**A combined liquid chromatography – trapped ion mobility – tandem high-resolution mass spectrometry and multivariate analysis approach for the determination of enzymatic reactivity descriptors in biomass hydrolysates**

**Ian Ramtanon1**, Alexandra Berlioz-Barbier1, Simon Remy2, Jean-Hugues Renault2, Agnès Le Masle1,\*

*1 IFP Energies nouvelles, rond-point de l’échangeur de Solaize, BP 3, 69360 Solaize, France*

*2* *Université de Reims Champagne-Ardenne, CNRS, ICMR 7312, 51097, Reims, France*

*∗ Corresponding author. E-mail address: agnes.le-masle@ifpen.fr (A. Le Masle)*

**Supplementary materials:**

**Graphical user interface

Description automatically generated with medium confidence**

Figure S1. Data processing steps for the compilation of the bucket table. (A) Bucketing of the adducts in positive and negative ionization modes: starting from the average mass spectrum of a chromatographic peak, adducts are merged under the most intense one. The RT and intensity of this ion is recorded. (B) Adduct filtering using KMD analysis: non-bucketed source dimers are visually identified and manually merged with their parent feature (C) Merging, annotation, and compilation of bucket table: the positive and negative bucket tables are merged. An average RT is calculated and the intensity of the prevalent adduct is recorded. A bucket table containing this ion’s RT, m/z, its intensity, and the annotation (molecular formula) of the parent feature is compiled.



Figure S2. Base peak chromatograms of pooled hydrolysate samples in (-) ESI (red) and (+) ESI (blue).

A screenshot of a computer screen

Description automatically generated with low confidence

Figure S3. Comparison of different scaling methods applied before PCA score plots projection (after class centroid centering). Class centroid scaling offered the best class separation according to biomass type in PC1/PC2 and according to enzymatic hydrolysis reactivity in PC1/PC3.

**Graphical user interface

Description automatically generated with medium confidence**

Figure S4. PCA score plots of the 66 hydrolysate and 11 QC samples with : (1) PC1/PC2 projection (95% explained variance) and (2) PC1/PC3 projection (94% explained variance).

Graphical user interface, qr code

Description automatically generated

Figure S5. Annotated MS/MS spectrum for the first mobility peak with corresponding structure hypotheses.

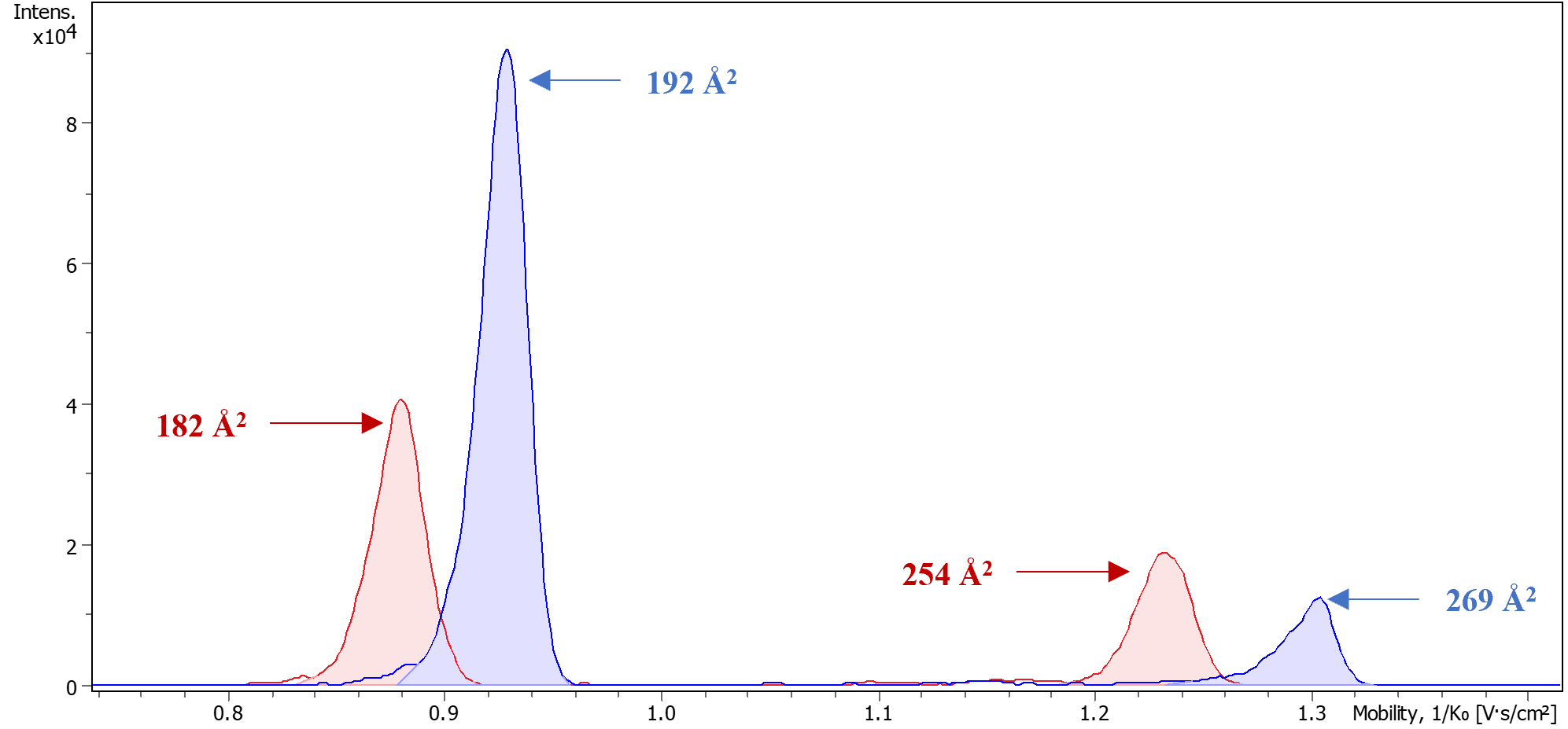
****

Figure S6. Mobility profiles of xylotriose (blue) and arabinotriose (red) showing mobility peaks with their associated collisional cross-sections.

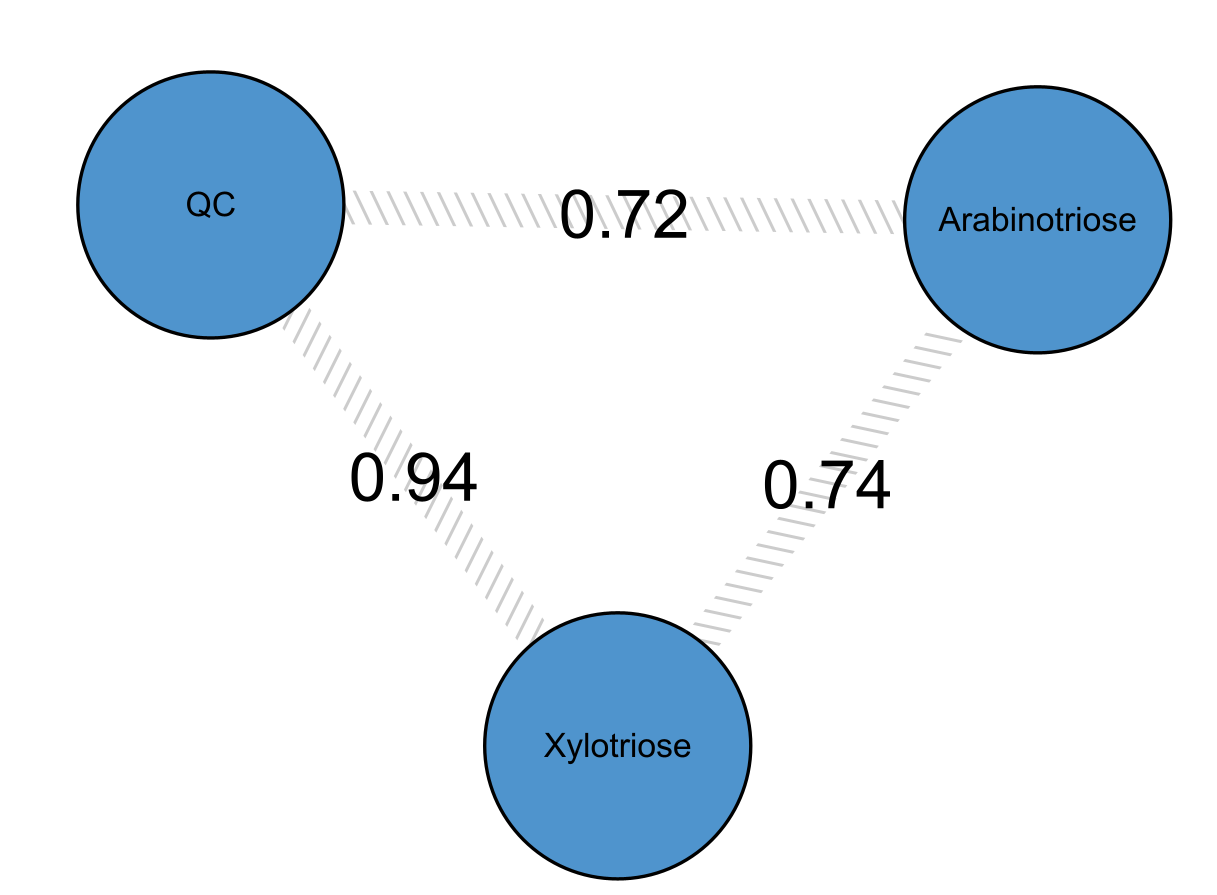


Figure S7. Miniature molecular network showing a stronger similarity between the fragmentation spectra of the most intense mobility peak at m/z 432.1714 and RT = 1.90 min for the quality control sample and the reference xylotriose (cosine score = 0.94) than with the reference arabinotriose (cosine score = 0.72). The molecular network was constructed on MetGem (DOI: 10.1021/acs.analchem.8b03099) with the following parameters. the data was filtered by removing all MS/MS fragment ions within ± 17 Da of the precursor m/z, and only the top 6 fragment ions in the ± 50 Da window were selected throughout the spectrum. The precursor ion mass tolerance was set at 0.02 Da, and a MS/MS fragment ion tolerance of 0.02 Da was used. A network was generated with edges filtered to have a cosine score above 0.7 and more than 6 matched peaks.

