NP/PN/PGG/GPG/GGP a |
| 189.0748 | 0.63 | 5 | 24567.84 | 10 | 7 | 4 | 1 | 0 | 1 | HG/GH b |
| 189.0999 | 0.35 | 4 | 79096.74 | 14 | 9 | 2 | 1 | 0 | 1 | PP b |
| 191.0792 | 0.53 | 4 | 993401.63 | 12 | 8 | 2 | 2 | 0 | 1 | NV/VN/VGG/GVG/AAA/GGV a / PA/AP c |
| 193.0949 | 0.79 | 3 | 218516.9 | 14 | 8 | 2 | 2 | 0 | 1 | KS/SK a /TP/PT b/LG/VA/AV/GL c |
| 194.0538 | 0.97 | 4 | 39557.32 | 9 | 6 | 3 | 3 | 0 | 1 | NG/GN/GGG c |
| 194.0902 | 1.05 | 3 | 385964.09 | 13 | 7 | 3 | 2 | 0 | 1 | QA/AQ/AAG/AGA/GAA b /PG/GP a-NH3 |
| 195.0742 | 0.96 | 3 | 12994.45 | 12 | 7 | 2 | 3 | 0 | 1 | EA/AE b/TA/AT c |
| 196.1058 | 0.78 | 2 | 15697.78 | 15 | 7 | 3 | 2 | 0 | 1 | VG/GV a-NH3 |
| 203.0792 | 0.50 | 5 | 90741.12 | 12 | 9 | 2 | 2 | 0 | 1 | QP/PQ/PAG/APG/PGA/GPA/AGP/GAP a |
| 203.0905 | 0.83 | 5 | 50988.64 | 12 | 8 | 4 | 1 | 0 | 1 | HA/AH b |
| 205.1060 | 0.09 | 4 | 31038.31 | 14 | 8 | 4 | 1 | 0 | 1 | RA/AR a |
| 206.0537 | 0.43 | 5 | 68818.51 | 9 | 7 | 3 | 3 | 0 | 1 | NN/NGG/GNG/GGN/GGGG a |
| 206.0901 | 0.50 | 4 | 256770.27 | 13 | 8 | 3 | 2 | 0 | 1 | NP/PN/PGG/GPG/GGP b |
| 208.0693 | 0.18 | 4 | 202729.3 | 11 | 7 | 3 | 3 | 0 | 1 | QG/NA/AN/GQ/AGG/GAG/GGA c |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 208.1057 | 0.25 | 3 | 279312.13 | 15 | 8 | 3 | 2 | 0 | 1 | NV/VN/VGG/GVG/AAA/GGV b /KG/GK c/PA/AP a-NH3 |
| 214.0951 | 0.08 | 6 | 20899.89 | 13 | 10 | 3 | 1 | 0 | 1 | HV/VH a |
| 215.0791 | 0.01 | 6 | 17214.95 | 12 | 10 | 2 | 2 | 0 | 1 | YG/GY b |
| 216.0743 | -0.22 | 6 | 32822.5 | 11 | 9 | 3 | 2 | 0 | 1 | HT/TH a |
| 217.0947 | -0.22 | 5 | 186713.49 | 14 | 10 | 2 | 2 | 0 | 1 | PAA/APA/AAP a /PP c |
| 219.0740 | -0.06 | 5 | 49085.82 | 12 | 9 | 2 | 3 | 0 | 1 | PSG/SPG/PGS/GPS/SGP/GSP a |
| 219.0852 | -0.21 | 5 | 14025.58 | 12 | 8 | 4 | 2 | 0 | 1 | HS/SH b |
| 222.0849 | -0.05 | 4 | 597805.78 | 13 | 8 | 3 | 3 | 0 | 1 | QA/AQ/AAG/AGA/GAA c |
| 223.0689 | -0.13 | 4 | 10003.22 | 12 | 8 | 2 | 4 | 0 | 1 | TSG/STG/SSA/TGS/SAS/ASS/GTS/SGT/GST a /EA/AE c |
| 223.0801 | -0.27 | 4 | 14349.11 | 12 | 7 | 4 | 3 | 0 | 1 | NN/NGG/GNG/GGN/GGGG b |
| 225.0957 | -0.49 | 3 | 28434.69 | 14 | 7 | 4 | 3 | 0 | 1 | QG/NA/AN/GQ/AGG/GAG/GGA a-NH3 |
| 227.0789 | -0.87 | 7 | 11943.93 | 12 | 11 | 2 | 2 | 0 | 1 | FG/GF c |
| 228.1109 | 0.74 | 6 | 25376.83 | 15 | 11 | 3 | 1 | 0 | 1 | HL/LH a |
| 229.0695 | -0.42 | 7 | 15465.57 | 10 | 9 | 4 | 2 | 0 | 1 | HN/NH/HGG/GHG/GGH a |
| 229.0947 | -0.21 | 6 | 20193.56 | 14 | 11 | 2 | 2 | 0 | 1 | PPG/PGP/GPP a /YA/FS/SF/AY b |
| 229.1059 | -0.35 | 6 | 55991.22 | 14 | 10 | 4 | 1 | 0 | 1 | HP/PH b |
| 231.0852 | -0.20 | 6 | 131113.65 | 12 | 9 | 4 | 2 | 0 | 1 | HA/AH c |
| 233.0896 | -0.27 | 5 | 93613.12 | 14 | 10 | 2 | 3 | 0 | 1 | TPG/PTG/PSA/SPA/PAS/APS/TGP/SAP/ASP/GTP/PGT/GPT a |
| 233.1008 | -0.41 | 5 | 141331.99 | 14 | 9 | 4 | 2 | 0 | 1 | HT/TH b |
| 234.0961 | -0.19 | 5 | 22013.49 | 13 | 8 | 5 | 2 | 0 | 1 | HG/GH a-NH3 |
| 236.0640 | -0.75 | 5 | 9704.15 | 11 | 8 | 3 | 4 | 0 | 1 | NSG/SNG/NGS/GNS/SGN/GSN/SGGG/GSGG/GGSG/GGGS a |
| 241.0946 | -0.61 | 7 | 41374.4 | 14 | 12 | 2 | 2 | 0 | 1 | FA/AF c |
| 243.0852 | -0.19 | 7 | 47233.49 | 12 | 10 | 4 | 2 | 0 | 1 | HQ/QH/HAG/AHG/HGA/GHA/AGH/GAH a |
| 244.1056 | -0.19 | 6 | 165225.9 | 15 | 11 | 3 | 2 | 0 | 1 | FG/GF a-NH3 |
| 245.0896 | -0.26 | 6 | 17957.79 | 14 | 11 | 2 | 3 | 0 | 1 | YS/SY b |
| 246.0848 | -0.46 | 6 | 165867.93 | 13 | 10 | 3 | 3 | 0 | 1 | NPG/PNG/NGP/GNP/PGN/GPN/PGGG/GPGG/GGPG/GGGP a |
| 246.0961 | -0.18 | 6 | 12297.54 | 13 | 9 | 5 | 2 | 0 | 1 | HN/NH/HGG/GHG/GGH b |
| 247.0800 | -0.65 | 6 | 11176.03 | 12 | 9 | 4 | 3 | 0 | 1 | HD/DH b/HS/SH c/ |
| 248.1117 | -0.38 | 5 | 34980.9 | 15 | 9 | 5 | 2 | 0 | 1 | RN/NR/RGG/GRG/GGR a /HA/AH a-NH3 |
| 249.0957 | -0.45 | 5 | 118316.54 | 14 | 9 | 4 | 3 | 0 | 1 | RD/DR a |

**Supplementary Table 4.** Assignments of abundant serum proteins, albumin, transferrin and fibronectin, enabled by SIMS-MFP and amino acid sequence search developed previously (code available on Github, https://github.com/guferraz/simsdenovo/).

**Human serum albumin**

| Mass (m/z) | Intensity | Assignment | Deviation (ppm) | DBE | Sequence assignment |
|---|---|---|---|---|---|
| 194.0902 | 385964.09 | $C_7H_{13}N_3O_2Na^+$ | 0.86 | 3 | QA a |
| 265.1270 | 436399.14 | $C_{10}H_{18}N_4O_3Na^+$ | -0.27 | 4 | QAA a |
| 378.2111 | 396449.82 | $C_{16}H_{29}N_5O_4Na^+$ | -0.29 | 5 | QAAL a |
| 435.2324 | 191754.07 | $C_{18}H_{32}N_6O_5Na^+$ | -0.46 | 6 | QAALG a |
| 548.3166 | 51031.77 | $C_{24}H_{43}N_7O_6Na^+$ | -0.17 | 7 | QAALGL a |
| 222.0849 | 597805.78 | $C_8H_{13}N_3O_3Na^+$ | -0.22 | 4 | QA b |
| 293.1219 | 337975.09 | $C_{11}H_{18}N_4O_4Na^+$ | -0.33 | 5 | QAA b |
| 406.2059 | 446712.66 | $C_{17}H_{29}N_5O_5Na^+$ | -0.38 | 6 | QAAL b |
| 463.2274 | 139180.91 | $C_{19}H_{32}N_6O_6Na^+$ | -0.37 | 7 | QAALG b |
| 576.3113 | 39553.65 | $C_{25}H_{43}N_7O_7Na^+$ | -0.49 | 8 | QAALGL b |
| 239.1113 | 15420.07 | $C_8H_{16}N_4O_3Na^+$ | -0.48 | 3 | QA c |
| 310.1488 | 11375.97 | $C_{11}H_{21}N_5O_4Na^+$ | 0.77 | 4 | QAA c |
| 423.2325 | 14456.29 | $C_{17}H_{32}N_6O_5Na^+$ | -0.29 | 5 | QAAL c |
| 480.2546 | 4832.96 | $C_{19}H_{35}N_7O_6Na^+$ | 1.03 | 6 | QAALG c |
| 177.0635 | 285218.19 | $C_7H_{10}N_2O_2Na^+$ | 0.48 | 4 | QA a-NH3 |
| 248.1005 | 119002.01 | $C_{10}H_{15}N_3O_3Na^+$ | -0.39 | 5 | QAA a-NH3 |
| 361.1846 | 827740.55 | $C_{16}H_{26}N_4O_4Na^+$ | -0.17 | 6 | QAAL a-NH3 |
| 418.2059 | 670771.72 | $C_{18}H_{29}N_5O_5Na^+$ | -0.36 | 7 | QAALG a-NH3 |
| 531.2899 | 96204.84 | $C_{24}H_{40}N_6O_6Na^+$ | -0.40 | 8 | QAALGL a-NH3 |
| 260.1482 | 9245.52 | $C_{11}H_{19}N_5ONa^+$ | 0.01 | 5 | HK a |
| 347.1801 | 101012.8 | $C_{14}H_{24}N_6O_3Na^+$ | -0.20 | 6 | HKS a |
| 476.2227 | 25134.05 | $C_{19}H_{31}N_7O_6Na^+$ | -0.22 | 8 | HKSE a |
| 575.2918 | 63260.83 | $C_{24}H_{40}N_8O_7Na^+$ | 0.98 | 9 | HKSEV a |
| 646.3296 | 8422.98 | $C_{27}H_{45}N_9O_8Na^+$ | 1.93 | 10 | HKSEVA a |
| 288.1430 | 58162.55 | $C_{12}H_{19}N_5O_2Na^+$ | -0.28 | 6 | HK b |
| 375.1751 | 22219.56 | $C_{15}H_{24}N_6O_4Na^+$ | -0.08 | 7 | HKS b |
| 504.2178 | 15102.82 | $C_{20}H_{31}N_7O_7Na^+$ | 0.10 | 9 | HKSE b |
| 603.2874 | 9395.91 | $C_{25}H_{40}N_8O_8Na^+$ | 2.03 | 10 | HKSEV b |
| 674.3257 | 5551.28 | $C_{28}H_{45}N_9O_9Na^+$ | 3.61 | 11 | HKSEVA b |
| 243.1216 | 16945.09 | $C_{11}H_{16}N_4ONa^+$ | -0.23 | 6 | HK a-NH3 |
| 330.1536 | 168744.97 | $C_{14}H_{21}N_5O_3Na^+$ | -0.03 | 7 | HKS a-NH3 |
| 459.1962 | 36073.28 | $C_{19}H_{28}N_6O_6Na^+$ | -0.17 | 9 | HKSE a-NH3 |
| 558.2648 | 26358.07 | $C_{24}H_{37}N_7O_7Na^+$ | 0.21 | 10 | HKSEV a-NH3 |
| 629.3020 | 10641.29 | $C_{27}H_{42}N_8O_8Na^+$ | 0.42 | 11 | HKSEVA a-NH3 |

**Human transferrin**

| Mass (m/z) | Intensity | Assignment | Deviation (ppm) | DBE | Sequence assignment |
|---|---|---|---|---|---|
| 531.3264 | 29307.12 | $C_{25}H_{44}N_6O_5Na^+$ | -0.29 | 7 | NLKPV a-NH3 |
| 630.3946 | 3680.45 | $C_{30}H_{53}N_7O_6Na^+$ | -0.53 | 8 | NLKPVV a-NH3 |
| 701.4318 | 1684.03 | $C_{33}H_{58}N_8O_7Na^+$ | -0.38 | 9 | NLKPVVA a-NH3 |
| 349.2209 | 204189.6 | $C_{16}H_{30}N_4O_3Na^+$ | -0.21 | 4 | LEK a-NH3 |
| 420.2580 | 48135.49 | $C_{19}H_{35}N_5O_4Na^+$ | -0.27 | 5 | LEKA a-NH3 |
| 519.3258 | 40499.77 | $C_{24}H_{44}N_6O_5Na^+$ | -1.36 | 6 | LEKAV a-NH3 |
| 590.3631 | 1955.09 | $C_{27}H_{49}N_7O_6Na^+$ | -0.91 | 7 | LEKAVA a-NH3 |

**Human fibronectin**

| Mass (m/z) | Intensity | Assignment | Deviation (ppm) | DBE | Sequence assignment |
|---|---|---|---|---|---|
| 233.1008 | 141331.99 | $C_9H_{14}N_4O_2Na^+$ | -0.23 | 5 | TT a |
| 346.1848 | 84358.43 | $C_{15}H_{25}N_5O_3Na^+$ | -0.36 | 6 | TTL a |
| 474.2434 | 13685.6 | $C_{20}H_{33}N_7O_5Na^+$ | -0.26 | 8 | TTLQ a |
| 571.2963 | 12205.61 | $C_{25}H_{40}N_8O_6Na^+$ | -0.08 | 10 | TTLQP a |
| 628.3178 | 7454.45 | $C_{27}H_{43}N_9O_7Na^+$ | -0.01 | 11 | TTLQPG a |
| 216.0743 | 32822.5 | $C_9H_{11}N_3O_2Na^+$ | -0.37 | 6 | TT a-NH3 |
| 329.1585 | 176485.78 | $C_{15}H_{22}N_4O_3Na^+$ | 0.12 | 7 | TTL a-NH3 |
| 457.2168 | 52780.46 | $C_{20}H_{30}N_6O_5Na^+$ | -0.44 | 9 | TTLQ a-NH3 |
| 554.2691 | 19494.24 | $C_{25}H_{37}N_7O_6Na^+$ | -1.16 | 11 | TTLQP a-NH3 |
| 611.2911 | 4651.97 | $C_{27}H_{40}N_8O_7Na^+$ | -0.13 | 12 | TTLQPG a-NH3 |

**Supplementary Table 5.** Assignments of 50 most abundant salt ions in the human serum spectrum assigned by formula search in a human serum peak list with elemental composition within limits: $C_0$, $H_{1\text{-}10}$, $N_{0\text{-}0}$, $O_{0\text{-}10}$, $S_{0\text{-}1}$, $P_{0\text{-}5}$, $Na_{0\text{-}5}$, $Ca_{0\text{-}5}$, $Cl_{0\text{-}5}$

| Mass (m/z) | Deviation (ppm) | DBE | Intensity | Assignment |
|---|---|---|---|---|
| 158.9131 | 0.27 | 1 | 17374.73 | $PO_4HNaCa^+$ |
| 163.9222 | 0.13 | 1.5 | 536719.5 | $PO_4Na_3^+$ |
| 164.9301 | 0.58 | 1 | 35374622 | $PO_4HNa_3^+$ |
| 174.8780 | -0.31 | 1.5 | 15440.77 | $PO_4Ca_2^+$ |
| 175.9461 | 2.19 | 0 | 103526.4 | $PO_6H_3Na_2^+$ |
| 176.8938 | 0.54 | 0.5 | 2173489 | $PO_4H_2Ca_2^+$ |
| 176.9237 | 0.44 | 0 | 119777.9 | $PO_5H_3NaCa^+$ |
| 180.8946 | -2.22 | 1.5 | 234310.8 | $PO_4H_0Na_2Ca^+$ |
| 182.8963 | 1.01 | 1 | 21241.72 | $PO_3Na_3Cl^+$ |
| 182.9108 | 0.81 | 0.5 | 980327.7 | $PO_4H_2Na_2Ca^+$ |
| 186.9121 | 0.81 | 1.5 | 29309137 | $PO_4Na_4^+$ |

| | | | | |
|---|---|---|---|---|
| 186.9172 | 1.21 | 0 | 304754 | $PO_6H_2NaCl^+$ |
| 189.9254 | 2.21 | 1 | 596262.3 | $PO_7HNa_2^+$ |
| 192.8888 | 0.94 | 0.5 | 1822408 | $PO_5H_2Ca_2^+$ |
| 198.9057 | 0.67 | 0.5 | 11958186 | $PO_5H_2Na_2Ca^+$ |
| 204.9226 | 0.42 | 0.5 | 17347588 | $PO_5H_2Na_4^+$ |
| 212.9149 | 0.71 | 1 | 4008325 | $PO_7HNa_3^+$ |
| 214.8706 | 0.17 | 1 | 61294.92 | $PO_5HNaCa_2^+$ |
| 216.8862 | -0.06 | 0 | 40272.44 | $PO_5H_3NaCa_2^+$ |
| 220.8874 | -0.50 | 1 | 516552.2 | $PO_5HNa_3Ca^+$ |
| 220.909 | -0.83 | 0.5 | 252973 | $P_2O_4H_3Na_4^+$ |
| 222.9031 | -0.27 | 0 | 230107.3 | $PO_5H_3Na_3Ca^+$ |
| 226.8857 | -0.31 | 2 | 109877.6 | $P_2O_6Na_3^+$ |
| 226.9044 | -0.25 | 1 | 380279.4 | $PO_5HNa_5^+$ |
| 228.9097 | 0.16 | 1 | 7492826 | $PO_8HNa_3^+$ |
| 230.9254 | 0.37 | 0 | 138934.4 | $PO_8H_3Na_3^+$ |
| 232.8811 | -0.12 | 0 | 830770.7 | $PO_6H_3NaCa_2^+$ |
| 234.8967 | 0.03 | 1.5 | 596586.5 | $PO_7Na_4^+$ |
| 238.8980 | -0.31 | 0 | 16007352 | $PO_6H_3Na_3Ca^+$ |
| 244.8705 | -0.28 | 1 | 1862251 | $PO_4Na_5Cl^+$ |
| 246.9202 | -0.12 | 0 | 13063913 | $PO_9H_3Na_3^+$ |
| 250.8833 | -0.26 | 1.5 | 93334.51 | $P_2O_6HNa_4^+$ |
| 250.8916 | -0.03 | 1.5 | 6897698 | $PO_8Na_4^+$ |
| 254.8845 | -0.97 | 0 | 112185.8 | $P_2O_5H_4Na_3Ca^+$ |
| 256.8641 | -0.34 | 0 | 6850488 | $PO_5H_2Na_3CaCl^+$ |
| 260.8800 | -0.07 | 0.5 | 1884970 | $PO_6H_2Na_4Ca^+$ |
| 263.8933 | 0.94 | 0 | 2484055 | $PO_9H_3Na_2Ca^+$ |
| 268.8723 | 0.17 | 1 | 1131889 | $PO_8HNa_3Ca^+$ |
| 276.8665 | -0.69 | 0.5 | 72838.71 | $P_2O_5H_3Na_4Ca^+$ |
| 286.8683 | 0.05 | 0.5 | 870317.9 | $PO_8HNa_4Cl^+$ |
| 288.8601 | -0.43 | 2 | 3335399 | $P_2O_7Na_5^+$ |
| 288.8653 | 0.18 | 0.5 | 112453 | $P_2O_9H_2Na_2Cl^+$ |
| 300.8538 | -0.14 | 1 | 1234999 | $P_2O_8H_2Na_3Ca^+$ |
| 318.8345 | 0.04 | 0.5 | 18006.9 | $P_2O_8H_3Na_2Ca_2^+$ |
| 318.8644 | -0.02 | 0 | 3033530 | $P_2O_9H_4Na_3Ca^+$ |
| 324.8812 | -0.47 | 0 | 46885.75 | $P_2O_9H_4Na_5^+$ |
| 374.8218 | 2.03 | 1 | 1826292 | $PO_6HNa_9Ca^+$ |
| 392.8324 | 2.03 | 0 | 2504059 | $PO_7H_3Na_9Ca^+$ |
| 396.8037 | 1.81 | 1.5 | 97944.77 | $PO_6Ca^+$ |

**Supplementary Table 6:** Output from SIMSMFP on carbonaceous ions ($C_nH_{<1}^-$) found in negative ion depth profile datasets from different engine deposits. a. injector tip 1, b. injector tip 2, c. injector needle 1

**a)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C |
|---|---|---|---|---|---|
| 84.0003 | -2.963075876 | 8 | 6612870.74 | 0 | 7 |
| 96.0004 | -1.551032798 | 9 | 220073965.8 | 0 | 8 |
| 97.0083 | -0.761789906 | 8.5 | 47997971.37 | 1 | 8 |
| 108.0005 | -0.452775477 | 10 | 84130360.44 | 0 | 9 |
| 109.0084 | 0.239431147 | 9.5 | 4132749.92 | 1 | 9 |
| 120.0005 | -0.407498136 | 11 | 78048155.01 | 0 | 10 |
| 121.0083 | -0.610701537 | 10.5 | 79168732.6 | 1 | 10 |
| 132.0005 | -0.370453005 | 12 | 30397142.14 | 0 | 11 |
| 133.0086 | 1.699892972 | 11.5 | 12830317.97 | 1 | 11 |
| 144.0004 | -1.034023836 | 13 | 152560782.5 | 0 | 12 |
| 145.0084 | 0.179989605 | 12.5 | 80177698.65 | 1 | 12 |
| 156.0005 | -0.313460436 | 14 | 25463202.22 | 0 | 13 |
| 157.0085 | 0.803141876 | 13.5 | 9373906.88 | 1 | 13 |
| 168.0005 | -0.291070478 | 15 | 10157390.85 | 0 | 14 |
| 169.0085 | 0.746116876 | 14.5 | 41521754.62 | 1 | 14 |
| 180.0005 | -0.271665838 | 16 | 2368939.23 | 0 | 15 |
| 181.0087 | 1.801574109 | 15.5 | 62770085.39 | 1 | 15 |
| 192.0005 | -0.254686772 | 17 | 3750276.95 | 0 | 16 |
| 193.0084 | 0.135227293 | 16.5 | 17708528.08 | 1 | 16 |
| 204.0005 | -0.239705238 | 18 | 12599560.26 | 0 | 17 |
| 205.0087 | 1.590666731 | 17.5 | 6013949.93 | 1 | 17 |
| 216.0005 | -0.226388314 | 19 | 1353836.11 | 0 | 18 |
| 217.0085 | 0.581083567 | 18.5 | 1720664.31 | 1 | 18 |
| 228.0006 | 0.224122267 | 20 | 2420252.62 | 0 | 19 |
| 229.0087 | 1.423965397 | 19.5 | 257766.72 | 1 | 19 |
| 240.0007 | 0.629581893 | 21 | 409189.44 | 0 | 20 |
| 241.0086 | 0.938141677 | 20.5 | 268580.7 | 1 | 20 |
| 252.0008 | 0.996426401 | 22 | 3238500.34 | 0 | 21 |
| 264.0009 | 1.329921477 | 23 | 202807.35 | 0 | 22 |
| 276.0007 | 0.547462679 | 24 | 657326.69 | 0 | 23 |
| 300.0006 | 0.170333022 | 26 | 462346.94 | 0 | 25 |
| 312.0008 | 0.804806276 | 27 | 54765.17 | 0 | 26 |
| 324.0006 | 0.157715782 | 28 | 110204.74 | 0 | 27 |
| 348.0007 | 0.434194717 | 30 | 74614.78 | 0 | 29 |

