**Supporting Information**

**Ultra-high resolution mass spectrometry explains changes in the optical properties of dissolved organic matter during drinking water production**

Lavonen, E.E,1,\* Kothawala, D.N.,2 Tranvik, L.J.,2 Gonsior, M.,3,4 Schmitt-Kopplin, P.,5,6 Köhler, S.J.1

1Department of Aquatic Sciences and Assessment, Swedish University of Agricultural Sciences (SLU), 75007, Uppsala, Sweden

2Department of Ecology and Genetics/Limnology, Uppsala University, 75236, Uppsala, Sweden

3Department of Thematic Studies, Unit of Environmental Change, Linköping University, 58183, Linköping, Sweden

4Chesapeake Biological Laboratory, University of Maryland Center for Environmental Science, Solomons, Maryland 20688, USA

5Analytical BioGeoChemistry, German Research Center for Environmental Health, Helmholtz Zentrum München, 85764, Neuherberg, Germany

6 Analytical Food Chemistry, Technische Universität München, 85354, Freising-Weihenstephan, Germany

\*Corresponding author: Phone: +46-18-67 30 59; fax: +46-18-67 31 56; e-mail: elin.lavonen@slu.se

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Figure A1 Map of southern Sweden showing the location of the four sampled WTPs.



Figure A2 Overview of treatment processes and the four WTPs. Sampling points are denoted by asterisks.

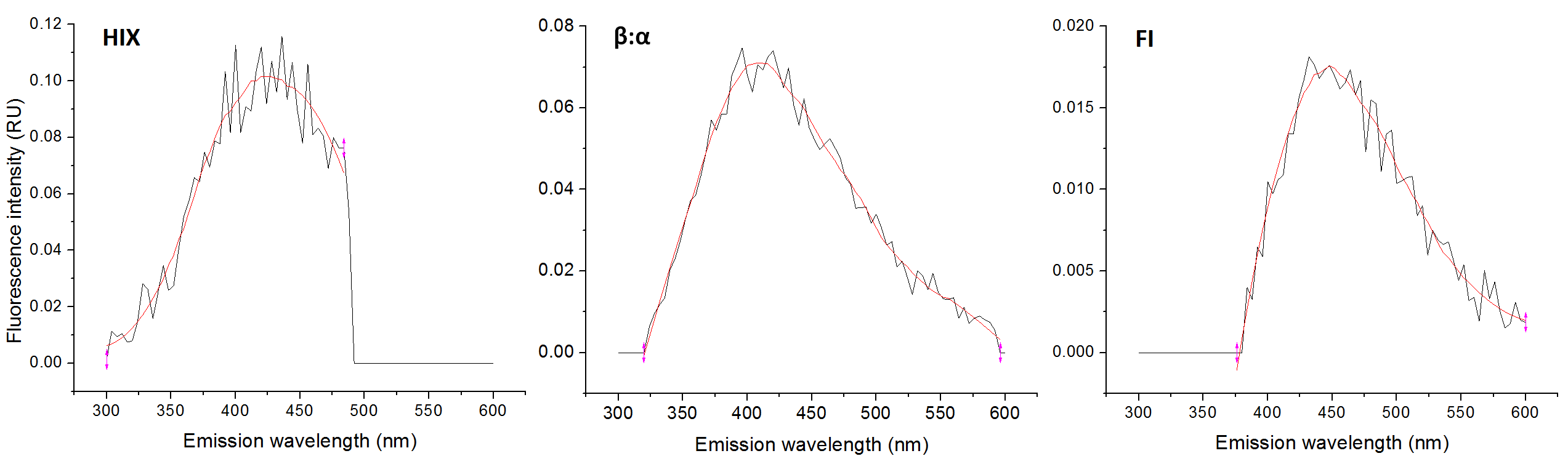


Figure A3 Examples of excitation spectra from a differential excitation emission matrix (EEM) for slow sand filtration from Lovö WTP (2011-07-11) that were used to calculate fluorescence indices for the calculated removed fluorescing dissolved organic matter. Black lines are extracted from the differential EEMs while red lines represent smoothed spectra. HIX = humification index (excitation = 254 nm), β:α = freshness index (excitation = 310 nm) and FI = fluorescence index, (excitation = 370 nm).

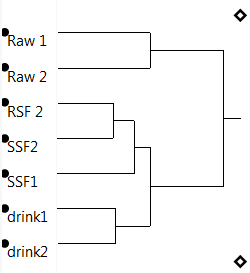


Figure A4 Dendrogram from hierarchial cluster analysis using Ward’s method of similarity which demonstrates the similarity of double samples from Lovö WTP taken for FT-ICR-MS analyses. Raw = untreated raw water, RSF = rapid sand filtrate (samples taken after coagulation treatment), SSF = slow sand filtrate, drink = drinking water, sampled after UV and monochloramine disinfection.

Table A1. Masses of singly negatively charged ions that are always present in DOM samples and were used for internal calibration of FT-ICR-MS data.

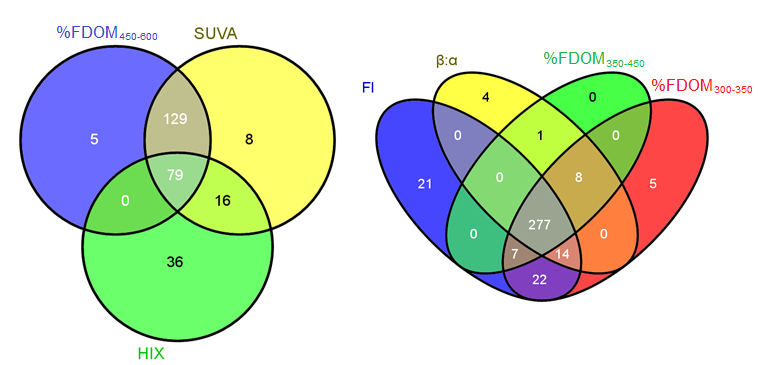
|  |  |
| --- | --- |
| Chemical formula | Theoretical mass |
| C11H13O6 | 241.071762 |
| C14H17O6 | 281.103062 |
| C14H17O7 | 297.097976 |
| C15H17O7 | 309.097976 |
| C15H17O8 | 325.092891 |
| C15H17O9 | 341.087806 |
| C17H19O8 | 351.108541 |
| C17H19O9 | 367.103456 |
| C19H23O8 | 379.139841 |
| C19H23O9 | 395.134756 |
| C19H21O10 | 409.114010 |
| C20H23O10 | 423.129671 |
| C21H25O10 | 437.145310 |
| C21H23O11 | 451.124585 |
| C22H25O11 | 465.140235 |
| C22H27O12 | 483.150800 |
| C24H29O12 | 509.166450 |
| C23H19O14 | 519.078029 |

Table A2 Number formulas correlated (p<0.05) with spectroscopic and fluorometric parameters that overlap between the measures. The percentage given in brackets represents the fraction of total formulas correlated with the parameter in the column to the far left. Numbers in italics show the amount and percentage of formulas uniquely correlated with the different parameters.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **HIX** | **SUVA** | **%FDOM450-600** | **β:α** | **FI** | **%FDOM350-450** | **%FDOM300-350** |
| **HIX** | *36 (27%)* | 95 (73%) | 79 (60%) | 0 | 0 | 0 | 0 |
| **SUVA** | 95 (41%) | *8 (3%)* | 208 (90%) | 0 | 0 | 0 | 0 |
| **%FDOM450-600** | 79 (37%) | 208 (98%) | *5 (2%)* | 0 | 0 | 0 | 0 |
| **β:α** | 0 | 0 | 0 | *4 (1%)* | 291 (96%) | 286 (94%) | 299 (98%) |
| **FI** | 0 | 0 | 0 | 291 (85%) | *21 (6%)* | 284 (83%) | 291 (85%) |
| **%FDOM350-450** | 0 | 0 | 0 | 286 (98%) | 284 (97%) | *0* | 292 (100%) |
| **%FDOM300-350** | 0 | 0 | 0 | 299 (90%) | 291 (87%) | 292 (88%) | *5 (2%)* |

Table A3 Average values (±SD) of oxygen to carbon and hydrogen to carbon ratios (O/C and H/C) as well as double bond equivalency per carbon (DBE/C) and average carbon oxidation state () for chemical formulas positively correlated (p<0.05) with single or groups of spectroscopic or fluorometric parameters.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Nr of formulas** | **O/C** | **H/C** | **DBE/C** |  |
| **HIX** | 131 | 0.698±0.081 | 0.978±0.141 | 0.568±0.069 | 0.418±0.198 |
| **SUVA** | 232 | 0.636±0.096 | 0.849±0.144 | 0.633±0.076 | 0.423±0.223 |
| **%FDOM450-600** | 213 | 0.623±0.096 | 0.827±0.134 | 0.643±0.072 | 0.418±0.226 |
| **%FDOM350-450** | 293 | 0.434±0.100 | 1.341±0.152 | 0.385±0.074 | -0.471±0.216 |
| **%FDOM300-350** | 333 | 0.439±0.098 | 1.318±0.160 | 0.396±0.078 | -0.439±0.225 |
| **FI** | 341 | 0.438±0.094 | 1.313±0.159 | 0.397±0.078 | -0.435±0.220 |
| **β:α** | 304 | 0.441±0.104 | 1.336±0.154 | 0.388±0.075 | -0.452±0.228 |
| **SUVA, %FDOM450-600, HIX** | 79 | 0.686±0.074 | 0.882±0.096 | 0.613±0.045 | 0.491±0.175 |
| **SUVA, %FDOM450-600** | 208 | 0.627±0.093 | 0.829±0.134 | 0.642±0.072 | 0.424±0.224 |
| **HIX – only** | 36 | 0.722±0.087 | 1.124±0.088 | 0.499±0.047 | 0.320±0.192 |
| **β:α, FI, %FDOM350-450, %FDOM300-350** | 277 | 0.433±0.098 | 1.341±0.153 | 0.385±0.075 | -0.472±0.216 |
| **FI – only** | 21 | 0.466±0.036 | 1.256±0.110 | 0.413±0.058 | -0.334±0.114 |



Oliveros, J.C. (2007) VENNY. An interactive tool for comparing lists with Venn Diagrams.

Figure A5 Venn diagrams ([Oliveros 2007](#_ENREF_1)) showing overlap of number of CHO-formulas that were significantly positively correlated with optical spectroscopic parameters



Figure A6 Differential absorbance spectra showing removed CDOM during (A) slow sand filtration at Lovö WTP, (B) disinfection with UV and monochloramine (NH2Cl) at Lovö WTP, and (C) disinfection with NH2Cl and UV at Kvarnagården WTP. Absorbance at approximately 260-270 nm was targeted in all cases, and the pattern in removal was consistent over the entire sampling period.

Table A4 List of CHO formulas for the neutral molecular components included in the rank correlation (and, hence, present in all samples or all samples except one) including oxygen to carbon and hydrogen to carbon ratios (O/C and H/C) as well as double bond equivalency per carbon (DBE/C) and the average carbon oxidation state (). Chemical formulas that were significantly positively correlated (p<0.05) with one or more of the spectroscopic parameters are marked with “x”. The table has been sorted based on decreasing .