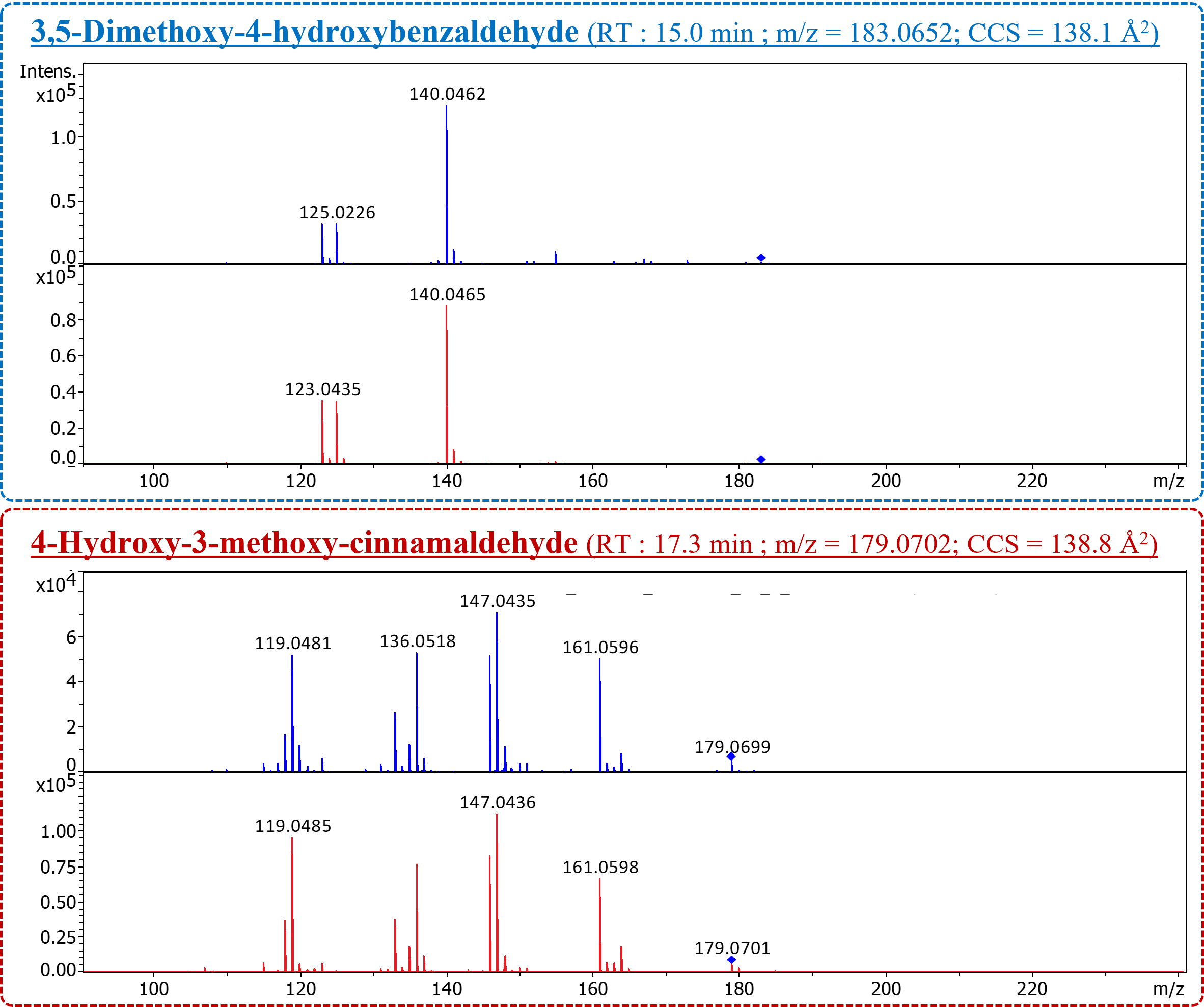


Figure S8. Comparison of HRMS/MS spectra for 3,5-Dimethoxy-4-hydroxybenzaldehyde (RT = 15.0 min, m/z 183.0652 and CCS =138 Å2) and 4-hydroxy-3-methoxy-cinnamaldehyde (RT = 17.3 min, m/z 179.0702 and CCS =139 Å2) in the pooled hydrolysate sample (blue) and the commercial standards present in an in-house system suitability test sample (red).

