

# **Supplementary Information**

## **Chemical Evolution Reimagined**

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## Methods

**Materials.** All chemicals and reagents were analytical grade, including glycolic acid (Acros Organics, #15451-0250), thioglycolic acid (Sigma-Aldrich, #528056), glycerol (Alfa Aesar #36646), adenine (Sigma-Aldrich, #A8626), urea (Alfa Aesar #A12360), glycine-1-<sup>13</sup>C,<sup>15</sup>N (Sigma-Aldrich, # 299340), decanoic acid-1-<sup>13</sup>C (Sigma-Aldrich, #488658), and D-glucose-<sup>13</sup>C<sub>6</sub> (Sigma-Aldrich, # 389374).

**High Performance Liquid Chromatography.** HPLC analyses were conducted with an Agilent 1260 quaternary pump and autosampler with DAD UV-vis detector at 210 nm, with a detection path length of 1.0 cm (Agilent Technologies, Santa Clara, CA) . Injection volume was 10  $\mu$ L with a H<sub>2</sub>O needle wash. Injection speed was 100  $\mu$ L/sec. Reaction mixtures were resolved by hydrophobicity on a Kinetex XB-C18 column (150 x 2.1 mm, 2.6  $\mu$ m particle size) with a 0.3 mL/min flow rate, constant 25°C column temperature. The solvent gradient used solution A) 0.1% formic acid in LC-MS grade water, and solution B) LC-MS grade acetonitrile. The gradient was 5 min 100% A, 0% B; 20 min ramp to 45% A, 55% B; 5 min ramp to 0% A, 100% B; 5 min 0% A, 100% B; 1 min ramp to 100% A, 0% B; 14 min 100% A, 0% B. Processing of HPLC data, filtering and blank subtraction was conducted using MATLAB version R2021a. The processed data were imported into Igor Pro9 and integrated using Multi-peak Fit.

**Liquid Chromatography Mass Spectrometry.** LC-MS data were collected on an Agilent 1260 HPLC coupled to an Agilent 6130 single quadrupole mass spectrometer and an inline Agilent UV absorbance detector (210 nm) using 2.0-kV electrospray ionization (ESI) capillary voltage. The path length was 0.6 cm. Mixtures were resolved on a Kinetex XB-C18 column (150 x 2.1 mm, 2.6  $\mu$ m particle size) under the conditions described for HPLC. Eluted peaks were detected in both negative and positive mode ESI-MS, scanning from 65-2000 m/z with 70V source fragmentation voltage.

**Single-step dry-down reactions.** Reactions were carried out by incubating mixtures at 45°C for 3 days under anoxia in open tubes. Mixtures contained 2 building-blocks (glycolic acid and thioglycolic acid, or glycolic acid or thioglycolic acid with either urea, glucose, glycerol, adenine, decanoic acid, or glycine) or 8 building-blocks (MFP Set 3; thioglycolic acid, glycolic acid, glycine, urea, MgCl<sub>2</sub>, glycerol, glucose, decanoic acid, and adenine, in addition to MgCl<sub>2</sub>).

**Wet-dry cycling experiments.** MFP Set 3 was made by combining reagents to achieve final concentrations of thioglycolic acid (125  $\mu$ mol, 192 mM), glycolic acid (125  $\mu$ mol, 192 mM), glycine (50  $\mu$ mol, 77 mM), urea (50  $\mu$ mol, 77 mM), MgCl<sub>2</sub> (50  $\mu$ mol, 77 mM), glycerol (5  $\mu$ mol, 7.7 mM), glucose (5  $\mu$ mol, 7.7 mM), decanoic acid (1.67  $\mu$ mol, 2.6 mM) and adenine (1.67  $\mu$ mol, 2.6 mM). Concentrations were constrained by solubility. MFP Set 3 was wet-dry cycled at 45°C in anoxia. Every 22 building-block mixture (MFP Set 4) was made by combining reagents to achieve final concentrations of thioglycolic acid (125  $\mu$ mol, 179 mM), lactic acid (62.5  $\mu$ mol, 89 mM), glycolic acid (62.5  $\mu$ mol, 89 mM), glycine (5  $\mu$ mol, 7.2 mM), serine (5  $\mu$ mol, 7.2 mM), threonine (5  $\mu$ mol, 7.2 mM), leucine (5  $\mu$ mol, 7.2 mM), valine (5  $\mu$ mol, 7.2 mM), proline (5  $\mu$ mol, 7.2 mM), glutamic acid (5  $\mu$ mol, 7.2 mM), alanine (5  $\mu$ mol, 7.2 mM), lysine (5  $\mu$ mol, 7.2 mM), Histidine (5  $\mu$ mol, 7.2 mM), urea (50  $\mu$ mol, 72 mM), KCl (12.5  $\mu$ mol, 18 mM), Na<sub>2</sub>HPO<sub>4</sub> (25  $\mu$ mol, 36mM), MgCl<sub>2</sub> (12.5  $\mu$ mol, 18 mM), glycerol (5  $\mu$ mol, 7.2 mM), thymine (0.83  $\mu$ mol, 1.2 mM), glucose <sup>13</sup>C<sub>6</sub> (1.25  $\mu$ mol, 1.8 mM), glucuronic acid (1.25  $\mu$ mol, 1.8 mM), ribose (1.25  $\mu$ mol,

1.8 mM), galactose (1.25  $\mu$ mol, 1.8 mM), decanoic acid (1.67  $\mu$ mol, 2.4 mM) and adenine (0.83  $\mu$ mol, 1.2 mM).

**Mass Spec combinatorial analysis.** Briefly, mass spectroscopy data were analyzed with in house MATLAB code. The code generates masses of all possible chemically linked building blocks (ignoring their order) to matches them with experimental MS peaks. An algorithm for detecting the molecular masses from mass spectroscopy analysis of fragments from mixture of amino acid and alpha-hydroxy acid-containing depsipeptides was originally designed by Forsythe *et al.* (PMID: 28847940) and modified for the purpose of this study.

The original code (Forsythe PNAS 2017) was adapted to apply to an expanded repertoire of building blocks. The revised code account for sugars, nucleobases, thioacids, fatty acids, glycerol and urea. A set of letters (capital or small) was arbitrarily assigned to each of the component of the mixtures along with its full mass and the mass of the corresponding residue within the polymer.

The initial set of the experimental frequencies has been filtered by applying the intensity threshold (set to 0.05). The resulting dataset was binned into histograms of width 1 m/z. Next, a mass defect filter was used to remove masses which were not compatible with product species based upon the combination of C, H, O, and N atoms. Observed m/z values were further filtered using the using a mass defect filter (absolute width 0.2 Da), such that the peaks with non-physical masses (containing high fractional digits, e.g. 0.65) were removed at this point. Candidate sequences, whose residues are encoded by single letters of a pre-defined alphabet were generated through a combinatorial approach (up to a specific length), and neutral masses were calculated. From the neutral masses, deprotonated or protonated ion m/z values were generated and were compared to the binned data (in the bin selected based on the mass of the candidate). Matches (within the relative  $\Delta m/m$  threshold of 0.003 for the negative mode and that of 0.0003 for the positive mode) between the binned experimental input data and computed for a given molecular composition were recorded, ignoring the specific order of the residues.

Assumptions about the nature of the interactions within the system were made, to account for the experimental mode (positive or negative), in which the measurements were performed, and the chemical nature of the components as specified by sequences using single letter alphabet. The molecules within a set were expected to form either linear or cyclic products. Due to presence of thioglycolic acid in the mixture, the formation of a disulfide bond between thiol groups of two thioglycolic acids was accounted for. The association of metal ions ionized molecular fragments was also taken into consideration based upon preliminary analyses of mass spectroscopy data from the simple depsipeptide systems. These options and filters accounting for certain chemical rules have been added into the current project in order to reduce the size of the combinatorial space.

**“Mode”:** Protonated molecules are observed in the positive mode while deprotonated molecules are observed in the negative mode. Each fragmentation of the initial peptide was analyzed using HRMS in both the positive and negative mode. There are sixteen fragments with a corresponding positive and negative mode data set. The “mode” option within the GUI is used to output accurate neutral masses of each sequence. Sequence matches have a single proton removed or added from the experimental m/z to generate the neutral m/z in the positive and negative mode, respectively. This is computationally equivalent to deprotonating positive ions or the protonation of negative ions.

**“Syntax”:** The Forsythe version of this code was used to identify peaks for alpha-hydroxy acid containing depsipeptides. In this version of the software, the fragmentation of the depsipeptides was known and understood to only begin with an oxo-acid. With this in mind, the molecules within alphabet files are abbreviated based on their classification (small letters for oxo-acids, capital letters for anything else). This led to two clear alphabets for the code to sort through. Sequences beginning with any molecule can be found in the output file using the “Syntax” mode.

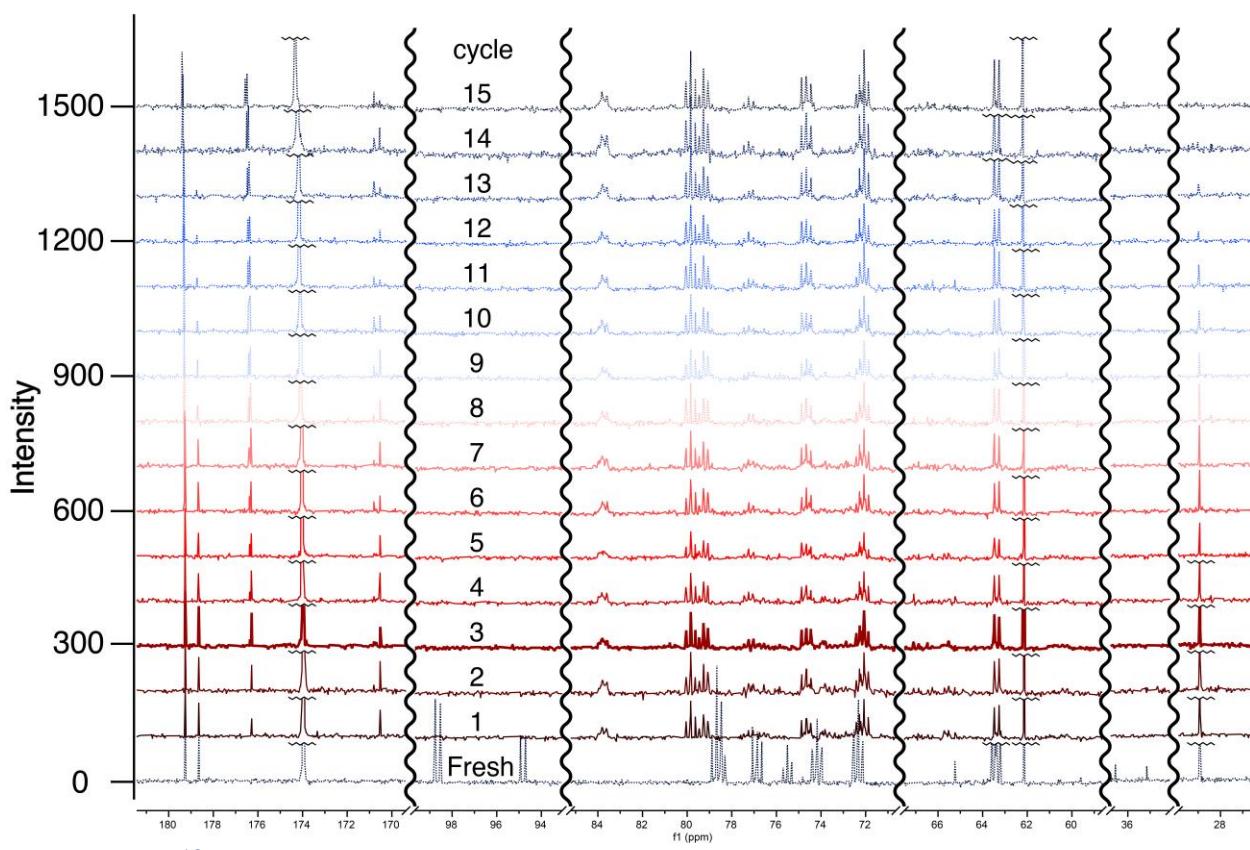
**“Order”:** The “All Perms” button shows every possible sequence combination for a match with an experimental m/z ratio. The “Combinations” option only shows unique sequence makeups for every match. For a sequence match of glycine and glucose (g’l’) the “All Perms” option will show g’l’ and l’g’. Comparatively, the “Combinations” option will only show g’l’.

**“Linearization”:** When selected, the software will also compare cyclic molecular sequence m/z to experimental m/z ratios. The cyclization of a molecular sequence is assumed to happen through dehydration: the loss of a water molecule (“H<sub>2</sub>O”, m/z of 18.0106 g/mol). Although cyclization can happen through the loss of various other molecules depending on the unique chemical composition, we found dehydration to be the most common form of cyclization within our data sets.

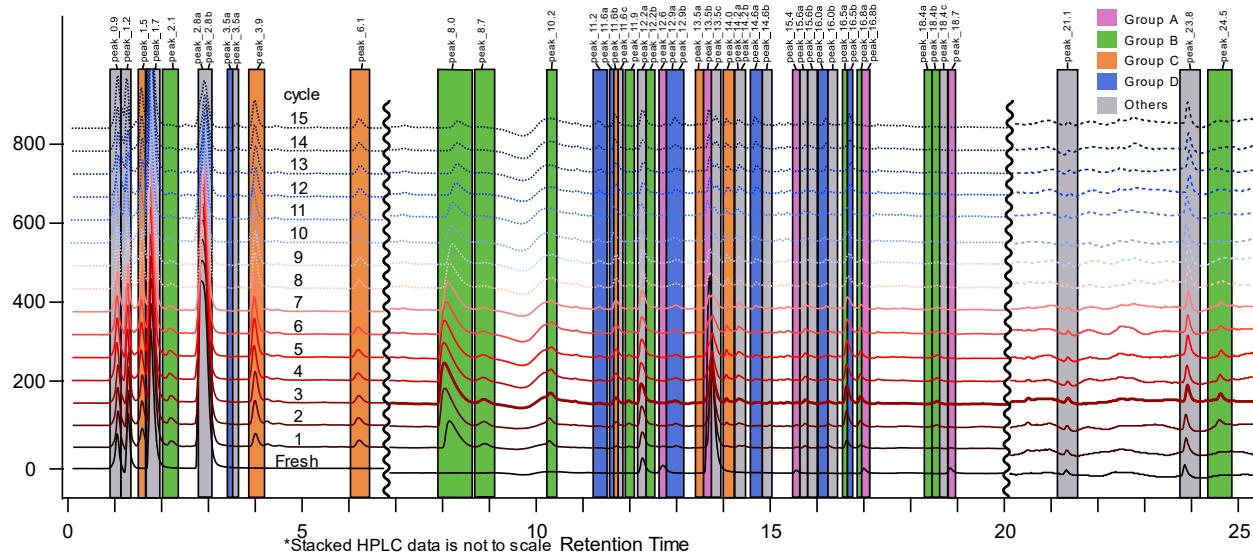
**“Disulfide Bond”:** A disulfide bond is commonly formed by the coupling of two thiols (R-SH, R-SH) to form the functional group R-S-S-R’. To find disulfide bonds, the code searches for any sequence that matches experimental m/z ratios without 2 hydrogen molecules (“H”, m/z of 1.0073 g/mol). Each of these distinctive “hits” were then filtered based on whether they contained at least two thioglycolic acids. Any sequence match containing two or more thioglycolic acids with a m/z ratio of the sequence minus 2.0146 g/mol (m/z of two hydrogen molecules) within the mass tolerance range is considered a likely match to that experimental peak. The software does not consider the possibility of two or more disulfide bonds. For example, the sequences t’t’ and t’t’t’t’ (two and four thioglycolic acids) are both considered to have one disulfide bond even though one has two more thiol groups. Additional disulfide bonds have not accounted for more unknown experimental peaks, thus being unnecessary for our current uses.

**“Ions”:** This functionality accounts for ion adducts, which occur when a molecule associates with an ion. If ions combine with molecules, experimental peaks would exist such that they cannot be considered likely matches to any permutation of building blocks within the alphabet file without using a statistically irrelevant mass tolerance filter. Four likely scenarios are considered: sequences that have an added magnesium minus hydrogen, magnesium minus hydrogen minus water, magnesium with an overall charge of two, and magnesium minus water with an overall charge of two. Magnesium and its associated effect on the overall charge are used as an example but can be changed on the GUI control page. This option has been activated for the positive mode and deactivated for the negative mode.

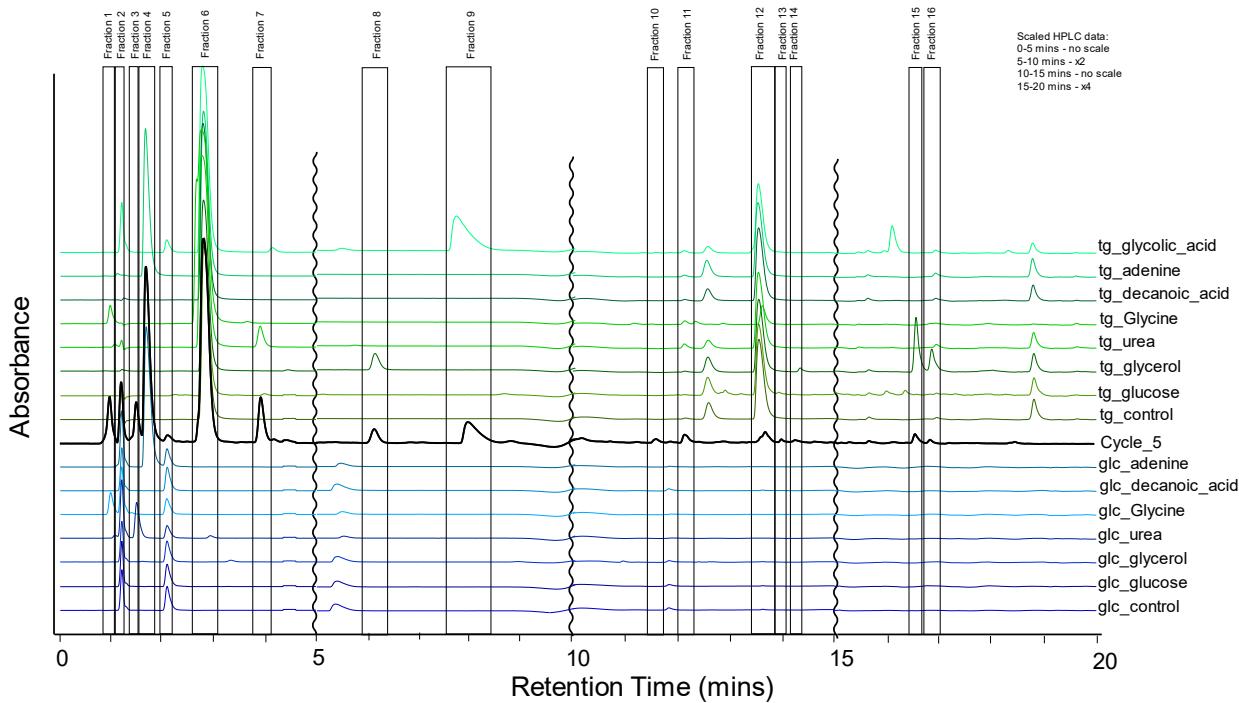
**“Residue Restrictions”:** When selected, the software will restrict the number of decanoic acids (“d”), ureas (“u”), and/or adenines (“n”) that can be in any output in any sequence. The user can select to restrict none, one, two, or all of the molecules and how many of each are allowed in any sequence. It was found that the three molecules listed above, especially with a polymer length greater than five, often formed chains of themselves. These chains typically did not show many more, if any, likely sequence m/z matches to experimental m/z as compared to when their output was restricted.



**Figure S1.  $^{13}\text{C}$  NMR spectra of 15 dry-wet cycles, initiating with MFP Set 3.** The input mixture was subjected to 15 dry-wet cycles at 45 °C under anoxia. Each cycle lasted two days. An aliquot was taken at the end of each cycle for analysis. No new carbon peaks are observed beyond cycle 3 demonstrating combinatorial compression.



**Figure S2. Chromatograms of 15 dry-wet cycles, initiating with MFP Set 3.** The input mixture was subjected to 15 dry-wet cycles at 45 °C under anoxia. Each cycle lasted two days. An aliquot was taken at the end of each cycle for analysis. The initial MFP Set 3 and the product mixture after each cycle were separated by C18-HPLC and monitored at 210 nM. Peaks that correspond Group A (shaded pink) consist primarily of starting materials. Peaks that correspond to Group B (reach maximum population at cycle 3) are shaded green. Species that grow in population and then maintain relatively constant population are Group C (shaded orange). Species that increase gradually beginning from cycle 2-3 correspond to Group D (shaded blue). Ungrouped peaks are shaded gray.



**Figure S3. HPLC chromatograms of Cycle 5 compared with 2-component dry-downs.** A comparison of the HPLC chromatogram of Cycle 5, with the HPLC Chromatograms of 2-component dry-downs of MFP Set 3 molecules with thioglycolic acid and glycolic acid. The 2-component mixtures were subject to 3 day dry-down at 45 °C under anoxia. The product mixtures were separated by C18-HPLC and monitored at 210 nm.

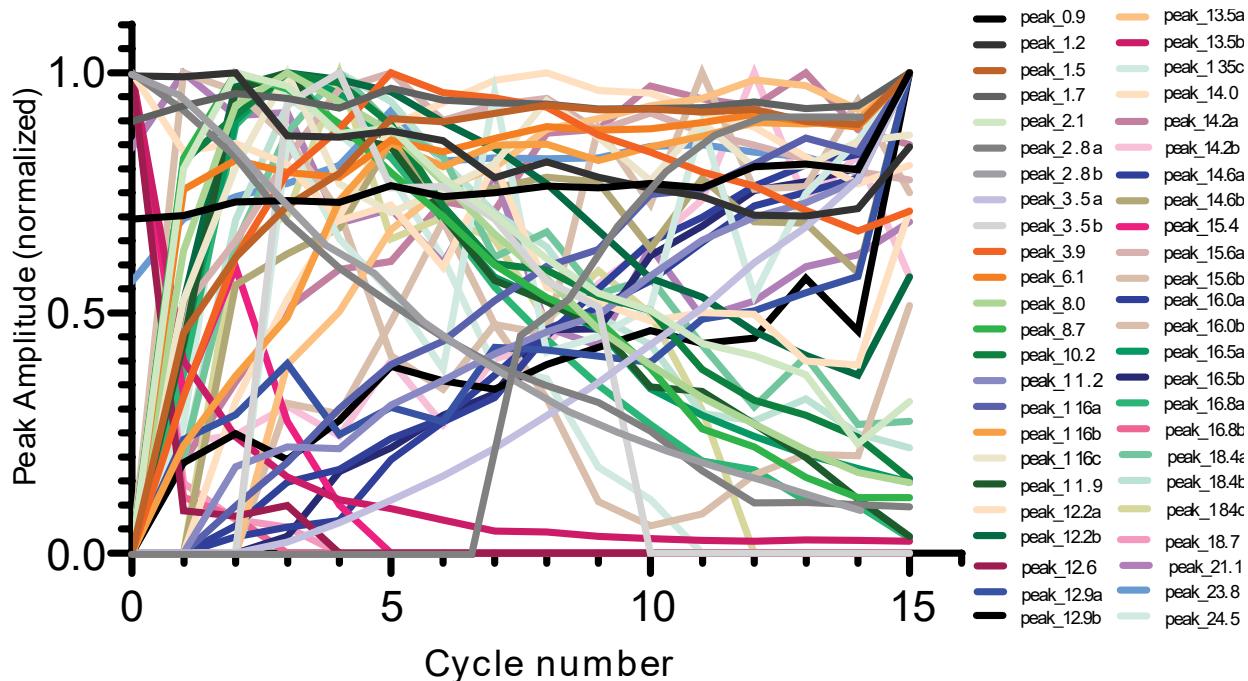
## **Building Blocks**

|                   |   |
|-------------------|---|
| Glycine           | G |
| glycolic acid     | g |
| thioglycolic acid | t |
| Glycerol          | y |
| Glucose           | l |
| decanoic acid     | d |
| adenine-glucose   | A |
| Urea              | u |
| Adenine           | n |

**Table S1. Peak Summary.**

Assignment of fractions 1 through 16 to peaks of different retention times. Characterization of these peaks into one of four groups is depicted. Extra peaks not depicted above: 3.5a, 3.5b, 8.7, 10.2, 11.2, 12.6, 12.9a, 12.9b, 14.6a, 14.6b, 15.4, 15.6a, 15.6b, 16.0a, 16.0b, 18.4a, 18.4b, 18.4c, 18.7, 21.1, 23.8, 24.5

| Fraction Number | Retention time (min)<br>Fractions | Peak ID  | Group                                   | Probable composition   |
|-----------------|-----------------------------------|--|---|--|
| 1               | 0.8056-1.1390                     | peak_0.9   | Others                                  | Glycine and various potential hydrophilic products   |
| 2               | 1.1390-1.3523                     | peak_1.2   | Others                                  | Glycolic acid and various potential hydrophilic products   |
| 3               | 1.4190-1.6056                     | peak_1.5   | Group C                                 | Co-oligomers composed of g and u in this fraction (such as gu and ggu)                                   |
| 4               | 1.6190-2.0056                     | peak_1.7   | Others                                  | Adenine and various potential hydrophilic products   |
| 5               | 2.0190-2.2990                     | peak_2.1   | Group B                                 | Various oligomers composed of g alone (e.g. gg) and other products composed of g and other constituents. |
| 6               | 2.6323-3.2723                     | peak_2.8a,<br>peak_2.8b                                | Others<br>Others                        | Thioglycolic acid and various possible products, such as tG.   |
| 7               | 3.8190-4.3523                     | peak_3.9   | Group C                                 | tu   |
| 8               | 5.9123-6.2190                     | peak_6.1   | Group C                                 | ty   |
| 9               | 7.8056-8.2056                     | peak_8.0   | Group B                                 | tg   |
| 10              | 11.2723-11.9790                   | peak_11.6a,<br>peak_11.6b,<br>peak_11.6c,<br>peak_11.9 | Group D<br>Group C<br>Others<br>Group B | Gtd  |
| 11              | 11.9923-12.3123                   | peak_12.2a,<br>peak_12.2b                              | Others<br>Group B                       | tg-S-S-tg  |
| 12              | 13.5123-13.8990                   | peak_13.5a,<br>peak_13.5b,<br>peak_13.5c               | Group C<br>Group A<br>Others            | (t)2 and co-oligomers of t and 1   |
| 13              | 13.9390-14.0990                   | peak_14.0  | Group C                                 | Co-oligomers of t and 1  |
| 14              | 14.0990-14.4190                   | peak_14.2a,<br>peak_14.2b                              | Others<br>Others                        | Co-oligomers of t and 1  |
| 15              | 16.4590-16.7523                   | peak_16.5a,<br>peak_16.5b                              | Group B<br>Group D                      | Co-oligomers of t and y, such as tyy and tty   |
| 16              | 16.7523-16.9390                   | peak_16.8a,<br>peak_16.8b                              | Group B<br>Group A                      | Co-oligomers of t and y, such as tyy and tty   |

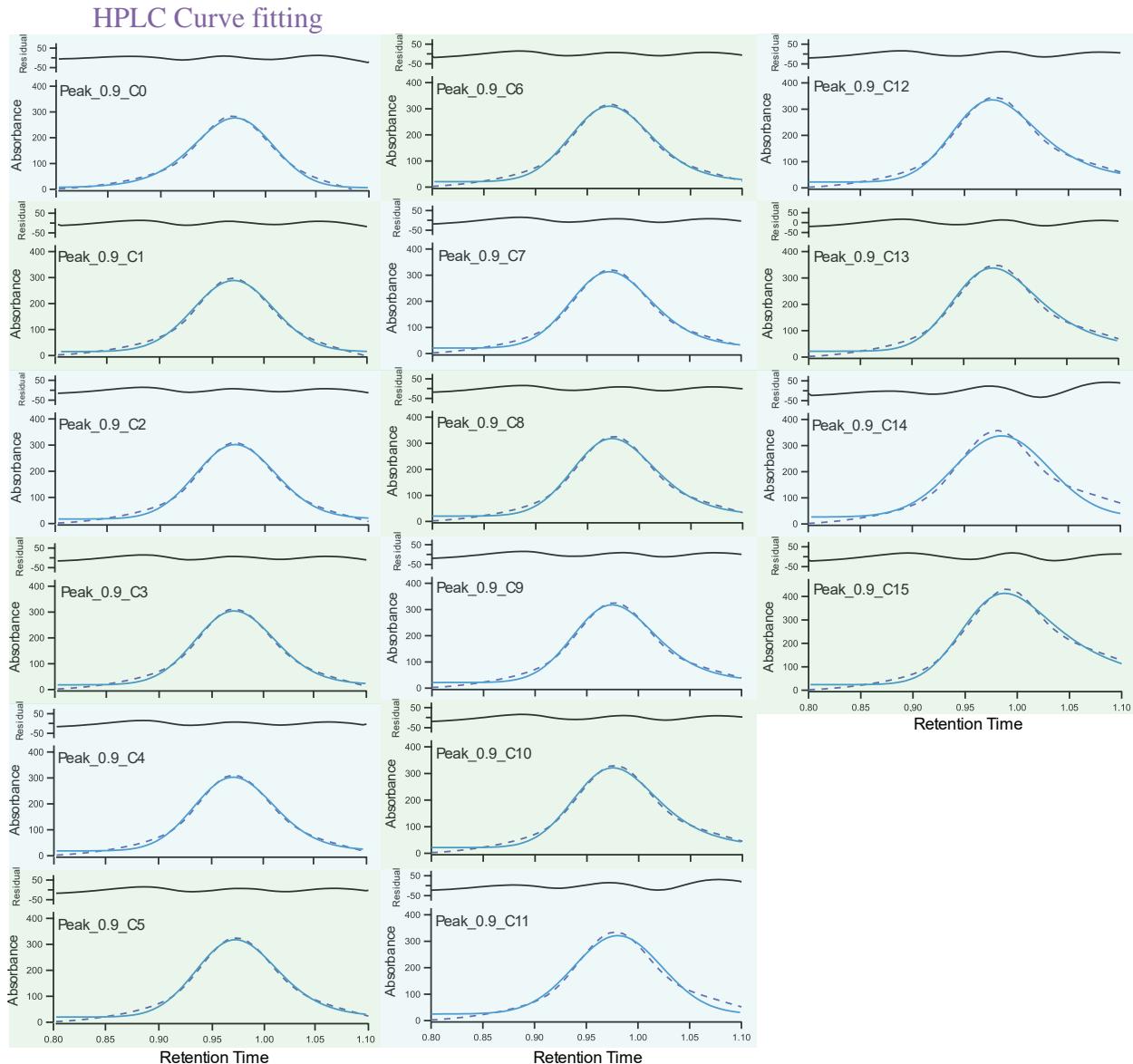


**Figure S4. HPLC Peak Amplitudes.** Peak Amplitude of the aliquots taken during the 15 dry-wet cycles, initiating with MFP Set 3. The peak intensities were calculated from the HPLC chromatogram using IgorPro 8. The initial MFP Set 3 and the product mixture after each cycle were separated by C18-HPLC and monitored at 210 nm. Peaks that correspond Group A (shaded pink) consist primarily of starting materials. Peaks that correspond to Group B (reach maximum population at cycle 3-5) are shaded green. Species that grow in population and then maintain concentration are Group C (shaded orange). Peaks that increase gradually beginning from cycle 2-3 correspond to Group D (shaded blue). Ungrouped peaks are shaded gray.