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Chemical formula** | **O/C** | **H/C** | **DBE/C** | **Cos** | **SUVA** | **%FDOM450-600** | **HIX** | **%FDOM350-450** | **%FDOM300-350** | **FI** | **β:α** |
| C12H8O10 | 0.83 | 0.67 | 0.75 | 1 | x | x |  |  |  |  |  |
| C15H12O13 | 0.87 | 0.8 | 0.667 | 0.933 | x | x | x |  |  |  |  |
| C13H8O10 | 0.77 | 0.62 | 0.769 | 0.923 | x | x |  |  |  |  |  |
| C13H10O11 | 0.85 | 0.77 | 0.692 | 0.923 | x | x |  |  |  |  |  |
| C11H8O9 | 0.82 | 0.73 | 0.727 | 0.909 | x | x |  |  |  |  |  |
| C14H8O10 | 0.71 | 0.57 | 0.786 | 0.857 | x | x |  |  |  |  |  |
| C14H12O12 | 0.86 | 0.86 | 0.643 | 0.857 | x |  |  |  |  |  |  |
| C14H10O11 | 0.79 | 0.71 | 0.714 | 0.857 | x | x |  |  |  |  |  |
| C12H8O9 | 0.75 | 0.67 | 0.75 | 0.833 |  |  |  |  |  |  |  |
| C12H10O10 | 0.83 | 0.83 | 0.667 | 0.833 |  |  |  |  |  |  |  |
| C17H14O14 | 0.82 | 0.82 | 0.647 | 0.824 | x | x | x |  |  |  |  |
| C17H12O13 | 0.76 | 0.71 | 0.706 | 0.824 | x | x | x |  |  |  |  |
| C17H10O12 | 0.71 | 0.59 | 0.765 | 0.824 | x | x |  |  |  |  |  |
| C15H14O13 | 0.87 | 0.93 | 0.6 | 0.8 | x |  | x |  |  |  |  |
| C15H12O12 | 0.8 | 0.8 | 0.667 | 0.8 | x | x | x |  |  |  |  |
| C15H10O11 | 0.73 | 0.67 | 0.733 | 0.8 | x | x |  |  |  |  |  |
| C18H14O14 | 0.78 | 0.78 | 0.667 | 0.778 | x | x | x |  |  |  |  |
| C18H12O13 | 0.72 | 0.67 | 0.722 | 0.778 | x | x |  |  |  |  |  |
| C13H8O9 | 0.69 | 0.62 | 0.769 | 0.769 | x | x |  |  |  |  |  |
| C13H12O11 | 0.85 | 0.92 | 0.615 | 0.769 |  |  | x |  |  |  |  |
| C13H10O10 | 0.77 | 0.77 | 0.692 | 0.769 | x | x |  |  |  |  |  |
| C16H14O13 | 0.81 | 0.88 | 0.625 | 0.75 | x | x | x |  |  |  |  |
| C16H12O12 | 0.75 | 0.75 | 0.688 | 0.75 | x | x |  |  |  |  |  |
| C16H10O11 | 0.69 | 0.63 | 0.75 | 0.75 | x | x |  |  |  |  |  |
| C19H16O15 | 0.79 | 0.84 | 0.632 | 0.737 | x | x | x |  |  |  |  |
| C19H14O14 | 0.74 | 0.74 | 0.684 | 0.737 | x | x | x |  |  |  |  |
| C19H12O13 | 0.68 | 0.63 | 0.737 | 0.737 | x | x |  |  |  |  |  |
| C11H8O8 | 0.73 | 0.73 | 0.727 | 0.727 |  |  |  |  |  |  |  |
| C11H10O9 | 0.82 | 0.91 | 0.636 | 0.727 |  |  |  |  |  |  |  |
| C14H8O9 | 0.64 | 0.57 | 0.786 | 0.714 | x | x |  |  |  |  |  |
| C14H14O12 | 0.86 | 1 | 0.571 | 0.714 |  |  | x |  |  |  |  |
| C14H12O11 | 0.79 | 0.86 | 0.643 | 0.714 | x | x |  |  |  |  |  |
| C14H10O10 | 0.71 | 0.71 | 0.714 | 0.714 | x | x |  |  |  |  |  |
| C17H16O14 | 0.82 | 0.94 | 0.588 | 0.706 | x | x | x |  |  |  |  |
| C17H14O13 | 0.76 | 0.82 | 0.647 | 0.706 | x | x | x |  |  |  |  |
| C17H12O12 | 0.71 | 0.71 | 0.706 | 0.706 | x | x |  |  |  |  |  |
| C17H10O11 | 0.65 | 0.59 | 0.765 | 0.706 | x | x |  |  |  |  |  |
| C20H16O15 | 0.75 | 0.8 | 0.65 | 0.7 | x | x | x |  |  |  |  |
| C20H14O14 | 0.7 | 0.7 | 0.7 | 0.7 | x | x |  |  |  |  |  |
| C21H16O15 | 0.71 | 0.76 | 0.667 | 0.667 | x | x | x |  |  |  |  |
| C21H14O14 | 0.67 | 0.67 | 0.714 | 0.667 | x | x |  |  |  |  |  |
| C18H16O14 | 0.78 | 0.89 | 0.611 | 0.667 | x | x | x |  |  |  |  |
| C18H14O13 | 0.72 | 0.78 | 0.667 | 0.667 | x | x | x |  |  |  |  |
| C18H12O12 | 0.67 | 0.67 | 0.722 | 0.667 | x | x |  |  |  |  |  |
| C15H8O9 | 0.6 | 0.53 | 0.8 | 0.667 | x | x |  |  |  |  |  |
| C15H16O13 | 0.87 | 1.07 | 0.533 | 0.667 |  |  | x |  |  |  |  |
| C15H14O12 | 0.8 | 0.93 | 0.6 | 0.667 | x |  | x |  |  |  |  |
| C15H12O11 | 0.73 | 0.8 | 0.667 | 0.667 | x | x | x |  |  |  |  |
| C15H10O10 | 0.67 | 0.67 | 0.733 | 0.667 | x | x |  |  |  |  |  |
| C12H8O8 | 0.67 | 0.67 | 0.75 | 0.667 |  |  |  |  |  |  |  |
| C12H12O10 | 0.83 | 1 | 0.583 | 0.667 |  |  |  |  |  |  |  |
| C12H10O9 | 0.75 | 0.83 | 0.667 | 0.667 | x |  |  |  |  |  |  |
| C19H18O15 | 0.79 | 0.95 | 0.579 | 0.632 | x | x | x |  |  |  |  |
| C19H16O14 | 0.74 | 0.84 | 0.632 | 0.632 | x | x | x |  |  |  |  |
| C19H14O13 | 0.68 | 0.74 | 0.684 | 0.632 | x | x |  |  |  |  |  |
| C16H16O13 | 0.81 | 1 | 0.563 | 0.625 | x |  | x |  |  |  |  |
| C16H14O12 | 0.75 | 0.88 | 0.625 | 0.625 | x | x | x |  |  |  |  |
| C16H12O11 | 0.69 | 0.75 | 0.688 | 0.625 | x | x |  |  |  |  |  |
| C16H10O10 | 0.63 | 0.63 | 0.75 | 0.625 | x | x |  |  |  |  |  |
| C13H8O8 | 0.62 | 0.62 | 0.769 | 0.615 | x | x |  |  |  |  |  |
| C13H14O11 | 0.85 | 1.08 | 0.538 | 0.615 |  |  |  |  |  |  |  |
| C13H12O10 | 0.77 | 0.92 | 0.615 | 0.615 | x |  |  |  |  |  |  |
| C13H10O9 | 0.69 | 0.77 | 0.692 | 0.615 | x | x |  |  |  |  |  |
| C20H18O15 | 0.75 | 0.9 | 0.6 | 0.6 | x | x | x |  |  |  |  |
| C20H16O14 | 0.7 | 0.8 | 0.65 | 0.6 | x | x | x |  |  |  |  |
| C20H14O13 | 0.65 | 0.7 | 0.7 | 0.6 | x | x |  |  |  |  |  |
| C10H8O7 | 0.7 | 0.8 | 0.7 | 0.6 |  |  |  |  |  |  |  |
| C10H10O8 | 0.8 | 1 | 0.6 | 0.6 |  |  |  |  |  |  |  |
| C17H18O14 | 0.82 | 1.06 | 0.529 | 0.588 | x |  | x |  |  |  |  |
| C17H16O13 | 0.76 | 0.94 | 0.588 | 0.588 | x | x | x |  |  |  |  |
| C17H14O12 | 0.71 | 0.82 | 0.647 | 0.588 | x | x | x |  |  |  |  |
| C17H12O11 | 0.65 | 0.71 | 0.706 | 0.588 | x | x |  |  |  |  |  |
| C17H10O10 | 0.59 | 0.59 | 0.765 | 0.588 | x | x |  |  |  |  |  |
| C21H18O15 | 0.71 | 0.86 | 0.619 | 0.571 | x | x | x |  |  |  |  |
| C21H16O14 | 0.67 | 0.76 | 0.667 | 0.571 | x | x |  |  |  |  |  |
| C14H8O8 | 0.57 | 0.57 | 0.786 | 0.571 | x | x |  |  |  |  |  |
| C14H16O12 | 0.86 | 1.14 | 0.5 | 0.571 |  |  | x |  |  |  |  |
| C14H14O11 | 0.79 | 1 | 0.571 | 0.571 |  |  | x |  |  |  |  |
| C14H12O10 | 0.71 | 0.86 | 0.643 | 0.571 | x | x |  |  |  |  |  |
| C14H10O9 | 0.64 | 0.71 | 0.714 | 0.571 | x | x |  |  |  |  |  |
| C18H18O14 | 0.78 | 1 | 0.556 | 0.556 | x | x | x |  |  |  |  |
| C18H16O13 | 0.72 | 0.89 | 0.611 | 0.556 | x | x | x |  |  |  |  |
| C18H14O12 | 0.67 | 0.78 | 0.667 | 0.556 | x | x | x |  |  |  |  |
| C18H12O11 | 0.61 | 0.67 | 0.722 | 0.556 | x | x |  |  |  |  |  |
| C22H16O14 | 0.64 | 0.73 | 0.682 | 0.545 | x | x |  |  |  |  |  |
| C11H8O7 | 0.64 | 0.73 | 0.727 | 0.545 |  |  |  |  |  |  |  |
| C11H12O9 | 0.82 | 1.09 | 0.545 | 0.545 |  |  |  |  |  |  |  |
| C11H10O8 | 0.73 | 0.91 | 0.636 | 0.545 |  |  |  |  |  |  |  |
| C15H8O8 | 0.53 | 0.53 | 0.8 | 0.533 | x | x |  |  |  |  |  |
| C15H16O12 | 0.8 | 1.07 | 0.533 | 0.533 |  |  | x |  |  |  |  |
| C15H14O11 | 0.73 | 0.93 | 0.6 | 0.533 | x | x | x |  |  |  |  |
| C15H12O10 | 0.67 | 0.8 | 0.667 | 0.533 | x | x |  |  |  |  |  |
| C15H10O9 | 0.6 | 0.67 | 0.733 | 0.533 | x | x |  |  |  |  |  |
| C19H18O14 | 0.74 | 0.95 | 0.579 | 0.526 | x | x | x |  |  |  |  |
| C19H16O13 | 0.68 | 0.84 | 0.632 | 0.526 | x | x | x |  |  |  |  |
| C19H14O12 | 0.63 | 0.74 | 0.684 | 0.526 | x | x | x |  |  |  |  |
| C19H12O11 | 0.58 | 0.63 | 0.737 | 0.526 | x | x |  |  |  |  |  |
| C20H20O15 | 0.75 | 1 | 0.55 | 0.5 | x | x | x |  |  |  |  |
| C20H18O14 | 0.7 | 0.9 | 0.6 | 0.5 | x | x | x |  |  |  |  |
| C20H16O13 | 0.65 | 0.8 | 0.65 | 0.5 | x | x |  |  |  |  |  |
| C20H14O12 | 0.6 | 0.7 | 0.7 | 0.5 | x | x |  |  |  |  |  |
| C16H18O13 | 0.81 | 1.13 | 0.5 | 0.5 |  |  | x |  |  |  |  |
| C16H16O12 | 0.75 | 1 | 0.563 | 0.5 | x |  | x |  |  |  |  |
| C16H14O11 | 0.69 | 0.88 | 0.625 | 0.5 | x | x | x |  |  |  |  |
| C16H12O10 | 0.63 | 0.75 | 0.688 | 0.5 | x | x |  |  |  |  |  |
| C16H10O9 | 0.56 | 0.63 | 0.75 | 0.5 | x | x |  |  |  |  |  |
| C12H8O7 | 0.58 | 0.67 | 0.75 | 0.5 |  |  |  |  |  |  |  |
| C12H14O10 | 0.83 | 1.17 | 0.5 | 0.5 |  |  |  |  |  |  |  |
| C12H12O9 | 0.75 | 1 | 0.583 | 0.5 |  |  |  |  |  |  |  |
| C12H10O8 | 0.67 | 0.83 | 0.667 | 0.5 | x | x |  |  |  |  |  |
| C21H20O15 | 0.71 | 0.95 | 0.571 | 0.476 | x | x | x |  |  |  |  |
| C21H18O14 | 0.67 | 0.86 | 0.619 | 0.476 | x | x | x |  |  |  |  |
| C21H16O13 | 0.62 | 0.76 | 0.667 | 0.476 | x | x | x |  |  |  |  |
| C21H14O12 | 0.57 | 0.67 | 0.714 | 0.476 | x | x |  |  |  |  |  |
| C17H18O13 | 0.76 | 1.06 | 0.529 | 0.471 |  |  | x |  |  |  |  |
| C17H16O12 | 0.71 | 0.94 | 0.588 | 0.471 | x | x | x |  |  |  |  |
| C17H14O11 | 0.65 | 0.82 | 0.647 | 0.471 | x | x | x |  |  |  |  |
| C17H12O10 | 0.59 | 0.71 | 0.706 | 0.471 | x | x |  |  |  |  |  |
| C17H10O9 | 0.53 | 0.59 | 0.765 | 0.471 | x | x |  |  |  |  |  |
| C13H8O7 | 0.54 | 0.62 | 0.769 | 0.462 | x | x |  |  |  |  |  |
| C13H16O11 | 0.85 | 1.23 | 0.462 | 0.462 |  |  |  |  |  |  |  |
| C13H14O10 | 0.77 | 1.08 | 0.538 | 0.462 |  |  | x |  |  |  |  |
| C13H12O9 | 0.69 | 0.92 | 0.615 | 0.462 | x |  |  |  |  |  |  |
| C13H10O8 | 0.62 | 0.77 | 0.692 | 0.462 | x | x |  |  |  |  |  |
| C22H20O15 | 0.68 | 0.91 | 0.591 | 0.455 | x | x | x |  |  |  |  |
| C22H18O14 | 0.64 | 0.82 | 0.636 | 0.455 | x | x | x |  |  |  |  |
| C22H16O13 | 0.59 | 0.73 | 0.682 | 0.455 | x | x |  |  |  |  |  |
| C9H10O7 | 0.78 | 1.11 | 0.556 | 0.444 |  |  |  |  |  |  |  |
| C18H20O14 | 0.78 | 1.11 | 0.5 | 0.444 |  |  | x |  |  |  |  |
| C18H18O13 | 0.72 | 1 | 0.556 | 0.444 | x |  | x |  |  |  |  |
| C18H16O12 | 0.67 | 0.89 | 0.611 | 0.444 | x | x | x |  |  |  |  |
| C18H14O11 | 0.61 | 0.78 | 0.667 | 0.444 | x | x |  |  |  |  |  |
| C18H12O10 | 0.56 | 0.67 | 0.722 | 0.444 | x | x | x |  |  |  |  |
| C14H8O7 | 0.5 | 0.57 | 0.786 | 0.429 | x | x |  |  |  |  |  |
| C14H16O11 | 0.79 | 1.14 | 0.5 | 0.429 |  |  | x |  |  |  |  |
| C14H14O10 | 0.71 | 1 | 0.571 | 0.429 | x | x | x |  |  |  |  |
| C14H12O9 | 0.64 | 0.86 | 0.643 | 0.429 | x | x |  |  |  |  |  |
| C14H10O8 | 0.57 | 0.71 | 0.714 | 0.429 | x | x |  |  |  |  |  |
| C19H20O14 | 0.74 | 1.05 | 0.526 | 0.421 | x |  | x |  |  |  |  |
| C19H18O13 | 0.68 | 0.95 | 0.579 | 0.421 | x | x | x |  |  |  |  |
| C19H16O12 | 0.63 | 0.84 | 0.632 | 0.421 | x | x | x |  |  |  |  |
| C19H14O11 | 0.58 | 0.74 | 0.684 | 0.421 | x | x | x |  |  |  |  |
| C20H22O15 | 0.75 | 1.1 | 0.5 | 0.4 | x | x | x |  |  |  |  |
| C20H20O14 | 0.7 | 1 | 0.55 | 0.4 | x | x | x |  |  |  |  |
| C20H18O13 | 0.65 | 0.9 | 0.6 | 0.4 | x | x | x |  |  |  |  |
| C20H16O12 | 0.6 | 0.8 | 0.65 | 0.4 | x | x | x |  |  |  |  |
| C20H14O11 | 0.55 | 0.7 | 0.7 | 0.4 | x | x | x |  |  |  |  |
| C15H18O12 | 0.8 | 1.2 | 0.467 | 0.4 |  |  | x |  |  |  |  |
| C15H16O11 | 0.73 | 1.07 | 0.533 | 0.4 | x |  | x |  |  |  |  |
| C15H14O10 | 0.67 | 0.93 | 0.6 | 0.4 | x | x | x |  |  |  |  |
| C15H12O9 | 0.6 | 0.8 | 0.667 | 0.4 | x | x |  |  |  |  |  |
| C15H10O8 | 0.53 | 0.67 | 0.733 | 0.4 | x | x |  |  |  |  |  |
| C10H8O6 | 0.6 | 0.8 | 0.7 | 0.4 |  |  |  |  |  |  |  |
| C10H12O8 | 0.8 | 1.2 | 0.5 | 0.4 |  |  |  |  |  |  |  |
| C10H10O7 | 0.7 | 1 | 0.6 | 0.4 |  |  |  |  |  |  |  |
| C21H22O15 | 0.71 | 1.05 | 0.524 | 0.381 | x | x | x |  |  |  |  |
| C21H20O14 | 0.67 | 0.95 | 0.571 | 0.381 | x | x | x |  |  |  |  |
| C21H18O13 | 0.62 | 0.86 | 0.619 | 0.381 | x | x |  |  |  |  |  |
| C21H16O12 | 0.57 | 0.76 | 0.667 | 0.381 | x | x |  |  |  |  |  |
| C16H18O12 | 0.75 | 1.13 | 0.5 | 0.375 |  |  | x |  |  |  |  |
| C16H16O11 | 0.69 | 1 | 0.563 | 0.375 | x | x | x |  |  |  |  |
| C16H14O10 | 0.63 | 0.88 | 0.625 | 0.375 | x | x | x |  |  |  |  |
| C16H12O9 | 0.56 | 0.75 | 0.688 | 0.375 | x | x |  |  |  |  |  |
| C16H10O8 | 0.5 | 0.63 | 0.75 | 0.375 | x | x |  |  |  |  |  |
| C22H22O15 | 0.68 | 1 | 0.545 | 0.364 | x | x | x |  |  |  |  |
| C22H20O14 | 0.64 | 0.91 | 0.591 | 0.364 | x |  | x |  |  |  |  |
| C22H18O13 | 0.59 | 0.82 | 0.636 | 0.364 | x | x | x |  |  |  |  |
| C22H16O12 | 0.55 | 0.73 | 0.682 | 0.364 | x | x |  |  |  |  |  |
| C11H8O6 | 0.55 | 0.73 | 0.727 | 0.364 |  |  |  |  |  |  |  |
| C11H14O9 | 0.82 | 1.27 | 0.455 | 0.364 |  |  |  |  |  |  |  |
| C11H12O8 | 0.73 | 1.09 | 0.545 | 0.364 |  |  |  |  |  |  |  |
| C11H10O7 | 0.64 | 0.91 | 0.636 | 0.364 |  |  |  |  |  |  |  |
| C17H20O13 | 0.76 | 1.18 | 0.471 | 0.353 |  |  | x |  |  |  |  |
| C17H18O12 | 0.71 | 1.06 | 0.529 | 0.353 |  |  | x |  |  |  |  |
| C17H16O11 | 0.65 | 0.94 | 0.588 | 0.353 | x | x |  |  |  |  |  |
| C17H14O10 | 0.59 | 0.82 | 0.647 | 0.353 | x | x |  |  |  |  |  |
| C17H12O9 | 0.53 | 0.71 | 0.706 | 0.353 | x | x |  |  |  |  |  |
| C23H18O13 | 0.57 | 0.78 | 0.652 | 0.348 | x | x |  |  |  |  |  |
| C18H20O13 | 0.72 | 1.11 | 0.5 | 0.333 |  |  | x |  |  |  |  |
| C18H18O12 | 0.67 | 1 | 0.556 | 0.333 | x | x | x |  |  |  |  |
| C18H16O11 | 0.61 | 0.89 | 0.611 | 0.333 | x | x | x |  |  |  |  |
| C18H14O10 | 0.56 | 0.78 | 0.667 | 0.333 | x | x |  |  |  |  |  |
| C18H12O9 | 0.5 | 0.67 | 0.722 | 0.333 | x | x |  |  |  |  |  |
| C12H8O6 | 0.5 | 0.67 | 0.75 | 0.333 |  |  |  |  |  |  |  |
| C12H14O9 | 0.75 | 1.17 | 0.5 | 0.333 |  |  |  |  |  |  |  |
| C12H12O8 | 0.67 | 1 | 0.583 | 0.333 | x |  |  |  |  |  |  |
| C12H10O7 | 0.58 | 0.83 | 0.667 | 0.333 | x |  |  |  |  |  |  |
| C19H22O14 | 0.74 | 1.16 | 0.474 | 0.316 |  |  | x |  |  |  |  |
| C19H20O13 | 0.68 | 1.05 | 0.526 | 0.316 | x |  | x |  |  |  |  |
| C19H18O12 | 0.63 | 0.95 | 0.579 | 0.316 | x | x |  |  |  |  |  |
| C19H16O11 | 0.58 | 0.84 | 0.632 | 0.316 | x | x |  |  |  |  |  |
| C19H14O10 | 0.53 | 0.74 | 0.684 | 0.316 | x | x |  |  |  |  |  |
| C13H8O6 | 0.46 | 0.62 | 0.769 | 0.308 |  | x |  |  |  |  |  |
| C13H16O10 | 0.77 | 1.23 | 0.462 | 0.308 |  |  | x |  |  |  |  |
| C13H14O9 | 0.69 | 1.08 | 0.538 | 0.308 |  |  |  |  |  |  |  |
| C13H12O8 | 0.62 | 0.92 | 0.615 | 0.308 | x | x |  |  |  |  |  |
| C13H10O7 | 0.54 | 0.77 | 0.692 | 0.308 | x | x |  |  |  |  |  |
| C20H22O14 | 0.7 | 1.1 | 0.5 | 0.3 | x |  | x |  |  |  |  |
| C20H20O13 | 0.65 | 1 | 0.55 | 0.3 | x | x | x |  |  |  |  |
| C20H18O12 | 0.6 | 0.9 | 0.6 | 0.3 | x | x | x |  |  |  |  |
| C20H16O11 | 0.55 | 0.8 | 0.65 | 0.3 | x | x |  |  |  |  |  |
| C21H24O15 | 0.71 | 1.14 | 0.476 | 0.286 | x | x | x |  |  |  |  |
| C21H22O14 | 0.67 | 1.05 | 0.524 | 0.286 | x | x | x |  |  |  |  |
| C21H20O13 | 0.62 | 0.95 | 0.571 | 0.286 | x | x | x |  |  |  |  |
| C21H18O12 | 0.57 | 0.86 | 0.619 | 0.286 | x | x | x |  |  |  |  |
| C21H16O11 | 0.52 | 0.76 | 0.667 | 0.286 | x | x |  |  |  |  |  |
| C14H18O11 | 0.79 | 1.29 | 0.429 | 0.286 |  |  |  |  |  |  |  |
| C14H16O10 | 0.71 | 1.14 | 0.5 | 0.286 | x |  | x |  |  |  |  |
| C14H14O9 | 0.64 | 1 | 0.571 | 0.286 | x |  | x |  |  |  |  |
| C14H12O8 | 0.57 | 0.86 | 0.643 | 0.286 | x | x |  |  |  |  |  |
| C14H10O7 | 0.5 | 0.71 | 0.714 | 0.286 | x | x |  |  |  |  |  |
| C22H24O15 | 0.68 | 1.09 | 0.5 | 0.273 | x | x | x |  |  |  |  |
| C22H22O14 | 0.64 | 1 | 0.545 | 0.273 | x | x | x |  |  |  |  |
| C22H20O13 | 0.59 | 0.91 | 0.591 | 0.273 | x | x |  |  |  |  |  |
| C22H18O12 | 0.55 | 0.82 | 0.636 | 0.273 | x | x |  |  |  |  |  |
| C15H18O11 | 0.73 | 1.2 | 0.467 | 0.267 |  |  |  |  |  |  |  |
| C15H16O10 | 0.67 | 1.07 | 0.533 | 0.267 | x |  | x |  |  |  |  |
| C15H14O9 | 0.6 | 0.93 | 0.6 | 0.267 | x | x | x |  |  |  |  |
| C15H12O8 | 0.53 | 0.8 | 0.667 | 0.267 | x | x |  |  |  |  |  |
| C15H10O7 | 0.47 | 0.67 | 0.733 | 0.267 |  | x |  |  |  |  |  |
| C23H22O14 | 0.61 | 0.96 | 0.565 | 0.261 | x | x |  |  |  |  |  |
| C23H20O13 | 0.57 | 0.87 | 0.609 | 0.261 | x | x |  |  |  |  |  |
| C23H18O12 | 0.52 | 0.78 | 0.652 | 0.261 | x | x | x |  |  |  |  |
| C16H20O12 | 0.75 | 1.25 | 0.438 | 0.25 |  |  |  |  |  |  |  |
| C16H18O11 | 0.69 | 1.13 | 0.5 | 0.25 |  |  | x |  |  |  |  |
| C16H16O10 | 0.63 | 1 | 0.563 | 0.25 | x | x | x |  |  |  |  |
| C16H14O9 | 0.56 | 0.88 | 0.625 | 0.25 | x | x |  |  |  |  |  |
| C16H12O8 | 0.5 | 0.75 | 0.688 | 0.25 | x | x |  |  |  |  |  |
| C17H22O13 | 0.76 | 1.29 | 0.412 | 0.235 |  |  | x |  |  |  |  |
| C17H20O12 | 0.71 | 1.18 | 0.471 | 0.235 |  |  | x |  |  |  |  |
| C17H18O11 | 0.65 | 1.06 | 0.529 | 0.235 |  |  | x |  |  |  |  |
| C17H16O10 | 0.59 | 0.94 | 0.588 | 0.235 | x | x |  |  |  |  |  |
| C17H14O9 | 0.53 | 0.82 | 0.647 | 0.235 | x | x |  |  |  |  |  |
| C17H12O8 | 0.47 | 0.71 | 0.706 | 0.235 | x | x |  |  |  |  |  |
| C9H10O6 | 0.67 | 1.11 | 0.556 | 0.222 |  |  |  |  |  |  |  |
| C18H22O13 | 0.72 | 1.22 | 0.444 | 0.222 |  |  | x |  |  |  |  |
| C18H20O12 | 0.67 | 1.11 | 0.5 | 0.222 |  |  |  |  |  |  |  |
| C18H18O11 | 0.61 | 1 | 0.556 | 0.222 | x | x | x |  |  |  |  |
| C18H16O10 | 0.56 | 0.89 | 0.611 | 0.222 | x | x |  |  |  |  |  |
| C18H14O9 | 0.5 | 0.78 | 0.667 | 0.222 | x | x |  |  |  |  |  |
| C19H22O13 | 0.68 | 1.16 | 0.474 | 0.211 |  |  | x |  |  |  |  |
| C19H20O12 | 0.63 | 1.05 | 0.526 | 0.211 |  |  | x |  |  |  |  |
| C19H18O11 | 0.58 | 0.95 | 0.579 | 0.211 | x | x | x |  |  |  |  |
| C19H16O10 | 0.53 | 0.84 | 0.632 | 0.211 | x | x |  |  |  |  |  |
| C19H14O9 | 0.47 | 0.74 | 0.684 | 0.211 | x | x |  |  |  |  |  |
| C20H24O14 | 0.7 | 1.2 | 0.45 | 0.2 |  |  | x |  |  |  |  |
| C20H22O13 | 0.65 | 1.1 | 0.5 | 0.2 |  |  | x |  |  |  |  |
| C20H20O12 | 0.6 | 1 | 0.55 | 0.2 | x | x | x |  |  |  |  |
| C20H18O11 | 0.55 | 0.9 | 0.6 | 0.2 | x | x |  |  |  |  |  |
| C20H16O10 | 0.5 | 0.8 | 0.65 | 0.2 | x | x |  |  |  |  |  |
| C10H14O8 | 0.8 | 1.4 | 0.4 | 0.2 |  |  |  |  |  |  |  |
| C10H12O7 | 0.7 | 1.2 | 0.5 | 0.2 |  |  |  |  |  |  |  |
| C10H10O6 | 0.6 | 1 | 0.6 | 0.2 |  |  |  |  |  |  |  |
| C21H24O14 | 0.67 | 1.14 | 0.476 | 0.19 |  |  | x |  |  |  |  |
| C21H22O13 | 0.62 | 1.05 | 0.524 | 0.19 |  |  | x |  |  |  |  |
| C21H20O12 | 0.57 | 0.95 | 0.571 | 0.19 | x | x |  |  |  |  |  |
| C21H18O11 | 0.52 | 0.86 | 0.619 | 0.19 | x | x |  |  |  |  |  |
| C21H16O10 | 0.48 | 0.76 | 0.667 | 0.19 | x | x |  |  |  |  |  |
| C22H26O15 | 0.68 | 1.18 | 0.455 | 0.182 | x |  |  |  |  |  |  |
| C22H24O14 | 0.64 | 1.09 | 0.5 | 0.182 |  |  | x |  |  |  |  |
| C22H22O13 | 0.59 | 1 | 0.545 | 0.182 | x | x | x |  |  |  |  |
| C22H20O12 | 0.55 | 0.91 | 0.591 | 0.182 | x | x |  |  |  |  |  |
| C22H18O11 | 0.5 | 0.82 | 0.636 | 0.182 | x | x |  |  |  |  |  |
| C11H8O5 | 0.45 | 0.73 | 0.727 | 0.182 |  |  |  |  |  |  |  |
| C11H14O8 | 0.73 | 1.27 | 0.455 | 0.182 |  |  |  |  |  |  |  |
| C11H12O7 | 0.64 | 1.09 | 0.545 | 0.182 |  |  |  |  |  |  |  |
| C11H10O6 | 0.55 | 0.91 | 0.636 | 0.182 |  |  |  |  |  |  |  |
| C23H26O15 | 0.65 | 1.13 | 0.478 | 0.174 | x | x |  |  |  |  |  |
| C23H24O14 | 0.61 | 1.04 | 0.522 | 0.174 | x | x | x |  |  |  |  |
| C23H22O13 | 0.57 | 0.96 | 0.565 | 0.174 | x | x |  |  |  |  |  |
| C23H20O12 | 0.52 | 0.87 | 0.609 | 0.174 | x | x |  |  |  |  |  |
| C24H26O15 | 0.63 | 1.08 | 0.5 | 0.167 | x | x |  |  |  |  |  |
| C24H24O14 | 0.58 | 1 | 0.542 | 0.167 | x | x |  |  |  |  |  |
| C24H22O13 | 0.54 | 0.92 | 0.583 | 0.167 | x | x |  |  |  |  |  |
| C12H14O8 | 0.67 | 1.17 | 0.5 | 0.167 |  |  |  |  |  |  |  |
| C12H12O7 | 0.58 | 1 | 0.583 | 0.167 | x | x |  |  |  |  |  |
| C12H10O6 | 0.5 | 0.83 | 0.667 | 0.167 |  |  |  |  |  |  |  |
| C12H16O9 | 0.75 | 1.33 | 0.417 | 0.167 |  |  |  |  |  |  | x |
| C25H26O15 | 0.6 | 1.04 | 0.52 | 0.16 | x | x |  |  |  |  |  |
| C13H18O10 | 0.77 | 1.38 | 0.385 | 0.154 |  |  |  |  |  |  |  |
| C13H16O9 | 0.69 | 1.23 | 0.462 | 0.154 |  |  |  |  |  |  |  |
| C13H14O8 | 0.62 | 1.08 | 0.538 | 0.154 |  |  |  |  |  |  |  |
| C13H12O7 | 0.54 | 0.92 | 0.615 | 0.154 | x | x |  |  |  |  |  |
| C13H10O6 | 0.46 | 0.77 | 0.692 | 0.154 |  |  |  |  |  |  |  |
| C14H18O10 | 0.71 | 1.29 | 0.429 | 0.143 |  |  | x |  |  |  |  |
| C14H16O9 | 0.64 | 1.14 | 0.5 | 0.143 | x |  | x |  |  |  |  |
| C14H14O8 | 0.57 | 1 | 0.571 | 0.143 | x | x |  |  |  |  |  |
| C14H12O7 | 0.5 | 0.86 | 0.643 | 0.143 |  |  |  |  |  |  |  |
| C14H10O6 | 0.43 | 0.71 | 0.714 | 0.143 |  |  |  |  |  |  |  |
| C15H20O11 | 0.73 | 1.33 | 0.4 | 0.133 |  |  |  |  |  |  |  |
| C15H18O10 | 0.67 | 1.2 | 0.467 | 0.133 |  |  | x |  |  |  |  |
| C15H16O9 | 0.6 | 1.07 | 0.533 | 0.133 | x | x | x |  |  |  |  |
| C15H14O8 | 0.53 | 0.93 | 0.6 | 0.133 | x | x |  |  |  |  |  |
| C15H12O7 | 0.47 | 0.8 | 0.667 | 0.133 |  |  |  |  |  |  |  |
| C16H20O11 | 0.69 | 1.25 | 0.438 | 0.125 |  |  |  |  |  |  |  |
| C16H18O10 | 0.63 | 1.13 | 0.5 | 0.125 |  |  |  |  |  |  |  |
| C16H16O9 | 0.56 | 1 | 0.563 | 0.125 | x | x |  |  |  |  |  |
| C16H14O8 | 0.5 | 0.88 | 0.625 | 0.125 | x | x |  |  |  |  |  |
| C16H12O7 | 0.44 | 0.75 | 0.688 | 0.125 | x | x |  |  |  |  |  |
| C17H22O12 | 0.71 | 1.29 | 0.412 | 0.118 |  |  |  |  |  |  |  |
| C17H20O11 | 0.65 | 1.18 | 0.471 | 0.118 |  |  |  |  |  |  |  |
| C17H18O10 | 0.59 | 1.06 | 0.529 | 0.118 |  |  |  |  |  |  |  |
| C17H16O9 | 0.53 | 0.94 | 0.588 | 0.118 | x | x |  |  |  |  |  |
| C17H14O8 | 0.47 | 0.82 | 0.647 | 0.118 |  | x |  |  |  |  |  |
| C17H12O7 | 0.41 | 0.71 | 0.706 | 0.118 | x | x |  |  |  |  |  |
| C18H22O12 | 0.67 | 1.22 | 0.444 | 0.111 |  |  |  |  |  |  |  |
| C18H20O11 | 0.61 | 1.11 | 0.5 | 0.111 |  |  |  |  |  |  |  |
| C18H18O10 | 0.56 | 1 | 0.556 | 0.111 |  |  |  |  |  |  |  |
| C18H16O9 | 0.5 | 0.89 | 0.611 | 0.111 | x | x |  |  |  |  |  |
| C18H14O8 | 0.44 | 0.78 | 0.667 | 0.111 | x | x |  |  |  |  |  |
| C19H24O13 | 0.68 | 1.26 | 0.421 | 0.105 |  |  |  |  |  |  |  |
| C19H22O12 | 0.63 | 1.16 | 0.474 | 0.105 |  |  |  |  |  |  |  |
| C19H20O11 | 0.58 | 1.05 | 0.526 | 0.105 |  |  |  |  |  |  |  |
| C19H18O10 | 0.53 | 0.95 | 0.579 | 0.105 |  |  |  |  |  |  |  |
| C19H16O9 | 0.47 | 0.84 | 0.632 | 0.105 |  | x |  |  |  |  |  |
| C20H26O14 | 0.7 | 1.3 | 0.4 | 0.1 | x |  | x |  |  |  |  |
| C20H24O13 | 0.65 | 1.2 | 0.45 | 0.1 |  |  |  |  |  |  |  |
| C20H22O12 | 0.6 | 1.1 | 0.5 | 0.1 |  |  |  |  |  |  |  |
| C20H20O11 | 0.55 | 1 | 0.55 | 0.1 |  |  |  |  |  |  |  |
| C20H18O10 | 0.5 | 0.9 | 0.6 | 0.1 |  |  |  |  |  |  |  |
| C20H16O9 | 0.45 | 0.8 | 0.65 | 0.1 | x | x |  |  |  |  |  |
| C21H26O14 | 0.67 | 1.24 | 0.429 | 0.095 |  |  | x |  |  |  |  |
| C21H24O13 | 0.62 | 1.14 | 0.476 | 0.095 |  |  |  |  |  |  |  |
| C21H22O12 | 0.57 | 1.05 | 0.524 | 0.095 |  |  |  |  |  |  |  |
| C21H20O11 | 0.52 | 0.95 | 0.571 | 0.095 |  |  |  |  |  |  |  |
| C21H18O10 | 0.48 | 0.86 | 0.619 | 0.095 | x | x |  |  |  |  |  |
| C22H26O14 | 0.64 | 1.18 | 0.455 | 0.091 |  |  |  |  |  |  |  |
| C22H24O13 | 0.59 | 1.09 | 0.5 | 0.091 |  |  |  |  |  |  |  |
| C22H22O12 | 0.55 | 1 | 0.545 | 0.091 |  |  |  |  |  |  |  |
| C22H20O11 | 0.5 | 0.91 | 0.591 | 0.091 | x | x |  |  |  |  |  |
| C23H26O14 | 0.61 | 1.13 | 0.478 | 0.087 |  |  |  |  |  |  |  |
| C23H24O13 | 0.57 | 1.04 | 0.522 | 0.087 |  |  |  |  |  |  |  |
| C23H22O12 | 0.52 | 0.96 | 0.565 | 0.087 | x | x |  |  |  |  |  |
| C23H20O11 | 0.48 | 0.87 | 0.609 | 0.087 | x | x | x |  |  |  |  |
| C24H28O15 | 0.63 | 1.17 | 0.458 | 0.083 |  |  |  |  |  |  |  |
| C24H26O14 | 0.58 | 1.08 | 0.5 | 0.083 | x | x | x |  |  |  |  |
| C24H24O13 | 0.54 | 1 | 0.542 | 0.083 | x | x |  |  |  |  |  |
| C24H22O12 | 0.5 | 0.92 | 0.583 | 0.083 | x | x |  |  |  |  |  |
| C25H28O15 | 0.6 | 1.12 | 0.48 | 0.08 |  |  |  |  |  |  |  |
| C25H26O14 | 0.56 | 1.04 | 0.52 | 0.08 | x | x |  |  |  |  |  |
| C25H24O13 | 0.52 | 0.96 | 0.56 | 0.08 | x | x |  |  |  |  |  |
| C9H12O6 | 0.67 | 1.33 | 0.444 | 0 |  |  |  |  |  |  |  |
| C26H30O15 | 0.58 | 1.15 | 0.462 | 0 |  |  |  |  |  |  |  |
| C26H28O14 | 0.54 | 1.08 | 0.5 | 0 |  |  |  |  |  |  |  |
| C25H30O15 | 0.6 | 1.2 | 0.44 | 0 |  |  |  |  |  |  |  |
| C25H26O13 | 0.52 | 1.04 | 0.52 | 0 | x | x |  |  |  |  |  |
| C24H28O14 | 0.58 | 1.17 | 0.458 | 0 |  |  |  |  |  |  |  |
| C24H26O13 | 0.54 | 1.08 | 0.5 | 0 |  |  |  |  |  |  |  |
| C24H24O12 | 0.5 | 1 | 0.542 | 0 |  |  | x |  |  |  |  |
| C23H28O14 | 0.61 | 1.22 | 0.435 | 0 |  |  |  |  |  |  |  |
| C23H26O13 | 0.57 | 1.13 | 0.478 | 0 |  |  |  |  |  |  |  |
| C23H24O12 | 0.52 | 1.04 | 0.522 | 0 |  |  |  |  |  |  |  |
| C23H22O11 | 0.48 | 0.96 | 0.565 | 0 |  |  |  |  |  |  |  |
| C22H28O14 | 0.64 | 1.27 | 0.409 | 0 |  |  |  |  |  |  |  |
| C22H22O11 | 0.5 | 1 | 0.545 | 0 |  |  |  |  |  |  |  |
| C22H20O10 | 0.45 | 0.91 | 0.591 | 0 |  |  |  |  |  |  |  |
| C21H22O11 | 0.52 | 1.05 | 0.524 | 0 |  |  |  |  |  |  |  |
| C21H20O10 | 0.48 | 0.95 | 0.571 | 0 |  |  |  |  |  |  |  |
| C21H18O9 | 0.43 | 0.86 | 0.619 | 0 |  | x |  |  |  |  |  |
| C20H26O13 | 0.65 | 1.3 | 0.4 | 0 |  |  |  |  |  |  |  |
| C20H22O11 | 0.55 | 1.1 | 0.5 | 0 |  |  |  |  |  |  |  |
| C20H20O10 | 0.5 | 1 | 0.55 | 0 |  |  |  |  |  |  |  |
| C20H18O9 | 0.45 | 0.9 | 0.6 | 0 |  |  |  |  |  |  |  |
| C19H26O13 | 0.68 | 1.37 | 0.368 | 0 |  |  |  |  |  |  |  |
| C19H20O10 | 0.53 | 1.05 | 0.526 | 0 |  |  |  |  |  |  |  |
| C19H18O9 | 0.47 | 0.95 | 0.579 | 0 |  |  |  |  |  |  |  |
| C19H16O8 | 0.42 | 0.84 | 0.632 | 0 |  |  |  |  |  |  |  |
| C18H20O10 | 0.56 | 1.11 | 0.5 | 0 |  |  |  |  |  |  |  |
| C18H18O9 | 0.5 | 1 | 0.556 | 0 |  |  |  |  |  |  |  |
| C18H16O8 | 0.44 | 0.89 | 0.611 | 0 |  |  |  |  |  |  |  |
| C17H20O10 | 0.59 | 1.18 | 0.471 | 0 |  |  |  |  |  |  |  |
| C17H18O9 | 0.53 | 1.06 | 0.529 | 0 |  |  |  |  |  |  |  |
| C17H16O8 | 0.47 | 0.94 | 0.588 | 0 |  |  |  |  |  |  |  |
| C17H14O7 | 0.41 | 0.82 | 0.647 | 0 |  |  |  |  |  |  |  |
| C16H20O10 | 0.63 | 1.25 | 0.438 | 0 |  |  |  |  |  |  |  |
| C16H18O9 | 0.56 | 1.13 | 0.5 | 0 |  |  |  |  |  |  |  |
| C16H16O8 | 0.5 | 1 | 0.563 | 0 |  |  |  |  |  |  |  |
| C16H14O7 | 0.44 | 0.88 | 0.625 | 0 |  |  |  |  |  |  |  |
| C16H12O6 | 0.38 | 0.75 | 0.688 | 0 |  |  |  |  |  |  |  |
| C15H20O10 | 0.67 | 1.33 | 0.4 | 0 |  |  |  |  |  |  |  |
| C15H18O9 | 0.6 | 1.2 | 0.467 | 0 |  |  |  |  |  |  |  |
| C15H16O8 | 0.53 | 1.07 | 0.533 | 0 | x | x |  |  |  |  |  |
| C15H14O7 | 0.47 | 0.93 | 0.6 | 0 |  |  |  |  |  |  |  |
| C15H12O6 | 0.4 | 0.8 | 0.667 | 0 |  |  |  |  |  |  |  |
| C14H20O10 | 0.71 | 1.43 | 0.357 | 0 |  |  |  |  |  |  |  |
| C14H18O9 | 0.64 | 1.29 | 0.429 | 0 |  |  | x |  |  |  |  |
| C14H16O8 | 0.57 | 1.14 | 0.5 | 0 | x |  |  |  |  |  |  |
| C14H14O7 | 0.5 | 1 | 0.571 | 0 |  |  |  |  |  |  |  |
| C14H12O6 | 0.43 | 0.86 | 0.643 | 0 |  |  |  |  |  |  |  |
| C13H16O8 | 0.62 | 1.23 | 0.462 | 0 |  |  |  |  |  |  |  |
| C13H14O7 | 0.54 | 1.08 | 0.538 | 0 |  |  |  |  |  |  |  |
| C13H12O6 | 0.46 | 0.92 | 0.615 | 0 |  |  |  |  |  |  |  |
| C12H16O8 | 0.67 | 1.33 | 0.417 | 0 |  |  |  |  |  |  |  |
| C12H14O7 | 0.58 | 1.17 | 0.5 | 0 |  |  |  |  |  |  |  |
| C12H12O6 | 0.5 | 1 | 0.583 | 0 |  |  |  |  |  |  |  |
| C12H10O5 | 0.42 | 0.83 | 0.667 | 0 |  |  |  |  |  |  |  |
| C11H16O8 | 0.73 | 1.45 | 0.364 | 0 |  |  |  |  |  |  |  |
| C11H14O7 | 0.64 | 1.27 | 0.455 | 0 |  |  |  |  |  |  |  |
| C11H12O6 | 0.55 | 1.09 | 0.545 | 0 |  |  |  |  |  |  |  |
| C11H10O5 | 0.45 | 0.91 | 0.636 | 0 |  |  |  |  |  |  |  |
| C10H12O6 | 0.6 | 1.2 | 0.5 | 0 |  |  |  |  |  |  |  |
| C10H10O5 | 0.5 | 1 | 0.6 | 0 |  |  | x |  |  |  |  |
| C22H24O12 | 0.55 | 1.09 | 0.5 | 0 |  |  |  |  | x | x |  |
| C19H22O11 | 0.58 | 1.16 | 0.474 | 0 |  |  |  |  | x | x |  |
| C25H32O9 | 0.36 | 1.28 | 0.4 | 0 |  |  |  | x | x | x | x |
| C22H26O13 | 0.59 | 1.18 | 0.455 | 0 |  |  |  | x | x | x | x |
| C21H26O13 | 0.62 | 1.24 | 0.429 | 0 |  |  |  | x | x | x | x |
| C21H24O12 | 0.57 | 1.14 | 0.476 | 0 |  |  |  |  | x | x | x |
| C20H24O12 | 0.6 | 1.2 | 0.45 | 0 |  |  |  |  | x | x | x |
| C19H24O12 | 0.63 | 1.26 | 0.421 | 0 |  |  |  | x | x | x | x |
| C18H24O12 | 0.67 | 1.33 | 0.389 | 0 |  |  |  | x | x | x | x |
| C18H22O11 | 0.61 | 1.22 | 0.444 | 0 |  |  |  |  | x | x | x |
| C17H22O11 | 0.65 | 1.29 | 0.412 | 0 |  |  |  | x | x | x | x |
| C16H22O11 | 0.69 | 1.38 | 0.375 | 0 |  |  |  | x | x | x | x |
| C13H18O9 | 0.69 | 1.38 | 0.385 | 0 |  |  |  |  |  |  | x |
| C10H14O7 | 0.7 | 1.4 | 0.4 | 0 |  |  |  |  |  |  | x |
| C27H30O14 | 0.52 | 1.11 | 0.481 | -0.07 |  |  |  |  |  |  |  |
| C26H30O14 | 0.54 | 1.15 | 0.462 | -0.08 |  |  |  |  |  |  |  |
| C25H30O14 | 0.56 | 1.2 | 0.44 | -0.08 |  |  |  |  |  |  |  |
| C25H28O13 | 0.52 | 1.12 | 0.48 | -0.08 |  |  |  |  |  |  |  |
| C25H26O12 | 0.48 | 1.04 | 0.52 | -0.08 | x | x |  |  |  |  |  |
| C25H24O11 | 0.44 | 0.96 | 0.56 | -0.08 |  |  |  |  |  |  |  |
| C24H30O14 | 0.58 | 1.25 | 0.417 | -0.08 |  |  |  |  |  |  |  |
| C24H28O13 | 0.54 | 1.17 | 0.458 | -0.08 |  |  |  |  |  |  |  |
| C24H24O11 | 0.46 | 1 | 0.542 | -0.08 |  |  |  |  |  |  |  |
| C24H26O12 | 0.5 | 1.08 | 0.5 | -0.08 |  |  |  |  | x |  |  |
| C23H22O10 | 0.43 | 0.96 | 0.565 | -0.09 |  |  |  |  |  |  |  |
| C23H24O11 | 0.48 | 1.04 | 0.522 | -0.09 |  |  |  |  | x |  |  |
| C23H28O13 | 0.57 | 1.22 | 0.435 | -0.09 |  |  |  |  | x | x | x |
| C23H26O12 | 0.52 | 1.13 | 0.478 | -0.09 |  |  |  |  | x | x | x |
| C22H22O10 | 0.45 | 1 | 0.545 | -0.09 |  |  |  |  |  |  |  |
| C22H20O9 | 0.41 | 0.91 | 0.591 | -0.09 |  |  |  |  |  |  |  |
| C22H28O13 | 0.59 | 1.27 | 0.409 | -0.09 |  |  |  | x | x | x | x |
| C22H26O12 | 0.55 | 1.18 | 0.455 | -0.09 |  |  |  | x | x | x | x |