Table S1. Summary the 618 annotated features that were associated to low enzymatic reactivity with 95% confidence in the PC1/PC3 projection.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RT (min) | m/z | Molecular formula |  | PC 1 (35%) | PC 3 (11%) | O/C | H/C | DBE |
| 1.51 | 471.1357 | C17H28O15 |  | -0.05861 | -0.94234 | 0.9 | 1.6 | 4 |
| 1.95 | 207.0512 | C7H12O7 |  | 0.057597 | -0.92864 | 1.0 | 1.7 | 2 |
| 16.27 | 401.1594 | C22H24O7 |  | 0.003248 | -0.92727 | 0.3 | 1.1 | 11 |
| 1.21 | 355.0886 | C12H20O12 |  | -0.13008 | -0.8972 | 1.0 | 1.7 | 3 |
| 11.73 | 331.1191 | C18H20O6 |  | -0.12082 | -0.88408 | 0.3 | 1.1 | 9 |
| 1.85 | 281.0883 | C10H18O9 |  | -0.14618 | -0.88 | 0.9 | 1.8 | 2 |
| 2.05 | 471.1359 | C17H28O15 |  | -0.04927 | -0.87689 | 0.9 | 1.6 | 4 |
| 5.91 | 227.0915 | C11H14O5 |  | -0.01094 | -0.87672 | 0.5 | 1.3 | 5 |
| 12.36 | 379.1398 | C19H24O8 |  | -0.12497 | -0.87333 | 0.4 | 1.3 | 8 |
| 12.37 | 331.1192 | C18H20O6 |  | -0.09343 | -0.86894 | 0.3 | 1.1 | 9 |
| 11.73 | 379.1398 | C19H24O8 |  | -0.12804 | -0.86831 | 0.4 | 1.3 | 8 |
| 7.57 | 227.0915 | C11H14O5 |  | -0.02484 | -0.86779 | 0.5 | 1.3 | 5 |
| 1.88 | 283.1023 | C10H18O9 |  | -0.13965 | -0.86416 | 0.9 | 1.8 | 2 |
| 1.57 | 131.0353 | C5H8O4 |  | -0.14931 | -0.86392 | 0.8 | 1.6 | 2 |
| 1.88 | 229.0706 | C10H12O6 |  | -0.14402 | -0.84948 | 0.6 | 1.2 | 5 |
| 5.9 | 167.0702 | C9H10O3 |  | -0.00632 | -0.84607 | 0.3 | 1.1 | 5 |
| 11.73 | 167.0702 | C9H10O3 |  | -0.1176 | -0.84558 | 0.3 | 1.1 | 5 |
| 2.18 | 413.1305 | C15H26O13 |  | -0.12211 | -0.84061 | 0.9 | 1.7 | 3 |
| 12.71 | 197.0807 | C10H12O4 |  | 0.044691 | -0.84011 | 0.4 | 1.2 | 5 |
| 1.65 | 471.1357 | C17H28O15 |  | -0.09349 | -0.83342 | 0.9 | 1.6 | 4 |
| 11.73 | 363.1439 | C19H22O7 |  | -0.1294 | -0.8333 | 0.4 | 1.2 | 9 |
| 7.57 | 167.0703 | C9H10O3 |  | -0.00234 | -0.82714 | 0.3 | 1.1 | 5 |
| 13.28 | 227.0914 | C11H14O5 |  | -0.00467 | -0.8244 | 0.5 | 1.3 | 5 |
| 7.56 | 177.0547 | C10H8O3 |  | -0.01166 | -0.82219 | 0.3 | 0.8 | 7 |
| 1.24 | 453.0561 | C33H10O3 |  | -0.12107 | -0.8217 | 0.1 | 0.3 | 29 |
| 1.39 | 471.1359 | C17H28O15 |  | -0.06296 | -0.82123 | 0.9 | 1.6 | 4 |
| 1.89 | 265.0917 | C15H26O13 |  | -0.14248 | -0.81791 | 0.9 | 1.7 | 3 |
| 12.36 | 363.1439 | C19H22O7 |  | -0.12572 | -0.81772 | 0.4 | 1.2 | 9 |
| 1.39 | 327.0933 | C11H20O11 |  | -0.17502 | -0.81465 | 1.0 | 1.8 | 2 |
| 12.36 | 167.0702 | C9H10O3 |  | -0.1167 | -0.81421 | 0.3 | 1.1 | 5 |
| 2.22 | 485.1519 | C18H30O15 |  | -0.06583 | -0.80806 | 0.8 | 1.7 | 4 |
| 6.82 | 545.1725 | C20H34O17 |  | -0.07939 | -0.79755 | 0.9 | 1.7 | 4 |
| 2.17 | 459.1357 | C16H28O15 |  | -0.12578 | -0.79732 | 0.9 | 1.8 | 3 |
| 1.23 | 517.1415 | C18H30O17 |  | -0.15126 | -0.79166 | 0.9 | 1.7 | 4 |
| 1.56 | 229.0707 | C10H12O6 |  | -0.18244 | -0.78414 | 0.6 | 1.2 | 5 |
| 1.39 | 229.0706 | C10H12O6 |  | -0.15756 | -0.78015 | 0.6 | 1.2 | 5 |
| 1.3 | 281.088 | C10H18O9 |  | -0.18002 | -0.77639 | 0.9 | 1.8 | 2 |
| 2.08 | 603.1779 | C22H36O19 |  | -0.0636 | -0.7762 | 0.9 | 1.6 | 5 |
| 18.32 | 505.1701 | C25H28O11 |  | -0.32403 | -0.77222 | 0.4 | 1.1 | 12 |
| 4.39 | 325.1126 | C12H20O10 |  | -0.08321 | -0.77088 | 0.8 | 1.7 | 3 |
| 1.29 | 563.1831 | C20H36O18 |  | -0.219 | -0.76616 | 0.9 | 1.8 | 3 |
| 5.95 | 209.0809 | C11H12O4 |  | -0.01393 | -0.76613 | 0.4 | 1.1 | 6 |
| 1.57 | 379.0563 | C31H8 |  | -0.13767 | -0.76232 | 0.0 | 0.3 | 28 |
| 18.29 | 487.1595 | C25H26O10 |  | -0.34402 | -0.76079 | 0.4 | 1.0 | 13 |
| 1.39 | 265.0917 | C10H16O8 |  | -0.15061 | -0.76069 | 0.8 | 1.6 | 3 |
| 1.3 | 265.0917 | C10H18O9 |  | -0.173 | -0.76038 | 0.9 | 1.8 | 2 |
| 1.55 | 97.02836 | C5H4O2 |  | -0.14488 | -0.75937 | 0.4 | 0.8 | 4 |
| 13.33 | 309.0967 | C25H34O16 |  | -0.15301 | -0.75783 | 0.6 | 1.4 | 9 |
| 1.3 | 229.0706 | C10H12O6 |  | -0.17293 | -0.75769 | 0.6 | 1.2 | 5 |
| 1.27 | 149.0458 | C5H10O5 |  | -0.15313 | -0.75682 | 1.0 | 2.0 | 1 |
| 2.06 | 459.1357 | C15H26O13 |  | -0.15264 | -0.75618 | 0.9 | 1.7 | 3 |
| 7.26 | 265.0917 | C10H16O8 |  | -0.18538 | -0.75608 | 0.8 | 1.6 | 3 |
| 21.11 | 371.1138 | C20H20O7 |  | -0.21138 | -0.75516 | 0.4 | 1.0 | 11 |
| 16.28 | 167.0701 | C9H10O3 |  | 0.045649 | -0.75084 | 0.3 | 1.1 | 5 |
| 14.87 | 589.1777 | C25H34O16 |  | -0.14411 | -0.74964 | 0.6 | 1.4 | 9 |
| 13.16 | 589.1777 | C25H34O16 |  | -0.12763 | -0.74939 | 0.6 | 1.4 | 9 |
| 1.94 | 485.1524 | C18H30O15 |  | -0.0717 | -0.74757 | 0.8 | 1.7 | 4 |
| 13.33 | 589.1776 | C25H34O16 |  | -0.12848 | -0.74755 | 0.6 | 1.4 | 9 |
| 18.31 | 355.1175 | C20H18O6 |  | -0.35538 | -0.7441 | 0.3 | 0.9 | 12 |
| 4.41 | 229.0704 | C10H12O6 |  | -0.11335 | -0.74305 | 0.6 | 1.2 | 5 |
| 1.39 | 281.0881 | C10H18O9 |  | -0.16065 | -0.74188 | 0.9 | 1.8 | 2 |
| 14.41 | 559.1674 | C24H32O15 |  | -0.09873 | -0.73959 | 0.6 | 1.3 | 9 |
| 20.99 | 371.1139 | C20H20O7 |  | -0.1667 | -0.73798 | 0.4 | 1.0 | 11 |
| 12.03 | 271.098 | C16H16O4 |  | -0.0986 | -0.73672 | 0.3 | 1.0 | 9 |
| 1.45 | 517.1416 | C18H30O17 |  | -0.02576 | -0.73638 | 0.9 | 1.7 | 4 |
| 12.19 | 271.098 | C16H16O4 |  | -0.09749 | -0.73352 | 0.3 | 1.0 | 9 |
| 1.4 | 97.02837 | C5H4O2 |  | -0.1211 | -0.73206 | 0.4 | 0.8 | 4 |
| 1.28 | 457.1202 | C16H26O15 |  | -0.23854 | -0.73054 | 0.9 | 1.6 | 4 |
| 13.91 | 521.1664 | C25H30O12 |  | -0.12995 | -0.72958 | 0.5 | 1.2 | 11 |
| 20.99 | 387.1437 | C21H22O7 |  | 0.094625 | -0.72945 | 0.3 | 1.0 | 11 |
| 13.95 | 205.051 | C11H10O4 |  | -0.26438 | -0.72891 | 0.4 | 0.9 | 7 |
| 12.61 | 279.0861 | C14H14O6 |  | -0.11154 | -0.72876 | 0.4 | 1.0 | 8 |
| 14.38 | 441.139 | C20H24O11 |  | -0.27526 | -0.72707 | 0.6 | 1.2 | 9 |
| 1.89 | 353.1098 | C13H22O11 |  | -0.09587 | -0.72691 | 0.8 | 1.7 | 3 |
| 17.65 | 337.0931 | C16H18O8 |  | -0.20863 | -0.72684 | 0.5 | 1.1 | 8 |
| 15.48 | 209.0808 | C11H12O4 |  | 0.214687 | -0.72614 | 0.4 | 1.1 | 6 |
| 14.42 | 565.1548 | C26H28O14 |  | -0.12386 | -0.72541 | 0.5 | 1.1 | 13 |
| 1.28 | 369.068 | C12H18O13 |  | -0.03746 | -0.72338 | 1.1 | 1.5 | 4 |
| 1.5 | 459.1356 | C15H26O13 |  | -0.11281 | -0.72161 | 0.9 | 1.7 | 3 |
| 15.39 | 209.0809 | C11H12O4 |  | 0.221009 | -0.72053 | 0.4 | 1.1 | 6 |
| 1.32 | 221.0669 | C8H14O7 |  | -0.13706 | -0.71998 | 0.9 | 1.8 | 2 |
| 15.47 | 363.1086 | C18H20O8 |  | 0.217802 | -0.7199 | 0.4 | 1.1 | 9 |
| 1.96 | 564.2129 | C20H34O17 |  | -0.10672 | -0.71567 | 0.9 | 1.7 | 4 |
| 7.38 | 281.0885 | C10H18O9 |  | -0.17085 | -0.71369 | 0.9 | 1.8 | 2 |
| 1.39 | 432.171 | C15H26O13 |  | -0.12517 | -0.7136 | 0.9 | 1.7 | 3 |
| 2.19 | 564.2131 | C20H34O17 |  | -0.09663 | -0.71252 | 0.9 | 1.7 | 4 |
| 1.39 | 353.1098 | C13H22O11 |  | -0.09814 | -0.71224 | 0.8 | 1.7 | 3 |
| 1.89 | 511.0985 | C36H16O4 |  | -0.15385 | -0.71186 | 0.1 | 0.4 | 29 |
| 7 | 545.1726 | C20H34O17 |  | -0.0353 | -0.70954 | 0.9 | 1.7 | 4 |
| 2.59 | 564.2129 | C20H34O17 |  | -0.09657 | -0.70843 | 0.9 | 1.7 | 4 |
| 1.23 | 193.0354 | C6H10O7 |  | 0.04456 | -0.7074 | 1.2 | 1.7 | 2 |
| 1.29 | 97.02838 | C5H4O2 |  | -0.15419 | -0.70518 | 0.4 | 0.8 | 4 |
| 2.29 | 459.1356 | C15H26O13 |  | -0.16666 | -0.70388 | 0.9 | 1.7 | 3 |
| 1.51 | 547.1517 | C19H32O18 |  | -0.12928 | -0.70347 | 0.9 | 1.7 | 4 |
| 14.12 | 363.1085 | C18H20O8 |  | 0.190572 | -0.70345 | 0.4 | 1.1 | 9 |
| 15.15 | 451.1611 | C22H28O10 |  | 0.142029 | -0.70333 | 0.5 | 1.3 | 9 |
| 20.99 | 367.1188 | C21H20O6 |  | 0.121211 | -0.70324 | 0.3 | 1.0 | 12 |
| 1.25 | 341.1092 | C12H22O11 |  | 0.117741 | -0.70247 | 0.9 | 1.8 | 2 |
| 16.04 | 389.1247 | C20H22O8 |  | -0.08849 | -0.70191 | 0.4 | 1.1 | 10 |
| 7.75 | 483.1381 | C36H20O2 |  | -0.09092 | -0.70163 | 0.1 | 0.6 | 27 |