## Chemical Analysis

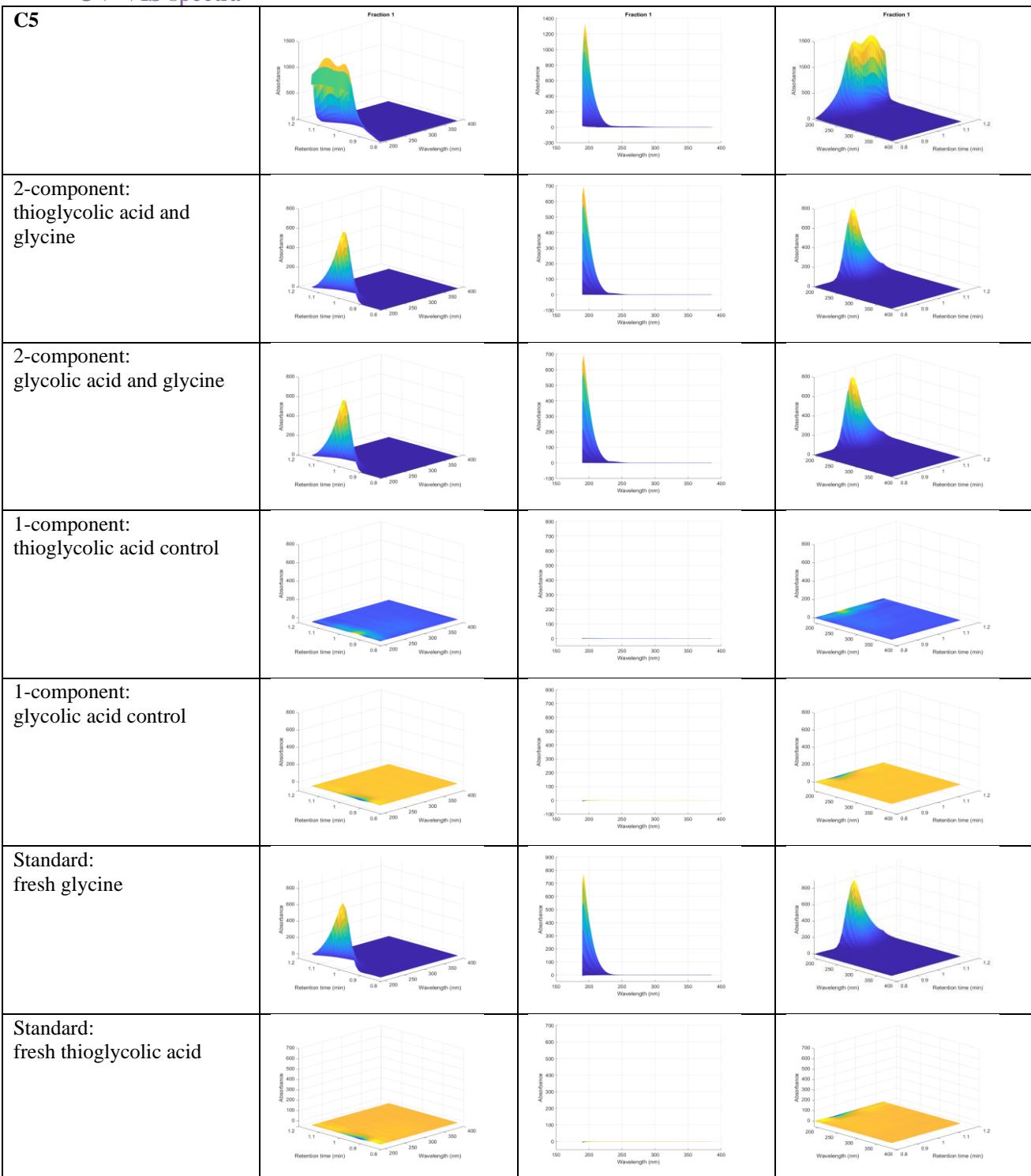
### Fraction 1 (retention time = 0.9 min)

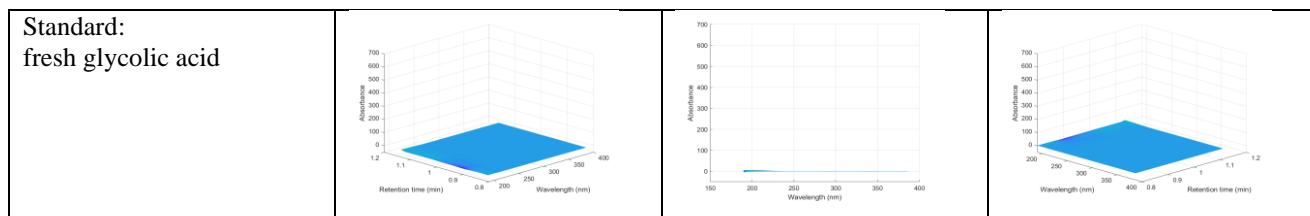
Initially, fraction 1 is composed of glycine only. Over cycles the absorbance peak goes up, indicating the appearance of new hydrophilic products that are not retained on the C18 column. The MS data indicates a variety of possible co-elutants in this fraction.



**Figure S5. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 1 which has a retention time of about 0.9 minutes.

## UV-VIS spectra





**Figure S6. UV-Vis absorbance.** UV-vis absorbance spectra of Cycle 5 (C5) fraction 1 and relevant fresh, 1-, and 2-component drydowns.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula     | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-------------|-------------------|-------------------|------------|----------|
| t        | 91.9926      | C2H4O2S1    | 90.9848           | 91.0              | 0.0152     | 87.1957  |
| y        | 92.0478      | C3H8O3      | 91.0400           | 91.0              | 0.0400     | 87.1957  |
| gt       | 149.9980     | C4H6O4S1    | 148.9902          | 149.0             | 0.0098     | 9.5710   |
| gy       | 150.0532     | C5H10O5     | 149.0454          | 149.0             | 0.0454     | 9.5710   |
| tt-H2    | 163.9595     | C4H4O3S2    | 162.9517          | 163.0             | 0.0483     | 13.6739  |
| ty       | 166.0293     | C5H10O4S1   | 165.0215          | 165.0             | 0.0215     | 10.5323  |
| tt       | 165.9741     | C4H6O3S2    | 164.9663          | 165.0             | 0.0337     | 10.5323  |
| yy       | 166.0845     | C6H14O5     | 165.0767          | 165.1             | 0.0233     | 8.5480   |
| d        | 173.1502     | C10H20O2    | 172.1424          | 172.3             | 0.1576     | 5.9285   |
| ggu      | 176.0437     | C5H8O5N2    | 175.0359          | 175.0             | 0.0359     | 32.6400  |
| gtu      | 192.0198     | C5H8O4N2S1  | 191.0120          | 191.0             | 0.0120     | 7.0806   |
| ggg      | 192.0273     | C6H8O7      | 191.0195          | 191.0             | 0.0195     | 7.0806   |
| gyu      | 192.0750     | C6H12O5N2   | 191.0672          | 191.1             | 0.0328     | 6.4598   |
| ggt      | 208.0034     | C6H8O6S1    | 206.9956          | 207.0             | 0.0044     | 17.6181  |
| ttu      | 207.9959     | C5H8O3N2S2  | 206.9881          | 207.0             | 0.0119     | 17.6181  |
| tyu      | 208.0511     | C6H12O4N2S1 | 207.0433          | 207.0             | 0.0433     | 17.6181  |
| yyu      | 208.1063     | C7H16O5N2   | 207.0985          | 207.1             | 0.0015     | 16.9093  |
| ggy      | 208.0586     | C7H12O7     | 207.0508          | 207.1             | 0.0492     | 16.9093  |
| GGGG     | 254.0983     | C8H14O5N4   | 253.0905          | 253.1             | 0.0095     | 21.2307  |
| gttu-H2  | 263.9867     | C7H8O5N2S2  | 262.9789          | 263.0             | 0.0211     | 26.7129  |
| Gttu-H2  | 265.0031     | C7H9O4N3S2  | 263.9953          | 264.0             | 0.0047     | 5.5022   |
| gggt     | 266.0088     | C8H10O8S1   | 265.0010          | 265.0             | 0.0010     | 12.3011  |
| gttu     | 266.0013     | C7H10O5N2S2 | 264.9935          | 265.0             | 0.0065     | 12.3011  |

|         |          |              |          |       |        |         |
|---------|----------|--------------|----------|-------|--------|---------|
| gtyu    | 266.0565 | C8H14O6N2S1  | 265.0487 | 265.0 | 0.0487 | 12.3011 |
| gyyu    | 266.1117 | C9H18O7N2    | 265.1039 | 265.1 | 0.0039 | 12.0685 |
| gggy    | 266.0640 | C9H14O9      | 265.0562 | 265.1 | 0.0438 | 12.0685 |
| gdu     | 273.1774 | C13H24O4N2   | 272.1696 | 272.4 | 0.2304 | 5.0075  |
| Gdu     | 274.1938 | C13H25O3N3   | 273.1860 | 273.2 | 0.0140 | 21.8536 |
| ttyu-H2 | 280.0180 | C8H12O5N2S2  | 279.0102 | 279.0 | 0.0102 | 6.8872  |
| ggtt-H2 | 279.9703 | C8H8O7S2     | 278.9625 | 279.0 | 0.0375 | 6.8872  |
| tttu-H2 | 279.9628 | C7H8O4N2S3   | 278.9550 | 279.0 | 0.0450 | 6.8872  |
| Glu     | 287.1276 | C9H17O7N3    | 286.1198 | 286.1 | 0.0198 | 8.4127  |
| dn      | 290.1941 | C15H23O1N5   | 289.1863 | 289.2 | 0.0137 | 13.7279 |
| Ggd     | 290.1774 | C14H25O5N1   | 289.1696 | 289.2 | 0.0304 | 13.7279 |
| GGGgu   | 295.1037 | C9H15O6N5    | 294.0959 | 294.1 | 0.0041 | 8.8238  |
| GGun    | 295.1204 | C10H13O2N9   | 294.1126 | 294.1 | 0.0126 | 8.8238  |
| Gtty-H2 | 297.0180 | C9H13O6N1S2  | 296.0102 | 296.0 | 0.0102 | 6.4883  |
| Gttt-H2 | 296.9628 | C8H9O5N1S3   | 295.9550 | 296.0 | 0.0450 | 6.4883  |
| gtd     | 305.1371 | C14H24O5S1   | 304.1293 | 304.1 | 0.0293 | 8.5051  |
| gyd     | 305.1923 | C15H28O6     | 304.1845 | 304.2 | 0.0155 | 6.6776  |
| Gtd     | 306.1535 | C14H25O4N1S1 | 305.1457 | 305.1 | 0.0457 | 10.3031 |
| Gyd     | 306.2087 | C15H29O5N1   | 305.2009 | 305.2 | 0.0009 | 8.6819  |
| gggtu   | 308.0306 | C9H12O8N2S1  | 307.0228 | 307.0 | 0.0228 | 8.6301  |
| ggggg   | 308.0381 | C10H12O11    | 307.0303 | 307.0 | 0.0303 | 8.6301  |
| gggyu   | 308.0858 | C10H16O9N2   | 307.0780 | 307.1 | 0.0220 | 7.054.0 |
| ttd     | 321.1132 | C14H24O4S2   | 320.1054 | 320.1 | 0.0054 | 6.0036  |
| yyd     | 321.2236 | C16H32O6     | 320.2158 | 320.2 | 0.0158 | 5.2885  |
| tyd     | 321.1684 | C15H28O5S1   | 320.1606 | 320.2 | 0.0394 | 5.2885  |
| GGttu   | 326.0395 | C9H14O5N4S2  | 325.0317 | 325.0 | 0.0317 | 7.1645  |
| GGggt   | 326.0470 | C10H14O8N2S1 | 325.0392 | 325.0 | 0.0392 | 7.1645  |
| GGggy   | 326.1022 | C11H18O9N2   | 325.0944 | 325.1 | 0.0056 | 6.1481  |
| GGtyu   | 326.0947 | C10H18O6N4S1 | 325.0869 | 325.1 | 0.0131 | 6.1481  |
| Ggttn   | 326.0637 | C11H12O4N6S1 | 325.0559 | 325.1 | 0.0441 | 6.1481  |

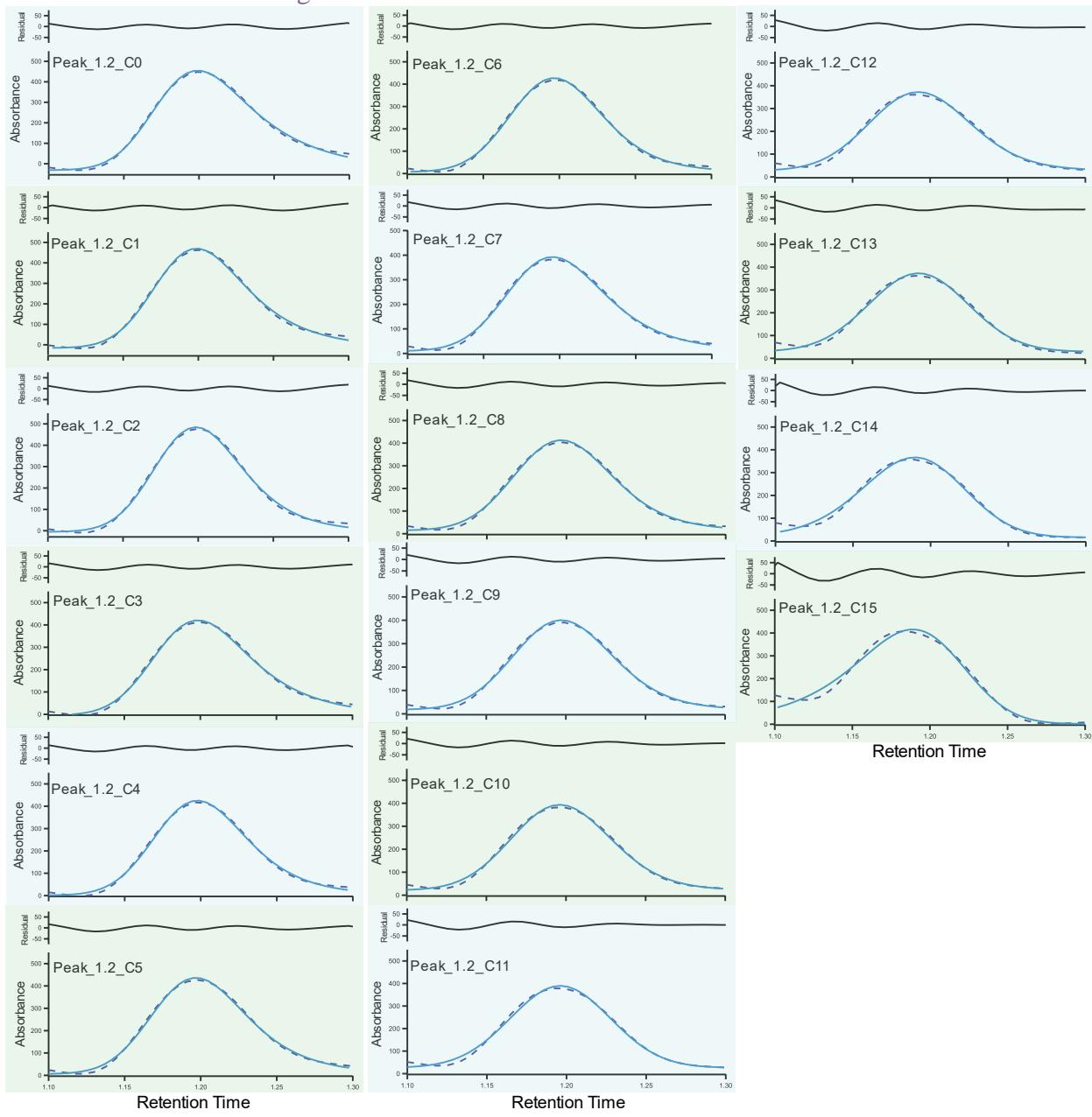
### HPLC MS – positive mode

| <b>Sequence</b> | <b>Neutral Mass</b> | <b>Formula</b> | <b>Deprotonated Mass</b> | <b>Experimental Mass</b> | <b>Difference</b> | <b>Relative</b> |
|-----------------|---------------------|----------------|--------------------------|--------------------------|-------------------|-----------------|
| yy              | 166.0835            | C6H14O5        | 167.0913                 | 167.1                    | 0.0087            | 11.3976         |
| gyu-H2O         | 174.0634            | C6H10O4N2      | 175.0712                 | 175.1                    | 0.0288            | 8.9444          |
| yn-H2O          | 191.0801            | C8H9O1N5       | 192.0879                 | 192.1                    | 0.0121            | 30.0954         |
| Ggy-H2O         | 191.0634            | C7H11O5N1      | 192.0712                 | 192.1                    | 0.0288            | 30.0954         |
| yl-H2O          | 242.1091            | C9H16O7        | 243.1169                 | 243.1                    | 0.0169            | 5.3535          |
| tl-H2O          | 242.0539            | C8H12O6S1      | 243.0617                 | 243.1                    | 0.0383            | 5.3535          |
| ynn-H2O         | 265.1168            | C11H15O3N5     | 266.1246                 | 266.1                    | 0.0246            | 5.2571          |
| tyn-H2O         | 265.0616            | C10H11O2N5S1   | 266.0694                 | 266.1                    | 0.0306            | 5.2571          |
| Gyyy-H2O        | 265.1001            | C10H17O7N1     | 266.1079                 | 266.1                    | 0.0079            | 5.2571          |
| GGGtn           | 386.1009            | C13H16O4N8S1   | 387.1087                 | 387.1                    | 0.0087            | 6.5772          |
| GGGGgy          | 386.1394            | C13H22O9N4     | 387.1472                 | 387.1                    | 0.0472            | 6.5772          |
| GGGGgt          | 386.0842            | C12H18O8N4S1   | 387.0920                 | 387.1                    | 0.0080            | 6.5772          |
| GGGyn           | 386.1561            | C14H20O5N8     | 387.1639                 | 387.2                    | 0.0361            | 6.1804          |

## Fraction 2 (retention time = 1.2 min)

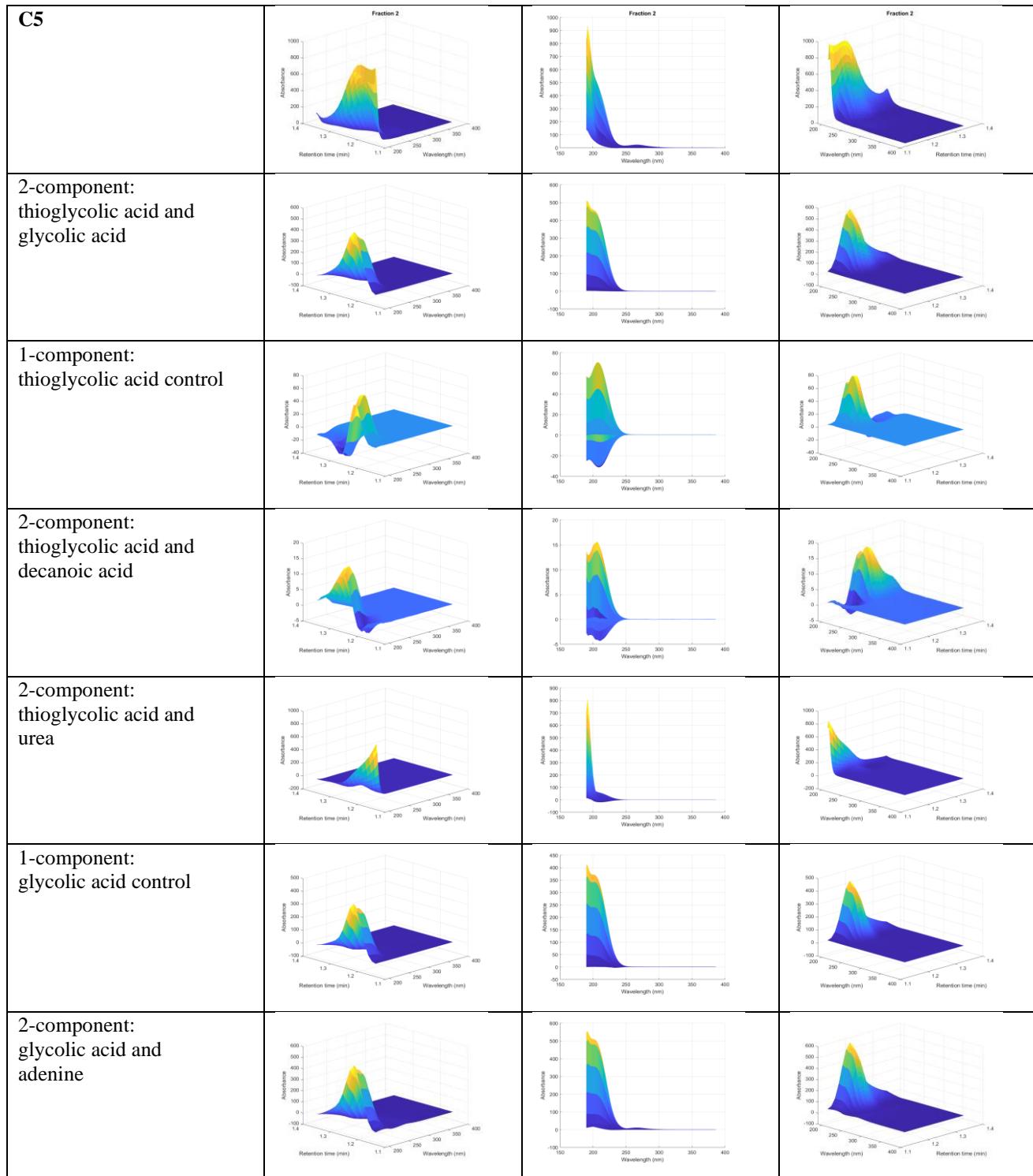
Initially, fraction 2 is composed of glycolic acid only. Over cycles the absorbance peak goes down and then goes up, indicating the consumption of glycolic acid and appearance of new hydrophilic products that are not retained on the C18 column. The MS data indicates a variety of possible co-elutants in this fraction.

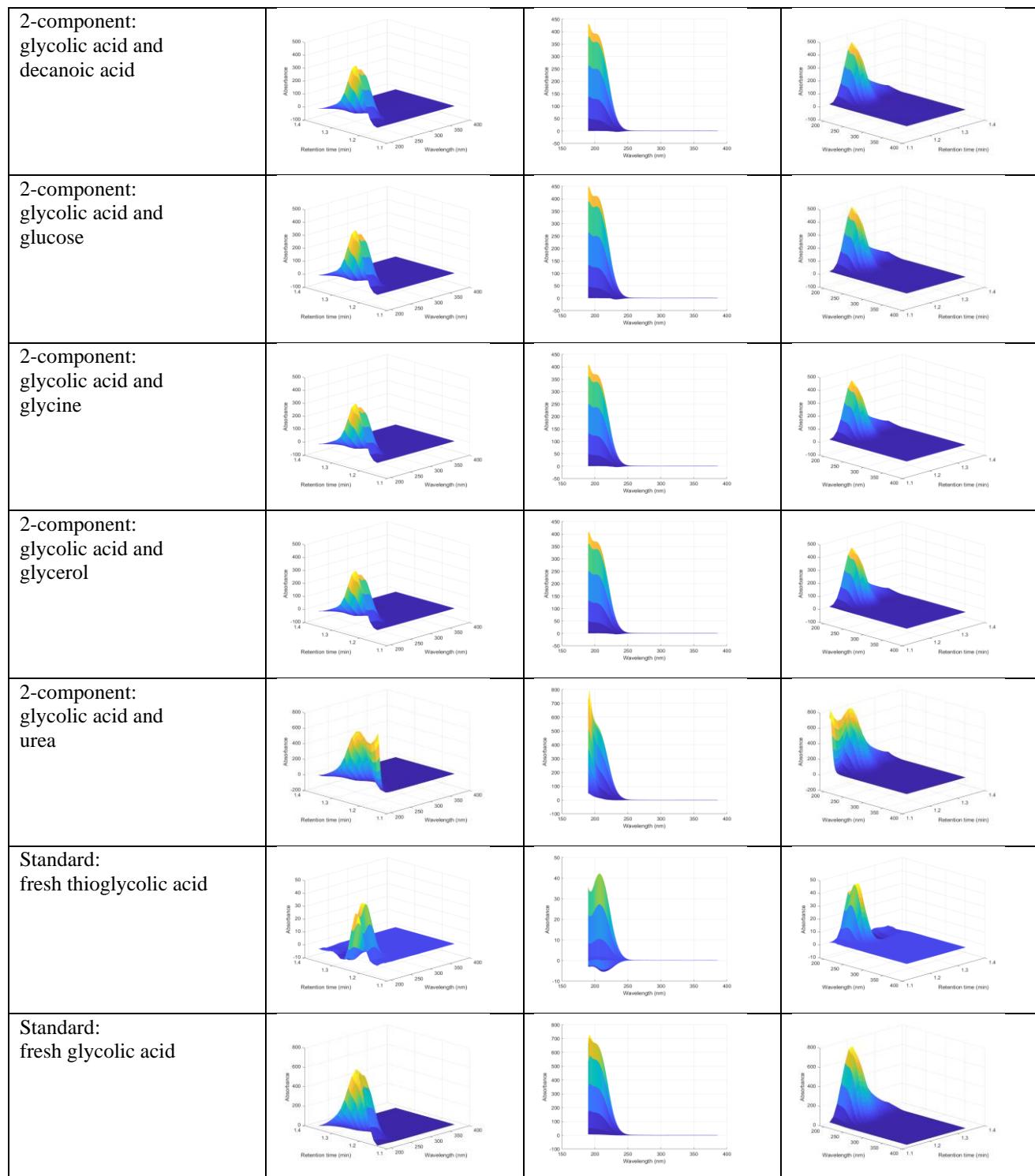
HPLC Curve fitting



**Figure S7. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 2 which has a retention time of about 1.2 minutes.

## UV-VIS spectrum





**Figure S8. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 2 and relevant fresh, control, and 2 building-block dry-downs.