**b)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C |
|---|---|---|---|---|---|
| 84.0003 | -2.963075876 | 8 | 233008645 | 0 | 7 |
| 96.0004 | -1.551032798 | 9 | 1577618743 | 0 | 8 |
| 97.0082 | -1.792628749 | 8.5 | 566131085.7 | 1 | 8 |

| | | | | | |
|---|---|---|---|---|---|
| 108.0005 | -0.452775477 | 10 | 423487212.1 | 0 | 9 |
| 109.0083 | -0.677929569 | 9.5 | 71678193.06 | 1 | 9 |
| 120.0005 | -0.407498136 | 11 | 343602244.3 | 0 | 10 |
| 121.0083 | -0.610701537 | 10.5 | 399600885 | 1 | 10 |
| 132.0004 | -1.128025612 | 12 | 137607509.1 | 0 | 11 |
| 133.0083 | -0.555604116 | 11.5 | 45786573.46 | 1 | 11 |
| 144.0004 | -1.034023836 | 13 | 428616341.1 | 0 | 12 |
| 145.0082 | -1.199241088 | 12.5 | 245485284.7 | 1 | 12 |
| 156.0004 | -0.954483821 | 14 | 90655083.09 | 0 | 13 |
| 157.0082 | -1.107584237 | 13.5 | 21511039.46 | 1 | 13 |
| 168.0004 | -0.886306628 | 15 | 45016093.82 | 0 | 14 |
| 169.0082 | -1.028943099 | 14.5 | 91134843.84 | 1 | 14 |
| 180.0004 | -0.8272197 | 16 | 14954606.88 | 0 | 15 |
| 181.0083 | -0.408268405 | 15.5 | 11988359.59 | 1 | 15 |
| 192.0004 | -0.775518616 | 17 | 18492551.57 | 0 | 16 |
| 193.0082 | -0.900997177 | 16.5 | 43210306.29 | 1 | 16 |
| 204.0003 | -1.220094756 | 18 | 35551840.38 | 0 | 17 |
| 205.0082 | -0.848258033 | 17.5 | 4315434.88 | 1 | 17 |
| 216.0003 | -1.152311887 | 19 | 12037073.81 | 0 | 18 |
| 217.0082 | -0.801351565 | 18.5 | 7850087.8 | 1 | 18 |
| 228.0004 | -0.653068603 | 20 | 12510637.33 | 0 | 19 |
| 229.0082 | -0.759360879 | 19.5 | 1970917.51 | 1 | 19 |
| 240.0005 | -0.203749534 | 21 | 4900414.46 | 0 | 20 |
| 241.0083 | -0.30662835 | 20.5 | 2772360.22 | 1 | 20 |
| 252.0005 | -0.194047196 | 22 | 12129226.89 | 0 | 21 |
| 253.0084 | 0.103158641 | 21.5 | 658870.99 | 1 | 21 |
| 264.0005 | -0.185226888 | 23 | 2528673.91 | 0 | 22 |
| 265.0085 | 0.47583402 | 22.5 | 214436.82 | 1 | 22 |
| 276.0004 | -0.539491681 | 24 | 4555222.04 | 0 | 23 |
| 277.0083 | -0.266778939 | 23.5 | 247192.07 | 1 | 23 |
| 288.0005 | -0.169791343 | 25 | 388118.88 | 0 | 24 |
| 289.0084 | 0.090308802 | 24.5 | 19991.96 | 1 | 24 |
| 300.0004 | -0.496332425 | 26 | 3071755.38 | 0 | 25 |
| 301.0083 | -0.24550812 | 25.5 | 44661.78 | 1 | 25 |
| 312.0005 | -0.156730494 | 27 | 76152.22 | 0 | 26 |
| 324.0003 | -0.768208575 | 28 | 603586.75 | 0 | 27 |
| 325.0082 | -0.535063137 | 27.5 | 16584.61 | 1 | 27 |
| 336.0005 | -0.145535477 | 29 | 15204.51 | 0 | 28 |
| 348.0003 | -0.715228757 | 30 | 233488.43 | 0 | 29 |
| 349.0089 | 1.507413688 | 29.5 | 8312.38 | 1 | 29 |
| 372.0001 | -1.20671865 | 32 | 24876.07 | 0 | 31 |
| 373.0078 | -1.538571357 | 31.5 | 9411.76 | 1 | 31 |
| 396.0001 | -1.133584287 | 34 | 11083.39 | 0 | 33 |
| 397.0084 | 0.065741686 | 33.5 | 5663.28 | 1 | 33 |
| 421.0089 | 1.24961885 | 35.5 | 9737.02 | 1 | 35 |
| 816 | -0.672671116 | 69 | 6518.44 | 0 | 68 |

| | | | | | |
|---|---|---|---|---|---|
| 911.9995 | -1.150108957 | 77 | 6587.79 | 0 | 76 |
| 935.9997 | -0.906943913 | 79 | 6150.25 | 0 | 78 |
| 1032 | -0.144282869 | 87 | 6210.61 | 0 | 86 |

**c)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C |
|---|---|---|---|---|---|
| 84.0003 | -2.96308 | 8 | 220744.68 | 0 | 7 |
| 85.0082 | -2.04568 | 7.5 | 88965.29 | 1 | 7 |
| 96.0005 | -0.50937 | 9 | 2081249.49 | 0 | 8 |
| 97.0084 | 0.269049 | 8.5 | 2095862.24 | 1 | 8 |
| 108.0006 | 0.473146 | 10 | 427641.02 | 0 | 9 |
| 109.0085 | 1.156792 | 9.5 | 197975.13 | 1 | 9 |
| 120.0005 | -0.4075 | 11 | 231114.71 | 0 | 10 |
| 121.0084 | 0.215688 | 10.5 | 666231.3 | 1 | 10 |
| 132.0006 | 0.38712 | 12 | 51597.92 | 0 | 11 |
| 133.0085 | 0.948061 | 11.5 | 69689.98 | 1 | 11 |
| 144.0005 | -0.33958 | 13 | 148719.99 | 0 | 12 |
| 145.0084 | 0.17999 | 12.5 | 166873.93 | 1 | 12 |
| 156.0005 | -0.31346 | 14 | 11353.74 | 0 | 13 |
| 157.0085 | 0.803142 | 13.5 | 17278.84 | 1 | 13 |
| 168.0006 | 0.304166 | 15 | 4698.32 | 0 | 14 |
| 169.0086 | 1.337804 | 14.5 | 43480.13 | 1 | 14 |
| 181.0088 | 2.354035 | 15.5 | 25599.2 | 1 | 15 |
| 193.0086 | 1.171452 | 16.5 | 12505.87 | 1 | 16 |
| 205.0087 | 1.590667 | 17.5 | 6963.24 | 1 | 17 |

**Supplementary Table 7:** Output from SIMSMFP on all species containing two oxygen atoms ($C_nH_nO_2^-$) found in negative ion depth profile datasets from different engine deposits. a. injector tip 1, b. injector tip 2, c. injector needle 1.

**a)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O |
|---|---|---|---|---|---|---|
| 85.0293 | -2.397991175 | 2.5 | 1370786.86 | 5 | 4 | 2 |
| 87.045 | -1.768047882 | 1.5 | 113545.11 | 7 | 4 | 2 |
| 92.9981 | -1.117225878 | 5.5 | 344621.86 | 1 | 5 | 2 |
| 95.0138 | -0.567285693 | 4.5 | 9766088.82 | 3 | 5 | 2 |
| 97.0295 | -0.04019396 | 3.5 | 4687395.61 | 5 | 5 | 2 |
| 99.0451 | -0.544196237 | 2.5 | 915249.95 | 7 | 5 | 2 |
| 101.0608 | -0.038590629 | 1.5 | 557410.88 | 9 | 5 | 2 |
| 106.0061 | 0.670716569 | 6 | 66532.37 | 2 | 6 | 2 |
| 107.0139 | 0.430785345 | 5.5 | 2497676.93 | 3 | 6 | 2 |
| 108.0217 | 0.195331161 | 5 | 17538290.93 | 4 | 6 | 2 |
| 109.0296 | 0.881412797 | 4.5 | 34608272.52 | 5 | 6 | 2 |
| 111.0452 | 0.415146437 | 3.5 | 5720464.39 | 7 | 6 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 113.0609 | 0.849985111 | 2.5 | 393019.77 | 9 | 6 | 2 |
| 115.0765 | 0.400603238 | 1.5 | 128886.08 | 11 | 6 | 2 |
| 119.0139 | 0.387349863 | 6.5 | 9266409.52 | 3 | 7 | 2 |
| 120.0217 | 0.175801573 | 6 | 192608.51 | 4 | 7 | 2 |
| 121.0295 | -0.032223548 | 5.5 | 91263656.71 | 5 | 7 | 2 |
| 122.0374 | 0.582608622 | 5 | 11642479.93 | 6 | 7 | 2 |
| 123.0452 | 0.374659209 | 4.5 | 26783866.46 | 7 | 7 | 2 |
| 125.0608 | -0.031184831 | 3.5 | 2146662.77 | 9 | 7 | 2 |
| 127.0765 | 0.362773737 | 2.5 | 245015.27 | 11 | 7 | 2 |
| 129.0921 | -0.030210988 | 1.5 | 128085.53 | 13 | 7 | 2 |
| 131.0139 | 0.351871185 | 7.5 | 698269.57 | 3 | 8 | 2 |
| 132.0217 | 0.159822237 | 7 | 3597370.41 | 4 | 8 | 2 |
| 133.0295 | -0.029316805 | 6.5 | 26633213.8 | 5 | 8 | 2 |
| 134.0374 | 0.530449246 | 6 | 2325149.15 | 6 | 8 | 2 |
| 135.0452 | 0.341367303 | 5.5 | 53350172.68 | 7 | 8 | 2 |
| 136.053 | 0.155086644 | 5 | 1194002.74 | 8 | 8 | 2 |
| 137.0608 | -0.028454525 | 4.5 | 8268800.02 | 9 | 8 | 2 |
| 139.0765 | 0.331472357 | 3.5 | 508869.49 | 11 | 8 | 2 |
| 141.0921 | -0.027641519 | 2.5 | 345456.94 | 13 | 8 | 2 |
| 143.0138 | -0.376886564 | 8.5 | 690911.49 | 3 | 9 | 2 |
| 143.1077 | -0.37663927 | 1.5 | 187329.08 | 15 | 8 | 2 |
| 144.0217 | 0.146505722 | 8 | 103408.16 | 4 | 9 | 2 |
| 145.0295 | -0.02689108 | 7.5 | 66960312.63 | 5 | 9 | 2 |
| 146.0373 | -0.197894608 | 7 | 2886402.26 | 6 | 9 | 2 |
| 147.0452 | 0.313509142 | 6.5 | 38229562.84 | 7 | 9 | 2 |
| 148.053 | 0.142516551 | 6 | 583201.08 | 8 | 9 | 2 |
| 149.0608 | -0.02616382 | 5.5 | 18190842.79 | 9 | 9 | 2 |
| 150.0686 | -0.192578557 | 5 | 51051.78 | 10 | 9 | 2 |
| 151.0764 | -0.356773002 | 4.5 | 1507044.97 | 11 | 9 | 2 |
| 153.0921 | -0.025474861 | 3.5 | 123122.68 | 13 | 9 | 2 |
| 155.0139 | 0.297392774 | 9.5 | 70235.07 | 3 | 10 | 2 |
| 155.1078 | 0.297212737 | 2.5 | 227709.1 | 15 | 9 | 2 |
| 156.0217 | 0.135237617 | 9 | 292229.67 | 4 | 10 | 2 |
| 157.0295 | -0.024836097 | 8.5 | 5363201.25 | 5 | 10 | 2 |
| 157.1234 | -0.024821255 | 1.5 | 102641.27 | 17 | 9 | 2 |
| 158.0373 | -0.182868188 | 8 | 14616324.53 | 6 | 10 | 2 |
| 159.0451 | -0.338897469 | 7.5 | 67934079.9 | 7 | 10 | 2 |
| 160.053 | 0.131831348 | 7 | 841279.15 | 8 | 10 | 2 |
| 161.0608 | -0.024214458 | 6.5 | 16069563.51 | 9 | 10 | 2 |
| 162.0687 | 0.438703039 | 6 | 69756.26 | 10 | 10 | 2 |
| 163.0765 | 0.282689492 | 5.5 | 4319741.06 | 11 | 10 | 2 |
| 165.0921 | -0.023623177 | 4.5 | 374114.11 | 13 | 10 | 2 |
| 167.0139 | 0.276025006 | 10.5 | 51033.91 | 3 | 11 | 2 |
| 167.1079 | 0.874286181 | 3.5 | 63447.8 | 15 | 10 | 2 |
| 168.0218 | 0.720740328 | 10 | 52137.72 | 4 | 11 | 2 |
| 169.0295 | -0.023072895 | 9.5 | 14368242.29 | 5 | 11 | 2 |

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|---|---|---|---|---|---|---|
| 169.1235 | 0.568224136 | 2.5 | 70100.72 | 17 | 10 | 2 |
| 170.0374 | 0.418143477 | 9 | 673414.04 | 6 | 11 | 2 |
| 171.0452 | 0.269519474 | 8.5 | 36042795.12 | 7 | 11 | 2 |
| 171.1391 | 0.269371595 | 1.5 | 86044.63 | 19 | 10 | 2 |
| 172.053 | 0.122636644 | 8 | 6038646.1 | 8 | 11 | 2 |
| 173.0608 | -0.022535432 | 7.5 | 32364607.72 | 9 | 11 | 2 |
| 174.0687 | 0.408459585 | 7 | 110152.31 | 10 | 11 | 2 |
| 175.0765 | 0.263313535 | 6.5 | 6766009.57 | 11 | 11 | 2 |
| 177.0921 | -0.022022439 | 5.5 | 831946.41 | 13 | 11 | 2 |
| 179.1078 | 0.257386958 | 4.5 | 86495.8 | 15 | 11 | 2 |
| 180.0218 | 0.672696759 | 11 | 53101.4 | 4 | 12 | 2 |
| 181.0296 | 0.530852695 | 10.5 | 783907.56 | 5 | 12 | 2 |
| 181.1236 | 1.082687249 | 3.5 | 58836.73 | 17 | 11 | 2 |
| 182.0374 | 0.390579231 | 10 | 10125092.38 | 6 | 12 | 2 |
| 183.0452 | 0.251850426 | 9.5 | 23542331.2 | 7 | 12 | 2 |
| 183.1391 | 0.251721296 | 2.5 | 61896.11 | 19 | 11 | 2 |
| 184.053 | 0.114640904 | 9 | 2104816.94 | 8 | 12 | 2 |
| 185.0608 | -0.021074155 | 8.5 | 27829054.48 | 9 | 12 | 2 |
| 186.0687 | 0.382117074 | 8 | 713322.75 | 10 | 12 | 2 |
| 187.0765 | 0.246423315 | 7.5 | 9680661.89 | 11 | 12 | 2 |
| 189.0922 | 0.508217942 | 6.5 | 1388969.73 | 13 | 12 | 2 |
| 191.1079 | 0.764490174 | 5.5 | 173384.08 | 15 | 12 | 2 |
| 193.0296 | 0.497851354 | 11.5 | 2033022.41 | 5 | 13 | 2 |
| 194.0374 | 0.366424339 | 11 | 144953.03 | 6 | 13 | 2 |
| 195.0452 | 0.236355526 | 10.5 | 35123799.92 | 7 | 13 | 2 |
| 196.053 | 0.10762397 | 10 | 5062305.47 | 8 | 13 | 2 |
| 197.0609 | 0.487666741 | 9.5 | 23947939.87 | 9 | 13 | 2 |
| 197.1547 | -0.01978142 | 2.5 | 55766.83 | 21 | 12 | 2 |
| 198.0687 | 0.358966487 | 9 | 603286.59 | 10 | 13 | 2 |
| 199.0765 | 0.231569325 | 8.5 | 11645711.12 | 11 | 13 | 2 |
| 199.1704 | 0.23146015 | 1.5 | 201411.21 | 23 | 12 | 2 |
| 200.0843 | 0.105455562 | 8 | 104307.92 | 12 | 13 | 2 |
| 200.9986 | 1.970664376 | 14.5 | 4144506.24 | 1 | 14 | 2 |
| 201.0922 | 0.47789047 | 7.5 | 1941899.94 | 13 | 13 | 2 |
| 203.1079 | 0.719322612 | 6.5 | 249008.21 | 15 | 13 | 2 |
| 205.0298 | 1.444182395 | 12.5 | 372502.28 | 5 | 14 | 2 |
| 205.1235 | 0.468498466 | 5.5 | 75703.69 | 17 | 13 | 2 |
| 206.0374 | 0.345083099 | 12 | 808583.65 | 6 | 14 | 2 |
| 207.0453 | 0.705643176 | 11.5 | 5424227.8 | 7 | 14 | 2 |
| 208.0531 | 0.582063283 | 11 | 7496205.51 | 8 | 14 | 2 |
| 209.0609 | 0.45967488 | 10.5 | 36149233.92 | 9 | 14 | 2 |
| 210.0688 | 0.814495724 | 10 | 1144842.82 | 10 | 14 | 2 |
| 211.0766 | 0.692166262 | 9.5 | 12943201.22 | 11 | 14 | 2 |
| 211.9908 | 1.986410903 | 16 | 180827.36 | 0 | 15 | 2 |
| 212.0844 | 0.570999419 | 9 | 114943.38 | 12 | 14 | 2 |
| 213.0923 | 0.920259345 | 8.5 | 3224798.66 | 13 | 14 | 2 |

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|---|---|---|---|---|---|---|
| 213.1862 | 0.919854007 | 1.5 | 150912.62 | 25 | 13 | 2 |
| 215.1079 | 0.679194484 | 7.5 | 384361.48 | 15 | 14 | 2 |
| 217.0298 | 1.364330631 | 13.5 | 619337.83 | 5 | 15 | 2 |
| 217.1235 | 0.442605441 | 6.5 | 100676 | 17 | 14 | 2 |
| 219.0453 | 0.666985767 | 12.5 | 11856452.61 | 7 | 15 | 2 |
| 220.0531 | 0.550322021 | 12 | 1095059.26 | 8 | 15 | 2 |
| 221.0609 | 0.434722023 | 11.5 | 19126275.94 | 9 | 15 | 2 |
| 222.0688 | 0.770482534 | 11 | 3674850.47 | 10 | 15 | 2 |
| 223.0766 | 0.654932412 | 10.5 | 18604856.98 | 11 | 15 | 2 |
| 224.0844 | 0.540421669 | 10 | 189793.4 | 12 | 15 | 2 |
| 225.0923 | 0.87119893 | 9.5 | 4348558.36 | 13 | 15 | 2 |
| 226.0998 | -0.570101904 | 9 | 55326.29 | 14 | 15 | 2 |
| 227.1079 | 0.643306965 | 8.5 | 693649.79 | 15 | 15 | 2 |
| 227.2019 | 1.083178735 | 1.5 | 600449.28 | 27 | 14 | 2 |
| 229.1236 | 0.855870665 | 7.5 | 86977.52 | 17 | 15 | 2 |
| 230.0376 | 1.178504381 | 14 | 87711.84 | 6 | 16 | 2 |
| 231.0455 | 1.497975587 | 13.5 | 1029999.59 | 7 | 16 | 2 |
| 232.0532 | 0.952799662 | 13 | 7158741.86 | 8 | 16 | 2 |
| 233.061 | 0.841411326 | 12.5 | 15655435.8 | 9 | 16 | 2 |
| 234.0689 | 1.158207323 | 12 | 1310555.21 | 10 | 16 | 2 |
| 235.0767 | 1.046893451 | 11.5 | 15885080.07 | 11 | 16 | 2 |
| 236.0845 | 0.936529959 | 11 | 560575.64 | 12 | 16 | 2 |
| 237.0923 | 0.827104727 | 10.5 | 5782637.63 | 13 | 16 | 2 |
| 238.0065 | 1.979361624 | 17 | 115434.36 | 2 | 17 | 2 |
| 239.108 | 1.029243075 | 9.5 | 906362.57 | 15 | 16 | 2 |
| 241.1237 | 1.228001908 | 8.5 | 138032.18 | 17 | 16 | 2 |
| 241.2176 | 1.227523877 | 1.5 | 758434.11 | 29 | 15 | 2 |
| 243.0456 | 1.835461406 | 14.5 | 3920649.03 | 7 | 17 | 2 |
| 244.0534 | 1.725445032 | 14 | 161794.79 | 8 | 17 | 2 |
| 245.0611 | 1.208271561 | 13.5 | 16839310.86 | 9 | 17 | 2 |
| 246.0689 | 1.101725162 | 13 | 4026534.08 | 10 | 17 | 2 |
| 247.0768 | 1.400780991 | 12.5 | 12615759.47 | 11 | 17 | 2 |
| 248.0845 | 0.891229388 | 12 | 508334.1 | 12 | 17 | 2 |
| 249.0924 | 1.188716926 | 11.5 | 6605464.18 | 13 | 17 | 2 |
| 250.1001 | 0.684126544 | 11 | 94738.28 | 14 | 17 | 2 |
| 251.1081 | 1.378292763 | 10.5 | 1044726.48 | 15 | 17 | 2 |
| 253.1238 | 1.564849373 | 9.5 | 164502.19 | 17 | 17 | 2 |
| 253.2177 | 1.564269084 | 2.5 | 212453.93 | 29 | 16 | 2 |
| 255.2333 | 1.356016121 | 1.5 | 21770341.06 | 31 | 16 | 2 |
| 256.0533 | 1.254037353 | 15 | 1482357.34 | 8 | 18 | 2 |
| 257.0613 | 1.929893599 | 14.5 | 5213393.92 | 9 | 18 | 2 |
| 258.069 | 1.437989583 | 14 | 2298345.42 | 10 | 18 | 2 |
| 259.0769 | 1.721885541 | 13.5 | 16964829.89 | 11 | 18 | 2 |
| 260.0846 | 1.234599805 | 13 | 859755.17 | 12 | 18 | 2 |
| 261.0925 | 1.517089158 | 12.5 | 5998090.21 | 13 | 18 | 2 |
| 262.1 | 0.271270581 | 12 | 124828.65 | 14 | 18 | 2 |