| C22H24O11 | 0.5 | 1.09 | 0.5 | -0.09 |  |  |  |  | x | x | x |
| C21H28O13 | 0.62 | 1.33 | 0.381 | -0.1 |  |  |  |  |  |  |  |
| C21H20O9 | 0.43 | 0.95 | 0.571 | -0.1 |  |  |  |  |  |  |  |
| C21H24O11 | 0.52 | 1.14 | 0.476 | -0.1 |  |  |  |  | x | x |  |
| C21H22O10 | 0.48 | 1.05 | 0.524 | -0.1 |  |  |  |  | x | x |  |
| C21H26O12 | 0.57 | 1.24 | 0.429 | -0.1 |  |  |  | x | x | x | x |
| C20H18O8 | 0.4 | 0.9 | 0.6 | -0.1 |  |  |  |  |  |  |  |
| C20H22O10 | 0.5 | 1.1 | 0.5 | -0.1 |  |  |  |  | x | x |  |
| C20H20O9 | 0.45 | 1 | 0.55 | -0.1 |  |  |  |  | x | x |  |
| C20H26O12 | 0.6 | 1.3 | 0.4 | -0.1 |  |  |  | x | x | x | x |
| C20H24O11 | 0.55 | 1.2 | 0.45 | -0.1 |  |  |  | x | x | x | x |
| C19H20O9 | 0.47 | 1.05 | 0.526 | -0.11 |  |  |  |  |  |  |  |
| C19H22O10 | 0.53 | 1.16 | 0.474 | -0.11 |  |  |  |  | x | x |  |
| C19H18O8 | 0.42 | 0.95 | 0.579 | -0.11 |  |  |  |  |  | x |  |
| C19H26O12 | 0.63 | 1.37 | 0.368 | -0.11 |  |  |  | x | x | x | x |
| C19H24O11 | 0.58 | 1.26 | 0.421 | -0.11 |  |  |  | x | x | x | x |
| C18H22O10 | 0.56 | 1.22 | 0.444 | -0.11 |  |  |  |  |  |  |  |
| C18H20O9 | 0.5 | 1.11 | 0.5 | -0.11 |  |  |  |  |  |  |  |
| C18H16O7 | 0.39 | 0.89 | 0.611 | -0.11 |  |  |  |  |  |  |  |
| C18H18O8 | 0.44 | 1 | 0.556 | -0.11 |  |  |  |  |  | x |  |
| C18H24O11 | 0.61 | 1.33 | 0.389 | -0.11 |  |  |  | x | x | x | x |
| C17H22O10 | 0.59 | 1.29 | 0.412 | -0.12 |  |  |  |  |  |  |  |
| C17H20O9 | 0.53 | 1.18 | 0.471 | -0.12 |  |  |  |  |  |  |  |
| C17H18O8 | 0.47 | 1.06 | 0.529 | -0.12 |  |  |  |  |  |  |  |
| C17H16O7 | 0.41 | 0.94 | 0.588 | -0.12 |  |  |  |  |  |  |  |
| C17H14O6 | 0.35 | 0.82 | 0.647 | -0.12 |  |  |  |  |  |  |  |
| C17H24O11 | 0.65 | 1.41 | 0.353 | -0.12 |  |  |  | x | x | x | x |
| C16H20O9 | 0.56 | 1.25 | 0.438 | -0.13 |  |  |  |  |  |  |  |
| C16H18O8 | 0.5 | 1.13 | 0.5 | -0.13 |  |  |  |  |  |  |  |
| C16H16O7 | 0.44 | 1 | 0.563 | -0.13 |  |  |  |  |  |  |  |
| C16H22O10 | 0.63 | 1.38 | 0.375 | -0.13 |  |  |  | x | x | x | x |
| C16H14O6 | 0.38 | 0.88 | 0.625 | -0.13 |  |  |  | x | x | x | x |
| C15H20O9 | 0.6 | 1.33 | 0.4 | -0.13 |  |  |  |  |  |  |  |
| C15H18O8 | 0.53 | 1.2 | 0.467 | -0.13 |  |  |  |  |  |  |  |
| C15H16O7 | 0.47 | 1.07 | 0.533 | -0.13 |  |  |  |  |  |  |  |
| C15H14O6 | 0.4 | 0.93 | 0.6 | -0.13 |  |  |  |  |  |  |  |
| C15H12O5 | 0.33 | 0.8 | 0.667 | -0.13 |  |  |  |  |  |  |  |
| C15H22O10 | 0.67 | 1.47 | 0.333 | -0.13 |  |  |  | x | x | x | x |
| C28H34O15 | 0.54 | 1.21 | 0.429 | -0.14 |  |  |  |  |  |  |  |
| C28H32O14 | 0.5 | 1.14 | 0.464 | -0.14 |  |  |  |  |  |  |  |
| C14H18O8 | 0.57 | 1.29 | 0.429 | -0.14 |  |  |  |  |  |  |  |
| C14H14O6 | 0.43 | 1 | 0.571 | -0.14 |  |  |  |  |  |  |  |
| C14H12O5 | 0.36 | 0.86 | 0.643 | -0.14 |  |  |  |  |  |  |  |
| C14H20O9 | 0.64 | 1.43 | 0.357 | -0.14 |  |  |  | x | x | x | x |
| C14H16O7 | 0.5 | 1.14 | 0.5 | -0.14 |  |  |  | x | x | x | x |
| C27H34O15 | 0.56 | 1.26 | 0.407 | -0.15 |  |  |  |  |  |  |  |
| C27H32O14 | 0.52 | 1.19 | 0.444 | -0.15 |  |  |  |  |  |  |  |
| C27H30O13 | 0.48 | 1.11 | 0.481 | -0.15 |  |  |  |  |  |  |  |
| C26H32O14 | 0.54 | 1.23 | 0.423 | -0.15 |  |  |  |  |  |  |  |
| C26H30O13 | 0.5 | 1.15 | 0.462 | -0.15 |  |  |  |  |  |  |  |
| C26H28O12 | 0.46 | 1.08 | 0.5 | -0.15 |  |  |  |  |  |  |  |
| C13H16O7 | 0.54 | 1.23 | 0.462 | -0.15 |  |  |  |  |  |  |  |
| C13H14O6 | 0.46 | 1.08 | 0.538 | -0.15 |  |  |  |  |  |  |  |
| C13H12O5 | 0.38 | 0.92 | 0.615 | -0.15 |  |  |  |  |  |  |  |
| C13H20O9 | 0.69 | 1.54 | 0.308 | -0.15 |  |  |  | x | x |  | x |
| C13H18O8 | 0.62 | 1.38 | 0.385 | -0.15 |  |  |  |  |  |  | x |
| C25H32O14 | 0.56 | 1.28 | 0.4 | -0.16 |  |  |  |  |  |  |  |
| C25H30O13 | 0.52 | 1.2 | 0.44 | -0.16 |  |  |  |  |  |  |  |
| C25H28O12 | 0.48 | 1.12 | 0.48 | -0.16 |  |  |  |  |  |  |  |
| C25H26O11 | 0.44 | 1.04 | 0.52 | -0.16 |  |  |  |  |  |  |  |
| C24H30O13 | 0.54 | 1.25 | 0.417 | -0.17 |  |  |  |  |  |  |  |
| C24H26O11 | 0.46 | 1.08 | 0.5 | -0.17 |  |  |  |  |  |  |  |
| C24H24O10 | 0.42 | 1 | 0.542 | -0.17 |  |  |  |  |  |  |  |
| C12H14O6 | 0.5 | 1.17 | 0.5 | -0.17 |  |  |  |  | x | x |  |
| C24H28O12 | 0.5 | 1.17 | 0.458 | -0.17 |  |  |  | x | x | x | x |
| C12H18O8 | 0.67 | 1.5 | 0.333 | -0.17 |  |  |  | x | x | x | x |
| C12H16O7 | 0.58 | 1.33 | 0.417 | -0.17 |  |  |  | x | x |  | x |
| C12H12O5 | 0.42 | 1 | 0.583 | -0.17 |  |  |  | x | x | x | x |
| C23H30O13 | 0.57 | 1.3 | 0.391 | -0.17 |  |  |  |  |  |  |  |
| C23H24O10 | 0.43 | 1.04 | 0.522 | -0.17 |  |  |  |  |  |  |  |
| C23H28O12 | 0.52 | 1.22 | 0.435 | -0.17 |  |  |  | x | x | x | x |
| C23H26O11 | 0.48 | 1.13 | 0.478 | -0.17 |  |  |  | x | x | x | x |
| C22H22O9 | 0.41 | 1 | 0.545 | -0.18 |  |  |  |  |  |  |  |
| C22H30O13 | 0.59 | 1.36 | 0.364 | -0.18 |  |  |  |  | x |  |  |
| C11H14O6 | 0.55 | 1.27 | 0.455 | -0.18 |  |  |  |  | x |  |  |
| C22H28O12 | 0.55 | 1.27 | 0.409 | -0.18 |  |  |  | x | x | x | x |
| C22H26O11 | 0.5 | 1.18 | 0.455 | -0.18 |  |  |  | x | x | x | x |
| C22H24O10 | 0.45 | 1.09 | 0.5 | -0.18 |  |  |  | x | x | x | x |
| C11H16O7 | 0.64 | 1.45 | 0.364 | -0.18 |  |  |  | x |  |  | x |
| C11H12O5 | 0.45 | 1.09 | 0.545 | -0.18 |  |  |  | x | x | x | x |
| C21H20O8 | 0.38 | 0.95 | 0.571 | -0.19 |  |  |  |  |  |  |  |
| C21H28O12 | 0.57 | 1.33 | 0.381 | -0.19 |  |  |  | x | x | x | x |
| C21H26O11 | 0.52 | 1.24 | 0.429 | -0.19 |  |  |  |  | x | x | x |
| C21H24O10 | 0.48 | 1.14 | 0.476 | -0.19 |  |  |  |  | x | x | x |
| C21H22O9 | 0.43 | 1.05 | 0.524 | -0.19 |  |  |  | x | x | x | x |
| C20H20O8 | 0.4 | 1 | 0.55 | -0.2 |  |  |  |  |  |  |  |
| C10H12O5 | 0.5 | 1.2 | 0.5 | -0.2 |  |  |  |  |  |  |  |
| C20H28O12 | 0.6 | 1.4 | 0.35 | -0.2 |  |  |  | x | x | x | x |
| C20H26O11 | 0.55 | 1.3 | 0.4 | -0.2 |  |  |  | x | x | x | x |
| C20H24O10 | 0.5 | 1.2 | 0.45 | -0.2 |  |  |  | x | x | x | x |
| C20H22O9 | 0.45 | 1.1 | 0.5 | -0.2 |  |  |  |  | x | x | x |
| C10H14O6 | 0.6 | 1.4 | 0.4 | -0.2 |  |  |  | x | x |  | x |
| C19H24O10 | 0.53 | 1.26 | 0.421 | -0.21 |  |  |  |  | x | x |  |
| C19H20O8 | 0.42 | 1.05 | 0.526 | -0.21 |  |  |  |  | x | x |  |
| C19H18O7 | 0.37 | 0.95 | 0.579 | -0.21 |  |  |  |  | x | x |  |
| C19H26O11 | 0.58 | 1.37 | 0.368 | -0.21 |  |  |  | x | x | x | x |
| C19H22O9 | 0.47 | 1.16 | 0.474 | -0.21 |  |  |  | x | x | x | x |
| C28H32O13 | 0.46 | 1.14 | 0.464 | -0.21 |  |  |  |  |  |  |  |
| C27H32O13 | 0.48 | 1.19 | 0.444 | -0.22 |  |  |  |  |  |  |  |
| C18H22O9 | 0.5 | 1.22 | 0.444 | -0.22 |  |  |  |  |  |  |  |
| C18H20O8 | 0.44 | 1.11 | 0.5 | -0.22 |  |  |  |  |  |  |  |
| C27H34O14 | 0.52 | 1.26 | 0.407 | -0.22 |  |  |  |  |  | x |  |
| C18H18O7 | 0.39 | 1 | 0.556 | -0.22 |  |  |  |  | x | x |  |
| C18H26O11 | 0.61 | 1.44 | 0.333 | -0.22 |  |  |  | x | x | x | x |
| C18H24O10 | 0.56 | 1.33 | 0.389 | -0.22 |  |  |  | x | x | x | x |
| C26H34O14 | 0.54 | 1.31 | 0.385 | -0.23 |  |  |  |  |  |  |  |
| C26H30O12 | 0.46 | 1.15 | 0.462 | -0.23 |  |  |  |  |  |  |  |
| C26H32O13 | 0.5 | 1.23 | 0.423 | -0.23 |  |  |  |  |  | x |  |
| C17H20O8 | 0.47 | 1.18 | 0.471 | -0.24 |  |  |  |  |  |  |  |
| C17H22O9 | 0.53 | 1.29 | 0.412 | -0.24 |  |  |  |  | x |  |  |
| C17H18O7 | 0.41 | 1.06 | 0.529 | -0.24 |  |  |  |  | x | x |  |
| C17H24O10 | 0.59 | 1.41 | 0.353 | -0.24 |  |  |  | x | x | x | x |
| C17H16O6 | 0.35 | 0.94 | 0.588 | -0.24 |  |  |  |  | x | x | x |
| C25H32O13 | 0.52 | 1.28 | 0.4 | -0.24 |  |  |  |  |  | x |  |
| C25H30O12 | 0.48 | 1.2 | 0.44 | -0.24 |  |  |  |  |  | x |  |
| C25H28O11 | 0.44 | 1.12 | 0.48 | -0.24 |  |  |  | x | x | x | x |
| C24H32O13 | 0.54 | 1.33 | 0.375 | -0.25 |  |  |  |  |  |  |  |
| C16H20O8 | 0.5 | 1.25 | 0.438 | -0.25 |  |  |  |  |  |  |  |
| C16H18O7 | 0.44 | 1.13 | 0.5 | -0.25 |  |  |  |  |  |  |  |
| C24H30O12 | 0.5 | 1.25 | 0.417 | -0.25 |  |  |  | x | x | x | x |
| C24H28O11 | 0.46 | 1.17 | 0.458 | -0.25 |  |  |  | x | x | x | x |
| C24H26O10 | 0.42 | 1.08 | 0.5 | -0.25 |  |  |  | x | x | x | x |
| C16H24O10 | 0.63 | 1.5 | 0.313 | -0.25 |  |  |  | x | x | x | x |
| C16H22O9 | 0.56 | 1.38 | 0.375 | -0.25 |  |  |  | x | x | x | x |
| C16H16O6 | 0.38 | 1 | 0.563 | -0.25 |  |  |  | x | x | x | x |
| C23H30O12 | 0.52 | 1.3 | 0.391 | -0.26 |  |  |  | x | x | x | x |
| C23H28O11 | 0.48 | 1.22 | 0.435 | -0.26 |  |  |  | x | x | x | x |
| C23H26O10 | 0.43 | 1.13 | 0.478 | -0.26 |  |  |  | x | x | x | x |
| C23H24O9 | 0.39 | 1.04 | 0.522 | -0.26 |  |  |  | x | x | x | x |
| C15H18O7 | 0.47 | 1.2 | 0.467 | -0.27 |  |  |  |  |  |  |  |
| C15H16O6 | 0.4 | 1.07 | 0.533 | -0.27 |  |  |  |  |  |  |  |
| C15H14O5 | 0.33 | 0.93 | 0.6 | -0.27 |  |  |  |  |  |  |  |
| C15H22O9 | 0.6 | 1.47 | 0.333 | -0.27 |  |  |  | x | x | x | x |
| C15H20O8 | 0.53 | 1.33 | 0.4 | -0.27 |  |  |  |  | x | x | x |
| C22H24O9 | 0.41 | 1.09 | 0.5 | -0.27 |  |  |  |  | x | x |  |
| C22H30O12 | 0.55 | 1.36 | 0.364 | -0.27 |  |  |  | x | x | x | x |
| C22H28O11 | 0.5 | 1.27 | 0.409 | -0.27 |  |  |  | x | x | x | x |
| C22H26O10 | 0.45 | 1.18 | 0.455 | -0.27 |  |  |  | x | x | x | x |
| C14H16O6 | 0.43 | 1.14 | 0.5 | -0.29 |  |  |  |  |  |  |  |
| C28H36O14 | 0.5 | 1.29 | 0.393 | -0.29 |  |  |  |  |  | x |  |
| C28H34O13 | 0.46 | 1.21 | 0.429 | -0.29 |  |  |  |  |  | x |  |
| C21H22O8 | 0.38 | 1.05 | 0.524 | -0.29 |  |  |  |  | x | x |  |
| C21H30O12 | 0.57 | 1.43 | 0.333 | -0.29 |  |  |  | x | x | x | x |
| C21H28O11 | 0.52 | 1.33 | 0.381 | -0.29 |  |  |  | x | x | x | x |
| C21H26O10 | 0.48 | 1.24 | 0.429 | -0.29 |  |  |  | x | x | x | x |
| C21H24O9 | 0.43 | 1.14 | 0.476 | -0.29 |  |  |  | x | x | x | x |
| C14H22O9 | 0.64 | 1.57 | 0.286 | -0.29 |  |  |  | x | x | x | x |
| C14H20O8 | 0.57 | 1.43 | 0.357 | -0.29 |  |  |  | x | x | x | x |
| C14H18O7 | 0.5 | 1.29 | 0.429 | -0.29 |  |  |  | x | x | x | x |
| C14H14O5 | 0.36 | 1 | 0.571 | -0.29 |  |  |  | x | x | x | x |
| C27H32O12 | 0.44 | 1.19 | 0.444 | -0.3 |  |  |  |  |  |  |  |
| C27H34O13 | 0.48 | 1.26 | 0.407 | -0.3 |  |  |  |  |  | x |  |
| C20H20O7 | 0.35 | 1 | 0.55 | -0.3 |  |  |  |  |  |  |  |
| C20H28O11 | 0.55 | 1.4 | 0.35 | -0.3 |  |  |  | x | x | x | x |
| C20H26O10 | 0.5 | 1.3 | 0.4 | -0.3 |  |  |  | x | x | x | x |
| C20H24O9 | 0.45 | 1.2 | 0.45 | -0.3 |  |  |  | x | x | x | x |
| C20H22O8 | 0.4 | 1.1 | 0.5 | -0.3 |  |  |  | x | x | x | x |
| C13H16O6 | 0.46 | 1.23 | 0.462 | -0.31 |  |  |  |  |  |  |  |
| C13H14O5 | 0.38 | 1.08 | 0.538 | -0.31 |  |  |  |  |  |  |  |
| C26H34O13 | 0.5 | 1.31 | 0.385 | -0.31 |  |  |  |  |  | x |  |
| C26H32O12 | 0.46 | 1.23 | 0.423 | -0.31 |  |  |  |  |  | x |  |
| C26H30O11 | 0.42 | 1.15 | 0.462 | -0.31 |  |  |  |  |  | x |  |
| C13H20O8 | 0.62 | 1.54 | 0.308 | -0.31 |  |  |  | x | x | x | x |
| C13H18O7 | 0.54 | 1.38 | 0.385 | -0.31 |  |  |  | x | x | x | x |
| C19H20O7 | 0.37 | 1.05 | 0.526 | -0.32 |  |  |  |  | x | x |  |
| C19H28O11 | 0.58 | 1.47 | 0.316 | -0.32 |  |  |  | x | x | x | x |
| C19H26O10 | 0.53 | 1.37 | 0.368 | -0.32 |  |  |  | x | x | x | x |
| C19H24O9 | 0.47 | 1.26 | 0.421 | -0.32 |  |  |  | x | x | x | x |
| C19H22O8 | 0.42 | 1.16 | 0.474 | -0.32 |  |  |  | x | x | x | x |
| C25H34O13 | 0.52 | 1.36 | 0.36 | -0.32 |  |  |  |  |  | x |  |
| C25H32O12 | 0.48 | 1.28 | 0.4 | -0.32 |  |  |  |  | x | x |  |
| C25H28O10 | 0.4 | 1.12 | 0.48 | -0.32 |  |  |  |  | x | x |  |
| C25H30O11 | 0.44 | 1.2 | 0.44 | -0.32 |  |  |  | x | x | x | x |
| C12H16O6 | 0.5 | 1.33 | 0.417 | -0.33 |  |  |  |  |  |  |  |
| C12H12O4 | 0.33 | 1 | 0.583 | -0.33 |  |  |  |  |  |  |  |
| C18H24O9 | 0.5 | 1.33 | 0.389 | -0.33 |  |  |  |  | x | x |  |
| C18H22O8 | 0.44 | 1.22 | 0.444 | -0.33 |  |  |  |  | x | x |  |
| C24H32O12 | 0.5 | 1.33 | 0.375 | -0.33 |  |  |  | x | x | x | x |
| C24H30O11 | 0.46 | 1.25 | 0.417 | -0.33 |  |  |  | x | x | x | x |
| C24H28O10 | 0.42 | 1.17 | 0.458 | -0.33 |  |  |  | x | x | x | x |
| C18H26O10 | 0.56 | 1.44 | 0.333 | -0.33 |  |  |  | x | x | x | x |
| C18H20O7 | 0.39 | 1.11 | 0.5 | -0.33 |  |  |  | x | x | x | x |
| C18H18O6 | 0.33 | 1 | 0.556 | -0.33 |  |  |  |  | x | x | x |
| C12H18O7 | 0.58 | 1.5 | 0.333 | -0.33 |  |  |  | x | x |  | x |
| C12H14O5 | 0.42 | 1.17 | 0.5 | -0.33 |  |  |  | x | x | x | x |
| C23H32O12 | 0.52 | 1.39 | 0.348 | -0.35 |  |  |  | x | x | x | x |
| C23H30O11 | 0.48 | 1.3 | 0.391 | -0.35 |  |  |  | x | x | x | x |
| C23H28O10 | 0.43 | 1.22 | 0.435 | -0.35 |  |  |  | x | x | x | x |
| C23H26O9 | 0.39 | 1.13 | 0.478 | -0.35 |  |  |  | x | x | x | x |
| C17H22O8 | 0.47 | 1.29 | 0.412 | -0.35 |  |  |  |  |  |  |  |
| C17H20O7 | 0.41 | 1.18 | 0.471 | -0.35 |  |  |  | x | x | x |  |
| C17H26O10 | 0.59 | 1.53 | 0.294 | -0.35 |  |  |  | x | x | x | x |
| C17H24O9 | 0.53 | 1.41 | 0.353 | -0.35 |  |  |  | x | x | x | x |
| C17H18O6 | 0.35 | 1.06 | 0.529 | -0.35 |  |  |  | x | x | x | x |
| C28H34O12 | 0.43 | 1.21 | 0.429 | -0.36 |  |  |  |  |  |  |  |
| C11H16O6 | 0.55 | 1.45 | 0.364 | -0.36 |  |  |  |  |  |  |  |
| C11H14O5 | 0.45 | 1.27 | 0.455 | -0.36 |  |  |  |  |  |  |  |
| C22H32O12 | 0.55 | 1.45 | 0.318 | -0.36 |  |  |  | x | x | x | x |
| C22H30O11 | 0.5 | 1.36 | 0.364 | -0.36 |  |  |  | x | x | x | x |
| C22H28O10 | 0.45 | 1.27 | 0.409 | -0.36 |  |  |  | x | x | x | x |
| C22H26O9 | 0.41 | 1.18 | 0.455 | -0.36 |  |  |  | x | x | x | x |
| C22H24O8 | 0.36 | 1.09 | 0.5 | -0.36 |  |  |  | x | x | x | x |
| C27H34O12 | 0.44 | 1.26 | 0.407 | -0.37 |  |  |  |  |  |  |  |
| C27H36O13 | 0.48 | 1.33 | 0.37 | -0.37 |  |  |  |  |  | x |  |
| C16H22O8 | 0.5 | 1.38 | 0.375 | -0.38 |  |  |  |  |  |  |  |
| C16H20O7 | 0.44 | 1.25 | 0.438 | -0.38 |  |  |  |  |  |  |  |
| C16H18O6 | 0.38 | 1.13 | 0.5 | -0.38 |  |  |  | x | x | x |  |
| C16H24O9 | 0.56 | 1.5 | 0.313 | -0.38 |  |  |  | x | x | x | x |
| C16H16O5 | 0.31 | 1 | 0.563 | -0.38 |  |  |  | x | x | x | x |
| C21H30O11 | 0.52 | 1.43 | 0.333 | -0.38 |  |  |  | x | x | x | x |
| C21H28O10 | 0.48 | 1.33 | 0.381 | -0.38 |  |  |  |  | x | x | x |
| C21H26O9 | 0.43 | 1.24 | 0.429 | -0.38 |  |  |  | x | x | x | x |
| C21H24O8 | 0.38 | 1.14 | 0.476 | -0.38 |  |  |  | x | x | x | x |
| C26H34O12 | 0.46 | 1.31 | 0.385 | -0.38 |  |  |  |  |  | x |  |
| C26H32O11 | 0.42 | 1.23 | 0.423 | -0.38 |  |  |  |  |  | x |  |
| C15H20O7 | 0.47 | 1.33 | 0.4 | -0.4 |  |  |  |  |  |  |  |
| C10H16O6 | 0.6 | 1.6 | 0.3 | -0.4 |  |  |  |  |  |  |  |
| C10H14O5 | 0.5 | 1.4 | 0.4 | -0.4 |  |  |  |  |  |  |  |
| C25H34O12 | 0.48 | 1.36 | 0.36 | -0.4 |  |  |  |  |  | x |  |
| C25H32O11 | 0.44 | 1.28 | 0.4 | -0.4 |  |  |  | x | x | x | x |
| C25H30O10 | 0.4 | 1.2 | 0.44 | -0.4 |  |  |  | x | x | x | x |
| C20H30O11 | 0.55 | 1.5 | 0.3 | -0.4 |  |  |  | x | x | x | x |
| C20H28O10 | 0.5 | 1.4 | 0.35 | -0.4 |  |  |  | x | x | x | x |
| C20H26O9 | 0.45 | 1.3 | 0.4 | -0.4 |  |  |  | x | x | x | x |
| C20H24O8 | 0.4 | 1.2 | 0.45 | -0.4 |  |  |  | x | x | x | x |
| C20H22O7 | 0.35 | 1.1 | 0.5 | -0.4 |  |  |  | x | x | x | x |
| C15H24O9 | 0.6 | 1.6 | 0.267 | -0.4 |  |  |  | x | x | x | x |
| C15H22O8 | 0.53 | 1.47 | 0.333 | -0.4 |  |  |  | x | x | x | x |
| C15H18O6 | 0.4 | 1.2 | 0.467 | -0.4 |  |  |  | x | x | x | x |
| C15H16O5 | 0.33 | 1.07 | 0.533 | -0.4 |  |  |  | x | x | x | x |
| C24H34O12 | 0.5 | 1.42 | 0.333 | -0.42 |  |  |  |  | x | x |  |
| C24H32O11 | 0.46 | 1.33 | 0.375 | -0.42 |  |  |  | x | x | x | x |
| C24H30O10 | 0.42 | 1.25 | 0.417 | -0.42 |  |  |  | x | x | x | x |
| C24H28O9 | 0.38 | 1.17 | 0.458 | -0.42 |  |  |  | x | x | x | x |
| C19H24O8 | 0.42 | 1.26 | 0.421 | -0.42 |  |  |  | x | x | x |  |
| C19H28O10 | 0.53 | 1.47 | 0.316 | -0.42 |  |  |  | x | x | x | x |
| C19H26O9 | 0.47 | 1.37 | 0.368 | -0.42 |  |  |  | x | x | x | x |
| C19H22O7 | 0.37 | 1.16 | 0.474 | -0.42 |  |  |  | x | x | x | x |
| C19H20O6 | 0.32 | 1.05 | 0.526 | -0.42 |  |  |  | x | x | x | x |
| C14H18O6 | 0.43 | 1.29 | 0.429 | -0.43 |  |  |  |  |  |  |  |
| C14H22O8 | 0.57 | 1.57 | 0.286 | -0.43 |  |  |  | x | x | x | x |
| C14H20O7 | 0.5 | 1.43 | 0.357 | -0.43 |  |  |  | x | x | x | x |
| C14H16O5 | 0.36 | 1.14 | 0.5 | -0.43 |  |  |  | x | x | x | x |
| C14H14O4 | 0.29 | 1 | 0.571 | -0.43 |  |  |  | x | x | x | x |
| C23H26O8 | 0.35 | 1.13 | 0.478 | -0.43 |  |  |  | x | x | x |  |
| C23H32O11 | 0.48 | 1.39 | 0.348 | -0.43 |  |  |  | x | x | x | x |
| C23H30O10 | 0.43 | 1.3 | 0.391 | -0.43 |  |  |  | x | x | x | x |
| C23H28O9 | 0.39 | 1.22 | 0.435 | -0.43 |  |  |  | x | x | x | x |
| C27H34O11 | 0.41 | 1.26 | 0.407 | -0.44 |  |  |  |  |  |  |  |
| C18H28O10 | 0.56 | 1.56 | 0.278 | -0.44 |  |  |  | x | x | x | x |
| C18H26O9 | 0.5 | 1.44 | 0.333 | -0.44 |  |  |  | x | x | x | x |
| C18H24O8 | 0.44 | 1.33 | 0.389 | -0.44 |  |  |  | x | x | x | x |
| C18H22O7 | 0.39 | 1.22 | 0.444 | -0.44 |  |  |  | x | x | x | x |
| C18H20O6 | 0.33 | 1.11 | 0.5 | -0.44 |  |  |  | x | x | x | x |
| C22H32O11 | 0.5 | 1.45 | 0.318 | -0.45 |  |  |  | x | x | x | x |
| C22H30O10 | 0.45 | 1.36 | 0.364 | -0.45 |  |  |  | x | x | x | x |
| C22H28O9 | 0.41 | 1.27 | 0.409 | -0.45 |  |  |  | x | x | x | x |
| C22H26O8 | 0.36 | 1.18 | 0.455 | -0.45 |  |  |  | x | x | x | x |
| C13H18O6 | 0.46 | 1.38 | 0.385 | -0.46 |  |  |  |  |  |  |  |
| C26H36O12 | 0.46 | 1.38 | 0.346 | -0.46 |  |  |  |  |  | x |  |
| C26H34O11 | 0.42 | 1.31 | 0.385 | -0.46 |  |  |  |  |  | x |  |
| C13H16O5 | 0.38 | 1.23 | 0.462 | -0.46 |  |  |  |  | x | x |  |
| C26H32O10 | 0.38 | 1.23 | 0.423 | -0.46 |  |  |  | x | x | x | x |
| C13H20O7 | 0.54 | 1.54 | 0.308 | -0.46 |  |  |  | x | x | x | x |
| C13H14O4 | 0.31 | 1.08 | 0.538 | -0.46 |  |  |  | x | x | x | x |
| C17H26O9 | 0.53 | 1.53 | 0.294 | -0.47 |  |  |  | x | x | x | x |
| C17H24O8 | 0.47 | 1.41 | 0.353 | -0.47 |  |  |  | x | x | x | x |
| C17H22O7 | 0.41 | 1.29 | 0.412 | -0.47 |  |  |  | x | x | x | x |
| C17H20O6 | 0.35 | 1.18 | 0.471 | -0.47 |  |  |  | x | x | x | x |
| C17H18O5 | 0.29 | 1.06 | 0.529 | -0.47 |  |  |  | x | x | x | x |
| C21H30O10 | 0.48 | 1.43 | 0.333 | -0.48 |  |  |  | x | x | x | x |
| C21H28O9 | 0.43 | 1.33 | 0.381 | -0.48 |  |  |  | x | x | x | x |
| C21H26O8 | 0.38 | 1.24 | 0.429 | -0.48 |  |  |  | x | x | x | x |
| C21H24O7 | 0.33 | 1.14 | 0.476 | -0.48 |  |  |  | x | x | x | x |
| C25H34O11 | 0.44 | 1.36 | 0.36 | -0.48 |  |  |  | x | x | x | x |
| C25H32O10 | 0.4 | 1.28 | 0.4 | -0.48 |  |  |  | x | x | x | x |
| C16H22O7 | 0.44 | 1.38 | 0.375 | -0.5 |  |  |  |  |  |  |  |
| C24H34O11 | 0.46 | 1.42 | 0.333 | -0.5 |  |  |  | x | x | x | x |
| C24H32O10 | 0.42 | 1.33 | 0.375 | -0.5 |  |  |  | x | x | x | x |
| C24H30O9 | 0.38 | 1.25 | 0.417 | -0.5 |  |  |  | x | x | x | x |
| C20H30O10 | 0.5 | 1.5 | 0.3 | -0.5 |  |  |  | x | x | x | x |
| C20H28O9 | 0.45 | 1.4 | 0.35 | -0.5 |  |  |  | x | x | x | x |
| C20H26O8 | 0.4 | 1.3 | 0.4 | -0.5 |  |  |  | x | x | x | x |
| C20H24O7 | 0.35 | 1.2 | 0.45 | -0.5 |  |  |  | x | x | x | x |
| C16H24O8 | 0.5 | 1.5 | 0.313 | -0.5 |  |  |  | x | x | x | x |
| C16H20O6 | 0.38 | 1.25 | 0.438 | -0.5 |  |  |  | x | x | x | x |
| C16H18O5 | 0.31 | 1.13 | 0.5 | -0.5 |  |  |  | x | x | x | x |
| C12H20O7 | 0.58 | 1.67 | 0.25 | -0.5 |  |  |  | x | x | x | x |
| C12H18O6 | 0.5 | 1.5 | 0.333 | -0.5 |  |  |  | x | x | x | x |
| C12H16O5 | 0.42 | 1.33 | 0.417 | -0.5 |  |  |  | x | x | x | x |
| C12H14O4 | 0.33 | 1.17 | 0.5 | -0.5 |  |  |  | x | x | x | x |
| C27H36O11 | 0.41 | 1.33 | 0.37 | -0.52 |  |  |  |  |  |  |  |
| C23H34O11 | 0.48 | 1.48 | 0.304 | -0.52 |  |  |  | x | x | x | x |
| C23H32O10 | 0.43 | 1.39 | 0.348 | -0.52 |  |  |  | x | x | x | x |
| C23H30O9 | 0.39 | 1.3 | 0.391 | -0.52 |  |  |  | x | x | x | x |
| C23H28O8 | 0.35 | 1.22 | 0.435 | -0.52 |  |  |  | x | x | x | x |
| C19H28O9 | 0.47 | 1.47 | 0.316 | -0.53 |  |  |  | x | x | x | x |
| C19H26O8 | 0.42 | 1.37 | 0.368 | -0.53 |  |  |  | x | x | x | x |
| C19H24O7 | 0.37 | 1.26 | 0.421 | -0.53 |  |  |  | x | x | x | x |
| C19H22O6 | 0.32 | 1.16 | 0.474 | -0.53 |  |  |  | x | x | x | x |
| C15H20O6 | 0.4 | 1.33 | 0.4 | -0.53 |  |  |  |  |  | x |  |
| C15H24O8 | 0.53 | 1.6 | 0.267 | -0.53 |  |  |  | x | x | x | x |
| C15H22O7 | 0.47 | 1.47 | 0.333 | -0.53 |  |  |  | x | x | x | x |
| C15H18O5 | 0.33 | 1.2 | 0.467 | -0.53 |  |  |  | x | x | x | x |
| C26H36O11 | 0.42 | 1.38 | 0.346 | -0.54 |  |  |  |  |  | x |  |
| C26H34O10 | 0.38 | 1.31 | 0.385 | -0.54 |  |  |  | x | x | x | x |
| C11H18O6 | 0.55 | 1.64 | 0.273 | -0.55 |  |  |  |  |  |  |  |
| C22H32O10 | 0.45 | 1.45 | 0.318 | -0.55 |  |  |  | x | x | x | x |
| C22H30O9 | 0.41 | 1.36 | 0.364 | -0.55 |  |  |  | x | x | x | x |
| C22H28O8 | 0.36 | 1.27 | 0.409 | -0.55 |  |  |  | x | x | x | x |
| C11H16O5 | 0.45 | 1.45 | 0.364 | -0.55 |  |  |  | x | x |  | x |
| C11H14O4 | 0.36 | 1.27 | 0.455 | -0.55 |  |  |  | x | x | x | x |
| C18H20O5 | 0.28 | 1.11 | 0.5 | -0.56 |  |  |  | x | x | x |  |
| C18H28O9 | 0.5 | 1.56 | 0.278 | -0.56 |  |  |  | x | x | x | x |
| C18H26O8 | 0.44 | 1.44 | 0.333 | -0.56 |  |  |  | x | x | x | x |
| C18H24O7 | 0.39 | 1.33 | 0.389 | -0.56 |  |  |  | x | x | x | x |
| C18H22O6 | 0.33 | 1.22 | 0.444 | -0.56 |  |  |  | x | x | x | x |
| C25H34O10 | 0.4 | 1.36 | 0.36 | -0.56 |  |  |  | x | x | x | x |
| C14H20O6 | 0.43 | 1.43 | 0.357 | -0.57 |  |  |  |  |  |  |  |
| C14H18O5 | 0.36 | 1.29 | 0.429 | -0.57 |  |  |  |  |  |  |  |
| C21H32O10 | 0.48 | 1.52 | 0.286 | -0.57 |  |  |  | x | x | x | x |
| C21H30O9 | 0.43 | 1.43 | 0.333 | -0.57 |  |  |  | x | x | x | x |
| C21H28O8 | 0.38 | 1.33 | 0.381 | -0.57 |  |  |  | x | x | x | x |
| C21H26O7 | 0.33 | 1.24 | 0.429 | -0.57 |  |  |  | x | x | x | x |
| C14H22O7 | 0.5 | 1.57 | 0.286 | -0.57 |  |  |  | x | x | x | x |
| C14H16O4 | 0.29 | 1.14 | 0.5 | -0.57 |  |  |  | x | x | x | x |
| C24H34O10 | 0.42 | 1.42 | 0.333 | -0.58 |  |  |  | x | x | x | x |
| C24H32O9 | 0.38 | 1.33 | 0.375 | -0.58 |  |  |  |  | x | x | x |
| C24H30O8 | 0.33 | 1.25 | 0.417 | -0.58 |  |  |  | x | x | x | x |
| C17H26O8 | 0.47 | 1.53 | 0.294 | -0.59 |  |  |  | x | x | x | x |
| C17H24O7 | 0.41 | 1.41 | 0.353 | -0.59 |  |  |  | x | x | x | x |
| C17H22O6 | 0.35 | 1.29 | 0.412 | -0.59 |  |  |  | x | x | x | x |
| C17H20O5 | 0.29 | 1.18 | 0.471 | -0.59 |  |  |  | x | x | x | x |
| C20H30O9 | 0.45 | 1.5 | 0.3 | -0.6 |  |  |  | x | x | x | x |
| C20H28O8 | 0.4 | 1.4 | 0.35 | -0.6 |  |  |  | x | x | x | x |
| C20H26O7 | 0.35 | 1.3 | 0.4 | -0.6 |  |  |  | x | x | x | x |
| C20H24O6 | 0.3 | 1.2 | 0.45 | -0.6 |  |  |  | x | x | x | x |
| C23H34O10 | 0.43 | 1.48 | 0.304 | -0.61 |  |  |  | x | x | x | x |
| C23H32O9 | 0.39 | 1.39 | 0.348 | -0.61 |  |  |  | x | x | x | x |
| C23H30O8 | 0.35 | 1.3 | 0.391 | -0.61 |  |  |  | x | x | x | x |
| C13H18O5 | 0.38 | 1.38 | 0.385 | -0.62 |  |  |  | x | x | x |  |
| C13H22O7 | 0.54 | 1.69 | 0.231 | -0.62 |  |  |  | x | x | x | x |
| C13H20O6 | 0.46 | 1.54 | 0.308 | -0.62 |  |  |  | x | x | x | x |
| C13H16O4 | 0.31 | 1.23 | 0.462 | -0.62 |  |  |  | x | x | x | x |
| C16H22O6 | 0.38 | 1.38 | 0.375 | -0.63 |  |  |  | x | x | x |  |
| C16H26O8 | 0.5 | 1.63 | 0.25 | -0.63 |  |  |  | x | x | x | x |
| C16H24O7 | 0.44 | 1.5 | 0.313 | -0.63 |  |  |  | x | x | x | x |
| C16H20O5 | 0.31 | 1.25 | 0.438 | -0.63 |  |  |  | x | x |  | x |
| C19H30O9 | 0.47 | 1.58 | 0.263 | -0.63 |  |  |  | x | x | x | x |
| C19H28O8 | 0.42 | 1.47 | 0.316 | -0.63 |  |  |  | x | x | x | x |
| C19H26O7 | 0.37 | 1.37 | 0.368 | -0.63 |  |  |  | x | x | x | x |
| C19H24O6 | 0.32 | 1.26 | 0.421 | -0.63 |  |  |  | x | x | x | x |
| C22H32O9 | 0.41 | 1.45 | 0.318 | -0.64 |  |  |  | x | x | x | x |
| C22H30O8 | 0.36 | 1.36 | 0.364 | -0.64 |  |  |  | x | x | x | x |
| C22H28O7 | 0.32 | 1.27 | 0.409 | -0.64 |  |  |  | x | x | x | x |
| C25H36O10 | 0.4 | 1.44 | 0.32 | -0.64 |  |  |  | x | x | x | x |
| C25H34O9 | 0.36 | 1.36 | 0.36 | -0.64 |  |  |  | x | x | x | x |
| C24H34O9 | 0.38 | 1.42 | 0.333 | -0.67 |  |  |  | x | x | x | x |
| C24H32O8 | 0.33 | 1.33 | 0.375 | -0.67 |  |  |  | x | x | x | x |
| C21H32O9 | 0.43 | 1.52 | 0.286 | -0.67 |  |  |  | x | x | x | x |
| C21H30O8 | 0.38 | 1.43 | 0.333 | -0.67 |  |  |  | x | x | x | x |
| C21H28O7 | 0.33 | 1.33 | 0.381 | -0.67 |  |  |  | x | x | x | x |
| C18H28O8 | 0.44 | 1.56 | 0.278 | -0.67 |  |  |  | x | x | x | x |
| C18H26O7 | 0.39 | 1.44 | 0.333 | -0.67 |  |  |  | x | x | x | x |
| C18H24O6 | 0.33 | 1.33 | 0.389 | -0.67 |  |  |  | x | x | x | x |
| C18H22O5 | 0.28 | 1.22 | 0.444 | -0.67 |  |  |  | x | x | x | x |
| C15H24O7 | 0.47 | 1.6 | 0.267 | -0.67 |  |  |  | x | x | x | x |
| C15H22O6 | 0.4 | 1.47 | 0.333 | -0.67 |  |  |  | x | x | x | x |
| C15H20O5 | 0.33 | 1.33 | 0.4 | -0.67 |  |  |  | x | x | x | x |
| C15H18O4 | 0.27 | 1.2 | 0.467 | -0.67 |  |  |  | x | x | x | x |
| C12H18O5 | 0.42 | 1.5 | 0.333 | -0.67 |  |  |  | x | x | x | x |
| C12H16O4 | 0.33 | 1.33 | 0.417 | -0.67 |  |  |  | x | x | x | x |
| C23H32O8 | 0.35 | 1.39 | 0.348 | -0.7 |  |  |  | x | x | x | x |
| C20H30O8 | 0.4 | 1.5 | 0.3 | -0.7 |  |  |  | x | x | x | x |
| C20H28O7 | 0.35 | 1.4 | 0.35 | -0.7 |  |  |  | x | x | x | x |
| C20H26O6 | 0.3 | 1.3 | 0.4 | -0.7 |  |  |  | x | x | x | x |
| C17H28O8 | 0.47 | 1.65 | 0.235 | -0.71 |  |  |  | x | x | x | x |
| C17H26O7 | 0.41 | 1.53 | 0.294 | -0.71 |  |  |  | x | x | x | x |
| C17H24O6 | 0.35 | 1.41 | 0.353 | -0.71 |  |  |  | x | x | x | x |
| C17H22O5 | 0.29 | 1.29 | 0.412 | -0.71 |  |  |  | x | x | x | x |
| C14H22O6 | 0.43 | 1.57 | 0.286 | -0.71 |  |  |  | x | x | x | x |
| C14H20O5 | 0.36 | 1.43 | 0.357 | -0.71 |  |  |  | x | x | x | x |
| C14H18O4 | 0.29 | 1.29 | 0.429 | -0.71 |  |  |  | x | x | x | x |
| C22H32O8 | 0.36 | 1.45 | 0.318 | -0.73 |  |  |  | x | x | x | x |
| C22H30O7 | 0.32 | 1.36 | 0.364 | -0.73 |  |  |  | x | x | x | x |
| C11H16O4 | 0.36 | 1.45 | 0.364 | -0.73 |  |  |  | x | x |  | x |
| C19H30O8 | 0.42 | 1.58 | 0.263 | -0.74 |  |  |  | x | x | x | x |
| C19H28O7 | 0.37 | 1.47 | 0.316 | -0.74 |  |  |  | x | x | x | x |
| C19H26O6 | 0.32 | 1.37 | 0.368 | -0.74 |  |  |  | x | x | x | x |
| C19H24O5 | 0.26 | 1.26 | 0.421 | -0.74 |  |  |  | x | x | x | x |
| C16H26O7 | 0.44 | 1.63 | 0.25 | -0.75 |  |  |  | x | x | x | x |
| C16H24O6 | 0.38 | 1.5 | 0.313 | -0.75 |  |  |  | x | x | x | x |
| C16H22O5 | 0.31 | 1.38 | 0.375 | -0.75 |  |  |  | x | x | x | x |
| C21H28O6 | 0.29 | 1.33 | 0.381 | -0.76 |  |  |  |  |  |  |  |
| C21H32O8 | 0.38 | 1.52 | 0.286 | -0.76 |  |  |  | x | x | x | x |
| C21H30O7 | 0.33 | 1.43 | 0.333 | -0.76 |  |  |  | x | x | x | x |
| C13H20O5 | 0.38 | 1.54 | 0.308 | -0.77 |  |  |  | x | x | x | x |
| C13H18O4 | 0.31 | 1.38 | 0.385 | -0.77 |  |  |  | x | x | x | x |
| C18H28O7 | 0.39 | 1.56 | 0.278 | -0.78 |  |  |  | x | x | x | x |
| C18H26O6 | 0.33 | 1.44 | 0.333 | -0.78 |  |  |  | x | x | x | x |
| C18H24O5 | 0.28 | 1.33 | 0.389 | -0.78 |  |  |  | x | x | x | x |
| C20H30O7 | 0.35 | 1.5 | 0.3 | -0.8 |  |  |  | x | x | x | x |
| C20H28O6 | 0.3 | 1.4 | 0.35 | -0.8 |  |  |  | x | x | x | x |
| C15H24O6 | 0.4 | 1.6 | 0.267 | -0.8 |  |  |  | x | x | x | x |
| C15H22O5 | 0.33 | 1.47 | 0.333 | -0.8 |  |  |  | x | x | x | x |
| C15H20O4 | 0.27 | 1.33 | 0.4 | -0.8 |  |  |  | x | x | x | x |
| C22H32O7 | 0.32 | 1.45 | 0.318 | -0.82 |  |  |  | x | x | x | x |
| C17H26O6 | 0.35 | 1.53 | 0.294 | -0.82 |  |  |  | x | x | x | x |
| C17H24O5 | 0.29 | 1.41 | 0.353 | -0.82 |  |  |  | x | x | x | x |
| C12H18O4 | 0.33 | 1.5 | 0.333 | -0.83 |  |  |  | x | x | x | x |
| C19H30O7 | 0.37 | 1.58 | 0.263 | -0.84 |  |  |  | x | x | x | x |
| C19H28O6 | 0.32 | 1.47 | 0.316 | -0.84 |  |  |  | x | x | x | x |
| C19H26O5 | 0.26 | 1.37 | 0.368 | -0.84 |  |  |  | x | x | x | x |
| C14H22O5 | 0.36 | 1.57 | 0.286 | -0.86 |  |  |  | x | x | x | x |
| C14H20O4 | 0.29 | 1.43 | 0.357 | -0.86 |  |  |  | x | x | x | x |
| C16H26O6 | 0.38 | 1.63 | 0.25 | -0.88 |  |  |  | x | x | x | x |
| C16H24O5 | 0.31 | 1.5 | 0.313 | -0.88 |  |  |  | x | x | x | x |
| C16H22O4 | 0.25 | 1.38 | 0.375 | -0.88 |  |  |  | x | x | x | x |
| C18H28O6 | 0.33 | 1.56 | 0.278 | -0.89 |  |  |  | x | x | x | x |
| C18H26O5 | 0.28 | 1.44 | 0.333 | -0.89 |  |  |  | x | x | x | x |
| C20H30O6 | 0.3 | 1.5 | 0.3 | -0.9 |  |  |  | x | x | x | x |
| C13H20O4 | 0.31 | 1.54 | 0.308 | -0.92 |  |  |  | x | x |  | x |
| C15H24O5 | 0.33 | 1.6 | 0.267 | -0.93 |  |  |  | x | x | x | x |
| C17H26O5 | 0.29 | 1.53 | 0.294 | -0.94 |  |  |  | x | x | x | x |