HPLC MS

**HPLC MS – negative mode**

| Sequence | Neutral Mass | Formula     | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-------------|-------------------|-------------------|------------|----------|
| g        | 76.0165      | C2H4O3      | 75.0087           | 75.0              | 0.0087     | 40.6811  |
| G        | 77.0329      | C2H5O2N1    | 76.0251           | 76.1              | 0.0749     | 5.0165   |
| y        | 92.0478      | C3H8O3      | 91.0400           | 91.0              | 0.0400     | 69.1785  |
| t        | 91.9926      | C2H4O2S1    | 90.9848           | 91.0              | 0.0152     | 69.1785  |
| tt-H2    | 163.9595     | C4H4O3S2    | 162.9517          | 163.0             | 0.0483     | 31.1444  |
| ty       | 166.0293     | C5H10O4S1   | 165.0215          | 165.0             | 0.0215     | 16.9789  |
| tt       | 165.9741     | C4H6O3S2    | 164.9663          | 165.0             | 0.0337     | 16.9789  |
| yy       | 166.0845     | C6H14O5     | 165.0767          | 165.1             | 0.0233     | 14.0888  |
| ggu      | 176.0437     | C5H8O5N2    | 175.0359          | 175.0             | 0.0359     | 17.9043  |
| l        | 186.0840     | C6H12O6     | 185.0762          | 185.1             | 0.0238     | 7.7172   |
| ttu-H2   | 205.9813     | C5H6O3N2S2  | 204.9735          | 205.0             | 0.0265     | 14.6329  |
| Gun      | 236.0986     | C8H10O1N8   | 235.0908          | 235.1             | 0.0092     | 7.1353   |
| GGgu     | 236.0819     | C7H12O5N4   | 235.0741          | 235.1             | 0.0259     | 7.1353   |
| GGGu     | 237.0983     | C7H13O4N5   | 236.0905          | 236.1             | 0.0095     | 5.3146   |
| gttu-H2  | 263.9867     | C7H8O5N2S2  | 262.9789          | 263.0             | 0.0211     | 31.1326  |
| gtyu     | 266.0565     | C8H14O6N2S1 | 265.0487          | 265.0             | 0.0487     | 16.4572  |
| gttu     | 266.0013     | C7H10O5N2S2 | 264.9935          | 265.0             | 0.0065     | 16.4572  |
| gggt     | 266.0088     | C8H10O8S1   | 265.0010          | 265.0             | 0.0010     | 16.4572  |
| gyyu     | 266.1117     | C9H18O7N2   | 265.1039          | 265.1             | 0.0039     | 16.7770  |
| gggy     | 266.0640     | C9H14O9     | 265.0562          | 265.1             | 0.0438     | 16.7770  |
| Gdu      | 274.1938     | C13H25O3N3  | 273.1860          | 273.2             | 0.0140     | 10.7649  |
| GGI      | 304.1276     | C10H18O8N2  | 303.1198          | 303.1             | 0.0198     | 5.3152   |

**HPLC MS – positive mode**

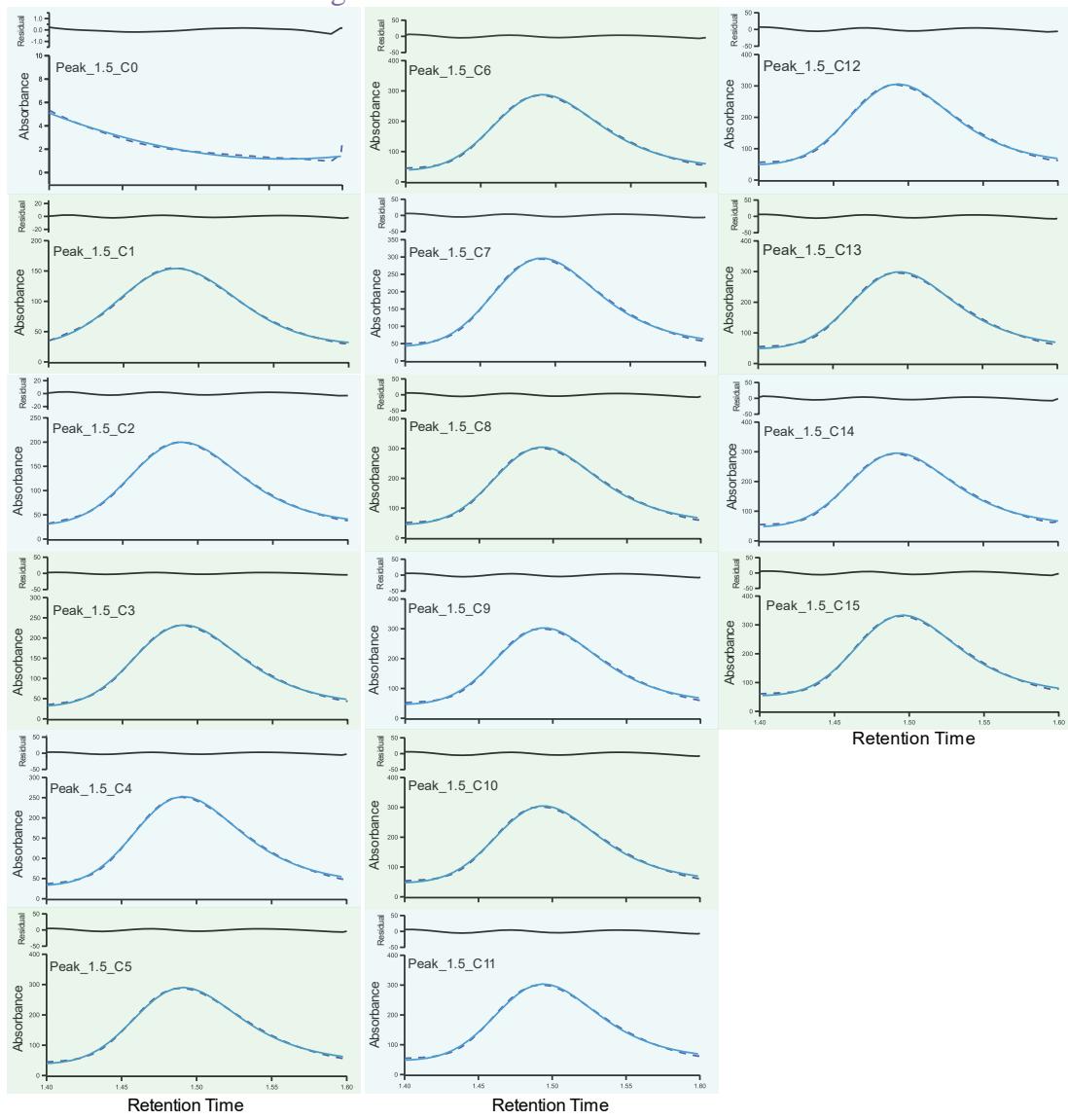
| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5   | 167.0913          | 167.1             | 0.0087     | 7.5030   |
| gyu-H2O  | 174.0634     | C6H10O4N2 | 175.0712          | 175.1             | 0.0288     | 9.0196   |
| yn-H2O   | 191.0801     | C8H9O1N5  | 192.0879          | 192.1             | 0.0121     | 14.7249  |

|          |          |              |          |       |        |         |
|----------|----------|--------------|----------|-------|--------|---------|
| Ggy-H2O  | 191.0634 | C7H11O5N1    | 192.0712 | 192.1 | 0.0288 | 14.7249 |
| Ggn-H2O  | 234.0706 | C9H8O2N6     | 235.0784 | 235.1 | 0.0216 | 5.1059  |
| GGyu-H2O | 234.1016 | C8H14O4N4    | 235.1094 | 235.1 | 0.0094 | 5.1059  |
| yl-H2O   | 242.1091 | C9H16O7      | 243.1169 | 243.1 | 0.0169 | 6.1085  |
| tl-H2O   | 242.0539 | C8H12O6S1    | 243.0617 | 243.1 | 0.0383 | 6.1085  |
| GGGGgt   | 386.0842 | C12H18O8N4S1 | 387.0920 | 387.1 | 0.0080 | 5.0021  |

### Fraction 3 (retention time = 1.5 min)

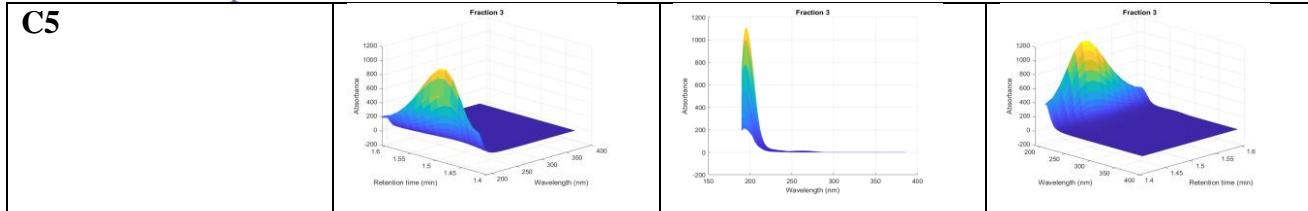
Fraction 3 is a product peak (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that this product is formed in cycle 1 and persists at comparable concentrations in all subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and a 2-component dry-down of glycolic acid and urea. Indeed, MS analysis confirms the presence of oligomers composed of g and u in this fraction (such as gu and ggu).

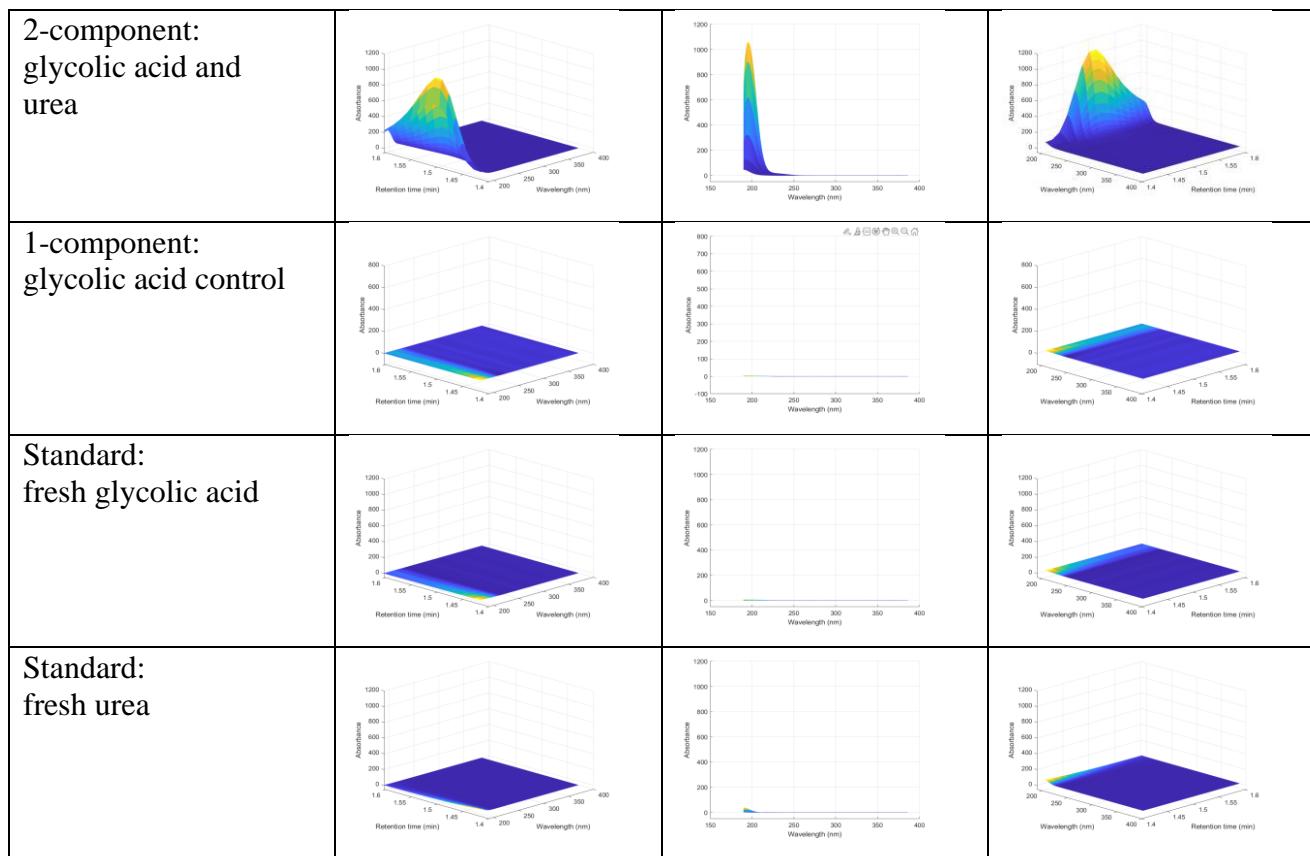
### HPLC Curve fitting



**Figure S9. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 3 which has a retention time of about 1.5 minutes.

### UV-VIS spectrum





**Figure S10. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 3 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula     | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-------------|-------------------|-------------------|------------|----------|
| g        | 76.0165      | C2H4O3      | 75.0087           | 75.1              | 0.0913     | 5.2359   |
| y        | 92.0478      | C3H8O3      | 91.0400           | 91.0              | 0.0400     | 88.1708  |
| t        | 91.9926      | C2H4O2S1    | 90.9848           | 91.0              | 0.0152     | 88.1708  |
| gu       | 118.0383     | C3H6O3N2    | 117.0305          | 117.0             | 0.0305     | 5.7023   |
| ggu      | 176.0437     | C5H8O5N2    | 175.0359          | 175.0             | 0.0359     | 49.4679  |
| ttu-H2   | 205.9813     | C5H6O3N2S2  | 204.9735          | 205.0             | 0.0265     | 9.7127   |
| gl       | 244.0894     | C8H14O8     | 243.0816          | 243.1             | 0.0184     | 6.0548   |
| ttyu-H2  | 280.0180     | C8H12O5N2S2 | 279.0102          | 279.0             | 0.0102     | 6.6568   |
| tttu-H2  | 279.9628     | C7H8O4N2S3  | 278.9550          | 279.0             | 0.0450     | 6.6568   |
| ggtt-H2  | 279.9703     | C8H8O7S2    | 278.9625          | 279.0             | 0.0375     | 6.6568   |

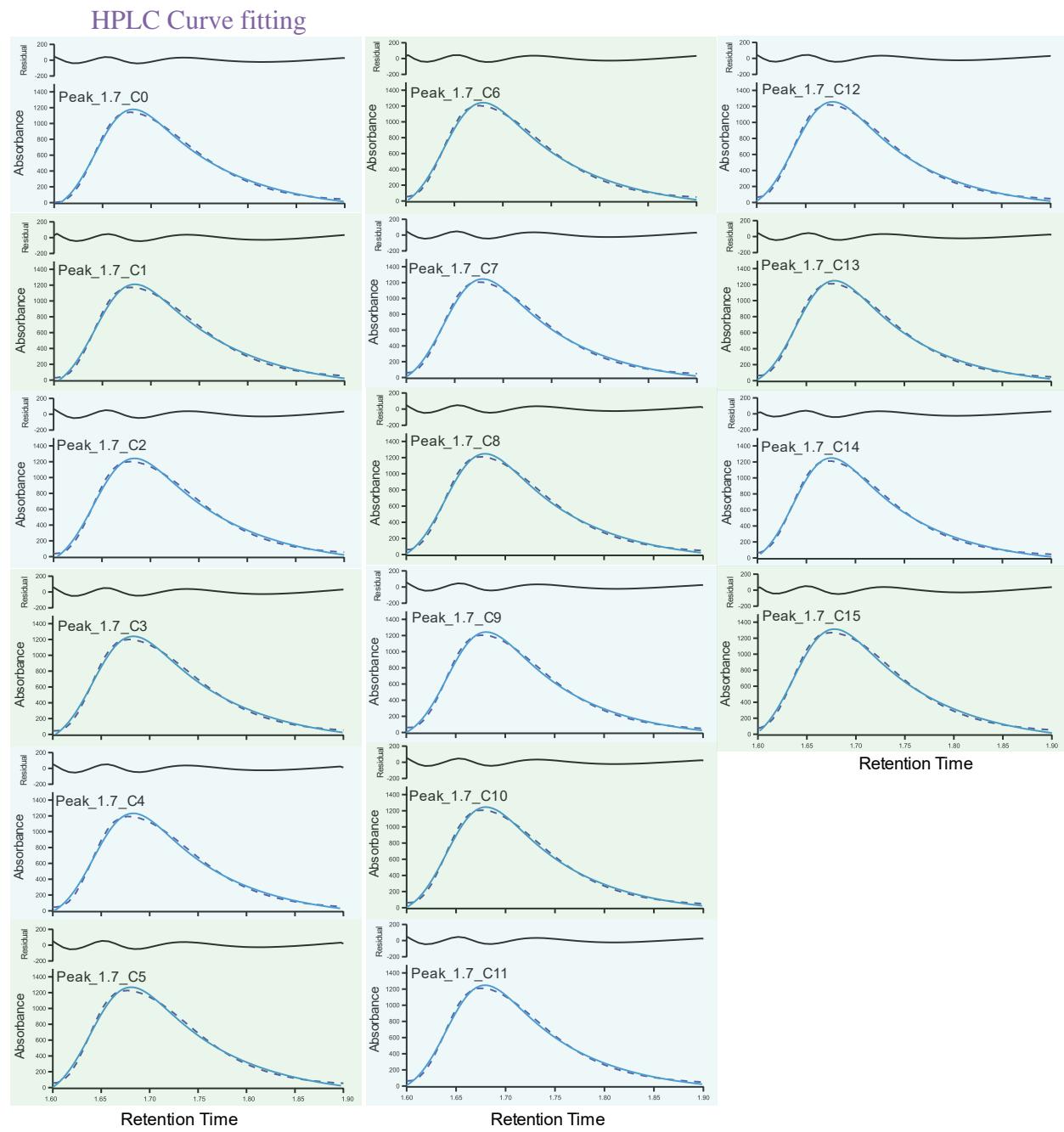
|     |          |              |          |       |        |         |
|-----|----------|--------------|----------|-------|--------|---------|
| gyd | 305.1923 | C15H28O6     | 304.1845 | 304.5 | 0.3155 | 6.4316  |
| gtd | 305.1371 | C14H24O5S1   | 304.1293 | 304.5 | 0.3707 | 6.4316  |
| Gtd | 306.1535 | C14H25O4N1S1 | 305.1457 | 305.1 | 0.0457 | 15.4957 |
| Gyd | 306.2087 | C15H29O5N1   | 305.2009 | 305.2 | 0.0009 | 12.7689 |

**HPLC MS – positive mode**

| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5   | 167.0913          | 167.1             | 0.0087     | 18.7152  |
| gyu-H2O  | 174.0634     | C6H10O4N2 | 175.0712          | 175.1             | 0.0288     | 8.9561   |
| yn-H2O   | 191.0801     | C8H9O1N5  | 192.0879          | 192.1             | 0.0121     | 17.6606  |
| Ggy-H2O  | 191.0634     | C7H11O5N1 | 192.0712          | 192.1             | 0.0288     | 17.6606  |

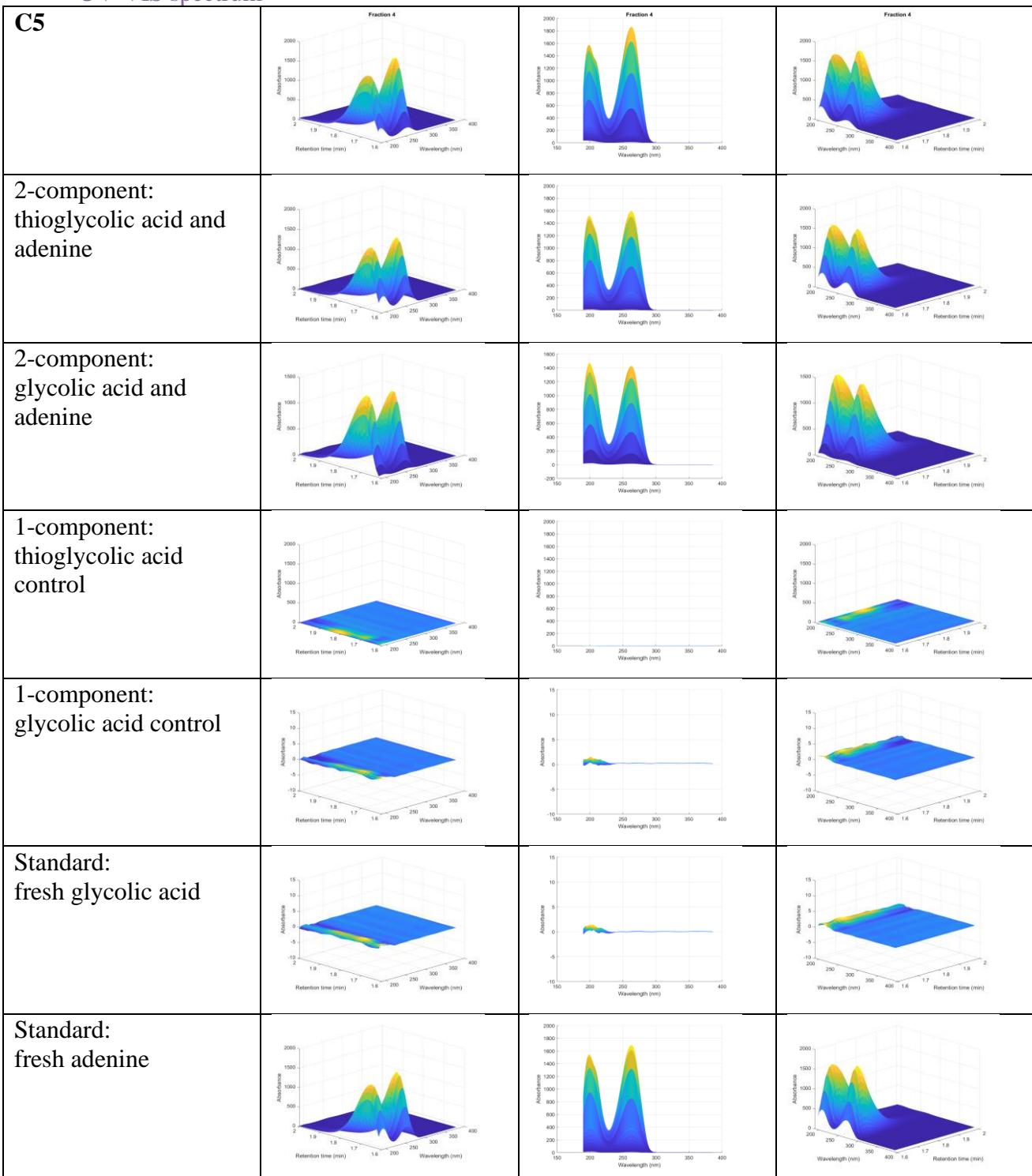
## Fraction 4 (retention time = 1.7 min)

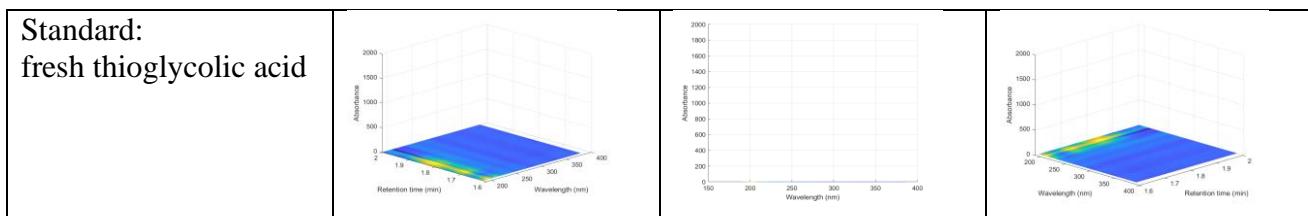
Fraction 4 is mostly adenine monomer. The HPLC curve fitting indicates an increase in the absorbance of this peak over cycles, indicating the formation of new hydrophilic species. MS analysis confirms the presence of various potential product peaks, such as heterodimers of glycolic acid and glycine (gG).



**Figure S11. Curve Fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 4 which has a retention time of about 1.7 minutes.