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|---|---|---|---|---|---|---|
| 263.1082 | 1.695503053 | 11.5 | 1519784.63 | 15 | 18 | 2 |
| 265.1239 | 1.871204098 | 10.5 | 223410.71 | 17 | 18 | 2 |
| 267.1395 | 1.669916822 | 9.5 | 64100.35 | 19 | 18 | 2 |
| 267.2334 | 1.669330049 | 2.5 | 53403.26 | 31 | 17 | 2 |
| 269.0613 | 1.843821147 | 15.5 | 8139332.96 | 9 | 19 | 2 |
| 269.2491 | 1.842535088 | 1.5 | 899511.9 | 33 | 17 | 2 |
| 270.069 | 1.374095175 | 15 | 1249119.48 | 10 | 19 | 2 |
| 272.0847 | 1.547682217 | 14 | 1254604.73 | 12 | 19 | 2 |
| 273.0926 | 1.816603237 | 13.5 | 7665320.29 | 13 | 19 | 2 |
| 274.1002 | 0.989055346 | 13 | 184187.79 | 14 | 19 | 2 |
| 275.1083 | 1.985040379 | 12.5 | 1515748.03 | 15 | 19 | 2 |
| 276.1155 | -0.285749903 | 12 | 51648.78 | 16 | 19 | 2 |
| 277.1237 | 1.06847706 | 11.5 | 263204.79 | 17 | 19 | 2 |
| 278.0377 | 1.334712865 | 18 | 81826.58 | 6 | 20 | 2 |
| 279.0457 | 1.957030941 | 17.5 | 1117703.37 | 7 | 20 | 2 |
| 279.1395 | 1.598128222 | 10.5 | 66130.92 | 19 | 19 | 2 |
| 279.2333 | 1.239466887 | 3.5 | 55781.5 | 31 | 18 | 2 |
| 280.0531 | 0.432418182 | 17 | 304538.02 | 8 | 20 | 2 |
| 281.0612 | 1.40930359 | 16.5 | 1231788.19 | 9 | 20 | 2 |
| 281.2489 | 1.052805226 | 2.5 | 802435.68 | 33 | 18 | 2 |
| 282.0689 | 0.961113616 | 16 | 2302779.69 | 10 | 20 | 2 |
| 283.0768 | 1.222637896 | 15.5 | 8351641.21 | 11 | 20 | 2 |
| 283.2646 | 1.221827305 | 1.5 | 29122657.2 | 35 | 18 | 2 |
| 283.9908 | 1.482796712 | 22 | 57618.58 | 0 | 21 | 2 |
| 284.0843 | 0.074273733 | 15 | 770373.76 | 12 | 20 | 2 |
| 285.0925 | 1.389375555 | 14.5 | 6146068.35 | 13 | 20 | 2 |
| 286.0066 | 1.996811054 | 21 | 112882.36 | 2 | 21 | 2 |
| 286.1 | 0.248514567 | 14 | 272042.35 | 14 | 20 | 2 |
| 287.1082 | 1.553772038 | 13.5 | 2082705.7 | 15 | 20 | 2 |
| 288.1155 | -0.273848434 | 13 | 58526.27 | 16 | 20 | 2 |
| 289.1239 | 1.715876312 | 12.5 | 334408.59 | 17 | 20 | 2 |
| 292.0524 | -1.982174612 | 18 | 222160.71 | 8 | 21 | 2 |
| 293.0613 | 1.692822764 | 17.5 | 2847064.56 | 9 | 21 | 2 |
| 294.0684 | -0.778389728 | 17 | 586418.83 | 10 | 21 | 2 |
| 295.0766 | 0.495125918 | 16.5 | 5218706.18 | 11 | 21 | 2 |
| 296.0843 | 0.071263493 | 16 | 1657166.45 | 12 | 21 | 2 |
| 296.9986 | 1.333678099 | 22.5 | 57881.28 | 1 | 22 | 2 |
| 297.0923 | 0.660064665 | 15.5 | 5123522.01 | 13 | 21 | 2 |
| 297.2799 | -0.013118949 | 1.5 | 70865.68 | 37 | 19 | 2 |
| 298.0065 | 1.580840501 | 22 | 79466.47 | 2 | 22 | 2 |
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| 301.1237 | 0.98331779 | 13.5 | 406744.62 | 17 | 21 | 2 |
| 301.2175 | 0.651025016 | 6.5 | 217653.22 | 29 | 20 | 2 |
| 302.0377 | 1.228656078 | 20 | 87640.55 | 6 | 22 | 2 |
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| 303.1395 | 1.471601875 | 12.5 | 98492.24 | 19 | 21 | 2 |
| 304.053 | 0.069395801 | 19 | 123798.29 | 8 | 22 | 2 |
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| 308.0841 | -0.580685261 | 17 | 903819.46 | 12 | 22 | 2 |
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| 310.0066 | 1.842222237 | 23 | 63516.81 | 2 | 23 | 2 |
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| 311.2958 | 0.790567025 | 1.5 | 1199608 | 39 | 20 | 2 |
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| 325.1235 | 0.295580075 | 15.5 | 445106.76 | 17 | 23 | 2 |
| 325.3114 | 0.602807397 | 1.5 | 101872.39 | 41 | 21 | 2 |
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| 338.0378 | 1.393633069 | 23 | 103406.21 | 6 | 25 | 2 |
| 339.0455 | 1.020807984 | 22.5 | 1182262.92 | 7 | 25 | 2 |
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| 358.0995 | -1.197710375 | 20 | 387054.96 | 14 | 26 | 2 |
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| 365.0611 | 0.811097759 | 23.5 | 370601.78 | 9 | 27 | 2 |
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| 386.0378 | 1.220348305 | 27 | 49762.55 | 6 | 29 | 2 |
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| 389.1552 | 1.274814348 | 18.5 | 51770.81 | 21 | 28 | 2 |
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| 391.0769 | 1.140697671 | 24.5 | 279578.37 | 11 | 29 | 2 |
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| 400.053 | 0.052743014 | 27 | 59292.4 | 8 | 30 | 2 |
| 401.0613 | 1.236969545 | 26.5 | 118873.48 | 9 | 30 | 2 |
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| 422.1315 | 0.642217352 | 23 | 96127.51 | 18 | 31 | 2 |
| 423.1393 | 0.581605498 | 22.5 | 99249.64 | 19 | 31 | 2 |
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| 426.0688 | 0.401578498 | 28 | 58625.35 | 10 | 32 | 2 |
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| 430.0996 | -0.764706009 | 26 | 152557.51 | 14 | 32 | 2 |
| 431.1079 | 0.338894392 | 25.5 | 214853.35 | 15 | 32 | 2 |
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| 438.0688 | 0.390578071 | 29 | 58837.24 | 10 | 33 | 2 |
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| 441.0929 | 1.804838475 | 27.5 | 130792.61 | 13 | 33 | 2 |
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| 459.1395 | 0.971601079 | 25.5 | 71370.66 | 19 | 34 | 2 |
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| 465.4678 | 0.206459007 | 1.5 | 306080.4 | 61 | 31 | 2 |
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| 467.1083 | 1.169109259 | 28.5 | 102548.4 | 15 | 35 | 2 |
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| 469.1237 | 0.631177207 | 27.5 | 109584.03 | 17 | 35 | 2 |
| 470.1317 | 1.00206064 | 27 | 88303.12 | 18 | 35 | 2 |
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| 477.093 | 1.87825368 | 30.5 | 57377.97 | 13 | 36 | 2 |
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| 479.4835 | 0.304702966 | 1.5 | 357146.62 | 63 | 32 | 2 |
| 480.1157 | 0.252230932 | 29 | 63950.21 | 16 | 36 | 2 |
| 481.1243 | 1.862515922 | 28.5 | 90211.99 | 17 | 36 | 2 |
| 482.1313 | 0.147470223 | 28 | 85373.84 | 18 | 36 | 2 |
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| 502.1004 | 0.938259444 | 32 | 55442 | 14 | 38 | 2 |
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| 518.1321 | 1.681234312 | 31 | 77025.92 | 18 | 39 | 2 |
| 520.1471 | 0.425072242 | 30 | 52639.3 | 20 | 39 | 2 |
| 521.5304 | 0.184265419 | 1.5 | 290001.02 | 69 | 35 | 2 |
| 526.1 | 0.135145428 | 34 | 60869.73 | 14 | 40 | 2 |
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| 532.1475 | 1.167158964 | 31 | 50981.2 | 20 | 40 | 2 |
| 535.5461 | 0.272805721 | 1.5 | 321750.18 | 71 | 36 | 2 |
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| 554.132 | 1.391547633 | 34 | 71158.26 | 18 | 42 | 2 |
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| 566.1319 | 1.185414204 | 35 | 76083.3 | 18 | 43 | 2 |
| 576.1167 | 1.945963694 | 37 | 73981.72 | 16 | 44 | 2 |
| 577.5932 | 0.512644802 | 1.5 | 170402.93 | 77 | 39 | 2 |
| 590.1314 | 0.289935512 | 37 | 57637.58 | 18 | 45 | 2 |
| 591.6089 | 0.585015206 | 1.5 | 190141.92 | 79 | 40 | 2 |
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| 602.132 | 1.28061785 | 38 | 74153.56 | 18 | 46 | 2 |
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| 605.0615 | 1.150462888 | 43.5 | 66227.28 | 9 | 47 | 2 |
| 605.6246 | 0.654035947 | 1.5 | 238251.24 | 81 | 41 | 2 |
| 616.1473 | 0.683440936 | 38 | 66796.18 | 20 | 47 | 2 |
| 619.6403 | 0.719934325 | 1.5 | 192396.52 | 83 | 42 | 2 |
| 624.1166 | 1.636075167 | 41 | 68595.17 | 16 | 48 | 2 |
| 630.1632 | 1.064963353 | 38 | 73795.34 | 22 | 48 | 2 |
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| 647.6712 | 0.071178097 | 1.5 | 119540.39 | 87 | 44 | 2 |
| 648.1165 | 1.421197129 | 43 | 60053.62 | 16 | 50 | 2 |
| 656.1784 | 0.336951162 | 39 | 56141.38 | 24 | 50 | 2 |
| 659.2025 | 1.283522265 | 37.5 | 49314.82 | 27 | 50 | 2 |
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| 681.1866 | 0.87509138 | 40.5 | 56649.98 | 25 | 52 | 2 |
| 684.2093 | -0.261469631 | 39 | 54755.34 | 28 | 52 | 2 |
| 688.1461 | -1.131880452 | 44 | 80288.63 | 20 | 53 | 2 |
| 689.1534 | -1.892028006 | 43.5 | 56763.24 | 21 | 53 | 2 |
| 689.7177 | -0.585601563 | 1.5 | 55542.41 | 93 | 47 | 2 |
| 690.1615 | -1.490808262 | 43 | 69251.81 | 22 | 53 | 2 |
| 692.1787 | 0.752840838 | 42 | 47005.37 | 24 | 53 | 2 |
| 694.1943 | 0.678628908 | 41 | 46388.2 | 26 | 53 | 2 |
| 695.1091 | 1.936534289 | 47.5 | 50140.71 | 15 | 54 | 2 |
| 698.1309 | -0.471114865 | 46 | 82980.56 | 18 | 54 | 2 |
| 702.1619 | -0.89566158 | 44 | 84680.02 | 22 | 54 | 2 |
| 703.1693 | -1.498783323 | 43.5 | 49481.73 | 23 | 54 | 2 |
| 703.7342 | 0.633904509 | 1.5 | 59833.43 | 95 | 48 | 2 |

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|---|---|---|---|---|---|---|
| 704.1769 | -1.816159657 | 43 | 69570.5 | 24 | 54 | 2 |
| 706.1945 | 0.95030567 | 42 | 61867.57 | 26 | 54 | 2 |
| 711.1382 | -1.200749692 | 46.5 | 60750.74 | 19 | 55 | 2 |
| 714.163 | 0.659653764 | 45 | 56841.1 | 22 | 55 | 2 |
| 716.1768 | -1.925358857 | 44 | 70949.19 | 24 | 55 | 2 |
| 717.7499 | 0.691188314 | 1.5 | 75422.15 | 97 | 49 | 2 |
| 718.1929 | -1.293383433 | 43 | 64133.12 | 26 | 55 | 2 |
| 724.7115 | 1.684949193 | 5 | 49721.44 | 92 | 50 | 2 |
| 727.1698 | -0.761719722 | 45.5 | 48398.77 | 23 | 56 | 2 |
| 728.1778 | -0.520339679 | 45 | 68222.71 | 24 | 56 | 2 |
| 730.193 | -1.135178041 | 44 | 68044.67 | 26 | 56 | 2 |
| 731.7661 | 1.429557198 | 1.5 | 65571.75 | 99 | 50 | 2 |
| 732.1149 | -0.927312599 | 50 | 49517.39 | 16 | 57 | 2 |
| 732.2095 | 0.02881689 | 43 | 52767.64 | 28 | 56 | 2 |
| 734.1305 | -0.992874259 | 49 | 49774.33 | 18 | 57 | 2 |
| 739.17 | -0.478780024 | 46.5 | 50217.17 | 23 | 57 | 2 |
| 740.1771 | -1.457622003 | 46 | 55376.08 | 24 | 57 | 2 |
| 742.1936 | -0.308410002 | 45 | 65647.77 | 26 | 57 | 2 |
| 745.2166 | -0.944556704 | 43.5 | 63061.59 | 29 | 57 | 2 |
| 750.1618 | -0.971656104 | 48 | 47957.57 | 22 | 58 | 2 |
| 759.1382 | -1.124826862 | 50.5 | 47658.5 | 19 | 59 | 2 |
| 759.7962 | -0.202554275 | 1.5 | 56165.65 | 103 | 52 | 2 |
| 762.1618 | -0.956357696 | 49 | 50626.98 | 22 | 59 | 2 |
| 773.8118 | -0.263500694 | 1.5 | 70874.84 | 105 | 53 | 2 |
| 774.1625 | -0.037330662 | 50 | 54845.81 | 22 | 60 | 2 |
| 776.1771 | -1.390015887 | 49 | 53364.88 | 24 | 60 | 2 |
| 779.201 | -0.839192264 | 47.5 | 64203.36 | 27 | 60 | 2 |
| 784.2414 | 0.791976159 | 45 | 49040.25 | 32 | 60 | 2 |
| 804.1147 | -1.09300208 | 56 | 55340.78 | 16 | 63 | 2 |
| 812.1768 | -1.697780162 | 52 | 49296.64 | 24 | 63 | 2 |
| 813.1846 | -1.726419286 | 51.5 | 58187.84 | 25 | 63 | 2 |
| 814.1954 | 1.929638796 | 51 | 76217.29 | 26 | 63 | 2 |
| 823.1692 | -1.401775458 | 53.5 | 51457.63 | 23 | 64 | 2 |
| 824.1774 | -0.945062633 | 53 | 48705.13 | 24 | 64 | 2 |
| 828.8684 | 1.95580284 | 2 | 53928.34 | 112 | 57 | 2 |
| 844.2423 | 1.80173718 | 50 | 52979.6 | 32 | 65 | 2 |
| 849.5629 | 1.525610378 | 26.5 | 45582.95 | 73 | 62 | 2 |
| 864.2084 | -1.248424168 | 54 | 78885.96 | 28 | 67 | 2 |
| 885.9379 | 0.785721603 | 1.5 | 52637.84 | 121 | 61 | 2 |
| 904.1485 | 1.792960898 | 62 | 67150.25 | 20 | 71 | 2 |
| 914.3185 | -0.578463297 | 50 | 47191.47 | 42 | 70 | 2 |
| 921.1866 | 0.647100583 | 60.5 | 55533.92 | 25 | 72 | 2 |
| 941.9988 | -1.065711475 | 1.5 | 48017.9 | 129 | 65 | 2 |
| 948.2109 | 1.498719462 | 61 | 46231.97 | 28 | 74 | 2 |
| 960.2079 | -1.644328696 | 62 | 60707.51 | 28 | 75 | 2 |
| 978.2557 | -0.74510116 | 60 | 47645.62 | 34 | 76 | 2 |

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|---|---|---|---|---|---|---|
| 1060.898 | 0.208408333 | 19 | 56938.83 | 116 | 76 | 2 |
| 1065.282 | 1.592163706 | 65.5 | 53788.39 | 37 | 83 | 2 |
| 1110.256 | -0.116099305 | 71 | 97550.39 | 34 | 87 | 2 |
| 1110.536 | -1.82695213 | 50 | 79565.7 | 70 | 84 | 2 |

**b)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O |
|---|---|---|---|---|---|---|
| 87.045 | -1.76805 | 1.5 | 32632.89 | 7 | 4 | 2 |
| 92.9981 | -1.11723 | 5.5 | 2510406.04 | 1 | 5 | 2 |
| 95.0138 | -0.56729 | 4.5 | 49008497.38 | 3 | 5 | 2 |
| 96.0216 | -0.82169 | 4 | 12130.25 | 4 | 5 | 2 |
| 97.0294 | -1.07081 | 3.5 | 4460634.73 | 5 | 5 | 2 |
| 99.0451 | -0.5442 | 2.5 | 150446.18 | 7 | 5 | 2 |
| 101.0607 | -1.02809 | 1.5 | 11398.67 | 9 | 5 | 2 |
| 101.061 | 1.940416 | 1.5 | 8125.29 | 9 | 5 | 2 |
| 106.0061 | 0.670717 | 6 | 675314.98 | 2 | 6 | 2 |
| 107.0139 | 0.430785 | 5.5 | 5655704.61 | 3 | 6 | 2 |
| 108.0217 | 0.195331 | 5 | 120220762.5 | 4 | 6 | 2 |
| 109.0295 | -0.03577 | 4.5 | 66956522.15 | 5 | 6 | 2 |
| 111.0452 | 0.415146 | 3.5 | 1337277.62 | 7 | 6 | 2 |
| 113.0609 | 0.849985 | 2.5 | 78093.24 | 9 | 6 | 2 |
| 115.0766 | 1.269591 | 1.5 | 14617.69 | 11 | 6 | 2 |
| 116.9983 | 0.82138 | 7.5 | 71533.86 | 1 | 7 | 2 |
| 118.0062 | 1.449926 | 7 | 20693.16 | 2 | 7 | 2 |
| 119.0139 | 0.38735 | 6.5 | 24789821.88 | 3 | 7 | 2 |
| 120.0217 | 0.175802 | 6 | 878751.67 | 4 | 7 | 2 |
| 121.0295 | -0.03222 | 5.5 | 252231185.3 | 5 | 7 | 2 |
| 122.0373 | -0.23681 | 5 | 43257141.72 | 6 | 7 | 2 |
| 123.0451 | -0.43805 | 4.5 | 32022317.56 | 7 | 7 | 2 |
| 125.0608 | -0.03118 | 3.5 | 145471.67 | 9 | 7 | 2 |
| 127.0765 | 0.362774 | 2.5 | 58241.47 | 11 | 7 | 2 |
| 129.0921 | -0.03021 | 1.5 | 12137.16 | 13 | 7 | 2 |
| 130.006 | -0.2223 | 8 | 23874.04 | 2 | 8 | 2 |
| 131.0138 | -0.41141 | 7.5 | 2487904.19 | 3 | 8 | 2 |
| 132.0216 | -0.59763 | 7 | 12130109.7 | 4 | 8 | 2 |
| 133.0295 | -0.02932 | 6.5 | 44765706.06 | 5 | 8 | 2 |
| 134.0373 | -0.21561 | 6 | 8182091.54 | 6 | 8 | 2 |
| 135.0452 | 0.341367 | 5.5 | 76581959.15 | 7 | 8 | 2 |
| 136.0529 | -0.57992 | 5 | 6879289.98 | 8 | 8 | 2 |
| 137.0607 | -0.75806 | 4.5 | 4381121.36 | 9 | 8 | 2 |
| 139.0765 | 0.331472 | 3.5 | 13913.28 | 11 | 8 | 2 |
| 141.0921 | -0.02764 | 2.5 | 47854.72 | 13 | 8 | 2 |
| 143.0138 | -0.37689 | 8.5 | 1796093.43 | 3 | 9 | 2 |
| 143.1077 | -0.37664 | 1.5 | 14201.31 | 15 | 8 | 2 |

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|---|---|---|---|---|---|---|
| 144.0216 | -0.54783 | 8 | 474223.11 | 4 | 9 | 2 |
| 145.0295 | -0.02689 | 7.5 | 114156368.9 | 5 | 9 | 2 |
| 146.0372 | -0.88265 | 7 | 4045198.57 | 6 | 9 | 2 |
| 147.0451 | -0.36655 | 6.5 | 45339388.22 | 7 | 9 | 2 |
| 148.0529 | -0.53292 | 6 | 1314491.57 | 8 | 9 | 2 |
| 149.0607 | -0.69703 | 5.5 | 11187649.3 | 9 | 9 | 2 |
| 150.0686 | -0.19258 | 5 | 244792.55 | 10 | 9 | 2 |
| 151.0764 | -0.35677 | 4.5 | 400249.75 | 11 | 9 | 2 |
| 155.0138 | -0.34771 | 9.5 | 157080.87 | 3 | 10 | 2 |
| 155.1078 | 0.297213 | 2.5 | 31482.26 | 15 | 9 | 2 |
| 156.0216 | -0.5057 | 9 | 1559949.42 | 4 | 10 | 2 |
| 157.0294 | -0.66166 | 8.5 | 8274169.94 | 5 | 10 | 2 |
| 157.1234 | -0.02482 | 1.5 | 9629.3 | 17 | 9 | 2 |
| 158.0372 | -0.81563 | 8 | 23696459.75 | 6 | 10 | 2 |
| 159.0451 | -0.3389 | 7.5 | 77592226.83 | 7 | 10 | 2 |
| 160.0529 | -0.49296 | 7 | 916042.15 | 8 | 10 | 2 |
| 161.0607 | -0.6451 | 6.5 | 9037669.24 | 9 | 10 | 2 |
| 162.0686 | -0.17832 | 6 | 50341.25 | 10 | 10 | 2 |
| 163.0764 | -0.33052 | 5.5 | 1198070.65 | 11 | 10 | 2 |
| 165.0921 | -0.02362 | 4.5 | 24272.68 | 13 | 10 | 2 |
| 167.0138 | -0.32273 | 10.5 | 102325.37 | 3 | 11 | 2 |
| 168.0216 | -0.46958 | 10 | 165697 | 4 | 11 | 2 |
| 169.0294 | -0.61469 | 9.5 | 20645875.57 | 5 | 11 | 2 |
| 169.1234 | -0.02306 | 2.5 | 31011.5 | 17 | 10 | 2 |
| 170.0372 | -0.75807 | 9 | 1768963.56 | 6 | 11 | 2 |
| 171.0451 | -0.31512 | 8.5 | 44238379.03 | 7 | 11 | 2 |
| 171.1391 | 0.269372 | 1.5 | 10114.23 | 19 | 10 | 2 |
| 172.0529 | -0.45858 | 8 | 5900749.93 | 8 | 11 | 2 |
| 173.0607 | -0.60037 | 7.5 | 21358168.03 | 9 | 11 | 2 |
| 174.0685 | -0.74051 | 7 | 73386.81 | 10 | 11 | 2 |
| 175.0763 | -0.87904 | 6.5 | 1964114.89 | 11 | 11 | 2 |
| 177.092 | -0.5867 | 5.5 | 180989.33 | 13 | 11 | 2 |
| 180.0216 | -0.43828 | 11 | 150736.05 | 4 | 12 | 2 |
| 181.0294 | -0.57394 | 10.5 | 2849268.18 | 5 | 12 | 2 |
| 182.0373 | -0.15876 | 10 | 14336632.62 | 6 | 12 | 2 |
| 183.045 | -0.84078 | 9.5 | 26254119.26 | 7 | 12 | 2 |
| 183.1389 | -0.84035 | 2.5 | 24588.34 | 19 | 11 | 2 |
| 184.0528 | -0.972 | 9 | 3081070.06 | 8 | 12 | 2 |
| 185.0607 | -0.56144 | 8.5 | 22518910.69 | 9 | 12 | 2 |
| 186.0685 | -0.69276 | 8 | 601306.81 | 10 | 12 | 2 |
| 187.0763 | -0.82266 | 7.5 | 4011019.01 | 11 | 12 | 2 |
| 188.9985 | 1.566682 | 13.5 | 48900.04 | 1 | 13 | 2 |
| 189.092 | -0.54947 | 6.5 | 326063.41 | 13 | 12 | 2 |
| 191.1078 | 0.241225 | 5.5 | 24362.51 | 15 | 12 | 2 |
| 192.0218 | 0.630658 | 12 | 20411.09 | 4 | 13 | 2 |
| 193.0293 | -1.05632 | 11.5 | 4327688.56 | 5 | 13 | 2 |