| 1.7 | 282.1182 | C5H8O4 |  | -0.15686 | -0.70134 | 0.8 | 1.6 | 2 |
| 20.44 | 469.1503 | C25H26O9 |  | 0.123334 | -0.69958 | 0.4 | 1.0 | 13 |
| 1.56 | 589.1626 | C21H34O19 |  | -0.10597 | -0.6991 | 0.9 | 1.6 | 5 |
| 1.33 | 383.0836 | C13H20O13 |  | 0.015709 | -0.69885 | 1.0 | 1.5 | 4 |
| 7.55 | 527.1632 | C20H32O16 |  | -0.17278 | -0.69767 | 0.8 | 1.6 | 5 |
| 18.08 | 533.1665 | C26H30O12 |  | -0.49215 | -0.69728 | 0.5 | 1.2 | 12 |
| 2.59 | 603.1781 | C22H36O19 |  | -0.08791 | -0.69684 | 0.9 | 1.6 | 5 |
| 12.22 | 277.1657 | C13H24O6 |  | -0.15867 | -0.69605 | 0.5 | 1.8 | 2 |
| 7.92 | 513.1465 | C19H30O16 |  | 0.116689 | -0.6956 | 0.8 | 1.6 | 5 |
| 14.7 | 476.1759 | C20H26O12 |  | -0.34506 | -0.69409 | 0.6 | 1.3 | 8 |
| 7.27 | 606.2237 | C22H36O18 |  | -0.17801 | -0.69323 | 0.8 | 1.6 | 5 |
| 1.3 | 115.0389 | C10H16O8 |  | -0.14392 | -0.69249 | 0.8 | 1.6 | 3 |
| 5.94 | 195.0664 | C10H12O4 |  | 0.125594 | -0.69124 | 0.4 | 1.2 | 5 |
| 8.34 | 606.2236 | C22H36O18 |  | -0.14902 | -0.69009 | 0.8 | 1.6 | 5 |
| 15.77 | 415.1399 | C22H24O8 |  | 0.196925 | -0.69003 | 0.4 | 1.1 | 11 |
| 1.25 | 487.1309 | C17H28O16 |  | -0.09044 | -0.68923 | 0.9 | 1.6 | 4 |
| 15.3 | 605.2241 | C30H38O13 |  | -0.08517 | -0.68792 | 0.4 | 1.3 | 12 |
| 1.34 | 487.1311 | C17H28O16 |  | -0.04829 | -0.68698 | 0.9 | 1.6 | 4 |
| 2.95 | 367.1232 | C14H22O11 |  | 0.116333 | -0.68673 | 0.8 | 1.6 | 4 |
| 19.56 | 345.133 | C19H20O6 |  | 0.148859 | -0.68643 | 0.3 | 1.1 | 10 |
| 16.57 | 439.1608 | C21H28O10 |  | 0.131383 | -0.6844 | 0.5 | 1.3 | 8 |
| 7.08 | 591.178 | C21H36O19 |  | 0.119034 | -0.68433 | 0.9 | 1.7 | 4 |
| 20.22 | 345.1331 | C19H20O6 |  | 0.15146 | -0.68358 | 0.3 | 1.1 | 10 |
| 14.51 | 437.1456 | C21H26O10 |  | 0.127485 | -0.68346 | 0.5 | 1.2 | 9 |
| 13.72 | 437.1457 | C21H26O10 |  | 0.202775 | -0.68284 | 0.5 | 1.2 | 9 |
| 21.54 | 371.1136 | C20H20O7 |  | -0.28907 | -0.68252 | 0.4 | 1.0 | 11 |
| 14.37 | 309.0964 | C20H26O12 |  | -0.20817 | -0.68112 | 0.6 | 1.3 | 8 |
| 1.38 | 489.1463 | C17H30O16 |  | -0.15207 | -0.68054 | 0.9 | 1.8 | 3 |
| 14.85 | 437.1458 | C21H26O10 |  | 0.127879 | -0.68051 | 0.5 | 1.2 | 9 |
| 7.36 | 229.0705 | C10H12O6 |  | -0.17701 | -0.68023 | 0.6 | 1.2 | 5 |
| 2.57 | 265.0916 | C10H16O8 |  | -0.08513 | -0.68007 | 0.8 | 1.6 | 3 |
| 14.32 | 279.0863 | C14H14O6 |  | -0.23916 | -0.67859 | 0.4 | 1.0 | 8 |
| 20.35 | 385.1642 | C22H24O6 |  | 0.154155 | -0.67793 | 0.3 | 1.1 | 11 |
| 1.56 | 247.0811 | C10H16O8 |  | -0.17626 | -0.6779 | 0.8 | 1.6 | 3 |
| 21.35 | 337.1085 | C20H18O5 |  | 0.118154 | -0.67769 | 0.3 | 0.9 | 12 |
| 13.81 | 563.1413 | C26H28O14 |  | -0.09353 | -0.67487 | 0.5 | 1.1 | 13 |
| 17.65 | 321.0967 | C16H16O7 |  | -0.23241 | -0.67476 | 0.4 | 1.0 | 9 |
| 15.5 | 295.0828 | C14H16O7 |  | 0.146768 | -0.67438 | 0.5 | 1.1 | 7 |
| 17.2 | 343.1193 | C19H20O6 |  | 0.210031 | -0.67197 | 0.3 | 1.1 | 10 |
| 14.51 | 279.0862 | C14H14O6 |  | -0.23449 | -0.67091 | 0.4 | 1.0 | 8 |
| 2.6 | 485.1521 | C18H30O15 |  | -0.08551 | -0.67037 | 0.8 | 1.7 | 4 |
| 19.52 | 329.1037 | C18H18O6 |  | 0.161082 | -0.6702 | 0.3 | 1.0 | 10 |
| 20.75 | 555.1877 | C29H32O11 |  | 0.109189 | -0.67018 | 0.4 | 1.1 | 14 |
| 13.95 | 147.0439 | C9H8O3 |  | -0.29073 | -0.66936 | 0.3 | 0.9 | 6 |
| 13.48 | 437.1456 | C21H26O10 |  | 0.208852 | -0.66932 | 0.5 | 1.2 | 9 |
| 1.35 | 339.0934 | C12H20O11 |  | 0.077568 | -0.66866 | 0.9 | 1.7 | 3 |
| 2.07 | 265.0919 | C15H26O13 |  | -0.13829 | -0.66822 | 0.9 | 1.7 | 3 |
| 1.39 | 297.0833 | C10H18O10 |  | -0.13159 | -0.66814 | 1.0 | 1.8 | 2 |
| 21.18 | 249.1119 | C14H16O4 |  | 0.153082 | -0.66719 | 0.3 | 1.1 | 7 |
| 21.5 | 385.1646 | C22H24O6 |  | 0.046996 | -0.66628 | 0.3 | 1.1 | 11 |
| 1.24 | 325.113 | C12H20O10 |  | 0.046703 | -0.66426 | 0.8 | 1.7 | 3 |
| 7.56 | 143.0338 | C6H6O4 |  | 0.124928 | -0.66396 | 0.7 | 1.0 | 4 |
| 20.99 | 355.119 | C20H20O6 |  | 0.14324 | -0.66325 | 0.3 | 1.0 | 11 |
| 20.96 | 355.1538 | C21H22O5 |  | 0.088174 | -0.66254 | 0.2 | 1.0 | 11 |
| 21.43 | 371.1488 | C21H22O6 |  | 0.132111 | -0.66192 | 0.3 | 1.0 | 11 |
| 15.8 | 379.1386 | C19H22O8 |  | 0.196412 | -0.66161 | 0.4 | 1.2 | 9 |
| 13.95 | 295.0822 | C14H16O7 |  | -0.32277 | -0.66157 | 0.5 | 1.1 | 7 |
| 20.35 | 420.2015 | C22H26O7 |  | 0.125722 | -0.66086 | 0.3 | 1.2 | 10 |
| 2.84 | 459.1356 | C16H28O15 |  | -0.08574 | -0.66082 | 0.9 | 1.8 | 3 |
| 2.45 | 429.125 | C15H26O14 |  | 0.114833 | -0.66027 | 0.9 | 1.7 | 3 |
| 15.01 | 275.0928 | C15H16O5 |  | 0.142321 | -0.65781 | 0.3 | 1.1 | 8 |
| 2.95 | 402.16 | C14H24O12 |  | 0.107195 | -0.65768 | 0.9 | 1.7 | 3 |
| 7.83 | 606.2237 | C22H36O18 |  | -0.17233 | -0.65763 | 0.8 | 1.6 | 5 |
| 13.95 | 119.049 | C8H6O |  | -0.28962 | -0.65751 | 0.1 | 0.8 | 6 |
| 13.94 | 279.0863 | C14H14O6 |  | -0.31702 | -0.65578 | 0.4 | 1.0 | 8 |
| 15.8 | 207.0651 | C11H10O4 |  | 0.222465 | -0.65552 | 0.4 | 0.9 | 7 |
| 10.28 | 269.0671 | C12H14O7 |  | 0.277953 | -0.65459 | 0.6 | 1.2 | 6 |
| 21.32 | 401.1241 | C21H22O8 |  | -0.41595 | -0.65438 | 0.4 | 1.0 | 11 |
| 15.73 | 347.1141 | C18H20O7 |  | 0.217899 | -0.6536 | 0.4 | 1.1 | 9 |
| 4.42 | 365.1076 | C14H20O11 |  | -0.05729 | -0.65293 | 0.8 | 1.4 | 5 |
| 2.18 | 383.1195 | C14H24O12 |  | 0.104947 | -0.65236 | 0.9 | 1.7 | 3 |
| 13.95 | 235.0616 | C12H12O5 |  | -0.32676 | -0.65167 | 0.4 | 1.0 | 7 |
| 16.07 | 347.1142 | C18H20O7 |  | 0.202593 | -0.65131 | 0.4 | 1.1 | 9 |
| 4.54 | 265.0916 | C10H16O8 |  | -0.15963 | -0.64949 | 0.8 | 1.6 | 3 |
| 7.12 | 532.1869 | C19H30O16 |  | -0.17234 | -0.64878 | 0.8 | 1.6 | 5 |
| 8.3 | 263.0778 | C10H16O8 |  | 0.059909 | -0.64864 | 0.8 | 1.6 | 3 |
| 4.42 | 532.1867 | C19H30O16 |  | -0.05735 | -0.6481 | 0.8 | 1.6 | 5 |
| 15.64 | 333.0984 | C17H18O7 |  | 0.113698 | -0.64602 | 0.4 | 1.1 | 9 |
| 14.58 | 195.0651 | C10H10O4 |  | -0.43076 | -0.64382 | 0.4 | 1.0 | 6 |
| 2.57 | 467.1412 | C18H28O14 |  | -0.07854 | -0.64305 | 0.8 | 1.6 | 5 |
| 17.22 | 355.1192 | C20H20O6 |  | 0.206349 | -0.64169 | 0.3 | 1.0 | 11 |
| 13.95 | 163.0404 | C9H8O3 |  | -0.32634 | -0.63957 | 0.3 | 0.9 | 6 |
| 14.69 | 441.1389 | C20H24O11 |  | -0.27925 | -0.63948 | 0.6 | 1.2 | 9 |
| 3.51 | 400.1448 | C14H22O12 |  | 0.03129 | -0.63776 | 0.9 | 1.6 | 4 |
| 17.06 | 385.1294 | C21H22O7 |  | 0.387861 | -0.63736 | 0.3 | 1.0 | 11 |
| 13.94 | 363.1087 | C18H20O8 |  | 0.12254 | -0.63683 | 0.4 | 1.1 | 9 |
| 9.55 | 245.0674 | C10H14O7 |  | 0.099277 | -0.6353 | 0.7 | 1.4 | 4 |
| 2.19 | 429.1248 | C15H26O14 |  | 0.112757 | -0.63502 | 0.9 | 1.7 | 3 |
| 18.08 | 385.1281 | C26H30O12 |  | -0.53749 | -0.63435 | 0.5 | 1.2 | 12 |
| 15.1 | 377.1247 | C19H22O8 |  | 0.195211 | -0.63394 | 0.4 | 1.2 | 9 |
| 11.57 | 453.1252 | C17H26O14 |  | 0.097996 | -0.63363 | 0.8 | 1.5 | 5 |
| 2.05 | 545.1727 | C20H34O17 |  | -0.07809 | -0.63273 | 0.9 | 1.7 | 4 |
| 12.07 | 453.1258 | C17H26O14 |  | 0.097576 | -0.63248 | 0.8 | 1.5 | 5 |
| 9.56 | 305.0881 | C12H18O9 |  | 0.097221 | -0.63072 | 0.8 | 1.5 | 4 |
| 7.47 | 621.2291 | C50H80O35 |  | -0.07571 | -0.62931 | 0.7 | 1.6 | 11 |
| 22.9 | 537.1769 | C29H30O10 |  | 0.092898 | -0.62924 | 0.3 | 1.0 | 15 |
| 15.52 | 333.0985 | C17H18O7 |  | 0.101641 | -0.62913 | 0.4 | 1.1 | 9 |
| 2.02 | 154.999 | C6H4O5 |  | 0.207999 | -0.62856 | 0.8 | 0.7 | 5 |
| 2.79 | 400.1448 | C14H22O12 |  | 0.034601 | -0.62781 | 0.9 | 1.6 | 4 |
| 7.22 | 591.1779 | C20H34O17 |  | 0.102555 | -0.62722 | 0.9 | 1.7 | 4 |
| 1.34 | 287.0759 | C12H14O8 |  | 0.071635 | -0.62593 | 0.7 | 1.2 | 6 |
| 9.66 | 263.0778 | C10H16O8 |  | 0.088559 | -0.62429 | 0.8 | 1.6 | 3 |
| 6.86 | 531.1569 | C19H32O17 |  | -0.16041 | -0.62413 | 0.9 | 1.7 | 4 |