UV-VIS spectrum





**Figure S12. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 4 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3       | 91.0400           | 91.0              | 0.0400     | 82.2071  |
| t        | 91.9926      | C2H4O2S1     | 90.9848           | 91.0              | 0.0152     | 82.2071  |
| n        | 135.0550     | C5H5N5       | 134.0472          | 134.0             | 0.0472     | 34.3871  |
| Gg       | 135.0383     | C4H7O4N1     | 134.0305          | 134.0             | 0.0305     | 34.3871  |
| ggu      | 176.0437     | C5H8O5N2     | 175.0359          | 175.0             | 0.0359     | 33.2801  |
| gyd      | 305.1923     | C15H28O6     | 304.1845          | 304.5             | 0.3155     | 5.6603   |
| gtd      | 305.1371     | C14H24O5S1   | 304.1293          | 304.5             | 0.3707     | 5.6603   |
| Gtd      | 306.1535     | C14H25O4N1S1 | 305.1457          | 305.1             | 0.0457     | 12.0432  |
| Gyd      | 306.2087     | C15H29O5N1   | 305.2009          | 305.2             | 0.0009     | 8.3741   |

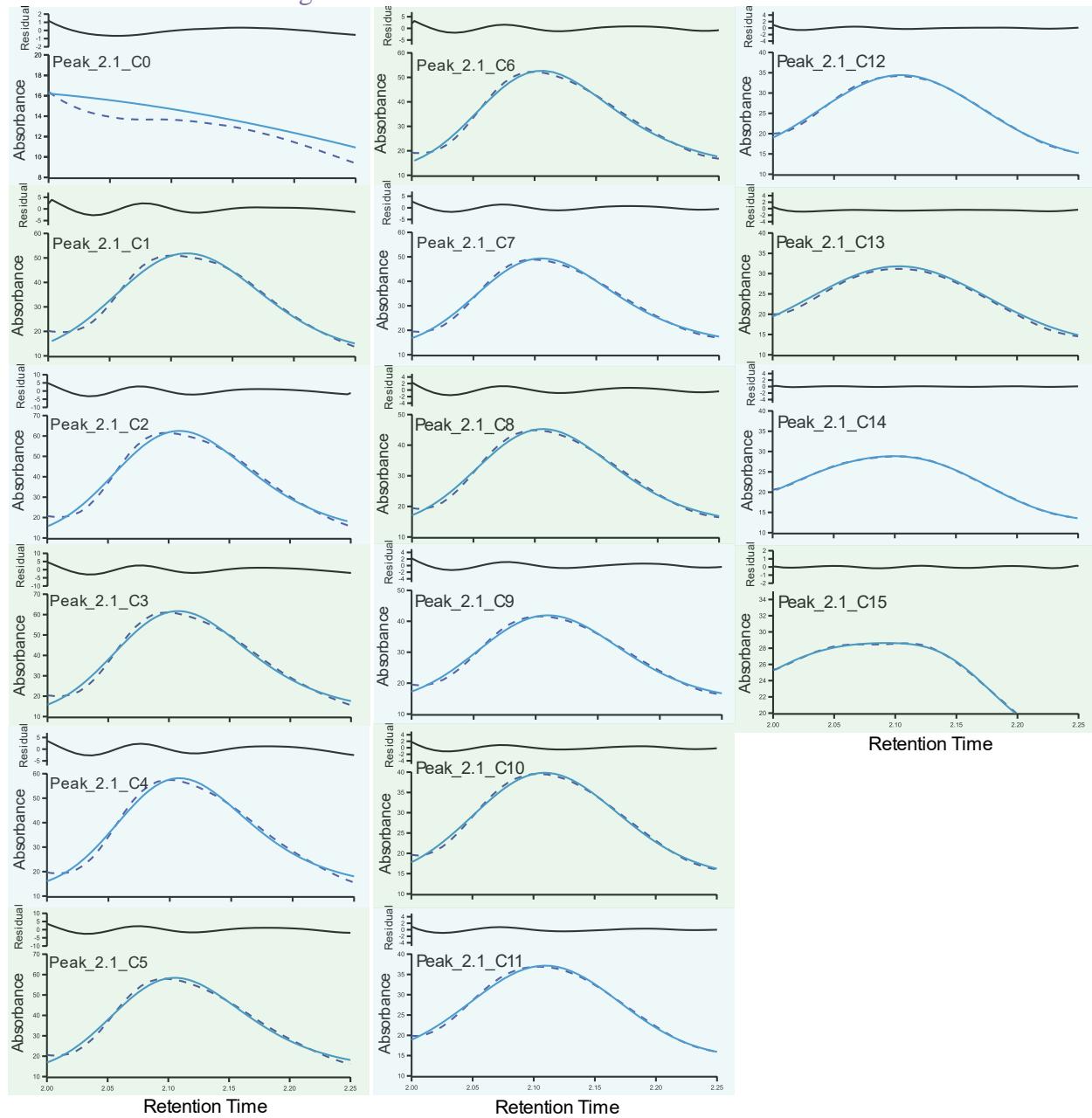
#### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5   | 167.0913          | 167.1             | 0.0087     | 16.1364  |
| gyu-H2O  | 174.0634     | C6H10O4N2 | 175.0712          | 175.1             | 0.0288     | 7.4952   |

### Fraction 5 (retention time = 2.1 min)

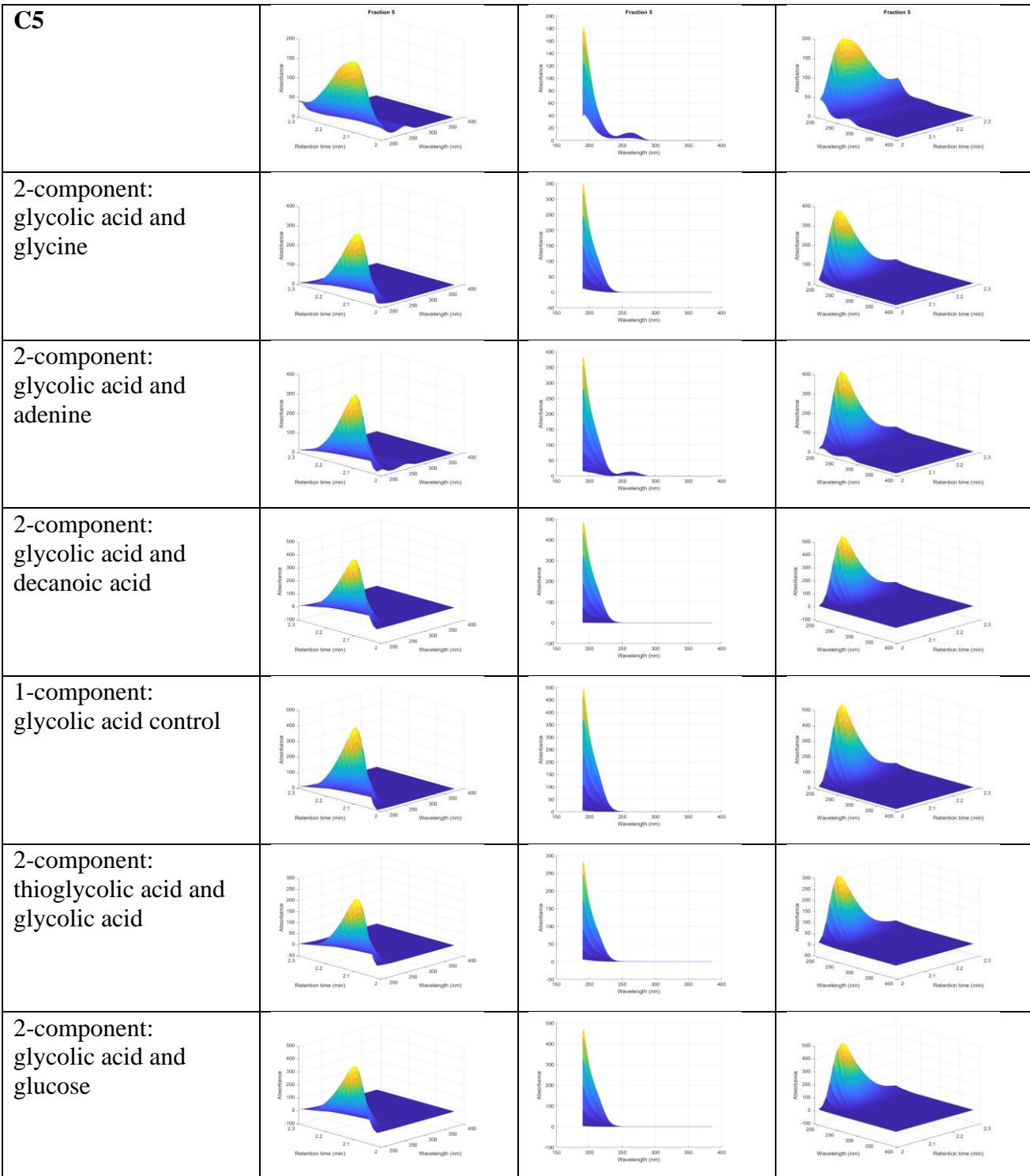
Fraction 5 is a product peak (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that this product is formed in cycle 1, reaches a maximum at cycle 2 and then decreases in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and all 2-component dry-down reactions involving glycolic acid. MS analysis suggests that various products are co-eluted in this fraction, such as oligomers composed of g alone (e.g. gg) and other products composed of g and other constituents.

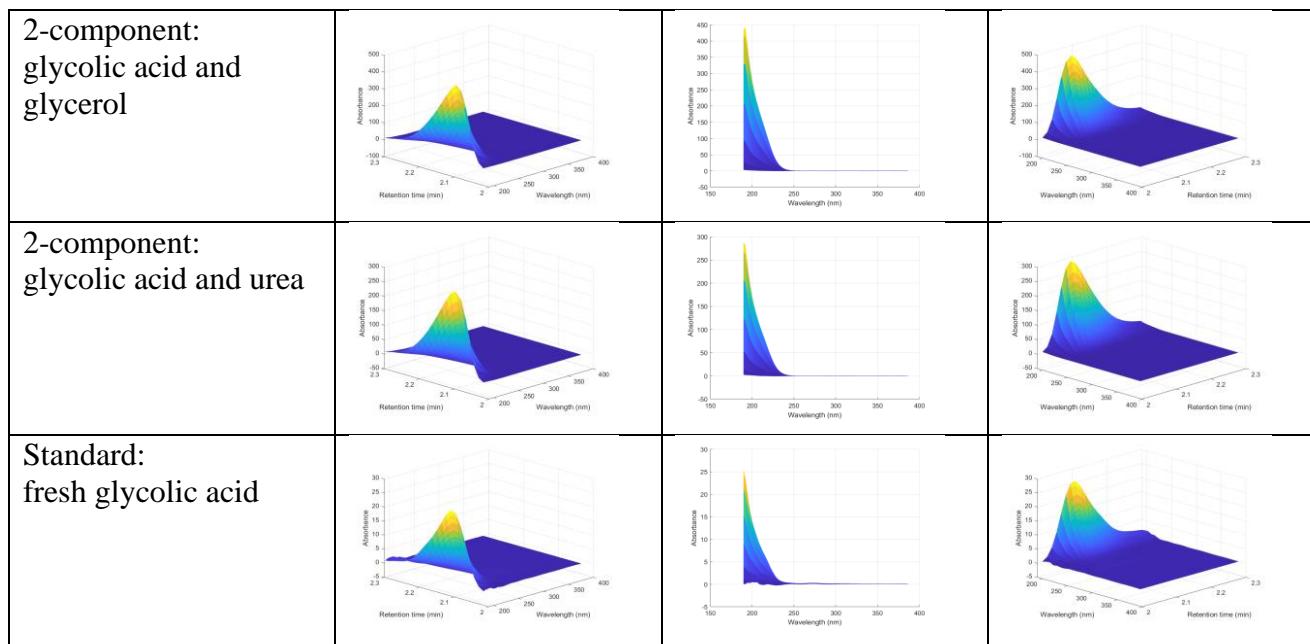
### HPLC Curve fitting



**Figure S13. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 5 which has a retention time of about 2.1 minutes.

### UV-VIS spectrum





**Figure S14. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 5 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula    | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3     | 91.0400           | 91.0              | 0.0400     | 83.8706  |
| t        | 91.9926      | C2H4O2S1   | 90.9848           | 91.0              | 0.0152     | 83.8706  |
| tu       | 134.0144     | C3H6O2N2S1 | 133.0066          | 133.0             | 0.0066     | 34.6192  |
| gg       | 134.0219     | C4H6O5     | 133.0141          | 133.0             | 0.0141     | 34.6192  |
| yu       | 134.0696     | C4H10O3N2  | 133.0618          | 133.1             | 0.0382     | 38.5615  |
| n        | 135.0550     | C5H5N5     | 134.0472          | 134.1             | 0.0528     | 5.0390   |
| Gg       | 135.0383     | C4H7O4N1   | 134.0305          | 134.1             | 0.0695     | 5.0390   |
| ty       | 166.0293     | C5H10O4S1  | 165.0215          | 165.0             | 0.0215     | 5.2849   |
| tt       | 165.9741     | C4H6O3S2   | 164.9663          | 165.0             | 0.0337     | 5.2849   |
| yy       | 166.0845     | C6H14O5    | 165.0767          | 165.1             | 0.0233     | 5.0991   |
| ggu      | 176.0437     | C5H8O5N2   | 175.0359          | 175.0             | 0.0359     | 16.0874  |
| gtu      | 192.0198     | C5H8O4N2S1 | 191.0120          | 191.0             | 0.0120     | 6.3238   |
| ggg      | 192.0273     | C6H8O7     | 191.0195          | 191.0             | 0.0195     | 6.3238   |
| gyu      | 192.0750     | C6H12O5N2  | 191.0672          | 191.1             | 0.0328     | 7.0675   |

|         |          |              |          |       |        |        |
|---------|----------|--------------|----------|-------|--------|--------|
| gl      | 244.0894 | C8H14O8      | 243.0816 | 243.1 | 0.0184 | 6.0085 |
| gttu-H2 | 263.9867 | C7H8O5N2S2   | 262.9789 | 263.0 | 0.0211 | 6.7287 |
| GGtl    | 378.1091 | C12H20O9N2S1 | 377.1013 | 377.1 | 0.0013 | 5.9109 |
| GGyl    | 378.1643 | C13H24O10N2  | 377.1565 | 377.2 | 0.0435 | 5.6242 |

### HPLC MS – positive mode

| Sequence   | Neutral Mass | Formula       | Deprotonated Mass | Experimental Mass | Difference | Relative |
|------------|--------------|---------------|-------------------|-------------------|------------|----------|
| yy         | 166.0835     | C6H14O5       | 167.0913          | 167.1             | 0.0087     | 16.1114  |
| gyu-H2O    | 174.0634     | C6H10O4N2     | 175.0712          | 175.1             | 0.0288     | 9.1055   |
| yn-H2O     | 191.0801     | C8H9O1N5      | 192.0879          | 192.1             | 0.0121     | 12.2546  |
| Ggy-H2O    | 191.0634     | C7H11O5N1     | 192.0712          | 192.1             | 0.0288     | 12.2546  |
| yl-H2O     | 242.1091     | C9H16O7       | 243.1169          | 243.1             | 0.0169     | 8.8441   |
| tl-H2O     | 242.0539     | C8H12O6S1     | 243.0617          | 243.1             | 0.0383     | 8.8441   |
| Gtyy       | 299.0868     | C10H19O7N1S1  | 300.0946          | 300.1             | 0.0054     | 7.7224   |
| gA-H2O     | 343.1208     | C13H15O6N5    | 344.1286          | 344.1             | 0.0286     | 9.5011   |
| gln-H2O    | 343.1217     | C13H15O6N5    | 344.1295          | 344.1             | 0.0295     | 9.5011   |
| Gtlu-H2O   | 343.0975     | C11H17O7N3S1  | 344.1053          | 344.1             | 0.0053     | 9.5011   |
| Gggl-H2O   | 343.1050     | C12H17O10N1   | 344.1128          | 344.1             | 0.0128     | 9.5011   |
| GGGty      | 343.0937     | C11H19O7N3S1  | 344.1015          | 344.1             | 0.0015     | 9.5011   |
| Gylu-H2O   | 343.1527     | C12H21O8N3    | 344.1605          | 344.2             | 0.0395     | 10.3329  |
| GGGyy      | 343.1489     | C12H23O8N3    | 344.1567          | 344.2             | 0.0433     | 10.3329  |
| gggyyu-H2O | 348.0796     | C12H16O10N2   | 349.0874          | 349.1             | 0.0126     | 5.4124   |
| gdn        | 348.1985     | C17H25O3N5    | 349.2063          | 349.2             | 0.0063     | 5.1804   |
| Gydu       | 348.2295     | C16H31O5N3    | 349.2373          | 349.2             | 0.0373     | 5.1804   |
| Gtdu       | 348.1743     | C15H27O4N3S1  | 349.1821          | 349.2             | 0.0179     | 5.1804   |
| Gggd       | 348.1818     | C16H27O7N1    | 349.1896          | 349.2             | 0.0104     | 5.1804   |
| Gtyy-H2    | 371.0537     | C12H19O8N1S2  | 372.0615          | 372.1             | 0.0385     | 8.5019   |
| GGGGn      | 371.1412     | C13H17O4N9    | 372.1490          | 372.1             | 0.0490     | 8.5019   |
| GGGGGg     | 371.1245     | C12H19O8N5    | 372.1323          | 372.1             | 0.0323     | 8.5019   |
| ggdu-H2O   | 371.1766     | C17H26O7N2    | 372.1844          | 372.2             | 0.0156     | 8.0031   |
| Gtyl-H2O   | 375.1124     | C13H21O90N1S1 | 376.1202          | 376.1             | 0.0202     | 8.6329   |
| Gttl-H2O   | 375.0572     | C12H17O8N1S2  | 376.0650          | 376.1             | 0.0350     | 8.6329   |
| Gyyl-H2O   | 375.1676     | C14H25O10N1   | 376.1754          | 376.2             | 0.0246     | 8.2678   |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| ttyy-H2     | 386.0686 | C13H22O9S2    | 387.0764 | 387.1 | 0.0236 | 11.1756 |
| GGGtn       | 386.1009 | C13H16O4N8S1  | 387.1087 | 387.1 | 0.0087 | 11.1756 |
| GGGGgy      | 386.1394 | C13H22O9N4    | 387.1472 | 387.1 | 0.0472 | 11.1756 |
| GGGGgt      | 386.0842 | C12H18O8N4S1  | 387.0920 | 387.1 | 0.0080 | 11.1756 |
| GAu-H2O     | 386.1590 | C14H18O5N8    | 387.1668 | 387.2 | 0.0332 | 9.8855  |
| Glun-H2O    | 386.1599 | C14H18O5N8    | 387.1677 | 387.2 | 0.0323 | 9.8855  |
| GGglu-H2O   | 386.1432 | C13H20O90N4   | 387.1510 | 387.2 | 0.0490 | 9.8855  |
| GGGyn       | 386.1561 | C14H20O5N8    | 387.1639 | 387.2 | 0.0361 | 9.8855  |
| GGGGGt      | 387.1006 | C12H19O7N5S1  | 388.1084 | 388.1 | 0.0084 | 16.1589 |
| ggydu-H2O   | 387.2079 | C18H30O7N2    | 388.2157 | 388.2 | 0.0157 | 15.6975 |
| ggtdu-H2O   | 387.1527 | C17H26O6N2S1  | 388.1605 | 388.2 | 0.0395 | 15.6975 |
| gggd-H2O    | 387.1602 | C18H26O9      | 388.1680 | 388.2 | 0.0320 | 15.6975 |
| GGGlu-H2O   | 387.1596 | C13H21O8N5    | 388.1674 | 388.2 | 0.0326 | 15.6975 |
| GGGGGy      | 387.1558 | C13H23O8N5    | 388.1636 | 388.2 | 0.0364 | 15.6975 |
| gtyl        | 392.1066 | C13H22O11S1   | 393.1144 | 393.1 | 0.0144 | 23.8418 |
| gttl        | 392.0514 | C12H18O10S2   | 393.0592 | 393.1 | 0.0408 | 23.8418 |
| Ggggun-H2O  | 392.1032 | C14H14O6N8    | 393.1110 | 393.1 | 0.0110 | 23.8418 |
| GGgggu-H2O  | 392.0865 | C13H16O10N4   | 393.0943 | 393.1 | 0.0057 | 23.8418 |
| gyyl        | 392.1618 | C14H26O12     | 393.1696 | 393.2 | 0.0304 | 24.9203 |
| GGGdu       | 392.2364 | C17H31O5N5    | 393.2442 | 393.2 | 0.0442 | 24.9203 |
| ttyd-H2     | 393.1343 | C17H28O6S2    | 394.1421 | 394.1 | 0.0421 | 6.7287  |
| tttd-H2     | 393.0791 | C16H24O5S3    | 394.0869 | 394.1 | 0.0131 | 6.7287  |
| Gtyl        | 393.1230 | C13H23O10N1S1 | 394.1308 | 394.1 | 0.0308 | 6.7287  |
| Gttl        | 393.0678 | C12H19O9N1S2  | 394.0756 | 394.1 | 0.0244 | 6.7287  |
| GGggun-H2O  | 393.1196 | C14H15O5N9    | 394.1274 | 394.1 | 0.0274 | 6.7287  |
| GGGgggu-H2O | 393.1029 | C13H17O90N5   | 394.1107 | 394.1 | 0.0107 | 6.7287  |
| Gyyl        | 393.1782 | C14H27O11N1   | 394.1860 | 394.2 | 0.0140 | 6.7217  |
| tyyl        | 408.1379 | C14H26O11S1   | 409.1457 | 409.1 | 0.0457 | 5.4006  |
| ttyl        | 408.0827 | C13H22O10S2   | 409.0905 | 409.1 | 0.0095 | 5.4006  |
| Gggyun-H2O  | 408.1345 | C15H18O6N8    | 409.1423 | 409.1 | 0.0423 | 5.4006  |
| Gggtun-H2O  | 408.0793 | C14H14O5N8S1  | 409.0871 | 409.1 | 0.0129 | 5.4006  |
| Ggggn-H2O   | 408.0868 | C15H14O8N6    | 409.0946 | 409.1 | 0.0054 | 5.4006  |
| gggggggu    | 408.0643 | C13H16O13N2   | 409.0721 | 409.1 | 0.0279 | 5.4006  |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| GGgggyu-H2O | 408.1178 | C14H20O10N4   | 409.1256 | 409.1 | 0.0256 | 5.4006  |
| GGgggtu-H2O | 408.0626 | C13H16O90N4S1 | 409.0704 | 409.1 | 0.0296 | 5.4006  |
| GGggggg-H2O | 408.0701 | C14H16O12N2   | 409.0779 | 409.1 | 0.0221 | 5.4006  |
| yyyl        | 408.1931 | C15H30O12     | 409.2009 | 409.2 | 0.0009 | 5.2244  |
| GGdn        | 408.2367 | C19H29O3N7    | 409.2445 | 409.2 | 0.0445 | 5.2244  |
| GGGgd       | 408.2200 | C18H31O7N3    | 409.2278 | 409.2 | 0.0278 | 5.2244  |
| Gttxyu      | 415.0349 | C12H19O7N3S3  | 416.0427 | 416.0 | 0.0427 | 10.7045 |
| gtyyn       | 415.1143 | C15H21O7N5S1  | 416.1221 | 416.1 | 0.0221 | 11.7990 |
| gttyn       | 415.0591 | C14H17O6N5S2  | 416.0669 | 416.1 | 0.0331 | 11.7990 |
| Gttxyu      | 415.0901 | C13H23O8N3S2  | 416.0979 | 416.1 | 0.0021 | 11.7990 |
| Gggtty      | 415.0976 | C14H23O11N1S1 | 416.1054 | 416.1 | 0.0054 | 11.7990 |
| Gggtty      | 415.0424 | C13H19O10N1S2 | 416.0502 | 416.1 | 0.0498 | 11.7990 |
| GGGttxy-H2  | 415.0606 | C13H19O8N3S2  | 416.0684 | 416.1 | 0.0316 | 11.7990 |
| tld         | 415.2036 | C18H32O8S1    | 416.2114 | 416.2 | 0.0114 | 12.0131 |
| gyyyyn      | 415.1695 | C16H25O8N5    | 416.1773 | 416.2 | 0.0227 | 12.0131 |
| Gyyyyu      | 415.2005 | C15H31O10N3   | 416.2083 | 416.2 | 0.0083 | 12.0131 |
| Gttxyu      | 415.1453 | C14H27O9N3S1  | 416.1531 | 416.2 | 0.0469 | 12.0131 |
| Gggyyy      | 415.1528 | C15H27O12N1   | 416.1606 | 416.2 | 0.0394 | 12.0131 |
| yld         | 415.2588 | C19H36O9      | 416.2666 | 416.3 | 0.0334 | 10.6106 |
| Gttd-H2     | 420.1412 | C17H27O5N3S2  | 421.1490 | 421.1 | 0.0490 | 6.7107  |
| Gtttd-H2O   | 420.1288 | C18H27O6N1S2  | 421.1366 | 421.1 | 0.0366 | 6.7107  |
| GGtlu       | 420.1299 | C13H22O9N4S1  | 421.1377 | 421.1 | 0.0377 | 6.7107  |
| GGggl       | 420.1374 | C14H22O12N2   | 421.1452 | 421.1 | 0.0452 | 6.7107  |
| An          | 420.1699 | C16H18O4N10   | 421.1777 | 421.2 | 0.0223 | 7.1056  |
| GgA         | 420.1532 | C15H20O8N6    | 421.1610 | 421.2 | 0.0390 | 7.1056  |
| tydn-H2O    | 420.2007 | C20H29O3N5S1  | 421.2085 | 421.2 | 0.0085 | 7.1056  |
| ttdn-H2O    | 420.1455 | C19H25O2N5S2  | 421.1533 | 421.2 | 0.0467 | 7.1056  |
| Ggln        | 420.1541 | C15H20O8N6    | 421.1619 | 421.2 | 0.0381 | 7.1056  |
| Ggyyd-H2O   | 420.2392 | C20H35O8N1    | 421.2470 | 421.2 | 0.0470 | 7.1056  |
| Ggtyd-H2O   | 420.1840 | C19H31O7N1S1  | 421.1918 | 421.2 | 0.0082 | 7.1056  |
| GGylu       | 420.1851 | C14H26O10N4   | 421.1929 | 421.2 | 0.0071 | 7.1056  |
| yydn-H2O    | 420.2559 | C21H33O4N5    | 421.2637 | 421.3 | 0.0363 | 6.6710  |
| tttyn       | 431.0352 | C14H17O5N5S3  | 432.0430 | 432.0 | 0.0430 | 15.4824 |

|            |          |               |          |       |        |         |
|------------|----------|---------------|----------|-------|--------|---------|
| ttyyn      | 431.0904 | C15H21O6N5S2  | 432.0982 | 432.1 | 0.0018 | 16.7985 |
| Ggtyyy     | 431.1289 | C15H27O11N1S1 | 432.1367 | 432.1 | 0.0367 | 16.7985 |
| Ggttyy     | 431.0737 | C14H23O10N1S2 | 432.0815 | 432.1 | 0.0185 | 16.7985 |
| yyyn       | 431.2008 | C17H29O8N5    | 432.2086 | 432.2 | 0.0086 | 17.3963 |
| ttyyn      | 431.1456 | C16H25O7N5S1  | 432.1534 | 432.2 | 0.0466 | 17.3963 |
| Ggdun-H2O  | 431.2315 | C20H28O3N8    | 432.2393 | 432.2 | 0.0393 | 17.3963 |
| Ggyyyy     | 431.1841 | C16H31O12N1   | 432.1919 | 432.2 | 0.0081 | 17.3963 |
| GGggdu-H2O | 431.2148 | C19H30O7N4    | 432.2226 | 432.2 | 0.0226 | 17.3963 |
| GGGGGGG    | 431.1627 | C14H23O8N7    | 432.1705 | 432.2 | 0.0295 | 17.3963 |
| ttlu-H2O   | 432.0387 | C13H18O8N2S3  | 433.0465 | 433.0 | 0.0465 | 5.2304  |
| GGtty      | 432.0349 | C13H20O8N2S3  | 433.0427 | 433.0 | 0.0427 | 5.2304  |
| tyylu-H2O  | 432.1491 | C15H26O10N2S1 | 433.1569 | 433.1 | 0.0569 | 5.1382  |
| ttylu-H2O  | 432.0939 | C14H22O90N2S2 | 433.1017 | 433.1 | 0.0017 | 5.1382  |
| gttu-H2    | 432.0586 | C13H18O10N2S2 | 433.0664 | 433.1 | 0.0336 | 5.1382  |
| ggyyl-H2O  | 432.1566 | C16H26O13     | 433.1644 | 433.1 | 0.0644 | 5.1382  |
| ggtyl-H2O  | 432.1014 | C15H22O12S1   | 433.1092 | 433.1 | 0.0092 | 5.1382  |
| ggttl-H2O  | 432.0462 | C14H18O11S2   | 433.0540 | 433.1 | 0.0460 | 5.1382  |
| GGtyyy     | 432.1453 | C15H28O10N2S1 | 433.1531 | 433.1 | 0.0531 | 5.1382  |
| GGttyy     | 432.0901 | C14H24O9N2S2  | 433.0979 | 433.1 | 0.0021 | 5.1382  |
| GtA        | 436.1293 | C15H20O7N6S1  | 437.1371 | 437.1 | 0.0371 | 7.6280  |
| ttdn-H2    | 436.1415 | C19H25O3N5S2  | 437.1493 | 437.1 | 0.0493 | 7.6280  |
| Gtln       | 436.1302 | C15H20O7N6S1  | 437.1380 | 437.1 | 0.0380 | 7.6280  |
| Gttd-H2O   | 436.1049 | C18H27O5N1S3  | 437.1127 | 437.1 | 0.0127 | 7.6280  |
| Ggtd-H2    | 436.1248 | C18H27O7N1S2  | 437.1326 | 437.1 | 0.0326 | 7.6280  |
| GGgtl      | 436.1135 | C14H22O11N2S1 | 437.1213 | 437.1 | 0.0213 | 7.6280  |
| GyA        | 436.1845 | C16H24O8N6    | 437.1923 | 437.2 | 0.0077 | 7.6977  |
| gllu-H2O   | 436.1725 | C15H24O12N2   | 437.1803 | 437.2 | 0.0197 | 7.6977  |
| Gyln       | 436.1854 | C16H24O8N6    | 437.1932 | 437.2 | 0.0068 | 7.6977  |
| Gtyyd-H2O  | 436.2153 | C20H35O7N1S1  | 437.2231 | 437.2 | 0.0231 | 7.6977  |
| Gttd-H2O   | 436.1601 | C19H31O6N1S2  | 437.1679 | 437.2 | 0.0321 | 7.6977  |
| GGgy1      | 436.1687 | C15H26O12N2   | 437.1765 | 437.2 | 0.0235 | 7.6977  |
| Gyyyd-H2O  | 436.2705 | C21H39O8N1    | 437.2783 | 437.3 | 0.0217 | 6.7750  |
| GGGttu     | 459.0418 | C13H19O7N5S3  | 460.0496 | 460.0 | 0.0496 | 14.8693 |