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|---|---|---|---|---|---|---|
| 194.0372 | -0.66431 | 11 | 575715.45 | 6 | 13 | 2 |
| 195.0451 | -0.27635 | 10.5 | 49550039.74 | 7 | 13 | 2 |
| 196.0528 | -0.91251 | 10 | 5788051.92 | 8 | 13 | 2 |
| 197.0607 | -0.52725 | 9.5 | 24802793.38 | 9 | 13 | 2 |
| 197.1547 | -0.01978 | 2.5 | 19968.97 | 21 | 12 | 2 |
| 198.0685 | -0.65078 | 9 | 1194307.31 | 10 | 13 | 2 |
| 199.0763 | -0.77307 | 8.5 | 6722982.27 | 11 | 13 | 2 |
| 199.1703 | -0.27062 | 1.5 | 65472.89 | 23 | 12 | 2 |
| 200.0842 | -0.39433 | 8 | 23589.9 | 12 | 13 | 2 |
| 200.9985 | 1.473147 | 14.5 | 41356.27 | 1 | 14 | 2 |
| 201.092 | -0.51668 | 7.5 | 636427.46 | 13 | 13 | 2 |
| 203.0141 | 1.212233 | 13.5 | 11916.62 | 3 | 14 | 2 |
| 203.1077 | -0.26538 | 6.5 | 37918.91 | 15 | 13 | 2 |
| 204.0215 | -0.87687 | 13 | 6269.89 | 4 | 14 | 2 |
| 205.0294 | -0.50676 | 12.5 | 316742.36 | 5 | 14 | 2 |
| 205.1233 | -0.50652 | 5.5 | 7179.14 | 17 | 13 | 2 |
| 206.0372 | -0.62561 | 12 | 1979681.34 | 6 | 14 | 2 |
| 207.045 | -0.74332 | 11.5 | 7317074.77 | 7 | 14 | 2 |
| 208.0528 | -0.85988 | 11 | 10209412.19 | 8 | 14 | 2 |
| 209.0608 | -0.01865 | 10.5 | 37916630.53 | 9 | 14 | 2 |
| 210.0685 | -0.61361 | 10 | 1918871.28 | 10 | 14 | 2 |
| 211.0763 | -0.72912 | 9.5 | 11287152.92 | 11 | 14 | 2 |
| 211.1704 | 0.218307 | 2.5 | 19042.96 | 23 | 13 | 2 |
| 212.0842 | -0.37202 | 9 | 324750.9 | 12 | 14 | 2 |
| 212.9985 | 1.390153 | 15.5 | 140452.96 | 1 | 15 | 2 |
| 213.092 | -0.48758 | 8.5 | 2027252.72 | 13 | 14 | 2 |
| 213.186 | -0.01829 | 1.5 | 18655.4 | 25 | 13 | 2 |
| 214.0063 | 1.266787 | 15 | 27146.14 | 2 | 15 | 2 |
| 215.0141 | 1.144577 | 14.5 | 15668.3 | 3 | 15 | 2 |
| 215.1077 | -0.25057 | 7.5 | 80077.25 | 15 | 14 | 2 |
| 217.0294 | -0.47874 | 13.5 | 376867.64 | 5 | 15 | 2 |
| 217.1233 | -0.47853 | 6.5 | 6636.58 | 17 | 14 | 2 |
| 218.0371 | -1.04982 | 13 | 117694.22 | 6 | 15 | 2 |
| 219.045 | -0.70259 | 12.5 | 10626841.42 | 7 | 15 | 2 |
| 219.1391 | 0.210369 | 5.5 | 6321.13 | 19 | 14 | 2 |
| 220.0528 | -0.81299 | 12 | 2070468.12 | 8 | 15 | 2 |
| 221.0607 | -0.47001 | 11.5 | 15813691.29 | 9 | 15 | 2 |
| 222.0685 | -0.58045 | 11 | 4427309.4 | 10 | 15 | 2 |
| 223.0764 | -0.24162 | 10.5 | 13743211.18 | 11 | 15 | 2 |
| 224.0842 | -0.3521 | 10 | 346952.05 | 12 | 15 | 2 |
| 224.9985 | 1.316011 | 16.5 | 245240.34 | 1 | 16 | 2 |
| 225.092 | -0.46159 | 9.5 | 3443446.1 | 13 | 15 | 2 |
| 225.186 | -0.01732 | 2.5 | 25874.01 | 25 | 14 | 2 |
| 226.0999 | -0.12782 | 9 | 44019.08 | 14 | 15 | 2 |
| 227.0141 | 1.084075 | 15.5 | 26856.84 | 3 | 16 | 2 |
| 227.1077 | -0.23733 | 8.5 | 549726.93 | 15 | 15 | 2 |

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|---|---|---|---|---|---|---|
| 227.2017 | 0.202903 | 1.5 | 81030.38 | 27 | 14 | 2 |
| 229.0296 | 0.419597 | 14.5 | 36405.05 | 5 | 16 | 2 |
| 229.1234 | -0.01702 | 7.5 | 9596.46 | 17 | 15 | 2 |
| 230.0373 | -0.12563 | 14 | 179071.39 | 6 | 16 | 2 |
| 231.0451 | -0.23329 | 13.5 | 1396611.69 | 7 | 16 | 2 |
| 232.0529 | -0.34001 | 13 | 6949066.55 | 8 | 16 | 2 |
| 233.0607 | -0.44581 | 12.5 | 11787259.72 | 9 | 16 | 2 |
| 234.0686 | -0.12347 | 12 | 1936728.04 | 10 | 16 | 2 |
| 235.0764 | -0.22929 | 11.5 | 11007783.05 | 11 | 16 | 2 |
| 236.0842 | -0.3342 | 11 | 704971.95 | 12 | 16 | 2 |
| 236.9985 | 1.249377 | 17.5 | 156344.72 | 1 | 17 | 2 |
| 237.0921 | -0.01645 | 10.5 | 3684971.5 | 13 | 16 | 2 |
| 238.0999 | -0.12138 | 10 | 30877.27 | 14 | 16 | 2 |
| 239.0143 | 1.866419 | 16.5 | 51656.92 | 3 | 17 | 2 |
| 239.1078 | 0.1928 | 9.5 | 845141.3 | 15 | 16 | 2 |
| 239.2016 | -0.22533 | 2.5 | 16020.28 | 27 | 15 | 2 |
| 240.1157 | 0.50434 | 9 | 12280.82 | 16 | 16 | 2 |
| 241.0298 | 1.22848 | 15.5 | 35873.76 | 5 | 17 | 2 |
| 241.1235 | 0.398551 | 8.5 | 76501.86 | 17 | 16 | 2 |
| 241.2174 | 0.398396 | 1.5 | 44780.96 | 29 | 15 | 2 |
| 242.0369 | -1.77204 | 15 | 24900.97 | 6 | 17 | 2 |
| 243.0451 | -0.22177 | 14.5 | 2102534.18 | 7 | 17 | 2 |
| 243.1392 | 0.600891 | 7.5 | 8987.04 | 19 | 16 | 2 |
| 244.0529 | -0.32329 | 14 | 494283.4 | 8 | 17 | 2 |
| 245.0608 | -0.01591 | 13.5 | 11147638.04 | 9 | 17 | 2 |
| 246.0686 | -0.11745 | 13 | 3653689.78 | 10 | 17 | 2 |
| 247.0764 | -0.21815 | 12.5 | 8174385.12 | 11 | 17 | 2 |
| 248.0843 | 0.085052 | 12 | 662778.62 | 12 | 17 | 2 |
| 248.9986 | 1.590775 | 18.5 | 2431429.2 | 1 | 18 | 2 |
| 249.0921 | -0.01566 | 11.5 | 4257498.35 | 13 | 17 | 2 |
| 250.1 | 0.284286 | 11 | 41693.26 | 14 | 17 | 2 |
| 251.0143 | 1.777193 | 17.5 | 79128.72 | 3 | 18 | 2 |
| 251.1078 | 0.183587 | 10.5 | 856869.36 | 15 | 17 | 2 |
| 253.03 | 1.960641 | 16.5 | 20407.25 | 5 | 18 | 2 |
| 253.1235 | 0.379657 | 9.5 | 128597.26 | 17 | 17 | 2 |
| 253.2175 | 0.774434 | 2.5 | 137916.96 | 29 | 16 | 2 |
| 254.0374 | 0.27988 | 16 | 26772.09 | 6 | 18 | 2 |
| 255.0453 | 0.57284 | 15.5 | 176412.36 | 7 | 18 | 2 |
| 255.1392 | 0.572629 | 8.5 | 8928.1 | 19 | 17 | 2 |
| 255.2333 | 1.356016 | 1.5 | 14970289.85 | 31 | 16 | 2 |
| 256.0531 | 0.472949 | 15 | 1896887.14 | 8 | 18 | 2 |
| 257.0609 | 0.373842 | 14.5 | 3569888.69 | 9 | 18 | 2 |
| 258.0686 | -0.11199 | 14 | 3012741.24 | 10 | 18 | 2 |
| 259.0765 | 0.17794 | 13.5 | 11210041.19 | 11 | 18 | 2 |
| 260.0843 | 0.081128 | 13 | 883593.16 | 12 | 18 | 2 |
| 261.0921 | -0.01494 | 12.5 | 3923854.55 | 13 | 18 | 2 |

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|---|---|---|---|---|---|---|
| 262.1001 | 0.652804 | 12 | 71385.25 | 14 | 18 | 2 |
| 263.0143 | 1.696108 | 18.5 | 396429.49 | 3 | 19 | 2 |
| 263.1078 | 0.175213 | 11.5 | 1130472.19 | 15 | 18 | 2 |
| 265.03 | 1.871867 | 17.5 | 48377.66 | 5 | 19 | 2 |
| 265.1236 | 0.739656 | 10.5 | 140471.84 | 17 | 18 | 2 |
| 266.0373 | -0.10863 | 17 | 11182.84 | 6 | 19 | 2 |
| 267.0454 | 0.921567 | 16.5 | 273838.66 | 7 | 19 | 2 |
| 267.1392 | 0.546906 | 9.5 | 21775.32 | 19 | 18 | 2 |
| 267.2332 | 0.920919 | 2.5 | 15715.72 | 31 | 17 | 2 |
| 268.0531 | 0.451776 | 16 | 99053.7 | 8 | 19 | 2 |
| 269.0609 | 0.357168 | 15.5 | 4659488.77 | 9 | 19 | 2 |
| 269.2489 | 1.099727 | 1.5 | 59864.39 | 33 | 17 | 2 |
| 270.0688 | 0.633543 | 15 | 1385371.11 | 10 | 19 | 2 |
| 271.0766 | 0.538962 | 14.5 | 4991019.39 | 11 | 19 | 2 |
| 272.0845 | 0.812616 | 14 | 1662027.92 | 12 | 19 | 2 |
| 273.0923 | 0.718073 | 13.5 | 5351710.97 | 13 | 19 | 2 |
| 274.1001 | 0.624225 | 13 | 131000.15 | 14 | 19 | 2 |
| 275.108 | 0.894559 | 12.5 | 1256905.35 | 15 | 19 | 2 |
| 276.1157 | 0.438584 | 12 | 11467.6 | 16 | 19 | 2 |
| 277.0299 | 1.429812 | 18.5 | 99159.93 | 5 | 20 | 2 |
| 277.1235 | 0.346777 | 11.5 | 221947.93 | 17 | 19 | 2 |
| 278.0374 | 0.255721 | 18 | 7321.45 | 6 | 20 | 2 |
| 279.0453 | 0.523571 | 17.5 | 59181.17 | 7 | 20 | 2 |
| 279.1389 | -0.55134 | 10.5 | 13571.49 | 19 | 19 | 2 |
| 279.2332 | 0.881343 | 3.5 | 21760.78 | 31 | 18 | 2 |
| 280.053 | 0.075343 | 17 | 268648.35 | 8 | 20 | 2 |
| 281.0609 | 0.341919 | 16.5 | 761454.89 | 9 | 20 | 2 |
| 281.2488 | 0.697248 | 2.5 | 392415.55 | 33 | 18 | 2 |
| 282.0687 | 0.252066 | 16 | 2328321.5 | 10 | 20 | 2 |
| 283.0765 | 0.162854 | 15.5 | 4554968.19 | 11 | 20 | 2 |
| 283.2646 | 1.221827 | 1.5 | 17489172.75 | 35 | 18 | 2 |
| 284.0843 | 0.074274 | 15 | 729186.35 | 12 | 20 | 2 |
| 285.0922 | 0.337084 | 14.5 | 3392643.77 | 13 | 20 | 2 |
| 286.0065 | 1.647168 | 21 | 26543.92 | 2 | 21 | 2 |
| 286.1 | 0.248515 | 14 | 268389.05 | 14 | 20 | 2 |
| 287.0144 | 1.902696 | 20.5 | 72116.08 | 3 | 21 | 2 |
| 287.1079 | 0.508868 | 13.5 | 1444429.7 | 15 | 20 | 2 |
| 288.1158 | 0.7674 | 13 | 11602.78 | 16 | 20 | 2 |
| 289.1236 | 0.678257 | 12.5 | 261659.2 | 17 | 20 | 2 |
| 291.0455 | 1.189163 | 18.5 | 77684.68 | 7 | 21 | 2 |
| 291.1393 | 0.845301 | 11.5 | 25514.6 | 19 | 20 | 2 |
| 292.0528 | -0.61256 | 18 | 20966.62 | 8 | 21 | 2 |
| 293.061 | 0.669144 | 17.5 | 1267911.87 | 9 | 21 | 2 |
| 294.0688 | 0.581837 | 17 | 381047.67 | 10 | 21 | 2 |
| 295.0764 | -0.18266 | 16.5 | 2906295.74 | 11 | 21 | 2 |
| 295.2644 | 0.494811 | 2.5 | 6470.21 | 35 | 19 | 2 |

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|---|---|---|---|---|---|---|
| 296.0842 | -0.26648 | 16 | 1473565.64 | 12 | 21 | 2 |
| 297.092 | -0.34972 | 15.5 | 2599834.63 | 13 | 21 | 2 |
| 297.2798 | -0.3495 | 1.5 | 18174.55 | 37 | 19 | 2 |
| 298.0999 | -0.09695 | 15 | 185363.47 | 14 | 21 | 2 |
| 299.0142 | 1.157471 | 21.5 | 248396.96 | 3 | 22 | 2 |
| 299.1077 | -0.1802 | 14.5 | 1300994.26 | 15 | 21 | 2 |
| 300.1157 | 0.403511 | 14 | 23822.73 | 16 | 21 | 2 |
| 301.0298 | 0.983625 | 20.5 | 68930.86 | 5 | 22 | 2 |
| 301.1234 | -0.01295 | 13.5 | 145014.63 | 17 | 21 | 2 |
| 302.0378 | 1.559741 | 20 | 6877.83 | 6 | 22 | 2 |
| 303.0455 | 1.142074 | 19.5 | 26266.01 | 7 | 22 | 2 |
| 303.1391 | 0.152075 | 12.5 | 40091.46 | 19 | 21 | 2 |
| 304.0531 | 0.398286 | 19 | 38696.83 | 8 | 22 | 2 |
| 305.0609 | 0.315019 | 18.5 | 150574.59 | 9 | 22 | 2 |
| 306.0687 | 0.232301 | 18 | 950890.19 | 10 | 22 | 2 |
| 307.0765 | 0.150125 | 17.5 | 1521620.13 | 11 | 22 | 2 |
| 308.0844 | 0.393074 | 17 | 628065.16 | 12 | 22 | 2 |
| 309.0922 | 0.310911 | 16.5 | 2486017.03 | 13 | 22 | 2 |
| 310.1001 | 0.551758 | 16 | 318412.41 | 14 | 22 | 2 |
| 311.1079 | 0.469612 | 15.5 | 1050477.64 | 15 | 22 | 2 |
| 311.2959 | 1.111805 | 1.5 | 29696.6 | 39 | 20 | 2 |
| 312.1157 | 0.387997 | 15 | 20994.44 | 16 | 22 | 2 |
| 313.0301 | 1.904293 | 21.5 | 138871.09 | 5 | 23 | 2 |
| 313.1236 | 0.626271 | 14.5 | 296210.58 | 17 | 22 | 2 |
| 315.0457 | 1.733402 | 20.5 | 45095.05 | 7 | 23 | 2 |
| 315.1394 | 1.098245 | 13.5 | 38281.87 | 19 | 22 | 2 |
| 316.0534 | 1.332372 | 20 | 17517.63 | 8 | 23 | 2 |
| 317.0607 | -0.3277 | 19.5 | 214814.65 | 9 | 23 | 2 |
| 318.0685 | -0.40526 | 19 | 73409.79 | 10 | 23 | 2 |
| 319.0763 | -0.48233 | 18.5 | 1360523.58 | 11 | 23 | 2 |
| 320.0842 | -0.2465 | 18 | 564754.84 | 12 | 23 | 2 |
| 321.092 | -0.32358 | 17.5 | 1226269.12 | 13 | 23 | 2 |
| 322.0999 | -0.08972 | 17 | 266446.6 | 14 | 23 | 2 |
| 323.1077 | -0.16682 | 16.5 | 1154236.24 | 15 | 23 | 2 |
| 324.1155 | -0.24343 | 16 | 21577.94 | 16 | 23 | 2 |
| 325.0299 | 1.218659 | 22.5 | 97476.77 | 5 | 24 | 2 |
| 325.1235 | 0.29558 | 15.5 | 236047.08 | 17 | 23 | 2 |
| 327.0455 | 1.058264 | 21.5 | 46582.47 | 7 | 24 | 2 |
| 327.1391 | 0.140919 | 14.5 | 34855.46 | 19 | 23 | 2 |
| 328.0533 | 0.978805 | 21 | 14119.97 | 8 | 24 | 2 |
| 329.0609 | 0.292043 | 20.5 | 30280.62 | 9 | 24 | 2 |
| 330.0687 | 0.21541 | 20 | 197858.59 | 10 | 24 | 2 |
| 331.0765 | 0.139243 | 19.5 | 331405.1 | 11 | 24 | 2 |
| 332.0843 | 0.063538 | 19 | 432145.83 | 12 | 24 | 2 |
| 333.0921 | -0.01171 | 18.5 | 1241361.03 | 13 | 24 | 2 |
| 334.1 | 0.212811 | 18 | 168764.26 | 14 | 24 | 2 |

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|---|---|---|---|---|---|---|
| 335.1079 | 0.435979 | 17.5 | 691055.72 | 15 | 24 | 2 |
| 336.1158 | 0.657809 | 17 | 36622.66 | 16 | 24 | 2 |
| 337.1236 | 0.581686 | 16.5 | 221767.69 | 17 | 24 | 2 |
| 339.0455 | 1.020808 | 22.5 | 60750.65 | 7 | 25 | 2 |
| 339.139 | -0.15893 | 15.5 | 38203.15 | 19 | 24 | 2 |
| 340.0535 | 1.532408 | 22 | 6537.05 | 8 | 25 | 2 |
| 341.0609 | 0.281768 | 21.5 | 63540.65 | 9 | 25 | 2 |
| 342.0685 | -0.37682 | 21 | 28117.36 | 10 | 25 | 2 |
| 343.0764 | -0.15711 | 20.5 | 475315.49 | 11 | 25 | 2 |
| 344.0843 | 0.061322 | 20 | 167060.55 | 12 | 25 | 2 |
| 345.0921 | -0.0113 | 19.5 | 615015.93 | 13 | 25 | 2 |
| 346.0999 | -0.0835 | 19 | 256687.33 | 14 | 25 | 2 |
| 347.1078 | 0.132812 | 18.5 | 616183 | 15 | 25 | 2 |
| 348.1159 | 0.922395 | 18 | 33900.87 | 16 | 25 | 2 |
| 349.1235 | 0.275261 | 17.5 | 189718.21 | 17 | 25 | 2 |
| 351.0458 | 1.840504 | 23.5 | 25801.66 | 7 | 26 | 2 |
| 351.1392 | 0.416074 | 16.5 | 35387.31 | 19 | 25 | 2 |
| 353.0611 | 0.838666 | 22.5 | 26102.84 | 9 | 26 | 2 |
| 353.1547 | -0.01104 | 15.5 | 6038.1 | 21 | 25 | 2 |
| 354.0688 | 0.48324 | 22 | 58678.11 | 10 | 26 | 2 |
| 355.0766 | 0.411461 | 21.5 | 94076.74 | 11 | 26 | 2 |
| 355.1705 | 0.411352 | 14.5 | 5983.27 | 23 | 25 | 2 |
| 356.0844 | 0.340088 | 21 | 230552.81 | 12 | 26 | 2 |
| 357.0922 | 0.269118 | 20.5 | 493303.4 | 13 | 26 | 2 |
| 358.1 | 0.198548 | 20 | 113401.71 | 14 | 26 | 2 |
| 359.1079 | 0.406842 | 19.5 | 424582.8 | 15 | 26 | 2 |
| 360.1157 | 0.336281 | 19 | 52408.39 | 16 | 26 | 2 |
| 361.1236 | 0.543028 | 18.5 | 150588.62 | 17 | 26 | 2 |
| 363.1393 | 0.677702 | 17.5 | 28467.87 | 19 | 26 | 2 |
| 365.0611 | 0.811098 | 23.5 | 25151.87 | 9 | 27 | 2 |
| 365.1551 | 1.084746 | 16.5 | 6775.92 | 21 | 26 | 2 |
| 366.0693 | 1.833263 | 23 | 9817.83 | 10 | 27 | 2 |
| 367.0765 | 0.125587 | 22.5 | 138272.51 | 11 | 27 | 2 |
| 368.0844 | 0.329001 | 22 | 45524.88 | 12 | 27 | 2 |
| 369.0921 | -0.01057 | 21.5 | 307562.38 | 13 | 27 | 2 |
| 370.0999 | -0.07809 | 21 | 150865.76 | 14 | 27 | 2 |
| 371.1078 | 0.124223 | 20.5 | 250871.15 | 15 | 27 | 2 |
| 372.1157 | 0.325437 | 20 | 33608.99 | 16 | 27 | 2 |
| 373.1235 | 0.257556 | 19.5 | 125919.84 | 17 | 27 | 2 |
| 375.1391 | 0.122888 | 18.5 | 32609.15 | 19 | 27 | 2 |
| 376.0536 | 1.651629 | 25 | 9223.65 | 8 | 28 | 2 |
| 377.1547 | -0.01034 | 17.5 | 7719.24 | 21 | 27 | 2 |
| 378.0691 | 1.24607 | 24 | 24221.94 | 10 | 28 | 2 |
| 379.0768 | 0.913008 | 23.5 | 23852.87 | 11 | 28 | 2 |
| 380.0846 | 0.844813 | 23 | 85827.74 | 12 | 28 | 2 |
| 381.0922 | 0.25217 | 22.5 | 134110.51 | 13 | 28 | 2 |

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|---|---|---|---|---|---|---|
| 382.1002 | 0.7095 | 22 | 75169.62 | 14 | 28 | 2 |
| 383.1079 | 0.381355 | 21.5 | 216212.65 | 15 | 28 | 2 |
| 384.1157 | 0.31527 | 21 | 37682.73 | 16 | 28 | 2 |
| 385.1237 | 0.768844 | 20.5 | 74988.58 | 17 | 28 | 2 |
| 386.1312 | -0.07485 | 20 | 6129.21 | 18 | 28 | 2 |
| 387.1393 | 0.635689 | 19.5 | 25825.89 | 19 | 28 | 2 |
| 389.0613 | 1.275122 | 25.5 | 20003.62 | 9 | 29 | 2 |
| 391.0768 | 0.884993 | 24.5 | 43154.76 | 11 | 29 | 2 |
| 392.0849 | 1.584098 | 24 | 23648.01 | 12 | 29 | 2 |
| 392.9989 | 1.771255 | 30.5 | 6989.24 | 1 | 30 | 2 |
| 393.0924 | 0.753259 | 23.5 | 120684.37 | 13 | 29 | 2 |
| 394.1001 | 0.434154 | 23 | 59161.15 | 14 | 29 | 2 |
| 395.1078 | 0.116677 | 22.5 | 107121.07 | 15 | 29 | 2 |
| 396.1157 | 0.305719 | 22 | 30011 | 16 | 29 | 2 |
| 397.1235 | 0.24199 | 21.5 | 74052.74 | 17 | 29 | 2 |
| 399.1391 | 0.115499 | 20.5 | 17255.75 | 19 | 29 | 2 |
| 403.0767 | 0.610554 | 25.5 | 19305.73 | 11 | 30 | 2 |
| 404.0848 | 1.289582 | 25 | 28274.86 | 12 | 30 | 2 |
| 405.0924 | 0.730945 | 24.5 | 38206.46 | 13 | 30 | 2 |
| 406.1003 | 0.913814 | 24 | 65094.2 | 14 | 30 | 2 |
| 407.1079 | 0.358873 | 23.5 | 85202.13 | 15 | 30 | 2 |
| 408.116 | 1.031816 | 23 | 28409.62 | 16 | 30 | 2 |
| 409.1235 | 0.234892 | 22.5 | 44096.6 | 17 | 30 | 2 |
| 410.131 | -0.55811 | 22 | 9462.91 | 18 | 30 | 2 |
| 411.1393 | 0.598581 | 21.5 | 20547.47 | 19 | 30 | 2 |
| 412.0536 | 1.50733 | 28 | 5817.52 | 8 | 31 | 2 |
| 413.1551 | 0.958721 | 20.5 | 6933.02 | 21 | 30 | 2 |
| 415.077 | 1.315661 | 26.5 | 24020.68 | 11 | 31 | 2 |
| 416.0844 | 0.291047 | 26 | 13538.58 | 12 | 31 | 2 |
| 417.0924 | 0.709915 | 25.5 | 56594.9 | 13 | 31 | 2 |
| 419.108 | 0.5872 | 24.5 | 62135.78 | 15 | 31 | 2 |
| 420.1162 | 1.478403 | 24 | 33215.02 | 16 | 31 | 2 |
| 421.1238 | 0.940579 | 23.5 | 32196.27 | 17 | 31 | 2 |
| 422.1319 | 1.58979 | 23 | 8484.87 | 18 | 31 | 2 |
| 423.1393 | 0.581605 | 22.5 | 16912.36 | 19 | 31 | 2 |
| 427.0772 | 1.746994 | 27.5 | 17924.5 | 11 | 32 | 2 |
| 428.0843 | 0.049289 | 27 | 20325.16 | 12 | 32 | 2 |
| 429.0924 | 0.690062 | 26.5 | 24798.53 | 13 | 32 | 2 |
| 430.1004 | 1.095327 | 26 | 28203.43 | 14 | 32 | 2 |
| 431.1077 | -0.12503 | 25.5 | 43857.5 | 15 | 32 | 2 |
| 432.1161 | 1.205927 | 25 | 22955.82 | 16 | 32 | 2 |
| 433.1237 | 0.683639 | 24.5 | 34002.76 | 17 | 32 | 2 |
| 434.1317 | 1.085156 | 24 | 7441.36 | 18 | 32 | 2 |
| 435.1386 | -1.04311 | 23.5 | 15138.02 | 19 | 32 | 2 |
| 436.0537 | 1.653698 | 30 | 6879.57 | 8 | 33 | 2 |
| 437.1553 | 1.36359 | 22.5 | 6906.11 | 21 | 32 | 2 |