| 13.28 | 225.0773 | C11H14O5 |  | 0.111736 | -0.62116 | 0.5 | 1.3 | 5 |
| 1.23 | 309.0817 | C11H16O10 |  | -0.22211 | -0.62002 | 0.9 | 1.5 | 4 |
| 1.29 | 207.0511 | C17H30O16 |  | 0.09718 | -0.61976 | 0.9 | 1.8 | 3 |
| 14.26 | 265.0723 | C13H14O6 |  | -0.39853 | -0.61954 | 0.5 | 1.1 | 7 |
| 1.77 | 187.0595 | C8H12O6 |  | 0.15265 | -0.61838 | 0.8 | 1.5 | 3 |
| 7.84 | 439.1442 | C27H44O22 |  | -0.18729 | -0.61749 | 0.8 | 1.6 | 6 |
| 9.66 | 191.0563 | C7H12O6 |  | 0.094075 | -0.61742 | 0.9 | 1.7 | 2 |
| 9.56 | 191.0562 | C7H12O6 |  | 0.082954 | -0.61597 | 0.9 | 1.7 | 2 |
| 13.38 | 349.1296 | C18H22O7 |  | 0.197342 | -0.61402 | 0.4 | 1.2 | 8 |
| 11.57 | 217.0707 | C9H12O6 |  | 0.084836 | -0.61345 | 0.7 | 1.3 | 4 |
| 8.42 | 513.1467 | C19H30O16 |  | 0.080705 | -0.61231 | 0.8 | 1.6 | 5 |
| 1.97 | 489.1461 | C17H30O16 |  | 0.082268 | -0.61198 | 0.9 | 1.8 | 3 |
| 3.67 | 205.0706 | C8H12O6 |  | 0.119749 | -0.61193 | 0.8 | 1.5 | 3 |
| 11.56 | 426.1606 | C8H12O6 |  | 0.088848 | -0.61185 | 0.8 | 1.5 | 3 |
| 9.66 | 251.0778 | C9H16O8 |  | 0.083842 | -0.61062 | 0.9 | 1.8 | 2 |
| 1.56 | 191.055 | C7H12O7 |  | 0.071406 | -0.61059 | 1.0 | 1.7 | 2 |
| 12.06 | 426.1605 | C16H24O12 |  | 0.08746 | -0.607 | 0.8 | 1.5 | 5 |
| 17.96 | 385.1294 | C21H22O7 |  | 0.223421 | -0.60571 | 0.3 | 1.0 | 11 |
| 1.4 | 207.0512 | C7H12O7 |  | 0.06256 | -0.60554 | 1.0 | 1.7 | 2 |
| 15.8 | 333.1326 | C18H20O6 |  | 0.195308 | -0.60483 | 0.3 | 1.1 | 9 |
| 20.76 | 401.1242 | C21H22O8 |  | -0.39321 | -0.60435 | 0.4 | 1.0 | 11 |
| 14.58 | 251.0567 | C12H12O6 |  | 0.170287 | -0.60273 | 0.5 | 1.0 | 7 |
| 12.01 | 585.1676 | C22H34O18 |  | 0.089513 | -0.60191 | 0.8 | 1.5 | 6 |
| 9.56 | 263.0777 | C10H16O8 |  | 0.083158 | -0.60191 | 0.8 | 1.6 | 3 |
| 14.84 | 457.135 | C20H26O12 |  | -0.30742 | -0.60145 | 0.6 | 1.3 | 8 |
| 7.07 | 131.0354 | C5H8O4 |  | -0.13566 | -0.60049 | 0.8 | 1.6 | 2 |
| 20.61 | 371.1488 | C21H22O6 |  | 0.12883 | -0.60018 | 0.3 | 1.0 | 11 |
| 11.89 | 453.1245 | C17H26O14 |  | 0.091342 | -0.59977 | 0.8 | 1.5 | 5 |
| 14.6 | 265.0721 | C13H14O6 |  | -0.46794 | -0.5991 | 0.5 | 1.1 | 7 |
| 8.34 | 527.1628 | C20H32O16 |  | -0.17577 | -0.59881 | 0.8 | 1.6 | 5 |
| 21.32 | 249.0756 | C13H12O5 |  | -0.39135 | -0.59739 | 0.4 | 0.9 | 8 |
| 14.61 | 193.0506 | C10H10O4 |  | -0.45853 | -0.59682 | 0.4 | 1.0 | 6 |
| 4.68 | 139.0041 | C6H4O4 |  | 0.065994 | -0.59669 | 0.7 | 0.7 | 5 |
| 4.4 | 307.1021 | C17H28O14 |  | 0.004977 | -0.59402 | 0.8 | 1.6 | 4 |
| 14.87 | 417.1556 | C22H26O8 |  | 0.291312 | -0.59384 | 0.4 | 1.2 | 10 |
| 4.69 | 429.1251 | C15H26O14 |  | 0.107097 | -0.59218 | 0.9 | 1.7 | 3 |
| 16.84 | 605.2223 | C30H36O13 |  | -0.17372 | -0.59177 | 0.4 | 1.2 | 13 |
| 3.52 | 255.0496 | C11H10O7 |  | 0.034696 | -0.59165 | 0.6 | 0.9 | 7 |
| 1.2 | 181.0707 | C6H12O6 |  | 0.146063 | -0.59153 | 1.0 | 2.0 | 1 |
| 12.8 | 225.0756 | C11H12O5 |  | 0.222337 | -0.59142 | 0.5 | 1.1 | 6 |
| 11.29 | 147.044 | C9H6O2 |  | 0.218629 | -0.59083 | 0.2 | 0.7 | 7 |
| 12.57 | 217.0707 | C9H12O6 |  | 0.06377 | -0.58604 | 0.7 | 1.3 | 4 |
| 14.61 | 149.0596 | C9H8O2 |  | -0.44521 | -0.58583 | 0.2 | 0.9 | 6 |
| 1.65 | 429.1255 | C15H26O14 |  | -0.06934 | -0.5848 | 0.9 | 1.7 | 3 |
| 3.07 | 411.1145 | C15H24O13 |  | 0.107872 | -0.58419 | 0.9 | 1.6 | 4 |
| 15.02 | 457.1352 | C20H26O12 |  | -0.29618 | -0.58384 | 0.6 | 1.3 | 8 |
| 14.6 | 235.0618 | C12H12O5 |  | -0.46748 | -0.58383 | 0.4 | 1.0 | 7 |
| 17.46 | 177.0545 | C10H8O3 |  | 0.041588 | -0.58348 | 0.3 | 0.8 | 7 |
| 11.53 | 165.0546 | C9H8O3 |  | 0.207219 | -0.58128 | 0.3 | 0.9 | 6 |
| 15.23 | 551.1771 | C26H32O13 |  | -0.10712 | -0.58034 | 0.5 | 1.2 | 11 |
| 21.27 | 265.1068 | C14H16O5 |  | 0.113913 | -0.58005 | 0.4 | 1.1 | 7 |
| 9.55 | 251.0773 | C9H16O8 |  | 0.068124 | -0.57938 | 0.9 | 1.8 | 2 |
| 7.25 | 411.114 | C15H24O13 |  | 0.088799 | -0.57801 | 0.9 | 1.6 | 4 |
| 6.83 | 265.0918 | C10H16O8 |  | -0.1779 | -0.57711 | 0.8 | 1.6 | 3 |
| 11.53 | 137.0596 | C8H8O2 |  | 0.210816 | -0.57656 | 0.3 | 1.0 | 5 |
| 2.04 | 589.1628 | C21H34O19 |  | -0.07582 | -0.57615 | 0.9 | 1.6 | 5 |
| 7.89 | 363.0935 | C14H20O11 |  | 0.116841 | -0.57566 | 0.8 | 1.4 | 5 |
| 15.58 | 303.0879 | C16H16O6 |  | 0.107352 | -0.5756 | 0.4 | 1.0 | 9 |
| 1.4 | 223.0463 | C7H12O8 |  | 0.154165 | -0.57517 | 1.1 | 1.7 | 2 |
| 1.43 | 323.097 | C12H18O10 |  | 0.023405 | -0.57429 | 0.8 | 1.5 | 4 |
| 7.84 | 175.06 | C7H10O5 |  | -0.107 | -0.57412 | 0.7 | 1.4 | 3 |
| 21.43 | 235.0964 | C13H14O4 |  | 0.128851 | -0.57404 | 0.3 | 1.1 | 7 |
| 19.33 | 335.1123 | C17H18O7 |  | 0.212477 | -0.57334 | 0.4 | 1.1 | 9 |
| 3.37 | 413.1302 | C15H26O13 |  | -0.08295 | -0.5732 | 0.9 | 1.7 | 3 |
| 7.57 | 195.0664 | C10H12O4 |  | 0.072219 | -0.57232 | 0.4 | 1.2 | 5 |
| 14.14 | 147.0439 | C9H6O2 |  | -0.25921 | -0.57192 | 0.2 | 0.7 | 7 |
| 7.83 | 527.163 | C20H32O16 |  | -0.18438 | -0.57161 | 0.8 | 1.6 | 5 |
| 3.6 | 545.1726 | C20H34O17 |  | -0.07503 | -0.57123 | 0.9 | 1.7 | 4 |
| 7.37 | 474.1815 | C17H28O14 |  | -0.19648 | -0.57041 | 0.8 | 1.6 | 4 |
| 3.59 | 591.1777 | C21H36O19 |  | -0.07306 | -0.56928 | 0.9 | 1.7 | 4 |
| 16.19 | 351.1072 | C27H36O17 |  | -0.15209 | -0.56917 | 0.6 | 1.3 | 10 |
| 6.15 | 265.0918 | C10H16O8 |  | -0.12836 | -0.56914 | 0.8 | 1.6 | 3 |
| 6.83 | 229.0707 | C10H12O6 |  | -0.14421 | -0.56871 | 0.6 | 1.2 | 5 |
| 1.36 | 387.1146 | C13H24O13 |  | -0.0545 | -0.56748 | 1.0 | 1.8 | 2 |
| 12.93 | 591.1728 | C28H32O14 |  | -0.07436 | -0.56644 | 0.5 | 1.1 | 13 |
| 7.41 | 591.1778 | C21H36O19 |  | 0.084058 | -0.56613 | 0.9 | 1.7 | 4 |
| 3.43 | 591.1777 | C21H36O19 |  | -0.06965 | -0.56171 | 0.9 | 1.7 | 4 |
| 17.08 | 387.1436 | C21H22O7 |  | 0.4879 | -0.56164 | 0.3 | 1.0 | 11 |
| 8.51 | 365.1078 | C14H20O11 |  | 0.096115 | -0.56022 | 0.8 | 1.4 | 5 |
| 3.08 | 193.0707 | C7H12O6 |  | -0.11767 | -0.55989 | 0.9 | 1.7 | 2 |
| 16.27 | 351.1073 | C27H36O17 |  | -0.15488 | -0.55948 | 0.6 | 1.3 | 10 |
| 7.37 | 545.1723 | C20H34O17 |  | -0.01416 | -0.5592 | 0.9 | 1.7 | 4 |
| 7.74 | 263.0778 | C10H16O8 |  | 0.043343 | -0.5591 | 0.8 | 1.6 | 3 |
| 9.11 | 153.0197 | C7H6O4 |  | 0.266908 | -0.55871 | 0.6 | 0.9 | 5 |
| 11.52 | 323.1122 | C16H18O7 |  | 0.358523 | -0.55859 | 0.4 | 1.1 | 8 |
| 15.54 | 347.1122 | C18H18O7 |  | 0.15889 | -0.55708 | 0.4 | 1.0 | 10 |
| 15.39 | 363.1087 | C18H20O8 |  | 0.182945 | -0.55609 | 0.4 | 1.1 | 9 |
| 3.76 | 474.1813 | C17H28O14 |  | -0.16113 | -0.55576 | 0.8 | 1.6 | 4 |
| 11.3 | 137.0247 | C7H6O3 |  | 0.602808 | -0.55314 | 0.4 | 0.9 | 5 |
| 12.68 | 265.0725 | C13H14O6 |  | 0.198385 | -0.55295 | 0.5 | 1.1 | 7 |
| 1.66 | 281.0883 | C10H18O9 |  | -0.12364 | -0.55263 | 0.9 | 1.8 | 2 |
| 2.12 | 205.0706 | C8H12O6 |  | 0.11116 | -0.55175 | 0.8 | 1.5 | 3 |
| 16.16 | 387.1437 | C21H22O7 |  | 0.469466 | -0.55167 | 0.3 | 1.0 | 11 |
| 4.41 | 513.1458 | C19H30O16 |  | -0.05039 | -0.55146 | 0.8 | 1.6 | 5 |
| 9.55 | 217.0706 | C14H22O11 |  | 0.063374 | -0.55118 | 0.8 | 1.6 | 4 |
| 9.65 | 217.0706 | C9H12O6 |  | 0.062934 | -0.55087 | 0.7 | 1.3 | 4 |
| 10.43 | 175.0601 | C7H10O5 |  | -0.00745 | -0.55009 | 0.7 | 1.4 | 3 |
| 8.99 | 648.2341 | C24H38O19 |  | -0.18565 | -0.54925 | 0.8 | 1.6 | 6 |
| 14.85 | 309.0967 | C20H26O12 |  | -0.30635 | -0.54805 | 0.6 | 1.3 | 8 |
| 9.65 | 384.15 | C14H22O11 |  | 0.064325 | -0.54787 | 0.8 | 1.6 | 4 |
| 16.52 | 403.14 | C21H24O8 |  | 0.269371 | -0.54586 | 0.4 | 1.1 | 10 |
| 8.51 | 255.0497 | C11H10O7 |  | 0.101105 | -0.5451 | 0.6 | 0.9 | 7 |
| 3.57 | 413.1304 | C15H26O13 |  | -0.08275 | -0.54353 | 0.9 | 1.7 | 3 |