Table A5 CHO formulas present before and after Al2(SO4)3 flocculation at Lovö WTP and the change in relative abundance during the treatment as well as correlation with optical parameters

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Decrease** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |  | **Increase** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |
| C14H16O10 | -21.932 |  | x |  | C15H20O7 | 9.682 |  |  |
| C14H14O10 | -21.090 |  | x |  | C15H18O7 | 7.672 |  |  |
| C13H14O9 | -20.837 |  |  |  | C14H18O7 | 6.705 | x |  |
| C13H14O10 | -19.789 |  | x |  | C15H20O6 | 6.204 |  |  |
| C13H16O9 | -18.718 |  |  |  | C16H20O8 | 5.799 |  |  |
| C15H14O10 | -18.208 |  | x |  | C17H20O8 | 5.494 |  |  |
| C15H14O11 | -18.039 |  | x |  | C17H22O8 | 4.219 |  |  |
| C14H14O9 | -17.640 |  | x |  | C16H22O7 | 4.119 |  |  |
| C15H16O11 | -17.469 |  | x |  | C15H22O6 | 4.061 | x |  |
| C15H16O10 | -17.388 |  | x |  | C12H16O6 | 3.406 |  |  |
| C16H14O11 | -17.006 |  | x |  | C17H24O8 | 3.333 | x |  |
| C12H14O9 | -16.996 |  |  |  | C14H20O7 | 3.319 | x |  |
| C15H18O10 | -16.560 |  | x |  | C16H20O7 | 3.220 |  |  |
| C14H12O10 | -16.462 |  | x |  | C15H22O7 | 3.188 | x |  |
| C14H14O11 | -16.337 |  | x |  | C16H22O8 | 3.015 |  |  |
| C16H16O11 | -15.670 |  | x |  | C18H22O8 | 2.760 |  |  |
| C15H12O11 | -15.468 |  | x |  | C14H20O6 | 2.727 |  |  |
| C13H12O9 | -15.388 |  | x |  | C14H18O8 | 2.706 |  |  |
| C15H12O10 | -15.055 |  | x |  | C17H24O7 | 2.666 | x |  |
| C13H16O10 | -14.986 |  | x |  | C17H22O7 | 2.454 | x |  |
| C14H18O9 | -14.853 |  | x |  | C19H24O8 | 2.434 | x |  |
| C14H12O9 | -14.818 |  | x |  | C16H22O6 | 2.339 |  |  |
| C16H14O10 | -14.585 |  | x |  | C18H24O8 | 2.153 | x |  |
| C16H12O11 | -14.371 |  | x |  | C18H24O7 | 2.150 | x |  |
| C13H12O10 | -14.010 |  | x |  | C19H24O9 | 1.802 | x |  |
| C12H14O8 | -13.871 |  |  |  | C14H22O7 | 1.740 | x |  |
| C17H14O11 | -13.373 |  | x |  | C17H20O7 | 1.523 | x |  |
| C16H16O10 | -13.342 |  | x |  | C18H22O9 | 1.462 |  |  |
| C17H14O12 | -13.240 |  | x |  | C13H20O7 | 1.421 | x |  |
| C17H16O11 | -13.127 |  | x |  | C19H26O8 | 1.333 | x |  |
| C14H12O11 | -13.057 |  | x |  | C18H26O7 | 1.321 | x |  |
| C14H18O10 | -12.977 |  | x |  | C19H22O9 | 1.230 | x |  |
| C16H14O12 | -12.735 |  | x |  | C18H22O7 | 1.196 | x |  |
| C16H18O11 | -12.642 |  | x |  | C19H22O8 | 1.171 | x |  |
| C17H16O12 | -12.483 |  | x |  | C18H20O8 | 1.168 |  |  |
| C14H16O11 | -12.479 |  | x |  | C20H24O8 | 1.155 | x |  |
| C16H16O12 | -12.316 |  | x |  | C19H24O7 | 1.127 | x |  |
| C12H12O8 | -12.244 |  | x |  | C15H18O6 | 1.011 | x |  |
| C12H12O9 | -12.130 |  |  |  | C14H16O6 | 0.971 |  |  |
| C15H18O11 | -12.103 |  |  |  | C14H16O7 | 0.946 | x |  |
| C14H16O9 | -11.497 |  | x |  | C15H16O6 | 0.894 |  |  |
| C16H18O10 | -11.377 |  |  |  | C18H26O8 | 0.820 | x |  |
| C13H10O9 | -11.336 |  | x |  | C16H18O8 | 0.804 |  |  |
| C18H16O12 | -11.075 |  | x |  | C15H18O8 | 0.799 |  |  |
| C16H12O12 | -10.592 |  | x |  | C17H20O9 | 0.794 |  |  |
| C15H14O9 | -10.508 |  | x |  | C16H24O8 | 0.754 | x |  |
| C15H14O12 | -10.405 |  | x |  | C12H18O6 | 0.746 | x |  |
| C18H14O12 | -10.376 |  | x |  | C20H26O8 | 0.741 | x |  |
| C19H16O13 | -10.365 |  | x |  | C14H18O5 | 0.741 |  |  |
| C17H18O12 | -10.361 |  | x |  | C17H26O7 | 0.698 | x |  |
| C14H10O9 | -10.282 |  | x |  | C19H22O7 | 0.681 | x |  |
| C15H16O12 | -10.222 |  | x |  | C14H16O8 | 0.669 |  |  |
| C11H14O8 | -10.155 |  |  |  | C17H26O8 | 0.651 | x |  |
| C17H18O11 | -10.153 |  | x |  | C19H26O7 | 0.628 | x |  |
| C16H18O12 | -10.002 |  | x |  | C20H26O7 | 0.628 | x |  |
| C15H12O9 | -9.969 |  | x |  | C20H24O9 | 0.614 | x |  |
| C14H10O10 | -9.900 |  | x |  | C16H20O6 | 0.603 |  |  |
| C13H10O10 | -9.890 |  | x |  | C18H26O6 | 0.597 | x |  |
| C16H12O10 | -9.890 |  | x |  | C13H18O6 | 0.595 |  |  |
| C17H12O12 | -9.864 |  | x |  | C20H28O8 | 0.592 | x |  |
| C17H12O11 | -9.780 |  | x |  | C21H26O9 | 0.591 | x |  |
| C18H14O13 | -9.682 |  | x |  | C17H22O9 | 0.579 |  |  |
| C17H16O13 | -9.345 |  | x |  | C17H18O8 | 0.558 |  |  |
| C16H20O10 | -9.334 |  |  |  | C16H20O9 | 0.551 |  |  |
| C12H12O10 | -9.224 |  |  |  | C14H22O6 | 0.535 | x |  |
| C15H12O12 | -9.184 |  | x |  | C19H26O9 | 0.518 | x |  |
| C17H16O10 | -9.179 |  | x |  | C15H24O6 | 0.510 | x |  |
| C18H16O13 | -9.161 |  | x |  | C17H18O6 | 0.500 | x |  |
| C15H10O11 | -9.141 |  | x |  | C16H18O6 | 0.484 | x |  |
| C11H12O8 | -9.055 |  |  |  | C16H22O5 | 0.478 | x |  |
| C18H16O11 | -9.014 |  | x |  | C20H26O9 | 0.466 | x |  |
| C17H14O13 | -9.012 |  | x |  | C16H24O5 | 0.454 | x |  |
| C13H14O11 | -8.965 |  |  |  | C17H26O6 | 0.446 | x |  |
| C13H12O8 | -8.919 |  | x |  | C15H22O5 | 0.440 | x |  |
| C19H14O13 | -8.861 |  | x |  | C16H20O5 | 0.426 |  |  |
| C13H12O11 | -8.838 |  | x |  | C16H24O6 | 0.424 | x |  |
| C13H14O8 | -8.818 |  |  |  | C15H16O7 | 0.420 |  |  |
| C19H16O14 | -8.782 |  | x |  | C15H24O7 | 0.419 | x |  |
| C18H18O12 | -8.734 |  | x |  | C23H30O10 | 0.414 | x |  |
| C14H10O11 | -8.688 |  | x |  | C16H26O7 | 0.405 | x |  |
| C12H16O8 | -8.686 |  |  |  | C19H26O6 | 0.397 | x |  |
| C19H16O12 | -8.664 |  | x |  | C22H26O9 | 0.371 | x |  |
| C16H20O11 | -8.633 |  |  |  | C22H28O9 | 0.369 | x |  |
| C19H18O13 | -8.609 |  | x |  | C13H20O5 | 0.354 | x |  |
| C15H20O10 | -8.608 |  |  |  | C17H22O5 | 0.354 | x |  |
| C18H14O11 | -8.388 |  | x |  | C18H28O7 | 0.351 | x |  |
| C17H14O10 | -8.342 |  | x |  | C20H22O8 | 0.342 | x |  |
| C11H12O9 | -8.332 |  |  |  | C13H16O4 | 0.327 | x |  |
| C17H18O13 | -8.319 |  | x |  | C21H28O9 | 0.315 | x |  |
| C20H18O13 | -8.069 |  | x |  | C21H26O8 | 0.314 | x |  |
| C18H18O13 | -7.940 |  | x |  | C23H28O10 | 0.314 | x |  |
| C19H18O14 | -7.896 |  | x |  | C20H28O7 | 0.299 | x |  |
| C18H18O11 | -7.883 |  | x |  | C16H16O6 | 0.284 | x |  |
| C17H20O12 | -7.875 |  | x |  | C17H24O5 | 0.282 | x |  |
| C12H16O9 | -7.835 | x |  |  | C21H24O9 | 0.280 | x |  |
| C20H18O14 | -7.833 |  | x |  | C15H24O8 | 0.274 | x |  |
| C12H14O7 | -7.805 |  |  |  | C29H36O15 | 0.272 |  |  |
| C20H16O14 | -7.759 |  | x |  | C22H26O10 | 0.263 | x |  |
| C12H10O8 | -7.748 |  | x |  | C18H22O6 | 0.262 | x |  |
| C16H10O11 | -7.679 |  | x |  | C18H24O9 | 0.262 | x |  |
| C17H20O11 | -7.679 |  |  |  | C27H34O13 | 0.257 |  |  |
| C20H16O13 | -7.665 |  | x |  | C27H36O14 | 0.254 |  |  |
| C16H16O13 | -7.620 |  | x |  | C18H20O7 | 0.253 | x |  |
| C12H14O10 | -7.584 |  |  |  | C27H34O12 | 0.248 |  |  |
| C19H18O12 | -7.549 |  | x |  | C29H36O13 | 0.247 |  |  |
| C15H10O10 | -7.456 |  | x |  | C13H18O4 | 0.247 |  |  |
| C15H16O9 | -7.324 |  | x |  | C19H28O8 | 0.244 | x |  |
| C19H14O14 | -7.249 |  | x |  | C28H38O12 | 0.244 |  |  |
| C14H14O8 | -7.201 |  | x |  | C19H28O7 | 0.244 | x |  |
| C18H20O12 | -7.170 |  |  |  | C24H32O9 | 0.242 | x |  |
| C16H14O13 | -7.163 |  | x |  | C28H36O13 | 0.239 |  |  |
| C19H14O12 | -7.088 |  | x |  | C21H24O8 | 0.238 | x |  |
| C12H10O9 | -7.066 |  | x |  | C23H30O9 | 0.238 | x |  |
| C18H12O12 | -7.028 |  | x |  | C12H20O6 | 0.237 |  |  |
| C20H20O13 | -6.965 |  | x |  | C28H36O12 | 0.237 |  |  |
| C17H18O10 | -6.939 |  |  |  | C22H26O8 | 0.230 | x |  |
| C18H16O14 | -6.809 |  | x |  | C29H40O13 | 0.230 |  |  |
| C14H14O12 | -6.791 |  | x |  | C29H38O14 | 0.229 |  |  |
| C18H12O13 | -6.749 |  | x |  | C22H24O9 | 0.228 | x |  |
| C18H14O14 | -6.626 |  | x |  | C27H34O14 | 0.223 |  |  |
| C20H20O14 | -6.615 |  | x |  | C29H36O14 | 0.223 |  |  |
| C17H12O13 | -6.511 |  | x |  | C30H38O15 | 0.219 |  |  |
| C19H20O13 | -6.458 |  | x |  | C23H28O9 | 0.217 | x |  |
| C11H10O8 | -6.270 |  |  |  | C29H38O15 | 0.217 |  |  |
| C15H10O9 | -6.261 |  | x |  | C15H26O6 | 0.217 |  |  |
| C18H20O13 | -6.234 |  | x |  | C14H14O5 | 0.210 |  |  |
| C12H16O7 | -6.055 | x |  |  | C22H28O8 | 0.208 | x |  |
| C21H18O14 | -5.945 |  | x |  | C17H20O5 | 0.206 | x |  |
| C13H18O9 | -5.927 | x |  |  | C26H36O12 | 0.204 |  |  |
| C19H20O12 | -5.920 |  | x |  | C19H26O10 | 0.199 | x |  |
| C16H14O9 | -5.878 |  | x |  | C28H34O14 | 0.198 |  |  |
| C20H18O12 | -5.869 |  | x |  | C21H22O9 | 0.198 | x |  |
| C18H18O14 | -5.767 |  | x |  | C20H28O9 | 0.198 | x |  |
| C19H20O14 | -5.759 |  | x |  | C27H36O12 | 0.192 |  |  |
| C13H10O8 | -5.727 |  | x |  | C21H28O8 | 0.191 | x |  |
| C20H14O13 | -5.714 |  | x |  | C21H26O7 | 0.191 | x |  |
| C11H12O7 | -5.712 |  |  |  | C20H30O9 | 0.191 | x |  |
| C17H12O10 | -5.705 |  | x |  | C21H28O7 | 0.191 | x |  |
| C14H12O12 | -5.699 |  | x |  | C24H30O9 | 0.188 | x |  |
| C21H16O14 | -5.670 |  | x |  | C29H36O16 | 0.187 |  |  |
| C15H18O12 | -5.608 |  | x |  | C22H28O7 | 0.186 | x |  |
| C20H16O12 | -5.596 |  | x |  | C25H34O11 | 0.186 | x |  |
| C20H22O13 | -5.569 |  | x |  | C23H28O8 | 0.184 | x |  |
| C20H18O15 | -5.555 |  | x |  | C20H24O7 | 0.184 | x |  |
| C16H20O12 | -5.543 |  |  |  | C21H30O9 | 0.181 | x |  |
| C20H14O14 | -5.533 |  | x |  | C28H36O14 | 0.180 |  |  |
| C16H10O12 | -5.515 |  |  |  | C30H38O13 | 0.178 |  |  |
| C19H18O11 | -5.481 |  | x |  | C21H26O10 | 0.174 | x |  |
| C18H12O11 | -5.474 |  | x |  | C22H30O8 | 0.173 | x |  |
| C16H12O13 | -5.473 |  |  |  | C27H36O11 | 0.173 |  |  |
| C19H16O11 | -5.468 |  | x |  | C16H18O7 | 0.171 |  |  |
| C20H16O15 | -5.440 |  | x |  | C20H28O6 | 0.169 | x |  |
| C19H16O15 | -5.419 |  | x |  | C27H36O13 | 0.169 |  |  |
| C12H12O7 | -5.414 |  | x |  | C28H36O15 | 0.168 |  |  |
| C17H16O14 | -5.403 |  | x |  | C16H26O8 | 0.166 | x |  |
| C21H18O15 | -5.375 |  | x |  | C26H34O11 | 0.165 | x |  |
| C18H16O10 | -5.371 |  | x |  | C28H38O14 | 0.163 |  |  |
| C18H20O11 | -5.349 |  |  |  | C26H34O14 | 0.162 |  |  |
| C19H12O13 | -5.316 |  | x |  | C27H38O13 | 0.161 |  |  |
| C21H20O14 | -5.296 |  | x |  | C28H38O13 | 0.160 |  |  |
| C17H20O10 | -5.286 |  |  |  | C23H26O9 | 0.158 | x |  |
| C13H10O11 | -5.269 |  | x |  | C24H30O10 | 0.153 | x |  |
| C18H22O12 | -5.228 |  |  |  | C19H24O6 | 0.151 | x |  |
| C12H10O10 | -5.195 |  |  |  | C13H18O5 | 0.150 | x |  |
| C11H10O9 | -5.191 |  |  |  | C24H34O8 | 0.149 |  |  |
| C16H18O13 | -5.187 |  | x |  | C20H28O10 | 0.147 | x |  |
| C16H10O10 | -5.161 |  | x |  | C26H34O12 | 0.146 |  |  |
| C20H20O12 | -5.159 |  | x |  | C23H26O10 | 0.144 | x |  |
| C14H20O9 | -5.151 | x |  |  | C25H34O10 | 0.143 | x |  |
| C21H18O13 | -5.131 |  | x |  | C27H36O10 | 0.143 |  |  |
| C17H20O13 | -5.115 |  | x |  | C24H34O9 | 0.142 | x |  |
| C19H18O15 | -5.110 |  | x |  | C30H36O14 | 0.141 |  |  |
| C17H22O11 | -5.080 | x |  |  | C22H26O7 | 0.141 |  |  |
| C13H18O8 | -5.070 | x |  |  | C18H28O8 | 0.140 | x |  |
| C16H12O9 | -5.067 |  | x |  | C25H30O10 | 0.139 | x |  |
| C21H16O15 | -5.062 |  | x |  | C28H34O15 | 0.139 |  |  |
| C21H20O13 | -4.979 |  | x |  | C22H32O9 | 0.138 | x |  |
| C15H14O13 | -4.977 |  | x |  | C25H32O10 | 0.135 | x |  |
| C17H10O12 | -4.843 |  | x |  | C19H24O5 | 0.132 | x |  |
| C19H12O12 | -4.829 |  |  |  | C19H26O5 | 0.130 | x |  |
| C11H14O9 | -4.768 |  |  |  | C17H26O5 | 0.128 | x |  |
| C14H18O11 | -4.758 |  |  |  | C18H26O9 | 0.126 | x |  |
| C22H18O15 | -4.757 |  |  |  | C20H30O8 | 0.126 | x |  |
| C20H22O14 | -4.746 |  | x |  | C29H38O11 | 0.126 |  |  |
| C20H20O15 | -4.727 |  | x |  | C26H32O11 | 0.125 |  |  |
| C22H18O14 | -4.725 |  | x |  | C20H30O7 | 0.125 | x |  |
| C17H14O14 | -4.682 |  | x |  | C19H20O9 | 0.122 |  |  |
| C21H16O13 | -4.662 |  | x |  | C26H32O12 | 0.120 |  |  |
| C13H8O9 | -4.633 |  | x |  | C22H24O8 | 0.118 | x |  |
| C14H10O8 | -4.581 |  | x |  | C25H34O12 | 0.117 |  |  |
| C10H12O7 | -4.580 |  |  |  | C18H24O6 | 0.116 | x |  |
| C15H20O11 | -4.577 |  |  |  | C16H26O9 | 0.115 |  |  |
| C22H20O15 | -4.555 |  | x |  | C29H34O15 | 0.111 |  |  |
| C21H20O15 | -4.545 |  | x |  | C18H28O9 | 0.110 | x |  |
| C15H10O12 | -4.524 |  |  |  | C28H34O13 | 0.105 |  |  |
| C19H22O13 | -4.520 |  | x |  | C26H36O11 | 0.104 |  |  |
| C13H12O7 | -4.485 |  | x |  | C23H30O8 | 0.103 | x |  |
| C17H10O11 | -4.472 |  | x |  | C14H24O7 | 0.102 |  |  |
| C21H14O14 | -4.428 |  | x |  | C25H34O9 | 0.099 | x |  |
| C17H18O14 | -4.427 |  | x |  | C27H38O11 | 0.098 |  |  |
| C19H14O11 | -4.419 |  | x |  | C19H22O5 | 0.096 |  |  |
| C18H18O10 | -4.405 |  |  |  | C26H34O10 | 0.096 | x |  |
| C14H12O8 | -4.401 |  | x |  | C18H26O5 | 0.095 | x |  |
| C11H14O6 | -4.349 | x |  |  | C21H32O9 | 0.094 | x |  |
| C20H14O12 | -4.336 |  | x |  | C22H28O10 | 0.093 | x |  |
| C22H16O14 | -4.327 |  | x |  | C25H32O11 | 0.092 | x |  |
| C19H22O12 | -4.311 |  |  |  | C22H32O8 | 0.091 | x |  |
| C14H16O12 | -4.292 |  | x |  | C27H34O15 | 0.091 |  |  |
| C21H22O14 | -4.257 |  | x |  | C28H34O12 | 0.090 |  |  |
| C18H14O10 | -4.239 |  | x |  | C24H32O10 | 0.090 | x |  |
| C19H14O15 | -4.237 |  |  |  | C26H38O11 | 0.089 |  |  |
| C22H20O14 | -4.237 |  | x |  | C24H30O8 | 0.089 | x |  |
| C16H22O10 | -4.228 | x |  |  | C23H32O9 | 0.087 | x |  |
| C22H16O15 | -4.212 |  |  |  | C26H34O13 | 0.086 |  |  |
| C15H16O13 | -4.209 |  | x |  | C27H32O13 | 0.085 |  |  |
| C11H10O7 | -4.192 |  |  |  | C23H24O9 | 0.085 | x |  |
| C15H12O8 | -4.121 |  | x |  | C27H36O15 | 0.084 |  |  |
| C18H20O14 | -4.096 |  | x |  | C19H28O6 | 0.083 | x |  |
| C20H14O15 | -4.081 |  |  |  | C19H22O6 | 0.083 | x |  |
| C16H16O9 | -4.064 |  | x |  | C20H22O7 | 0.082 | x |  |
| C21H22O13 | -4.052 |  | x |  | C26H36O10 | 0.076 |  |  |
| C17H22O12 | -4.044 |  |  |  | C19H30O9 | 0.075 | x |  |
| C19H12O14 | -4.027 |  |  |  | C25H36O12 | 0.074 |  |  |
| C18H16O15 | -3.984 |  |  |  | C24H30O11 | 0.073 | x |  |
| C12H10O7 | -3.940 |  | x |  | C21H22O8 | 0.073 | x |  |
| C19H20O11 | -3.921 |  |  |  | C27H32O12 | 0.072 |  |  |
| C12H8O8 | -3.920 |  |  |  | C28H32O12 | 0.071 |  |  |
| C18H22O13 | -3.892 |  | x |  | C27H38O10 | 0.069 |  |  |
| C11H8O9 | -3.872 |  | x |  | C20H24O6 | 0.069 | x |  |
| C15H14O8 | -3.856 |  | x |  | C22H30O7 | 0.068 | x |  |
| C14H8O9 | -3.809 |  | x |  | C28H34O16 | 0.068 |  |  |
| C14H8O10 | -3.800 |  | x |  | C29H34O14 | 0.067 |  |  |
| C13H10O7 | -3.799 |  | x |  | C19H30O8 | 0.066 | x |  |
| C19H20O15 | -3.798 |  |  |  | C14H18O6 | 0.063 |  |  |
| C13H18O10 | -3.779 |  |  |  | C25H32O12 | 0.062 |  |  |
| C20H22O12 | -3.761 |  |  |  | C13H22O5 | 0.060 |  |  |
| C11H16O8 | -3.758 |  |  |  | C21H30O8 | 0.060 | x |  |
| C12H8O9 | -3.704 |  |  |  | C23H26O8 | 0.059 | x |  |
| C13H16O11 | -3.681 |  |  |  | C26H36O13 | 0.058 |  |  |
| C17H16O9 | -3.680 |  | x |  | C25H34O13 | 0.058 |  |  |
| C22H18O13 | -3.646 |  | x |  | C17H28O8 | 0.058 | x |  |
| C20H24O13 | -3.641 |  |  |  | C25H36O10 | 0.056 | x |  |
| C13H14O7 | -3.638 |  |  |  | C27H34O10 | 0.056 |  |  |
| C21H14O15 | -3.630 |  |  |  | C28H32O14 | 0.053 |  |  |
| C11H8O8 | -3.630 |  |  |  | C23H32O8 | 0.052 | x |  |
| C20H18O11 | -3.592 |  | x |  | C20H26O6 | 0.050 | x |  |
| C16H16O14 | -3.555 |  |  |  | C22H30O9 | 0.049 | x |  |
| C21H14O13 | -3.549 |  |  |  | C17H18O5 | 0.048 | x |  |
| C14H20O8 | -3.545 | x |  |  | C23H34O10 | 0.047 | x |  |
| C22H22O15 | -3.540 |  | x |  | C25H30O11 | 0.046 | x |  |
| C21H18O16 | -3.529 |  |  |  | C13H22O7 | 0.046 | x |  |
| C18H14O15 | -3.504 |  |  |  | C25H36O11 | 0.046 |  |  |
| C22H18O16 | -3.501 |  |  |  | C18H20O6 | 0.045 | x |  |
| C21H22O15 | -3.481 |  | x |  | C26H32O10 | 0.044 | x |  |
| C18H22O11 | -3.477 | x |  |  | C20H26O5 | 0.044 |  |  |
| C22H22O14 | -3.465 |  | x |  | C28H36O11 | 0.044 |  |  |
| C21H20O12 | -3.463 |  | x |  | C23H32O10 | 0.043 | x |  |
| C15H12O13 | -3.446 |  | x |  | C19H30O10 | 0.043 |  |  |
| C13H8O8 | -3.434 |  | x |  | C26H30O12 | 0.042 |  |  |
| C22H16O13 | -3.423 |  | x |  | C24H36O9 | 0.041 |  |  |
| C13H8O10 | -3.416 |  | x |  | C20H20O7 | 0.038 |  |  |
| C23H20O15 | -3.414 |  |  |  | C20H22O9 | 0.037 | x |  |
| C16H22O11 | -3.411 | x |  |  | C21H24O7 | 0.036 | x |  |
| C22H20O16 | -3.407 |  |  |  | C24H26O9 | 0.036 |  |  |
| C16H14O8 | -3.389 |  | x |  | C22H30O10 | 0.034 | x |  |
| C16H14O14 | -3.374 |  |  |  | C27H30O11 | 0.033 |  |  |
| C19H22O14 | -3.371 |  | x |  | C19H30O6 | 0.033 |  |  |
| C22H14O14 | -3.370 |  |  |  | C24H36O11 | 0.029 |  |  |
| C18H10O12 | -3.364 |  |  |  | C22H32O10 | 0.028 | x |  |
| C10H12O8 | -3.356 |  |  |  | C25H36O9 | 0.026 |  |  |
| C23H18O15 | -3.342 |  |  |  | C16H26O6 | 0.025 | x |  |
| C16H10O9 | -3.340 |  | x |  | C19H30O7 | 0.024 | x |  |
| C20H12O13 | -3.326 |  |  |  | C18H28O6 | 0.022 | x |  |
| C17H22O10 | -3.323 |  |  |  | C15H26O7 | 0.022 |  |  |
| C21H18O12 | -3.322 |  | x |  | C17H28O7 | 0.021 |  |  |
| C22H20O13 | -3.307 |  | x |  | C27H32O14 | 0.017 |  |  |
| C21H24O13 | -3.299 |  |  |  | C22H32O7 | 0.016 | x |  |
| C21H16O16 | -3.286 |  |  |  | C19H18O7 | 0.013 | x |  |
| C12H12O11 | -3.278 |  |  |  | C24H28O10 | 0.013 | x |  |
| C12H18O7 | -3.273 | x |  |  | C26H38O10 | 0.011 |  |  |
| C21H24O14 | -3.270 |  | x |  | C23H28O11 | 0.010 | x |  |
| C20H22O15 | -3.255 |  | x |  | C27H34O11 | 0.010 |  |  |
| C14H20O10 | -3.224 |  |  |  | C24H32O8 | 0.009 | x |  |
| C15H10O8 | -3.217 |  | x |  | C28H30O13 | 0.009 |  |  |
| C23H20O14 | -3.215 |  |  |  | C18H28O10 | 0.007 | x |  |
| C18H20O10 | -3.173 |  |  |  | C27H30O12 | 0.007 |  |  |
| C18H18O15 | -3.100 |  |  |  | C19H18O6 | 0.007 |  |  |
| C20H18O16 | -3.091 |  |  |  | C15H24O5 | 0.005 | x |  |
| C17H14O9 | -3.089 |  | x |  | C24H28O9 | 0.004 | x |  |
| C23H18O14 | -3.087 |  |  |  | C22H20O9 | 0.003 |  |  |
| C21H16O12 | -3.069 |  | x |  | C21H30O7 | 0.002 | x |  |
| C20H16O11 | -3.069 |  | x |  | C20H26O10 | 0.001 | x |  |
| C21H20O16 | -3.062 |  |  |  | C26H30O13 | 0.001 |  |  |
| C13H16O7 | -3.056 |  |  |  | C24H34O11 | 0.001 | x |  |
| C10H10O7 | -3.054 |  |  |  | C28H32O13 | 0.0001 |  |  |
| C15H18O9 | -3.034 |  |  |  |  |  |  |  |
| C15H8O11 | -3.020 |  |  |  |  |  |  |  |
| C20H16O16 | -3.015 |  |  |  |  |  |  |  |
| C15H8O10 | -2.999 |  |  |  |  |  |  |  |
| C19H12O11 | -2.987 |  | x |  |  |  |  |  |
| C20H24O14 | -2.976 |  | x |  |  |  |  |  |
| C23H18O16 | -2.936 |  |  |  |  |  |  |  |
| C18H12O10 | -2.919 |  | x |  |  |  |  |  |
| C14H12O7 | -2.916 |  |  |  |  |  |  |  |
| C17H10O10 | -2.872 |  | x |  |  |  |  |  |
| C20H20O11 | -2.870 |  |  |  |  |  |  |  |
| C20H24O12 | -2.844 | x |  |  |  |  |  |  |
| C22H22O13 | -2.842 |  | x |  |  |  |  |  |
| C23H22O15 | -2.834 |  |  |  |  |  |  |  |
| C11H8O7 | -2.811 |  |  |  |  |  |  |  |
| C10H14O7 | -2.810 | x |  |  |  |  |  |  |
| C20H12O12 | -2.792 |  |  |  |  |  |  |  |
| C22H14O15 | -2.782 |  |  |  |  |  |  |  |
| C18H10O11 | -2.762 |  |  |  |  |  |  |  |
| C12H18O8 | -2.759 | x |  |  |  |  |  |  |
| C23H16O14 | -2.734 |  |  |  |  |  |  |  |
| C23H20O16 | -2.728 |  |  |  |  |  |  |  |
| C10H10O8 | -2.719 |  |  |  |  |  |  |  |
| C17H12O9 | -2.717 |  | x |  |  |  |  |  |
| C23H16O15 | -2.710 |  |  |  |  |  |  |  |
| C19H16O10 | -2.676 |  | x |  |  |  |  |  |
| C22H14O13 | -2.670 |  |  |  |  |  |  |  |
| C18H24O12 | -2.668 | x |  |  |  |  |  |  |
| C13H12O12 | -2.665 |  |  |  |  |  |  |  |
| C19H24O12 | -2.656 | x |  |  |  |  |  |  |
| C22H24O14 | -2.652 |  | x |  |  |  |  |  |
| C23H22O14 | -2.646 |  | x |  |  |  |  |  |
| C22H22O16 | -2.645 |  |  |  |  |  |  |  |
| C21H22O12 | -2.645 |  |  |  |  |  |  |  |
| C21H12O13 | -2.644 |  |  |  |  |  |  |  |
| C20H20O16 | -2.632 |  |  |  |  |  |  |  |
| C16H12O8 | -2.609 |  | x |  |  |  |  |  |
| C11H12O10 | -2.563 |  |  |  |  |  |  |  |
| C11H10O10 | -2.539 |  |  |  |  |  |  |  |
| C21H24O12 | -2.523 | x |  |  |  |  |  |  |
| C12H16O10 | -2.503 |  |  |  |  |  |  |  |
| C18H24O11 | -2.501 | x |  |  |  |  |  |  |
| C20H14O11 | -2.464 |  | x |  |  |  |  |  |
| C19H18O10 | -2.442 |  |  |  |  |  |  |  |
| C24H20O15 | -2.437 |  |  |  |  |  |  |  |
| C19H24O13 | -2.434 |  |  |  |  |  |  |  |
| C24H18O15 | -2.429 |  |  |  |  |  |  |  |
| C22H24O15 | -2.408 |  | x |  |  |  |  |  |
| C13H16O8 | -2.366 |  |  |  |  |  |  |  |
| C21H26O13 | -2.361 | x |  |  |  |  |  |  |
| C23H16O16 | -2.352 |  |  |  |  |  |  |  |
| C21H14O12 | -2.321 |  | x |  |  |  |  |  |
| C23H20O13 | -2.304 |  | x |  |  |  |  |  |
| C23H22O16 | -2.293 |  |  |  |  |  |  |  |
| C15H8O9 | -2.286 |  | x |  |  |  |  |  |
| C23H18O13 | -2.276 |  | x |  |  |  |  |  |
| C22H24O13 | -2.274 |  |  |  |  |  |  |  |
| C23H24O14 | -2.264 |  | x |  |  |  |  |  |
| C17H18O9 | -2.261 |  |  |  |  |  |  |  |
| C23H24O15 | -2.253 |  |  |  |  |  |  |  |
| C24H20O16 | -2.250 |  |  |  |  |  |  |  |
| C19H22O11 | -2.237 | x |  |  |  |  |  |  |
| C19H14O10 | -2.234 |  | x |  |  |  |  |  |
| C14H10O7 | -2.227 |  | x |  |  |  |  |  |
| C21H24O15 | -2.174 |  | x |  |  |  |  |  |
| C12H12O6 | -2.169 |  |  |  |  |  |  |  |
| C24H22O15 | -2.167 |  |  |  |  |  |  |  |
| C14H8O8 | -2.158 |  | x |  |  |  |  |  |
| C16H8O11 | -2.156 |  |  |  |  |  |  |  |
| C12H14O6 | -2.150 | x |  |  |  |  |  |  |
| C24H18O16 | -2.117 |  |  |  |  |  |  |  |
| C17H20O14 | -2.114 |  |  |  |  |  |  |  |
| C10H8O7 | -2.104 |  |  |  |  |  |  |  |
| C23H16O13 | -2.100 |  |  |  |  |  |  |  |
| C23H20O17 | -2.066 |  |  |  |  |  |  |  |
| C23H22O13 | -2.063 |  | x |  |  |  |  |  |
| C13H14O12 | -2.053 |  |  |  |  |  |  |  |
| C13H8O7 | -2.049 |  | x |  |  |  |  |  |
| C12H10O6 | -2.044 |  |  |  |  |  |  |  |
| C21H22O16 | -2.041 |  |  |  |  |  |  |  |
| C24H22O16 | -2.041 |  |  |  |  |  |  |  |
| C23H18O17 | -2.035 |  |  |  |  |  |  |  |
| C21H26O12 | -2.034 | x |  |  |  |  |  |  |
| C22H20O12 | -2.020 |  | x |  |  |  |  |  |
| C10H14O6 | -2.018 | x |  |  |  |  |  |  |
| C24H16O15 | -2.009 |  |  |  |  |  |  |  |
| C18H22O10 | -2.008 |  |  |  |  |  |  |  |
| C18H18O9 | -2.002 |  |  |  |  |  |  |  |
| C12H14O11 | -1.996 |  |  |  |  |  |  |  |
| C18H22O14 | -1.994 |  |  |  |  |  |  |  |
| C21H26O14 | -1.967 |  | x |  |  |  |  |  |
| C21H18O17 | -1.938 |  |  |  |  |  |  |  |
| C23H14O14 | -1.933 |  |  |  |  |  |  |  |
| C15H22O10 | -1.928 | x |  |  |  |  |  |  |
| C15H14O7 | -1.920 |  |  |  |  |  |  |  |
| C22H16O12 | -1.918 |  | x |  |  |  |  |  |
| C17H22O13 | -1.913 |  | x |  |  |  |  |  |
| C20H12O11 | -1.898 |  |  |  |  |  |  |  |
| C12H8O7 | -1.898 |  |  |  |  |  |  |  |
| C18H16O9 | -1.890 |  | x |  |  |  |  |  |
| C15H12O7 | -1.888 |  |  |  |  |  |  |  |
| C19H24O11 | -1.885 | x |  |  |  |  |  |  |