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|---|---|---|---|---|---|---|
| 441.0928 | 1.578128 | 27.5 | 41175.94 | 13 | 33 | 2 |
| 442.1004 | 1.065596 | 27 | 17435.93 | 14 | 33 | 2 |
| 443.1074 | -0.79868 | 26.5 | 42317.62 | 15 | 33 | 2 |
| 444.1163 | 1.623676 | 26 | 26291.48 | 16 | 33 | 2 |
| 445.1235 | 0.215895 | 25.5 | 26311.45 | 17 | 33 | 2 |
| 446.132 | 1.728415 | 25 | 8147.39 | 18 | 33 | 2 |
| 447.1388 | -0.56783 | 24.5 | 10065.93 | 19 | 33 | 2 |
| 454.1007 | 1.698084 | 28 | 21468.72 | 14 | 34 | 2 |
| 457.1239 | 1.085265 | 26.5 | 27919.32 | 17 | 34 | 2 |
| 459.1394 | 0.753802 | 25.5 | 13270.7 | 19 | 34 | 2 |
| 466.1008 | 1.868913 | 29 | 11721.4 | 14 | 35 | 2 |
| 468.1165 | 1.967676 | 28 | 22916.73 | 16 | 35 | 2 |
| 469.1238 | 0.844341 | 27.5 | 24721.86 | 17 | 35 | 2 |
| 470.1315 | 0.576648 | 27 | 11165.4 | 18 | 35 | 2 |
| 471.1397 | 1.371357 | 26.5 | 9657.76 | 19 | 35 | 2 |
| 473.1552 | 1.048494 | 25.5 | 5776.8 | 21 | 35 | 2 |
| 480.1163 | 1.50193 | 29 | 18352.92 | 16 | 36 | 2 |
| 482.132 | 1.599357 | 28 | 13010.22 | 18 | 36 | 2 |
| 483.1397 | 1.337296 | 27.5 | 11533.48 | 19 | 36 | 2 |
| 485.1541 | -1.24476 | 26.5 | 10602.79 | 21 | 36 | 2 |
| 490.1005 | 1.165273 | 31 | 6011.26 | 14 | 37 | 2 |
| 491.1086 | 1.72284 | 30.5 | 33391.99 | 15 | 37 | 2 |
| 492.1162 | 1.262102 | 30 | 7636.52 | 16 | 37 | 2 |
| 495.1396 | 1.102922 | 28.5 | 9400.03 | 19 | 37 | 2 |
| 497.154 | -1.41586 | 27.5 | 6996.11 | 21 | 37 | 2 |
| 506.1315 | 0.535632 | 30 | 12836.12 | 18 | 38 | 2 |
| 509.0616 | 1.56386 | 35.5 | 5762.2 | 9 | 39 | 2 |
| 512.0852 | 1.798727 | 34 | 5919.4 | 12 | 39 | 2 |
| 519.139 | -0.10383 | 30.5 | 22516.3 | 19 | 39 | 2 |
| 526.1001 | 0.325223 | 34 | 12470.83 | 14 | 40 | 2 |
| 528.1163 | 1.365421 | 33 | 11926.15 | 16 | 40 | 2 |
| 531.1395 | 0.839893 | 31.5 | 18465.45 | 19 | 40 | 2 |
| 536.085 | 1.345124 | 36 | 6987.35 | 12 | 41 | 2 |
| 538.101 | 1.990522 | 35 | 6377.42 | 14 | 41 | 2 |
| 556.1473 | 0.757174 | 33 | 9536.26 | 20 | 42 | 2 |
| 564.1153 | -0.4944 | 36 | 10620.19 | 16 | 43 | 2 |
| 566.1319 | 1.185414 | 35 | 7494.61 | 18 | 43 | 2 |
| 569.1557 | 1.750139 | 33.5 | 9730.4 | 21 | 43 | 2 |
| 572.0838 | -0.83711 | 39 | 8037.04 | 12 | 44 | 2 |
| 582.0694 | 1.324758 | 41 | 6111.26 | 10 | 45 | 2 |
| 586.1011 | 1.998123 | 39 | 7901.07 | 14 | 45 | 2 |
| 589.1238 | 0.672355 | 37.5 | 14347.41 | 17 | 45 | 2 |
| 591.1393 | 0.416315 | 36.5 | 15094.61 | 19 | 45 | 2 |
| 600.1159 | 0.535064 | 39 | 9230.81 | 16 | 46 | 2 |
| 606.1626 | 0.117295 | 36 | 9901.37 | 22 | 46 | 2 |
| 614.1302 | -1.67537 | 39 | 11384.74 | 18 | 47 | 2 |

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|---|---|---|---|---|---|---|
| 624.1152 | -0.6071 | 41 | 12996.99 | 16 | 48 | 2 |
| 628.1472 | 0.511186 | 39 | 9881.82 | 20 | 48 | 2 |
| 638.1315 | 0.424834 | 41 | 10566.55 | 18 | 49 | 2 |
| 648.1143 | -1.97326 | 43 | 8873.36 | 16 | 50 | 2 |
| 650.132 | 1.186068 | 42 | 8885.27 | 18 | 50 | 2 |
| 652.1474 | 0.799053 | 41 | 8068.4 | 20 | 50 | 2 |
| 654.1633 | 1.178759 | 40 | 7201.51 | 22 | 50 | 2 |
| 660.1161 | 0.789407 | 44 | 14544.18 | 16 | 51 | 2 |
| 664.1463 | -0.87164 | 42 | 13138.97 | 20 | 51 | 2 |
| 666.1624 | -0.1935 | 41 | 8310.93 | 22 | 51 | 2 |
| 676.1456 | -1.89145 | 43 | 11329.65 | 20 | 52 | 2 |
| 688.1472 | 0.466615 | 44 | 7751.35 | 20 | 53 | 2 |
| 698.1308 | -0.61435 | 46 | 6086 | 18 | 54 | 2 |
| 701.1557 | 1.420657 | 44.5 | 6861.29 | 21 | 54 | 2 |
| 702.1637 | 1.667847 | 44 | 7910.27 | 22 | 54 | 2 |
| 712.1482 | 1.855095 | 46 | 6414.92 | 20 | 55 | 2 |
| 724.1468 | -0.10896 | 47 | 8048.51 | 20 | 56 | 2 |
| 728.178 | -0.24568 | 45 | 8582.44 | 24 | 56 | 2 |
| 730.1938 | -0.03958 | 44 | 6572.63 | 26 | 56 | 2 |
| 738.1617 | -1.12292 | 47 | 7958.88 | 22 | 57 | 2 |
| 740.1769 | -1.72783 | 46 | 9127.52 | 24 | 57 | 2 |
| 742.1929 | -1.25156 | 45 | 7282.56 | 26 | 57 | 2 |
| 750.1613 | -1.63818 | 48 | 8023.76 | 22 | 58 | 2 |
| 754.1952 | 1.817968 | 46 | 6902.09 | 26 | 58 | 2 |
| 762.164 | 1.930166 | 49 | 10972.5 | 22 | 59 | 2 |
| 800.1788 | 0.776202 | 51 | 8680.43 | 24 | 62 | 2 |
| 804.2104 | 1.145348 | 49 | 7788.46 | 28 | 62 | 2 |
| 810.1619 | -0.77626 | 53 | 8727.41 | 22 | 63 | 2 |
| 824.1779 | -0.3384 | 53 | 7563.64 | 24 | 64 | 2 |
| 914.2243 | -0.90667 | 57 | 5690.78 | 30 | 71 | 2 |
| 924.2092 | -0.30177 | 59 | 6627.59 | 28 | 72 | 2 |
| 938.2241 | -1.09665 | 59 | 6559.14 | 30 | 73 | 2 |
| 963.2332 | 0.255494 | 60.5 | 8650.98 | 31 | 75 | 2 |
| 1045.31 | -1.63004 | 61.5 | 5910.21 | 41 | 81 | 2 |
| 1067.295 | -0.42528 | 64.5 | 11825.45 | 39 | 83 | 2 |
| 1080.303 | -0.07304 | 65 | 5961.58 | 40 | 84 | 2 |

**c)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O |
|---|---|---|---|---|---|---|
| 85.0293 | -2.39799 | 2.5 | 5050.53 | 5 | 4 | 2 |
| 92.9981 | -1.11723 | 5.5 | 8640.46 | 1 | 5 | 2 |
| 95.0138 | -0.56729 | 4.5 | 163947 | 3 | 5 | 2 |
| 97.0294 | -1.07081 | 3.5 | 26981.66 | 5 | 5 | 2 |
| 107.0139 | 0.430785 | 5.5 | 9091.68 | 3 | 6 | 2 |
| 108.0217 | 0.195331 | 5 | 263177.4 | 4 | 6 | 2 |

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|---|---|---|---|---|---|---|
| 109.0295 | -0.03577 | 4.5 | 135806.2 | 5 | 6 | 2 |
| 111.0452 | 0.415146 | 3.5 | 9863.44 | 7 | 6 | 2 |
| 119.0138 | -0.45289 | 6.5 | 102630.2 | 3 | 7 | 2 |
| 120.0217 | 0.175802 | 6 | 6527.03 | 4 | 7 | 2 |
| 121.0295 | -0.03222 | 5.5 | 784922.7 | 5 | 7 | 2 |
| 122.0373 | -0.23681 | 5 | 24277.07 | 6 | 7 | 2 |
| 123.0452 | 0.374659 | 4.5 | 58050.05 | 7 | 7 | 2 |
| 127.0764 | -0.42415 | 2.5 | 9011 | 11 | 7 | 2 |
| 131.0138 | -0.41141 | 7.5 | 3218.14 | 3 | 8 | 2 |
| 132.0216 | -0.59763 | 7 | 46426.82 | 4 | 8 | 2 |
| 133.0295 | -0.02932 | 6.5 | 160342.8 | 5 | 8 | 2 |
| 134.0373 | -0.21561 | 6 | 24906.3 | 6 | 8 | 2 |
| 135.0451 | -0.39913 | 5.5 | 1110759 | 7 | 8 | 2 |
| 137.0607 | -0.75806 | 4.5 | 5380.82 | 9 | 8 | 2 |
| 141.0921 | -0.02764 | 2.5 | 20434.78 | 13 | 8 | 2 |
| 143.0138 | -0.37689 | 8.5 | 8595.77 | 3 | 9 | 2 |
| 145.0294 | -0.71641 | 7.5 | 911478.3 | 5 | 9 | 2 |
| 146.0372 | -0.88265 | 7 | 13643.75 | 6 | 9 | 2 |
| 147.0451 | -0.36655 | 6.5 | 278396.5 | 7 | 9 | 2 |
| 148.053 | 0.142517 | 6 | 4084.72 | 8 | 9 | 2 |
| 149.0607 | -0.69703 | 5.5 | 121129.8 | 9 | 9 | 2 |
| 157.0294 | -0.66166 | 8.5 | 23894.17 | 5 | 10 | 2 |
| 158.0372 | -0.81563 | 8 | 164557.9 | 6 | 10 | 2 |
| 159.0451 | -0.3389 | 7.5 | 572742.6 | 7 | 10 | 2 |
| 161.0608 | -0.02421 | 6.5 | 64698.88 | 9 | 10 | 2 |
| 163.0764 | -0.33052 | 5.5 | 17548.85 | 11 | 10 | 2 |
| 169.0295 | -0.02307 | 9.5 | 148194.7 | 5 | 11 | 2 |
| 170.0373 | -0.16996 | 9 | 2779.99 | 6 | 11 | 2 |
| 171.0451 | -0.31512 | 8.5 | 294621.6 | 7 | 11 | 2 |
| 172.053 | 0.122637 | 8 | 32948.41 | 8 | 11 | 2 |
| 173.0607 | -0.60037 | 7.5 | 154942.7 | 9 | 11 | 2 |
| 175.0764 | -0.30787 | 6.5 | 11991.8 | 11 | 11 | 2 |
| 177.0921 | -0.02202 | 5.5 | 10203.86 | 13 | 11 | 2 |
| 181.0295 | -0.02154 | 10.5 | 3428.19 | 5 | 12 | 2 |
| 182.0374 | 0.390579 | 10 | 73657.85 | 6 | 12 | 2 |
| 183.0451 | -0.29446 | 9.5 | 137611.7 | 7 | 12 | 2 |
| 184.053 | 0.114641 | 9 | 16921.41 | 8 | 12 | 2 |
| 185.0607 | -0.56144 | 8.5 | 144204.4 | 9 | 12 | 2 |
| 187.0764 | -0.28812 | 7.5 | 14766.9 | 11 | 12 | 2 |
| 191.1078 | 0.241225 | 5.5 | 6478.64 | 15 | 12 | 2 |
| 193.0295 | -0.0202 | 11.5 | 17307.5 | 5 | 13 | 2 |
| 195.0451 | -0.27635 | 10.5 | 243982.1 | 7 | 13 | 2 |
| 196.053 | 0.107624 | 10 | 14768.3 | 8 | 13 | 2 |
| 197.0608 | -0.01979 | 9.5 | 93692.02 | 9 | 13 | 2 |
| 198.0686 | -0.14591 | 9 | 2814.82 | 10 | 13 | 2 |
| 199.0765 | 0.231569 | 8.5 | 30070.84 | 11 | 13 | 2 |

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|---|---|---|---|---|---|---|
| 200.9985 | 1.473147 | 14.5 | 3200 | 1 | 14 | 2 |
| 203.0142 | 1.70481 | 13.5 | 4005.04 | 3 | 14 | 2 |
| 205.1235 | 0.468498 | 5.5 | 3800.02 | 17 | 13 | 2 |
| 206.0374 | 0.345083 | 12 | 5692.27 | 6 | 14 | 2 |
| 207.0452 | 0.222657 | 11.5 | 22011.63 | 7 | 14 | 2 |
| 208.053 | 0.101416 | 11 | 42398.91 | 8 | 14 | 2 |
| 209.0608 | -0.01865 | 10.5 | 138609.8 | 9 | 14 | 2 |
| 210.0687 | 0.338461 | 10 | 5496.41 | 10 | 14 | 2 |
| 211.0765 | 0.218404 | 9.5 | 67111.91 | 11 | 14 | 2 |
| 217.0297 | 0.903564 | 13.5 | 3096.86 | 5 | 15 | 2 |
| 219.0452 | 0.210459 | 12.5 | 67372.44 | 7 | 15 | 2 |
| 220.053 | 0.095886 | 12 | 4789.21 | 8 | 15 | 2 |
| 221.0609 | 0.434722 | 11.5 | 82464.53 | 9 | 15 | 2 |
| 222.0687 | 0.320171 | 11 | 8889.72 | 10 | 15 | 2 |
| 223.0765 | 0.206656 | 10.5 | 35554.05 | 11 | 15 | 2 |
| 225.0922 | 0.426936 | 9.5 | 4172.78 | 13 | 15 | 2 |
| 231.0454 | 1.06516 | 13.5 | 2973.94 | 7 | 16 | 2 |
| 232.0531 | 0.521864 | 13 | 34340.85 | 8 | 16 | 2 |
| 233.0609 | 0.412339 | 12.5 | 43526.96 | 9 | 16 | 2 |
| 233.1548 | 0.412173 | 5.5 | 4146.5 | 21 | 15 | 2 |
| 234.0687 | 0.303757 | 12 | 6649.54 | 10 | 16 | 2 |
| 235.0766 | 0.6215 | 11.5 | 48522.84 | 11 | 16 | 2 |
| 237.0922 | 0.405328 | 10.5 | 6049.93 | 13 | 16 | 2 |
| 243.0453 | 0.601123 | 14.5 | 9284.64 | 7 | 17 | 2 |
| 245.061 | 0.80021 | 13.5 | 69178.84 | 9 | 17 | 2 |
| 246.0689 | 1.101725 | 13 | 7189.9 | 10 | 17 | 2 |
| 247.0766 | 0.591315 | 12.5 | 29720.69 | 11 | 17 | 2 |
| 249.0924 | 1.188717 | 11.5 | 12812.06 | 13 | 17 | 2 |
| 256.0532 | 0.863493 | 15 | 7627.48 | 8 | 18 | 2 |
| 257.0612 | 1.540881 | 14.5 | 10530.73 | 9 | 18 | 2 |
| 258.0689 | 1.050496 | 14 | 8817.35 | 10 | 18 | 2 |
| 259.0767 | 0.949913 | 13.5 | 36562.56 | 11 | 18 | 2 |
| 261.0924 | 1.134083 | 12.5 | 5859.32 | 13 | 18 | 2 |
| 269.0612 | 1.472158 | 15.5 | 31064.06 | 9 | 19 | 2 |
| 271.0768 | 1.276762 | 14.5 | 23825.15 | 11 | 19 | 2 |
| 273.0925 | 1.450426 | 13.5 | 7217.03 | 13 | 19 | 2 |
| 282.0688 | 0.60659 | 16 | 7777.3 | 10 | 20 | 2 |
| 283.0767 | 0.869376 | 15.5 | 15255.86 | 11 | 20 | 2 |
| 285.0923 | 0.687848 | 14.5 | 8391.99 | 13 | 20 | 2 |
| 293.0611 | 1.010371 | 17.5 | 5405.45 | 9 | 21 | 2 |
| 295.0765 | 0.156231 | 16.5 | 13105 | 11 | 21 | 2 |
| 297.0922 | 0.323469 | 15.5 | 6582.56 | 13 | 21 | 2 |
| 309.0921 | -0.01262 | 16.5 | 4581.85 | 13 | 22 | 2 |
| 319.0764 | -0.16893 | 18.5 | 6547.05 | 11 | 23 | 2 |

**Supplementary Table 8:** Output from SIMSMFP on all sulfonated species ($C_nH_nSO_3^-$) found in negative ion depth profile datasets from different engine deposits. a. injector tip 1, b. injector tip 2, c. injector needle 1.