|            |          |               |          |       |        |         |
|------------|----------|---------------|----------|-------|--------|---------|
| gtAu-H2O   | 459.1241 | C16H19O7N7S1  | 460.1319 | 460.1 | 0.0319 | 17.3395 |
| gggA-H2O   | 459.1316 | C17H19O10N5   | 460.1394 | 460.1 | 0.0394 | 17.3395 |
| gtlun-H2O  | 459.1250 | C16H19O7N7S1  | 460.1328 | 460.1 | 0.0328 | 17.3395 |
| ggglu-H2O  | 459.1325 | C17H19O10N5   | 460.1403 | 460.1 | 0.0403 | 17.3395 |
| Gggglu-H2O | 459.1083 | C15H21O11N3S1 | 460.1161 | 460.1 | 0.0161 | 17.3395 |
| Ggggl-H2O  | 459.1158 | C16H21O14N1   | 460.1236 | 460.1 | 0.0236 | 17.3395 |
| GGgtyn     | 459.1212 | C16H21O7N7S1  | 460.1290 | 460.1 | 0.0290 | 17.3395 |
| GGgttn     | 459.0660 | C15H17O6N7S2  | 460.0738 | 460.1 | 0.0262 | 17.3395 |
| GGGttyu    | 459.0970 | C14H23O8N5S2  | 460.1048 | 460.1 | 0.0048 | 17.3395 |
| GGGggy     | 459.1045 | C15H23O11N3S1 | 460.1123 | 460.1 | 0.0123 | 17.3395 |
| GGGggtt    | 459.0493 | C14H19O10N3S2 | 460.0571 | 460.1 | 0.0429 | 17.3395 |
| GGGGGtt-H2 | 459.0675 | C14H19O8N5S2  | 460.0753 | 460.1 | 0.0247 | 17.3395 |
| gyAu-H2O   | 459.1793 | C17H23O8N7    | 460.1871 | 460.2 | 0.0129 | 18.4190 |
| gylun-H2O  | 459.1802 | C17H23O8N7    | 460.1880 | 460.2 | 0.0120 | 18.4190 |
| Gggylu-H2O | 459.1635 | C16H25O12N3   | 460.1713 | 460.2 | 0.0287 | 18.4190 |
| GGgbyn     | 459.1764 | C17H25O8N7    | 460.1842 | 460.2 | 0.0158 | 18.4190 |
| GGGyyyu    | 459.2074 | C16H31O10N5   | 460.2152 | 460.2 | 0.0152 | 18.4190 |
| GGGttyu    | 459.1522 | C15H27O9N5S1  | 460.1600 | 460.2 | 0.0400 | 18.4190 |
| GGGggyy    | 459.1597 | C16H27O12N3   | 460.1675 | 460.2 | 0.0325 | 18.4190 |
| GGld       | 459.2657 | C20H36O9N2    | 460.2735 | 460.3 | 0.0265 | 16.8817 |
| GtAu-H2O   | 460.1405 | C16H20O6N8S1  | 461.1483 | 461.1 | 0.0483 | 5.7910  |
| Gtlun-H2O  | 460.1414 | C16H20O6N8S1  | 461.1492 | 461.1 | 0.0492 | 5.7910  |
| ttyyyy-H2  | 460.1053 | C16H28O11S2   | 461.1131 | 461.1 | 0.0131 | 5.7910  |
| tttyyy-H2  | 460.0501 | C15H24O10S3   | 461.0579 | 461.1 | 0.0421 | 5.7910  |
| gggglu     | 460.1264 | C15H22O14N2   | 461.1342 | 461.1 | 0.0342 | 5.7910  |
| GGgtlu-H2O | 460.1247 | C15H22O10N4S1 | 461.1325 | 461.1 | 0.0325 | 5.7910  |
| GGgggl-H2O | 460.1322 | C16H22O13N2   | 461.1400 | 461.1 | 0.0400 | 5.7910  |
| GGGtyn     | 460.1376 | C16H22O6N8S1  | 461.1454 | 461.1 | 0.0454 | 5.7910  |
| GGGttn     | 460.0824 | C15H18O5N8S2  | 461.0902 | 461.1 | 0.0098 | 5.7910  |
| GGGGgty    | 460.1209 | C15H24O10N4S1 | 461.1287 | 461.1 | 0.0287 | 5.7910  |
| GGGGggtt   | 460.0657 | C14H20O9N4S2  | 461.0735 | 461.1 | 0.0265 | 5.7910  |
| gAn-H2O    | 460.1647 | C18H18O5N10   | 461.1725 | 461.2 | 0.0275 | 5.7260  |
| GyAu-H2O   | 460.1957 | C17H24O7N8    | 461.2035 | 461.2 | 0.0035 | 5.7260  |

|            |          |               |          |       |        |         |
|------------|----------|---------------|----------|-------|--------|---------|
| GggA-H2O   | 460.1480 | C17H20O90N6   | 461.1558 | 461.2 | 0.0442 | 5.7260  |
| Gylun-H2O  | 460.1966 | C17H24O7N8    | 461.2044 | 461.2 | 0.0044 | 5.7260  |
| Gggln-H2O  | 460.1489 | C17H20O90N6   | 461.1567 | 461.2 | 0.0433 | 5.7260  |
| GGgylu-H2O | 460.1799 | C16H26O11N4   | 461.1877 | 461.2 | 0.0123 | 5.7260  |
| GGGbyn     | 460.1928 | C17H26O7N8    | 461.2006 | 461.2 | 0.0006 | 5.7260  |
| GGGGggyy   | 460.1761 | C16H28O11N4   | 461.1839 | 461.2 | 0.0161 | 5.7260  |
| GGtttn     | 475.0421 | C15H17O5N7S3  | 476.0499 | 476.0 | 0.0499 | 14.7118 |
| GGGgtt     | 475.0254 | C14H19O9N3S3  | 476.0332 | 476.0 | 0.0332 | 14.7118 |
| ttAu-H2O   | 475.1002 | C16H19O6N7S2  | 476.1080 | 476.1 | 0.0080 | 15.7115 |
| ggtA-H2O   | 475.1077 | C17H19O90N5S1 | 476.1155 | 476.1 | 0.0155 | 15.7115 |
| ttlun-H2O  | 475.1011 | C16H19O6N7S2  | 476.1089 | 476.1 | 0.0089 | 15.7115 |
| ggtln-H2O  | 475.1086 | C17H19O90N5S1 | 476.1164 | 476.1 | 0.0164 | 15.7115 |
| Ggtlu-H2O  | 475.1396 | C16H25O11N3S1 | 476.1474 | 476.1 | 0.0474 | 15.7115 |
| Ggtlu-H2O  | 475.0844 | C15H21O10N3S2 | 476.0922 | 476.1 | 0.0078 | 15.7115 |
| Ggggtl-H2O | 475.0919 | C16H21O13N1S1 | 476.0997 | 476.1 | 0.0003 | 15.7115 |
| GGttn      | 475.0973 | C16H21O6N7S2  | 476.1051 | 476.1 | 0.0051 | 15.7115 |
| GGGgtty    | 475.1358 | C16H27O11N3S1 | 476.1436 | 476.1 | 0.0436 | 15.7115 |
| GGGgtty    | 475.0806 | C15H23O10N3S2 | 476.0884 | 476.1 | 0.0116 | 15.7115 |
| yyAu-H2O   | 475.2106 | C18H27O8N7    | 476.2184 | 476.2 | 0.0184 | 15.8837 |
| tyAu-H2O   | 475.1554 | C17H23O7N7S1  | 476.1632 | 476.2 | 0.0368 | 15.8837 |
| ggyA-H2O   | 475.1629 | C18H23O10N5   | 476.1707 | 476.2 | 0.0293 | 15.8837 |
| yylun-H2O  | 475.2115 | C18H27O8N7    | 476.2193 | 476.2 | 0.0193 | 15.8837 |
| tylun-H2O  | 475.1563 | C17H23O7N7S1  | 476.1641 | 476.2 | 0.0359 | 15.8837 |
| ggyln-H2O  | 475.1638 | C18H23O10N5   | 476.1716 | 476.2 | 0.0284 | 15.8837 |
| Ggyylu-H2O | 475.1948 | C17H29O12N3   | 476.2026 | 476.2 | 0.0026 | 15.8837 |
| Ggggyl-H2O | 475.1471 | C17H25O14N1   | 476.1549 | 476.2 | 0.0451 | 15.8837 |
| GGyyyn     | 475.2077 | C18H29O8N7    | 476.2155 | 476.2 | 0.0155 | 15.8837 |
| GGtyn      | 475.1525 | C17H25O7N7S1  | 476.1603 | 476.2 | 0.0397 | 15.8837 |
| GGGgyyy    | 475.1910 | C17H31O12N3   | 476.1988 | 476.2 | 0.0012 | 15.8837 |
| tAn-H2O    | 476.1408 | C18H18O4N10S1 | 477.1486 | 477.1 | 0.0486 | 5.1420  |
| GgtA-H2O   | 476.1241 | C17H20O8N6S1  | 477.1319 | 477.1 | 0.0319 | 5.1420  |
| Ggtln-H2O  | 476.1250 | C17H20O8N6S1  | 477.1328 | 477.1 | 0.0328 | 5.1420  |
| gggtlu     | 476.1025 | C15H22O13N2S1 | 477.1103 | 477.1 | 0.0103 | 5.1420  |

|              |          |               |          |       |        |        |
|--------------|----------|---------------|----------|-------|--------|--------|
| gggggl       | 476.1100 | C16H22O16     | 477.1178 | 477.1 | 0.0178 | 5.1420 |
| GGtlu-H2O    | 476.1008 | C15H22O90N4S2 | 477.1086 | 477.1 | 0.0086 | 5.1420 |
| GGggtl-H2O   | 476.1083 | C16H22O12N2S1 | 477.1161 | 477.1 | 0.0161 | 5.1420 |
| GGGGtty      | 476.0970 | C15H24O9N4S2  | 477.1048 | 477.1 | 0.0048 | 5.1420 |
| GGGGttt      | 476.0418 | C14H20O8N4S3  | 477.0496 | 477.1 | 0.0504 | 5.1420 |
| yAn-H2O      | 476.1960 | C19H22O5N10   | 477.2038 | 477.2 | 0.0038 | 5.3589 |
| GgyA-H2O     | 476.1793 | C18H24O90N6   | 477.1871 | 477.2 | 0.0129 | 5.3589 |
| Ggyln-H2O    | 476.1802 | C18H24O90N6   | 477.1880 | 477.2 | 0.0120 | 5.3589 |
| ggylu        | 476.1577 | C16H26O14N2   | 477.1655 | 477.2 | 0.0345 | 5.3589 |
| GGyylu-H2O   | 476.2112 | C17H30O11N4   | 477.2190 | 477.2 | 0.0190 | 5.3589 |
| GGtylu-H2O   | 476.1560 | C16H26O10N4S1 | 477.1638 | 477.2 | 0.0362 | 5.3589 |
| GGggyl-H2O   | 476.1635 | C17H26O13N2   | 477.1713 | 477.2 | 0.0287 | 5.3589 |
| GGGGyyy      | 476.2074 | C17H32O11N4   | 477.2152 | 477.2 | 0.0152 | 5.3589 |
| GGGGtyy      | 476.1522 | C16H28O10N4S1 | 477.1600 | 477.2 | 0.0400 | 5.3589 |
| gggggggt-H2O | 480.0188 | C16H16O15S1   | 481.0266 | 481.0 | 0.0266 | 6.7125 |
| ttyyl-H2     | 480.1048 | C16H26O12S2   | 481.1126 | 481.1 | 0.0126 | 6.8265 |
| tttyl-H2     | 480.0496 | C15H22O11S3   | 481.0574 | 481.1 | 0.0426 | 6.8265 |
| gggggyyu-H2O | 480.1217 | C17H24O14N2   | 481.1295 | 481.1 | 0.0295 | 6.8265 |
| gggggtyu-H2O | 480.0665 | C16H20O13N2S1 | 481.0743 | 481.1 | 0.0257 | 6.8265 |
| gggggggy-H2O | 480.0740 | C17H20O16     | 481.0818 | 481.1 | 0.0182 | 6.8265 |
| GGGA         | 480.1914 | C17H24O8N8    | 481.1992 | 481.2 | 0.0008 | 5.9030 |
| tydun        | 480.2331 | C21H33O4N7S1  | 481.2409 | 481.2 | 0.0409 | 5.9030 |
| ttdun        | 480.1779 | C20H29O3N7S2  | 481.1857 | 481.2 | 0.0143 | 5.9030 |
| ggydn        | 480.2406 | C22H33O7N5    | 481.2484 | 481.2 | 0.0484 | 5.9030 |
| ggtdn        | 480.1854 | C21H29O6N5S1  | 481.1932 | 481.2 | 0.0068 | 5.9030 |
| GGGln        | 480.1923 | C17H24O8N8    | 481.2001 | 481.2 | 0.0001 | 5.9030 |
| Ggtydu       | 480.2164 | C20H35O8N3S1  | 481.2242 | 481.2 | 0.0242 | 5.9030 |
| Gttdu        | 480.1612 | C19H31O7N3S2  | 481.1690 | 481.2 | 0.0310 | 5.9030 |
| Gggyd        | 480.2239 | C21H35O11N1   | 481.2317 | 481.2 | 0.0317 | 5.9030 |
| Gggtd        | 480.1687 | C20H31O10N1S1 | 481.1765 | 481.2 | 0.0235 | 5.9030 |
| GGGtyd-H2O   | 480.2222 | C21H35O7N3S1  | 481.2300 | 481.2 | 0.0300 | 5.9030 |
| GGGttd-H2O   | 480.1670 | C20H31O6N3S2  | 481.1748 | 481.2 | 0.0252 | 5.9030 |
| GGGGgl       | 480.1756 | C16H26O12N4   | 481.1834 | 481.2 | 0.0166 | 5.9030 |

|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| Gtttvy-H2O   | 503.0207 | C16H23O90N1S4 | 504.0285 | 504.0 | 0.0285 | 17.2836 |
| Ggttyy-H2    | 503.0406 | C16H23O11N1S3 | 504.0484 | 504.0 | 0.0484 | 17.2836 |
| ttyyyn-H2    | 503.1125 | C18H25O8N5S2  | 504.1203 | 504.1 | 0.0203 | 19.7356 |
| ttyyyn-H2    | 503.0573 | C17H21O7N5S3  | 504.0651 | 504.1 | 0.0349 | 19.7356 |
| Gttyyy-H2O   | 503.1311 | C18H31O11N1S2 | 504.1389 | 504.1 | 0.0389 | 19.7356 |
| Gttyyy-H2O   | 503.0759 | C17H27O10N1S3 | 504.0837 | 504.1 | 0.0163 | 19.7356 |
| Ggttyy-H2    | 503.0958 | C17H27O12N1S2 | 504.1036 | 504.1 | 0.0036 | 19.7356 |
| GGGGgtn      | 503.1281 | C17H21O7N9S1  | 504.1359 | 504.1 | 0.0359 | 19.7356 |
| GGGGGttu     | 503.1039 | C15H23O8N7S2  | 504.1117 | 504.1 | 0.0117 | 19.7356 |
| GGGGGggt     | 503.1114 | C16H23O11N5S1 | 504.1192 | 504.1 | 0.0192 | 19.7356 |
| GAun-H2O     | 503.2029 | C19H21O4N13   | 504.2107 | 504.2 | 0.0107 | 19.9865 |
| GGgAu-H2O    | 503.1862 | C18H23O8N9    | 504.1940 | 504.2 | 0.0060 | 19.9865 |
| GGglun-H2O   | 503.1871 | C18H23O8N9    | 504.1949 | 504.2 | 0.0051 | 19.9865 |
| gggydu-H2O   | 503.2187 | C22H34O11N2   | 504.2265 | 504.2 | 0.0265 | 19.9865 |
| ggggtdu-H2O  | 503.1635 | C21H30O10N2S1 | 504.1713 | 504.2 | 0.0287 | 19.9865 |
| gggggd-H2O   | 503.1710 | C22H30O13     | 504.1788 | 504.2 | 0.0212 | 19.9865 |
| Gyyyyy-H2O   | 503.2415 | C20H39O13N1   | 504.2493 | 504.2 | 0.0493 | 19.9865 |
| Gt-yyyyy-H2O | 503.1863 | C19H35O12N1S1 | 504.1941 | 504.2 | 0.0059 | 19.9865 |
| GGGgglu-H2O  | 503.1704 | C17H25O12N5   | 504.1782 | 504.2 | 0.0218 | 19.9865 |
| GGGGgyn      | 503.1833 | C18H25O8N9    | 504.1911 | 504.2 | 0.0089 | 19.9865 |
| GGGGGyyu     | 503.2143 | C17H31O10N7   | 504.2221 | 504.2 | 0.0221 | 19.9865 |
| GGGGGtyu     | 503.1591 | C16H27O9N7S1  | 504.1669 | 504.2 | 0.0331 | 19.9865 |
| GGGGGggy     | 503.1666 | C17H27O12N5   | 504.1744 | 504.2 | 0.0256 | 19.9865 |
| ttttyyu      | 504.0313 | C15H24O9N2S4  | 505.0391 | 505.0 | 0.0391 | 5.9947  |
| ggttyy       | 504.0388 | C16H24O12S3   | 505.0466 | 505.0 | 0.0466 | 5.9947  |
| ttyyyyu      | 504.1417 | C17H32O11N2S2 | 505.1495 | 505.1 | 0.0495 | 6.3321  |
| ttyyyyu      | 504.0865 | C16H28O10N2S3 | 505.0943 | 505.1 | 0.0057 | 6.3321  |
| ggttyyy      | 504.0940 | C17H28O13S2   | 505.1018 | 505.1 | 0.0018 | 6.3321  |
| GGttyyy-H2   | 504.1122 | C17H28O11N2S2 | 505.1200 | 505.1 | 0.0200 | 6.3321  |
| GGttyyy-H2   | 504.0570 | C16H24O10N2S3 | 505.0648 | 505.1 | 0.0352 | 6.3321  |
| GGGGGGgt     | 504.1278 | C16H24O10N6S1 | 505.1356 | 505.1 | 0.0356 | 6.3321  |
| lll-H2O      | 504.2182 | C18H30O15     | 505.2260 | 505.2 | 0.0260 | 6.1297  |
| GGGAu-H2O    | 504.2026 | C18H24O7N10   | 505.2104 | 505.2 | 0.0104 | 6.1297  |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| ggtdun-H2O  | 504.1966 | C22H29O5N7S1  | 505.2044 | 505.2 | 0.0044 | 6.1297  |
| ggggdn-H2O  | 504.2041 | C23H29O8N5    | 505.2119 | 505.2 | 0.0119 | 6.1297  |
| GGGlun-H2O  | 504.2035 | C18H24O7N10   | 505.2113 | 505.2 | 0.0113 | 6.1297  |
| tyyyyyu     | 504.1969 | C18H36O12N2S1 | 505.2047 | 505.2 | 0.0047 | 6.1297  |
| ggyyyyyy    | 504.2044 | C19H36O15     | 505.2122 | 505.2 | 0.0122 | 6.1297  |
| ggtyyyy     | 504.1492 | C18H32O14S1   | 505.1570 | 505.2 | 0.0430 | 6.1297  |
| Ggggydu-H2O | 504.2351 | C22H35O10N3   | 505.2429 | 505.2 | 0.0429 | 6.1297  |
| Ggggtdu-H2O | 504.1799 | C21H31O90N3S1 | 505.1877 | 505.2 | 0.0123 | 6.1297  |
| Ggggggd-H2O | 504.1874 | C22H31O12N1   | 505.1952 | 505.2 | 0.0048 | 6.1297  |
| GGGGglu-H2O | 504.1868 | C17H26O11N6   | 505.1946 | 505.2 | 0.0054 | 6.1297  |
| GGGGGyn     | 504.1997 | C18H26O7N10   | 505.2075 | 505.2 | 0.0075 | 6.1297  |
| GGGGGtn     | 504.1445 | C17H22O6N10S1 | 505.1523 | 505.2 | 0.0477 | 6.1297  |
| GGGGGGgy    | 504.1830 | C17H28O11N6   | 505.1908 | 505.2 | 0.0092 | 6.1297  |
| ggydun-H2O  | 504.2518 | C23H33O6N7    | 505.2596 | 505.3 | 0.0404 | 5.3649  |
| yyyyyyu     | 504.2521 | C19H40O13N2   | 505.2599 | 505.3 | 0.0401 | 5.3649  |
| Gtttvy-H2   | 519.0167 | C16H23O10N1S4 | 520.0245 | 520.0 | 0.0245 | 11.9349 |
| gggtdu-H2O  | 519.1396 | C21H30O90N2S2 | 520.1474 | 520.1 | 0.0474 | 14.2127 |
| Gttxyy-H2   | 519.1271 | C18H31O12N1S2 | 520.1349 | 520.1 | 0.0349 | 14.2127 |
| Gttxyy-H2   | 519.0719 | C17H27O11N1S3 | 520.0797 | 520.1 | 0.0203 | 14.2127 |
| GGGGttn     | 519.1042 | C17H21O6N9S2  | 520.1120 | 520.1 | 0.0120 | 14.2127 |
| GGGGGgtt    | 519.0875 | C16H23O10N5S2 | 520.0953 | 520.1 | 0.0047 | 14.2127 |
| GgAn-H2O    | 519.1865 | C20H21O6N11   | 520.1943 | 520.2 | 0.0057 | 15.0502 |
| gggAu       | 519.1640 | C18H23O11N7   | 520.1718 | 520.2 | 0.0282 | 15.0502 |
| GGyAu-H2O   | 519.2175 | C19H27O8N9    | 520.2253 | 520.2 | 0.0253 | 15.0502 |
| GGtAu-H2O   | 519.1623 | C18H23O7N9S1  | 520.1701 | 520.2 | 0.0299 | 15.0502 |
| GGggA-H2O   | 519.1698 | C19H23O10N7   | 520.1776 | 520.2 | 0.0224 | 15.0502 |
| ggglun      | 519.1649 | C18H23O11N7   | 520.1727 | 520.2 | 0.0273 | 15.0502 |
| GGylun-H2O  | 519.2184 | C19H27O8N9    | 520.2262 | 520.2 | 0.0262 | 15.0502 |
| GGtlun-H2O  | 519.1632 | C18H23O7N9S1  | 520.1710 | 520.2 | 0.0290 | 15.0502 |
| GGggln-H2O  | 519.1707 | C19H23O10N7   | 520.1785 | 520.2 | 0.0215 | 15.0502 |
| gggtydu-H2O | 519.1948 | C22H34O10N2S1 | 520.2026 | 520.2 | 0.0026 | 15.0502 |
| gggggyd-H2O | 519.2023 | C23H34O13     | 520.2101 | 520.2 | 0.0101 | 15.0502 |
| gggggtd-H2O | 519.1471 | C22H30O12S1   | 520.1549 | 520.2 | 0.0451 | 15.0502 |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| Ggggglu     | 519.1482 | C17H25O15N3   | 520.1560 | 520.2 | 0.0440 | 15.0502 |
| GGGgylu-H2O | 519.2017 | C18H29O12N5   | 520.2095 | 520.2 | 0.0095 | 15.0502 |
| GGGgtlu-H2O | 519.1465 | C17H25O11N5S1 | 520.1543 | 520.2 | 0.0457 | 15.0502 |
| GGGgggl-H2O | 519.1540 | C18H25O14N3   | 520.1618 | 520.2 | 0.0382 | 15.0502 |
| GGGGyyn     | 519.2146 | C19H29O8N9    | 520.2224 | 520.2 | 0.0224 | 15.0502 |
| GGGGtyn     | 519.1594 | C18H25O7N9S1  | 520.1672 | 520.2 | 0.0328 | 15.0502 |
| GGGGGgyy    | 519.1979 | C18H31O12N5   | 520.2057 | 520.2 | 0.0057 | 15.0502 |
| GGGGGgty    | 519.1427 | C17H27O11N5S1 | 520.1505 | 520.2 | 0.0495 | 15.0502 |
| gggyydu-H2O | 519.2500 | C23H38O11N2   | 520.2578 | 520.3 | 0.0422 | 13.4732 |
| ttyylu      | 524.1412 | C17H30O12N2S2 | 525.1490 | 525.1 | 0.0490 | 5.2697  |
| tttylu      | 524.0860 | C16H26O11N2S3 | 525.0938 | 525.1 | 0.0062 | 5.2697  |
| tttlu       | 524.0308 | C15H22O10N2S4 | 525.0386 | 525.1 | 0.0614 | 5.2697  |
| ggttyl      | 524.0935 | C17H26O14S2   | 525.1013 | 525.1 | 0.0013 | 5.2697  |
| ggttl       | 524.0383 | C16H22O13S3   | 525.0461 | 525.1 | 0.0539 | 5.2697  |
| GGttyl-H2   | 524.1117 | C17H26O12N2S2 | 525.1195 | 525.1 | 0.0195 | 5.2697  |
| GGttl-H2    | 524.0565 | C16H22O11N2S3 | 525.0643 | 525.1 | 0.0357 | 5.2697  |
| Ggggtun-H2O | 524.0901 | C18H18O90N8S1 | 525.0979 | 525.1 | 0.0021 | 5.2697  |
| Ggggggn-H2O | 524.0976 | C19H18O12N6   | 525.1054 | 525.1 | 0.0054 | 5.2697  |
| yyyylu      | 524.2516 | C19H38O14N2   | 525.2594 | 525.2 | 0.0594 | 5.2199  |
| ttyylu      | 524.1964 | C18H34O13N2S1 | 525.2042 | 525.2 | 0.0042 | 5.2199  |
| ggyyl       | 524.2039 | C19H34O16     | 525.2117 | 525.2 | 0.0117 | 5.2199  |
| ggttyl      | 524.1487 | C18H30O15S1   | 525.1565 | 525.2 | 0.0435 | 5.2199  |
| GGtdun      | 524.2400 | C22H33O4N9S1  | 525.2478 | 525.2 | 0.0478 | 5.2199  |
| GGgdnd      | 524.2475 | C23H33O7N7    | 525.2553 | 525.2 | 0.0553 | 5.2199  |
| GGGgtdu     | 524.2233 | C21H35O8N5S1  | 525.2311 | 525.2 | 0.0311 | 5.2199  |
| GGGggd      | 524.2308 | C22H35O11N3   | 525.2386 | 525.2 | 0.0386 | 5.2199  |
| GGGGGtd-H2O | 524.2291 | C22H35O7N5S1  | 525.2369 | 525.2 | 0.0369 | 5.2199  |
| Ggggyun-H2O | 524.1453 | C19H22O10N8   | 525.1531 | 525.2 | 0.0469 | 5.2199  |
| tttyun      | 547.0385 | C17H21O6N7S4  | 548.0463 | 548.0 | 0.0463 | 19.2360 |
| Ggttyu      | 547.0218 | C16H23O10N3S4 | 548.0296 | 548.0 | 0.0296 | 19.2360 |
| Ggggtty     | 547.0293 | C17H23O13N1S3 | 548.0371 | 548.0 | 0.0371 | 19.2360 |
| GGGttty-H2O | 547.0276 | C17H23O90N3S4 | 548.0354 | 548.0 | 0.0354 | 19.2360 |
| tttyun      | 547.0937 | C18H25O7N7S3  | 548.1015 | 548.1 | 0.0015 | 22.2783 |