| C19H22O15 | -1.883 |  |  |  |  |  |  |  |
| C19H10O11 | -1.880 |  |  |  |  |  |  |  |
| C22H26O14 | -1.866 |  |  |  |  |  |  |  |
| C24H18O14 | -1.862 |  |  |  |  |  |  |  |
| C17H24O10 | -1.845 | x |  |  |  |  |  |  |
| C22H18O12 | -1.843 |  | x |  |  |  |  |  |
| C24H20O14 | -1.837 |  |  |  |  |  |  |  |
| C18H20O15 | -1.833 |  |  |  |  |  |  |  |
| C24H22O14 | -1.814 |  |  |  |  |  |  |  |
| C16H20O13 | -1.809 |  |  |  |  |  |  |  |
| C10H10O9 | -1.793 |  |  |  |  |  |  |  |
| C17H10O9 | -1.756 |  | x |  |  |  |  |  |
| C15H18O13 | -1.751 |  |  |  |  |  |  |  |
| C21H12O12 | -1.734 |  |  |  |  |  |  |  |
| C23H24O16 | -1.732 |  |  |  |  |  |  |  |
| C15H20O12 | -1.724 |  |  |  |  |  |  |  |
| C23H26O15 | -1.724 |  | x |  |  |  |  |  |
| C22H24O16 | -1.723 |  |  |  |  |  |  |  |
| C22H26O13 | -1.719 | x |  |  |  |  |  |  |
| C18H10O10 | -1.712 |  |  |  |  |  |  |  |
| C22H22O12 | -1.711 |  |  |  |  |  |  |  |
| C23H24O13 | -1.698 |  |  |  |  |  |  |  |
| C20H24O11 | -1.697 | x |  |  |  |  |  |  |
| C24H24O15 | -1.690 |  |  |  |  |  |  |  |
| C23H22O17 | -1.689 |  |  |  |  |  |  |  |
| C20H24O15 | -1.685 |  |  |  |  |  |  |  |
| C23H26O14 | -1.682 |  |  |  |  |  |  |  |
| C21H20O11 | -1.680 |  |  |  |  |  |  |  |
| C13H18O7 | -1.677 | x |  |  |  |  |  |  |
| C16H8O9 | -1.676 |  |  |  |  |  |  |  |
| C10H10O6 | -1.671 |  |  |  |  |  |  |  |
| C17H24O11 | -1.664 | x |  |  |  |  |  |  |
| C9H10O7 | -1.661 |  |  |  |  |  |  |  |
| C20H22O11 | -1.654 |  |  |  |  |  |  |  |
| C15H22O9 | -1.652 | x |  |  |  |  |  |  |
| C21H18O11 | -1.625 |  | x |  |  |  |  |  |
| C15H20O9 | -1.625 |  |  |  |  |  |  |  |
| C16H22O12 | -1.615 |  |  |  |  |  |  |  |
| C10H12O6 | -1.608 |  |  |  |  |  |  |  |
| C20H26O13 | -1.608 |  |  |  |  |  |  |  |
| C20H26O12 | -1.607 | x |  |  |  |  |  |  |
| C18H24O13 | -1.606 |  |  |  |  |  |  |  |
| C19H12O10 | -1.572 |  |  |  |  |  |  |  |
| C18H14O9 | -1.560 |  | x |  |  |  |  |  |
| C22H14O12 | -1.552 |  |  |  |  |  |  |  |
| C10H12O9 | -1.545 |  |  |  |  |  |  |  |
| C21H16O11 | -1.539 |  | x |  |  |  |  |  |
| C18H12O9 | -1.535 |  | x |  |  |  |  |  |
| C24H16O14 | -1.529 |  |  |  |  |  |  |  |
| C25H22O16 | -1.523 |  |  |  |  |  |  |  |
| C24H24O16 | -1.523 |  |  |  |  |  |  |  |
| C16H10O8 | -1.521 |  | x |  |  |  |  |  |
| C11H16O7 | -1.516 | x |  |  |  |  |  |  |
| C24H24O14 | -1.511 |  | x |  |  |  |  |  |
| C25H20O16 | -1.510 |  |  |  |  |  |  |  |
| C22H24O12 | -1.497 | x |  |  |  |  |  |  |
| C22H26O12 | -1.496 | x |  |  |  |  |  |  |
| C25H22O15 | -1.490 |  |  |  |  |  |  |  |
| C19H20O10 | -1.489 |  |  |  |  |  |  |  |
| C22H26O15 | -1.471 |  | x |  |  |  |  |  |
| C11H12O5 | -1.461 | x |  |  |  |  |  |  |
| C23H14O13 | -1.460 |  |  |  |  |  |  |  |
| C25H20O15 | -1.455 |  |  |  |  |  |  |  |
| C14H12O6 | -1.447 |  |  |  |  |  |  |  |
| C23H20O12 | -1.442 |  | x |  |  |  |  |  |
| C12H18O9 | -1.433 |  |  |  |  |  |  |  |
| C10H8O8 | -1.428 |  |  |  |  |  |  |  |
| C19H26O12 | -1.424 | x |  |  |  |  |  |  |
| C22H22O17 | -1.422 |  |  |  |  |  |  |  |
| C24H22O13 | -1.398 |  | x |  |  |  |  |  |
| C20H20O10 | -1.394 |  |  |  |  |  |  |  |
| C12H16O5 | -1.385 | x |  |  |  |  |  |  |
| C13H20O9 | -1.379 | x |  |  |  |  |  |  |
| C13H16O5 | -1.377 | x |  |  |  |  |  |  |
| C21H22O11 | -1.371 |  |  |  |  |  |  |  |
| C18H24O10 | -1.357 | x |  |  |  |  |  |  |
| C25H18O15 | -1.347 |  |  |  |  |  |  |  |
| C25H24O15 | -1.347 |  |  |  |  |  |  |  |
| C10H14O8 | -1.339 |  |  |  |  |  |  |  |
| C19H24O14 | -1.337 |  |  |  |  |  |  |  |
| C25H20O14 | -1.327 |  |  |  |  |  |  |  |
| C21H14O11 | -1.321 |  |  |  |  |  |  |  |
| C17H12O8 | -1.318 |  | x |  |  |  |  |  |
| C25H22O17 | -1.316 |  |  |  |  |  |  |  |
| C20H16O10 | -1.312 |  | x |  |  |  |  |  |
| C23H18O12 | -1.309 |  | x |  |  |  |  |  |
| C11H12O6 | -1.309 |  |  |  |  |  |  |  |
| C22H28O13 | -1.304 | x |  |  |  |  |  |  |
| C23H22O12 | -1.287 |  | x |  |  |  |  |  |
| C21H28O13 | -1.276 |  |  |  |  |  |  |  |
| C9H12O7 | -1.255 |  |  |  |  |  |  |  |
| C25H22O14 | -1.253 |  |  |  |  |  |  |  |
| C9H10O6 | -1.249 |  |  |  |  |  |  |  |
| C20H18O10 | -1.247 |  |  |  |  |  |  |  |
| C24H20O13 | -1.241 |  |  |  |  |  |  |  |
| C17H16O8 | -1.234 |  |  |  |  |  |  |  |
| C17H14O8 | -1.230 |  | x |  |  |  |  |  |
| C24H24O13 | -1.218 |  | x |  |  |  |  |  |
| C18H10O9 | -1.213 |  |  |  |  |  |  |  |
| C9H12O6 | -1.209 |  |  |  |  |  |  |  |
| C23H24O17 | -1.204 |  |  |  |  |  |  |  |
| C24H18O13 | -1.202 |  |  |  |  |  |  |  |
| C23H26O13 | -1.200 |  |  |  |  |  |  |  |
| C11H6O7 | -1.199 |  |  |  |  |  |  |  |
| C12H8O6 | -1.190 |  |  |  |  |  |  |  |
| C23H28O14 | -1.183 |  |  |  |  |  |  |  |
| C23H16O12 | -1.181 |  |  |  |  |  |  |  |
| C25H18O14 | -1.179 |  |  |  |  |  |  |  |
| C14H8O7 | -1.179 |  | x |  |  |  |  |  |
| C12H6O9 | -1.177 |  |  |  |  |  |  |  |
| C15H10O7 | -1.171 |  | x |  |  |  |  |  |
| C21H26O15 | -1.171 |  |  |  |  |  |  |  |
| C24H26O16 | -1.169 |  |  |  |  |  |  |  |
| C25H24O16 | -1.168 |  |  |  |  |  |  |  |
| C24H26O15 | -1.148 |  | x |  |  |  |  |  |
| C24H26O14 | -1.146 |  | x |  |  |  |  |  |
| C11H14O7 | -1.139 |  |  |  |  |  |  |  |
| C26H22O16 | -1.131 |  |  |  |  |  |  |  |
| C24H24O17 | -1.130 |  |  |  |  |  |  |  |
| C20H26O14 | -1.128 |  | x |  |  |  |  |  |
| C11H16O9 | -1.127 |  |  |  |  |  |  |  |
| C21H28O12 | -1.125 | x |  |  |  |  |  |  |
| C15H22O11 | -1.106 |  |  |  |  |  |  |  |
| C14H20O11 | -1.094 |  |  |  |  |  |  |  |
| C23H26O16 | -1.094 |  |  |  |  |  |  |  |
| C24H16O13 | -1.092 |  |  |  |  |  |  |  |
| C25H24O14 | -1.088 |  |  |  |  |  |  |  |
| C22H28O14 | -1.080 |  |  |  |  |  |  |  |
| C20H14O10 | -1.080 |  |  |  |  |  |  |  |
| C15H16O8 | -1.077 |  | x |  |  |  |  |  |
| C23H28O15 | -1.076 |  |  |  |  |  |  |  |
| C25H24O17 | -1.054 |  |  |  |  |  |  |  |
| C15H8O8 | -1.051 |  | x |  |  |  |  |  |
| C26H24O16 | -1.050 |  |  |  |  |  |  |  |
| C25H26O15 | -1.000 |  | x |  |  |  |  |  |
| C19H14O9 | -0.990 |  | x |  |  |  |  |  |
| C22H26O16 | -0.986 |  |  |  |  |  |  |  |
| C24H28O14 | -0.985 |  |  |  |  |  |  |  |
| C16H12O7 | -0.985 |  | x |  |  |  |  |  |
| C17H24O12 | -0.984 |  |  |  |  |  |  |  |
| C19H26O11 | -0.983 | x |  |  |  |  |  |  |
| C26H22O15 | -0.983 |  |  |  |  |  |  |  |
| C19H26O13 | -0.956 |  |  |  |  |  |  |  |
| C13H20O8 | -0.950 | x |  |  |  |  |  |  |
| C13H20O6 | -0.948 | x |  |  |  |  |  |  |
| C25H26O16 | -0.941 |  |  |  |  |  |  |  |
| C23H24O12 | -0.938 |  |  |  |  |  |  |  |
| C16H24O9 | -0.926 | x |  |  |  |  |  |  |
| C16H16O8 | -0.923 |  |  |  |  |  |  |  |
| C10H8O6 | -0.921 |  |  |  |  |  |  |  |
| C24H26O13 | -0.907 |  |  |  |  |  |  |  |
| C26H20O15 | -0.904 |  |  |  |  |  |  |  |
| C16H24O10 | -0.900 | x |  |  |  |  |  |  |
| C17H10O8 | -0.899 |  |  |  |  |  |  |  |
| C19H12O9 | -0.899 |  |  |  |  |  |  |  |
| C24H28O15 | -0.896 |  |  |  |  |  |  |  |
| C22H20O11 | -0.892 |  | x |  |  |  |  |  |
| C19H18O9 | -0.886 |  |  |  |  |  |  |  |
| C14H20O5 | -0.880 | x |  |  |  |  |  |  |
| C21H24O11 | -0.880 | x |  |  |  |  |  |  |
| C13H6O8 | -0.876 |  |  |  |  |  |  |  |
| C19H16O9 | -0.870 |  | x |  |  |  |  |  |
| C26H24O15 | -0.868 |  |  |  |  |  |  |  |
| C21H26O11 | -0.862 | x |  |  |  |  |  |  |
| C16H8O8 | -0.861 |  |  |  |  |  |  |  |
| C11H16O5 | -0.860 | x |  |  |  |  |  |  |
| C14H14O7 | -0.854 |  |  |  |  |  |  |  |
| C14H22O9 | -0.845 | x |  |  |  |  |  |  |
| C25H26O14 | -0.842 |  | x |  |  |  |  |  |
| C22H16O11 | -0.832 |  |  |  |  |  |  |  |
| C14H10O6 | -0.827 |  |  |  |  |  |  |  |
| C18H14O8 | -0.824 |  | x |  |  |  |  |  |
| C23H28O13 | -0.823 | x |  |  |  |  |  |  |
| C16H10O7 | -0.823 |  |  |  |  |  |  |  |
| C22H28O12 | -0.822 | x |  |  |  |  |  |  |
| C25H20O13 | -0.806 |  |  |  |  |  |  |  |
| C23H26O12 | -0.804 | x |  |  |  |  |  |  |
| C26H26O16 | -0.803 |  |  |  |  |  |  |  |
| C20H12O10 | -0.797 |  |  |  |  |  |  |  |
| C10H12O5 | -0.795 |  |  |  |  |  |  |  |
| C22H18O11 | -0.795 |  | x |  |  |  |  |  |
| C17H14O7 | -0.791 |  |  |  |  |  |  |  |
| C11H10O5 | -0.777 |  |  |  |  |  |  |  |
| C18H16O8 | -0.774 |  |  |  |  |  |  |  |
| C20H28O12 | -0.773 | x |  |  |  |  |  |  |
| C21H28O14 | -0.769 |  |  |  |  |  |  |  |
| C25H28O15 | -0.769 |  |  |  |  |  |  |  |
| C13H10O6 | -0.769 |  |  |  |  |  |  |  |
| C24H28O16 | -0.755 |  |  |  |  |  |  |  |
| C24H28O13 | -0.750 |  |  |  |  |  |  |  |
| C22H22O11 | -0.748 |  |  |  |  |  |  |  |
| C25H26O17 | -0.747 |  |  |  |  |  |  |  |
| C16H18O9 | -0.735 |  |  |  |  |  |  |  |
| C15H12O6 | -0.733 |  |  |  |  |  |  |  |
| C15H8O7 | -0.730 |  |  |  |  |  |  |  |
| C22H14O11 | -0.718 |  |  |  |  |  |  |  |
| C20H26O11 | -0.718 | x |  |  |  |  |  |  |
| C10H16O7 | -0.712 |  |  |  |  |  |  |  |
| C24H20O12 | -0.712 |  |  |  |  |  |  |  |
| C24H26O17 | -0.705 |  |  |  |  |  |  |  |
| C24H18O12 | -0.700 |  |  |  |  |  |  |  |
| C18H26O12 | -0.699 |  |  |  |  |  |  |  |
| C26H20O14 | -0.695 |  |  |  |  |  |  |  |
| C17H16O7 | -0.694 |  |  |  |  |  |  |  |
| C22H30O12 | -0.692 | x |  |  |  |  |  |  |
| C22H28O15 | -0.673 |  |  |  |  |  |  |  |
| C11H8O6 | -0.669 |  |  |  |  |  |  |  |
| C25H24O18 | -0.668 |  |  |  |  |  |  |  |
| C12H14O5 | -0.668 | x |  |  |  |  |  |  |
| C24H24O12 | -0.666 |  | x |  |  |  |  |  |
| C22H30O13 | -0.664 | x |  |  |  |  |  |  |
| C26H26O15 | -0.661 |  |  |  |  |  |  |  |
| C10H10O5 | -0.653 |  | x |  |  |  |  |  |
| C23H30O13 | -0.652 |  |  |  |  |  |  |  |
| C21H20O10 | -0.651 |  |  |  |  |  |  |  |
| C26H24O14 | -0.651 |  |  |  |  |  |  |  |
| C24H22O12 | -0.649 |  | x |  |  |  |  |  |
| C18H26O11 | -0.645 | x |  |  |  |  |  |  |
| C18H26O10 | -0.643 | x |  |  |  |  |  |  |
| C13H10O5 | -0.643 |  |  |  |  |  |  |  |
| C26H26O17 | -0.642 |  |  |  |  |  |  |  |
| C22H28O11 | -0.635 | x |  |  |  |  |  |  |
| C25H26O13 | -0.633 |  | x |  |  |  |  |  |
| C23H20O11 | -0.632 |  | x |  |  |  |  |  |
| C16H24O11 | -0.616 |  |  |  |  |  |  |  |
| C14H14O6 | -0.607 |  |  |  |  |  |  |  |
| C25H22O13 | -0.606 |  |  |  |  |  |  |  |
| C26H22O14 | -0.596 |  |  |  |  |  |  |  |
| C21H14O10 | -0.593 |  |  |  |  |  |  |  |
| C25H24O13 | -0.592 |  | x |  |  |  |  |  |
| C23H18O11 | -0.591 |  |  |  |  |  |  |  |
| C23H28O12 | -0.586 | x |  |  |  |  |  |  |
| C20H22O10 | -0.584 | x |  |  |  |  |  |  |
| C11H10O6 | -0.583 |  |  |  |  |  |  |  |
| C10H16O6 | -0.583 |  |  |  |  |  |  |  |
| C23H30O12 | -0.583 | x |  |  |  |  |  |  |
| C22H24O11 | -0.581 | x |  |  |  |  |  |  |
| C25H28O14 | -0.579 |  |  |  |  |  |  |  |
| C18H12O8 | -0.572 |  |  |  |  |  |  |  |
| C27H22O15 | -0.571 |  |  |  |  |  |  |  |
| C25H28O16 | -0.570 |  |  |  |  |  |  |  |
| C21H16O10 | -0.556 |  | x |  |  |  |  |  |
| C21H28O11 | -0.554 | x |  |  |  |  |  |  |
| C26H28O15 | -0.549 |  |  |  |  |  |  |  |
| C9H12O5 | -0.549 |  |  |  |  |  |  |  |
| C19H22O10 | -0.549 | x |  |  |  |  |  |  |
| C26H28O16 | -0.547 |  |  |  |  |  |  |  |
| C17H10O7 | -0.539 |  |  |  |  |  |  |  |
| C24H30O13 | -0.537 |  |  |  |  |  |  |  |
| C10H14O5 | -0.535 |  |  |  |  |  |  |  |
| C20H18O9 | -0.535 |  |  |  |  |  |  |  |
| C26H22O13 | -0.529 |  |  |  |  |  |  |  |
| C21H18O10 | -0.525 |  | x |  |  |  |  |  |
| C16H14O7 | -0.516 |  |  |  |  |  |  |  |
| C23H16O11 | -0.514 |  |  |  |  |  |  |  |
| C20H28O13 | -0.513 |  |  |  |  |  |  |  |
| C11H16O6 | -0.513 |  |  |  |  |  |  |  |
| C10H8O5 | -0.510 |  |  |  |  |  |  |  |
| C20H28O11 | -0.509 | x |  |  |  |  |  |  |
| C22H30O14 | -0.508 |  |  |  |  |  |  |  |
| C24H30O15 | -0.507 |  |  |  |  |  |  |  |
| C25H30O15 | -0.506 |  |  |  |  |  |  |  |
| C23H30O14 | -0.504 |  |  |  |  |  |  |  |
| C24H16O12 | -0.503 |  |  |  |  |  |  |  |
| C11H12O4 | -0.500 |  |  |  |  |  |  |  |
| C9H8O6 | -0.499 |  |  |  |  |  |  |  |
| C27H26O15 | -0.498 |  |  |  |  |  |  |  |
| C23H22O11 | -0.494 |  |  |  |  |  |  |  |
| C13H14O6 | -0.486 |  |  |  |  |  |  |  |
| C20H14O9 | -0.486 |  |  |  |  |  |  |  |
| C15H20O5 | -0.484 | x |  |  |  |  |  |  |
| C26H24O13 | -0.484 |  |  |  |  |  |  |  |
| C27H24O15 | -0.483 |  |  |  |  |  |  |  |
| C19H24O10 | -0.477 | x |  |  |  |  |  |  |
| C21H22O10 | -0.473 | x |  |  |  |  |  |  |
| C26H28O17 | -0.466 |  |  |  |  |  |  |  |
| C26H26O14 | -0.461 |  |  |  |  |  |  |  |
| C24H30O14 | -0.460 |  |  |  |  |  |  |  |
| C21H30O12 | -0.459 | x |  |  |  |  |  |  |
| C26H20O13 | -0.452 |  |  |  |  |  |  |  |
| C27H28O16 | -0.446 |  |  |  |  |  |  |  |
| C15H20O8 | -0.442 | x |  |  |  |  |  |  |
| C15H18O5 | -0.437 | x |  |  |  |  |  |  |
| C23H30O11 | -0.434 | x |  |  |  |  |  |  |
| C11H18O7 | -0.429 |  |  |  |  |  |  |  |
| C15H22O8 | -0.429 | x |  |  |  |  |  |  |
| C24H26O12 | -0.427 | x |  |  |  |  |  |  |
| C13H14O5 | -0.426 |  |  |  |  |  |  |  |
| C23H30O15 | -0.418 |  |  |  |  |  |  |  |
| C17H18O7 | -0.416 | x |  |  |  |  |  |  |
| C15H10O6 | -0.413 |  |  |  |  |  |  |  |
| C14H16O5 | -0.413 | x |  |  |  |  |  |  |
| C16H14O6 | -0.413 | x |  |  |  |  |  |  |
| C27H24O14 | -0.413 |  |  |  |  |  |  |  |
| C20H16O9 | -0.412 |  | x |  |  |  |  |  |
| C14H18O4 | -0.410 | x |  |  |  |  |  |  |
| C27H26O14 | -0.404 |  |  |  |  |  |  |  |
| C24H24O11 | -0.403 |  |  |  |  |  |  |  |
| C20H20O9 | -0.402 | x |  |  |  |  |  |  |
| C21H24O10 | -0.401 | x |  |  |  |  |  |  |
| C16H16O7 | -0.399 |  |  |  |  |  |  |  |
| C17H24O9 | -0.399 | x |  |  |  |  |  |  |
| C12H14O4 | -0.395 | x |  |  |  |  |  |  |
| C13H8O6 | -0.389 |  | x |  |  |  |  |  |
| C13H12O5 | -0.389 |  |  |  |  |  |  |  |
| C25H20O12 | -0.386 |  |  |  |  |  |  |  |
| C22H30O11 | -0.379 | x |  |  |  |  |  |  |
| C19H16O8 | -0.377 |  |  |  |  |  |  |  |
| C12H18O5 | -0.371 | x |  |  |  |  |  |  |
| C23H24O11 | -0.368 | x |  |  |  |  |  |  |
| C12H10O5 | -0.368 |  |  |  |  |  |  |  |
| C11H18O6 | -0.366 |  |  |  |  |  |  |  |
| C19H14O8 | -0.364 |  |  |  |  |  |  |  |
| C26H26O13 | -0.363 |  |  |  |  |  |  |  |
| C27H28O15 | -0.360 |  |  |  |  |  |  |  |
| C11H18O5 | -0.360 |  |  |  |  |  |  |  |
| C14H20O4 | -0.359 | x |  |  |  |  |  |  |
| C25H30O16 | -0.353 |  |  |  |  |  |  |  |
| C24H20O11 | -0.349 |  |  |  |  |  |  |  |
| C25H24O12 | -0.349 |  |  |  |  |  |  |  |
| C22H16O10 | -0.345 |  |  |  |  |  |  |  |
| C27H22O14 | -0.344 |  |  |  |  |  |  |  |
| C25H28O13 | -0.344 |  |  |  |  |  |  |  |
| C19H28O12 | -0.342 |  |  |  |  |  |  |  |
| C13H16O6 | -0.341 |  |  |  |  |  |  |  |
| C25H32O13 | -0.341 | x |  |  |  |  |  |  |
| C19H12O8 | -0.340 |  |  |  |  |  |  |  |
| C26H28O14 | -0.339 |  |  |  |  |  |  |  |
| C21H30O13 | -0.334 |  |  |  |  |  |  |  |
| C26H30O16 | -0.331 |  |  |  |  |  |  |  |
| C17H26O11 | -0.322 |  |  |  |  |  |  |  |
| C27H28O14 | -0.317 |  |  |  |  |  |  |  |
| C24H22O11 | -0.310 |  |  |  |  |  |  |  |
| C22H18O10 | -0.309 |  |  |  |  |  |  |  |
| C12H12O5 | -0.305 | x |  |  |  |  |  |  |
| C15H14O5 | -0.304 |  |  |  |  |  |  |  |
| C14H16O4 | -0.303 | x |  |  |  |  |  |  |
| C25H30O14 | -0.302 |  |  |  |  |  |  |  |
| C17H12O7 | -0.299 |  | x |  |  |  |  |  |
| C25H32O15 | -0.297 |  |  |  |  |  |  |  |
| C15H12O5 | -0.294 |  |  |  |  |  |  |  |
| C24H32O14 | -0.289 |  |  |  |  |  |  |  |
| C26H30O14 | -0.287 |  |  |  |  |  |  |  |
| C23H26O11 | -0.287 | x |  |  |  |  |  |  |
| C16H22O9 | -0.284 | x |  |  |  |  |  |  |
| C14H22O5 | -0.283 | x |  |  |  |  |  |  |
| C23H32O12 | -0.282 | x |  |  |  |  |  |  |
| C14H12O5 | -0.280 |  |  |  |  |  |  |  |
| C19H28O11 | -0.280 | x |  |  |  |  |  |  |
| C26H28O13 | -0.277 |  |  |  |  |  |  |  |
| C25H26O12 | -0.275 |  | x |  |  |  |  |  |
| C18H22O5 | -0.272 | x |  |  |  |  |  |  |
| C22H20O10 | -0.268 |  |  |  |  |  |  |  |
| C26H30O15 | -0.267 |  |  |  |  |  |  |  |
| C12H20O7 | -0.265 | x |  |  |  |  |  |  |
| C23H32O14 | -0.262 |  |  |  |  |  |  |  |
| C28H28O16 | -0.259 |  |  |  |  |  |  |  |
| C11H8O5 | -0.256 |  |  |  |  |  |  |  |
| C16H24O7 | -0.255 | x |  |  |  |  |  |  |
| C16H22O4 | -0.254 | x |  |  |  |  |  |  |
| C18H12O7 | -0.250 |  |  |  |  |  |  |  |
| C27H30O15 | -0.244 |  |  |  |  |  |  |  |
| C18H20O9 | -0.242 |  |  |  |  |  |  |  |
| C17H16O6 | -0.242 | x |  |  |  |  |  |  |
| C14H22O8 | -0.240 | x |  |  |  |  |  |  |
| C23H32O13 | -0.238 |  |  |  |  |  |  |  |
| C22H32O12 | -0.238 | x |  |  |  |  |  |  |
| C24H30O12 | -0.234 | x |  |  |  |  |  |  |
| C11H16O4 | -0.232 | x |  |  |  |  |  |  |
| C12H8O5 | -0.231 |  |  |  |  |  |  |  |
| C25H22O11 | -0.228 |  |  |  |  |  |  |  |
| C13H12O4 | -0.224 |  |  |  |  |  |  |  |
| C13H12O6 | -0.224 |  |  |  |  |  |  |  |
| C24H32O13 | -0.221 |  |  |  |  |  |  |  |
| C21H30O11 | -0.219 | x |  |  |  |  |  |  |
| C24H28O12 | -0.213 | x |  |  |  |  |  |  |
| C17H26O10 | -0.212 | x |  |  |  |  |  |  |
| C12H20O5 | -0.211 |  |  |  |  |  |  |  |
| C27H30O16 | -0.208 |  |  |  |  |  |  |  |
| C25H30O13 | -0.202 |  |  |  |  |  |  |  |
| C16H14O5 | -0.201 |  |  |  |  |  |  |  |
| C25H32O14 | -0.200 |  |  |  |  |  |  |  |
| C20H16O8 | -0.199 |  |  |  |  |  |  |  |
| C18H14O7 | -0.199 |  |  |  |  |  |  |  |
| C21H18O9 | -0.197 |  | x |  |  |  |  |  |
| C12H16O4 | -0.192 | x |  |  |  |  |  |  |
| C26H26O12 | -0.190 |  |  |  |  |  |  |  |
| C25H28O12 | -0.188 |  |  |  |  |  |  |  |
| C16H10O6 | -0.187 |  |  |  |  |  |  |  |
| C18H18O6 | -0.186 | x |  |  |  |  |  |  |
| C12H18O4 | -0.185 | x |  |  |  |  |  |  |
| C11H14O5 | -0.184 |  |  |  |  |  |  |  |
| C10H12O4 | -0.179 |  |  |  |  |  |  |  |
| C27H28O13 | -0.178 |  |  |  |  |  |  |  |
| C16H18O4 | -0.177 |  |  |  |  |  |  |  |
| C13H18O3 | -0.176 |  |  |  |  |  |  |  |
| C13H22O6 | -0.175 |  |  |  |  |  |  |  |
| C22H32O11 | -0.175 | x |  |  |  |  |  |  |
| C10H14O4 | -0.171 |  |  |  |  |  |  |  |
| C19H18O8 | -0.169 | x |  |  |  |  |  |  |
| C12H12O4 | -0.167 |  |  |  |  |  |  |  |
| C20H30O12 | -0.164 |  |  |  |  |  |  |  |
| C23H22O10 | -0.161 |  |  |  |  |  |  |  |
| C15H16O5 | -0.161 | x |  |  |  |  |  |  |
| C15H24O9 | -0.160 | x |  |  |  |  |  |  |
| C16H12O6 | -0.159 |  |  |  |  |  |  |  |
| C20H18O8 | -0.156 |  |  |  |  |  |  |  |
| C16H20O4 | -0.156 |  |  |  |  |  |  |  |
| C25H24O11 | -0.155 |  |  |  |  |  |  |  |
| C17H12O6 | -0.153 |  |  |  |  |  |  |  |
| C14H22O4 | -0.150 |  |  |  |  |  |  |  |
| C26H28O12 | -0.148 |  |  |  |  |  |  |  |
| C27H30O14 | -0.145 |  |  |  |  |  |  |  |
| C24H26O11 | -0.144 |  |  |  |  |  |  |  |
| C24H24O10 | -0.141 |  |  |  |  |  |  |  |
| C16H24O4 | -0.138 |  |  |  |  |  |  |  |
| C25H34O15 | -0.134 |  |  |  |  |  |  |  |
| C11H14O4 | -0.133 | x |  |  |  |  |  |  |
| C28H26O14 | -0.132 |  |  |  |  |  |  |  |
| C22H22O10 | -0.131 |  |  |  |  |  |  |  |
| C20H30O11 | -0.129 | x |  |  |  |  |  |  |
| C18H24O5 | -0.126 | x |  |  |  |  |  |  |
| C21H20O9 | -0.125 |  |  |  |  |  |  |  |
| C26H32O16 | -0.123 |  |  |  |  |  |  |  |
| C25H26O11 | -0.123 |  |  |  |  |  |  |  |
| C19H16O7 | -0.122 |  |  |  |  |  |  |  |
| C28H30O14 | -0.121 |  |  |  |  |  |  |  |
| C10H16O5 | -0.120 |  |  |  |  |  |  |  |
| C22H26O11 | -0.116 | x |  |  |  |  |  |  |
| C15H18O4 | -0.112 | x |  |  |  |  |  |  |
| C17H24O4 | -0.112 |  |  |  |  |  |  |  |
| C26H26O11 | -0.111 |  |  |  |  |  |  |  |
| C29H32O17 | -0.106 |  |  |  |  |  |  |  |
| C24H32O12 | -0.103 | x |  |  |  |  |  |  |
| C17H20O6 | -0.102 | x |  |  |  |  |  |  |
| C14H14O4 | -0.099 | x |  |  |  |  |  |  |
| C23H34O12 | -0.099 |  |  |  |  |  |  |  |
| C16H18O5 | -0.094 | x |  |  |  |  |  |  |
| C27H30O13 | -0.094 |  |  |  |  |  |  |  |
| C11H14O3 | -0.087 |  |  |  |  |  |  |  |
| C29H30O15 | -0.086 |  |  |  |  |  |  |  |
| C26H32O14 | -0.085 |  |  |  |  |  |  |  |
| C17H26O9 | -0.085 | x |  |  |  |  |  |  |
| C27H32O15 | -0.082 |  |  |  |  |  |  |  |
| C28H32O16 | -0.081 |  |  |  |  |  |  |  |
| C25H26O10 | -0.080 |  |  |  |  |  |  |  |
| C26H32O15 | -0.078 |  |  |  |  |  |  |  |
| C18H16O7 | -0.075 |  |  |  |  |  |  |  |
| C21H30O10 | -0.075 | x |  |  |  |  |  |  |
| C23H32O11 | -0.072 | x |  |  |  |  |  |  |
| C25H34O14 | -0.071 |  |  |  |  |  |  |  |
| C27H32O16 | -0.070 |  |  |  |  |  |  |  |
| C14H10O5 | -0.070 |  |  |  |  |  |  |  |
| C15H20O4 | -0.070 | x |  |  |  |  |  |  |
| C18H18O7 | -0.066 | x |  |  |  |  |  |  |
| C15H14O6 | -0.065 |  |  |  |  |  |  |  |
| C17H14O6 | -0.065 |  |  |  |  |  |  |  |
| C26H34O15 | -0.064 |  |  |  |  |  |  |  |
| C24H34O12 | -0.063 | x |  |  |  |  |  |  |
| C22H24O10 | -0.061 | x |  |  |  |  |  |  |
| C17H22O6 | -0.060 | x |  |  |  |  |  |  |
| C24H28O11 | -0.057 | x |  |  |  |  |  |  |
| C19H20O7 | -0.049 | x |  |  |  |  |  |  |
| C20H30O10 | -0.049 | x |  |  |  |  |  |  |
| C20H20O8 | -0.049 |  |  |  |  |  |  |  |
| C19H28O10 | -0.045 | x |  |  |  |  |  |  |
| C19H28O9 | -0.044 | x |  |  |  |  |  |  |
| C29H34O17 | -0.043 |  |  |  |  |  |  |  |
| C14H24O6 | -0.042 |  |  |  |  |  |  |  |
| C24H34O13 | -0.039 |  |  |  |  |  |  |  |
| C21H20O8 | -0.038 |  |  |  |  |  |  |  |
| C21H26O6 | -0.035 |  |  |  |  |  |  |  |
| C20H24O10 | -0.034 | x |  |  |  |  |  |  |
| C21H32O8 | -0.034 | x |  |  |  |  |  |  |
| C13H14O4 | -0.033 | x |  |  |  |  |  |  |
| C21H28O6 | -0.033 |  |  |  |  |  |  |  |
| C18H20O5 | -0.032 | x |  |  |  |  |  |  |
| C20H30O6 | -0.031 | x |  |  |  |  |  |  |
| C16H16O5 | -0.029 | x |  |  |  |  |  |  |
| C23H34O11 | -0.028 | x |  |  |  |  |  |  |
| C28H32O15 | -0.024 |  |  |  |  |  |  |  |
| C21H28O10 | -0.023 | x |  |  |  |  |  |  |
| C25H28O10 | -0.020 | x |  |  |  |  |  |  |
| C27H38O14 | -0.020 |  |  |  |  |  |  |  |
| C24H26O10 | -0.018 | x |  |  |  |  |  |  |
| C19H20O8 | -0.018 | x |  |  |  |  |  |  |
| C17H24O6 | -0.018 | x |  |  |  |  |  |  |
| C24H34O10 | -0.016 | x |  |  |  |  |  |  |
| C25H28O11 | -0.014 | x |  |  |  |  |  |  |
| C24H32O11 | -0.013 | x |  |  |  |  |  |  |
| C18H18O8 | -0.012 | x |  |  |  |  |  |  |
| C19H28O5 | -0.010 |  |  |  |  |  |  |  |
| C13H20O4 | -0.010 | x |  |  |  |  |  |  |
| C26H32O13 | -0.010 | x |  |  |  |  |  |  |
| C23H24O10 | -0.010 |  |  |  |  |  |  |  |
| C17H22O4 | -0.009 |  |  |  |  |  |  |  |
| C21H32O10 | -0.009 | x |  |  |  |  |  |  |
| C20H28O5 | -0.007 |  |  |  |  |  |  |  |
| C22H22O9 | -0.007 |  |  |  |  |  |  |  |
| C26H34O9 | -0.007 |  |  |  |  |  |  |  |
| C26H28O11 | -0.005 |  |  |  |  |  |  |  |
| C26H30O11 | -0.005 | x |  |  |  |  |  |  |
| C19H20O6 | -0.003 | x |  |  |  |  |  |  |
| C23H34O9 | -0.003 |  |  |  |  |  |  |  |
| C25H30O12 | -0.002 | x |  |  |  |  |  |  |