**a)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O | S |
|---|---|---|---|---|---|---|---|
| 94.9808 | -0.420084725 | 0.5 | 261373.59 | 3 | 1 | 3 | 1 |
| 106.9809 | 0.561782839 | 1.5 | 129002.6 | 3 | 2 | 3 | 1 |
| 108.9966 | 1.010124272 | 0.5 | 86666.45 | 5 | 2 | 3 | 1 |
| 120.9964 | -0.74299676 | 1.5 | 51336.2 | 5 | 3 | 3 | 1 |
| 123.0122 | 0.488569665 | 0.5 | 112313.66 | 7 | 3 | 3 | 1 |
| 155.9884 | -1.698200316 | 5 | 514526.43 | 4 | 6 | 3 | 1 |
| 156.9965 | 0.064332648 | 4.5 | 4905764.45 | 5 | 6 | 3 | 1 |
| 165.9727 | -1.897296378 | 7 | 54647.67 | 2 | 7 | 3 | 1 |
| 170.0041 | -1.264085563 | 5 | 8642757.7 | 6 | 7 | 3 | 1 |
| 171.0122 | 0.351437038 | 4.5 | 7770542.57 | 7 | 7 | 3 | 1 |
| 179.9884 | -1.471759348 | 7 | 215954.85 | 4 | 8 | 3 | 1 |
| 180.9964 | -0.496694715 | 6.5 | 504599.65 | 5 | 8 | 3 | 1 |
| 182.004 | -1.730178761 | 6 | 1633013.89 | 6 | 8 | 3 | 1 |
| 183.0121 | -0.218018324 | 5.5 | 141185515.7 | 7 | 8 | 3 | 1 |
| 184.0198 | -0.896098421 | 5 | 4768474.31 | 8 | 8 | 3 | 1 |
| 185.0279 | 0.59504575 | 4.5 | 149150.56 | 9 | 8 | 3 | 1 |
| 191.9884 | -1.379768957 | 8 | 73957.05 | 4 | 9 | 3 | 1 |
| 194.004 | -1.623159775 | 7 | 3651125.19 | 6 | 9 | 3 | 1 |
| 195.0122 | 0.308185942 | 6.5 | 2232912.79 | 7 | 9 | 3 | 1 |
| 196.0198 | -0.84124084 | 6 | 4518536.76 | 8 | 9 | 3 | 1 |
| 197.0279 | 0.558804421 | 5.5 | 5889233.53 | 9 | 9 | 3 | 1 |
| 198.0353 | -1.590118021 | 5 | 450776.03 | 10 | 9 | 3 | 1 |
| 206.004 | -1.528608758 | 8 | 1789043.18 | 6 | 10 | 3 | 1 |
| 207.0121 | -0.19274232 | 7.5 | 443281.45 | 7 | 10 | 3 | 1 |
| 208.0197 | -1.273435462 | 7 | 2634609.47 | 8 | 10 | 3 | 1 |
| 209.0279 | 0.526724222 | 6.5 | 13389238.08 | 9 | 10 | 3 | 1 |
| 210.0353 | -1.499269541 | 6 | 3005210.96 | 10 | 10 | 3 | 1 |
| 211.0436 | 0.758611592 | 5.5 | 620065.12 | 11 | 10 | 3 | 1 |
| 218.004 | -1.444466822 | 9 | 583541.52 | 6 | 11 | 3 | 1 |
| 220.0197 | -1.203981648 | 8 | 5633611.37 | 8 | 11 | 3 | 1 |
| 221.0279 | 0.498127408 | 7.5 | 367301.03 | 9 | 11 | 3 | 1 |
| 222.0354 | -0.967862746 | 7 | 1121719.73 | 10 | 11 | 3 | 1 |
| 223.0435 | 0.269454237 | 6.5 | 1126679.25 | 11 | 11 | 3 | 1 |
| 224.051 | -1.182318699 | 6 | 486228.23 | 12 | 11 | 3 | 1 |
| 225.059 | -0.399450651 | 5.5 | 877724.88 | 13 | 11 | 3 | 1 |
| 230.0042 | -0.499555846 | 10 | 244845.09 | 6 | 12 | 3 | 1 |
| 231.0119 | -1.038473563 | 9.5 | 292789.85 | 7 | 12 | 3 | 1 |
| 232.0196 | -1.572709487 | 9 | 2679452.26 | 8 | 12 | 3 | 1 |
| 233.028 | 0.901609203 | 8.5 | 6192113.08 | 9 | 12 | 3 | 1 |
| 234.0354 | -0.918236312 | 8 | 4144505.16 | 10 | 12 | 3 | 1 |
| 234.1293 | -0.917868045 | 1 | 57271.17 | 22 | 11 | 3 | 1 |
| 235.0437 | 1.106603954 | 7.5 | 184100.2 | 11 | 12 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 236.0509 | -1.545850645 | 7 | 1945855.88 | 12 | 12 | 3 | 1 |
| 237.0591 | 0.042605411 | 6.5 | 234055.77 | 13 | 12 | 3 | 1 |
| 238.0665 | -1.742787318 | 6 | 3204620.22 | 14 | 12 | 3 | 1 |
| 239.075 | 1.087944298 | 5.5 | 908240.48 | 15 | 12 | 3 | 1 |
| 240.0821 | -1.936417166 | 5 | 2293880.34 | 16 | 12 | 3 | 1 |
| 242.0043 | -0.06156915 | 11 | 72926.15 | 6 | 13 | 3 | 1 |
| 242.0978 | -1.713767283 | 4 | 430383.1 | 18 | 12 | 3 | 1 |
| 243.0121 | -0.164189328 | 10.5 | 78745.32 | 7 | 13 | 3 | 1 |
| 244.0199 | -0.265961845 | 10 | 2261087.22 | 8 | 13 | 3 | 1 |
| 244.1135 | -1.494794244 | 3 | 176207.31 | 20 | 12 | 3 | 1 |
| 245.0277 | -0.366897159 | 9.5 | 135539.44 | 9 | 13 | 3 | 1 |
| 246.0355 | -0.46700556 | 9 | 1987727.63 | 10 | 13 | 3 | 1 |
| 246.1291 | -1.685697874 | 2 | 167600.15 | 22 | 12 | 3 | 1 |
| 248.0512 | -0.261639464 | 8 | 710262.41 | 12 | 13 | 3 | 1 |
| 248.1448 | -1.470510216 | 1 | 146361.33 | 24 | 12 | 3 | 1 |
| 249.0588 | -1.163980805 | 7.5 | 203898.84 | 13 | 13 | 3 | 1 |
| 250.0667 | -0.859369982 | 7 | 245514.21 | 14 | 13 | 3 | 1 |
| 251.0745 | -0.955492377 | 6.5 | 816037.41 | 15 | 13 | 3 | 1 |
| 252.0822 | -1.447541603 | 6 | 465611.5 | 16 | 13 | 3 | 1 |
| 253.0905 | 0.435022444 | 5.5 | 547578.17 | 17 | 13 | 3 | 1 |
| 254.0044 | 0.335033679 | 12 | 51305.21 | 6 | 14 | 3 | 1 |
| 254.0979 | -1.239284582 | 5 | 718169.71 | 18 | 13 | 3 | 1 |
| 255.0124 | 1.019951443 | 11.5 | 75634.71 | 7 | 14 | 3 | 1 |
| 255.1058 | -0.940393258 | 4.5 | 48493.42 | 19 | 13 | 3 | 1 |
| 256.02 | 0.137098683 | 11 | 754968.79 | 8 | 14 | 3 | 1 |
| 256.1136 | -1.034305582 | 4 | 156492.67 | 20 | 13 | 3 | 1 |
| 257.0279 | 0.42835835 | 10.5 | 311800.3 | 9 | 14 | 3 | 1 |
| 258.0356 | -0.057743967 | 10 | 2716975.76 | 10 | 14 | 3 | 1 |
| 258.1294 | -0.445125386 | 3 | 54171.49 | 22 | 13 | 3 | 1 |
| 259.0434 | -0.15402822 | 9.5 | 130235.78 | 11 | 14 | 3 | 1 |
| 260.0512 | -0.249566177 | 9 | 2173572.54 | 12 | 14 | 3 | 1 |
| 261.0586 | -1.876586639 | 8.5 | 199613.79 | 13 | 14 | 3 | 1 |
| 262.0667 | -0.820019574 | 8 | 1924422 | 14 | 14 | 3 | 1 |
| 263.0747 | -0.151667925 | 7.5 | 81159.9 | 15 | 14 | 3 | 1 |
| 264.0823 | -1.003095377 | 7 | 1908615.45 | 16 | 14 | 3 | 1 |
| 265.0906 | 0.792559851 | 6.5 | 310650.91 | 17 | 14 | 3 | 1 |
| 266.098 | -0.807596549 | 6 | 468105.99 | 18 | 14 | 3 | 1 |
| 267.0126 | 1.723142626 | 12.5 | 51235.91 | 7 | 15 | 3 | 1 |
| 267.1063 | 0.973770567 | 5.5 | 234859.39 | 19 | 14 | 3 | 1 |
| 268.0201 | 0.504066927 | 12 | 511258.9 | 8 | 15 | 3 | 1 |
| 268.1137 | -0.615037197 | 5 | 165512.75 | 20 | 14 | 3 | 1 |
| 269.0282 | 1.524377835 | 11.5 | 104144.08 | 9 | 15 | 3 | 1 |
| 270.0357 | 0.315143615 | 11 | 2582643.49 | 10 | 15 | 3 | 1 |
| 270.1292 | -1.16573711 | 4 | 66318.94 | 22 | 14 | 3 | 1 |
| 271.0438 | 1.328569325 | 10.5 | 166619.54 | 11 | 15 | 3 | 1 |
| 272.0514 | 0.496597581 | 10 | 991200.32 | 12 | 15 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 272.145 | -0.605926621 | 3 | 53103.06 | 24 | 14 | 3 | 1 |
| 273.0591 | 0.036988331 | 9.5 | 131410.49 | 13 | 15 | 3 | 1 |
| 274.067 | 0.310508111 | 9 | 376499.58 | 14 | 15 | 3 | 1 |
| 275.0745 | -0.872126609 | 8.5 | 393037.77 | 15 | 15 | 3 | 1 |
| 276.0823 | -0.959495578 | 8 | 243170.22 | 16 | 15 | 3 | 1 |
| 277.09 | -1.407122059 | 7.5 | 286926.09 | 17 | 15 | 3 | 1 |
| 278.0978 | -1.491918962 | 7 | 480990.74 | 18 | 15 | 3 | 1 |
| 279.1061 | 0.215330345 | 6.5 | 116820.85 | 19 | 15 | 3 | 1 |
| 280.0199 | -0.231769188 | 13 | 219786.3 | 8 | 16 | 3 | 1 |
| 280.1135 | -1.302684536 | 6 | 186446.52 | 20 | 15 | 3 | 1 |
| 281.028 | 0.747612896 | 12.5 | 260817.56 | 9 | 16 | 3 | 1 |
| 281.1219 | 0.74736318 | 5.5 | 160669.64 | 21 | 15 | 3 | 1 |
| 282.0355 | -0.407395357 | 12 | 1344841.97 | 10 | 16 | 3 | 1 |
| 282.1292 | -1.116154048 | 5 | 52881.08 | 22 | 15 | 3 | 1 |
| 283.0436 | 0.565637558 | 11.5 | 188267.27 | 11 | 16 | 3 | 1 |
| 284.0512 | -0.228479884 | 11 | 2464660.86 | 12 | 16 | 3 | 1 |
| 285.0595 | 1.438649089 | 10.5 | 78606.51 | 13 | 16 | 3 | 1 |
| 286.0667 | -0.751222839 | 10 | 1405087.16 | 14 | 16 | 3 | 1 |
| 287.0751 | 1.254377171 | 9.5 | 68547.05 | 15 | 16 | 3 | 1 |
| 288.0823 | -0.919528053 | 9 | 1443678.34 | 16 | 16 | 3 | 1 |
| 290.098 | -0.7407836 | 8 | 521613.2 | 18 | 16 | 3 | 1 |
| 291.106 | -0.137063457 | 7.5 | 77671.13 | 19 | 16 | 3 | 1 |
| 291.2004 | 1.580014062 | 0.5 | 51973.11 | 31 | 15 | 3 | 1 |
| 292.0202 | 0.80508194 | 14 | 100077.29 | 8 | 17 | 3 | 1 |
| 292.1136 | -0.906838161 | 7 | 146163.73 | 20 | 16 | 3 | 1 |
| 293.122 | 1.057922394 | 6.5 | 72925.86 | 21 | 16 | 3 | 1 |
| 294.0357 | 0.289420722 | 13 | 1292145.6 | 10 | 17 | 3 | 1 |
| 294.1293 | -0.730630519 | 6 | 64152.45 | 22 | 16 | 3 | 1 |
| 295.0435 | 0.203698818 | 12.5 | 175075.09 | 11 | 17 | 3 | 1 |
| 295.1375 | 0.542459317 | 5.5 | 161630.07 | 23 | 16 | 3 | 1 |
| 296.0511 | -0.556998127 | 12 | 1309967.94 | 12 | 17 | 3 | 1 |
| 297.0591 | 0.03399997 | 11.5 | 140930.05 | 13 | 17 | 3 | 1 |
| 297.1532 | 0.707043197 | 4.5 | 1738427.73 | 25 | 16 | 3 | 1 |
| 298.0667 | -0.720979046 | 11 | 629919.73 | 14 | 17 | 3 | 1 |
| 299.0745 | -0.802140629 | 10.5 | 157535.58 | 15 | 17 | 3 | 1 |
| 300.0823 | -0.882757051 | 10 | 195072.46 | 16 | 17 | 3 | 1 |
| 301.0901 | -0.962833786 | 9.5 | 238337.35 | 17 | 17 | 3 | 1 |
| 302.0978 | -1.373394411 | 9 | 301179.34 | 18 | 17 | 3 | 1 |
| 303.1058 | -0.791472186 | 8.5 | 68034.14 | 19 | 17 | 3 | 1 |
| 304.0201 | 0.444378711 | 15 | 91314.69 | 8 | 18 | 3 | 1 |
| 304.1135 | -1.199879526 | 8 | 205149.56 | 20 | 17 | 3 | 1 |
| 305.0282 | 1.344467664 | 14.5 | 82749.99 | 9 | 18 | 3 | 1 |
| 305.2158 | 0.688365886 | 0.5 | 82267.79 | 33 | 16 | 3 | 1 |
| 306.0355 | -0.375446498 | 14 | 524107.65 | 10 | 18 | 3 | 1 |
| 306.1292 | -1.02864959 | 7 | 62049.07 | 22 | 17 | 3 | 1 |
| 307.0437 | 0.847111406 | 13.5 | 222771.1 | 11 | 18 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 307.1376 | 0.846852421 | 6.5 | 58172.15 | 23 | 17 | 3 | 1 |
| 308.0511 | -0.535300512 | 13 | 1693945.61 | 12 | 18 | 3 | 1 |
| 309.0596 | 1.650493438 | 12.5 | 111657.77 | 13 | 18 | 3 | 1 |
| 309.1533 | 1.003063241 | 5.5 | 226643.29 | 25 | 17 | 3 | 1 |
| 310.0668 | -0.370565173 | 12 | 1450304.07 | 14 | 18 | 3 | 1 |
| 311.1689 | 0.835881148 | 4.5 | 14513907.43 | 27 | 17 | 3 | 1 |
| 312.0823 | -0.848813839 | 11 | 1027687.77 | 16 | 18 | 3 | 1 |
| 313.0909 | 1.629241958 | 10.5 | 48643.8 | 17 | 18 | 3 | 1 |
| 314.0979 | -1.002552657 | 10 | 576457.83 | 18 | 18 | 3 | 1 |
| 315.1063 | 0.825436415 | 9.5 | 48362.04 | 19 | 18 | 3 | 1 |
| 318.0354 | -0.675710486 | 15 | 265197.81 | 10 | 19 | 3 | 1 |
| 318.1289 | -1.932860584 | 8 | 56900.84 | 22 | 18 | 3 | 1 |
| 319.0438 | 1.128686426 | 14.5 | 88635.29 | 11 | 19 | 3 | 1 |
| 319.2312 | -0.124987767 | 0.5 | 72543.83 | 35 | 17 | 3 | 1 |
| 320.051 | -0.827679903 | 14 | 788120.88 | 12 | 19 | 3 | 1 |
| 321.0592 | 0.342927528 | 13.5 | 148364.39 | 13 | 19 | 3 | 1 |
| 322.0666 | -0.977747125 | 13 | 546664.31 | 14 | 19 | 3 | 1 |
| 323.0747 | -0.123500835 | 12.5 | 103513.8 | 15 | 19 | 3 | 1 |
| 323.1687 | 0.185971015 | 5.5 | 206446 | 27 | 18 | 3 | 1 |
| 324.0823 | -0.817384299 | 12 | 222583.98 | 16 | 19 | 3 | 1 |
| 325.0901 | -0.891751983 | 11.5 | 153514.74 | 17 | 19 | 3 | 1 |
| 325.1844 | 0.338577242 | 4.5 | 16960296.04 | 29 | 18 | 3 | 1 |
| 326.0978 | -1.272316072 | 11 | 156397.35 | 18 | 19 | 3 | 1 |
| 327.106 | -0.121978793 | 10.5 | 63592.44 | 19 | 19 | 3 | 1 |
| 328.1134 | -1.416886178 | 10 | 146004.87 | 20 | 19 | 3 | 1 |
| 330.0354 | -0.651141848 | 16 | 143744.04 | 10 | 20 | 3 | 1 |
| 330.1292 | -0.95386806 | 9 | 61468.58 | 22 | 19 | 3 | 1 |
| 331.0438 | 1.08777265 | 15.5 | 123458.7 | 11 | 20 | 3 | 1 |
| 332.0511 | -0.496610064 | 15 | 593290.66 | 12 | 20 | 3 | 1 |
| 333.0596 | 1.531560061 | 14.5 | 110457.53 | 13 | 20 | 3 | 1 |
| 333.2473 | 1.230619137 | 0.5 | 69943.32 | 37 | 18 | 3 | 1 |
| 334.0667 | -0.643284296 | 14 | 958405.41 | 14 | 20 | 3 | 1 |
| 334.2541 | -1.839615038 | 0 | 50802.7 | 38 | 18 | 3 | 1 |
| 335.0753 | 1.671567365 | 13.5 | 55788.79 | 15 | 20 | 3 | 1 |
| 336.0823 | -0.788199174 | 13 | 701764.14 | 16 | 20 | 3 | 1 |
| 337.1845 | 0.623101391 | 5.5 | 136200.17 | 29 | 19 | 3 | 1 |
| 338.0979 | -0.931386166 | 12 | 477642.44 | 18 | 20 | 3 | 1 |
| 339.2 | 0.177181635 | 4.5 | 6239694.28 | 31 | 19 | 3 | 1 |
| 340.1133 | -1.660914354 | 11 | 130392.74 | 20 | 20 | 3 | 1 |
| 342.0356 | -0.043562715 | 17 | 75819.28 | 10 | 21 | 3 | 1 |
| 342.129 | -1.50498562 | 10 | 56089.23 | 22 | 20 | 3 | 1 |
| 343.0439 | 1.341229554 | 16.5 | 62972.34 | 11 | 21 | 3 | 1 |
| 344.0511 | -0.479289039 | 16 | 373787.13 | 12 | 21 | 3 | 1 |
| 345.0595 | 1.188492093 | 15.5 | 107713.77 | 13 | 21 | 3 | 1 |
| 346.0667 | -0.620978171 | 15 | 386268.1 | 14 | 21 | 3 | 1 |
| 347.075 | 0.749406309 | 14.5 | 112298.69 | 15 | 21 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 348.0826 | 0.100838144 | 14 | 3774944.25 | 16 | 21 | 3 | 1 |
| 349.0906 | 0.601849853 | 13.5 | 84705.78 | 17 | 21 | 3 | 1 |
| 350.0979 | -0.899461884 | 13 | 128879.47 | 18 | 21 | 3 | 1 |
| 351.106 | -0.113640882 | 12.5 | 79597.43 | 19 | 21 | 3 | 1 |
| 351.2 | 0.171127592 | 5.5 | 79729.82 | 31 | 20 | 3 | 1 |
| 352.1134 | -1.320311542 | 12 | 126597.34 | 20 | 21 | 3 | 1 |
| 354.0357 | 0.240371297 | 18 | 65176.01 | 10 | 22 | 3 | 1 |
| 354.1292 | -0.88922269 | 11 | 63907.33 | 22 | 21 | 3 | 1 |
| 356.0511 | -0.463135555 | 17 | 217657.22 | 12 | 22 | 3 | 1 |
| 357.0596 | 1.428615079 | 16.5 | 98215.94 | 13 | 22 | 3 | 1 |
| 358.0668 | -0.320889742 | 16 | 583451.77 | 14 | 22 | 3 | 1 |
| 359.0754 | 1.838335941 | 15.5 | 68978.29 | 15 | 22 | 3 | 1 |
| 360.0824 | -0.457950526 | 15 | 483244.8 | 16 | 22 | 3 | 1 |
| 362.0979 | -0.869653556 | 14 | 373951.78 | 18 | 22 | 3 | 1 |
| 364.1135 | -1.002159037 | 13 | 160929.89 | 20 | 22 | 3 | 1 |
| 365.2157 | 0.301465773 | 5.5 | 63505.06 | 33 | 21 | 3 | 1 |
| 366.1289 | -1.679460341 | 12 | 57665.28 | 22 | 22 | 3 | 1 |
| 368.0512 | -0.176334131 | 18 | 134523.93 | 12 | 23 | 3 | 1 |
| 369.0596 | 1.382163491 | 17.5 | 75368.22 | 13 | 23 | 3 | 1 |
| 370.0667 | -0.58070579 | 17 | 258332.04 | 14 | 23 | 3 | 1 |
| 371.0751 | 0.970424449 | 16.5 | 86815.16 | 15 | 23 | 3 | 1 |
| 372.0824 | -0.443181207 | 16 | 178903.16 | 16 | 23 | 3 | 1 |
| 374.098 | -0.574448077 | 15 | 112004.21 | 18 | 23 | 3 | 1 |
| 376.1135 | -0.97018492 | 14 | 102930.09 | 20 | 23 | 3 | 1 |
| 378.1291 | -1.097243097 | 13 | 58249.44 | 22 | 23 | 3 | 1 |
| 379.2314 | 0.422169861 | 5.5 | 184481.72 | 35 | 22 | 3 | 1 |
| 380.0513 | 0.092355961 | 19 | 89982.23 | 12 | 24 | 3 | 1 |
| 381.247 | 0.288789241 | 4.5 | 9662373.54 | 37 | 22 | 3 | 1 |
| 382.0668 | -0.300732661 | 18 | 272405.64 | 14 | 24 | 3 | 1 |
| 384.0824 | -0.429334771 | 17 | 343753.12 | 16 | 24 | 3 | 1 |
| 386.0979 | -0.815595587 | 16 | 316014.57 | 18 | 24 | 3 | 1 |
| 388.1135 | -0.940188004 | 15 | 157230.41 | 20 | 24 | 3 | 1 |
| 390.1294 | -0.294517578 | 14 | 60786.9 | 22 | 24 | 3 | 1 |
| 392.0517 | 1.109803842 | 20 | 58962.85 | 12 | 25 | 3 | 1 |
| 393.247 | 0.279976785 | 5.5 | 57952.11 | 37 | 23 | 3 | 1 |
| 394.0668 | -0.291574846 | 19 | 150920.78 | 14 | 25 | 3 | 1 |
| 395.0753 | 1.417706432 | 18.5 | 67698.03 | 15 | 25 | 3 | 1 |
| 396.0826 | 0.088617887 | 18 | 139302.36 | 16 | 25 | 3 | 1 |
| 398.0983 | 0.213766344 | 17 | 106090.03 | 18 | 25 | 3 | 1 |
| 400.1137 | -0.412132682 | 16 | 79313.46 | 20 | 25 | 3 | 1 |
| 402.1292 | -0.783081043 | 15 | 57559.4 | 22 | 25 | 3 | 1 |
| 404.0513 | 0.086870165 | 21 | 62247.49 | 12 | 26 | 3 | 1 |
| 406.0668 | -0.28295829 | 20 | 136513.89 | 14 | 26 | 3 | 1 |
| 407.2627 | 0.393112512 | 5.5 | 5732989.9 | 39 | 24 | 3 | 1 |
| 408.0825 | -0.159036444 | 19 | 230788.43 | 16 | 26 | 3 | 1 |
| 409.2783 | 0.269010181 | 4.5 | 8039727.68 | 41 | 24 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 410.098 | -0.524020813 | 18 | 230235.98 | 18 | 26 | 3 | 1 |
| 412.1136 | -0.642783518 | 17 | 143848.03 | 20 | 26 | 3 | 1 |
| 414.1294 | -0.277449435 | 16 | 57987.43 | 22 | 26 | 3 | 1 |
| 418.067 | 0.203555931 | 21 | 82882.18 | 14 | 27 | 3 | 1 |
| 420.0827 | 0.321603445 | 20 | 110641.48 | 16 | 27 | 3 | 1 |
| 421.2785 | 0.736093174 | 5.5 | 106901.87 | 41 | 25 | 3 | 1 |
| 422.0986 | 0.912346905 | 19 | 85641.62 | 18 | 27 | 3 | 1 |
| 424.1142 | 0.790118003 | 18 | 67881.51 | 20 | 27 | 3 | 1 |
| 426.1294 | -0.269636334 | 17 | 51848.13 | 22 | 27 | 3 | 1 |
| 430.067 | 0.197876184 | 22 | 83696.75 | 14 | 28 | 3 | 1 |
| 432.0825 | -0.150202775 | 21 | 148378.58 | 16 | 28 | 3 | 1 |
| 433.2786 | 0.946505062 | 6.5 | 51109.21 | 41 | 26 | 3 | 1 |
| 434.098 | -0.49504926 | 20 | 178896.87 | 18 | 28 | 3 | 1 |
| 435.2939 | 0.138067655 | 5.5 | 3852620.9 | 43 | 26 | 3 | 1 |
| 436.1137 | -0.378112262 | 19 | 126579.72 | 20 | 28 | 3 | 1 |
| 437.3096 | 0.251766775 | 4.5 | 4690758.18 | 45 | 26 | 3 | 1 |
| 438.1294 | -0.262251221 | 18 | 75989.59 | 22 | 28 | 3 | 1 |
| 442.0674 | 1.097345184 | 23 | 50473.5 | 14 | 29 | 3 | 1 |
| 444.083 | 0.979772759 | 22 | 83331.62 | 16 | 29 | 3 | 1 |
| 446.0987 | 1.087428696 | 21 | 74751.87 | 18 | 29 | 3 | 1 |
| 448.1141 | 0.524643441 | 20 | 69050.31 | 20 | 29 | 3 | 1 |
| 449.3096 | 0.245042676 | 5.5 | 139211.38 | 45 | 27 | 3 | 1 |
| 450.1297 | 0.411214981 | 19 | 56669.77 | 22 | 29 | 3 | 1 |
| 452.0518 | 1.183715303 | 25 | 45316.75 | 12 | 30 | 3 | 1 |
| 454.0674 | 1.06834474 | 24 | 43834.49 | 14 | 30 | 3 | 1 |
| 456.0828 | 0.515476841 | 23 | 99690.81 | 16 | 30 | 3 | 1 |
| 458.0983 | 0.185768024 | 22 | 126315.82 | 18 | 30 | 3 | 1 |
| 460.1137 | -0.358389548 | 21 | 146097.21 | 20 | 30 | 3 | 1 |
| 462.1295 | -0.032242044 | 20 | 89493.38 | 22 | 30 | 3 | 1 |
| 463.3255 | 0.777207988 | 5.5 | 1945050.99 | 47 | 28 | 3 | 1 |
| 465.3408 | 0.021704523 | 4.5 | 1865174.22 | 49 | 28 | 3 | 1 |
| 468.0827 | 0.288624294 | 24 | 47688.3 | 16 | 31 | 3 | 1 |
| 470.0984 | 0.393747507 | 23 | 72481.41 | 18 | 31 | 3 | 1 |
| 472.1144 | 1.133413017 | 22 | 58411.33 | 20 | 31 | 3 | 1 |
| 477.3408 | 0.021158887 | 5.5 | 99606.31 | 49 | 29 | 3 | 1 |
| 480.0823 | -0.551780088 | 25 | 59986.45 | 16 | 32 | 3 | 1 |
| 482.0979 | -0.653186405 | 24 | 101231.75 | 18 | 32 | 3 | 1 |
| 484.1134 | -0.960311269 | 23 | 142643.81 | 20 | 32 | 3 | 1 |
| 486.1298 | 0.586469225 | 22 | 80203.01 | 22 | 32 | 3 | 1 |
| 490.0662 | -1.458780379 | 27 | 50508.57 | 14 | 33 | 3 | 1 |
| 491.3566 | 0.325832709 | 5.5 | 614139.53 | 51 | 30 | 3 | 1 |
| 492.0833 | 1.493855 | 26 | 41565.78 | 16 | 33 | 3 | 1 |
| 493.3723 | 0.425844924 | 4.5 | 107251.41 | 53 | 30 | 3 | 1 |
| 495.1063 | 0.525342005 | 24.5 | 75906.85 | 19 | 33 | 3 | 1 |
| 496.1144 | 1.078583039 | 24 | 41621.94 | 20 | 33 | 3 | 1 |
| 504.0825 | -0.12874875 | 27 | 51486.8 | 16 | 34 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 505.3725 | 0.811481299 | 5.5 | 82702.38 | 53 | 31 | 3 | 1 |
| 506.0976 | -1.214981563 | 26 | 83179.76 | 18 | 34 | 3 | 1 |
| 508.1137 | -0.324533557 | 25 | 84929.44 | 20 | 34 | 3 | 1 |
| 510.1291 | -0.813322868 | 24 | 101042.86 | 22 | 34 | 3 | 1 |
| 512.1452 | 0.068535256 | 23 | 45608.48 | 24 | 34 | 3 | 1 |
| 516.082 | -1.094592297 | 28 | 49137.36 | 16 | 35 | 3 | 1 |
| 519.388 | 0.50078194 | 5.5 | 129251.8 | 55 | 32 | 3 | 1 |
| 522.1301 | 1.12060319 | 25 | 41030.58 | 22 | 35 | 3 | 1 |
| 526.0661 | -1.549042483 | 30 | 59219.43 | 14 | 36 | 3 | 1 |
| 528.0817 | -1.637812073 | 29 | 66016.54 | 16 | 36 | 3 | 1 |
| 530.0981 | -0.216752286 | 28 | 63393.37 | 18 | 36 | 3 | 1 |
| 533.4041 | 1.33126263 | 5.5 | 63744.18 | 57 | 33 | 3 | 1 |
| 543.0124 | 0.478994816 | 35.5 | 51645.75 | 7 | 38 | 3 | 1 |
| 543.106 | -0.073466316 | 28.5 | 114859.75 | 19 | 37 | 3 | 1 |
| 544.1148 | 1.718574108 | 28 | 44462.29 | 20 | 37 | 3 | 1 |
| 544.3952 | -0.670284667 | 7 | 68789.96 | 56 | 34 | 3 | 1 |
| 545.1219 | 0.385418529 | 27.5 | 103633.6 | 21 | 37 | 3 | 1 |
| 547.1381 | 1.389230719 | 26.5 | 126365.06 | 23 | 37 | 3 | 1 |
| 547.4196 | 1.023164996 | 5.5 | 66903.96 | 59 | 34 | 3 | 1 |
| 554.0977 | -0.929257641 | 30 | 44069.03 | 18 | 38 | 3 | 1 |
| 556.1132 | -1.195618455 | 29 | 75926.23 | 20 | 38 | 3 | 1 |
| 558.1292 | -0.564205962 | 28 | 101246.45 | 22 | 38 | 3 | 1 |
| 560.1442 | -1.72258918 | 27 | 95040.54 | 24 | 38 | 3 | 1 |
| 569.1224 | 1.247712067 | 29.5 | 125253.21 | 21 | 39 | 3 | 1 |
| 571.1376 | 0.455407101 | 28.5 | 117601.57 | 23 | 39 | 3 | 1 |
| 573.1541 | 1.936830165 | 27.5 | 81851.96 | 25 | 39 | 3 | 1 |
| 575.1681 | -0.938681219 | 26.5 | 60272.26 | 27 | 39 | 3 | 1 |
| 579.1996 | -0.586843983 | 24.5 | 52323.79 | 31 | 39 | 3 | 1 |
| 580.1133 | -0.973774347 | 31 | 85402.53 | 20 | 40 | 3 | 1 |
| 584.1448 | -0.624673492 | 29 | 95058.37 | 24 | 40 | 3 | 1 |
| 586.1619 | 1.851198464 | 28 | 53055.69 | 26 | 40 | 3 | 1 |
| 589.4667 | 1.204649652 | 5.5 | 49525.38 | 65 | 37 | 3 | 1 |
| 591.106 | -0.067500579 | 32.5 | 50804.26 | 19 | 41 | 3 | 1 |
| 593.1228 | 1.871622669 | 31.5 | 94118.24 | 21 | 41 | 3 | 1 |
| 595.1376 | 0.437041978 | 30.5 | 114406.59 | 23 | 41 | 3 | 1 |
| 597.1528 | -0.318008958 | 29.5 | 103836.94 | 25 | 41 | 3 | 1 |
| 600.082 | -0.94137046 | 35 | 53273.93 | 16 | 42 | 3 | 1 |
| 603.482 | 0.596704152 | 5.5 | 111686.08 | 67 | 38 | 3 | 1 |
| 604.1132 | -1.100620328 | 33 | 81791.48 | 20 | 42 | 3 | 1 |
| 605.4977 | 0.677294526 | 4.5 | 5098216.39 | 69 | 38 | 3 | 1 |
| 606.1295 | -0.024582205 | 32 | 83575.51 | 22 | 42 | 3 | 1 |
| 615.1065 | 0.748001109 | 34.5 | 49487.8 | 19 | 43 | 3 | 1 |
| 617.1222 | 0.826579277 | 33.5 | 66183.66 | 21 | 43 | 3 | 1 |
| 619.137 | -0.548989664 | 32.5 | 75816.91 | 23 | 43 | 3 | 1 |
| 621.1535 | 0.821214754 | 31.5 | 75509.38 | 25 | 43 | 3 | 1 |
| 623.1693 | 1.05926383 | 30.5 | 52075.71 | 27 | 43 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 628.113 | -1.376979634 | 35 | 72551.78 | 20 | 44 | 3 | 1 |
| 631.1384 | 1.679666109 | 33.5 | 65084.04 | 23 | 44 | 3 | 1 |
| 631.5133 | 0.570217928 | 5.5 | 234160.71 | 71 | 40 | 3 | 1 |
| 633.529 | 0.647326745 | 4.5 | 9966396.25 | 73 | 40 | 3 | 1 |
| 634.162 | 1.868768887 | 32 | 48933.64 | 26 | 44 | 3 | 1 |
| 637.0892 | -1.867709855 | 37.5 | 45912.57 | 17 | 45 | 3 | 1 |
| 641.1215 | -0.296199619 | 35.5 | 107537.04 | 21 | 45 | 3 | 1 |
| 643.1374 | 0.093448158 | 34.5 | 90740.3 | 23 | 45 | 3 | 1 |
| 645.1541 | 1.720677138 | 33.5 | 74297.35 | 25 | 45 | 3 | 1 |
| 647.1691 | 0.710942978 | 32.5 | 97186.07 | 27 | 45 | 3 | 1 |
| 651.1994 | -0.829084843 | 30.5 | 52916.94 | 31 | 45 | 3 | 1 |
| 652.113 | -1.326302118 | 37 | 59533.69 | 20 | 46 | 3 | 1 |
| 654.129 | -0.787152985 | 36 | 46391.96 | 22 | 46 | 3 | 1 |
| 657.1542 | 1.841428128 | 34.5 | 64527.34 | 25 | 46 | 3 | 1 |
| 659.5446 | 0.545983087 | 5.5 | 228138.41 | 75 | 42 | 3 | 1 |
| 660.1765 | 0.053167603 | 33 | 50308.52 | 28 | 46 | 3 | 1 |
| 661.5604 | 0.771056419 | 4.5 | 10070947.77 | 77 | 42 | 3 | 1 |
| 664.2087 | 1.40784262 | 31 | 46839.5 | 32 | 46 | 3 | 1 |
| 665.1212 | -0.736556945 | 37.5 | 49548 | 21 | 47 | 3 | 1 |
| 667.1371 | -0.359596122 | 36.5 | 64274.5 | 23 | 47 | 3 | 1 |
| 669.1527 | -0.433234259 | 35.5 | 58879.92 | 25 | 47 | 3 | 1 |
| 671.1687 | 0.089545304 | 34.5 | 63946.75 | 27 | 47 | 3 | 1 |
| 678.1288 | -1.054223396 | 38 | 54873.96 | 22 | 48 | 3 | 1 |
| 680.1443 | -1.271640298 | 37 | 55373.96 | 24 | 48 | 3 | 1 |
| 683.1673 | -1.961301971 | 35.5 | 94994.42 | 27 | 48 | 3 | 1 |
| 684.1753 | -1.702630914 | 35 | 78953.48 | 28 | 48 | 3 | 1 |
| 687.5755 | -0.058029987 | 5.5 | 163286.46 | 79 | 44 | 3 | 1 |
| 689.1225 | 1.17555435 | 39.5 | 50395.05 | 21 | 49 | 3 | 1 |
| 689.5915 | 0.449686719 | 4.5 | 7035275.46 | 81 | 44 | 3 | 1 |
| 691.1368 | -0.781176141 | 38.5 | 62187.38 | 23 | 49 | 3 | 1 |
| 695.1683 | -0.488946107 | 36.5 | 60616.44 | 27 | 49 | 3 | 1 |
| 700.2078 | 0.050127979 | 34 | 59085.25 | 32 | 49 | 3 | 1 |
| 702.2228 | -0.875647247 | 33 | 50406.64 | 34 | 49 | 3 | 1 |
| 703.1376 | 0.369913508 | 39.5 | 45134.49 | 23 | 50 | 3 | 1 |
| 715.6071 | 0.363467739 | 5.5 | 70470.4 | 83 | 46 | 3 | 1 |
| 717.6229 | 0.571470384 | 4.5 | 2979082.76 | 85 | 46 | 3 | 1 |
| 727.136 | -1.842705534 | 41.5 | 45401.41 | 23 | 52 | 3 | 1 |
| 740.2402 | 1.53342353 | 35 | 58930.96 | 36 | 52 | 3 | 1 |
| 741.153 | 0.013627416 | 41.5 | 64637.56 | 25 | 53 | 3 | 1 |
| 743.1672 | -1.937514479 | 40.5 | 59147.32 | 27 | 53 | 3 | 1 |
| 745.6542 | 0.549987146 | 4.5 | 770967.23 | 89 | 48 | 3 | 1 |
| 758.1911 | -1.338578943 | 40 | 64345.79 | 30 | 54 | 3 | 1 |
| 765.1528 | -0.24818566 | 43.5 | 55043.73 | 25 | 55 | 3 | 1 |
| 769.1831 | -1.546963473 | 41.5 | 56811.22 | 29 | 55 | 3 | 1 |
| 773.685 | -0.116197147 | 4.5 | 123934.27 | 93 | 50 | 3 | 1 |
| 782.1919 | -0.274740688 | 42 | 81313.49 | 30 | 56 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 787.1368 | -0.685903174 | 46.5 | 56346.5 | 23 | 57 | 3 | 1 |
| 798.2227 | -0.895613918 | 41 | 48048.26 | 34 | 57 | 3 | 1 |
| 819.2014 | 1.782348764 | 44.5 | 93672.11 | 31 | 59 | 3 | 1 |
| 827.1689 | 0.314446157 | 47.5 | 54025.35 | 27 | 60 | 3 | 1 |
| 829.7478 | 0.132690939 | 4.5 | 66919.48 | 101 | 54 | 3 | 1 |
| 833.215 | -0.707980032 | 44.5 | 46428.72 | 33 | 60 | 3 | 1 |
| 849.5274 | -1.400659159 | 22.5 | 78258.68 | 73 | 58 | 3 | 1 |
| 856.2086 | 0.97534738 | 47 | 67073.71 | 32 | 62 | 3 | 1 |
| 857.7793 | 0.361515033 | 4.5 | 145566.82 | 105 | 56 | 3 | 1 |
| 863.1703 | 1.923262643 | 50.5 | 50111.18 | 27 | 63 | 3 | 1 |
| 867.2923 | -1.775522815 | 41.5 | 51119.66 | 43 | 62 | 3 | 1 |
| 872.2382 | -0.991585948 | 46 | 48968.25 | 36 | 63 | 3 | 1 |
| 874.1612 | 0.440536791 | 52 | 67302.48 | 26 | 64 | 3 | 1 |
| 878.1928 | 0.780125429 | 50 | 62816.43 | 30 | 64 | 3 | 1 |
| 885.2454 | -1.683033306 | 46.5 | 50371.25 | 37 | 64 | 3 | 1 |
| 885.8106 | 0.350074958 | 4.5 | 246736.83 | 109 | 58 | 3 | 1 |
| 898.161 | 0.206087815 | 54 | 52645.29 | 26 | 66 | 3 | 1 |
| 904.2075 | -0.292963642 | 51 | 84271.73 | 32 | 66 | 3 | 1 |
| 911.1701 | 1.6024476 | 54.5 | 53353.97 | 27 | 67 | 3 | 1 |
| 913.1832 | -1.193515933 | 53.5 | 51322.11 | 29 | 67 | 3 | 1 |
| 913.8419 | 0.339336712 | 4.5 | 274144.67 | 113 | 60 | 3 | 1 |
| 915.6685 | -1.026462126 | 17.5 | 49820.45 | 91 | 62 | 3 | 1 |
| 916.2077 | -0.070835462 | 52 | 50684.95 | 32 | 67 | 3 | 1 |
| 920.2409 | 1.994155725 | 50 | 98477.13 | 36 | 67 | 3 | 1 |
| 926.1917 | -0.447963218 | 54 | 50986.54 | 30 | 68 | 3 | 1 |
| 941.8733 | 0.435409071 | 4.5 | 180774.58 | 117 | 62 | 3 | 1 |
| 944.2396 | 0.566699705 | 52 | 60647.54 | 36 | 69 | 3 | 1 |
| 948.2708 | 0.458835387 | 50 | 47639.67 | 40 | 69 | 3 | 1 |
| 962.2862 | 0.192354453 | 50 | 51579.19 | 42 | 70 | 3 | 1 |
| 966.3177 | 0.398523336 | 48 | 49583.8 | 46 | 70 | 3 | 1 |
| 967.2307 | -0.558191235 | 54.5 | 84671.47 | 35 | 71 | 3 | 1 |
| 969.9042 | 0.0104134 | 4.5 | 73990.54 | 121 | 64 | 3 | 1 |
| 991.6999 | -0.846928883 | 21.5 | 51806.8 | 95 | 68 | 3 | 1 |
| 1004.241 | 1.926931612 | 57 | 47898.82 | 36 | 74 | 3 | 1 |
| 1007.734 | 1.44889707 | 20.5 | 53217.47 | 99 | 69 | 3 | 1 |
| 1026.319 | 1.641889867 | 53 | 52590.06 | 46 | 75 | 3 | 1 |
| 1029.246 | -0.767454347 | 58.5 | 46597.14 | 37 | 76 | 3 | 1 |
| 1062.225 | 1.77467374 | 63 | 53077.42 | 34 | 79 | 3 | 1 |
| 1082.031 | 1.857712941 | 4.5 | 61439.88 | 137 | 72 | 3 | 1 |
| 1082.192 | -0.568198559 | 67 | 46703.34 | 30 | 81 | 3 | 1 |
| 1083.037 | -0.290756398 | 4 | 51926.15 | 138 | 72 | 3 | 1 |
| 1109.054 | 1.29398701 | 5 | 59990.23 | 140 | 74 | 3 | 1 |
| 1109.497 | -0.351420417 | 46.5 | 46109.29 | 69 | 80 | 3 | 1 |
| 1109.779 | 0.279425005 | 25.5 | 53329.64 | 105 | 77 | 3 | 1 |
| 1110.062 | 0.819865083 | 4.5 | 89107.88 | 141 | 74 | 3 | 1 |
| 1110.881 | 0.256643217 | 18 | 75897.26 | 118 | 76 | 3 | 1 |