|               |          |               |          |       |        |         |
|---------------|----------|---------------|----------|-------|--------|---------|
| ggtyyn        | 547.1012 | C19H25O10N5S2 | 548.1090 | 548.1 | 0.0090 | 22.2783 |
| ggttyn        | 547.0460 | C18H21O9N5S3  | 548.0538 | 548.1 | 0.0462 | 22.2783 |
| GGt yyn-H2    | 547.1194 | C19H25O8N7S2  | 548.1272 | 548.1 | 0.0272 | 22.2783 |
| GGttyn-H2     | 547.0642 | C18H21O7N7S3  | 548.0720 | 548.1 | 0.0280 | 22.2783 |
| Ggt yyyu      | 547.1322 | C18H31O12N3S2 | 548.1400 | 548.1 | 0.0400 | 22.2783 |
| Ggt yyyu      | 547.0770 | C17H27O11N3S3 | 548.0848 | 548.1 | 0.0152 | 22.2783 |
| Ggggtyyy      | 547.1397 | C19H31O15N1S1 | 548.1475 | 548.1 | 0.0475 | 22.2783 |
| Ggggtyy       | 547.0845 | C18H27O14N1S2 | 548.0923 | 548.1 | 0.0077 | 22.2783 |
| GGGt yyyy-H2O | 547.1380 | C19H31O11N3S2 | 548.1458 | 548.1 | 0.0458 | 22.2783 |
| GGGt tyy-H2O  | 547.0828 | C18H27O10N3S3 | 548.0906 | 548.1 | 0.0094 | 22.2783 |
| GGGgt yy-H2   | 547.1027 | C18H27O12N3S2 | 548.1105 | 548.1 | 0.0105 | 22.2783 |
| GGGgt ty-H2   | 547.0475 | C17H23O11N3S3 | 548.0553 | 548.1 | 0.0447 | 22.2783 |
| gttld         | 547.1905 | C22H36O11S2   | 548.1983 | 548.2 | 0.0017 | 23.1101 |
| ttyyun        | 547.2041 | C20H33O9N7S1  | 548.2119 | 548.2 | 0.0119 | 23.1101 |
| ttyyun        | 547.1489 | C19H29O8N7S2  | 548.1567 | 548.2 | 0.0433 | 23.1101 |
| ggyyyyn       | 547.2116 | C21H33O12N5   | 548.2194 | 548.2 | 0.0194 | 23.1101 |
| ggt yyyn      | 547.1564 | C20H29O11N5S1 | 548.1642 | 548.2 | 0.0358 | 23.1101 |
| Ggt yyyu      | 547.1874 | C19H35O13N3S1 | 548.1952 | 548.2 | 0.0048 | 23.1101 |
| Gggg yyyy     | 547.1949 | C20H35O16N1   | 548.2027 | 548.2 | 0.0027 | 23.1101 |
| GGgggdu-H2O   | 547.2256 | C23H34O11N4   | 548.2334 | 548.2 | 0.0334 | 23.1101 |
| GGGt yyyy-H2O | 547.1932 | C20H35O12N3S1 | 548.2010 | 548.2 | 0.0010 | 23.1101 |
| GGGGGGgn      | 547.1902 | C19H25O8N11   | 548.1980 | 548.2 | 0.0020 | 23.1101 |
| gyyld         | 547.3009 | C24H44O13     | 548.3087 | 548.3 | 0.0087 | 20.4719 |
| gtyld         | 547.2457 | C23H40O12S1   | 548.2535 | 548.3 | 0.0465 | 20.4719 |
| yyyyyun       | 547.2593 | C21H37O10N7   | 548.2671 | 548.3 | 0.0329 | 20.4719 |
| Ggggdun-H2O   | 547.2423 | C24H32O7N8    | 548.2501 | 548.3 | 0.0499 | 20.4719 |
| Ggyyyyyu      | 547.2426 | C20H39O14N3   | 548.2504 | 548.3 | 0.0496 | 20.4719 |
| GGGyyyyy-H2O  | 547.2484 | C21H39O13N3   | 548.2562 | 548.3 | 0.0438 | 20.4719 |
| GGtttyu       | 548.0382 | C16H24O9N4S4  | 549.0460 | 549.0 | 0.0460 | 5.2354  |
| ggtylu-H2O    | 548.1047 | C18H26O13N2S2 | 549.1125 | 549.1 | 0.0125 | 5.6840  |
| ggttlu-H2O    | 548.0495 | C17H22O12N2S3 | 549.0573 | 549.1 | 0.0427 | 5.6840  |
| gggtlu-H2     | 548.0694 | C17H22O14N2S2 | 549.0772 | 549.1 | 0.0228 | 5.6840  |
| ggggtl-H2O    | 548.1122 | C19H26O16S1   | 549.1200 | 549.1 | 0.0200 | 5.6840  |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| gggttl-H2O  | 548.0570 | C18H22O15S2   | 549.0648 | 549.1 | 0.0352 | 5.6840  |
| Ggttyn      | 548.1176 | C19H26O9N6S2  | 549.1254 | 549.1 | 0.0254 | 5.6840  |
| Gtttyn      | 548.0624 | C18H22O8N6S3  | 549.0702 | 549.1 | 0.0298 | 5.6840  |
| GGttyyu     | 548.0934 | C17H28O10N4S3 | 549.1012 | 549.1 | 0.0012 | 5.6840  |
| GGggttyy    | 548.1009 | C18H28O13N2S2 | 549.1087 | 549.1 | 0.0087 | 5.6840  |
| GGggttyy    | 548.0457 | C17H24O12N2S3 | 549.0535 | 549.1 | 0.0465 | 5.6840  |
| GGGGttyy-H2 | 548.1191 | C18H28O11N4S2 | 549.1269 | 549.1 | 0.0269 | 5.6840  |
| GGGGttyy-H2 | 548.0639 | C17H24O10N4S3 | 549.0717 | 549.1 | 0.0283 | 5.6840  |
| Gtld        | 548.2069 | C22H37O10N1S2 | 549.2147 | 549.2 | 0.0147 | 5.9260  |
| ggyylu-H2O  | 548.2151 | C20H34O15N2   | 549.2229 | 549.2 | 0.0229 | 5.9260  |
| ggttylu-H2O | 548.1599 | C19H30O14N2S1 | 549.1677 | 549.2 | 0.0323 | 5.9260  |
| gggyyl-H2O  | 548.1674 | C20H30O17     | 549.1752 | 549.2 | 0.0248 | 5.9260  |
| Ggyyyyn     | 548.2280 | C21H34O11N6   | 549.2358 | 549.2 | 0.0358 | 5.9260  |
| Ggttyyn     | 548.1728 | C20H30O10N6S1 | 549.1806 | 549.2 | 0.0194 | 5.9260  |
| GGttyyyu    | 548.2038 | C19H36O12N4S1 | 549.2116 | 549.2 | 0.0116 | 5.9260  |
| GGttyyyu    | 548.1486 | C18H32O11N4S2 | 549.1564 | 549.2 | 0.0436 | 5.9260  |
| GGggyyyy    | 548.2113 | C20H36O15N2   | 549.2191 | 549.2 | 0.0191 | 5.9260  |
| GGggttyy    | 548.1561 | C19H32O14N2S1 | 549.1639 | 549.2 | 0.0361 | 5.9260  |
| GGGggdu-H2O | 548.2420 | C23H35O10N5   | 549.2498 | 549.2 | 0.0498 | 5.9260  |
| GGGGGGGn    | 548.2066 | C19H26O7N12   | 549.2144 | 549.2 | 0.0144 | 5.9260  |
| Gyld        | 548.3173 | C24H45O12N1   | 549.3251 | 549.3 | 0.0251 | 5.5631  |
| Gtyld       | 548.2621 | C23H41O11N1S1 | 549.2699 | 549.3 | 0.0301 | 5.5631  |
| GGggdun-H2O | 548.2587 | C24H33O6N9    | 549.2665 | 549.3 | 0.0335 | 5.5631  |
| GGyyyyyu    | 548.2590 | C20H40O13N4   | 549.2668 | 549.3 | 0.0332 | 5.5631  |
| gtttyn      | 563.0221 | C18H21O8N5S4  | 564.0299 | 564.0 | 0.0299 | 10.9232 |
| GGGttyy-H2  | 563.0236 | C17H23O10N3S4 | 564.0314 | 564.0 | 0.0314 | 10.9232 |
| gttyyyyn    | 563.1325 | C20H29O10N5S2 | 564.1403 | 564.1 | 0.0403 | 12.2821 |
| gttyny      | 563.0773 | C19H25O9N5S3  | 564.0851 | 564.1 | 0.0149 | 12.2821 |
| Gtttyyu     | 563.1083 | C18H31O11N3S3 | 564.1161 | 564.1 | 0.0161 | 12.2821 |
| Gtttyyu     | 563.0531 | C17H27O10N3S4 | 564.0609 | 564.1 | 0.0391 | 12.2821 |
| Gggttyy     | 563.1158 | C19H31O14N1S2 | 564.1236 | 564.1 | 0.0236 | 12.2821 |
| Gggtttyy    | 563.0606 | C18H27O13N1S3 | 564.0684 | 564.1 | 0.0316 | 12.2821 |
| GGGttyyy-H2 | 563.1340 | C19H31O12N3S2 | 564.1418 | 564.1 | 0.0418 | 12.2821 |

|               |          |               |          |       |        |         |
|---------------|----------|---------------|----------|-------|--------|---------|
| GGGttyy-H2    | 563.0788 | C18H27O11N3S3 | 564.0866 | 564.1 | 0.0134 | 12.2821 |
| Glll-H2O      | 563.2400 | C20H33O16N1   | 564.2478 | 564.2 | 0.0478 | 12.2543 |
| ttyld         | 563.2218 | C23H40O11S2   | 564.2296 | 564.2 | 0.0296 | 12.2543 |
| ttld          | 563.1666 | C22H36O10S3   | 564.1744 | 564.2 | 0.0256 | 12.2543 |
| GGGGAu-H2O    | 563.2244 | C20H27O8N11   | 564.2322 | 564.2 | 0.0322 | 12.2543 |
| gttyyn        | 563.1877 | C21H33O11N5S1 | 564.1955 | 564.2 | 0.0045 | 12.2543 |
| Ggtdun-H2O    | 563.2184 | C24H32O6N8S1  | 564.2262 | 564.2 | 0.0262 | 12.2543 |
| Ggggdn-H2O    | 563.2259 | C25H32O90N6   | 564.2337 | 564.2 | 0.0337 | 12.2543 |
| GGGGlun-H2O   | 563.2253 | C20H27O8N11   | 564.2331 | 564.2 | 0.0331 | 12.2543 |
| gggggdgu      | 563.2034 | C23H34O14N2   | 564.2112 | 564.2 | 0.0112 | 12.2543 |
| Gt-yyyyyu     | 563.2187 | C20H39O13N3S1 | 564.2265 | 564.2 | 0.0265 | 12.2543 |
| Gt-yyyyyu     | 563.1635 | C19H35O12N3S2 | 564.1713 | 564.2 | 0.0287 | 12.2543 |
| Ggyyyyyy      | 563.2262 | C21H39O16N1   | 564.2340 | 564.2 | 0.0340 | 12.2543 |
| Gggtyyyy      | 563.1710 | C20H35O15N1S1 | 564.1788 | 564.2 | 0.0212 | 12.2543 |
| GGggtdu-H2O   | 563.2017 | C23H34O10N4S1 | 564.2095 | 564.2 | 0.0095 | 12.2543 |
| GGgggggd-H2O  | 563.2092 | C24H34O13N2   | 564.2170 | 564.2 | 0.0170 | 12.2543 |
| GGGGGglu-H2O  | 563.2086 | C19H29O12N7   | 564.2164 | 564.2 | 0.0164 | 12.2543 |
| GGGGGGGyn     | 563.2215 | C20H29O8N11   | 564.2293 | 564.2 | 0.0293 | 12.2543 |
| GGGGGGGtn     | 563.1663 | C19H25O7N11S1 | 564.1741 | 564.2 | 0.0259 | 12.2543 |
| yyld          | 563.3322 | C25H48O13     | 564.3400 | 564.3 | 0.0400 | 10.4719 |
| tyld          | 563.2770 | C24H44O12S1   | 564.2848 | 564.3 | 0.0152 | 10.4719 |
| gyyyyyn       | 563.2429 | C22H37O12N5   | 564.2507 | 564.3 | 0.0493 | 10.4719 |
| Gggydun-H2O   | 563.2736 | C25H36O7N8    | 564.2814 | 564.3 | 0.0186 | 10.4719 |
| Gyyyyyyu      | 563.2739 | C21H43O14N3   | 564.2817 | 564.3 | 0.0183 | 10.4719 |
| GGgggydu-H2O  | 563.2569 | C24H38O11N4   | 564.2647 | 564.3 | 0.0353 | 10.4719 |
| ttAn          | 568.1329 | C20H22O6N10S2 | 569.1407 | 569.1 | 0.0407 | 5.0305  |
| GgtA          | 568.1714 | C20H28O11N6S1 | 569.1792 | 569.1 | 0.0792 | 5.0305  |
| GtgtA         | 568.1162 | C19H24O10N6S2 | 569.1240 | 569.1 | 0.0240 | 5.0305  |
| tttydn-H2O    | 568.1637 | C24H33O5N5S3  | 569.1715 | 569.1 | 0.0715 | 5.0305  |
| tttdn-H2O     | 568.1085 | C23H29O4N5S4  | 569.1163 | 569.1 | 0.0163 | 5.0305  |
| gttdn-H2      | 568.1284 | C23H29O6N5S3  | 569.1362 | 569.1 | 0.0362 | 5.0305  |
| ggtllu-H2-H2O | 568.1594 | C19H26O15N2S1 | 569.1672 | 569.1 | 0.0672 | 5.0305  |
| ggggll-H2-H2O | 568.1669 | C20H26O18     | 569.1747 | 569.1 | 0.0747 | 5.0305  |

|                |          |               |          |       |        |         |
|----------------|----------|---------------|----------|-------|--------|---------|
| Ggtyn          | 568.1723 | C20H28O11N6S1 | 569.1801 | 569.1 | 0.0801 | 5.0305  |
| Ggtln          | 568.1171 | C19H24O10N6S2 | 569.1249 | 569.1 | 0.0249 | 5.0305  |
| Gttdydu-H2-H2O | 568.1594 | C22H33O7N3S3  | 569.1672 | 569.1 | 0.0672 | 5.0305  |
| Gttdu-H2       | 568.1042 | C21H31O7N3S4  | 569.1120 | 569.1 | 0.0120 | 5.0305  |
| Gtttyd-H2O     | 568.1470 | C23H35O90N1S3 | 569.1548 | 569.1 | 0.0548 | 5.0305  |
| Gtttd-H2O      | 568.0918 | C22H31O8N1S4  | 569.0996 | 569.1 | 0.0004 | 5.0305  |
| Gggttd-H2-H2O  | 568.1669 | C23H33O10N1S2 | 569.1747 | 569.1 | 0.0747 | 5.0305  |
| Gggtd-H2       | 568.1117 | C22H31O10N1S3 | 569.1195 | 569.1 | 0.0195 | 5.0305  |
| GGttylu        | 568.1481 | C18H30O12N4S2 | 569.1559 | 569.1 | 0.0559 | 5.0305  |
| GGtllu         | 568.0929 | C17H26O11N4S3 | 569.1007 | 569.1 | 0.0007 | 5.0305  |
| GGggtyl        | 568.1556 | C19H30O15N2S1 | 569.1634 | 569.1 | 0.0634 | 5.0305  |
| GGggtl         | 568.1004 | C18H26O14N2S2 | 569.1082 | 569.1 | 0.0082 | 5.0305  |
| GGGGttl-H2     | 568.1186 | C18H26O12N4S2 | 569.1264 | 569.1 | 0.0264 | 5.0305  |
| ggttAu-H2O     | 591.1110 | C20H23O10N7S2 | 592.1188 | 592.1 | 0.0188 | 20.9635 |
| gggttA-H2O     | 591.1185 | C21H23O13N5S1 | 592.1263 | 592.1 | 0.0263 | 20.9635 |
| ggttlun-H2O    | 591.1119 | C20H23O10N7S2 | 592.1197 | 592.1 | 0.0197 | 20.9635 |
| gggtln-H2O     | 591.1194 | C21H23O13N5S1 | 592.1272 | 592.1 | 0.0272 | 20.9635 |
| Ggggtlu-H2O    | 591.0952 | C19H25O14N3S2 | 592.1030 | 592.1 | 0.0030 | 20.9635 |
| Gggggtl-H2O    | 591.1027 | C20H25O17N1S1 | 592.1105 | 592.1 | 0.0105 | 20.9635 |
| GGttypn        | 591.1006 | C19H25O7N9S3  | 592.1084 | 592.1 | 0.0084 | 20.9635 |
| GGtttun        | 591.0454 | C18H21O6N9S4  | 592.0532 | 592.1 | 0.0468 | 20.9635 |
| GGggtyn        | 591.1081 | C20H25O10N7S2 | 592.1159 | 592.1 | 0.0159 | 20.9635 |
| GGggttn        | 591.0529 | C19H21O9N7S3  | 592.0607 | 592.1 | 0.0393 | 20.9635 |
| GGGGttn-H2     | 591.1263 | C20H25O8N9S2  | 592.1341 | 592.1 | 0.0341 | 20.9635 |
| GGGGtttn-H2    | 591.0711 | C19H21O7N9S3  | 592.0789 | 592.1 | 0.0211 | 20.9635 |
| ggyyAu-H2O     | 591.2214 | C22H31O12N7   | 592.2292 | 592.2 | 0.0292 | 21.6550 |
| ggytAu-H2O     | 591.1662 | C21H27O11N7S1 | 592.1740 | 592.2 | 0.0260 | 21.6550 |
| gggyA-H2O      | 591.1737 | C22H27O14N5   | 592.1815 | 592.2 | 0.0185 | 21.6550 |
| ggyylun-H2O    | 591.2223 | C22H31O12N7   | 592.2301 | 592.2 | 0.0301 | 21.6550 |
| ggtlyn-H2O     | 591.1671 | C21H27O11N7S1 | 592.1749 | 592.2 | 0.0251 | 21.6550 |
| gggyln-H2O     | 591.1746 | C22H27O14N5   | 592.1824 | 592.2 | 0.0176 | 21.6550 |
| Ggggyylu-H2O   | 591.2056 | C21H33O16N3   | 592.2134 | 592.2 | 0.0134 | 21.6550 |
| Ggggtlu-H2O    | 591.1504 | C20H29O15N3S1 | 592.1582 | 592.2 | 0.0418 | 21.6550 |

|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| Ggggggyl-H2O | 591.1579 | C21H29O18N1   | 592.1657 | 592.2 | 0.0343 | 21.6550 |
| GGttyyun     | 591.2110 | C21H33O9N9S1  | 592.2188 | 592.2 | 0.0188 | 21.6550 |
| GGttyun      | 591.1558 | C20H29O8N9S2  | 592.1636 | 592.2 | 0.0364 | 21.6550 |
| GGggyyn      | 591.2185 | C22H33O12N7   | 592.2263 | 592.2 | 0.0263 | 21.6550 |
| GGggtyn      | 591.1633 | C21H29O11N7S1 | 592.1711 | 592.2 | 0.0289 | 21.6550 |
| GydA         | 591.3236 | C26H42O9N6    | 592.3314 | 592.3 | 0.0314 | 20.0530 |
| GtdA         | 591.2684 | C25H38O8N6S1  | 592.2762 | 592.3 | 0.0238 | 20.0530 |
| gldu-H2O     | 591.3116 | C25H42O13N2   | 592.3194 | 592.3 | 0.0194 | 20.0530 |
| Gyldn        | 591.3245 | C26H42O9N6    | 592.3323 | 592.3 | 0.0323 | 20.0530 |
| Gtldn        | 591.2693 | C25H38O8N6S1  | 592.2771 | 592.3 | 0.0229 | 20.0530 |
| GGgyld       | 591.3078 | C25H44O13N2   | 592.3156 | 592.3 | 0.0156 | 20.0530 |
| GGgtld       | 591.2526 | C24H40O12N2S1 | 592.2604 | 592.3 | 0.0396 | 20.0530 |
| GGyyyyun     | 591.2662 | C22H37O10N9   | 592.2740 | 592.3 | 0.0260 | 20.0530 |
| GgttAu-H2O   | 592.1274 | C20H24O90N8S2 | 593.1352 | 593.1 | 0.0352 | 5.7218  |
| GgggtA-H2O   | 592.1349 | C21H24O12N6S1 | 593.1427 | 593.1 | 0.0427 | 5.7218  |
| Ggtlun-H2O   | 592.1283 | C20H24O90N8S2 | 593.1361 | 593.1 | 0.0361 | 5.7218  |
| Ggggtln-H2O  | 592.1358 | C21H24O12N6S1 | 593.1436 | 593.1 | 0.0436 | 5.7218  |
| tttyyyyy-H2O | 592.1275 | C21H36O13S3   | 593.1353 | 593.1 | 0.0353 | 5.7218  |
| tttyyyyy-H2O | 592.0723 | C20H32O12S4   | 593.0801 | 593.1 | 0.0199 | 5.7218  |
| tttttyyy-H2O | 592.0171 | C19H28O11S5   | 593.0249 | 593.1 | 0.0751 | 5.7218  |
| gtttxyyy-H2  | 592.0922 | C20H32O14S3   | 593.1000 | 593.1 | 0.0000 | 5.7218  |
| gtttxyyy-H2  | 592.0370 | C19H28O13S4   | 593.0448 | 593.1 | 0.0552 | 5.7218  |
| gggggtlu     | 592.1133 | C19H26O17N2S1 | 593.1211 | 593.1 | 0.0211 | 5.7218  |
| gggggggl     | 592.1208 | C20H26O20     | 593.1286 | 593.1 | 0.0286 | 5.7218  |
| GGggtlu-H2O  | 592.1116 | C19H26O13N4S2 | 593.1194 | 593.1 | 0.0194 | 5.7218  |
| GGgggtl-H2O  | 592.1191 | C20H26O16N2S1 | 593.1269 | 593.1 | 0.0269 | 5.7218  |
| GGGgttn      | 592.1245 | C20H26O9N8S2  | 593.1323 | 593.1 | 0.0323 | 5.7218  |
| GGGgttn      | 592.0693 | C19H22O8N8S3  | 593.0771 | 593.1 | 0.0229 | 5.7218  |
| tyAun-H2O    | 592.1993 | C22H26O6N12S1 | 593.2071 | 593.2 | 0.0071 | 6.3383  |
| ttAun-H2O    | 592.1441 | C21H22O5N12S2 | 593.1519 | 593.2 | 0.0481 | 6.3383  |
| ggyAn-H2O    | 592.2068 | C23H26O90N10  | 593.2146 | 593.2 | 0.0146 | 6.3383  |
| ggtAn-H2O    | 592.1516 | C22H22O8N10S1 | 593.1594 | 593.2 | 0.0406 | 6.3383  |
| GgyyAu-H2O   | 592.2378 | C22H32O11N8   | 593.2456 | 593.2 | 0.0456 | 6.3383  |

|               |          |               |          |       |        |        |
|---------------|----------|---------------|----------|-------|--------|--------|
| GgttyAu-H2O   | 592.1826 | C21H28O10N8S1 | 593.1904 | 593.2 | 0.0096 | 6.3383 |
| GgggyA-H2O    | 592.1901 | C22H28O13N6   | 593.1979 | 593.2 | 0.0021 | 6.3383 |
| Ggyylun-H2O   | 592.2387 | C22H32O11N8   | 593.2465 | 593.2 | 0.0465 | 6.3383 |
| Ggtylun-H2O   | 592.1835 | C21H28O10N8S1 | 593.1913 | 593.2 | 0.0087 | 6.3383 |
| Ggggyln-H2O   | 592.1910 | C22H28O13N6   | 593.1988 | 593.2 | 0.0012 | 6.3383 |
| ttyyyyyy-H2O  | 592.2379 | C23H44O15S1   | 593.2457 | 593.2 | 0.0457 | 6.3383 |
| ttyyyyyy-H2O  | 592.1827 | C22H40O14S2   | 593.1905 | 593.2 | 0.0095 | 6.3383 |
| gtyyyyyy-H2   | 592.1474 | C21H36O15S2   | 593.1552 | 593.2 | 0.0448 | 6.3383 |
| gggggylu      | 592.1685 | C20H30O18N2   | 593.1763 | 593.2 | 0.0237 | 6.3383 |
| GGggyylu-H2O  | 592.2220 | C21H34O15N4   | 593.2298 | 593.2 | 0.0298 | 6.3383 |
| GGggttylu-H2O | 592.1668 | C20H30O14N4S1 | 593.1746 | 593.2 | 0.0254 | 6.3383 |
| GGggggyl-H2O  | 592.1743 | C21H30O17N2   | 593.1821 | 593.2 | 0.0179 | 6.3383 |
| GGGgtyyn      | 592.2349 | C22H34O11N8   | 593.2427 | 593.2 | 0.0427 | 6.3383 |
| GGGgtyn       | 592.1797 | C21H30O10N8S1 | 593.1875 | 593.2 | 0.0125 | 6.3383 |
| yyAun-H2O     | 592.2545 | C23H30O7N12   | 593.2623 | 593.3 | 0.0377 | 6.1874 |
| Glldu-H2O     | 592.3280 | C25H43O12N3   | 593.3358 | 593.3 | 0.0358 | 6.1874 |
| GGGyld        | 592.3242 | C25H45O12N3   | 593.3320 | 593.3 | 0.0320 | 6.1874 |
| GGGtld        | 592.2690 | C24H41O11N3S1 | 593.2768 | 593.3 | 0.0232 | 6.1874 |
| yyyyyyyy-H2O  | 592.2931 | C24H48O16     | 593.3009 | 593.3 | 0.0009 | 6.1874 |
| GGgttn        | 607.0290 | C19H21O8N7S4  | 608.0368 | 608.0 | 0.0368 | 6.5908 |
| gtttAu-H2O    | 607.0871 | C20H23O90N7S3 | 608.0949 | 608.1 | 0.0051 | 8.3323 |
| ggttAu-H2     | 607.1070 | C20H23O11N7S2 | 608.1148 | 608.1 | 0.0148 | 8.3323 |
| gggttA-H2O    | 607.0946 | C21H23O12N5S2 | 608.1024 | 608.1 | 0.0024 | 8.3323 |
| gttlun-H2O    | 607.0880 | C20H23O90N7S3 | 608.0958 | 608.1 | 0.0042 | 8.3323 |
| ggtlun-H2     | 607.1079 | C20H23O11N7S2 | 608.1157 | 608.1 | 0.0157 | 8.3323 |
| gggtln-H2O    | 607.0955 | C21H23O12N5S2 | 608.1033 | 608.1 | 0.0033 | 8.3323 |
| Ggttylu-H2O   | 607.1265 | C20H29O14N3S2 | 608.1343 | 608.1 | 0.0343 | 8.3323 |
| Gggttlu-H2O   | 607.0713 | C19H25O13N3S3 | 608.0791 | 608.1 | 0.0209 | 8.3323 |
| Ggggtlu-H2    | 607.0912 | C19H25O15N3S2 | 608.0990 | 608.1 | 0.0010 | 8.3323 |
| Ggggtyl-H2O   | 607.1340 | C21H29O17N1S1 | 608.1418 | 608.1 | 0.0418 | 8.3323 |
| Ggggttl-H2O   | 607.0788 | C20H25O16N1S2 | 608.0866 | 608.1 | 0.0134 | 8.3323 |
| GGgttyyn      | 607.1394 | C21H29O10N7S2 | 608.1472 | 608.1 | 0.0472 | 8.3323 |
| GGgttytn      | 607.0842 | C20H25O9N7S3  | 608.0920 | 608.1 | 0.0080 | 8.3323 |