Table A6 CHO formulas present before and after NH2Cl and UV disinfection at Kvarnagården WTP and the change in relative abundance during the treatment as well as correlation with optical parameters

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Decrease** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |  | **Increase** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |
| C15H20O6 | -23.991 | x |  |  | C16H14O10 | 18.121 |  | x |
| C15H20O7 | -19.683 |  |  |  | C16H16O10 | 17.881 |  | x |
| C12H16O6 | -19.474 |  |  |  | C16H18O10 | 17.124 |  |  |
| C14H18O7 | -19.363 | x |  |  | C16H14O11 | 16.832 |  | x |
| C14H20O6 | -18.021 |  |  |  | C16H12O11 | 16.738 |  | x |
| C15H22O6 | -15.997 | x |  |  | C15H12O10 | 16.662 |  | x |
| C13H16O8 | -14.028 |  |  |  | C13H10O9 | 16.096 |  | x |
| C16H22O7 | -13.806 |  |  |  | C15H12O11 | 15.802 |  | x |
| C15H18O7 | -13.174 |  |  |  | C14H14O9 | 15.726 |  | x |
| C13H18O6 | -12.415 |  |  |  | C17H18O10 | 15.473 |  |  |
| C11H14O7 | -11.329 |  |  |  | C15H16O10 | 15.008 |  | x |
| C14H20O7 | -11.276 | x |  |  | C16H18O9 | 14.542 |  |  |
| C16H20O7 | -10.929 |  |  |  | C17H16O10 | 14.523 |  | x |
| C14H16O6 | -10.100 |  |  |  | C15H14O10 | 14.472 |  | x |
| C16H22O6 | -9.778 | x |  |  | C17H16O11 | 14.146 |  | x |
| C14H18O6 | -9.456 |  |  |  | C17H14O11 | 14.084 |  | x |
| C13H18O5 | -9.157 | x |  |  | C15H10O11 | 13.947 |  | x |
| C15H22O7 | -9.153 | x |  |  | C14H12O9 | 13.227 |  | x |
| C15H18O6 | -9.006 | x |  |  | C17H12O11 | 13.048 |  | x |
| C17H24O7 | -8.546 | x |  |  | C14H10O9 | 12.940 |  | x |
| C17H22O7 | -8.379 | x |  |  | C17H20O10 | 12.650 |  |  |
| C12H18O6 | -7.881 | x |  |  | C15H18O10 | 12.450 |  | x |
| C15H22O5 | -7.585 | x |  |  | C16H12O10 | 12.275 |  | x |
| C13H20O7 | -7.585 | x |  |  | C15H14O9 | 12.127 |  | x |
| C16H20O8 | -7.552 |  |  |  | C17H18O9 | 12.066 |  |  |
| C11H16O6 | -7.319 |  |  |  | C16H20O10 | 12.047 |  |  |
| C13H16O6 | -7.264 |  |  |  | C13H12O9 | 12.037 |  | x |
| C13H18O7 | -7.246 | x |  |  | C16H16O11 | 11.910 |  | x |
| C14H18O5 | -6.904 |  |  |  | C17H14O12 | 11.780 |  | x |
| C15H16O6 | -6.833 |  |  |  | C14H12O10 | 11.671 |  | x |
| C12H14O6 | -6.263 | x |  |  | C15H14O11 | 11.531 |  | x |
| C14H22O7 | -6.168 | x |  |  | C13H14O9 | 11.511 |  |  |
| C15H20O5 | -6.161 | x |  |  | C14H10O11 | 11.386 |  | x |
| C18H24O7 | -6.119 | x |  |  | C17H14O10 | 11.367 |  | x |
| C12H16O8 | -5.909 |  |  |  | C16H10O11 | 11.360 |  | x |
| C14H22O6 | -5.897 | x |  |  | C16H12O12 | 11.300 |  | x |
| C16H22O8 | -5.424 |  |  |  | C17H18O11 | 10.977 |  | x |
| C11H14O5 | -4.929 |  |  |  | C15H10O10 | 10.945 |  | x |
| C14H16O7 | -4.799 | x |  |  | C18H14O12 | 10.849 |  | x |
| C16H22O5 | -4.762 | x |  |  | C13H10O10 | 10.828 |  | x |
| C16H20O5 | -4.541 | x |  |  | C14H18O9 | 10.731 |  | x |
| C16H20O6 | -4.513 | x |  |  | C14H10O10 | 10.639 |  | x |
| C17H20O8 | -4.124 |  |  |  | C14H14O8 | 10.614 |  | x |
| C13H20O5 | -4.087 | x |  |  | C18H20O10 | 10.560 |  |  |
| C16H24O6 | -4.084 | x |  |  | C11H8O8 | 10.396 |  |  |
| C11H16O7 | -3.926 | x |  |  | C17H12O12 | 10.205 |  | x |
| C14H18O8 | -3.878 |  |  |  | C16H16O9 | 10.172 |  | x |
| C13H16O5 | -3.778 | x |  |  | C12H8O8 | 10.108 |  |  |
| C17H24O8 | -3.762 | x |  |  | C15H12O9 | 9.971 |  | x |
| C16H18O6 | -3.615 | x |  |  | C19H16O13 | 9.807 |  | x |
| C18H26O6 | -3.520 | x |  |  | C18H16O12 | 9.710 |  | x |
| C17H24O6 | -3.458 | x |  |  | C17H20O9 | 9.655 |  |  |
| C17H20O7 | -3.455 | x |  |  | C13H8O10 | 9.582 |  | x |
| C13H18O8 | -3.450 | x |  |  | C16H10O10 | 9.577 |  | x |
| C19H24O7 | -3.421 | x |  |  | C18H18O11 | 9.567 |  | x |
| C12H14O8 | -3.416 |  |  |  | C13H16O9 | 9.557 |  |  |
| C15H24O6 | -3.376 | x |  |  | C18H18O10 | 9.387 |  |  |
| C19H24O8 | -3.307 | x |  |  | C15H16O9 | 9.283 |  | x |
| C12H18O5 | -3.307 | x |  |  | C19H16O12 | 9.220 |  | x |
| C10H14O5 | -3.262 |  |  |  | C18H20O11 | 9.123 |  |  |
| C19H26O8 | -3.247 | x |  |  | C12H10O7 | 9.119 |  | x |
| C18H26O7 | -3.182 | x |  |  | C18H16O11 | 9.066 |  | x |
| C17H22O6 | -3.151 | x |  |  | C19H14O13 | 8.955 |  | x |
| C14H14O7 | -3.144 |  |  |  | C13H8O9 | 8.894 |  | x |
| C18H24O6 | -3.141 | x |  |  | C18H14O13 | 8.875 |  | x |
| C15H18O5 | -3.111 | x |  |  | C18H14O11 | 8.871 |  | x |
| C18H22O7 | -3.050 | x |  |  | C15H16O11 | 8.763 |  | x |
| C12H12O9 | -2.983 |  |  |  | C16H14O9 | 8.749 |  | x |
| C18H24O8 | -2.961 | x |  |  | C16H14O12 | 8.733 |  | x |
| C10H14O6 | -2.774 | x |  |  | C16H18O11 | 8.668 |  | x |
| C19H26O7 | -2.702 | x |  |  | C11H8O7 | 8.658 |  |  |
| C15H24O5 | -2.665 | x |  |  | C19H14O12 | 8.522 |  | x |
| C13H20O6 | -2.650 | x |  |  | C20H16O13 | 8.458 |  | x |
| C17H22O5 | -2.601 | x |  |  | C17H16O12 | 8.326 |  | x |
| C20H26O8 | -2.584 | x |  |  | C18H20O9 | 8.306 |  |  |
| C16H24O5 | -2.537 | x |  |  | C17H16O9 | 8.259 |  | x |
| C18H22O6 | -2.476 | x |  |  | C20H18O13 | 8.182 |  | x |
| C16H24O8 | -2.459 | x |  |  | C10H8O7 | 8.085 |  |  |
| C13H20O8 | -2.447 | x |  |  | C18H12O12 | 7.940 |  | x |
| C20H28O7 | -2.379 | x |  |  | C19H18O12 | 7.910 |  | x |
| C20H26O7 | -2.354 | x |  |  | C16H20O9 | 7.910 |  |  |
| C11H14O8 | -2.347 |  |  |  | C14H8O10 | 7.881 |  | x |
| C12H18O8 | -2.330 | x |  |  | C16H10O12 | 7.855 |  |  |
| C20H28O8 | -2.313 | x |  |  | C19H14O14 | 7.798 |  | x |
| C14H22O8 | -2.306 | x |  |  | C11H6O8 | 7.795 |  |  |
| C17H26O7 | -2.292 | x |  |  | C19H16O14 | 7.791 |  | x |
| C17H24O5 | -2.228 | x |  |  | C16H12O9 | 7.780 |  | x |
| C12H18O7 | -2.213 | x |  |  | C20H20O12 | 7.646 |  | x |
| C10H16O6 | -2.207 |  |  |  | C14H10O8 | 7.577 |  | x |
| C17H22O8 | -2.194 |  |  |  | C18H16O10 | 7.516 |  | x |
| C17H26O6 | -2.180 | x |  |  | C19H18O13 | 7.477 |  | x |
| C19H26O6 | -2.064 | x |  |  | C20H16O14 | 7.471 |  | x |
| C14H20O5 | -2.058 | x |  |  | C18H16O13 | 7.412 |  | x |
| C14H14O6 | -2.028 |  |  |  | C17H12O10 | 7.409 |  | x |
| C15H24O7 | -1.978 | x |  |  | C19H20O11 | 7.389 |  |  |
| C15H14O6 | -1.969 |  |  |  | C15H10O8 | 7.355 |  | x |
| C20H24O8 | -1.967 | x |  |  | C15H12O12 | 7.351 |  | x |
| C13H18O4 | -1.923 | x |  |  | C14H12O11 | 7.343 |  | x |
| C13H16O4 | -1.918 | x |  |  | C19H18O11 | 7.293 |  | x |
| C16H24O7 | -1.861 | x |  |  | C20H20O13 | 7.271 |  | x |
| C13H18O9 | -1.826 | x |  |  | C21H16O14 | 7.246 |  | x |
| C16H18O5 | -1.791 | x |  |  | C15H10O9 | 7.210 |  | x |
| C17H18O6 | -1.785 | x |  |  | C20H18O14 | 7.183 |  | x |
| C17H20O5 | -1.755 | x |  |  | C14H8O11 | 7.111 |  |  |
| C16H26O7 | -1.651 | x |  |  | C18H12O13 | 7.102 |  | x |
| C13H14O5 | -1.651 |  |  |  | C12H8O10 | 7.006 |  | x |
| C19H24O6 | -1.562 | x |  |  | C19H20O12 | 7.000 |  | x |
| C15H16O5 | -1.555 | x |  |  | C19H16O11 | 6.996 |  | x |
| C12H14O5 | -1.552 | x |  |  | C12H8O9 | 6.996 |  |  |
| C19H28O6 | -1.537 | x |  |  | C17H10O11 | 6.974 |  | x |
| C20H28O6 | -1.495 | x |  |  | C15H18O9 | 6.961 |  |  |
| C19H28O7 | -1.472 | x |  |  | C18H22O10 | 6.950 |  |  |
| C12H16O5 | -1.436 | x |  |  | C18H18O12 | 6.925 |  | x |
| C16H16O6 | -1.423 | x |  |  | C17H20O11 | 6.904 |  |  |
| C18H28O6 | -1.423 | x |  |  | C17H10O12 | 6.904 |  | x |
| C11H12O7 | -1.403 |  |  |  | C18H12O11 | 6.826 |  | x |
| C14H22O5 | -1.402 | x |  |  | C12H8O7 | 6.821 |  |  |
| C21H28O7 | -1.389 | x |  |  | C13H10O7 | 6.771 |  | x |
| C11H14O4 | -1.384 | x |  |  | C19H12O13 | 6.755 |  | x |
| C12H16O4 | -1.384 | x |  |  | C20H22O12 | 6.747 |  |  |
| C14H20O4 | -1.281 | x |  |  | C14H8O9 | 6.646 |  | x |
| C13H14O6 | -1.258 |  |  |  | C17H12O13 | 6.559 |  | x |
| C17H20O6 | -1.251 | x |  |  | C18H18O9 | 6.541 |  |  |
| C14H16O5 | -1.242 | x |  |  | C9H6O7 | 6.525 |  |  |
| C19H26O5 | -1.208 | x |  |  | C20H16O12 | 6.513 |  | x |
| C18H22O8 | -1.162 | x |  |  | C20H18O12 | 6.511 |  | x |
| C22H28O8 | -1.146 | x |  |  | C16H10O9 | 6.389 |  | x |
| C11H12O6 | -1.138 |  |  |  | C21H14O14 | 6.317 |  | x |
| C21H28O8 | -1.132 | x |  |  | C20H14O13 | 6.252 |  | x |
| C11H16O5 | -1.114 | x |  |  | C21H18O13 | 6.209 |  | x |
| C15H24O8 | -1.112 | x |  |  | C21H18O14 | 6.182 |  | x |
| C11H18O6 | -1.106 |  |  |  | C17H14O13 | 6.169 |  | x |
| C18H26O5 | -1.079 | x |  |  | C20H14O14 | 6.162 |  | x |
| C20H30O7 | -1.068 | x |  |  | C15H20O10 | 6.159 |  |  |
| C21H26O8 | -1.058 | x |  |  | C17H22O9 | 6.072 | x |  |
| C19H24O5 | -1.048 | x |  |  | C21H16O13 | 6.012 |  | x |
| C21H30O8 | -1.030 | x |  |  | C19H12O12 | 6.010 |  |  |
| C13H20O4 | -1.023 | x |  |  | C18H14O10 | 5.988 |  | x |
| C18H20O6 | -1.014 | x |  |  | C15H10O12 | 5.984 |  |  |
| C10H14O4 | -1.008 |  |  |  | C22H18O15 | 5.970 |  |  |
| C23H30O8 | -1.002 | x |  |  | C17H14O9 | 5.898 |  | x |
| C19H22O7 | -0.985 | x |  |  | C22H16O14 | 5.880 |  | x |
| C18H24O5 | -0.981 | x |  |  | C12H10O8 | 5.834 |  | x |
| C19H22O6 | -0.979 | x |  |  | C22H18O14 | 5.808 |  | x |
| C22H30O8 | -0.979 | x |  |  | C13H8O8 | 5.793 |  | x |
| C18H28O7 | -0.952 | x |  |  | C11H8O9 | 5.775 |  | x |
| C21H30O7 | -0.928 | x |  |  | C21H20O13 | 5.726 |  | x |
| C20H24O7 | -0.919 | x |  |  | C21H16O15 | 5.702 |  | x |
| C12H12O6 | -0.918 |  |  |  | C21H22O13 | 5.690 |  | x |
| C20H26O6 | -0.917 | x |  |  | C15H12O8 | 5.666 |  | x |
| C22H28O7 | -0.906 | x |  |  | C17H10O10 | 5.659 |  | x |
| C13H14O7 | -0.906 |  |  |  | C19H20O10 | 5.638 |  |  |
| C13H14O4 | -0.905 | x |  |  | C18H14O14 | 5.615 |  | x |
| C21H26O7 | -0.893 | x |  |  | C20H22O13 | 5.529 |  | x |
| C23H32O8 | -0.878 | x |  |  | C22H16O15 | 5.519 |  |  |
| C24H32O9 | -0.832 | x |  |  | C11H6O7 | 5.424 |  |  |
| C12H12O5 | -0.788 | x |  |  | C14H14O11 | 5.410 |  | x |
| C17H26O8 | -0.785 | x |  |  | C20H20O11 | 5.390 |  |  |
| C18H26O8 | -0.770 | x |  |  | C17H10O13 | 5.362 |  |  |
| C16H16O5 | -0.770 | x |  |  | C21H20O14 | 5.345 |  | x |
| C23H30O9 | -0.769 | x |  |  | C13H14O10 | 5.342 |  | x |
| C21H30O9 | -0.766 | x |  |  | C14H14O10 | 5.339 |  | x |
| C16H18O7 | -0.753 |  |  |  | C19H18O14 | 5.330 |  | x |
| C12H18O4 | -0.743 | x |  |  | C15H8O11 | 5.320 |  |  |
| C15H20O4 | -0.739 | x |  |  | C21H22O12 | 5.290 |  |  |
| C22H30O7 | -0.713 | x |  |  | C20H18O11 | 5.277 |  | x |
| C11H16O4 | -0.712 | x |  |  | C9H6O8 | 5.276 |  |  |
| C10H10O8 | -0.706 |  |  |  | C22H20O15 | 5.262 |  | x |
| C20H30O8 | -0.694 | x |  |  | C14H16O10 | 5.251 |  | x |
| C22H32O8 | -0.690 | x |  |  | C19H22O10 | 5.249 | x |  |
| C19H28O8 | -0.660 | x |  |  | C13H12O8 | 5.237 |  | x |
| C20H26O9 | -0.590 | x |  |  | C21H18O15 | 5.213 |  | x |
| C23H32O9 | -0.587 | x |  |  | C11H6O9 | 5.191 |  |  |
| C21H28O9 | -0.576 | x |  |  | C22H20O14 | 5.176 |  | x |
| C15H16O7 | -0.576 |  |  |  | C21H24O12 | 5.158 | x |  |
| C23H28O8 | -0.570 | x |  |  | C15H8O10 | 5.128 |  |  |
| C10H12O8 | -0.562 |  |  |  | C12H10O6 | 5.104 |  |  |
| C11H16O8 | -0.550 |  |  |  | C13H12O7 | 5.094 |  | x |
| C22H26O8 | -0.548 | x |  |  | C21H14O15 | 5.052 |  |  |
| C21H28O6 | -0.535 |  |  |  | C12H6O10 | 5.051 |  |  |
| C24H34O9 | -0.533 | x |  |  | C20H16O15 | 5.020 |  | x |
| C20H30O9 | -0.521 | x |  |  | C19H12O14 | 5.018 |  |  |
| C22H28O9 | -0.505 | x |  |  | C20H22O11 | 5.014 |  |  |
| C19H30O7 | -0.504 | x |  |  | C17H12O9 | 5.008 |  | x |
| C19H20O6 | -0.503 | x |  |  | C17H22O10 | 4.986 |  |  |
| C17H18O5 | -0.493 | x |  |  | C18H12O14 | 4.981 |  |  |
| C10H14O7 | -0.481 | x |  |  | C11H10O8 | 4.962 |  |  |
| C22H30O9 | -0.457 | x |  |  | C18H10O12 | 4.958 |  |  |
| C10H12O5 | -0.447 |  |  |  | C16H12O8 | 4.947 |  | x |
| C24H30O9 | -0.408 | x |  |  | C22H20O13 | 4.937 |  | x |
| C24H30O8 | -0.406 | x |  |  | C22H14O14 | 4.931 |  |  |
| C21H24O8 | -0.405 | x |  |  | C21H20O12 | 4.927 |  | x |
| C21H26O9 | -0.403 | x |  |  | C21H14O13 | 4.901 |  |  |
| C20H24O6 | -0.393 | x |  |  | C16H12O13 | 4.829 |  |  |
| C11H14O9 | -0.388 |  |  |  | C22H18O13 | 4.807 |  | x |
| C22H32O9 | -0.387 | x |  |  | C19H18O10 | 4.777 |  |  |
| C10H12O6 | -0.377 |  |  |  | C20H14O12 | 4.754 |  | x |
| C22H26O9 | -0.366 | x |  |  | C18H20O12 | 4.751 |  |  |
| C12H16O9 | -0.362 | x |  |  | C20H12O13 | 4.731 |  |  |
| C12H16O7 | -0.345 | x |  |  | C12H8O6 | 4.705 |  |  |
| C25H34O9 | -0.326 | x |  |  | C19H22O12 | 4.694 |  |  |
| C23H30O10 | -0.312 | x |  |  | C19H14O11 | 4.682 |  | x |
| C13H12O6 | -0.310 |  |  |  | C20H12O14 | 4.679 |  |  |
| C11H12O5 | -0.298 | x |  |  | C20H20O14 | 4.674 |  | x |
| C15H22O8 | -0.284 | x |  |  | C16H8O11 | 4.671 |  |  |
| C15H20O9 | -0.281 |  |  |  | C21H12O14 | 4.667 |  |  |
| C21H24O7 | -0.268 | x |  |  | C16H14O8 | 4.663 |  | x |
| C22H24O8 | -0.251 | x |  |  | C19H20O13 | 4.650 |  | x |
| C16H22O4 | -0.251 | x |  |  | C23H20O14 | 4.641 |  |  |
| C23H28O9 | -0.250 | x |  |  | C13H8O7 | 4.631 |  | x |
| C10H14O8 | -0.240 |  |  |  | C16H8O9 | 4.609 |  |  |
| C24H32O10 | -0.235 | x |  |  | C16H20O11 | 4.604 |  |  |
| C12H10O5 | -0.219 |  |  |  | C18H22O9 | 4.592 |  |  |
| C25H34O10 | -0.207 | x |  |  | C22H16O13 | 4.583 |  | x |
| C18H22O5 | -0.192 | x |  |  | C18H10O13 | 4.557 |  |  |
| C23H26O8 | -0.183 | x |  |  | C12H6O9 | 4.504 |  |  |
| C21H32O9 | -0.183 | x |  |  | C22H14O13 | 4.501 |  |  |
| C13H16O7 | -0.179 |  |  |  | C17H8O11 | 4.497 |  |  |
| C27H36O10 | -0.168 |  |  |  | C16H8O10 | 4.493 |  |  |
| C22H32O10 | -0.164 | x |  |  | C23H18O14 | 4.479 |  |  |
| C23H32O10 | -0.158 | x |  |  | C18H10O11 | 4.434 |  |  |
| C18H28O8 | -0.142 | x |  |  | C10H6O7 | 4.428 |  |  |
| C16H26O8 | -0.140 | x |  |  | C15H8O9 | 4.422 |  | x |
| C20H22O7 | -0.139 | x |  |  | C19H22O11 | 4.420 | x |  |
| C26H34O10 | -0.111 | x |  |  | C17H18O12 | 4.418 |  | x |
| C14H18O4 | -0.107 | x |  |  | C20H14O15 | 4.417 |  |  |
| C18H28O9 | -0.092 | x |  |  | C15H14O12 | 4.397 |  | x |
| C19H30O9 | -0.086 | x |  |  | C21H24O13 | 4.391 |  |  |
| C27H36O11 | -0.085 |  |  |  | C18H12O10 | 4.355 |  | x |
| C20H22O8 | -0.083 | x |  |  | C21H22O14 | 4.336 |  | x |
| C25H32O10 | -0.078 | x |  |  | C19H12O11 | 4.316 |  | x |
| C20H28O9 | -0.060 | x |  |  | C19H10O13 | 4.286 |  |  |
| C18H16O7 | -0.059 |  |  |  | C23H22O14 | 4.257 |  | x |
| C19H28O9 | -0.052 | x |  |  | C14H8O8 | 4.250 |  | x |
| C18H20O7 | -0.051 | x |  |  | C16H16O12 | 4.209 |  | x |
| C26H36O11 | -0.048 | x |  |  | C21H18O12 | 4.207 |  | x |
| C23H28O10 | -0.038 | x |  |  | C23H18O15 | 4.193 |  |  |
| C12H14O4 | -0.030 | x |  |  | C15H18O8 | 4.193 |  |  |
| C23H26O9 | -0.021 | x |  |  | C22H22O13 | 4.192 |  | x |
| C21H32O10 | -0.018 | x |  |  | C10H6O6 | 4.188 |  |  |
| C25H32O9 | -0.015 | x |  |  | C14H20O8 | 4.184 | x |  |
|  |  |  |  |  | C23H20O15 | 4.183 |  |  |
|  |  |  |  |  | C22H22O14 | 4.171 |  | x |
|  |  |  |  |  | C15H8O12 | 4.170 |  |  |
|  |  |  |  |  | C15H18O11 | 4.161 |  |  |
|  |  |  |  |  | C18H22O11 | 4.144 | x |  |
|  |  |  |  |  | C15H14O8 | 4.118 |  | x |
|  |  |  |  |  | C17H8O12 | 4.076 |  |  |
|  |  |  |  |  | C17H10O9 | 4.076 |  | x |
|  |  |  |  |  | C22H14O15 | 4.063 |  |  |
|  |  |  |  |  | C19H16O15 | 4.063 |  | x |
|  |  |  |  |  | C20H18O15 | 4.054 |  | x |
|  |  |  |  |  | C20H24O11 | 4.017 | x |  |
|  |  |  |  |  | C20H20O10 | 4.012 |  |  |
|  |  |  |  |  | C18H16O14 | 4.005 |  | x |
|  |  |  |  |  | C18H18O13 | 3.997 |  | x |
|  |  |  |  |  | C19H10O12 | 3.988 |  |  |
|  |  |  |  |  | C18H16O9 | 3.981 |  | x |
|  |  |  |  |  | C15H16O8 | 3.965 |  | x |
|  |  |  |  |  | C12H12O7 | 3.945 |  | x |
|  |  |  |  |  | C10H6O9 | 3.944 |  |  |
|  |  |  |  |  | C13H8O11 | 3.938 |  |  |
|  |  |  |  |  | C23H16O15 | 3.903 |  |  |
|  |  |  |  |  | C16H22O9 | 3.903 | x |  |
|  |  |  |  |  | C19H14O15 | 3.902 |  |  |
|  |  |  |  |  | C18H10O10 | 3.881 |  |  |
|  |  |  |  |  | C12H14O7 | 3.879 |  |  |
|  |  |  |  |  | C21H22O11 | 3.877 |  |  |
|  |  |  |  |  | C22H24O13 | 3.839 |  |  |
|  |  |  |  |  | C11H8O10 | 3.839 |  |  |
|  |  |  |  |  | C13H10O11 | 3.838 |  | x |
|  |  |  |  |  | C17H8O10 | 3.832 |  |  |
|  |  |  |  |  | C17H22O11 | 3.811 | x |  |
|  |  |  |  |  | C20H12O12 | 3.808 |  |  |
|  |  |  |  |  | C21H16O16 | 3.807 |  |  |
|  |  |  |  |  | C23H18O13 | 3.788 |  | x |
|  |  |  |  |  | C22H22O15 | 3.777 |  | x |
|  |  |  |  |  | C19H16O10 | 3.765 |  | x |
|  |  |  |  |  | C21H12O13 | 3.748 |  |  |
|  |  |  |  |  | C21H20O15 | 3.742 |  | x |
|  |  |  |  |  | C20H24O12 | 3.737 | x |  |
|  |  |  |  |  | C22H18O16 | 3.714 |  |  |
|  |  |  |  |  | C23H18O16 | 3.702 |  |  |
|  |  |  |  |  | C23H24O14 | 3.684 |  | x |
|  |  |  |  |  | C21H16O12 | 3.680 |  | x |
|  |  |  |  |  | C16H22O10 | 3.679 | x |  |
|  |  |  |  |  | C21H24O11 | 3.675 | x |  |
|  |  |  |  |  | C12H10O10 | 3.670 |  |  |
|  |  |  |  |  | C23H20O13 | 3.670 |  | x |
|  |  |  |  |  | C19H24O10 | 3.636 | x |  |
|  |  |  |  |  | C15H14O7 | 3.612 |  |  |
|  |  |  |  |  | C20H22O14 | 3.599 |  | x |
|  |  |  |  |  | C22H22O12 | 3.598 |  |  |
|  |  |  |  |  | C23H16O14 | 3.594 |  |  |
|  |  |  |  |  | C17H16O13 | 3.567 |  | x |
|  |  |  |  |  | C14H10O12 | 3.561 |  |  |
|  |  |  |  |  | C17H16O8 | 3.553 |  |  |
|  |  |  |  |  | C17H20O12 | 3.550 |  | x |
|  |  |  |  |  | C21H12O15 | 3.544 |  |  |
|  |  |  |  |  | C12H6O8 | 3.491 |  |  |
|  |  |  |  |  | C23H22O15 | 3.477 |  |  |
|  |  |  |  |  | C24H20O15 | 3.471 |  |  |
|  |  |  |  |  | C22H16O16 | 3.465 |  |  |
|  |  |  |  |  | C16H8O12 | 3.455 |  |  |
|  |  |  |  |  | C20H16O11 | 3.444 |  | x |
|  |  |  |  |  | C18H14O9 | 3.435 |  | x |
|  |  |  |  |  | C20H22O10 | 3.417 | x |  |
|  |  |  |  |  | C22H26O12 | 3.411 | x |  |
|  |  |  |  |  | C22H20O12 | 3.383 |  | x |
|  |  |  |  |  | C21H20O11 | 3.383 |  |  |
|  |  |  |  |  | C20H10O13 | 3.380 |  |  |
|  |  |  |  |  | C24H18O15 | 3.376 |  |  |
|  |  |  |  |  | C23H16O13 | 3.372 |  |  |
|  |  |  |  |  | C18H12O9 | 3.361 |  | x |
|  |  |  |  |  | C19H10O11 | 3.348 |  |  |
|  |  |  |  |  | C16H10O13 | 3.340 |  |  |
|  |  |  |  |  | C15H12O7 | 3.338 |  |  |
|  |  |  |  |  | C17H24O9 | 3.332 | x |  |
|  |  |  |  |  | C14H16O11 | 3.315 |  | x |
|  |  |  |  |  | C12H10O9 | 3.278 |  | x |
|  |  |  |  |  | C23H16O16 | 3.248 |  |  |
|  |  |  |  |  | C22H24O14 | 3.247 |  | x |
|  |  |  |  |  | C16H18O12 | 3.244 |  | x |
|  |  |  |  |  | C23H22O13 | 3.239 |  | x |
|  |  |  |  |  | C22H12O14 | 3.227 |  |  |
|  |  |  |  |  | C21H14O12 | 3.216 |  | x |
|  |  |  |  |  | C24H16O15 | 3.163 |  |  |
|  |  |  |  |  | C14H18O10 | 3.158 |  | x |
|  |  |  |  |  | C12H12O8 | 3.132 |  | x |
|  |  |  |  |  | C22H26O13 | 3.127 | x |  |
|  |  |  |  |  | C21H26O11 | 3.124 | x |  |
|  |  |  |  |  | C21H18O16 | 3.121 |  |  |
|  |  |  |  |  | C24H22O15 | 3.119 |  |  |
|  |  |  |  |  | C22H24O12 | 3.113 | x |  |
|  |  |  |  |  | C24H20O16 | 3.097 |  |  |
|  |  |  |  |  | C19H18O9 | 3.093 |  |  |
|  |  |  |  |  | C21H26O12 | 3.081 | x |  |
|  |  |  |  |  | C17H14O8 | 3.077 |  | x |
|  |  |  |  |  | C23H24O13 | 3.075 |  |  |
|  |  |  |  |  | C18H24O10 | 3.026 | x |  |
|  |  |  |  |  | C10H6O8 | 3.013 |  |  |
|  |  |  |  |  | C22H20O16 | 3.008 |  |  |
|  |  |  |  |  | C22H18O12 | 3.007 |  | x |
|  |  |  |  |  | C20H24O13 | 2.981 |  |  |
|  |  |  |  |  | C20H20O15 | 2.978 |  | x |
|  |  |  |  |  | C23H14O15 | 2.975 |  |  |
|  |  |  |  |  | C14H10O7 | 2.964 |  | x |
|  |  |  |  |  | C14H6O9 | 2.962 |  |  |
|  |  |  |  |  | C20H12O15 | 2.959 |  |  |
|  |  |  |  |  | C19H10O14 | 2.959 |  |  |
|  |  |  |  |  | C16H18O8 | 2.944 |  |  |
|  |  |  |  |  | C16H10O8 | 2.933 |  | x |
|  |  |  |  |  | C21H24O14 | 2.933 |  | x |
|  |  |  |  |  | C21H14O16 | 2.927 |  |  |
|  |  |  |  |  | C19H24O11 | 2.921 | x |  |
|  |  |  |  |  | C23H20O16 | 2.914 |  |  |
|  |  |  |  |  | C13H16O10 | 2.914 |  | x |
|  |  |  |  |  | C24H18O16 | 2.908 |  |  |
|  |  |  |  |  | C17H18O8 | 2.871 |  |  |
|  |  |  |  |  | C15H8O8 | 2.843 |  | x |
|  |  |  |  |  | C19H20O9 | 2.839 |  |  |
|  |  |  |  |  | C16H14O13 | 2.772 |  | x |
|  |  |  |  |  | C23H14O14 | 2.770 |  |  |
|  |  |  |  |  | C15H10O7 | 2.764 |  | x |
|  |  |  |  |  | C21H26O13 | 2.740 | x |  |
|  |  |  |  |  | C22H12O13 | 2.738 |  |  |
|  |  |  |  |  | C14H8O7 | 2.735 |  | x |
|  |  |  |  |  | C14H8O12 | 2.734 |  |  |
|  |  |  |  |  | C24H22O14 | 2.730 |  |  |
|  |  |  |  |  | C20H14O11 | 2.724 |  | x |
|  |  |  |  |  | C23H24O15 | 2.724 |  |  |
|  |  |  |  |  | C18H10O14 | 2.721 |  |  |
|  |  |  |  |  | C23H26O14 | 2.693 |  |  |
|  |  |  |  |  | C24H18O14 | 2.682 |  |  |
|  |  |  |  |  | C22H14O12 | 2.668 |  |  |
|  |  |  |  |  | C19H14O10 | 2.661 |  | x |
|  |  |  |  |  | C13H6O7 | 2.651 |  |  |
|  |  |  |  |  | C22H12O15 | 2.643 |  |  |
|  |  |  |  |  | C16H12O7 | 2.637 |  | x |
|  |  |  |  |  | C19H12O10 | 2.627 |  |  |
|  |  |  |  |  | C22H14O16 | 2.626 |  |  |
|  |  |  |  |  | C9H6O9 | 2.623 |  |  |
|  |  |  |  |  | C17H12O14 | 2.623 |  |  |
|  |  |  |  |  | C19H12O15 | 2.621 |  |  |
|  |  |  |  |  | C24H20O14 | 2.618 |  |  |
|  |  |  |  |  | C19H18O15 | 2.614 |  | x |
|  |  |  |  |  | C17H10O8 | 2.595 |  |  |
|  |  |  |  |  | C22H16O12 | 2.582 |  | x |
|  |  |  |  |  | C23H24O12 | 2.576 |  |  |
|  |  |  |  |  | C19H22O9 | 2.561 | x |  |
|  |  |  |  |  | C24H24O13 | 2.560 |  | x |
|  |  |  |  |  | C21H12O12 | 2.560 |  |  |
|  |  |  |  |  | C10H4O8 | 2.553 |  |  |
|  |  |  |  |  | C24H24O15 | 2.546 |  |  |
|  |  |  |  |  | C23H14O16 | 2.544 |  |  |
|  |  |  |  |  | C14H12O6 | 2.540 |  |  |
|  |  |  |  |  | C17H24O10 | 2.540 | x |  |
|  |  |  |  |  | C15H16O12 | 2.536 |  | x |
|  |  |  |  |  | C20H10O14 | 2.528 |  |  |
|  |  |  |  |  | C24H16O16 | 2.525 |  |  |
|  |  |  |  |  | C17H12O8 | 2.503 |  | x |
|  |  |  |  |  | C23H20O12 | 2.491 |  | x |
|  |  |  |  |  | C18H24O11 | 2.488 | x |  |
|  |  |  |  |  | C18H16O8 | 2.477 |  |  |
|  |  |  |  |  | C18H10O9 | 2.477 |  |  |
|  |  |  |  |  | C20H24O10 | 2.459 | x |  |
|  |  |  |  |  | C23H22O12 | 2.456 |  | x |
|  |  |  |  |  | C19H22O13 | 2.449 |  | x |
|  |  |  |  |  | C23H26O13 | 2.447 |  |  |
|  |  |  |  |  | C18H24O9 | 2.441 | x |  |
|  |  |  |  |  | C13H10O6 | 2.430 |  |  |
|  |  |  |  |  | C8H6O7 | 2.426 |  |  |
|  |  |  |  |  | C20H12O11 | 2.426 |  |  |
|  |  |  |  |  | C20H16O16 | 2.424 |  |  |
|  |  |  |  |  | C24H24O14 | 2.418 |  | x |
|  |  |  |  |  | C19H20O14 | 2.417 |  | x |
|  |  |  |  |  | C16H10O7 | 2.417 |  |  |
|  |  |  |  |  | C23H22O16 | 2.414 |  |  |
|  |  |  |  |  | C22H24O11 | 2.401 | x |  |
|  |  |  |  |  | C21H10O14 | 2.392 |  |  |
|  |  |  |  |  | C18H14O15 | 2.391 |  |  |
|  |  |  |  |  | C18H8O12 | 2.390 |  |  |
|  |  |  |  |  | C25H20O14 | 2.389 |  |  |
|  |  |  |  |  | C13H12O11 | 2.364 |  | x |
|  |  |  |  |  | C13H12O10 | 2.363 |  | x |
|  |  |  |  |  | C24H26O13 | 2.361 |  |  |
|  |  |  |  |  | C24H16O14 | 2.360 |  |  |
|  |  |  |  |  | C24H22O13 | 2.357 |  | x |
|  |  |  |  |  | C21H22O15 | 2.351 |  | x |
|  |  |  |  |  | C23H18O12 | 2.345 |  | x |
|  |  |  |  |  | C20H10O12 | 2.344 |  |  |
|  |  |  |  |  | C25H22O15 | 2.339 |  |  |
|  |  |  |  |  | C23H26O12 | 2.333 | x |  |
|  |  |  |  |  | C14H6O10 | 2.329 |  |  |
|  |  |  |  |  | C21H18O11 | 2.327 |  | x |
|  |  |  |  |  | C18H8O13 | 2.322 |  |  |
|  |  |  |  |  | C21H22O10 | 2.321 | x |  |
|  |  |  |  |  | C17H8O13 | 2.320 |  |  |
|  |  |  |  |  | C18H22O12 | 2.309 |  |  |
|  |  |  |  |  | C18H20O13 | 2.305 |  | x |
|  |  |  |  |  | C17H14O14 | 2.303 |  | x |
|  |  |  |  |  | C16H8O8 | 2.298 |  |  |
|  |  |  |  |  | C21H24O10 | 2.296 | x |  |
|  |  |  |  |  | C14H12O12 | 2.282 |  | x |
|  |  |  |  |  | C12H14O9 | 2.277 |  |  |