| 10.97 | 243.0864 | C11H14O6 |  | 0.293282 | -0.54333 | 0.5 | 1.3 | 5 |
| 2.6 | 413.1305 | C15H26O13 |  | -0.10686 | -0.543 | 0.9 | 1.7 | 3 |
| 11.4 | 455.1556 | C21H28O11 |  | 0.074672 | -0.54265 | 0.5 | 1.3 | 8 |
| 20.34 | 173.0596 | C11H8O2 |  | 0.028974 | -0.54259 | 0.2 | 0.7 | 8 |
| 7.21 | 205.0707 | C8H12O6 |  | 0.088816 | -0.54212 | 0.8 | 1.5 | 3 |
| 2.92 | 331.1019 | C14H18O9 |  | 0.098588 | -0.5397 | 0.6 | 1.3 | 6 |
| 8.52 | 363.0935 | C14H20O11 |  | 0.110512 | -0.53869 | 0.8 | 1.4 | 5 |
| 15.55 | 319.1172 | C17H18O6 |  | 0.154805 | -0.53862 | 0.4 | 1.1 | 9 |
| 16.07 | 209.0807 | C11H12O4 |  | 0.004731 | -0.53847 | 0.4 | 1.1 | 6 |
| 9.65 | 157.0494 | C7H8O4 |  | 0.061799 | -0.5383 | 0.6 | 1.1 | 4 |
| 7.58 | 325.1124 | C12H20O10 |  | -0.22523 | -0.53772 | 0.8 | 1.7 | 3 |
| 11.89 | 585.1677 | C22H34O18 |  | 0.067675 | -0.53766 | 0.8 | 1.5 | 6 |
| 7.37 | 265.0917 | C10H16O8 |  | -0.21341 | -0.53655 | 0.8 | 1.6 | 3 |
| 10.15 | 213.0758 | C10H12O5 |  | 0.283952 | -0.5364 | 0.5 | 1.2 | 5 |
| 1.41 | 379.0566 | C31H8 |  | -0.21397 | -0.53622 | 0.0 | 0.3 | 28 |
| 15.03 | 309.0968 | C20H26O12 |  | -0.29262 | -0.53458 | 0.6 | 1.3 | 8 |
| 3.89 | 129.0181 | C5H4O4 |  | 0.069551 | -0.53337 | 0.8 | 0.8 | 4 |
| 16 | 317.1034 | C17H18O6 |  | 0.178971 | -0.53292 | 0.4 | 1.1 | 9 |
| 1.5 | 221.0672 | C8H14O7 |  | -0.11755 | -0.53187 | 0.9 | 1.8 | 2 |
| 1.34 | 358.1343 | C12H20O11 |  | 0.084692 | -0.53089 | 0.9 | 1.7 | 3 |
| 12.66 | 217.0708 | C9H12O6 |  | 0.057707 | -0.53084 | 0.7 | 1.3 | 4 |
| 1.58 | 381.1044 | C14H22O12 |  | 0.099091 | -0.53015 | 0.9 | 1.6 | 4 |
| 20.34 | 235.0963 | C13H14O4 |  | 0.02561 | -0.52994 | 0.3 | 1.1 | 7 |
| 9.56 | 157.0494 | C7H8O4 |  | 0.060129 | -0.52991 | 0.6 | 1.1 | 4 |
| 16.37 | 347.1121 | C18H18O7 |  | 0.196448 | -0.52911 | 0.4 | 1.0 | 10 |
| 16.24 | 391.1386 | C20H22O8 |  | 0.465034 | -0.528 | 0.4 | 1.1 | 10 |
| 16.39 | 177.0545 | C10H8O3 |  | -0.39388 | -0.52731 | 0.3 | 0.8 | 7 |
| 14.56 | 255.0518 | C11H12O7 |  | 0.159706 | -0.52724 | 0.6 | 1.1 | 6 |
| 7.75 | 384.15 | C14H22O11 |  | 0.008495 | -0.52642 | 0.8 | 1.6 | 4 |
| 6.81 | 115.0389 | C5H6O3 |  | -0.14606 | -0.52488 | 0.6 | 1.2 | 3 |
| 6.99 | 591.178 | C21H36O19 |  | 0.088877 | -0.52341 | 0.9 | 1.7 | 4 |
| 14.58 | 177.0546 | C15H18O8 |  | -0.35783 | -0.52174 | 0.5 | 1.2 | 7 |
| 8.29 | 411.1143 | C14H22O11 |  | 0.007972 | -0.5202 | 0.8 | 1.6 | 4 |
| 10.19 | 251.0568 | C12H12O6 |  | 0.074155 | -0.51976 | 0.5 | 1.0 | 7 |
| 11.12 | 585.1675 | C22H34O18 |  | 0.021438 | -0.51802 | 0.8 | 1.5 | 6 |
| 11.55 | 539.1624 | C21H32O16 |  | 0.057018 | -0.51704 | 0.8 | 1.5 | 6 |
| 9.1 | 175.06 | C7H10O5 |  | -0.00637 | -0.51612 | 0.7 | 1.4 | 3 |
| 9.56 | 131.0352 | C5H8O4 |  | 0.070395 | -0.51589 | 0.8 | 1.6 | 2 |
| 15.06 | 247.0961 | C14H14O4 |  | 0.128095 | -0.51557 | 0.3 | 1.0 | 8 |
| 23.97 | 181.1223 | C11H16O2 |  | -0.20116 | -0.51386 | 0.2 | 1.5 | 4 |
| 20.34 | 265.1071 | C14H16O5 |  | 0.038044 | -0.5132 | 0.4 | 1.1 | 7 |
| 20.34 | 205.0859 | C12H12O3 |  | 0.039747 | -0.51315 | 0.3 | 1.0 | 7 |
| 20.63 | 249.1119 | C14H16O4 |  | 0.12822 | -0.51314 | 0.3 | 1.1 | 7 |
| 14.27 | 325.093 | C15H18O8 |  | -0.54125 | -0.51294 | 0.5 | 1.2 | 7 |
| 7.16 | 131.0354 | C5H8O4 |  | -0.08767 | -0.51159 | 0.8 | 1.6 | 2 |
| 3.5 | 321.0831 | C12H18O10 |  | 0.027129 | -0.51037 | 0.8 | 1.5 | 4 |
| 17.35 | 209.0808 | C11H12O4 |  | 0.018861 | -0.51019 | 0.4 | 1.1 | 6 |
| 6.85 | 325.1129 | C12H20O10 |  | -0.17927 | -0.50968 | 0.8 | 1.7 | 3 |
| 14.86 | 401.1594 | C22H24O7 |  | 0.414047 | -0.50862 | 0.3 | 1.1 | 11 |
| 17.02 | 392.1701 | C20H22O7 |  | 0.126002 | -0.50586 | 0.4 | 1.1 | 10 |
| 8.28 | 131.0354 | C5H8O4 |  | 0.053509 | -0.50553 | 0.8 | 1.6 | 2 |
| 15.28 | 401.1594 | C22H24O7 |  | 0.324853 | -0.50398 | 0.3 | 1.1 | 11 |
| 14.09 | 205.0857 | C12H12O3 |  | 0.157355 | -0.50372 | 0.3 | 1.0 | 7 |
| 2.76 | 381.1039 | C14H22O12 |  | 0.007584 | -0.50321 | 0.9 | 1.6 | 4 |
| 12.9 | 585.1674 | C22H34O18 |  | 0.064317 | -0.50286 | 0.8 | 1.5 | 6 |
| 8.58 | 263.0782 | C10H16O8 |  | 0.064293 | -0.50229 | 0.8 | 1.6 | 3 |
| 14.51 | 459.1314 | C23H24O10 |  | -0.17497 | -0.50147 | 0.4 | 1.0 | 12 |
| 6.85 | 307.1024 | C17H28O14 |  | -0.17183 | -0.50016 | 0.8 | 1.6 | 4 |
| 18.13 | 177.0545 | C10H8O3 |  | -0.29958 | -0.49893 | 0.3 | 0.8 | 7 |
| 2.95 | 383.119 | C14H24O12 |  | 0.101601 | -0.49694 | 0.9 | 1.7 | 3 |
| 11.67 | 206.0812 | C11H8O3 |  | -0.30797 | -0.4949 | 0.3 | 0.7 | 8 |
| 16.83 | 373.1296 | C20H22O7 |  | 0.167659 | -0.49347 | 0.4 | 1.1 | 10 |
| 22.7 | 643.2382 | C33H38O13 |  | -0.03878 | -0.49273 | 0.4 | 1.2 | 15 |
| 8.29 | 349.1128 | C14H20O10 |  | -0.01629 | -0.49112 | 0.7 | 1.4 | 5 |
| 2.06 | 473.1511 | C17H30O15 |  | -0.11625 | -0.491 | 0.9 | 1.8 | 3 |
| 8.66 | 349.1126 | C24H38O19 |  | -0.10681 | -0.49026 | 0.8 | 1.6 | 6 |
| 14.86 | 307.1175 | C16H18O6 |  | 0.094793 | -0.48874 | 0.4 | 1.1 | 8 |
| 10.61 | 341.0883 | C15H18O9 |  | 0.238214 | -0.48858 | 0.6 | 1.2 | 7 |
| 2.51 | 205.0707 | C8H12O6 |  | 0.092993 | -0.48805 | 0.8 | 1.5 | 3 |
| 8.29 | 193.0707 | C7H12O6 |  | -0.00755 | -0.48753 | 0.9 | 1.7 | 2 |
| 20.84 | 249.1119 | C14H16O4 |  | 0.108314 | -0.4873 | 0.3 | 1.1 | 7 |
| 16.33 | 219.1016 | C13H16O4 |  | 0.119218 | -0.48703 | 0.3 | 1.2 | 6 |
| 7.36 | 501.146 | C17H28O14 |  | -0.17942 | -0.48636 | 0.8 | 1.6 | 4 |
| 18.13 | 361.1662 | C20H26O6 |  | 0.082973 | -0.48624 | 0.3 | 1.3 | 8 |
| 2.06 | 575.1832 | C21H36O18 |  | -0.05808 | -0.48573 | 0.9 | 1.7 | 4 |
| 7.08 | 175.06 | C7H10O5 |  | -0.20352 | -0.48431 | 0.7 | 1.4 | 3 |
| 7.75 | 411.1143 | C15H24O13 |  | 0.024859 | -0.48429 | 0.9 | 1.6 | 4 |
| 15.78 | 417.1542 | C22H26O9 |  | 0.135053 | -0.48376 | 0.4 | 1.2 | 10 |
| 1.35 | 249.0624 | C9H14O8 |  | 0.116742 | -0.48309 | 0.9 | 1.6 | 3 |
| 6.82 | 175.0601 | C7H12O6 |  | -0.13115 | -0.4829 | 0.9 | 1.7 | 2 |
| 6.82 | 131.0354 | C5H8O4 |  | -0.0824 | -0.48153 | 0.8 | 1.6 | 2 |
| 7.09 | 545.1725 | C20H34O17 |  | -0.03458 | -0.48097 | 0.9 | 1.7 | 4 |
| 21.34 | 357.133 | C20H20O6 |  | 0.060565 | -0.47968 | 0.3 | 1.0 | 11 |
| 16 | 177.0545 | C10H8O3 |  | -0.07607 | -0.47828 | 0.3 | 0.8 | 7 |
| 3.35 | 187.0599 | C8H10O5 |  | 0.176291 | -0.47714 | 0.6 | 1.3 | 4 |
| 1.38 | 263.0777 | C10H16O8 |  | -0.0684 | -0.47607 | 0.8 | 1.6 | 3 |
| 14.46 | 197.0819 | C10H14O4 |  | 0.246525 | -0.47536 | 0.4 | 1.4 | 4 |
| 20.16 | 373.1645 | C21H24O6 |  | 0.015544 | -0.47532 | 0.3 | 1.1 | 10 |
| 1.9 | 97.02834 | C5H4O2 |  | -0.01179 | -0.47499 | 0.4 | 0.8 | 4 |
| 10.6 | 543.1568 | C20H32O17 |  | 0.031725 | -0.47498 | 0.9 | 1.6 | 5 |
| 8.17 | 229.0705 | C10H12O6 |  | 0.018389 | -0.47466 | 0.6 | 1.2 | 5 |
| 3.51 | 381.1038 | C14H22O12 |  | 0.023832 | -0.47446 | 0.9 | 1.6 | 4 |
| 15.96 | 223.06 | C11H10O5 |  | 0.231571 | -0.47072 | 0.5 | 0.9 | 7 |
| 1.31 | 535.1522 | C18H32O18 |  | 0.058551 | -0.47056 | 1.0 | 1.8 | 3 |
| 5.34 | 381.1038 | C14H22O12 |  | 0.028076 | -0.47017 | 0.9 | 1.6 | 4 |
| 8.84 | 389.1053 | C14H22O11 |  | -0.00983 | -0.46854 | 0.8 | 1.6 | 4 |
| 2.19 | 402.1604 | C14H24O12 |  | 0.076564 | -0.46481 | 0.9 | 1.7 | 3 |
| 9.4 | 411.114 | C15H24O13 |  | 0.017837 | -0.46432 | 0.9 | 1.6 | 4 |
| 20.35 | 249.1119 | C14H16O4 |  | 0.119789 | -0.46348 | 0.3 | 1.1 | 7 |
| 2.06 | 281.0881 | C10H18O9 |  | -0.20464 | -0.46018 | 0.9 | 1.8 | 2 |
| 8.77 | 411.1142 | C15H24O13 |  | 0.002606 | -0.46006 | 0.9 | 1.6 | 4 |
| 20.34 | 383.1487 | C22H22O6 |  | 0.068557 | -0.45803 | 0.3 | 1.0 | 12 |
| 9.11 | 245.0675 | C10H14O7 |  | 0.056298 | -0.45641 | 0.7 | 1.4 | 4 |
| 21.1 | 205.0859 | C12H12O3 |  | 0.057228 | -0.45601 | 0.3 | 1.0 | 7 |