**b)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O | S |
|---|---|---|---|---|---|---|---|
| 93.9728 | -2.28683 | 1 | 2333199.5 | 2 | 1 | 3 | 1 |
| 94.9807 | -1.47293 | 0.5 | 21072048.92 | 3 | 1 | 3 | 1 |
| 104.9653 | 1.048919 | 2.5 | 10841.24 | 1 | 2 | 3 | 1 |
| 106.9809 | 0.561783 | 1.5 | 7320835.87 | 3 | 2 | 3 | 1 |
| 108.9966 | 1.010124 | 0.5 | 2712140.45 | 5 | 2 | 3 | 1 |
| 119.9887 | 0.292528 | 2 | 62284.8 | 4 | 3 | 3 | 1 |
| 120.9965 | 0.083473 | 1.5 | 1697099.17 | 5 | 3 | 3 | 1 |
| 123.0121 | -0.32436 | 0.5 | 1404597.5 | 7 | 3 | 3 | 1 |
| 132.9965 | 0.075942 | 2.5 | 24202.44 | 5 | 4 | 3 | 1 |
| 137.0276 | -1.38585 | 0.5 | 200061.48 | 9 | 4 | 3 | 1 |
| 143.9884 | -1.83973 | 4 | 56083.07 | 4 | 5 | 3 | 1 |
| 149.0276 | -1.27426 | 1.5 | 63754.96 | 9 | 5 | 3 | 1 |
| 154.9809 | 0.38779 | 5.5 | 38011.86 | 3 | 6 | 3 | 1 |
| 155.9886 | -0.41606 | 5 | 604358.14 | 4 | 6 | 3 | 1 |
| 156.9964 | -0.57262 | 4.5 | 6660420.78 | 5 | 6 | 3 | 1 |
| 168.9966 | 0.651493 | 5.5 | 39442.63 | 5 | 7 | 3 | 1 |
| 170.0043 | -0.08764 | 5 | 20941188.06 | 6 | 7 | 3 | 1 |
| 171.0121 | -0.23332 | 4.5 | 2905824.73 | 7 | 7 | 3 | 1 |
| 180.9965 | 0.055802 | 6.5 | 3698739.11 | 5 | 8 | 3 | 1 |
| 183.0122 | 0.328394 | 5.5 | 511433348.8 | 7 | 8 | 3 | 1 |
| 184.0198 | -0.8961 | 5 | 20270630.3 | 8 | 8 | 3 | 1 |
| 185.0276 | -1.02633 | 4.5 | 1067406.08 | 9 | 8 | 3 | 1 |
| 191.0746 | -0.73217 | 1.5 | 382828.95 | 15 | 8 | 3 | 1 |
| 191.9883 | -1.90063 | 8 | 13177.45 | 4 | 9 | 3 | 1 |
| 192.9962 | -1.5021 | 7.5 | 21178.78 | 5 | 9 | 3 | 1 |
| 193.0902 | -0.98348 | 0.5 | 24524.73 | 17 | 8 | 3 | 1 |
| 194.004 | -1.62316 | 7 | 593122.87 | 6 | 9 | 3 | 1 |
| 195.0122 | 0.308186 | 6.5 | 20162138.29 | 7 | 9 | 3 | 1 |
| 196.0199 | -0.33109 | 6 | 8197732.64 | 8 | 9 | 3 | 1 |
| 197.0279 | 0.558804 | 5.5 | 56843043.79 | 9 | 9 | 3 | 1 |
| 198.0355 | -0.5802 | 5 | 1712417.22 | 10 | 9 | 3 | 1 |
| 199.0432 | -1.20526 | 4.5 | 432480.05 | 11 | 9 | 3 | 1 |
| 205.0902 | -0.92593 | 1.5 | 62430.93 | 17 | 9 | 3 | 1 |
| 207.0121 | -0.19274 | 7.5 | 8243816.36 | 7 | 10 | 3 | 1 |
| 208.0196 | -1.75416 | 7 | 150988.63 | 8 | 10 | 3 | 1 |
| 209.0278 | 0.048319 | 6.5 | 8199712.19 | 9 | 10 | 3 | 1 |
| 210.0352 | -1.97538 | 6 | 1510177.41 | 10 | 10 | 3 | 1 |
| 211.0433 | -0.6629 | 5.5 | 4734852.41 | 11 | 10 | 3 | 1 |
| 213.0588 | -1.36066 | 4.5 | 252480.22 | 13 | 10 | 3 | 1 |
| 219.1059 | -0.6385 | 1.5 | 24954.98 | 19 | 10 | 3 | 1 |
| 220.0198 | -0.74948 | 8 | 445468.79 | 8 | 11 | 3 | 1 |
| 221.0278 | 0.045696 | 7.5 | 1054986.51 | 9 | 11 | 3 | 1 |