|  |  |  |  |  | C25H20O16 | 2.267 |  |  |
|  |  |  |  |  | C21H16O11 | 2.257 |  | x |
|  |  |  |  |  | C25H20O15 | 2.255 |  |  |
|  |  |  |  |  | C24H22O16 | 2.245 |  |  |
|  |  |  |  |  | C16H8O13 | 2.239 |  |  |
|  |  |  |  |  | C23H18O17 | 2.201 |  |  |
|  |  |  |  |  | C21H10O13 | 2.198 |  |  |
|  |  |  |  |  | C25H22O16 | 2.185 |  |  |
|  |  |  |  |  | C25H18O15 | 2.170 |  |  |
|  |  |  |  |  | C24H20O13 | 2.170 |  |  |
|  |  |  |  |  | C19H24O12 | 2.162 | x |  |
|  |  |  |  |  | C25H18O16 | 2.142 |  |  |
|  |  |  |  |  | C25H22O14 | 2.129 |  |  |
|  |  |  |  |  | C23H14O13 | 2.126 |  |  |
|  |  |  |  |  | C23H20O17 | 2.102 |  |  |
|  |  |  |  |  | C22H24O15 | 2.089 |  | x |
|  |  |  |  |  | C20H16O10 | 2.087 |  | x |
|  |  |  |  |  | C24H14O15 | 2.087 |  |  |
|  |  |  |  |  | C23H16O17 | 2.067 |  |  |
|  |  |  |  |  | C13H10O8 | 2.067 |  | x |
|  |  |  |  |  | C24H18O17 | 2.066 |  |  |
|  |  |  |  |  | C24H28O13 | 2.033 |  |  |
|  |  |  |  |  | C25H18O14 | 2.028 |  |  |
|  |  |  |  |  | C18H18O14 | 2.028 |  | x |
|  |  |  |  |  | C25H24O15 | 2.021 |  |  |
|  |  |  |  |  | C22H22O11 | 2.020 |  |  |
|  |  |  |  |  | C13H6O9 | 2.019 |  |  |
|  |  |  |  |  | C24H26O14 | 2.016 |  | x |
|  |  |  |  |  | C22H28O11 | 2.012 | x |  |
|  |  |  |  |  | C22H22O16 | 2.011 |  |  |
|  |  |  |  |  | C19H16O9 | 2.007 |  | x |
|  |  |  |  |  | C17H18O13 | 1.986 |  | x |
|  |  |  |  |  | C18H14O8 | 1.974 |  | x |
|  |  |  |  |  | C13H6O10 | 1.972 |  |  |
|  |  |  |  |  | C14H10O6 | 1.971 |  |  |
|  |  |  |  |  | C13H6O8 | 1.968 |  |  |
|  |  |  |  |  | C24H18O13 | 1.963 |  |  |
|  |  |  |  |  | C24H20O17 | 1.948 |  |  |
|  |  |  |  |  | C21H10O15 | 1.945 |  |  |
|  |  |  |  |  | C15H22O9 | 1.937 | x |  |
|  |  |  |  |  | C12H12O10 | 1.931 |  |  |
|  |  |  |  |  | C19H14O9 | 1.929 |  | x |
|  |  |  |  |  | C24H22O12 | 1.925 |  | x |
|  |  |  |  |  | C24H24O16 | 1.924 |  |  |
|  |  |  |  |  | C22H26O11 | 1.890 | x |  |
|  |  |  |  |  | C25H20O17 | 1.885 |  |  |
|  |  |  |  |  | C22H20O11 | 1.870 |  | x |
|  |  |  |  |  | C18H12O8 | 1.865 |  |  |
|  |  |  |  |  | C22H18O17 | 1.858 |  |  |
|  |  |  |  |  | C25H16O16 | 1.857 |  |  |
|  |  |  |  |  | C20H14O16 | 1.855 |  |  |
|  |  |  |  |  | C11H10O5 | 1.851 |  |  |
|  |  |  |  |  | C22H16O17 | 1.848 |  |  |
|  |  |  |  |  | C25H18O17 | 1.830 |  |  |
|  |  |  |  |  | C15H6O11 | 1.827 |  |  |
|  |  |  |  |  | C17H8O9 | 1.825 |  |  |
|  |  |  |  |  | C18H12O15 | 1.823 |  |  |
|  |  |  |  |  | C10H8O6 | 1.813 |  |  |
|  |  |  |  |  | C24H16O17 | 1.811 |  |  |
|  |  |  |  |  | C14H20O9 | 1.804 | x |  |
|  |  |  |  |  | C23H28O12 | 1.802 | x |  |
|  |  |  |  |  | C15H10O13 | 1.802 |  |  |
|  |  |  |  |  | C20H18O16 | 1.797 |  |  |
|  |  |  |  |  | C23H16O12 | 1.778 |  |  |
|  |  |  |  |  | C20H18O10 | 1.776 |  |  |
|  |  |  |  |  | C24H14O14 | 1.774 |  |  |
|  |  |  |  |  | C13H10O5 | 1.768 |  |  |
|  |  |  |  |  | C22H26O14 | 1.757 |  |  |
|  |  |  |  |  | C21H20O16 | 1.755 |  |  |
|  |  |  |  |  | C17H10O14 | 1.747 |  |  |
|  |  |  |  |  | C25H24O14 | 1.746 |  |  |
|  |  |  |  |  | C21H12O16 | 1.736 |  |  |
|  |  |  |  |  | C19H12O9 | 1.735 |  |  |
|  |  |  |  |  | C25H24O16 | 1.731 |  |  |
|  |  |  |  |  | C18H18O8 | 1.726 | x |  |
|  |  |  |  |  | C22H28O12 | 1.725 | x |  |
|  |  |  |  |  | C22H28O13 | 1.714 | x |  |
|  |  |  |  |  | C19H10O10 | 1.706 |  |  |
|  |  |  |  |  | C24H28O14 | 1.691 |  |  |
|  |  |  |  |  | C24H16O13 | 1.687 |  |  |
|  |  |  |  |  | C26H22O16 | 1.682 |  |  |
|  |  |  |  |  | C18H8O11 | 1.678 |  |  |
|  |  |  |  |  | C24H14O16 | 1.673 |  |  |
|  |  |  |  |  | C11H8O6 | 1.668 |  |  |
|  |  |  |  |  | C24H26O15 | 1.664 |  | x |
|  |  |  |  |  | C22H12O16 | 1.659 |  |  |
|  |  |  |  |  | C24H24O12 | 1.656 |  | x |
|  |  |  |  |  | C20H22O15 | 1.653 |  | x |
|  |  |  |  |  | C9H8O7 | 1.650 |  |  |
|  |  |  |  |  | C25H26O15 | 1.641 |  | x |
|  |  |  |  |  | C17H14O7 | 1.629 |  |  |
|  |  |  |  |  | C16H24O9 | 1.624 | x |  |
|  |  |  |  |  | C24H26O12 | 1.619 | x |  |
|  |  |  |  |  | C21H14O11 | 1.613 |  |  |
|  |  |  |  |  | C14H12O8 | 1.610 |  | x |
|  |  |  |  |  | C20H10O15 | 1.607 |  |  |
|  |  |  |  |  | C20H26O12 | 1.606 | x |  |
|  |  |  |  |  | C15H8O7 | 1.601 |  |  |
|  |  |  |  |  | C23H12O15 | 1.598 |  |  |
|  |  |  |  |  | C23H12O16 | 1.595 |  |  |
|  |  |  |  |  | C25H26O14 | 1.593 |  | x |
|  |  |  |  |  | C21H20O10 | 1.590 |  |  |
|  |  |  |  |  | C25H22O17 | 1.583 |  |  |
|  |  |  |  |  | C25H16O15 | 1.582 |  |  |
|  |  |  |  |  | C14H12O7 | 1.579 |  |  |
|  |  |  |  |  | C20H24O14 | 1.577 |  | x |
|  |  |  |  |  | C16H16O13 | 1.577 |  | x |
|  |  |  |  |  | C23H28O13 | 1.577 | x |  |
|  |  |  |  |  | C23H26O15 | 1.575 |  | x |
|  |  |  |  |  | C21H28O12 | 1.570 | x |  |
|  |  |  |  |  | C26H20O15 | 1.564 |  |  |
|  |  |  |  |  | C14H8O6 | 1.559 |  |  |
|  |  |  |  |  | C16H16O8 | 1.557 |  |  |
|  |  |  |  |  | C25H16O17 | 1.535 |  |  |
|  |  |  |  |  | C24H20O12 | 1.525 |  |  |
|  |  |  |  |  | C22H12O12 | 1.525 |  |  |
|  |  |  |  |  | C23H12O14 | 1.516 |  |  |
|  |  |  |  |  | C21H26O14 | 1.498 |  | x |
|  |  |  |  |  | C20H14O10 | 1.480 |  |  |
|  |  |  |  |  | C18H20O8 | 1.474 |  |  |
|  |  |  |  |  | C26H24O16 | 1.472 |  |  |
|  |  |  |  |  | C23H22O17 | 1.464 |  |  |
|  |  |  |  |  | C26H22O15 | 1.454 |  |  |
|  |  |  |  |  | C14H6O8 | 1.452 |  |  |
|  |  |  |  |  | C26H18O16 | 1.447 |  |  |
|  |  |  |  |  | C25H18O13 | 1.441 |  |  |
|  |  |  |  |  | C10H8O5 | 1.441 |  |  |
|  |  |  |  |  | C24H30O13 | 1.438 |  |  |
|  |  |  |  |  | C19H24O13 | 1.435 |  |  |
|  |  |  |  |  | C15H12O13 | 1.428 |  | x |
|  |  |  |  |  | C20H18O9 | 1.424 |  |  |
|  |  |  |  |  | C26H20O16 | 1.413 |  |  |
|  |  |  |  |  | C23H24O16 | 1.412 |  |  |
|  |  |  |  |  | C18H16O15 | 1.410 |  |  |
|  |  |  |  |  | C20H20O9 | 1.410 | x |  |
|  |  |  |  |  | C25H22O13 | 1.401 |  |  |
|  |  |  |  |  | C24H28O15 | 1.400 |  |  |
|  |  |  |  |  | C19H14O16 | 1.397 |  |  |
|  |  |  |  |  | C26H26O14 | 1.388 |  |  |
|  |  |  |  |  | C17H16O14 | 1.388 |  | x |
|  |  |  |  |  | C26H18O15 | 1.386 |  |  |
|  |  |  |  |  | C20H10O11 | 1.382 |  |  |
|  |  |  |  |  | C19H8O13 | 1.381 |  |  |
|  |  |  |  |  | C14H14O12 | 1.379 |  | x |
|  |  |  |  |  | C20H26O11 | 1.378 | x |  |
|  |  |  |  |  | C26H26O16 | 1.376 |  |  |
|  |  |  |  |  | C23H28O14 | 1.372 |  |  |
|  |  |  |  |  | C21H16O17 | 1.370 |  |  |
|  |  |  |  |  | C23H14O12 | 1.370 |  |  |
|  |  |  |  |  | C23H24O11 | 1.368 | x |  |
|  |  |  |  |  | C22H10O14 | 1.367 |  |  |
|  |  |  |  |  | C23H26O11 | 1.366 | x |  |
|  |  |  |  |  | C18H22O13 | 1.361 |  | x |
|  |  |  |  |  | C22H24O16 | 1.357 |  |  |
|  |  |  |  |  | C25H28O12 | 1.357 |  |  |
|  |  |  |  |  | C11H12O8 | 1.355 |  |  |
|  |  |  |  |  | C21H18O17 | 1.352 |  |  |
|  |  |  |  |  | C24H20O18 | 1.349 |  |  |
|  |  |  |  |  | C18H10O8 | 1.346 |  |  |
|  |  |  |  |  | C19H18O8 | 1.346 | x |  |
|  |  |  |  |  | C21H28O13 | 1.345 |  |  |
|  |  |  |  |  | C26H22O14 | 1.345 |  |  |
|  |  |  |  |  | C25H28O14 | 1.340 |  |  |
|  |  |  |  |  | C24H22O17 | 1.335 |  |  |
|  |  |  |  |  | C19H16O8 | 1.332 |  |  |
|  |  |  |  |  | C24H18O12 | 1.329 |  |  |
|  |  |  |  |  | C20H12O10 | 1.324 |  |  |
|  |  |  |  |  | C19H20O8 | 1.322 | x |  |
|  |  |  |  |  | C26H20O17 | 1.320 |  |  |
|  |  |  |  |  | C22H20O17 | 1.319 |  |  |
|  |  |  |  |  | C18H8O10 | 1.318 |  |  |
|  |  |  |  |  | C22H16O11 | 1.311 |  |  |
|  |  |  |  |  | C26H26O15 | 1.309 |  |  |
|  |  |  |  |  | C21H12O11 | 1.307 |  |  |
|  |  |  |  |  | C25H16O14 | 1.307 |  |  |
|  |  |  |  |  | C17H16O7 | 1.306 |  |  |
|  |  |  |  |  | C25H30O13 | 1.305 |  |  |
|  |  |  |  |  | C17H10O7 | 1.299 |  |  |
|  |  |  |  |  | C15H20O8 | 1.296 | x |  |
|  |  |  |  |  | C26H24O15 | 1.295 |  |  |
|  |  |  |  |  | C24H28O11 | 1.290 | x |  |
|  |  |  |  |  | C10H10O7 | 1.288 |  |  |
|  |  |  |  |  | C24H14O17 | 1.288 |  |  |
|  |  |  |  |  | C10H12O7 | 1.288 |  |  |
|  |  |  |  |  | C26H24O13 | 1.287 |  |  |
|  |  |  |  |  | C26H24O14 | 1.282 |  |  |
|  |  |  |  |  | C21H10O12 | 1.281 |  |  |
|  |  |  |  |  | C24H28O12 | 1.278 | x |  |
|  |  |  |  |  | C22H14O17 | 1.277 |  |  |
|  |  |  |  |  | C25H26O13 | 1.275 |  | x |
|  |  |  |  |  | C18H26O10 | 1.275 | x |  |
|  |  |  |  |  | C13H14O11 | 1.252 |  |  |
|  |  |  |  |  | C25H24O13 | 1.247 |  | x |
|  |  |  |  |  | C25H24O17 | 1.242 |  |  |
|  |  |  |  |  | C23H14O17 | 1.234 |  |  |
|  |  |  |  |  | C25H26O16 | 1.232 |  |  |
|  |  |  |  |  | C18H24O12 | 1.225 | x |  |
|  |  |  |  |  | C25H14O16 | 1.217 |  |  |
|  |  |  |  |  | C19H26O11 | 1.214 | x |  |
|  |  |  |  |  | C20H26O13 | 1.213 |  |  |
|  |  |  |  |  | C22H30O12 | 1.203 | x |  |
|  |  |  |  |  | C23H18O11 | 1.189 |  |  |
|  |  |  |  |  | C23H20O11 | 1.187 |  | x |
|  |  |  |  |  | C19H26O12 | 1.177 | x |  |
|  |  |  |  |  | C22H18O11 | 1.177 |  | x |
|  |  |  |  |  | C25H28O15 | 1.176 |  |  |
|  |  |  |  |  | C24H26O11 | 1.174 |  |  |
|  |  |  |  |  | C16H22O11 | 1.166 | x |  |
|  |  |  |  |  | C20H12O16 | 1.163 |  |  |
|  |  |  |  |  | C26H16O16 | 1.161 |  |  |
|  |  |  |  |  | C25H20O13 | 1.158 |  |  |
|  |  |  |  |  | C26H20O14 | 1.158 |  |  |
|  |  |  |  |  | C12H8O5 | 1.148 |  |  |
|  |  |  |  |  | C22H22O10 | 1.147 |  |  |
|  |  |  |  |  | C25H28O13 | 1.145 |  |  |
|  |  |  |  |  | C26H22O17 | 1.143 |  |  |
|  |  |  |  |  | C26H28O14 | 1.130 |  |  |
|  |  |  |  |  | C24H30O12 | 1.118 | x |  |
|  |  |  |  |  | C24H30O14 | 1.118 |  |  |
|  |  |  |  |  | C23H22O11 | 1.117 |  |  |
|  |  |  |  |  | C25H18O18 | 1.115 |  |  |
|  |  |  |  |  | C23H28O15 | 1.110 |  |  |
|  |  |  |  |  | C21H24O15 | 1.108 |  | x |
|  |  |  |  |  | C24H18O18 | 1.108 |  |  |
|  |  |  |  |  | C20H16O9 | 1.106 |  | x |
|  |  |  |  |  | C24H12O15 | 1.106 |  |  |
|  |  |  |  |  | C18H10O15 | 1.102 |  |  |
|  |  |  |  |  | C22H10O15 | 1.097 |  |  |
|  |  |  |  |  | C20H22O9 | 1.096 | x |  |
|  |  |  |  |  | C20H20O16 | 1.095 |  |  |
|  |  |  |  |  | C19H16O16 | 1.092 |  |  |
|  |  |  |  |  | C11H6O6 | 1.091 |  |  |
|  |  |  |  |  | C21H18O10 | 1.090 |  | x |
|  |  |  |  |  | C26H26O13 | 1.088 |  |  |
|  |  |  |  |  | C15H12O6 | 1.081 |  |  |
|  |  |  |  |  | C19H20O15 | 1.079 |  |  |
|  |  |  |  |  | C23H30O13 | 1.079 |  |  |
|  |  |  |  |  | C23H28O11 | 1.078 | x |  |
|  |  |  |  |  | C19H14O8 | 1.078 |  |  |
|  |  |  |  |  | C22H28O14 | 1.076 |  |  |
|  |  |  |  |  | C26H24O17 | 1.075 |  |  |
|  |  |  |  |  | C22H26O15 | 1.075 |  | x |
|  |  |  |  |  | C14H20O10 | 1.074 |  |  |
|  |  |  |  |  | C25H14O15 | 1.072 |  |  |
|  |  |  |  |  | C11H12O9 | 1.071 |  |  |
|  |  |  |  |  | C16H16O7 | 1.070 |  |  |
|  |  |  |  |  | C17H22O12 | 1.069 |  |  |
|  |  |  |  |  | C25H26O12 | 1.067 |  | x |
|  |  |  |  |  | C27H26O16 | 1.064 |  |  |
|  |  |  |  |  | C19H12O8 | 1.062 |  |  |
|  |  |  |  |  | C27H22O16 | 1.057 |  |  |
|  |  |  |  |  | C25H16O13 | 1.057 |  |  |
|  |  |  |  |  | C23H12O13 | 1.052 |  |  |
|  |  |  |  |  | C15H10O6 | 1.052 |  |  |
|  |  |  |  |  | C27H20O16 | 1.052 |  |  |
|  |  |  |  |  | C26H18O17 | 1.051 |  |  |
|  |  |  |  |  | C19H22O14 | 1.051 |  | x |
|  |  |  |  |  | C24H26O16 | 1.048 |  |  |
|  |  |  |  |  | C25H20O18 | 1.045 |  |  |
|  |  |  |  |  | C13H8O6 | 1.043 |  | x |
|  |  |  |  |  | C11H10O9 | 1.041 |  |  |
|  |  |  |  |  | C15H20O11 | 1.040 |  |  |
|  |  |  |  |  | C27H18O16 | 1.039 |  |  |
|  |  |  |  |  | C18H20O14 | 1.037 |  | x |
|  |  |  |  |  | C26H16O15 | 1.032 |  |  |
|  |  |  |  |  | C16H12O14 | 1.022 |  |  |
|  |  |  |  |  | C13H14O8 | 1.018 |  |  |
|  |  |  |  |  | C26H18O14 | 1.015 |  |  |
|  |  |  |  |  | C25H24O12 | 1.008 |  |  |
|  |  |  |  |  | C24H24O17 | 1.001 |  |  |
|  |  |  |  |  | C24H24O11 | 0.994 |  |  |
|  |  |  |  |  | C9H8O6 | 0.994 |  |  |
|  |  |  |  |  | C27H24O15 | 0.988 |  |  |
|  |  |  |  |  | C10H8O8 | 0.985 |  |  |
|  |  |  |  |  | C25H26O17 | 0.979 |  |  |
|  |  |  |  |  | C11H8O5 | 0.974 |  |  |
|  |  |  |  |  | C23H26O16 | 0.973 |  |  |
|  |  |  |  |  | C22H10O13 | 0.971 |  |  |
|  |  |  |  |  | C23H30O12 | 0.971 | x |  |
|  |  |  |  |  | C27H28O15 | 0.971 |  |  |
|  |  |  |  |  | C10H6O5 | 0.965 |  |  |
|  |  |  |  |  | C15H8O6 | 0.960 |  |  |
|  |  |  |  |  | C24H16O12 | 0.957 |  |  |
|  |  |  |  |  | C26H16O17 | 0.945 |  |  |
|  |  |  |  |  | C22H24O10 | 0.943 | x |  |
|  |  |  |  |  | C27H24O17 | 0.940 |  |  |
|  |  |  |  |  | C16H14O7 | 0.928 |  |  |
|  |  |  |  |  | C25H30O12 | 0.928 | x |  |
|  |  |  |  |  | C26H28O15 | 0.921 |  |  |
|  |  |  |  |  | C27H26O15 | 0.921 |  |  |
|  |  |  |  |  | C10H10O9 | 0.919 |  |  |
|  |  |  |  |  | C17H24O11 | 0.918 | x |  |
|  |  |  |  |  | C26H28O13 | 0.917 |  |  |
|  |  |  |  |  | C21H28O11 | 0.914 | x |  |
|  |  |  |  |  | C26H30O14 | 0.910 |  |  |
|  |  |  |  |  | C21H22O16 | 0.907 |  |  |
|  |  |  |  |  | C27H20O17 | 0.900 |  |  |
|  |  |  |  |  | C25H30O15 | 0.894 |  |  |
|  |  |  |  |  | C22H14O11 | 0.889 |  |  |
|  |  |  |  |  | C26H20O18 | 0.886 |  |  |
|  |  |  |  |  | C23H18O18 | 0.885 |  |  |
|  |  |  |  |  | C21H20O9 | 0.880 |  |  |
|  |  |  |  |  | C17H20O13 | 0.878 |  | x |
|  |  |  |  |  | C25H22O12 | 0.871 |  |  |
|  |  |  |  |  | C21H16O10 | 0.863 |  | x |
|  |  |  |  |  | C27H24O14 | 0.861 |  |  |
|  |  |  |  |  | C23H16O11 | 0.849 |  |  |
|  |  |  |  |  | C24H22O11 | 0.846 |  |  |
|  |  |  |  |  | C27H24O16 | 0.841 |  |  |
|  |  |  |  |  | C21H14O10 | 0.831 |  |  |
|  |  |  |  |  | C27H28O14 | 0.830 |  |  |
|  |  |  |  |  | C23H24O17 | 0.829 |  |  |
|  |  |  |  |  | C27H32O15 | 0.829 |  |  |
|  |  |  |  |  | C25H32O13 | 0.820 | x |  |
|  |  |  |  |  | C25H30O14 | 0.820 |  |  |
|  |  |  |  |  | C16H24O10 | 0.808 | x |  |
|  |  |  |  |  | C16H20O12 | 0.808 |  |  |
|  |  |  |  |  | C24H28O16 | 0.808 |  |  |
|  |  |  |  |  | C15H22O10 | 0.808 | x |  |
|  |  |  |  |  | C22H30O13 | 0.807 | x |  |
|  |  |  |  |  | C22H20O10 | 0.806 |  |  |
|  |  |  |  |  | C27H26O17 | 0.803 |  |  |
|  |  |  |  |  | C27H22O17 | 0.803 |  |  |
|  |  |  |  |  | C26H22O13 | 0.800 |  |  |
|  |  |  |  |  | C11H10O10 | 0.799 |  |  |
|  |  |  |  |  | C15H14O13 | 0.797 |  | x |
|  |  |  |  |  | C26H32O14 | 0.796 |  |  |
|  |  |  |  |  | C23H30O11 | 0.793 | x |  |
|  |  |  |  |  | C26H22O18 | 0.792 |  |  |
|  |  |  |  |  | C10H10O6 | 0.787 |  |  |
|  |  |  |  |  | C17H18O14 | 0.784 |  | x |
|  |  |  |  |  | C28H32O14 | 0.781 |  |  |
|  |  |  |  |  | C21H26O10 | 0.776 | x |  |
|  |  |  |  |  | C25H22O18 | 0.776 |  |  |
|  |  |  |  |  | C20H14O9 | 0.775 |  |  |
|  |  |  |  |  | C26H24O18 | 0.768 |  |  |
|  |  |  |  |  | C25H28O11 | 0.766 | x |  |
|  |  |  |  |  | C26H32O13 | 0.763 | x |  |
|  |  |  |  |  | C15H18O12 | 0.763 |  | x |
|  |  |  |  |  | C22H26O10 | 0.762 | x |  |
|  |  |  |  |  | C26H20O13 | 0.762 |  |  |
|  |  |  |  |  | C18H12O7 | 0.760 |  |  |
|  |  |  |  |  | C20H26O10 | 0.757 | x |  |
|  |  |  |  |  | C20H18O8 | 0.756 |  |  |
|  |  |  |  |  | C23H20O18 | 0.743 |  |  |
|  |  |  |  |  | C25H28O16 | 0.742 |  |  |
|  |  |  |  |  | C27H20O18 | 0.739 |  |  |
|  |  |  |  |  | C26H30O13 | 0.738 |  |  |
|  |  |  |  |  | C23H24O10 | 0.722 |  |  |
|  |  |  |  |  | C18H26O11 | 0.721 | x |  |
|  |  |  |  |  | C27H30O16 | 0.720 |  |  |
|  |  |  |  |  | C26H30O15 | 0.714 |  |  |
|  |  |  |  |  | C27H20O15 | 0.711 |  |  |
|  |  |  |  |  | C25H32O12 | 0.708 | x |  |
|  |  |  |  |  | C24H20O11 | 0.703 |  |  |
|  |  |  |  |  | C25H26O11 | 0.700 |  |  |
|  |  |  |  |  | C28H22O18 | 0.687 |  |  |
|  |  |  |  |  | C20H20O8 | 0.686 |  |  |
|  |  |  |  |  | C25H24O11 | 0.682 |  |  |
|  |  |  |  |  | C26H28O16 | 0.680 |  |  |
|  |  |  |  |  | C14H16O8 | 0.676 |  | x |
|  |  |  |  |  | C22H30O11 | 0.675 | x |  |
|  |  |  |  |  | C9H10O6 | 0.671 |  |  |
|  |  |  |  |  | C17H14O6 | 0.669 |  |  |
|  |  |  |  |  | C13H12O5 | 0.668 |  |  |
|  |  |  |  |  | C27H18O17 | 0.668 |  |  |
|  |  |  |  |  | C17H12O7 | 0.667 |  | x |
|  |  |  |  |  | C27H30O15 | 0.664 |  |  |
|  |  |  |  |  | C26H18O13 | 0.663 |  |  |
|  |  |  |  |  | C17H18O7 | 0.656 | x |  |
|  |  |  |  |  | C23H32O12 | 0.652 | x |  |
|  |  |  |  |  | C17H12O6 | 0.650 |  |  |
|  |  |  |  |  | C27H30O13 | 0.648 |  |  |
|  |  |  |  |  | C27H32O14 | 0.646 |  |  |
|  |  |  |  |  | C25H32O14 | 0.639 |  |  |
|  |  |  |  |  | C20H28O12 | 0.626 | x |  |
|  |  |  |  |  | C27H20O14 | 0.624 |  |  |
|  |  |  |  |  | C19H18O7 | 0.618 | x |  |
|  |  |  |  |  | C26H32O15 | 0.617 |  |  |
|  |  |  |  |  | C18H14O7 | 0.613 |  |  |
|  |  |  |  |  | C19H26O10 | 0.607 | x |  |
|  |  |  |  |  | C16H14O6 | 0.602 | x |  |
|  |  |  |  |  | C27H24O13 | 0.601 |  |  |
|  |  |  |  |  | C20H26O14 | 0.600 |  | x |
|  |  |  |  |  | C26H28O12 | 0.600 |  |  |
|  |  |  |  |  | C25H16O18 | 0.598 |  |  |
|  |  |  |  |  | C24H32O14 | 0.597 |  |  |
|  |  |  |  |  | C15H12O5 | 0.595 |  |  |
|  |  |  |  |  | C24H32O12 | 0.591 | x |  |
|  |  |  |  |  | C27H28O16 | 0.589 |  |  |
|  |  |  |  |  | C28H26O16 | 0.587 |  |  |
|  |  |  |  |  | C27H30O14 | 0.577 |  |  |
|  |  |  |  |  | C26H24O12 | 0.577 |  |  |
|  |  |  |  |  | C26H30O12 | 0.571 |  |  |
|  |  |  |  |  | C26H26O17 | 0.571 |  |  |
|  |  |  |  |  | C26H26O12 | 0.565 |  |  |
|  |  |  |  |  | C21H18O9 | 0.561 |  | x |
|  |  |  |  |  | C24H24O10 | 0.555 |  |  |
|  |  |  |  |  | C27H28O12 | 0.550 |  |  |
|  |  |  |  |  | C25H20O12 | 0.549 |  |  |
|  |  |  |  |  | C28H28O14 | 0.547 |  |  |
|  |  |  |  |  | C28H30O14 | 0.545 |  |  |
|  |  |  |  |  | C23H22O10 | 0.539 |  |  |
|  |  |  |  |  | C25H34O14 | 0.538 |  |  |
|  |  |  |  |  | C28H30O15 | 0.531 |  |  |
|  |  |  |  |  | C25H30O11 | 0.530 | x |  |
|  |  |  |  |  | C14H18O11 | 0.530 |  |  |
|  |  |  |  |  | C24H26O17 | 0.527 |  |  |
|  |  |  |  |  | C20H16O8 | 0.526 |  |  |
|  |  |  |  |  | C24H30O11 | 0.525 | x |  |
|  |  |  |  |  | C27H32O12 | 0.521 |  |  |
|  |  |  |  |  | C18H26O9 | 0.521 | x |  |
|  |  |  |  |  | C27H34O13 | 0.517 | x |  |
|  |  |  |  |  | C18H18O15 | 0.517 |  |  |
|  |  |  |  |  | C28H28O15 | 0.516 |  |  |
|  |  |  |  |  | C11H10O7 | 0.516 |  |  |
|  |  |  |  |  | C28H28O16 | 0.513 |  |  |
|  |  |  |  |  | C23H30O14 | 0.507 |  |  |
|  |  |  |  |  | C14H16O9 | 0.503 |  | x |
|  |  |  |  |  | C12H14O10 | 0.496 |  |  |
|  |  |  |  |  | C28H32O15 | 0.496 |  |  |
|  |  |  |  |  | C22H18O10 | 0.494 |  |  |
|  |  |  |  |  | C23H26O10 | 0.494 | x |  |
|  |  |  |  |  | C26H34O14 | 0.491 |  |  |
|  |  |  |  |  | C21H16O9 | 0.490 |  |  |
|  |  |  |  |  | C17H16O6 | 0.488 | x |  |
|  |  |  |  |  | C25H18O12 | 0.488 |  |  |
|  |  |  |  |  | C17H26O9 | 0.487 | x |  |
|  |  |  |  |  | C25H32O15 | 0.487 |  |  |
|  |  |  |  |  | C28H24O18 | 0.486 |  |  |
|  |  |  |  |  | C25H34O12 | 0.483 | x |  |
|  |  |  |  |  | C27H34O14 | 0.481 | x |  |
|  |  |  |  |  | C21H28O14 | 0.479 |  |  |
|  |  |  |  |  | C27H30O12 | 0.477 |  |  |
|  |  |  |  |  | C11H10O6 | 0.466 |  |  |
|  |  |  |  |  | C24H32O13 | 0.465 |  |  |
|  |  |  |  |  | C27H26O13 | 0.464 |  |  |
|  |  |  |  |  | C19H26O9 | 0.455 | x |  |
|  |  |  |  |  | C25H22O11 | 0.436 |  |  |
|  |  |  |  |  | C13H18O10 | 0.427 |  |  |
|  |  |  |  |  | C14H12O5 | 0.423 |  |  |
|  |  |  |  |  | C16H18O13 | 0.423 |  | x |
|  |  |  |  |  | C21H24O9 | 0.422 | x |  |
|  |  |  |  |  | C20H28O10 | 0.421 | x |  |
|  |  |  |  |  | C14H16O4 | 0.421 | x |  |
|  |  |  |  |  | C17H26O10 | 0.419 | x |  |
|  |  |  |  |  | C19H28O11 | 0.418 | x |  |
|  |  |  |  |  | C28H34O15 | 0.415 |  |  |
|  |  |  |  |  | C27H32O13 | 0.411 |  |  |
|  |  |  |  |  | C28H28O17 | 0.406 |  |  |
|  |  |  |  |  | C25H34O13 | 0.403 | x |  |
|  |  |  |  |  | C28H34O13 | 0.398 | x |  |
|  |  |  |  |  | C21H28O10 | 0.397 | x |  |
|  |  |  |  |  | C27H34O15 | 0.393 |  |  |
|  |  |  |  |  | C15H16O13 | 0.393 |  | x |
|  |  |  |  |  | C11H14O6 | 0.384 | x |  |
|  |  |  |  |  | C15H14O5 | 0.374 |  |  |
|  |  |  |  |  | C17H22O13 | 0.370 |  | x |
|  |  |  |  |  | C27H28O13 | 0.369 |  |  |
|  |  |  |  |  | C28H36O14 | 0.367 | x |  |
|  |  |  |  |  | C19H26O13 | 0.363 |  |  |
|  |  |  |  |  | C12H12O4 | 0.361 |  |  |
|  |  |  |  |  | C21H22O9 | 0.359 | x |  |
|  |  |  |  |  | C26H28O11 | 0.357 |  |  |
|  |  |  |  |  | C24H26O10 | 0.355 | x |  |
|  |  |  |  |  | C19H20O7 | 0.346 | x |  |
|  |  |  |  |  | C26H34O13 | 0.340 | x |  |
|  |  |  |  |  | C28H32O13 | 0.336 |  |  |
|  |  |  |  |  | C21H30O11 | 0.325 | x |  |
|  |  |  |  |  | C19H16O7 | 0.325 |  |  |
|  |  |  |  |  | C29H34O15 | 0.324 |  |  |
|  |  |  |  |  | C22H32O11 | 0.324 | x |  |
|  |  |  |  |  | C28H34O16 | 0.323 |  |  |
|  |  |  |  |  | C27H36O13 | 0.323 | x |  |
|  |  |  |  |  | C26H26O18 | 0.321 |  |  |
|  |  |  |  |  | C22H32O12 | 0.319 | x |  |
|  |  |  |  |  | C29H30O17 | 0.319 |  |  |
|  |  |  |  |  | C26H32O12 | 0.318 | x |  |
|  |  |  |  |  | C29H24O16 | 0.316 |  |  |
|  |  |  |  |  | C20H28O11 | 0.316 | x |  |
|  |  |  |  |  | C26H30O11 | 0.312 | x |  |
|  |  |  |  |  | C22H30O10 | 0.308 | x |  |
|  |  |  |  |  | C26H34O12 | 0.286 | x |  |
|  |  |  |  |  | C19H28O10 | 0.285 | x |  |
|  |  |  |  |  | C25H30O10 | 0.278 | x |  |
|  |  |  |  |  | C21H20O8 | 0.261 |  |  |
|  |  |  |  |  | C22H28O10 | 0.260 | x |  |
|  |  |  |  |  | C18H18O6 | 0.257 | x |  |
|  |  |  |  |  | C14H16O12 | 0.257 |  | x |
|  |  |  |  |  | C14H10O5 | 0.251 |  |  |
|  |  |  |  |  | C24H32O11 | 0.251 | x |  |
|  |  |  |  |  | C19H22O8 | 0.249 | x |  |
|  |  |  |  |  | C22H20O9 | 0.248 |  |  |
|  |  |  |  |  | C10H10O5 | 0.248 |  | x |
|  |  |  |  |  | C29H26O16 | 0.245 |  |  |
|  |  |  |  |  | C26H32O11 | 0.241 | x |  |
|  |  |  |  |  | C25H32O11 | 0.240 | x |  |
|  |  |  |  |  | C28H34O12 | 0.235 |  |  |
|  |  |  |  |  | C20H20O7 | 0.228 |  |  |
|  |  |  |  |  | C26H34O11 | 0.205 | x |  |
|  |  |  |  |  | C23H24O9 | 0.199 | x |  |
|  |  |  |  |  | C23H32O11 | 0.196 | x |  |
|  |  |  |  |  | C29H32O16 | 0.194 |  |  |
|  |  |  |  |  | C24H34O11 | 0.194 | x |  |
|  |  |  |  |  | C29H36O13 | 0.192 |  |  |
|  |  |  |  |  | C29H34O16 | 0.191 |  |  |
|  |  |  |  |  | C29H32O15 | 0.180 |  |  |
|  |  |  |  |  | C26H36O12 | 0.175 | x |  |
|  |  |  |  |  | C30H38O14 | 0.173 |  |  |
|  |  |  |  |  | C24H28O10 | 0.164 | x |  |
|  |  |  |  |  | C22H24O9 | 0.160 | x |  |
|  |  |  |  |  | C20H18O7 | 0.157 |  |  |
|  |  |  |  |  | C21H22O8 | 0.153 | x |  |
|  |  |  |  |  | C27H32O11 | 0.144 |  |  |
|  |  |  |  |  | C18H28O10 | 0.141 | x |  |
|  |  |  |  |  | C18H18O7 | 0.141 | x |  |
|  |  |  |  |  | C27H34O12 | 0.133 |  |  |
|  |  |  |  |  | C25H34O11 | 0.130 | x |  |
|  |  |  |  |  | C24H30O10 | 0.125 | x |  |
|  |  |  |  |  | C16H12O6 | 0.119 |  |  |
|  |  |  |  |  | C13H12O4 | 0.116 |  |  |
|  |  |  |  |  | C27H36O12 | 0.109 |  |  |
|  |  |  |  |  | C20H24O9 | 0.108 | x |  |
|  |  |  |  |  | C21H30O10 | 0.107 | x |  |
|  |  |  |  |  | C27H34O11 | 0.093 |  |  |
|  |  |  |  |  | C25H28O10 | 0.091 | x |  |
|  |  |  |  |  | C22H22O9 | 0.089 |  |  |
|  |  |  |  |  | C20H30O11 | 0.086 | x |  |
|  |  |  |  |  | C23H34O11 | 0.085 | x |  |
|  |  |  |  |  | C14H14O4 | 0.080 | x |  |
|  |  |  |  |  | C26H26O10 | 0.076 |  |  |
|  |  |  |  |  | C19H24O9 | 0.073 | x |  |
|  |  |  |  |  | C24H34O12 | 0.070 | x |  |
|  |  |  |  |  | C29H38O13 | 0.064 |  |  |
|  |  |  |  |  | C11H10O4 | 0.062 |  |  |
|  |  |  |  |  | C30H36O13 | 0.054 |  |  |
|  |  |  |  |  | C17H28O8 | 0.039 | x |  |
|  |  |  |  |  | C29H36O12 | 0.032 |  |  |
|  |  |  |  |  | C24H34O10 | 0.008 | x |  |
|  |  |  |  |  | C20H30O10 | 0.007 | x |  |