| 1.23 | 147.0651 | C6H10O4 |  | -0.05916 | -0.45585 | 0.7 | 1.7 | 2 |
| 9.55 | 389.1053 | C14H22O11 |  | 0.044613 | -0.45467 | 0.8 | 1.6 | 4 |
| 20.99 | 385.1296 | C21H22O7 |  | 0.063345 | -0.45354 | 0.3 | 1.0 | 11 |
| 15.77 | 405.1541 | C21H24O8 |  | 0.087941 | -0.45331 | 0.4 | 1.1 | 10 |
| 1.22 | 163.0601 | C6H10O5 |  | 0.165456 | -0.45256 | 0.8 | 1.7 | 2 |
| 21.1 | 265.1071 | C14H16O5 |  | 0.056628 | -0.45131 | 0.4 | 1.1 | 7 |
| 11.59 | 175.0601 | C7H10O5 |  | -0.00079 | -0.45055 | 0.7 | 1.4 | 3 |
| 1.23 | 200.1125 | C6H14O6 |  | -0.14657 | -0.44952 | 1.0 | 2.3 | 0 |
| 7.06 | 537.1465 | C21H30O16 |  | 0.07691 | -0.44934 | 0.8 | 1.4 | 7 |
| 2.02 | 97.02832 | C5H4O2 |  | 0.004805 | -0.449 | 0.4 | 0.8 | 4 |
| 4.14 | 381.1039 | C14H22O12 |  | 0.021035 | -0.44828 | 0.9 | 1.6 | 4 |
| 9.11 | 411.1143 | C15H24O13 |  | 0.010812 | -0.448 | 0.9 | 1.6 | 4 |
| 16.61 | 219.1016 | C13H16O4 |  | 0.152353 | -0.44736 | 0.3 | 1.2 | 6 |
| 6.84 | 271.0807 | C12H14O7 |  | -0.15557 | -0.44672 | 0.6 | 1.2 | 6 |
| 15.62 | 401.1594 | C22H24O7 |  | -0.01212 | -0.44654 | 0.3 | 1.1 | 11 |
| 17.41 | 417.1542 | C22H24O8 |  | 0.409786 | -0.44522 | 0.4 | 1.1 | 11 |
| 5.64 | 591.1778 | C21H36O19 |  | 0.059472 | -0.44502 | 0.9 | 1.7 | 4 |
| 8.29 | 389.1053 | C14H22O11 |  | -0.00313 | -0.44424 | 0.8 | 1.6 | 4 |
| 2.93 | 179.0564 | C6H12O6 |  | 0.092499 | -0.44399 | 1.0 | 2.0 | 1 |
| 1.9 | 115.0389 | C5H6O3 |  | -0.00791 | -0.44309 | 0.6 | 1.2 | 3 |
| 16.08 | 435.1648 | C22H26O9 |  | 0.084816 | -0.44304 | 0.4 | 1.2 | 10 |
| 11.14 | 209.0461 | C10H10O5 |  | 0.127801 | -0.44291 | 0.5 | 1.0 | 6 |
| 19.77 | 249.1119 | C14H16O4 |  | 0.147845 | -0.44286 | 0.3 | 1.1 | 7 |
| 2.94 | 429.1249 | C15H26O14 |  | 0.09218 | -0.44223 | 0.9 | 1.7 | 3 |
| 22 | 265.1069 | C14H16O5 |  | -0.15188 | -0.44183 | 0.4 | 1.1 | 7 |
| 12.45 | 558.2023 | C21H32O16 |  | -0.00075 | -0.44073 | 0.8 | 1.5 | 6 |
| 13.72 | 311.1118 | C15H18O7 |  | 0.227412 | -0.4385 | 0.5 | 1.2 | 7 |
| 16.08 | 405.1542 | C21H24O8 |  | 0.080851 | -0.43781 | 0.4 | 1.1 | 10 |
| 4.44 | 281.0885 | C10H18O9 |  | -0.13446 | -0.43769 | 0.9 | 1.8 | 2 |
| 14.09 | 551.1771 | C26H32O13 |  | -0.1312 | -0.43677 | 0.5 | 1.2 | 11 |
| 16.79 | 235.0599 | C12H10O5 |  | 0.127822 | -0.43622 | 0.4 | 0.8 | 8 |
| 20.34 | 436.1964 | C22H26O8 |  | 0.085529 | -0.43509 | 0.4 | 1.2 | 10 |
| 21.11 | 436.1963 | C22H26O8 |  | 0.067724 | -0.43448 | 0.4 | 1.2 | 10 |
| 15.81 | 601.1784 | C26H34O16 |  | -0.07154 | -0.43435 | 0.6 | 1.3 | 10 |
| 13.29 | 179.0355 | C9H8O4 |  | 0.087134 | -0.43353 | 0.4 | 0.9 | 6 |
| 1.32 | 519.1566 | C18H32O17 |  | 0.186055 | -0.43343 | 0.9 | 1.8 | 3 |
| 20.49 | 551.1413 | C25H28O14 |  | -0.07166 | -0.43132 | 0.6 | 1.1 | 12 |
| 8.35 | 323.0987 | C12H20O10 |  | -0.02016 | -0.43072 | 0.8 | 1.7 | 3 |
| 21.43 | 265.1069 | C14H16O5 |  | 0.06568 | -0.43005 | 0.4 | 1.1 | 7 |
| 6.08 | 229.0705 | C10H12O6 |  | -0.13982 | -0.42879 | 0.6 | 1.2 | 5 |
| 8.57 | 307.1023 | C27H44O22 |  | -0.11544 | -0.4286 | 0.8 | 1.6 | 6 |
| 9 | 307.1022 | C12H20O10 |  | -0.13936 | -0.42793 | 0.8 | 1.7 | 3 |
| 1.84 | 191.055 | C7H10O6 |  | 0.003121 | -0.42769 | 0.9 | 1.4 | 3 |
| 13.35 | 401.1592 | C22H24O7 |  | 0.219125 | -0.42743 | 0.3 | 1.1 | 11 |
| 2.08 | 295.1022 | C16H28O14 |  | 0.074998 | -0.42648 | 0.9 | 1.8 | 3 |
| 12.2 | 209.0807 | C11H12O4 |  | 0.028551 | -0.42355 | 0.4 | 1.1 | 6 |
| 1.44 | 339.0935 | C11H18O9 |  | 0.16329 | -0.42303 | 0.8 | 1.6 | 3 |
| 15.89 | 601.1781 | C26H34O16 |  | -0.06941 | -0.42146 | 0.6 | 1.3 | 10 |
| 8.85 | 411.1143 | C14H22O11 |  | -0.00353 | -0.42139 | 0.8 | 1.6 | 4 |
| 17 | 137.0596 | C8H8O2 |  | 0.046226 | -0.42118 | 0.3 | 1.0 | 5 |
| 2.69 | 115.0389 | C5H6O3 |  | -0.01835 | -0.42071 | 0.6 | 1.2 | 3 |
| 14.34 | 311.0781 | C14H16O8 |  | 0.214341 | -0.42006 | 0.6 | 1.1 | 7 |
| 7.47 | 175.06 | C7H10O5 |  | -0.08084 | -0.41912 | 0.7 | 1.4 | 3 |
| 16.26 | 247.0962 | C14H14O4 |  | 0.512096 | -0.41755 | 0.3 | 1.0 | 8 |
| 11.33 | 341.0882 | C15H18O9 |  | 0.194596 | -0.41597 | 0.6 | 1.2 | 7 |
| 11.87 | 341.0881 | C15H18O9 |  | 0.191361 | -0.41574 | 0.6 | 1.2 | 7 |
| 13.91 | 197.0807 | C10H12O4 |  | 0.425857 | -0.41291 | 0.4 | 1.2 | 5 |
| 17.25 | 147.0439 | C9H6O2 |  | 0.033733 | -0.40986 | 0.2 | 0.7 | 7 |
| 2.13 | 245.0635 | C8H14O7 |  | 0.286191 | -0.40884 | 0.9 | 1.8 | 2 |
| 2.07 | 229.0707 | C10H14O7 |  | -0.08778 | -0.40573 | 0.7 | 1.4 | 4 |
| 2.68 | 459.1356 | C16H28O15 |  | -0.06458 | -0.40538 | 0.9 | 1.8 | 3 |
| 2.65 | 471.1358 | C17H28O15 |  | 0.054539 | -0.40524 | 0.9 | 1.6 | 4 |
| 21.39 | 361.1281 | C19H20O7 |  | 0.106283 | -0.40511 | 0.4 | 1.1 | 10 |
| 17.53 | 345.1329 | C19H20O6 |  | -0.12323 | -0.40372 | 0.3 | 1.1 | 10 |
| 10.77 | 343.138 | C16H22O8 |  | 0.109201 | -0.40274 | 0.5 | 1.4 | 6 |
| 1.36 | 255.0498 | C11H12O8 |  | 0.146547 | -0.40232 | 0.7 | 1.1 | 6 |
| 13.11 | 227.0913 | C11H14O5 |  | 0.110334 | -0.40093 | 0.5 | 1.3 | 5 |
| 4.71 | 381.1044 | C14H22O12 |  | 0.051565 | -0.39851 | 0.9 | 1.6 | 4 |
| 18.1 | 435.165 | C22H26O9 |  | -0.07879 | -0.39475 | 0.4 | 1.2 | 10 |
| 14.14 | 345.1336 | C19H20O6 |  | 0.026365 | -0.39434 | 0.3 | 1.1 | 10 |
| 16.83 | 375.1437 | C20H22O7 |  | 0.126425 | -0.39431 | 0.4 | 1.1 | 10 |
| 11.38 | 209.0808 | C11H12O4 |  | 0.07455 | -0.39287 | 0.4 | 1.1 | 6 |
| 9.1 | 389.1052 | C14H22O11 |  | -0.00977 | -0.3925 | 0.8 | 1.6 | 4 |
| 14.23 | 227.0912 | C11H14O5 |  | 0.095518 | -0.39227 | 0.5 | 1.3 | 5 |
| 1.32 | 191.055 | C7H10O6 |  | 0.1135 | -0.3911 | 0.9 | 1.4 | 3 |
| 1.26 | 259.0813 | C11H14O7 |  | 0.13942 | -0.38874 | 0.6 | 1.3 | 5 |
| 16.82 | 385.1294 | C21H24O8 |  | 0.141989 | -0.38773 | 0.4 | 1.1 | 10 |
| 6.91 | 527.1631 | C20H32O16 |  | -0.07189 | -0.38665 | 0.8 | 1.6 | 5 |
| 1.19 | 91.03897 | C3H6O3 |  | -0.04652 | -0.38315 | 1.0 | 2.0 | 1 |
| 17.25 | 179.0702 | C10H10O3 |  | 0.037703 | -0.38126 | 0.3 | 1.0 | 6 |
| 8.38 | 381.1045 | C14H22O12 |  | 0.028126 | -0.3811 | 0.9 | 1.6 | 4 |
| 20.35 | 219.1013 | C13H14O3 |  | 0.085627 | -0.37889 | 0.2 | 1.1 | 7 |
| 2.11 | 97.02833 | C5H6O3 |  | 0.051325 | -0.37847 | 0.6 | 1.2 | 3 |
| 5.89 | 545.1724 | C20H34O17 |  | -0.07032 | -0.37491 | 0.9 | 1.7 | 4 |
| 2.69 | 339.0935 | C12H20O11 |  | 0.043284 | -0.37278 | 0.9 | 1.7 | 3 |
| 12.03 | 167.0702 | C9H10O3 |  | 0.39204 | -0.37148 | 0.3 | 1.1 | 5 |
| 16.87 | 235.0963 | C13H14O4 |  | 0.531383 | -0.36798 | 0.3 | 1.1 | 7 |
| 9.09 | 217.0706 | C9H12O6 |  | 0.039152 | -0.36739 | 0.7 | 1.3 | 4 |
| 17.97 | 387.1438 | C21H22O7 |  | 0.136271 | -0.36737 | 0.3 | 1.0 | 11 |
| 3.28 | 295.1021 | C11H18O9 |  | 0.121767 | -0.36616 | 0.8 | 1.6 | 3 |
| 9.41 | 501.1467 | C18H30O16 |  | -0.04048 | -0.36119 | 0.9 | 1.7 | 4 |
| 2.63 | 205.0707 | C8H14O7 |  | 0.073997 | -0.35824 | 0.9 | 1.8 | 2 |
| 10.15 | 181.051 | C9H10O4 |  | 0.467141 | -0.35423 | 0.4 | 1.1 | 5 |
| 1.3 | 193.0354 | C6H10O7 |  | 0.082488 | -0.35162 | 1.2 | 1.7 | 2 |
| 7.61 | 211.06 | C10H10O5 |  | -0.00809 | -0.34928 | 0.5 | 1.0 | 6 |
| 21.73 | 301.0723 | C16H14O6 |  | 0.246474 | -0.34823 | 0.4 | 0.9 | 10 |
| 1.36 | 519.1569 | C18H32O17 |  | 0.03235 | -0.34665 | 0.9 | 1.8 | 3 |
| 2.09 | 340.1239 | C12H18O10 |  | 0.180451 | -0.34421 | 0.8 | 1.5 | 4 |
| 2.02 | 115.0389 | C5H6O3 |  | -0.01898 | -0.34408 | 0.6 | 1.2 | 3 |
| 12.03 | 227.0915 | C11H14O5 |  | 0.381255 | -0.34376 | 0.5 | 1.3 | 5 |
| 7.77 | 363.0936 | C14H20O11 |  | 0.087126 | -0.34083 | 0.8 | 1.4 | 5 |
| 8.61 | 411.1143 | C15H24O13 |  | -0.00802 | -0.34058 | 0.9 | 1.6 | 4 |
| 10.77 | 193.0858 | C11H12O3 |  | 0.144076 | -0.33948 | 0.3 | 1.1 | 6 |
| 16.83 | 405.1543 | C21H24O8 |  | 0.098129 | -0.33947 | 0.4 | 1.1 | 10 |