|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| gtyyAu-H2O   | 607.1975 | C22H31O11N7S1 | 608.2053 | 608.2 | 0.0053 | 9.1123  |
| gttyAu-H2O   | 607.1423 | C21H27O10N7S2 | 608.1501 | 608.2 | 0.0499 | 9.1123  |
| gggyyA-H2O   | 607.2050 | C23H31O14N5   | 608.2128 | 608.2 | 0.0128 | 9.1123  |
| gggytA-H2O   | 607.1498 | C22H27O13N5S1 | 608.1576 | 608.2 | 0.0424 | 9.1123  |
| GGttlD       | 607.2287 | C24H40O11N2S2 | 608.2365 | 608.2 | 0.0365 | 9.1123  |
| gttylun-H2O  | 607.1984 | C22H31O11N7S1 | 608.2062 | 608.2 | 0.0062 | 9.1123  |
| gttylun-H2O  | 607.1432 | C21H27O10N7S2 | 608.1510 | 608.2 | 0.0490 | 9.1123  |
| gggyyln-H2O  | 607.2059 | C23H31O14N5   | 608.2137 | 608.2 | 0.0137 | 9.1123  |
| gggyln-H2O   | 607.1507 | C22H27O13N5S1 | 608.1585 | 608.2 | 0.0415 | 9.1123  |
| Gggyyylu-H2O | 607.2369 | C22H37O16N3   | 608.2447 | 608.2 | 0.0447 | 9.1123  |
| Gggyylu-H2O  | 607.1817 | C21H33O15N3S1 | 608.1895 | 608.2 | 0.0105 | 9.1123  |
| Ggggyyl-H2O  | 607.1892 | C22H33O18N1   | 608.1970 | 608.2 | 0.0030 | 9.1123  |
| GGgtyyn      | 607.1946 | C22H33O11N7S1 | 608.2024 | 608.2 | 0.0024 | 9.1123  |
| tlldu-H2O    | 607.2877 | C25H42O12N2S1 | 608.2955 | 608.3 | 0.0045 | 8.2813  |
| ggld-H2-H2O  | 607.2952 | C26H40O15     | 608.3030 | 608.3 | 0.0030 | 8.2813  |
| gyyyAu-H2O   | 607.2527 | C23H35O12N7   | 608.2605 | 608.3 | 0.0395 | 8.2813  |
| GGyyld       | 607.3391 | C26H48O13N2   | 608.3469 | 608.3 | 0.0469 | 8.2813  |
| GGtyld       | 607.2839 | C25H44O12N2S1 | 608.2917 | 608.3 | 0.0083 | 8.2813  |
| gyylyn-H2O   | 607.2536 | C23H35O12N7   | 608.2614 | 608.3 | 0.0386 | 8.2813  |
| GGgtyyy      | 607.2498 | C23H37O12N7   | 608.2576 | 608.3 | 0.0424 | 8.2813  |
| GGGggdun-H2O | 607.2805 | C26H36O7N10   | 608.2883 | 608.3 | 0.0117 | 8.2813  |
| ylldu-H2O    | 607.3429 | C26H46O13N2   | 608.3507 | 608.4 | 0.0493 | 6.1277  |
| tttttyyn-H2O | 635.0243 | C21H25O8N5S5  | 636.0321 | 636.0 | 0.0321 | 12.6512 |
| tttld-H2     | 635.1335 | C24H36O11S4   | 636.1413 | 636.1 | 0.0413 | 15.3676 |
| Gttll        | 635.1222 | C20H31O15N1S3 | 636.1300 | 636.1 | 0.0300 | 15.3676 |
| tttyyyyn-H2O | 635.1347 | C23H33O10N5S3 | 636.1425 | 636.1 | 0.0425 | 15.3676 |
| tttyyyyn-H2O | 635.0795 | C22H29O90N5S4 | 636.0873 | 636.1 | 0.0127 | 15.3676 |
| gttynyyn-H2  | 635.0994 | C22H29O11N5S3 | 636.1072 | 636.1 | 0.0072 | 15.3676 |
| gttynyyn-H2  | 635.0442 | C21H25O10N5S4 | 636.0520 | 636.1 | 0.0480 | 15.3676 |
| tttyld-H2    | 635.1887 | C25H40O12S3   | 636.1965 | 636.2 | 0.0035 | 16.5720 |
| Gtyll        | 635.2326 | C22H39O17N1S1 | 636.2404 | 636.2 | 0.0404 | 16.5720 |
| Gtyll        | 635.1774 | C21H35O16N1S2 | 636.1852 | 636.2 | 0.0148 | 16.5720 |
| GgtAun-H2O   | 635.1898 | C23H25O7N13S1 | 636.1976 | 636.2 | 0.0024 | 16.5720 |

|              |          |                |          |       |        |         |
|--------------|----------|----------------|----------|-------|--------|---------|
| GgggAn-H2O   | 635.1973 | C24H25O10N11   | 636.2051 | 636.2 | 0.0051 | 16.5720 |
| gggggAu      | 635.1748 | C22H27O15N7    | 636.1826 | 636.2 | 0.0174 | 16.5720 |
| GGggyAu-H2O  | 635.2283 | C23H31O12N9    | 636.2361 | 636.2 | 0.0361 | 16.5720 |
| GGggtAu-H2O  | 635.1731 | C22H27O11N9S1  | 636.1809 | 636.2 | 0.0191 | 16.5720 |
| GGgggA-H2O   | 635.1806 | C23H27O14N7    | 636.1884 | 636.2 | 0.0116 | 16.5720 |
| ttyyyyyn-H2O | 635.1899 | C24H37O11N5S2  | 636.1977 | 636.2 | 0.0023 | 16.5720 |
| gttyyyyyn-H2 | 635.1546 | C23H33O12N5S2  | 636.1624 | 636.2 | 0.0376 | 16.5720 |
| ggggglun     | 635.1757 | C22H27O15N7    | 636.1835 | 636.2 | 0.0165 | 16.5720 |
| GGggylun-H2O | 635.2292 | C23H31O12N9    | 636.2370 | 636.2 | 0.0370 | 16.5720 |
| GGggtlun-H2O | 635.1740 | C22H27O11N9S1  | 636.1818 | 636.2 | 0.0182 | 16.5720 |
| GGgggln-H2O  | 635.1815 | C23H27O14N7    | 636.1893 | 636.2 | 0.0107 | 16.5720 |
| GGGdA        | 635.3305 | C27H42O9N8     | 636.3383 | 636.3 | 0.0383 | 15.2039 |
| ttyyld-H2    | 635.2439 | C26H44O13S2    | 636.2517 | 636.3 | 0.0483 | 15.2039 |
| Gyyyll       | 635.2878 | C23H43O18N1    | 636.2956 | 636.3 | 0.0044 | 15.2039 |
| GgyAun-H2O   | 635.2450 | C24H29O8N13    | 636.2528 | 636.3 | 0.0472 | 15.2039 |
| GGGIldn      | 635.3314 | C27H42O9N8     | 636.3392 | 636.3 | 0.0392 | 15.2039 |
| GGGGgld      | 635.3147 | C26H44O13N4    | 636.3225 | 636.3 | 0.0225 | 15.2039 |
| yyyyyyyn-H2O | 635.3003 | C26H45O13N5    | 636.3081 | 636.3 | 0.0081 | 15.2039 |
| ttyyyyyn-H2O | 635.2451 | C25H41O12N5S1  | 636.2529 | 636.3 | 0.0471 | 15.2039 |
| Gttttn-H2    | 636.0054 | C20H22O8N6S5   | 637.0132 | 637.0 | 0.0132 | 5.6953  |
| Gtttyyn-H2   | 636.1158 | C22H30O10N6S3  | 637.1236 | 637.1 | 0.0236 | 6.1489  |
| Gtttyn-H2    | 636.0606 | C21H26O9N6S4   | 637.0684 | 637.1 | 0.0316 | 6.1489  |
| gtlll-H2O    | 636.2051 | C22H34O18S1    | 637.2129 | 637.2 | 0.0129 | 6.1274  |
| gggAun       | 636.2079 | C23H26O10N12   | 637.2157 | 637.2 | 0.0157 | 6.1274  |
| GGtAun-H2O   | 636.2062 | C23H26O6N14S1  | 637.2140 | 637.2 | 0.0140 | 6.1274  |
| GGggAn-H2O   | 636.2137 | C24H26O90N12   | 637.2215 | 637.2 | 0.0215 | 6.1274  |
| GggggAu      | 636.1912 | C22H28O14N8    | 637.1990 | 637.2 | 0.0010 | 6.1274  |
| GGGgtAu-H2O  | 636.1895 | C22H28O10N10S1 | 637.1973 | 637.2 | 0.0027 | 6.1274  |
| GGGgggA-H2O  | 636.1970 | C23H28O13N8    | 637.2048 | 637.2 | 0.0048 | 6.1274  |
| gggydun-H2O  | 636.2387 | C27H37O90N7S1  | 637.2465 | 637.2 | 0.0465 | 6.1274  |
| gggttdun-H2O | 636.1835 | C26H33O8N7S2   | 637.1913 | 637.2 | 0.0087 | 6.1274  |
| ggggtdn-H2O  | 636.1910 | C27H33O11N5S1  | 637.1988 | 637.2 | 0.0012 | 6.1274  |
| Gttyyyn-H2   | 636.1710 | C23H34O11N6S2  | 637.1788 | 637.2 | 0.0212 | 6.1274  |

|              |          |                |          |       |        |        |
|--------------|----------|----------------|----------|-------|--------|--------|
| Gggglun      | 636.1921 | C22H28O14N8    | 637.1999 | 637.2 | 0.0001 | 6.1274 |
| GGGgtlun-H2O | 636.1904 | C22H28O10N10S1 | 637.1982 | 637.2 | 0.0018 | 6.1274 |
| GGGggln-H2O  | 636.1979 | C23H28O13N8    | 637.2057 | 637.2 | 0.0057 | 6.1274 |
| gylll-H2O    | 636.2603 | C23H38O19      | 637.2681 | 637.3 | 0.0319 | 5.5093 |
| GGyAun-H2O   | 636.2614 | C24H30O7N14    | 637.2692 | 637.3 | 0.0308 | 5.5093 |
| GGGgyAu-H2O  | 636.2447 | C23H32O11N10   | 637.2525 | 637.3 | 0.0475 | 5.5093 |
| GGGGGld      | 636.3311 | C26H45O12N5    | 637.3389 | 637.3 | 0.0389 | 5.5093 |
| ggyydun-H2O  | 636.2939 | C28H41O10N7    | 637.3017 | 637.3 | 0.0017 | 5.5093 |
| ggggydn-H2O  | 636.2462 | C28H37O12N5    | 637.2540 | 637.3 | 0.0460 | 5.5093 |
| GGGgylun-H2O | 636.2456 | C23H32O11N10   | 637.2534 | 637.3 | 0.0466 | 5.5093 |
| GtyAun-H2O   | 651.2211 | C24H29O7N13S1  | 652.2289 | 652.2 | 0.0289 | 5.0032 |
| GttAun-H2O   | 651.1659 | C23H25O6N13S2  | 652.1737 | 652.2 | 0.0263 | 5.0032 |
| GggyAn-H2O   | 651.2286 | C25H29O10N11   | 652.2364 | 652.2 | 0.0364 | 5.0032 |
| GggtAn-H2O   | 651.1734 | C24H25O90N11S1 | 652.1812 | 652.2 | 0.0188 | 5.0032 |
| ggggyAu      | 651.2061 | C23H31O15N7    | 652.2139 | 652.2 | 0.0139 | 5.0032 |
| ggggtAu      | 651.1509 | C22H27O14N7S1  | 652.1587 | 652.2 | 0.0413 | 5.0032 |
| ggggggA      | 651.1584 | C23H27O17N5    | 652.1662 | 652.2 | 0.0338 | 5.0032 |
| GGgtyAu-H2O  | 651.2044 | C23H31O11N9S1  | 652.2122 | 652.2 | 0.0122 | 5.0032 |
| GGgttAu-H2O  | 651.1492 | C22H27O10N9S2  | 652.1570 | 652.2 | 0.0430 | 5.0032 |
| GGgggyA-H2O  | 651.2119 | C24H31O14N7    | 652.2197 | 652.2 | 0.0197 | 5.0032 |
| GGgggtA-H2O  | 651.1567 | C23H27O13N7S1  | 652.1645 | 652.2 | 0.0355 | 5.0032 |
| ttyyyyyn-H2  | 651.1859 | C24H37O12N5S2  | 652.1937 | 652.2 | 0.0063 | 5.0032 |
| ttyyyyyn-H2  | 651.1307 | C23H33O11N5S3  | 652.1385 | 652.2 | 0.0615 | 5.0032 |
| ggggylun     | 651.2070 | C23H31O15N7    | 652.2148 | 652.2 | 0.0148 | 5.0032 |
| ggggtlun     | 651.1518 | C22H27O14N7S1  | 652.1596 | 652.2 | 0.0404 | 5.0032 |
| ggggggln     | 651.1593 | C23H27O17N5    | 652.1671 | 652.2 | 0.0329 | 5.0032 |
| GGgtlun-H2O  | 651.2053 | C23H31O11N9S1  | 652.2131 | 652.2 | 0.0131 | 5.0032 |
| GGgtlun-H2O  | 651.1501 | C22H27O10N9S2  | 652.1579 | 652.2 | 0.0421 | 5.0032 |
| GGgggyln-H2O | 651.2128 | C24H31O14N7    | 652.2206 | 652.2 | 0.0206 | 5.0032 |
| GGgggtln-H2O | 651.1576 | C23H27O13N7S1  | 652.1654 | 652.2 | 0.0346 | 5.0032 |
| GyyAun-H2O   | 651.2763 | C25H33O8N13    | 652.2841 | 652.3 | 0.0159 | 5.0627 |
| GGlldu-H2O   | 651.3498 | C27H46O13N4    | 652.3576 | 652.3 | 0.0576 | 5.0627 |
| GGggyAu-H2O  | 651.2596 | C24H35O12N9    | 652.2674 | 652.3 | 0.0326 | 5.0627 |

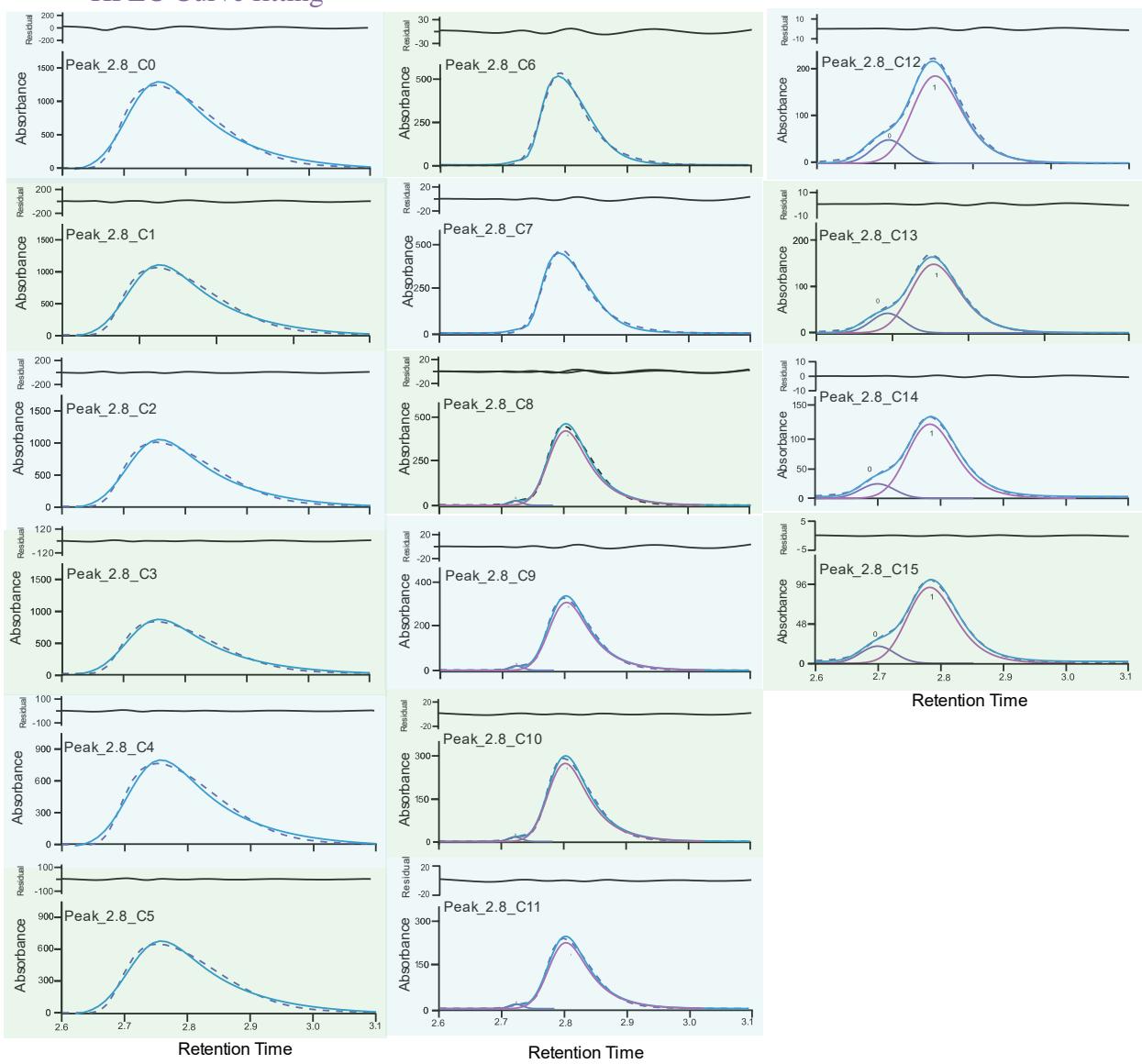
|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| GGGGyld      | 651.3460 | C27H48O13N4   | 652.3538 | 652.3 | 0.0538 | 5.0627  |
| GGGGtld      | 651.2908 | C26H44O12N4S1 | 652.2986 | 652.3 | 0.0014 | 5.0627  |
| GGgyylun-H2O | 651.2605 | C24H35O12N9   | 652.2683 | 652.3 | 0.0317 | 5.0627  |
| ttyyldu      | 679.2251 | C26H44O12N2S3 | 680.2329 | 680.2 | 0.0329 | 13.7809 |
| tttldu       | 679.1699 | C25H40O11N2S4 | 680.1777 | 680.2 | 0.0223 | 13.7809 |
| ggtyyld      | 679.2326 | C27H44O15S2   | 680.2404 | 680.2 | 0.0404 | 13.7809 |
| ggttld       | 679.1774 | C26H40O14S3   | 680.1852 | 680.2 | 0.0148 | 13.7809 |
| GGttld-H2    | 679.1956 | C26H40O12N2S3 | 680.2034 | 680.2 | 0.0034 | 13.7809 |
| GGGtyll      | 679.2395 | C23H39O17N3S1 | 680.2473 | 680.2 | 0.0473 | 13.7809 |
| GGGtll       | 679.1843 | C22H35O16N3S2 | 680.1921 | 680.2 | 0.0079 | 13.7809 |
| GGGGggAu-H2O | 679.2352 | C24H31O12N11  | 680.2430 | 680.2 | 0.0430 | 13.7809 |
| gllA-H2O     | 679.2666 | C25H35O16N5   | 680.2744 | 680.3 | 0.0256 | 12.5362 |
| gllln-H2O    | 679.2675 | C25H35O16N5   | 680.2753 | 680.3 | 0.0247 | 12.5362 |
| Gylllu-H2O   | 679.2985 | C24H41O18N3   | 680.3063 | 680.3 | 0.0063 | 12.5362 |
| Gtlllu-H2O   | 679.2433 | C23H37O17N3S1 | 680.2511 | 680.3 | 0.0489 | 12.5362 |
| Ggglll-H2O   | 679.2508 | C24H37O20N1   | 680.2586 | 680.3 | 0.0414 | 12.5362 |
| ttyyldu      | 679.3355 | C28H52O14N2S1 | 680.3433 | 680.3 | 0.0433 | 12.5362 |
| ttyyldu      | 679.2803 | C27H48O13N2S2 | 680.2881 | 680.3 | 0.0119 | 12.5362 |
| ggtyyld      | 679.2878 | C28H48O16S1   | 680.2956 | 680.3 | 0.0044 | 12.5362 |
| GGttyld-H2   | 679.2508 | C27H44O13N2S2 | 680.2586 | 680.3 | 0.0414 | 12.5362 |
| GGGtyll      | 679.2947 | C24H43O18N3   | 680.3025 | 680.3 | 0.0025 | 12.5362 |
| GGGgAun-H2O  | 679.2519 | C25H29O8N15   | 680.2597 | 680.3 | 0.0403 | 12.5362 |
| yyyyldu      | 679.3907 | C29H56O15N2   | 680.3985 | 680.4 | 0.0015 | 9.5806  |
| gyyyld       | 679.3430 | C29H52O17     | 680.3508 | 680.4 | 0.0492 | 9.5806  |
| GllA-H2O     | 680.2830 | C25H36O15N6   | 681.2908 | 681.2 | 0.0908 | 5.1742  |
| ttydA        | 680.2648 | C28H43O10N5S2 | 681.2726 | 681.2 | 0.0726 | 5.1742  |
| tttdA        | 680.2096 | C27H39O9N5S3  | 681.2174 | 681.2 | 0.0174 | 5.1742  |
| Gllln-H2O    | 680.2839 | C25H36O15N6   | 681.2917 | 681.2 | 0.0917 | 5.1742  |
| ttyldn       | 680.2657 | C28H43O10N5S2 | 681.2735 | 681.2 | 0.0735 | 5.1742  |
| tttdln       | 680.2105 | C27H39O9N5S3  | 681.2183 | 681.2 | 0.0183 | 5.1742  |
| glllu        | 680.2614 | C23H38O20N2   | 681.2692 | 681.2 | 0.0692 | 5.1742  |
| GGglll-H2O   | 680.2672 | C24H38O19N2   | 681.2750 | 681.2 | 0.0750 | 5.1742  |
| Ggttyld      | 680.2490 | C27H45O14N1S2 | 681.2568 | 681.2 | 0.0568 | 5.1742  |

|              |          |               |          |       |        |        |
|--------------|----------|---------------|----------|-------|--------|--------|
| Ggttld       | 680.1938 | C26H41O13N1S3 | 681.2016 | 681.2 | 0.0016 | 5.1742 |
| GGGGAun-H2O  | 680.2683 | C25H30O7N16   | 681.2761 | 681.2 | 0.0761 | 5.1742 |
| GGGGGgAu-H2O | 680.2516 | C24H32O11N12  | 681.2594 | 681.2 | 0.0594 | 5.1742 |
| GGttldu      | 723.2320 | C27H44O12N4S3 | 724.2398 | 724.2 | 0.0398 | 8.1596 |
| GGggttld     | 723.2395 | C28H44O15N2S2 | 724.2473 | 724.2 | 0.0473 | 8.1596 |
| tydAn        | 723.3272 | C31H44O8N10S1 | 724.3350 | 724.3 | 0.0350 | 7.5750 |
| ttdAn        | 723.2720 | C30H40O7N10S2 | 724.2798 | 724.3 | 0.0202 | 7.5750 |
| GgtydA       | 723.3105 | C30H46O12N6S1 | 724.3183 | 724.3 | 0.0183 | 7.5750 |
| GgttdA       | 723.2553 | C29H42O11N6S2 | 724.2631 | 724.3 | 0.0369 | 7.5750 |
| Ggtylnd      | 723.3114 | C30H46O12N6S1 | 724.3192 | 724.3 | 0.0192 | 7.5750 |
| Ggtldn       | 723.2562 | C29H42O11N6S2 | 724.2640 | 724.3 | 0.0360 | 7.5750 |
| GGttyldu     | 723.2872 | C28H48O13N4S2 | 724.2950 | 724.3 | 0.0050 | 7.5750 |
| GGggttyld    | 723.2947 | C29H48O16N2S1 | 724.3025 | 724.3 | 0.0025 | 7.5750 |
| GGGGGyll     | 723.3016 | C25H43O18N5   | 724.3094 | 724.3 | 0.0094 | 7.5750 |
| GGGGGtll     | 723.2464 | C24H39O17N5S1 | 724.2542 | 724.3 | 0.0458 | 7.5750 |
| yydAn        | 723.3824 | C32H48O9N10   | 724.3902 | 724.4 | 0.0098 | 6.0274 |
| GgyydA       | 723.3657 | C31H50O13N6   | 724.3735 | 724.4 | 0.0265 | 6.0274 |
| Ggyylnd      | 723.3666 | C31H50O13N6   | 724.3744 | 724.4 | 0.0256 | 6.0274 |
| GGtyyldu     | 723.3424 | C29H52O14N4S1 | 724.3502 | 724.4 | 0.0498 | 6.0274 |
| GGggyyld     | 723.3499 | C30H52O17N2   | 724.3577 | 724.4 | 0.0423 | 6.0274 |

### Fraction 6 (retention time = 2.8 min)

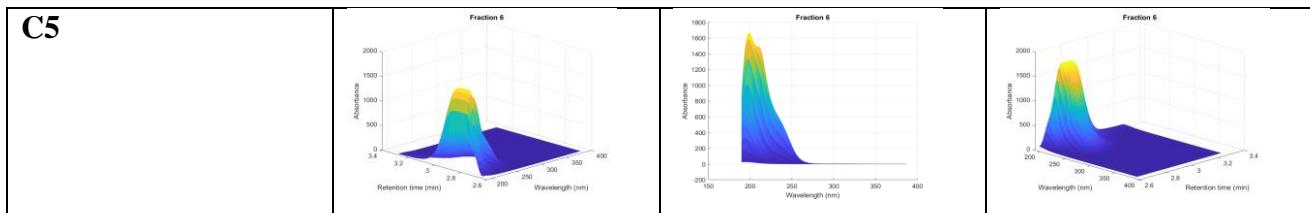
Initially, fraction 6 is composed of thioglycolic acid alone. Over cycles the absorbance peak goes down and then a shoulder appears on the left that goes up over cycles, indicating the consumption of thioglycolic acid and appearance of new hydrophilic products that are not retained well on the C18 column. The MS data indicate a variety of possible products in this fraction, such as tG.