Table A7 CHO formulas present before and after UV and NH2Cl disinfection at Lovö WTP and the change in relative abundance during the treatment as well as correlation with optical parameters

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Decrease** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |  | **Increase** | Change % | FI, β:α, %FDOM300-350 or %FDOM350-450 | SUVA, HIX or %FDOM450-600 |
| C14H18O7 | -10.036 | x |  |  | C14H18O9 | 12.148 |  | x |
| C15H18O7 | -9.433 |  |  |  | C12H16O7 | 9.648 | x |  |
| C15H20O6 | -8.456 | x |  |  | C12H14O7 | 9.647 |  |  |
| C17H20O8 | -5.175 |  |  |  | C12H14O8 | 9.452 |  |  |
| C14H16O7 | -4.947 | x |  |  | C13H16O9 | 8.938 |  |  |
| C15H22O6 | -4.365 | x |  |  | C15H18O9 | 8.614 |  |  |
| C15H18O6 | -4.143 | x |  |  | C13H16O7 | 8.602 |  |  |
| C16H20O6 | -3.857 | x |  |  | C15H18O8 | 8.394 |  |  |
| C15H20O7 | -3.584 |  |  |  | C15H20O8 | 7.691 | x |  |
| C18H22O8 | -3.520 | x |  |  | C15H18O10 | 6.834 |  | x |
| C14H16O6 | -3.157 |  |  |  | C14H16O10 | 6.791 |  | x |
| C14H18O5 | -2.981 |  |  |  | C16H20O10 | 6.699 |  |  |
| C16H22O7 | -2.816 |  |  |  | C12H16O8 | 6.646 |  |  |
| C18H24O8 | -2.798 | x |  |  | C14H16O9 | 6.475 |  | x |
| C15H16O7 | -2.718 |  |  |  | C15H16O9 | 6.418 |  | x |
| C19H24O8 | -2.705 | x |  |  | C12H12O8 | 6.143 |  | x |
| C16H22O6 | -2.515 | x |  |  | C15H16O10 | 6.142 |  | x |
| C17H22O7 | -2.402 | x |  |  | C13H14O9 | 6.095 |  |  |
| C19H24O7 | -2.333 | x |  |  | C14H14O9 | 6.021 |  | x |
| C16H20O7 | -2.331 |  |  |  | C13H14O10 | 6.011 |  | x |
| C17H24O7 | -2.217 | x |  |  | C11H14O6 | 5.820 | x |  |
| C17H20O9 | -2.196 |  |  |  | C16H18O10 | 5.284 |  |  |
| C18H24O7 | -2.145 | x |  |  | C11H14O8 | 4.893 |  |  |
| C17H24O8 | -1.901 | x |  |  | C13H18O8 | 4.883 | x |  |
| C14H20O7 | -1.807 | x |  |  | C15H16O11 | 4.840 |  | x |
| C16H22O5 | -1.792 | x |  |  | C13H16O10 | 4.701 |  | x |
| C15H16O6 | -1.788 |  |  |  | C17H20O10 | 4.453 |  |  |
| C20H24O8 | -1.740 | x |  |  | C15H20O10 | 4.294 |  |  |
| C16H16O8 | -1.677 |  |  |  | C18H22O10 | 4.104 |  |  |
| C16H18O6 | -1.671 | x |  |  | C17H18O10 | 4.097 |  |  |
| C16H20O5 | -1.643 | x |  |  | C14H14O10 | 4.044 |  | x |
| C14H12O8 | -1.569 |  | x |  | C13H14O7 | 4.041 |  |  |
| C17H22O6 | -1.564 | x |  |  | C17H18O11 | 4.004 |  | x |
| C12H14O5 | -1.535 | x |  |  | C12H18O7 | 3.905 | x |  |
| C14H16O8 | -1.465 |  | x |  | C16H20O11 | 3.828 |  |  |
| C19H22O8 | -1.459 | x |  |  | C11H12O7 | 3.793 |  |  |
| C17H22O5 | -1.450 | x |  |  | C11H14O7 | 3.766 |  |  |
| C16H24O6 | -1.392 | x |  |  | C13H18O7 | 3.764 | x |  |
| C19H26O7 | -1.385 | x |  |  | C14H20O9 | 3.753 | x |  |
| C14H20O6 | -1.363 |  |  |  | C12H14O6 | 3.746 | x |  |
| C19H22O9 | -1.340 | x |  |  | C12H14O9 | 3.711 |  |  |
| C19H26O8 | -1.333 | x |  |  | C16H18O11 | 3.681 |  | x |
| C17H18O6 | -1.259 | x |  |  | C15H22O8 | 3.679 | x |  |
| C17H20O6 | -1.225 | x |  |  | C11H12O8 | 3.627 |  |  |
| C16H16O6 | -1.219 | x |  |  | C14H18O10 | 3.565 |  | x |
| C18H26O7 | -1.212 | x |  |  | C15H16O8 | 3.396 |  | x |
| C20H26O7 | -1.198 | x |  |  | C17H22O11 | 3.322 | x |  |
| C14H14O7 | -1.169 |  |  |  | C15H14O11 | 3.174 |  | x |
| C17H20O7 | -1.162 | x |  |  | C14H14O11 | 3.123 |  | x |
| C18H26O6 | -1.071 | x |  |  | C18H20O10 | 3.114 |  |  |
| C14H14O5 | -1.069 | x |  |  | C16H16O11 | 3.019 |  | x |
| C15H22O5 | -1.054 | x |  |  | C10H12O7 | 2.999 |  |  |
| C14H22O7 | -1.039 | x |  |  | C14H20O8 | 2.954 | x |  |
| C15H20O5 | -1.032 | x |  |  | C16H18O12 | 2.954 |  | x |
| C17H24O5 | -0.962 | x |  |  | C15H22O9 | 2.877 | x |  |
| C18H24O6 | -0.955 | x |  |  | C17H16O11 | 2.872 |  | x |
| C15H18O5 | -0.947 | x |  |  | C11H16O6 | 2.833 |  |  |
| C15H24O6 | -0.939 | x |  |  | C16H18O9 | 2.830 |  |  |
| C21H26O9 | -0.932 | x |  |  | C13H12O10 | 2.692 |  | x |
| C18H22O6 | -0.928 | x |  |  | C15H20O9 | 2.690 |  |  |
| C20H26O8 | -0.899 | x |  |  | C13H12O9 | 2.678 |  | x |
| C18H20O8 | -0.876 |  |  |  | C16H16O10 | 2.673 |  | x |
| C14H16O5 | -0.854 | x |  |  | C14H16O11 | 2.621 |  | x |
| C18H18O8 | -0.829 | x |  |  | C17H24O10 | 2.577 | x |  |
| C13H16O4 | -0.807 | x |  |  | C10H14O6 | 2.414 | x |  |
| C17H20O5 | -0.802 | x |  |  | C17H20O11 | 2.393 |  |  |
| C13H12O6 | -0.798 |  |  |  | C12H12O7 | 2.364 |  | x |
| C13H18O4 | -0.790 | x |  |  | C18H24O9 | 2.363 | x |  |
| C15H14O7 | -0.787 |  |  |  | C15H18O11 | 2.352 |  |  |
| C20H28O8 | -0.777 | x |  |  | C17H20O12 | 2.347 |  | x |
| C20H22O10 | -0.768 | x |  |  | C16H20O9 | 2.288 |  |  |
| C19H26O6 | -0.765 | x |  |  | C16H22O10 | 2.257 | x |  |
| C19H24O6 | -0.745 | x |  |  | C14H12O9 | 2.211 |  | x |
| C17H24O6 | -0.722 | x |  |  | C16H14O11 | 2.095 |  | x |
| C14H14O8 | -0.713 |  | x |  | C12H12O6 | 2.050 |  |  |
| C16H16O7 | -0.695 |  |  |  | C16H14O10 | 2.046 |  | x |
| C18H22O7 | -0.674 | x |  |  | C11H10O8 | 2.000 |  |  |
| C22H26O9 | -0.668 | x |  |  | C15H14O12 | 1.949 |  | x |
| C20H28O7 | -0.657 | x |  |  | C13H12O7 | 1.919 |  | x |
| C15H20O4 | -0.633 | x |  |  | C17H24O9 | 1.911 | x |  |
| C18H26O8 | -0.629 | x |  |  | C11H16O8 | 1.902 |  |  |
| C19H22O7 | -0.623 | x |  |  | C11H10O7 | 1.894 |  |  |
| C18H20O6 | -0.583 | x |  |  | C15H20O11 | 1.864 |  |  |
| C15H14O8 | -0.577 |  | x |  | C11H12O9 | 1.846 |  |  |
| C16H18O5 | -0.569 | x |  |  | C13H20O6 | 1.843 | x |  |
| C19H20O9 | -0.549 |  |  |  | C17H22O10 | 1.832 |  |  |
| C21H26O7 | -0.535 | x |  |  | C16H22O8 | 1.807 |  |  |
| C21H24O9 | -0.533 | x |  |  | C11H8O7 | 1.795 |  |  |
| C16H24O5 | -0.528 | x |  |  | C16H16O12 | 1.774 |  | x |
| C20H28O6 | -0.522 | x |  |  | C14H12O10 | 1.767 |  | x |
| C22H26O11 | -0.506 | x |  |  | C18H24O10 | 1.745 | x |  |
| C20H24O7 | -0.498 | x |  |  | C14H12O11 | 1.728 |  | x |
| C18H24O5 | -0.491 | x |  |  | C13H16O8 | 1.711 |  |  |
| C21H26O10 | -0.488 | x |  |  | C16H14O12 | 1.705 |  | x |
| C21H24O8 | -0.488 | x |  |  | C15H12O10 | 1.685 |  | x |
| C14H18O6 | -0.487 |  |  |  | C10H14O7 | 1.681 | x |  |
| C17H14O8 | -0.476 |  | x |  | C15H16O12 | 1.681 |  | x |
| C15H14O6 | -0.471 |  |  |  | C18H24O11 | 1.657 | x |  |
| C20H22O8 | -0.470 | x |  |  | C16H20O8 | 1.647 |  |  |
| C13H14O6 | -0.467 |  |  |  | C12H16O6 | 1.632 |  |  |
| C22H28O8 | -0.442 | x |  |  | C15H12O11 | 1.631 |  | x |
| C23H24O12 | -0.441 |  |  |  | C16H22O11 | 1.625 | x |  |
| C24H28O11 | -0.439 | x |  |  | C12H14O10 | 1.610 |  |  |
| C23H30O8 | -0.438 | x |  |  | C12H18O8 | 1.606 | x |  |
| C20H20O9 | -0.436 | x |  |  | C12H12O10 | 1.585 |  |  |
| C18H22O5 | -0.431 | x |  |  | C17H18O12 | 1.584 |  | x |
| C22H26O10 | -0.420 | x |  |  | C12H10O8 | 1.567 |  | x |
| C15H18O4 | -0.420 | x |  |  | C13H18O6 | 1.543 |  |  |
| C20H18O10 | -0.417 |  |  |  | C18H20O11 | 1.530 |  |  |
| C17H18O8 | -0.416 |  |  |  | C14H20O10 | 1.510 |  |  |
| C16H14O7 | -0.413 |  |  |  | C17H16O10 | 1.501 |  | x |
| C20H22O9 | -0.412 | x |  |  | C12H16O9 | 1.498 | x |  |
| C23H28O10 | -0.409 | x |  |  | C13H10O9 | 1.479 |  | x |
| C21H22O10 | -0.401 | x |  |  | C19H24O11 | 1.409 | x |  |
| C20H26O6 | -0.400 | x |  |  | C19H24O10 | 1.408 | x |  |
| C17H26O6 | -0.396 | x |  |  | C17H16O12 | 1.398 |  | x |
| C16H14O6 | -0.395 | x |  |  | C20H24O11 | 1.397 | x |  |
| C21H28O7 | -0.388 | x |  |  | C13H14O11 | 1.386 |  |  |
| C16H16O5 | -0.388 | x |  |  | C13H12O11 | 1.379 |  | x |
| C26H34O10 | -0.387 | x |  |  | C13H10O10 | 1.374 |  | x |
| C15H12O7 | -0.387 |  |  |  | C13H16O5 | 1.374 | x |  |
| C25H32O10 | -0.380 | x |  |  | C12H12O9 | 1.333 |  |  |
| C25H28O11 | -0.379 | x |  |  | C19H20O12 | 1.332 |  | x |
| C19H24O9 | -0.370 | x |  |  | C15H18O12 | 1.314 |  | x |
| C21H22O9 | -0.369 | x |  |  | C13H18O9 | 1.312 | x |  |
| C25H30O12 | -0.369 | x |  |  | C13H18O10 | 1.305 |  |  |
| C16H14O9 | -0.365 |  | x |  | C18H26O10 | 1.259 | x |  |
| C23H30O9 | -0.354 | x |  |  | C16H24O10 | 1.247 | x |  |
| C25H34O11 | -0.346 | x |  |  | C10H10O7 | 1.233 |  |  |
| C26H32O13 | -0.344 | x |  |  | C16H24O9 | 1.211 | x |  |
| C23H28O11 | -0.341 | x |  |  | C18H20O12 | 1.208 |  |  |
| C19H26O5 | -0.340 | x |  |  | C11H8O8 | 1.155 |  |  |
| C23H26O13 | -0.339 |  |  |  | C17H14O11 | 1.138 |  | x |
| C27H34O12 | -0.336 |  |  |  | C15H22O10 | 1.135 | x |  |
| C14H22O6 | -0.336 | x |  |  | C13H16O6 | 1.124 |  |  |
| C22H22O10 | -0.335 |  |  |  | C16H20O12 | 1.120 |  |  |
| C25H32O12 | -0.333 | x |  |  | C11H16O7 | 1.110 | x |  |
| C21H20O10 | -0.333 |  |  |  | C12H10O7 | 1.097 |  | x |
| C23H26O11 | -0.331 | x |  |  | C15H14O10 | 1.095 |  | x |
| C16H18O7 | -0.330 |  |  |  | C14H14O12 | 1.070 |  | x |
| C22H26O8 | -0.324 | x |  |  | C13H10O7 | 1.065 |  | x |
| C24H28O10 | -0.323 | x |  |  | C11H10O9 | 1.063 |  |  |
| C23H22O13 | -0.322 |  | x |  | C11H14O9 | 1.061 |  |  |
| C22H18O13 | -0.321 |  | x |  | C18H22O12 | 1.054 |  |  |
| C12H12O5 | -0.321 | x |  |  | C16H12O11 | 1.052 |  | x |
| C24H28O12 | -0.320 | x |  |  | C10H12O6 | 1.034 |  |  |
| C26H32O11 | -0.318 | x |  |  | C17H22O12 | 1.025 |  |  |
| C22H24O9 | -0.316 | x |  |  | C12H10O9 | 1.017 |  | x |
| C23H28O12 | -0.313 | x |  |  | C14H10O9 | 1.016 |  | x |
| C18H16O7 | -0.313 |  |  |  | C17H26O9 | 1.013 | x |  |
| C24H30O12 | -0.313 | x |  |  | C16H22O9 | 1.013 | x |  |
| C25H30O11 | -0.310 | x |  |  | C18H26O9 | 1.011 | x |  |
| C23H24O11 | -0.310 | x |  |  | C18H22O9 | 1.011 |  |  |
| C23H20O13 | -0.306 |  | x |  | C18H18O11 | 0.982 |  | x |
| C18H20O5 | -0.304 | x |  |  | C16H16O13 | 0.979 |  | x |
| C17H14O9 | -0.304 |  | x |  | C17H24O11 | 0.979 | x |  |
| C20H22O7 | -0.303 | x |  |  | C18H24O12 | 0.973 | x |  |
| C25H28O12 | -0.300 |  |  |  | C13H12O8 | 0.972 |  | x |
| C23H22O12 | -0.299 |  | x |  | C15H14O9 | 0.966 |  | x |
| C24H22O14 | -0.297 |  |  |  | C16H12O12 | 0.942 |  | x |
| C17H26O7 | -0.297 | x |  |  | C18H22O11 | 0.942 | x |  |
| C22H20O10 | -0.297 |  |  |  | C15H12O12 | 0.933 |  | x |
| C17H22O4 | -0.296 |  |  |  | C19H28O9 | 0.926 | x |  |
| C16H16O9 | -0.296 |  | x |  | C20H28O10 | 0.922 | x |  |
| C22H22O11 | -0.293 |  |  |  | C20H22O13 | 0.912 |  | x |
| C25H32O11 | -0.292 | x |  |  | C18H18O12 | 0.903 |  | x |
| C20H22O6 | -0.288 |  |  |  | C18H18O13 | 0.900 |  | x |
| C22H24O14 | -0.286 |  | x |  | C10H14O5 | 0.896 |  |  |
| C18H28O7 | -0.285 | x |  |  | C14H18O11 | 0.886 |  |  |
| C17H26O5 | -0.283 | x |  |  | C17H14O12 | 0.883 |  | x |
| C24H30O10 | -0.282 | x |  |  | C12H18O5 | 0.873 | x |  |
| C24H32O9 | -0.278 | x |  |  | C10H10O6 | 0.869 |  |  |
| C26H36O9 | -0.277 |  |  |  | C14H10O10 | 0.866 |  | x |
| C26H30O12 | -0.276 |  |  |  | C19H26O11 | 0.862 | x |  |
| C19H22O6 | -0.275 | x |  |  | C12H8O8 | 0.849 |  |  |
| C15H16O5 | -0.275 | x |  |  | C18H16O10 | 0.841 |  | x |
| C28H32O13 | -0.274 |  |  |  | C20H22O12 | 0.838 |  |  |
| C27H34O11 | -0.273 |  |  |  | C10H8O7 | 0.824 |  |  |
| C28H36O11 | -0.272 |  |  |  | C19H22O13 | 0.818 |  | x |
| C20H14O12 | -0.272 |  | x |  | C17H12O11 | 0.807 |  | x |
| C25H24O13 | -0.272 |  | x |  | C15H12O9 | 0.802 |  | x |
| C26H32O12 | -0.272 | x |  |  | C17H16O9 | 0.798 |  | x |
| C30H40O13 | -0.271 |  |  |  | C12H10O10 | 0.797 |  |  |
| C26H34O12 | -0.270 | x |  |  | C9H10O6 | 0.790 |  |  |
| C19H28O6 | -0.270 | x |  |  | C17H18O13 | 0.782 |  | x |
| C24H32O11 | -0.270 | x |  |  | C19H22O12 | 0.781 |  |  |
| C18H26O5 | -0.270 | x |  |  | C17H14O10 | 0.780 |  | x |
| C17H18O5 | -0.269 | x |  |  | C12H10O6 | 0.768 |  |  |
| C22H28O7 | -0.267 | x |  |  | C14H22O9 | 0.764 | x |  |
| C24H26O12 | -0.267 | x |  |  | C16H14O13 | 0.759 |  | x |
| C22H20O12 | -0.267 |  | x |  | C21H24O12 | 0.757 | x |  |
| C13H20O7 | -0.267 | x |  |  | C19H20O13 | 0.749 |  | x |
| C19H18O8 | -0.267 | x |  |  | C10H12O8 | 0.747 |  |  |
| C23H28O9 | -0.265 | x |  |  | C19H26O12 | 0.738 | x |  |
| C18H18O7 | -0.265 | x |  |  | C19H26O9 | 0.735 | x |  |
| C24H26O11 | -0.264 |  |  |  | C11H16O5 | 0.730 | x |  |
| C29H36O13 | -0.264 |  |  |  | C18H22O13 | 0.729 |  | x |
| C28H34O15 | -0.264 |  |  |  | C11H12O5 | 0.720 | x |  |
| C29H34O14 | -0.260 |  |  |  | C13H8O8 | 0.716 |  | x |
| C26H34O11 | -0.260 | x |  |  | C18H16O12 | 0.714 |  | x |
| C25H30O13 | -0.260 |  |  |  | C10H8O6 | 0.713 |  |  |
| C28H36O14 | -0.259 | x |  |  | C14H16O12 | 0.710 |  | x |
| C20H30O7 | -0.258 | x |  |  | C13H18O5 | 0.706 | x |  |
| C17H24O4 | -0.258 |  |  |  | C10H10O8 | 0.702 |  |  |
| C24H28O13 | -0.257 |  |  |  | C17H16O13 | 0.701 |  | x |
| C24H32O8 | -0.257 | x |  |  | C19H20O11 | 0.687 |  |  |
| C23H20O11 | -0.256 |  | x |  | C14H12O12 | 0.670 |  | x |
| C18H22O4 | -0.255 |  |  |  | C15H24O8 | 0.666 | x |  |
| C28H32O14 | -0.255 |  |  |  | C12H12O11 | 0.664 |  |  |
| C30H36O14 | -0.254 |  |  |  | C21H26O11 | 0.659 | x |  |
| C26H30O11 | -0.254 | x |  |  | C19H24O13 | 0.652 |  |  |
| C20H28O5 | -0.253 |  |  |  | C12H8O9 | 0.648 |  |  |
| C24H30O11 | -0.253 | x |  |  | C20H22O14 | 0.647 |  | x |
| C25H28O13 | -0.253 |  |  |  | C9H10O7 | 0.647 |  |  |
| C22H28O9 | -0.253 | x |  |  | C18H20O13 | 0.646 |  | x |
| C25H30O14 | -0.251 |  |  |  | C11H8O9 | 0.646 |  | x |
| C24H22O15 | -0.250 |  |  |  | C10H16O6 | 0.643 |  |  |
| C23H26O10 | -0.250 | x |  |  | C20H28O9 | 0.638 | x |  |
| C20H14O11 | -0.250 |  | x |  | C15H14O13 | 0.637 |  | x |
| C22H18O12 | -0.249 |  | x |  | C18H14O12 | 0.631 |  | x |
| C27H30O15 | -0.247 |  |  |  | C9H12O6 | 0.628 |  |  |
| C27H32O14 | -0.245 |  |  |  | C19H22O11 | 0.624 | x |  |
| C20H26O5 | -0.244 |  |  |  | C15H10O11 | 0.623 |  | x |
| C22H30O8 | -0.244 | x |  |  | C19H18O13 | 0.622 |  | x |
| C12H14O4 | -0.243 | x |  |  | C13H20O9 | 0.609 | x |  |
| C18H20O7 | -0.242 | x |  |  | C18H16O13 | 0.600 |  | x |
| C25H22O13 | -0.242 |  |  |  | C12H16O10 | 0.599 |  |  |
| C25H32O8 | -0.242 |  |  |  | C19H20O10 | 0.598 |  |  |
| C24H26O10 | -0.242 | x |  |  | C20H20O13 | 0.595 |  | x |
| C27H32O12 | -0.240 |  |  |  | C20H26O9 | 0.589 | x |  |
| C23H26O12 | -0.239 | x |  |  | C13H16O11 | 0.585 |  |  |
| C19H14O11 | -0.239 |  | x |  | C20H24O13 | 0.576 |  |  |
| C28H36O12 | -0.239 |  |  |  | C16H10O11 | 0.571 |  | x |
| C24H24O14 | -0.236 |  | x |  | C14H12O6 | 0.568 |  |  |
| C16H12O6 | -0.236 |  |  |  | C12H16O5 | 0.560 | x |  |
| C19H24O5 | -0.235 | x |  |  | C17H14O13 | 0.559 |  | x |
| C21H30O6 | -0.233 |  |  |  | C17H26O10 | 0.559 | x |  |
| C23H22O14 | -0.233 |  | x |  | C18H28O9 | 0.555 | x |  |
| C27H34O10 | -0.232 |  |  |  | C19H18O14 | 0.554 |  | x |
| C19H18O7 | -0.229 | x |  |  | C11H14O5 | 0.553 |  |  |
| C31H40O16 | -0.229 |  |  |  | C12H18O6 | 0.551 | x |  |
| C20H24O6 | -0.228 | x |  |  | C21H26O12 | 0.549 | x |  |
| C19H28O7 | -0.227 | x |  |  | C16H18O13 | 0.546 |  | x |
| C20H16O11 | -0.227 |  | x |  | C16H12O10 | 0.545 |  | x |
| C23H20O14 | -0.224 |  |  |  | C19H28O8 | 0.540 | x |  |
| C27H36O11 | -0.224 |  |  |  | C19H18O12 | 0.535 |  | x |
| C24H30O8 | -0.224 | x |  |  | C14H8O10 | 0.535 |  | x |
| C22H22O13 | -0.223 |  | x |  | C15H24O9 | 0.526 | x |  |
| C24H32O10 | -0.223 | x |  |  | C20H20O11 | 0.525 |  |  |
| C17H14O6 | -0.222 |  |  |  | C20H24O12 | 0.517 | x |  |
| C25H26O12 | -0.221 |  | x |  | C16H14O8 | 0.516 |  | x |
| C27H36O12 | -0.220 |  |  |  | C17H20O13 | 0.516 |  | x |
| C26H28O11 | -0.220 |  |  |  | C11H18O6 | 0.515 |  |  |
| C21H28O6 | -0.219 |  |  |  | C14H10O11 | 0.512 |  | x |
| C27H36O9 | -0.219 |  |  |  | C18H18O9 | 0.507 |  |  |
| C28H36O15 | -0.218 |  |  |  | C18H20O14 | 0.496 |  | x |
| C14H20O5 | -0.218 | x |  |  | C12H8O6 | 0.494 |  |  |
| C21H18O11 | -0.217 |  | x |  | C12H8O7 | 0.493 |  |  |
| C23H22O11 | -0.217 |  |  |  | C13H8O7 | 0.489 |  | x |
| C22H22O14 | -0.217 |  | x |  | C13H10O11 | 0.488 |  | x |
| C26H28O12 | -0.216 |  |  |  | C20H26O12 | 0.482 | x |  |
| C15H24O5 | -0.215 | x |  |  | C15H10O9 | 0.482 |  | x |
| C23H24O13 | -0.214 |  |  |  | C18H18O14 | 0.476 |  | x |
| C22H24O13 | -0.213 |  |  |  | C20H28O12 | 0.474 | x |  |
| C27H34O14 | -0.213 | x |  |  | C12H20O7 | 0.472 | x |  |
| C25H34O10 | -0.212 | x |  |  | C21H28O10 | 0.470 | x |  |
| C26H32O9 | -0.212 |  |  |  | C15H22O11 | 0.470 |  |  |
| C27H36O10 | -0.211 |  |  |  | C15H16O13 | 0.468 |  | x |
| C27H32O11 | -0.211 |  |  |  | C15H10O10 | 0.467 |  | x |
| C21H18O13 | -0.211 |  | x |  | C9H12O7 | 0.464 |  |  |
| C24H24O10 | -0.211 |  |  |  | C18H26O11 | 0.457 | x |  |
| C22H18O10 | -0.211 |  |  |  | C17H24O12 | 0.457 |  |  |
| C29H36O15 | -0.210 |  |  |  | C13H8O10 | 0.455 |  | x |
| C15H16O4 | -0.208 |  |  |  | C13H8O9 | 0.453 |  | x |
| C23H22O10 | -0.207 |  |  |  | C19H28O11 | 0.449 | x |  |
| C26H30O13 | -0.206 |  |  |  | C21H28O12 | 0.448 | x |  |
| C23H18O14 | -0.206 |  |  |  | C16H26O8 | 0.445 | x |  |
| C21H16O11 | -0.205 |  | x |  | C20H26O13 | 0.438 |  |  |
| C22H20O13 | -0.204 |  | x |  | C16H18O8 | 0.438 |  |  |
| C27H32O13 | -0.204 |  |  |  | C19H24O12 | 0.437 | x |  |
| C24H26O14 | -0.204 |  | x |  | C19H16O13 | 0.434 |  | x |
| C22H22O12 | -0.203 |  |  |  | C14H22O8 | 0.422 | x |  |
| C24H22O11 | -0.202 |  |  |  | C19H20O14 | 0.422 |  | x |
| C22H24O12 | -0.201 | x |  |  | C21H28O13 | 0.407 |  |  |
| C28H34O13 | -0.201 | x |  |  | C22H30O10 | 0.404 | x |  |
| C25H32O9 | -0.201 | x |  |  | C15H12O13 | 0.404 |  | x |
| C26H28O13 | -0.201 |  |  |  | C17H22O13 | 0.402 |  | x |
| C23H24O10 | -0.201 |  |  |  | C11H18O5 | 0.397 |  |  |
| C23H28O8 | -0.200 | x |  |  | C18H16O14 | 0.393 |  | x |
| C25H20O15 | -0.199 |  |  |  | C15H20O12 | 0.390 |  |  |
| C14H12O5 | -0.199 |  |  |  | C18H16O9 | 0.390 |  | x |
| C29H34O15 | -0.198 |  |  |  | C12H18O9 | 0.387 |  |  |
| C25H36O11 | -0.197 |  |  |  | C18H14O13 | 0.387 |  | x |
| C25H20O13 | -0.196 |  |  |  | C19H22O10 | 0.386 | x |  |
| C24H24O13 | -0.196 |  | x |  | C13H20O8 | 0.386 | x |  |
| C25H26O13 | -0.195 |  | x |  | C16H22O12 | 0.385 |  |  |
| C27H38O12 | -0.195 |  |  |  | C18H18O10 | 0.384 |  |  |
| C23H30O10 | -0.194 | x |  |  | C14H8O9 | 0.382 |  | x |
| C17H16O6 | -0.193 | x |  |  | C16H12O8 | 0.381 |  | x |
| C24H32O12 | -0.192 | x |  |  | C21H24O11 | 0.376 | x |  |
| C17H20O4 | -0.191 |  |  |  | C18H24O13 | 0.372 |  |  |
| C22H24O8 | -0.191 | x |  |  | C11H12O10 | 0.368 |  |  |
| C27H30O13 | -0.191 |  |  |  | C17H12O12 | 0.368 |  | x |
| C22H20O14 | -0.190 |  | x |  | C13H22O6 | 0.367 |  |  |
| C22H28O12 | -0.190 | x |  |  | C20H28O11 | 0.363 | x |  |
| C24H22O13 | -0.190 |  | x |  | C22H28O11 | 0.362 | x |  |
| C24H34O9 | -0.189 | x |  |  | C20H30O10 | 0.359 | x |  |
| C24H20O15 | -0.188 |  |  |  | C19H26O10 | 0.359 | x |  |
| C29H34O13 | -0.186 |  |  |  | C20H26O10 | 0.358 | x |  |
| C24H26O13 | -0.185 |  |  |  | C19H16O14 | 0.348 |  | x |
| C26H32O10 | -0.185 | x |  |  | C20H20O14 | 0.346 |  | x |
| C21H18O10 | -0.185 |  | x |  | C21H26O13 | 0.345 | x |  |
| C17H12O7 | -0.185 |  | x |  | C17H14O14 | 0.344 |  | x |
| C29H38O14 | -0.184 |  |  |  | C19H28O12 | 0.342 |  |  |
| C27H34O13 | -0.184 | x |  |  | C12H20O5 | 0.341 |  |  |
| C21H22O12 | -0.184 |  |  |  | C10H14O8 | 0.335 |  |  |
| C21H20O13 | -0.183 |  | x |  | C18H14O10 | 0.329 |  | x |
| C22H18O14 | -0.182 |  | x |  | C17H18O14 | 0.328 |  | x |
| C27H30O11 | -0.182 |  |  |  | C16H12O13 | 0.327 |  |  |
| C28H34O12 | -0.181 |  |  |  | C20H24O14 | 0.319 |  | x |
| C26H34O9 | -0.180 |  |  |  | C20H20O12 | 0.310 |  | x |
| C19H20O6 | -0.180 | x |  |  | C19H20O15 | 0.309 |  |  |
| C25H26O11 | -0.180 |  |  |  | C19H18O15 | 0.307 |  | x |
| C30H40O14 | -0.179 |  |  |  | C15H22O7 | 0.303 | x |  |
| C22H20O11 | -0.179 |  | x |  | C16H24O8 | 0.297 | x |  |
| C15H8O8 | -0.178 |  | x |  | C19H16O12 | 0.294 |  | x |
| C23H20O12 | -0.177 |  | x |  | C16H10O10 | 0.291 |  | x |
| C17H22O8 | -0.177 |  |  |  | C17H26O11 | 0.291 |  |  |
| C30H36O16 | -0.176 |  |  |  | C12H8O10 | 0.290 |  | x |
| C31H38O15 | -0.174 |  |  |  | C14H10O6 | 0.290 |  |  |
| C28H32O16 | -0.172 |  |  |  | C16H24O7 | 0.288 | x |  |
| C26H36O10 | -0.171 |  |  |  | C20H30O9 | 0.287 | x |  |
| C23H22O15 | -0.171 |  |  |  | C11H8O6 | 0.286 |  |  |
| C26H30O10 | -0.170 |  |  |  | C21H28O11 | 0.285 | x |  |
| C30H38O16 | -0.170 |  |  |  | C10H10O5 | 0.284 |  | x |
| C16H12O9 | -0.168 |  | x |  | C12H16O4 | 0.283 | x |  |
| C25H30O10 | -0.167 | x |  |  | C15H12O8 | 0.282 |  | x |
| C25H24O12 | -0.167 |  |  |  | C21H30O9 | 0.279 | x |  |
| C29H36O14 | -0.167 |  |  |  | C22H30O12 | 0.277 | x |  |
| C22H30O7 | -0.166 | x |  |  | C14H12O7 | 0.277 |  |  |
| C30H38O15 | -0.166 |  |  |  | C10H12O5 | 0.276 |  |  |
| C29H38O12 | -0.165 |  |  |  | C11H10O5 | 0.276 |  |  |
| C22H22O9 | -0.164 |  |  |  | C22H32O11 | 0.275 | x |  |
| C21H24O10 | -0.164 | x |  |  | C20H24O9 | 0.274 | x |  |
| C22H24O11 | -0.163 | x |  |  | C19H28O10 | 0.274 | x |  |
| C25H24O11 | -0.162 |  |  |  | C16H26O7 | 0.271 | x |  |
| C26H30O14 | -0.159 |  |  |  | C19H18O11 | 0.269 |  | x |
| C26H34O13 | -0.159 | x |  |  | C18H28O10 | 0.269 | x |  |
| C23H20O15 | -0.159 |  |  |  | C16H16O14 | 0.267 |  |  |
| C22H18O15 | -0.159 |  |  |  | C17H16O14 | 0.266 |  | x |
| C21H18O9 | -0.159 |  | x |  | C21H24O13 | 0.255 |  |  |
| C13H20O4 | -0.158 | x |  |  | C18H26O12 | 0.252 |  |  |
| C29H38O15 | -0.158 |  |  |  | C21H30O10 | 0.250 | x |  |
| C24H28O9 | -0.158 | x |  |  | C17H18O9 | 0.250 |  |  |
| C22H16O12 | -0.157 |  | x |  | C16H20O13 | 0.248 |  |  |
| C28H32O12 | -0.157 |  |  |  | C22H28O13 | 0.247 | x |  |
| C28H38O11 | -0.157 |  |  |  | C19H16O11 | 0.240 |  | x |
| C15H24O7 | -0.156 | x |  |  | C20H26O14 | 0.239 |  | x |
| C17H16O8 | -0.156 |  |  |  | C20H24O10 | 0.238 | x |  |
| C19H28O5 | -0.156 |  |  |  | C20H26O11 | 0.235 | x |  |
| C26H24O14 | -0.156 |  |  |  | C18H28O8 | 0.234 | x |  |
| C26H26O14 | -0.154 |  |  |  | C16H24O11 | 0.230 |  |  |
| C19H18O10 | -0.154 |  |  |  | C20H30O8 | 0.230 | x |  |
| C24H20O13 | -0.154 |  |  |  | C14H8O8 | 0.226 |  | x |
| C29H38O11 | -0.154 |  |  |  | C18H22O14 | 0.223 |  |  |
| C21H30O7 | -0.153 | x |  |  | C19H24O14 | 0.221 |  |  |
| C22H26O7 | -0.153 |  |  |  | C15H10O8 | 0.220 |  | x |
| C15H10O7 | -0.153 |  | x |  | C23H32O10 | 0.215 | x |  |
| C19H30O6 | -0.152 |  |  |  | C14H20O11 | 0.214 |  |  |
| C28H30O12 | -0.151 |  |  |  | C20H22O15 | 0.213 |  | x |
| C29H38O13 | -0.151 |  |  |  | C11H12O6 | 0.210 |  |  |
| C32H42O14 | -0.150 |  |  |  | C20H30O11 | 0.201 | x |  |
| C13H16O3 | -0.150 |  |  |  | C17H12O13 | 0.200 |  | x |
| C29H40O13 | -0.150 |  |  |  | C19H26O13 | 0.200 |  |  |
| C21H20O8 | -0.149 |  |  |  | C11H10O6 | 0.199 |  |  |
| C31H40O15 | -0.149 |  |  |  | C19H16O15 | 0.194 |  | x |
| C31H42O14 | -0.148 |  |  |  | C14H22O5 | 0.192 | x |  |
| C21H14O13 | -0.147 |  |  |  | C22H32O9 | 0.190 | x |  |
| C27H36O14 | -0.147 |  |  |  | C13H10O8 | 0.190 |  | x |
| C23H26O9 | -0.146 | x |  |  | C20H20O15 | 0.190 |  | x |
| C29H34O16 | -0.144 |  |  |  | C18H12O12 | 0.189 |  | x |
| C13H14O8 | -0.143 |  |  |  | C14H20O4 | 0.186 | x |  |
| C21H18O12 | -0.143 |  | x |  | C20H20O10 | 0.186 |  |  |
| C23H18O11 | -0.142 |  |  |  | C16H26O9 | 0.181 |  |  |
| C28H38O13 | -0.141 |  |  |  | C17H22O9 | 0.181 | x |  |
| C22H16O13 | -0.140 |  | x |  | C21H24O14 | 0.178 |  | x |
| C24H30O9 | -0.140 | x |  |  | C16H14O14 | 0.176 |  |  |
| C30H38O14 | -0.139 |  |  |  | C20H16O13 | 0.174 |  | x |
| C17H26O8 | -0.139 | x |  |  | C18H16O15 | 0.173 |  |  |
| C27H28O14 | -0.138 |  |  |  | C19H22O14 | 0.171 |  | x |
| C23H18O13 | -0.138 |  | x |  | C21H32O9 | 0.167 | x |  |
| C20H16O12 | -0.137 |  | x |  | C13H22O7 | 0.166 | x |  |
| C27H28O16 | -0.137 |  |  |  | C13H12O4 | 0.166 |  |  |
| C26H36O11 | -0.136 | x |  |  | C23H30O11 | 0.163 | x |  |
| C27H30O14 | -0.136 |  |  |  | C21H30O11 | 0.162 | x |  |
| C23H24O9 | -0.136 | x |  |  | C22H30O13 | 0.162 | x |  |
| C23H18O15 | -0.135 |  |  |  | C18H14O14 | 0.160 |  | x |
| C21H28O8 | -0.134 | x |  |  | C19H20O8 | 0.159 | x |  |
| C30H38O12 | -0.133 |  |  |  | C22H30O11 | 0.159 | x |  |
| C29H40O14 | -0.133 |  |  |  | C18H16O11 | 0.156 |  | x |
| C18H28O6 | -0.132 | x |  |  | C21H30O12 | 0.155 | x |  |
| C19H18O6 | -0.132 |  |  |  | C21H26O14 | 0.154 |  | x |
| C22H18O11 | -0.132 |  | x |  | C20H18O14 | 0.151 |  | x |
| C28H36O13 | -0.131 |  |  |  | C15H8O9 | 0.150 |  | x |
| C22H16O14 | -0.130 |  | x |  | C15H14O5 | 0.149 |  |  |
| C25H26O14 | -0.130 |  | x |  | C19H30O10 | 0.149 |  |  |
| C25H26O15 | -0.130 |  | x |  | C17H28O8 | 0.141 | x |  |
| C25H34O8 | -0.129 |  |  |  | C20H18O9 | 0.139 |  |  |
| C22H22O8 | -0.129 |  |  |  | C22H32O8 | 0.139 | x |  |
| C24H20O14 | -0.129 |  |  |  | C14H10O8 | 0.138 |  | x |
| C23H18O12 | -0.129 |  | x |  | C21H28O14 | 0.137 |  |  |
| C30H40O15 | -0.129 |  |  |  | C21H32O10 | 0.137 | x |  |
| C28H38O10 | -0.129 |  |  |  | C14H24O5 | 0.135 |  |  |
| C25H34O9 | -0.128 | x |  |  | C18H12O13 | 0.132 |  | x |
| C17H16O7 | -0.128 |  |  |  | C18H18O15 | 0.129 |  |  |
| C27H34O15 | -0.127 |  |  |  | C20H32O9 | 0.126 |  |  |
| C31H36O15 | -0.127 |  |  |  | C20H18O15 | 0.125 |  | x |
| C15H26O6 | -0.127 |  |  |  | C25H32O15 | 0.125 |  |  |
| C28H32O11 | -0.127 |  |  |  | C23H34O9 | 0.119 |  |  |
| C25H22O14 | -0.126 |  |  |  | C20H28O13 | 0.118 |  |  |
| C29H36O17 | -0.125 |  |  |  | C17H10O11 | 0.118 |  | x |
| C22H20O9 | -0.124 |  |  |  | C14H14O6 | 0.117 |  |  |
| C27H30O10 | -0.123 |  |  |  | C18H14O9 | 0.116 |  | x |
| C23H28O13 | -0.123 | x |  |  | C15H26O7 | 0.116 |  |  |
| C15H12O6 | -0.123 |  |  |  | C19H30O8 | 0.113 | x |  |
| C21H14O11 | -0.122 |  |  |  | C19H14O14 | 0.108 |  | x |
| C30H32O15 | -0.121 |  |  |  | C23H28O15 | 0.106 |  |  |
| C27H38O10 | -0.121 |  |  |  | C21H26O15 | 0.103 |  |  |
| C25H28O14 | -0.120 |  |  |  | C17H28O7 | 0.099 |  |  |
| C25H34O13 | -0.120 | x |  |  | C21H28O9 | 0.099 | x |  |
| C21H16O10 | -0.120 |  | x |  | C21H18O16 | 0.098 |  |  |
| C28H40O11 | -0.120 |  |  |  | C21H32O8 | 0.093 | x |  |
| C28H34O11 | -0.119 |  |  |  | C21H22O14 | 0.087 |  | x |
| C30H40O11 | -0.118 |  |  |  | C22H28O10 | 0.085 | x |  |
| C25H24O14 | -0.118 |  |  |  | C17H14O7 | 0.085 |  |  |
| C23H20O16 | -0.118 |  |  |  | C19H30O9 | 0.082 | x |  |
| C21H26O6 | -0.118 |  |  |  | C24H34O10 | 0.082 | x |  |
| C24H20O12 | -0.115 |  |  |  | C19H16O10 | 0.079 |  | x |
| C27H36O13 | -0.115 | x |  |  | C22H32O12 | 0.079 | x |  |
| C24H22O12 | -0.115 |  | x |  | C16H10O9 | 0.079 |  | x |
| C28H34O14 | -0.115 |  |  |  | C23H32O13 | 0.079 |  |  |
| C28H40O12 | -0.115 |  |  |  | C19H14O12 | 0.078 |  | x |
| C20H18O11 | -0.114 |  | x |  | C11H12O4 | 0.078 |  |  |
| C21H26O8 | -0.114 | x |  |  | C20H16O15 | 0.077 |  | x |
| C23H32O7 | -0.113 |  |  |  | C21H24O15 | 0.076 |  | x |
| C26H38O11 | -0.113 |  |  |  | C20H18O12 | 0.071 |  | x |
| C22H32O7 | -0.113 | x |  |  | C16H20O4 | 0.068 |  |  |
| C19H22O5 | -0.112 |  |  |  | C21H22O15 | 0.068 |  | x |
| C29H32O15 | -0.111 |  |  |  | C11H18O7 | 0.067 |  |  |
| C31H42O13 | -0.111 |  |  |  | C19H14O9 | 0.066 |  | x |
| C25H28O9 | -0.111 |  |  |  | C18H12O9 | 0.064 |  | x |
| C32H42O16 | -0.110 |  |  |  | C14H14O4 | 0.063 | x |  |
| C16H10O8 | -0.110 |  | x |  | C21H20O12 | 0.063 |  | x |
| C16H22O4 | -0.109 | x |  |  | C14H22O4 | 0.063 |  |  |
| C26H26O13 | -0.108 |  |  |  | C23H32O12 | 0.061 | x |  |
| C21H20O9 | -0.105 |  |  |  | C14H16O4 | 0.060 | x |  |
| C27H26O14 | -0.105 |  |  |  | C22H32O10 | 0.058 | x |  |
| C18H12O10 | -0.104 |  | x |  | C22H30O14 | 0.054 |  |  |
| C21H18O14 | -0.104 |  | x |  | C18H14O11 | 0.053 |  | x |
| C30H36O13 | -0.103 |  |  |  | C23H30O14 | 0.052 |  |  |
| C24H24O12 | -0.102 |  | x |  | C22H28O15 | 0.051 |  |  |
| C24H20O16 | -0.101 |  |  |  | C21H20O14 | 0.048 |  | x |
| C24H36O9 | -0.101 |  |  |  | C23H28O14 | 0.048 |  |  |
| C28H34O16 | -0.100 |  |  |  | C17H12O10 | 0.046 |  | x |
| C26H36O13 | -0.099 |  |  |  | C16H18O4 | 0.046 |  |  |
| C26H28O14 | -0.098 |  |  |  | C23H26O15 | 0.046 |  | x |
| C25H36O10 | -0.098 | x |  |  | C17H28O6 | 0.046 |  |  |
| C26H28O15 | -0.097 |  |  |  | C22H34O9 | 0.045 |  |  |
| C24H22O16 | -0.097 |  |  |  | C23H30O15 | 0.044 |  |  |
| C22H26O12 | -0.097 | x |  |  | C18H12O11 | 0.044 |  | x |
| C20H14O14 | -0.097 |  | x |  | C25H30O15 | 0.044 |  |  |
| C27H30O16 | -0.096 |  |  |  | C14H8O7 | 0.040 |  | x |
| C16H14O5 | -0.096 |  |  |  | C24H24O16 | 0.040 |  |  |
| C25H22O15 | -0.096 |  |  |  | C20H20O7 | 0.037 |  |  |
| C29H36O12 | -0.096 |  |  |  | C23H32O11 | 0.033 | x |  |
| C19H12O12 | -0.095 |  |  |  | C21H22O11 | 0.032 |  |  |
| C19H20O7 | -0.095 | x |  |  | C19H14O10 | 0.030 |  | x |
| C27H38O11 | -0.095 |  |  |  | C18H14O8 | 0.029 |  | x |
| C30H42O14 | -0.094 |  |  |  | C13H20O5 | 0.027 | x |  |
| C24H30O13 | -0.093 |  |  |  | C21H22O13 | 0.027 |  | x |
| C29H40O15 | -0.092 |  |  |  | C24H36O12 | 0.026 |  |  |
| C25H28O10 | -0.091 | x |  |  | C21H32O11 | 0.025 |  |  |
| C27H30O12 | -0.091 |  |  |  | C23H34O11 | 0.024 | x |  |
| C24H26O15 | -0.090 |  | x |  | C20H24O15 | 0.021 |  |  |
| C15H12O5 | -0.090 |  |  |  | C11H16O4 | 0.020 | x |  |
| C24H28O15 | -0.088 |  |  |  | C22H30O9 | 0.020 | x |  |
| C28H38O12 | -0.087 |  |  |  | C27H38O13 | 0.019 |  |  |
| C18H16O6 | -0.087 |  |  |  | C14H24O6 | 0.019 |  |  |
| C25H36O8 | -0.086 |  |  |  | C17H12O8 | 0.016 |  | x |
| C23H26O8 | -0.085 | x |  |  | C26H32O14 | 0.015 |  |  |
| C27H36O15 | -0.085 |  |  |  | C23H30O13 | 0.015 |  |  |
| C26H34O14 | -0.084 |  |  |  | C12H10O5 | 0.014 |  |  |
| C23H32O9 | -0.082 | x |  |  | C21H32O7 | 0.013 |  |  |
| C25H26O10 | -0.081 |  |  |  | C19H12O13 | 0.013 |  | x |
| C25H32O13 | -0.081 | x |  |  | C25H28O15 | 0.012 |  |  |
| C27H32O16 | -0.080 |  |  |  | C28H36O16 | 0.011 |  |  |
| C22H24O10 | -0.080 | x |  |  | C27H40O11 | 0.010 |  |  |
| C21H16O12 | -0.079 |  | x |  | C21H16O14 | 0.010 |  | x |
| C26H30O15 | -0.078 |  |  |  | C12H8O5 | 0.010 |  |  |
| C16H24O4 | -0.078 |  |  |  | C24H32O13 | 0.009 |  |  |
| C22H28O14 | -0.077 |  |  |  | C23H34O12 | 0.009 |  |  |
| C26H26O15 | -0.076 |  |  |  | C20H16O10 | 0.007 |  | x |
| C24H30O15 | -0.074 |  |  |  | C19H16O8 | 0.007 |  |  |
| C29H34O12 | -0.074 |  |  |  | C17H10O12 | 0.006 |  | x |
| C20H22O11 | -0.074 |  |  |  | C24H36O11 | 0.005 |  |  |
| C27H28O15 | -0.073 |  |  |  | C22H24O15 | 0.005 |  | x |
| C28H38O14 | -0.073 |  |  |  | C21H18O15 | 0.005 |  | x |
| C27H32O10 | -0.072 |  |  |  | C19H30O7 | 0.004 | x |  |
| C24H24O15 | -0.070 |  |  |  | C14H24O7 | 0.002 |  |  |
| C26H30O16 | -0.069 |  |  |  | C20H18O8 | 0.001 |  |  |
| C24H32O14 | -0.069 |  |  |  | C25H36O9 | 0.001 |  |  |
| C22H24O7 | -0.067 |  |  |  | C23H34O8 | 0.0004 |  |  |
| C28H32O15 | -0.067 |  |  |  |  |  |  |  |
| C17H10O9 | -0.067 |  | x |  |  |  |  |  |
| C21H20O11 | -0.066 |  |  |  |  |  |  |  |
| C25H32O14 | -0.065 |  |  |  |  |  |  |  |
| C20H14O13 | -0.063 |  | x |  |  |  |  |  |
| C15H8O7 | -0.063 |  |  |  |  |  |  |  |
| C24H34O11 | -0.063 | x |  |  |  |  |  |  |
| C18H16O8 | -0.061 |  |  |  |  |  |  |  |
| C18H20O9 | -0.061 |  |  |  |  |  |  |  |
| C26H38O12 | -0.060 |  |  |  |  |  |  |  |
| C30H34O15 | -0.059 |  |  |  |  |  |  |  |
| C12H18O4 | -0.058 | x |  |  |  |  |  |  |
| C23H24O14 | -0.057 |  | x |  |  |  |  |  |
| C21H22O8 | -0.056 | x |  |  |  |  |  |  |
| C19H12O11 | -0.055 |  | x |  |  |  |  |  |
| C18H18O6 | -0.054 | x |  |  |  |  |  |  |
| C15H20O3 | -0.054 |  |  |  |  |  |  |  |
| C27H32O15 | -0.054 |  |  |  |  |  |  |  |
| C21H14O12 | -0.054 |  | x |  |  |  |  |  |
| C23H32O8 | -0.053 | x |  |  |  |  |  |  |
| C13H14O5 | -0.053 |  |  |  |  |  |  |  |
| C24H18O15 | -0.053 |  |  |  |  |  |  |  |
| C16H12O7 | -0.052 |  | x |  |  |  |  |  |
| C24H24O11 | -0.051 |  |  |  |  |  |  |  |
| C10H12O4 | -0.050 |  |  |  |  |  |  |  |
| C20H16O14 | -0.050 |  | x |  |  |  |  |  |
| C23H32O14 | -0.050 |  |  |  |  |  |  |  |
| C23H22O16 | -0.049 |  |  |  |  |  |  |  |
| C17H18O7 | -0.048 | x |  |  |  |  |  |  |
| C25H34O14 | -0.047 |  |  |  |  |  |  |  |
| C22H26O14 | -0.047 |  |  |  |  |  |  |  |
| C26H26O12 | -0.046 |  |  |  |  |  |  |  |
| C23H30O7 | -0.046 |  |  |  |  |  |  |  |
| C23H16O15 | -0.045 |  |  |  |  |  |  |  |
| C23H26O14 | -0.043 |  |  |  |  |  |  |  |
| C16H26O6 | -0.042 | x |  |  |  |  |  |  |
| C29H40O11 | -0.042 |  |  |  |  |  |  |  |
| C22H16O15 | -0.042 |  |  |  |  |  |  |  |
| C19H16O9 | -0.039 |  | x |  |  |  |  |  |
| C28H32O10 | -0.038 |  |  |  |  |  |  |  |
| C22H26O13 | -0.036 | x |  |  |  |  |  |  |
| C15H22O4 | -0.035 |  |  |  |  |  |  |  |
| C20H18O13 | -0.035 |  | x |  |  |  |  |  |
| C23H30O12 | -0.035 | x |  |  |  |  |  |  |
| C26H36O14 | -0.035 |  |  |  |  |  |  |  |
| C24H34O8 | -0.034 |  |  |  |  |  |  |  |
| C11H14O4 | -0.034 | x |  |  |  |  |  |  |
| C20H30O6 | -0.034 | x |  |  |  |  |  |  |
| C19H14O13 | -0.032 |  | x |  |  |  |  |  |
| C24H30O14 | -0.032 |  |  |  |  |  |  |  |
| C22H22O15 | -0.032 |  | x |  |  |  |  |  |
| C21H16O15 | -0.031 |  | x |  |  |  |  |  |
| C22H14O13 | -0.030 |  |  |  |  |  |  |  |
| C24H34O13 | -0.029 |  |  |  |  |  |  |  |
| C26H36O12 | -0.029 | x |  |  |  |  |  |  |
| C25H34O12 | -0.029 | x |  |  |  |  |  |  |
| C21H20O15 | -0.028 |  | x |  |  |  |  |  |
| C22H34O10 | -0.028 |  |  |  |  |  |  |  |
| C25H22O16 | -0.026 |  |  |  |  |  |  |  |
| C23H24O16 | -0.024 |  |  |  |  |  |  |  |
| C23H34O10 | -0.023 | x |  |  |  |  |  |  |
| C23H24O15 | -0.023 |  |  |  |  |  |  |  |
| C21H14O14 | -0.023 |  | x |  |  |  |  |  |
| C26H34O15 | -0.023 |  |  |  |  |  |  |  |
| C24H34O12 | -0.022 | x |  |  |  |  |  |  |
| C22H26O15 | -0.022 |  | x |  |  |  |  |  |
| C26H32O15 | -0.021 |  |  |  |  |  |  |  |
| C24H36O10 | -0.021 |  |  |  |  |  |  |  |
| C13H10O6 | -0.021 |  |  |  |  |  |  |  |
| C31H40O17 | -0.020 |  |  |  |  |  |  |  |
| C21H24O7 | -0.018 | x |  |  |  |  |  |  |
| C20H20O8 | -0.018 |  |  |  |  |  |  |  |
| C22H22O16 | -0.018 |  |  |  |  |  |  |  |
| C21H30O8 | -0.018 | x |  |  |  |  |  |  |
| C13H14O4 | -0.018 | x |  |  |  |  |  |  |
| C12H20O6 | -0.017 |  |  |  |  |  |  |  |
| C20H16O9 | -0.015 |  | x |  |  |  |  |  |
| C14H18O4 | -0.012 | x |  |  |  |  |  |  |
| C14H10O7 | -0.011 |  | x |  |  |  |  |  |
| C25H36O12 | -0.011 |  |  |  |  |  |  |  |
| C21H16O13 | -0.010 |  | x |  |  |  |  |  |
| C22H20O15 | -0.009 |  | x |  |  |  |  |  |
| C21H20O16 | -0.008 |  |  |  |  |  |  |  |
| C13H12O5 | -0.008 |  |  |  |  |  |  |  |
| C17H10O10 | -0.007 |  | x |  |  |  |  |  |
| C12H10O4 | -0.007 |  |  |  |  |  |  |  |
| C24H28O16 | -0.007 |  |  |  |  |  |  |  |
| C24H28O14 | -0.005 |  |  |  |  |  |  |  |
| C19H18O9 | -0.001 |  |  |  |  |  |  |  |
| C17H12O9 | -0.001 |  | x |  |  |  |  |  |