| 4.19 | 113.0233 | C5H4O3 |  | 0.068883 | -0.33834 | 0.6 | 0.8 | 4 |
| 20.35 | 145.0647 | C10H8O |  | 0.045378 | -0.33618 | 0.1 | 0.8 | 7 |
| 4.54 | 413.1308 | C15H26O13 |  | -0.05447 | -0.33456 | 0.9 | 1.7 | 3 |
| 2.7 | 455.1406 | C17H28O14 |  | -0.00754 | -0.33437 | 0.8 | 1.6 | 4 |
| 10.31 | 543.1565 | C20H32O17 |  | -0.04939 | -0.33355 | 0.9 | 1.6 | 5 |
| 21.11 | 235.0963 | C13H14O4 |  | 0.061425 | -0.33287 | 0.3 | 1.1 | 7 |
| 12.78 | 401.1591 | C22H24O7 |  | 0.229391 | -0.32884 | 0.3 | 1.1 | 11 |
| 21.11 | 173.0596 | C11H8O2 |  | 0.06098 | -0.32875 | 0.2 | 0.7 | 8 |
| 15.48 | 177.0546 | C10H8O3 |  | 0.075476 | -0.3282 | 0.3 | 0.8 | 7 |
| 2 | 282.1184 | C5H8O4 |  | 0.031484 | -0.32749 | 0.8 | 1.6 | 2 |
| 7.85 | 225.0408 | C10H10O6 |  | 0.590498 | -0.32477 | 0.6 | 1.0 | 6 |
| 12.81 | 183.0651 | C9H10O4 |  | 0.007658 | -0.32376 | 0.4 | 1.1 | 5 |
| 15.81 | 219.1014 | C13H14O3 |  | 0.044952 | -0.3223 | 0.2 | 1.1 | 7 |
| 2.68 | 97.02834 | C5H4O2 |  | -0.02442 | -0.32179 | 0.4 | 0.8 | 4 |
| 3.46 | 175.0601 | C7H10O5 |  | 0.040863 | -0.32031 | 0.7 | 1.4 | 3 |
| 16.6 | 359.1502 | C20H24O6 |  | 0.195452 | -0.31869 | 0.3 | 1.2 | 9 |
| 1.48 | 273.0603 | C11H12O8 |  | 0.008568 | -0.31854 | 0.7 | 1.1 | 6 |
| 2.1 | 273.0604 | C11H12O8 |  | 0.182301 | -0.31854 | 0.7 | 1.1 | 6 |
| 2.11 | 269.0655 | C12H12O7 |  | 0.174817 | -0.31747 | 0.6 | 1.0 | 7 |
| 2.12 | 157.0495 | C7H8O4 |  | 0.00112 | -0.31732 | 0.6 | 1.1 | 4 |
| 7.24 | 187.0608 | C8H10O5 |  | 0.040042 | -0.31711 | 0.6 | 1.3 | 4 |
| 4.85 | 263.0776 | C10H16O8 |  | -0.02659 | -0.31487 | 0.8 | 1.6 | 3 |
| 10.97 | 241.0719 | C11H14O6 |  | 0.348875 | -0.31458 | 0.5 | 1.3 | 5 |
| 15.36 | 289.1069 | C16H16O5 |  | 0.092792 | -0.31386 | 0.3 | 1.0 | 9 |
| 1.57 | 351.0576 | C12H16O12 |  | 0.203327 | -0.31344 | 1.0 | 1.3 | 5 |
| 17.36 | 191.07 | C11H10O3 |  | 0.01773 | -0.31257 | 0.3 | 0.9 | 7 |
| 2.12 | 131.0353 | C5H8O4 |  | 0.084825 | -0.3107 | 0.8 | 1.6 | 2 |
| 11.5 | 269.0672 | C12H14O7 |  | 0.16881 | -0.30803 | 0.6 | 1.2 | 6 |
| 2.03 | 311.0989 | C11H20O10 |  | 0.19818 | -0.30685 | 0.9 | 1.8 | 2 |
| 4.85 | 149.0459 | C5H10O5 |  | -9E-05 | -0.30498 | 1.0 | 2.0 | 1 |
| 15.36 | 307.1173 | C16H18O6 |  | 0.06988 | -0.30364 | 0.4 | 1.1 | 8 |
| 2.94 | 381.1039 | C14H22O12 |  | 0.004963 | -0.29796 | 0.9 | 1.6 | 4 |
| 3.56 | 205.0705 | C8H12O6 |  | 0.065 | -0.29738 | 0.8 | 1.5 | 3 |
| 16.04 | 307.1171 | C16H18O6 |  | 0.021142 | -0.2928 | 0.4 | 1.1 | 8 |
| 20.84 | 265.1069 | C14H16O5 |  | 0.069012 | -0.28851 | 0.4 | 1.1 | 7 |
| 20.84 | 205.0857 | C12H12O3 |  | 0.06284 | -0.28726 | 0.3 | 1.0 | 7 |
| 16.19 | 219.1013 | C13H14O3 |  | 0.071698 | -0.28725 | 0.2 | 1.1 | 7 |
| 7.45 | 471.1361 | C17H28O15 |  | 0.000831 | -0.28705 | 0.9 | 1.6 | 4 |
| 12.03 | 241.0721 | C11H14O6 |  | 0.277354 | -0.28681 | 0.5 | 1.3 | 5 |
| 10.97 | 225.0757 | C11H12O5 |  | 0.283924 | -0.28462 | 0.5 | 1.1 | 6 |
| 11.75 | 209.0807 | C11H12O4 |  | 0.089649 | -0.28344 | 0.4 | 1.1 | 6 |
| 17 | 345.1332 | C19H20O6 |  | 0.05842 | -0.28213 | 0.3 | 1.1 | 10 |
| 21.11 | 383.1486 | C22H22O6 |  | 0.061346 | -0.27691 | 0.3 | 1.0 | 12 |
| 3.45 | 115.0389 | C5H6O3 |  | 0.011409 | -0.27665 | 0.6 | 1.2 | 3 |
| 13.88 | 467.156 | C22H28O11 |  | 0.166064 | -0.27209 | 0.5 | 1.3 | 9 |
| 21.48 | 361.0935 | C18H18O8 |  | 0.184388 | -0.27193 | 0.4 | 1.0 | 10 |
| 1.8 | 149.0461 | C5H10O5 |  | 0.097539 | -0.26803 | 1.0 | 2.0 | 1 |
| 3.43 | 181.0145 | C8H6O5 |  | 0.053094 | -0.26791 | 0.6 | 0.8 | 6 |
| 10.97 | 211.0617 | C10H12O5 |  | 0.398158 | -0.26778 | 0.5 | 1.2 | 5 |
| 2.1 | 175.06 | C7H10O5 |  | 0.002734 | -0.26645 | 0.7 | 1.4 | 3 |
| 13.89 | 469.1702 | C22H28O11 |  | 0.124804 | -0.26537 | 0.5 | 1.3 | 9 |
| 2.19 | 473.1511 | C17H30O15 |  | 0.005948 | -0.26522 | 0.9 | 1.8 | 3 |
| 20.84 | 436.1966 | C22H26O8 |  | 0.056016 | -0.26503 | 0.4 | 1.2 | 10 |
| 3.68 | 321.083 | C12H18O10 |  | 0.016703 | -0.26472 | 0.8 | 1.5 | 4 |
| 1.28 | 133.0495 | C5H8O4 |  | 0.00976 | -0.26446 | 0.8 | 1.6 | 2 |
| 12.29 | 213.0756 | C10H12O5 |  | 0.52089 | -0.26378 | 0.5 | 1.2 | 5 |
| 4.03 | 531.1564 | C19H32O17 |  | 0.010566 | -0.26367 | 0.9 | 1.7 | 4 |
| 2.21 | 207.0515 | C7H12O7 |  | 0.212868 | -0.26305 | 1.0 | 1.7 | 2 |
| 21.61 | 331.0829 | C17H16O7 |  | 0.179485 | -0.26001 | 0.4 | 0.9 | 10 |
| 1.39 | 351.0574 | C12H16O12 |  | 0.341736 | -0.25973 | 1.0 | 1.3 | 5 |
| 1.74 | 207.0514 | C7H12O7 |  | 0.147282 | -0.25887 | 1.0 | 1.7 | 2 |
| 10.97 | 155.0702 | C8H10O3 |  | 0.314176 | -0.257 | 0.4 | 1.3 | 4 |
| 1.37 | 357.104 | C12H22O12 |  | 0.124659 | -0.2555 | 1.0 | 1.8 | 2 |
| 26.36 | 385.1646 | C22H24O6 |  | 0.017191 | -0.25214 | 0.3 | 1.1 | 11 |
| 7.48 | 485.1518 | C18H30O15 |  | 0.022883 | -0.24967 | 0.8 | 1.7 | 4 |
| 2.1 | 231.0862 | C10H14O6 |  | 0.194848 | -0.24905 | 0.6 | 1.4 | 4 |
| 1.47 | 437.0619 | C33H10O2 |  | 0.174294 | -0.2457 | 0.1 | 0.3 | 29 |
| 1.51 | 287.0759 | C12H14O8 |  | 0.087492 | -0.24314 | 0.7 | 1.2 | 6 |
| 21.11 | 145.0647 | C10H8O |  | 0.055897 | -0.24054 | 0.1 | 0.8 | 7 |
| 2.15 | 489.1462 | C17H30O16 |  | 0.07439 | -0.23792 | 0.9 | 1.8 | 3 |
| 1.21 | 378.1606 | C6H12O6 |  | 0.032465 | -0.23548 | 1.0 | 2.0 | 1 |
| 21.57 | 345.0981 | C18H18O7 |  | 0.517901 | -0.23339 | 0.4 | 1.0 | 10 |
| 9.65 | 341.0882 | C15H18O9 |  | 0.1653 | -0.23299 | 0.6 | 1.2 | 7 |
| 15.01 | 183.0652 | C9H10O4 |  | 0.340464 | -0.23163 | 0.4 | 1.1 | 5 |
| 7.93 | 305.0885 | C12H18O9 |  | 0.030645 | -0.22545 | 0.8 | 1.5 | 4 |
| 12.69 | 325.093 | C15H18O8 |  | 0.046548 | -0.22436 | 0.5 | 1.2 | 7 |
| 2.53 | 295.1019 | C11H18O9 |  | 0.180096 | -0.22389 | 0.8 | 1.6 | 3 |
| 3.16 | 205.0705 | C8H12O6 |  | 0.041094 | -0.22093 | 0.8 | 1.5 | 3 |
| 16.35 | 363.1091 | C18H20O8 |  | 0.066008 | -0.22084 | 0.4 | 1.1 | 9 |
| 11.29 | 219.0633 | C10H12O4 |  | 0.316039 | -0.22016 | 0.4 | 1.2 | 5 |
| 1.23 | 295.1025 | C11H18O9 |  | 0.026355 | -0.21944 | 0.8 | 1.6 | 3 |
| 13.1 | 379.14 | C19H24O8 |  | 0.123306 | -0.21835 | 0.4 | 1.3 | 8 |
| 17.37 | 233.0806 | C13H12O4 |  | 0.293338 | -0.21694 | 0.3 | 0.9 | 8 |
| 2.06 | 211.0603 | C10H10O5 |  | 0.0368 | -0.21476 | 0.5 | 1.0 | 6 |
| 10.39 | 341.0881 | C15H18O9 |  | 0.178133 | -0.2135 | 0.6 | 1.2 | 7 |
| 16.86 | 167.0701 | C9H10O3 |  | 0.149117 | -0.2094 | 0.3 | 1.1 | 5 |
| 2.06 | 163.0601 | C6H10O5 |  | 0.227385 | -0.20386 | 0.8 | 1.7 | 2 |
| 5.14 | 211.06 | C10H10O5 |  | 0.126039 | -0.19852 | 0.5 | 1.0 | 6 |
| 4.66 | 471.1359 | C17H28O15 |  | 0.039417 | -0.1965 | 0.9 | 1.6 | 4 |
| 17.01 | 375.1434 | C20H22O7 |  | 0.052392 | -0.1941 | 0.4 | 1.1 | 10 |
| 11.38 | 227.0914 | C11H14O5 |  | 0.114892 | -0.19212 | 0.5 | 1.3 | 5 |
| 19.88 | 319.1175 | C17H18O6 |  | 0.429644 | -0.1901 | 0.4 | 1.1 | 9 |
| 2.4 | 205.0707 | C8H12O6 |  | 0.286422 | -0.18969 | 0.8 | 1.5 | 3 |
| 21.48 | 181.0494 | C9H8O4 |  | 0.590904 | -0.18786 | 0.4 | 0.9 | 6 |
| 17.23 | 327.1221 | C19H18O5 |  | 0.061394 | -0.18693 | 0.3 | 0.9 | 11 |
| 15.01 | 155.0702 | C8H10O3 |  | 0.357383 | -0.18583 | 0.4 | 1.3 | 4 |
| 12.17 | 297.0986 | C14H18O7 |  | 0.059659 | -0.18211 | 0.5 | 1.3 | 6 |
| 20.2 | 289.107 | C16H16O5 |  | 0.381253 | -0.1798 | 0.3 | 1.0 | 9 |
| 12.03 | 181.0858 | C10H12O3 |  | 0.381125 | -0.17376 | 0.3 | 1.2 | 5 |
| 17.69 | 345.1329 | C19H20O6 |  | 0.05166 | -0.17317 | 0.3 | 1.1 | 10 |
| 15.02 | 123.0439 | C7H6O2 |  | 0.337589 | -0.16126 | 0.3 | 0.9 | 5 |
| 9.84 | 269.0671 | C12H14O7 |  | 0.640653 | -0.13811 | 0.6 | 1.2 | 6 |
| 12.03 | 191.0701 | C11H10O3 |  | 0.334143 | -0.13137 | 0.3 | 0.9 | 7 |
| 17.71 | 239.0912 | C12H16O6 |  | 0.667564 | -0.11492 | 0.5 | 1.3 | 5 |