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|---|---|---|---|---|---|---|---|
| 222.0354 | -0.96786 | 7 | 75002.56 | 10 | 11 | 3 | 1 |
| 223.0434 | -0.17889 | 6.5 | 1401504.48 | 11 | 11 | 3 | 1 |
| 224.0509 | -1.62865 | 6 | 145168.54 | 12 | 11 | 3 | 1 |
| 225.059 | -0.39945 | 5.5 | 3809232.44 | 13 | 11 | 3 | 1 |
| 226.0666 | -1.39295 | 5 | 275629.01 | 14 | 11 | 3 | 1 |
| 227.0743 | -1.93725 | 4.5 | 473793.94 | 15 | 11 | 3 | 1 |
| 231.1059 | -0.60535 | 2.5 | 5917.13 | 19 | 11 | 3 | 1 |
| 233.0281 | 1.330743 | 8.5 | 478860.27 | 9 | 12 | 3 | 1 |
| 233.1217 | 0.043325 | 1.5 | 12195.94 | 21 | 11 | 3 | 1 |
| 235.0436 | 0.681151 | 7.5 | 343335.91 | 11 | 12 | 3 | 1 |
| 237.0591 | 0.042605 | 6.5 | 563291.92 | 13 | 12 | 3 | 1 |
| 239.0748 | 0.251386 | 5.5 | 3755693.56 | 15 | 12 | 3 | 1 |
| 241.0904 | 0.041893 | 4.5 | 253578.98 | 17 | 12 | 3 | 1 |
| 243.0125 | 1.481819 | 10.5 | 34732.24 | 7 | 13 | 3 | 1 |
| 244.0198 | -0.67576 | 10 | 89207.49 | 8 | 13 | 3 | 1 |
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| 247.0437 | 1.052851 | 8.5 | 241655.09 | 11 | 13 | 3 | 1 |
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| 248.0515 | 0.947788 | 8 | 25259.55 | 12 | 13 | 3 | 1 |
| 248.9653 | 0.44223 | 14.5 | 14001.6 | 1 | 14 | 3 | 1 |
| 249.0591 | 0.040553 | 7.5 | 155630.22 | 13 | 13 | 3 | 1 |
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| 251.0746 | -0.5572 | 6.5 | 399589.43 | 15 | 13 | 3 | 1 |
| 253.0904 | 0.039907 | 5.5 | 2191250.63 | 17 | 13 | 3 | 1 |
| 254.0039 | -1.63344 | 12 | 13149.49 | 6 | 14 | 3 | 1 |
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| 262.0664 | -1.96477 | 8 | 409036.77 | 14 | 14 | 3 | 1 |
| 263.075 | 0.988692 | 7.5 | 42291.37 | 15 | 14 | 3 | 1 |
| 265.0906 | 0.79256 | 6.5 | 118004.94 | 17 | 14 | 3 | 1 |
| 266.0977 | -1.935 | 6 | 88060.24 | 18 | 14 | 3 | 1 |
| 267.0122 | 0.225083 | 12.5 | 16746.63 | 7 | 15 | 3 | 1 |
| 267.1062 | 0.599387 | 5.5 | 1125887.07 | 19 | 14 | 3 | 1 |
| 268.0202 | 0.877173 | 12 | 39860.53 | 8 | 15 | 3 | 1 |
| 268.1135 | -1.36099 | 5 | 28165.31 | 20 | 14 | 3 | 1 |
| 269.1219 | 0.780688 | 4.5 | 222767.53 | 21 | 14 | 3 | 1 |
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| 277.0902 | -0.68534 | 7.5 | 53883.88 | 17 | 15 | 3 | 1 |
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| 283.1375 | 0.56545 | 4.5 | 516173.71 | 23 | 15 | 3 | 1 |
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| 284.9655 | 1.088203 | 17.5 | 9179.16 | 1 | 17 | 3 | 1 |
| 286.0665 | -1.45036 | 10 | 184593 | 14 | 16 | 3 | 1 |
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| 290.0977 | -1.77492 | 8 | 75511.22 | 18 | 16 | 3 | 1 |
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| 295.1373 | -0.13519 | 5.5 | 793677.3 | 23 | 16 | 3 | 1 |
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| 297.1531 | 0.370516 | 4.5 | 11867614.88 | 25 | 16 | 3 | 1 |
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| 301.0908 | 1.362049 | 9.5 | 112263.21 | 17 | 17 | 3 | 1 |
| 301.1845 | 0.69758 | 2.5 | 8529.25 | 29 | 16 | 3 | 1 |
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| 303.2001 | 0.528034 | 1.5 | 72062.85 | 31 | 16 | 3 | 1 |
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| 304.1133 | -1.85753 | 8 | 21093.8 | 20 | 17 | 3 | 1 |
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| 306.0356 | -0.04869 | 14 | 57885.23 | 10 | 18 | 3 | 1 |
| 307.1376 | 0.846852 | 6.5 | 46177.14 | 23 | 17 | 3 | 1 |
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| 310.0668 | -0.37057 | 12 | 78343.28 | 14 | 18 | 3 | 1 |
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| 317.0278 | 0.031858 | 15.5 | 8987.97 | 9 | 19 | 3 | 1 |
| 317.122 | 0.977858 | 8.5 | 8356.7 | 21 | 18 | 3 | 1 |
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| 319.1376 | 0.81501 | 7.5 | 8342.32 | 23 | 18 | 3 | 1 |
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| 321.153 | 0.031449 | 6.5 | 22855.27 | 25 | 18 | 3 | 1 |
| 323.1687 | 0.185971 | 5.5 | 1063626.52 | 27 | 18 | 3 | 1 |
| 325.1846 | 0.953613 | 4.5 | 43762883.49 | 29 | 18 | 3 | 1 |
| 328.1133 | -1.72166 | 10 | 15200.99 | 20 | 19 | 3 | 1 |
| 330.0361 | 1.469841 | 16 | 33860.29 | 10 | 20 | 3 | 1 |
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| 357.1535 | 1.428239 | 9.5 | 6947.24 | 25 | 21 | 3 | 1 |
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| 359.2628 | 0.723983 | 1.5 | 232395.49 | 39 | 20 | 3 | 1 |
| 361.2784 | 0.581546 | 0.5 | 48368.69 | 41 | 20 | 3 | 1 |
| 364.1133 | -1.55144 | 13 | 12805.88 | 20 | 22 | 3 | 1 |
| 365.2159 | 0.849088 | 5.5 | 35034.18 | 33 | 21 | 3 | 1 |
| 367.2315 | 0.708273 | 4.5 | 79992.21 | 35 | 21 | 3 | 1 |
| 368.0513 | 0.095367 | 18 | 17964.41 | 12 | 23 | 3 | 1 |
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| 379.2314 | 0.42217 | 5.5 | 25040.17 | 35 | 22 | 3 | 1 |
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|---|---|---|---|---|---|---|---|
| 387.2003 | 0.93001 | 8.5 | 20635.54 | 31 | 23 | 3 | 1 |
| 387.2941 | 0.671583 | 1.5 | 102315.52 | 43 | 22 | 3 | 1 |
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| 392.052 | 1.87501 | 20 | 11169.09 | 12 | 25 | 3 | 1 |
| 393.247 | 0.279977 | 5.5 | 8403.54 | 37 | 23 | 3 | 1 |
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| 395.2626 | 0.152051 | 4.5 | 14189.72 | 39 | 23 | 3 | 1 |
| 401.3097 | 0.523536 | 1.5 | 135061.61 | 45 | 23 | 3 | 1 |
| 403.3253 | 0.39695 | 0.5 | 56359.48 | 47 | 23 | 3 | 1 |
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| 407.2627 | 0.393113 | 5.5 | 10014.45 | 39 | 24 | 3 | 1 |
| 409.2784 | 0.513343 | 4.5 | 33817.13 | 41 | 24 | 3 | 1 |
| 413.3097 | 0.508336 | 2.5 | 6415.23 | 45 | 24 | 3 | 1 |
| 415.3255 | 0.867032 | 1.5 | 216112.79 | 47 | 24 | 3 | 1 |
| 417.3412 | 0.98265 | 0.5 | 81190.38 | 49 | 24 | 3 | 1 |
| 421.2786 | 0.973466 | 5.5 | 6238.92 | 41 | 25 | 3 | 1 |
| 423.2943 | 1.086952 | 4.5 | 12375.7 | 43 | 25 | 3 | 1 |
| 428.052 | 1.717318 | 23 | 5820.86 | 12 | 28 | 3 | 1 |
| 429.2471 | 0.489462 | 8.5 | 6083.06 | 37 | 26 | 3 | 1 |
| 429.3409 | 0.25644 | 1.5 | 122144.16 | 49 | 25 | 3 | 1 |
| 430.0664 | -1.19726 | 22 | 17394.26 | 14 | 28 | 3 | 1 |
| 431.3566 | 0.371155 | 0.5 | 81827.43 | 51 | 25 | 3 | 1 |
| 435.2944 | 1.286717 | 5.5 | 20293.95 | 43 | 26 | 3 | 1 |
| 437.3097 | 0.480438 | 4.5 | 1988029.08 | 45 | 26 | 3 | 1 |
| 443.3567 | 0.586661 | 1.5 | 114260.66 | 51 | 26 | 3 | 1 |
| 444.0823 | -0.59651 | 22 | 12508.27 | 16 | 29 | 3 | 1 |
| 445.3726 | 1.145334 | 0.5 | 109120.09 | 53 | 26 | 3 | 1 |
| 448.0195 | -1.03768 | 27 | 7153.55 | 8 | 30 | 3 | 1 |
| 449.31 | 1.135298 | 5.5 | 23729.22 | 45 | 27 | 3 | 1 |
| 451.3255 | 0.797873 | 4.5 | 2617857.06 | 47 | 27 | 3 | 1 |
| 452.051 | -0.586 | 25 | 7224.87 | 12 | 30 | 3 | 1 |
| 455.3564 | -0.08762 | 2.5 | 7275.4 | 51 | 27 | 3 | 1 |
| 457.2788 | 1.334199 | 8.5 | 15325.34 | 41 | 28 | 3 | 1 |
| 457.3726 | 1.115284 | 1.5 | 120449.42 | 53 | 27 | 3 | 1 |
| 459.2944 | 1.219481 | 7.5 | 651176.31 | 43 | 28 | 3 | 1 |
| 459.3883 | 1.219231 | 0.5 | 142314.86 | 55 | 27 | 3 | 1 |
| 465.3411 | 0.666393 | 4.5 | 684957.93 | 49 | 28 | 3 | 1 |
| 467.3566 | 0.342565 | 3.5 | 6840.47 | 51 | 28 | 3 | 1 |
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| 473.3101 | 1.289009 | 7.5 | 11082.68 | 45 | 29 | 3 | 1 |
| 473.4038 | 0.86628 | 0.5 | 161982.11 | 57 | 28 | 3 | 1 |
| 477.3415 | 1.487616 | 5.5 | 9168.48 | 49 | 29 | 3 | 1 |
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| 480.0819 | -1.38497 | 25 | 14425.82 | 16 | 32 | 3 | 1 |
| 482.0978 | -0.86061 | 24 | 19727.41 | 18 | 32 | 3 | 1 |
| 485.4039 | 1.050879 | 1.5 | 107258.4 | 57 | 29 | 3 | 1 |
| 487.4197 | 1.354276 | 0.5 | 130349.37 | 59 | 29 | 3 | 1 |
| 490.0662 | -1.45878 | 27 | 6310.72 | 14 | 33 | 3 | 1 |
| 491.075 | 0.529655 | 26.5 | 15165.39 | 15 | 33 | 3 | 1 |
| 493.3726 | 1.033905 | 4.5 | 79552.2 | 53 | 30 | 3 | 1 |
| 497.122 | 0.623791 | 23.5 | 50024.57 | 21 | 33 | 3 | 1 |
| 497.4032 | -0.38178 | 2.5 | 6537.69 | 57 | 30 | 3 | 1 |
| 499.4196 | 1.121503 | 1.5 | 98611.89 | 59 | 30 | 3 | 1 |
| 501.0596 | 1.018044 | 28.5 | 8247.73 | 13 | 34 | 3 | 1 |
| 501.4353 | 1.216709 | 0.5 | 73903 | 61 | 30 | 3 | 1 |
| 503.0739 | -1.66953 | 27.5 | 11454.75 | 15 | 34 | 3 | 1 |
| 504.0819 | -1.31903 | 27 | 5297.95 | 16 | 34 | 3 | 1 |
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| 507.3882 | 0.906802 | 4.5 | 276096.17 | 55 | 31 | 3 | 1 |
| 513.4351 | 0.798738 | 1.5 | 81362.23 | 61 | 31 | 3 | 1 |
| 515.4507 | 0.698612 | 0.5 | 50979 | 63 | 31 | 3 | 1 |
| 517.0894 | -1.91437 | 27.5 | 17617.95 | 17 | 35 | 3 | 1 |
| 519.1053 | -1.42533 | 26.5 | 32974.64 | 19 | 35 | 3 | 1 |
| 521.122 | 0.595063 | 25.5 | 48072.17 | 21 | 35 | 3 | 1 |
| 523.4198 | 1.452183 | 3.5 | 9818.56 | 59 | 32 | 3 | 1 |
| 525.4347 | 0.019222 | 2.5 | 6332.5 | 61 | 32 | 3 | 1 |
| 527.4507 | 0.682718 | 1.5 | 62272.22 | 63 | 32 | 3 | 1 |
| 529.0909 | 0.964107 | 28.5 | 27382.01 | 17 | 36 | 3 | 1 |
| 529.4666 | 1.152293 | 0.5 | 27894.39 | 65 | 32 | 3 | 1 |
| 531.1057 | -0.63999 | 27.5 | 36187.36 | 19 | 36 | 3 | 1 |
| 532.1136 | -0.49783 | 27 | 16607.4 | 20 | 36 | 3 | 1 |
| 533.1225 | 1.519541 | 26.5 | 35800.24 | 21 | 36 | 3 | 1 |
| 534.1286 | -1.71288 | 26 | 19849.63 | 22 | 36 | 3 | 1 |
| 536.1442 | -1.7997 | 25 | 10514.56 | 24 | 36 | 3 | 1 |
| 541.4663 | 0.572704 | 1.5 | 35543.72 | 65 | 33 | 3 | 1 |
| 543.1052 | -1.54648 | 28.5 | 24889.43 | 19 | 37 | 3 | 1 |
| 543.4822 | 1.030578 | 0.5 | 15459.14 | 67 | 33 | 3 | 1 |
| 545.1211 | -1.08214 | 27.5 | 36949.83 | 21 | 37 | 3 | 1 |
| 547.1364 | -1.71785 | 26.5 | 24484.76 | 23 | 37 | 3 | 1 |
| 555.4822 | 1.008314 | 1.5 | 14634.89 | 67 | 34 | 3 | 1 |
| 557.1225 | 1.454081 | 28.5 | 28581.11 | 21 | 38 | 3 | 1 |
| 557.4973 | 0.018117 | 0.5 | 6507.39 | 69 | 34 | 3 | 1 |
| 558.1292 | -0.56421 | 28 | 13578.17 | 22 | 38 | 3 | 1 |
| 563.0757 | 1.705102 | 32.5 | 5534.08 | 15 | 39 | 3 | 1 |
| 565.0908 | 0.725725 | 31.5 | 14214.81 | 17 | 39 | 3 | 1 |
| 566.0982 | -0.02632 | 31 | 14442.08 | 18 | 39 | 3 | 1 |
| 567.1065 | 0.811312 | 30.5 | 17315.17 | 19 | 39 | 3 | 1 |
| 569.4977 | 0.720109 | 1.5 | 17623.75 | 69 | 35 | 3 | 1 |
| 571.1366 | -1.29549 | 28.5 | 27920 | 23 | 39 | 3 | 1 |

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| 572.1463 | 1.983937 | 28 | 10832.4 | 24 | 39 | 3 | 1 |
| 573.1528 | -0.33133 | 27.5 | 28036.72 | 25 | 39 | 3 | 1 |
| 575.1686 | -0.06937 | 26.5 | 6390.75 | 27 | 39 | 3 | 1 |
| 575.3557 | -1.28599 | 12.5 | 372785.12 | 51 | 37 | 3 | 1 |
| 577.0914 | 1.750332 | 32.5 | 5846.93 | 17 | 40 | 3 | 1 |
| 579.1056 | -0.75962 | 31.5 | 11019.95 | 19 | 40 | 3 | 1 |
| 581.1216 | -0.1547 | 30.5 | 26001.99 | 21 | 40 | 3 | 1 |
| 582.1288 | -1.22808 | 30 | 13463.09 | 22 | 40 | 3 | 1 |
| 583.514 | 1.816755 | 1.5 | 7690.78 | 71 | 36 | 3 | 1 |
| 584.1458 | 1.08723 | 29 | 19214.85 | 24 | 40 | 3 | 1 |
| 585.1537 | 1.213529 | 28.5 | 26074.06 | 25 | 40 | 3 | 1 |
| 586.0658 | -1.90234 | 35 | 6245.74 | 14 | 41 | 3 | 1 |
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| 587.1679 | -1.26011 | 27.5 | 12745.46 | 27 | 40 | 3 | 1 |
| 589.09 | -0.66187 | 33.5 | 20175.48 | 17 | 41 | 3 | 1 |
| 591.1053 | -1.25172 | 32.5 | 12807.28 | 19 | 41 | 3 | 1 |
| 595.1368 | -0.90719 | 30.5 | 21930.32 | 23 | 41 | 3 | 1 |
| 597.1529 | -0.15055 | 29.5 | 22352.35 | 25 | 41 | 3 | 1 |
| 604.1131 | -1.26615 | 33 | 13160.63 | 20 | 42 | 3 | 1 |
| 605.1218 | 0.181947 | 32.5 | 16097.41 | 21 | 42 | 3 | 1 |
| 606.1286 | -1.50941 | 32 | 7101.29 | 22 | 42 | 3 | 1 |
| 607.1375 | 0.263697 | 31.5 | 21543.71 | 23 | 42 | 3 | 1 |
| 608.1443 | -1.42219 | 31 | 11416.41 | 24 | 42 | 3 | 1 |
| 609.1537 | 1.165717 | 30.5 | 17784.96 | 25 | 42 | 3 | 1 |
| 611.1693 | 1.080062 | 29.5 | 13154.39 | 27 | 42 | 3 | 1 |
| 613.0912 | 1.321339 | 35.5 | 7337.75 | 17 | 43 | 3 | 1 |
| 613.1843 | 0.016471 | 28.5 | 11908.85 | 29 | 42 | 3 | 1 |
| 615.1054 | -1.04031 | 34.5 | 15611.97 | 19 | 43 | 3 | 1 |
| 617.1209 | -1.27997 | 33.5 | 16836.95 | 21 | 43 | 3 | 1 |
| 619.1363 | -1.6796 | 32.5 | 15732.65 | 23 | 43 | 3 | 1 |
| 621.1539 | 1.465178 | 31.5 | 24963.84 | 25 | 43 | 3 | 1 |
| 624.1754 | -1.70609 | 30 | 6402.81 | 28 | 43 | 3 | 1 |
| 627.1072 | 1.849926 | 35.5 | 10334.94 | 19 | 44 | 3 | 1 |
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| 631.1382 | 1.362778 | 33.5 | 15190.7 | 23 | 44 | 3 | 1 |
| 634.1614 | 0.922637 | 32 | 7880.19 | 26 | 44 | 3 | 1 |
| 637.1843 | 0.015851 | 30.5 | 8270.88 | 29 | 44 | 3 | 1 |
| 639.1065 | 0.719912 | 36.5 | 7097.69 | 19 | 45 | 3 | 1 |
| 640.1148 | 1.460834 | 36 | 6840.82 | 20 | 45 | 3 | 1 |
| 643.1365 | -1.30594 | 34.5 | 16331.6 | 23 | 45 | 3 | 1 |
| 645.152 | -1.53436 | 33.5 | 12488.47 | 25 | 45 | 3 | 1 |
| 647.1681 | -0.83425 | 32.5 | 7629.16 | 27 | 45 | 3 | 1 |
| 648.1754 | -1.64292 | 32 | 7210.56 | 28 | 45 | 3 | 1 |
| 651.1992 | -1.13621 | 30.5 | 5884.31 | 31 | 45 | 3 | 1 |
| 669.1524 | -0.88156 | 35.5 | 12905.8 | 25 | 47 | 3 | 1 |
| 672.1777 | 1.837464 | 34 | 7430.7 | 28 | 47 | 3 | 1 |

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| 673.1841 | -0.28209 | 33.5 | 6532.81 | 29 | 47 | 3 | 1 |
| 675.2006 | 0.977636 | 32.5 | 7080.86 | 31 | 47 | 3 | 1 |
| 678.129 | -0.75929 | 38 | 9133.38 | 22 | 48 | 3 | 1 |
| 683.1673 | -1.9613 | 35.5 | 11916.82 | 27 | 48 | 3 | 1 |
| 685.0905 | 0.160709 | 41.5 | 5929.28 | 17 | 49 | 3 | 1 |
| 687.2007 | 1.106083 | 33.5 | 8159.32 | 31 | 48 | 3 | 1 |
| 695.168 | -0.9205 | 36.5 | 7184.02 | 27 | 49 | 3 | 1 |
| 710.1907 | -1.99228 | 36 | 9552.82 | 30 | 50 | 3 | 1 |
| 713.2168 | 1.696682 | 34.5 | 6108.4 | 33 | 50 | 3 | 1 |
| 719.1682 | -0.61168 | 38.5 | 11162.79 | 27 | 51 | 3 | 1 |
| 725.1225 | 1.117192 | 42.5 | 7221.15 | 21 | 52 | 3 | 1 |
| 728.1447 | -0.63847 | 41 | 10874.23 | 24 | 52 | 3 | 1 |
| 735.2001 | 0.217764 | 37.5 | 7090.21 | 31 | 52 | 3 | 1 |
| 745.1832 | -1.46259 | 39.5 | 6343.57 | 29 | 53 | 3 | 1 |
| 754.1606 | -0.28495 | 42 | 15076.34 | 26 | 54 | 3 | 1 |
| 756.1751 | -1.805 | 41 | 16690.33 | 28 | 54 | 3 | 1 |
| 764.1437 | -1.91704 | 44 | 9661.12 | 24 | 55 | 3 | 1 |
| 765.1528 | -0.24819 | 43.5 | 6110.99 | 25 | 55 | 3 | 1 |
| 766.16 | -1.06361 | 43 | 5977.72 | 26 | 55 | 3 | 1 |
| 776.1448 | -0.47014 | 45 | 8115.8 | 24 | 56 | 3 | 1 |
| 784.2077 | -0.08276 | 41 | 6414.21 | 32 | 56 | 3 | 1 |
| 792.1757 | -0.96557 | 44 | 8651.25 | 28 | 57 | 3 | 1 |
| 802.1611 | 0.355415 | 46 | 10177.1 | 26 | 58 | 3 | 1 |
| 835.6999 | -1.00502 | 8.5 | 46269.73 | 95 | 55 | 3 | 1 |
| 848.2381 | -1.13753 | 44 | 6680.94 | 36 | 61 | 3 | 1 |
| 854.1915 | -0.71986 | 48 | 8329.56 | 30 | 62 | 3 | 1 |
| 855.1995 | -0.51438 | 47.5 | 6358.64 | 31 | 62 | 3 | 1 |
| 863.7323 | 0.301135 | 8.5 | 58091.3 | 99 | 57 | 3 | 1 |
| 891.7626 | -0.8297 | 8.5 | 11985.84 | 103 | 59 | 3 | 1 |
| 893.2155 | -0.10065 | 49.5 | 6064.56 | 33 | 65 | 3 | 1 |
| 898.1599 | -1.01864 | 54 | 6883.31 | 26 | 66 | 3 | 1 |
| 941.2164 | 0.860695 | 53.5 | 5976.65 | 33 | 69 | 3 | 1 |
| 948.269 | -1.43936 | 50 | 6427.31 | 40 | 69 | 3 | 1 |
| 993.2453 | -1.60071 | 55.5 | 7737.8 | 37 | 73 | 3 | 1 |
| 1028.239 | -0.54939 | 59 | 5882.74 | 36 | 76 | 3 | 1 |

**c)**

| Mass (m/z) | Deviation (ppm) | DBE | Intensity (AU) | H | C | O | S |
|---|---|---|---|---|---|---|---|
| 106.9809 | 0.561782839 | 1.5 | 11985.31 | 3 | 2 | 3 | 1 |
| 156.9964 | -0.572624268 | 4.5 | 85848.85 | 5 | 6 | 3 | 1 |
| 171.0121 | -0.233316769 | 4.5 | 8278.56 | 7 | 7 | 3 | 1 |
| 297.1531 | 0.370516211 | 4.5 | 75644.46 | 25 | 16 | 3 | 1 |
| 311.1688 | 0.514512002 | 4.5 | 295070.3 | 27 | 17 | 3 | 1 |
| 325.1843 | 0.031059311 | 4.5 | 275892.6 | 29 | 18 | 3 | 1 |
| 339.2 | 0.177181635 | 4.5 | 68174.87 | 31 | 19 | 3 | 1 |
| 155.9886 | -0.416055872 | 5 | 50009.39 | 4 | 6 | 3 | 1 |
| 170.0043 | -0.087644834 | 5 | 193261.1 | 6 | 7 | 3 | 1 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 184.0199 | -0.352679124 | 5 | 94614.58 | 8 | 8 | 3 | 1 |
| 198.0355 | -0.580198668 | 5 | 3177.24 | 10 | 9 | 3 | 1 |
| 183.0121 | -0.218018324 | 5.5 | 5819652 | 7 | 8 | 3 | 1 |
| 197.0278 | 0.051261804 | 5.5 | 409289 | 9 | 9 | 3 | 1 |
| 211.0435 | 0.284775495 | 5.5 | 38650.67 | 11 | 10 | 3 | 1 |
| 225.0591 | 0.044877103 | 5.5 | 28921.2 | 13 | 11 | 3 | 1 |
| 239.0749 | 0.66966506 | 5.5 | 29204.32 | 15 | 12 | 3 | 1 |
| 253.0905 | 0.435022444 | 5.5 | 11567.52 | 17 | 13 | 3 | 1 |
| 267.1064 | 1.348153715 | 5.5 | 2877.42 | 19 | 14 | 3 | 1 |
| 295.1375 | 0.542459317 | 5.5 | 6298.23 | 23 | 16 | 3 | 1 |
| 309.1532 | 0.679598797 | 5.5 | 9376.64 | 25 | 17 | 3 | 1 |
| 323.1686 | -0.12346495 | 5.5 | 9393.61 | 27 | 18 | 3 | 1 |
| 196.0199 | -0.331088724 | 6 | 86192.03 | 8 | 9 | 3 | 1 |
| 210.0353 | -1.499269541 | 6 | 4897.37 | 10 | 10 | 3 | 1 |
| 180.9965 | 0.055802187 | 6.5 | 100900.8 | 5 | 8 | 3 | 1 |
| 195.0121 | -0.204602647 | 6.5 | 306767.7 | 7 | 9 | 3 | 1 |
| 209.0278 | 0.048318934 | 6.5 | 172641.7 | 9 | 10 | 3 | 1 |
| 223.0436 | 0.717797394 | 6.5 | 17874.88 | 11 | 11 | 3 | 1 |
| 237.0591 | 0.042605411 | 6.5 | 5164.54 | 13 | 12 | 3 | 1 |
| 194.0042 | -0.592254869 | 7 | 5085.41 | 6 | 9 | 3 | 1 |
| 207.0122 | 0.290321138 | 7.5 | 36289.6 | 7 | 10 | 3 | 1 |
| 221.0279 | 0.498127408 | 7.5 | 22893.32 | 9 | 11 | 3 | 1 |
| 235.0436 | 0.681150685 | 7.5 | 3652.35 | 11 | 12 | 3 | 1 |
| 233.028 | 0.901609203 | 8.5 | 3000.88 | 9 | 12 | 3 | 1 |
| 252.9961 | -1.541128101 | 12.5 | 5215.16 | 5 | 14 | 3 | 1 |
| 250.9804 | -1.752723436 | 13.5 | 3296.72 | 3 | 14 | 3 | 1 |