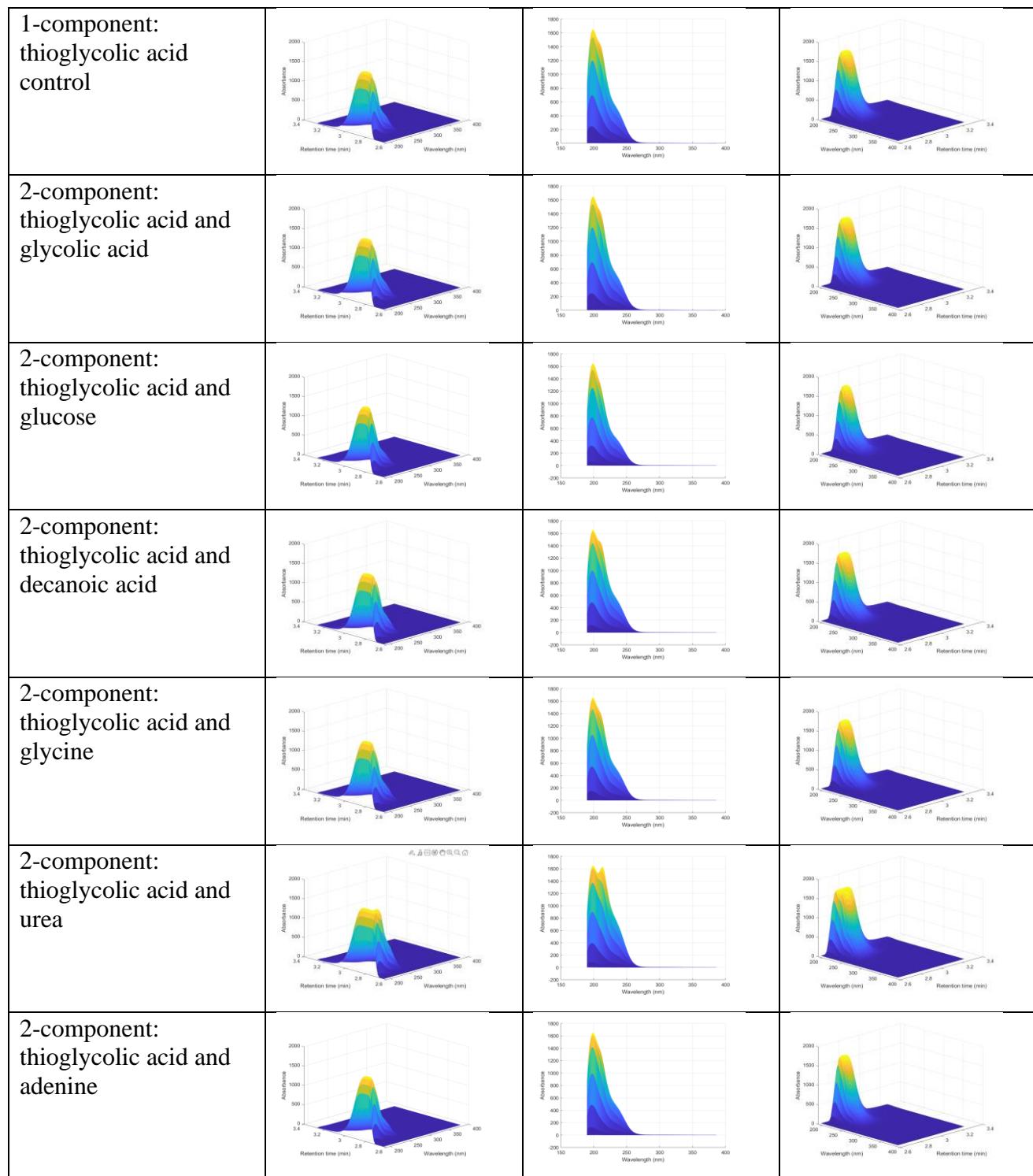
### HPLC Curve fitting

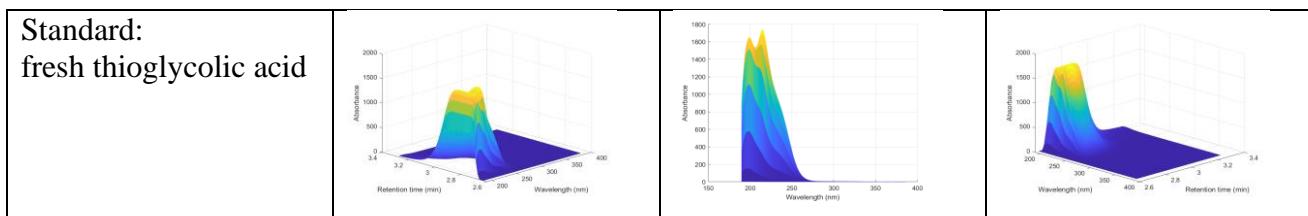


**Figure S15. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 6 which has a retention time of about 2.8 minutes at (230 nm)

### UV-VIS spectrum







**Figure S16. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 6 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula    | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3     | 91.0400           | 91.0              | 0.0400     | 88.3612  |
| t        | 91.9926      | C2H4O2S1   | 90.9848           | 91.0              | 0.0152     | 88.3612  |
| Gy       | 151.0696     | C5H11O4N1  | 150.0618          | 150.1             | 0.0382     | 5.6331   |
| Gt       | 151.0144     | C4H7O3N1S1 | 150.0066          | 150.0             | 0.0066     | 5.1004   |
| tyyy     | 314.1027     | C11H22O8S1 | 313.0949          | 313.1             | 0.0051     | 6.4879   |
| ttyy     | 314.0475     | C10H18O7S2 | 313.0397          | 313.0             | 0.0397     | 7.2445   |
| ttty     | 313.9923     | C9H14O6S3  | 312.9845          | 313.0             | 0.0155     | 7.2445   |
| tttt     | 313.9371     | C8H10O5S4  | 312.9293          | 312.9             | 0.0293     | 7.1988   |

#### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 11.7795  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 9.0169   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 14.0370  |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 14.0370  |
| yl-H2O   | 242.1091     | C9H16O7      | 243.1169          | 243.1             | 0.0169     | 7.6000   |
| tl-H2O   | 242.0539     | C8H12O6S1    | 243.0617          | 243.1             | 0.0383     | 7.6000   |
| Gtyy     | 299.0868     | C10H19O7N1S1 | 300.0946          | 300.1             | 0.0054     | 5.5070   |
| Gyn-H2O  | 324.1386     | C13H18O4N6   | 325.1464          | 325.1             | 0.0464     | 7.1433   |
| Gtyn-H2O | 324.0834     | C12H14O3N6S1 | 325.0912          | 325.1             | 0.0088     | 7.1433   |
| ggyyu    | 324.1161     | C11H20O9N2   | 325.1239          | 325.1             | 0.0239     | 7.1433   |
| ggtyu    | 324.0609     | C10H16O8N2S1 | 325.0687          | 325.1             | 0.0313     | 7.1433   |
| ggggy    | 324.0684     | C11H16O11    | 325.0762          | 325.1             | 0.0238     | 7.1433   |

|            |          |              |          |       |        |         |
|------------|----------|--------------|----------|-------|--------|---------|
| GGgyy-H2O  | 324.1219 | C12H20O8N2   | 325.1297 | 325.1 | 0.0297 | 7.1433  |
| GGgty-H2O  | 324.0667 | C11H16O7N2S1 | 325.0745 | 325.1 | 0.0255 | 7.1433  |
| gA-H2O     | 343.1208 | C13H15O6N5   | 344.1286 | 344.1 | 0.0286 | 8.3824  |
| gln-H2O    | 343.1217 | C13H15O6N5   | 344.1295 | 344.1 | 0.0295 | 8.3824  |
| Gtlu-H2O   | 343.0975 | C11H17O7N3S1 | 344.1053 | 344.1 | 0.0053 | 8.3824  |
| Gggl-H2O   | 343.1050 | C12H17O10N1  | 344.1128 | 344.1 | 0.0128 | 8.3824  |
| GGGty      | 343.0937 | C11H19O7N3S1 | 344.1015 | 344.1 | 0.0015 | 8.3824  |
| Gylu-H2O   | 343.1527 | C12H21O8N3   | 344.1605 | 344.2 | 0.0395 | 8.8074  |
| GGGyy      | 343.1489 | C12H23O8N3   | 344.1567 | 344.2 | 0.0433 | 8.8074  |
| ttyyy-H2   | 386.0686 | C13H22O9S2   | 387.0764 | 387.1 | 0.0236 | 6.3106  |
| GGGtn      | 386.1009 | C13H16O4N8S1 | 387.1087 | 387.1 | 0.0087 | 6.3106  |
| GGGGgy     | 386.1394 | C13H22O9N4   | 387.1472 | 387.1 | 0.0472 | 6.3106  |
| GGGGgt     | 386.0842 | C12H18O8N4S1 | 387.0920 | 387.1 | 0.0080 | 6.3106  |
| GAu-H2O    | 386.1590 | C14H18O5N8   | 387.1668 | 387.2 | 0.0332 | 5.6268  |
| Glun-H2O   | 386.1599 | C14H18O5N8   | 387.1677 | 387.2 | 0.0323 | 5.6268  |
| GGglu-H2O  | 386.1432 | C13H20O90N4  | 387.1510 | 387.2 | 0.0490 | 5.6268  |
| GGGyn      | 386.1561 | C14H20O5N8   | 387.1639 | 387.2 | 0.0361 | 5.6268  |
| GGGGGt     | 387.1006 | C12H19O7N5S1 | 388.1084 | 388.1 | 0.0084 | 9.7033  |
| ggydu-H2O  | 387.2079 | C18H30O7N2   | 388.2157 | 388.2 | 0.0157 | 9.5524  |
| ggtdu-H2O  | 387.1527 | C17H26O6N2S1 | 388.1605 | 388.2 | 0.0395 | 9.5524  |
| gggd-H2O   | 387.1602 | C18H26O9     | 388.1680 | 388.2 | 0.0320 | 9.5524  |
| GGGlu-H2O  | 387.1596 | C13H21O8N5   | 388.1674 | 388.2 | 0.0326 | 9.5524  |
| GGGGGy     | 387.1558 | C13H23O8N5   | 388.1636 | 388.2 | 0.0364 | 9.5524  |
| gtyl       | 392.1066 | C13H22O11S1  | 393.1144 | 393.1 | 0.0144 | 13.1878 |
| gttl       | 392.0514 | C12H18O10S2  | 393.0592 | 393.1 | 0.0408 | 13.1878 |
| Ggggun-H2O | 392.1032 | C14H14O6N8   | 393.1110 | 393.1 | 0.0110 | 13.1878 |
| GGgggu-H2O | 392.0865 | C13H16O10N4  | 393.0943 | 393.1 | 0.0057 | 13.1878 |
| gyyl       | 392.1618 | C14H26O12    | 393.1696 | 393.2 | 0.0304 | 14.0618 |
| GGGdu      | 392.2364 | C17H31O5N5   | 393.2442 | 393.2 | 0.0442 | 14.0618 |
| Gttyu      | 415.0349 | C12H19O7N3S3 | 416.0427 | 416.0 | 0.0427 | 7.0827  |
| gtyyn      | 415.1143 | C15H21O7N5S1 | 416.1221 | 416.1 | 0.0221 | 7.6470  |
| gttyn      | 415.0591 | C14H17O6N5S2 | 416.0669 | 416.1 | 0.0331 | 7.6470  |
| Gttyyu     | 415.0901 | C13H23O8N3S2 | 416.0979 | 416.1 | 0.0021 | 7.6470  |

|            |          |               |          |       |        |         |
|------------|----------|---------------|----------|-------|--------|---------|
| Gggtyy     | 415.0976 | C14H23O11N1S1 | 416.1054 | 416.1 | 0.0054 | 7.6470  |
| Gggtty     | 415.0424 | C13H19O10N1S2 | 416.0502 | 416.1 | 0.0498 | 7.6470  |
| GGGtty-H2  | 415.0606 | C13H19O8N3S2  | 416.0684 | 416.1 | 0.0316 | 7.6470  |
| tld        | 415.2036 | C18H32O8S1    | 416.2114 | 416.2 | 0.0114 | 7.4309  |
| gyyyyn     | 415.1695 | C16H25O8N5    | 416.1773 | 416.2 | 0.0227 | 7.4309  |
| Gyyyyu     | 415.2005 | C15H31O10N3   | 416.2083 | 416.2 | 0.0083 | 7.4309  |
| Gtyyyu     | 415.1453 | C14H27O9N3S1  | 416.1531 | 416.2 | 0.0469 | 7.4309  |
| Gggyyy     | 415.1528 | C15H27O12N1   | 416.1606 | 416.2 | 0.0394 | 7.4309  |
| yld        | 415.2588 | C19H36O9      | 416.2666 | 416.3 | 0.0334 | 6.1309  |
| tttyn      | 431.0352 | C14H17O5N5S3  | 432.0430 | 432.0 | 0.0430 | 9.6941  |
| ttyyn      | 431.0904 | C15H21O6N5S2  | 432.0982 | 432.1 | 0.0018 | 11.0371 |
| Ggtyyy     | 431.1289 | C15H27O11N1S1 | 432.1367 | 432.1 | 0.0367 | 11.0371 |
| Ggttyy     | 431.0737 | C14H23O10N1S2 | 432.0815 | 432.1 | 0.0185 | 11.0371 |
| yyyyn      | 431.2008 | C17H29O8N5    | 432.2086 | 432.2 | 0.0086 | 11.7540 |
| tyyyn      | 431.1456 | C16H25O7N5S1  | 432.1534 | 432.2 | 0.0466 | 11.7540 |
| Ggdun-H2O  | 431.2315 | C20H28O3N8    | 432.2393 | 432.2 | 0.0393 | 11.7540 |
| Ggyyyy     | 431.1841 | C16H31O12N1   | 432.1919 | 432.2 | 0.0081 | 11.7540 |
| GGggdu-H2O | 431.2148 | C19H30O7N4    | 432.2226 | 432.2 | 0.0226 | 11.7540 |
| GGGGGGGG   | 431.1627 | C14H23O8N7    | 432.1705 | 432.2 | 0.0295 | 11.7540 |
| GGGtttu    | 459.0418 | C13H19O7N5S3  | 460.0496 | 460.0 | 0.0496 | 8.9130  |
| gtAu-H2O   | 459.1241 | C16H19O7N7S1  | 460.1319 | 460.1 | 0.0319 | 9.9979  |
| gggA-H2O   | 459.1316 | C17H19O10N5   | 460.1394 | 460.1 | 0.0394 | 9.9979  |
| gtlun-H2O  | 459.1250 | C16H19O7N7S1  | 460.1328 | 460.1 | 0.0328 | 9.9979  |
| gggln-H2O  | 459.1325 | C17H19O10N5   | 460.1403 | 460.1 | 0.0403 | 9.9979  |
| Gggtlu-H2O | 459.1083 | C15H21O11N3S1 | 460.1161 | 460.1 | 0.0161 | 9.9979  |
| Gggggl-H2O | 459.1158 | C16H21O14N1   | 460.1236 | 460.1 | 0.0236 | 9.9979  |
| GGgtyn     | 459.1212 | C16H21O7N7S1  | 460.1290 | 460.1 | 0.0290 | 9.9979  |
| GGgttn     | 459.0660 | C15H17O6N7S2  | 460.0738 | 460.1 | 0.0262 | 9.9979  |
| GGGttyu    | 459.0970 | C14H23O8N5S2  | 460.1048 | 460.1 | 0.0048 | 9.9979  |
| GGGggt     | 459.1045 | C15H23O11N3S1 | 460.1123 | 460.1 | 0.0123 | 9.9979  |
| GGGggtt    | 459.0493 | C14H19O10N3S2 | 460.0571 | 460.1 | 0.0429 | 9.9979  |
| GGGGGtt-H2 | 459.0675 | C14H19O8N5S2  | 460.0753 | 460.1 | 0.0247 | 9.9979  |
| gyAu-H2O   | 459.1793 | C17H23O8N7    | 460.1871 | 460.2 | 0.0129 | 9.8986  |

|            |          |               |          |       |        |         |
|------------|----------|---------------|----------|-------|--------|---------|
| gylun-H2O  | 459.1802 | C17H23O8N7    | 460.1880 | 460.2 | 0.0120 | 9.8986  |
| Gggylu-H2O | 459.1635 | C16H25O12N3   | 460.1713 | 460.2 | 0.0287 | 9.8986  |
| GGgyn      | 459.1764 | C17H25O8N7    | 460.1842 | 460.2 | 0.0158 | 9.8986  |
| GGGyyu     | 459.2074 | C16H31O10N5   | 460.2152 | 460.2 | 0.0152 | 9.8986  |
| GGGtyyu    | 459.1522 | C15H27O9N5S1  | 460.1600 | 460.2 | 0.0400 | 9.8986  |
| GGGggyy    | 459.1597 | C16H27O12N3   | 460.1675 | 460.2 | 0.0325 | 9.8986  |
| GGld       | 459.2657 | C20H36O9N2    | 460.2735 | 460.3 | 0.0265 | 7.9929  |
| GGtttn     | 475.0421 | C15H17O5N7S3  | 476.0499 | 476.0 | 0.0499 | 9.7430  |
| GGGgttt    | 475.0254 | C14H19O9N3S3  | 476.0332 | 476.0 | 0.0332 | 9.7430  |
| ttAu-H2O   | 475.1002 | C16H19O6N7S2  | 476.1080 | 476.1 | 0.0080 | 10.1806 |
| ggtA-H2O   | 475.1077 | C17H19O90N5S1 | 476.1155 | 476.1 | 0.0155 | 10.1806 |
| ttlun-H2O  | 475.1011 | C16H19O6N7S2  | 476.1089 | 476.1 | 0.0089 | 10.1806 |
| ggtln-H2O  | 475.1086 | C17H19O90N5S1 | 476.1164 | 476.1 | 0.0164 | 10.1806 |
| Ggtlu-H2O  | 475.1396 | C16H25O11N3S1 | 476.1474 | 476.1 | 0.0474 | 10.1806 |
| Ggtlu-H2O  | 475.0844 | C15H21O10N3S2 | 476.0922 | 476.1 | 0.0078 | 10.1806 |
| Ggggtl-H2O | 475.0919 | C16H21O13N1S1 | 476.0997 | 476.1 | 0.0003 | 10.1806 |
| GGttn      | 475.0973 | C16H21O6N7S2  | 476.1051 | 476.1 | 0.0051 | 10.1806 |
| GGGgtyy    | 475.1358 | C16H27O11N3S1 | 476.1436 | 476.1 | 0.0436 | 10.1806 |
| GGGgtty    | 475.0806 | C15H23O10N3S2 | 476.0884 | 476.1 | 0.0116 | 10.1806 |
| yyAu-H2O   | 475.2106 | C18H27O8N7    | 476.2184 | 476.2 | 0.0184 | 9.8019  |
| tyAu-H2O   | 475.1554 | C17H23O7N7S1  | 476.1632 | 476.2 | 0.0368 | 9.8019  |
| ggyA-H2O   | 475.1629 | C18H23O10N5   | 476.1707 | 476.2 | 0.0293 | 9.8019  |
| yylyn-H2O  | 475.2115 | C18H27O8N7    | 476.2193 | 476.2 | 0.0193 | 9.8019  |
| tylyn-H2O  | 475.1563 | C17H23O7N7S1  | 476.1641 | 476.2 | 0.0359 | 9.8019  |
| ggyln-H2O  | 475.1638 | C18H23O10N5   | 476.1716 | 476.2 | 0.0284 | 9.8019  |
| Ggyylu-H2O | 475.1948 | C17H29O12N3   | 476.2026 | 476.2 | 0.0026 | 9.8019  |
| Gggyl-H2O  | 475.1471 | C17H25O14N1   | 476.1549 | 476.2 | 0.0451 | 9.8019  |
| GGyyyn     | 475.2077 | C18H29O8N7    | 476.2155 | 476.2 | 0.0155 | 9.8019  |
| GGtyn      | 475.1525 | C17H25O7N7S1  | 476.1603 | 476.2 | 0.0397 | 9.8019  |
| GGGgyyy    | 475.1910 | C17H31O12N3   | 476.1988 | 476.2 | 0.0012 | 9.8019  |
| Gtttyy-H2O | 503.0207 | C16H23O90N1S4 | 504.0285 | 504.0 | 0.0285 | 9.6504  |
| Gtttyy-H2  | 503.0406 | C16H23O11N1S3 | 504.0484 | 504.0 | 0.0484 | 9.6504  |
| ttyyyn-H2  | 503.1125 | C18H25O8N5S2  | 504.1203 | 504.1 | 0.0203 | 10.9071 |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| tttynn-H2   | 503.0573 | C17H21O7N5S3  | 504.0651 | 504.1 | 0.0349 | 10.9071 |
| Gttyyy-H2O  | 503.1311 | C18H31O11N1S2 | 504.1389 | 504.1 | 0.0389 | 10.9071 |
| Gttyyy-H2O  | 503.0759 | C17H27O10N1S3 | 504.0837 | 504.1 | 0.0163 | 10.9071 |
| Ggttyy-H2   | 503.0958 | C17H27O12N1S2 | 504.1036 | 504.1 | 0.0036 | 10.9071 |
| GGGGgtn     | 503.1281 | C17H21O7N9S1  | 504.1359 | 504.1 | 0.0359 | 10.9071 |
| GGGGGttu    | 503.1039 | C15H23O8N7S2  | 504.1117 | 504.1 | 0.0117 | 10.9071 |
| GGGGGggt    | 503.1114 | C16H23O11N5S1 | 504.1192 | 504.1 | 0.0192 | 10.9071 |
| GAun-H2O    | 503.2029 | C19H21O4N13   | 504.2107 | 504.2 | 0.0107 | 10.6896 |
| GGgAu-H2O   | 503.1862 | C18H23O8N9    | 504.1940 | 504.2 | 0.0060 | 10.6896 |
| GGglun-H2O  | 503.1871 | C18H23O8N9    | 504.1949 | 504.2 | 0.0051 | 10.6896 |
| gggyydu-H2O | 503.2187 | C22H34O11N2   | 504.2265 | 504.2 | 0.0265 | 10.6896 |
| gggtdu-H2O  | 503.1635 | C21H30O10N2S1 | 504.1713 | 504.2 | 0.0287 | 10.6896 |
| gggggd-H2O  | 503.1710 | C22H30O13     | 504.1788 | 504.2 | 0.0212 | 10.6896 |
| Gyyyyy-H2O  | 503.2415 | C20H39O13N1   | 504.2493 | 504.2 | 0.0493 | 10.6896 |
| Gtffffy-H2O | 503.1863 | C19H35O12N1S1 | 504.1941 | 504.2 | 0.0059 | 10.6896 |
| GGGgglu-H2O | 503.1704 | C17H25O12N5   | 504.1782 | 504.2 | 0.0218 | 10.6896 |
| GGGGgyn     | 503.1833 | C18H25O8N9    | 504.1911 | 504.2 | 0.0089 | 10.6896 |
| GGGGGyyu    | 503.2143 | C17H31O10N7   | 504.2221 | 504.2 | 0.0221 | 10.6896 |
| GGGGGtyu    | 503.1591 | C16H27O9N7S1  | 504.1669 | 504.2 | 0.0331 | 10.6896 |
| GGGGGggy    | 503.1666 | C17H27O12N5   | 504.1744 | 504.2 | 0.0256 | 10.6896 |
| Gtttyy-H2   | 519.0167 | C16H23O10N1S4 | 520.0245 | 520.0 | 0.0245 | 8.1458  |
| gggtdu-H2O  | 519.1396 | C21H30O90N2S2 | 520.1474 | 520.1 | 0.0474 | 8.9994  |
| Gtffffy-H2  | 519.1271 | C18H31O12N1S2 | 520.1349 | 520.1 | 0.0349 | 8.9994  |
| Gtffffy-H2  | 519.0719 | C17H27O11N1S3 | 520.0797 | 520.1 | 0.0203 | 8.9994  |
| GGGGttn     | 519.1042 | C17H21O6N9S2  | 520.1120 | 520.1 | 0.0120 | 8.9994  |
| GGGGGggt    | 519.0875 | C16H23O10N5S2 | 520.0953 | 520.1 | 0.0047 | 8.9994  |
| GgAn-H2O    | 519.1865 | C20H21O6N11   | 520.1943 | 520.2 | 0.0057 | 9.4078  |
| gggAu       | 519.1640 | C18H23O11N7   | 520.1718 | 520.2 | 0.0282 | 9.4078  |
| GGyAu-H2O   | 519.2175 | C19H27O8N9    | 520.2253 | 520.2 | 0.0253 | 9.4078  |
| GGtAu-H2O   | 519.1623 | C18H23O7N9S1  | 520.1701 | 520.2 | 0.0299 | 9.4078  |
| GGggA-H2O   | 519.1698 | C19H23O10N7   | 520.1776 | 520.2 | 0.0224 | 9.4078  |
| ggglun      | 519.1649 | C18H23O11N7   | 520.1727 | 520.2 | 0.0273 | 9.4078  |
| GGylun-H2O  | 519.2184 | C19H27O8N9    | 520.2262 | 520.2 | 0.0262 | 9.4078  |

|               |          |               |          |       |        |         |
|---------------|----------|---------------|----------|-------|--------|---------|
| GGtlun-H2O    | 519.1632 | C18H23O7N9S1  | 520.1710 | 520.2 | 0.0290 | 9.4078  |
| GGggln-H2O    | 519.1707 | C19H23O10N7   | 520.1785 | 520.2 | 0.0215 | 9.4078  |
| gggydu-H2O    | 519.1948 | C22H34O10N2S1 | 520.2026 | 520.2 | 0.0026 | 9.4078  |
| ggggyd-H2O    | 519.2023 | C23H34O13     | 520.2101 | 520.2 | 0.0101 | 9.4078  |
| ggggtd-H2O    | 519.1471 | C22H30O12S1   | 520.1549 | 520.2 | 0.0451 | 9.4078  |
| Ggggglu       | 519.1482 | C17H25O15N3   | 520.1560 | 520.2 | 0.0440 | 9.4078  |
| GGGgylu-H2O   | 519.2017 | C18H29O12N5   | 520.2095 | 520.2 | 0.0095 | 9.4078  |
| GGGgtlu-H2O   | 519.1465 | C17H25O11N5S1 | 520.1543 | 520.2 | 0.0457 | 9.4078  |
| GGGgggl-H2O   | 519.1540 | C18H25O14N3   | 520.1618 | 520.2 | 0.0382 | 9.4078  |
| GGGGyyn       | 519.2146 | C19H29O8N9    | 520.2224 | 520.2 | 0.0224 | 9.4078  |
| GGGGtyn       | 519.1594 | C18H25O7N9S1  | 520.1672 | 520.2 | 0.0328 | 9.4078  |
| GGGGGgyy      | 519.1979 | C18H31O12N5   | 520.2057 | 520.2 | 0.0057 | 9.4078  |
| GGGGGgty      | 519.1427 | C17H27O11N5S1 | 520.1505 | 520.2 | 0.0495 | 9.4078  |
| ggyydu-H2O    | 519.2500 | C23H38O11N2   | 520.2578 | 520.3 | 0.0422 | 8.6323  |
| ttyyun        | 547.0385 | C17H21O6N7S4  | 548.0463 | 548.0 | 0.0463 | 9.2919  |
| Gttttyu       | 547.0218 | C16H23O10N3S4 | 548.0296 | 548.0 | 0.0296 | 9.2919  |
| Ggggtty       | 547.0293 | C17H23O13N1S3 | 548.0371 | 548.0 | 0.0371 | 9.2919  |
| GGGttty-H2O   | 547.0276 | C17H23O90N3S4 | 548.0354 | 548.0 | 0.0354 | 9.2919  |
| ttyyun        | 547.0937 | C18H25O7N7S3  | 548.1015 | 548.1 | 0.0015 | 10.7508 |
| ggttyn        | 547.1012 | C19H25O10N5S2 | 548.1090 | 548.1 | 0.0090 | 10.7508 |
| ggttyn        | 547.0460 | C18H21O9N5S3  | 548.0538 | 548.1 | 0.0462 | 10.7508 |
| GGt yyn-H2    | 547.1194 | C19H25O8N7S2  | 548.1272 | 548.1 | 0.0272 | 10.7508 |
| GGttyn-H2     | 547.0642 | C18H21O7N7S3  | 548.0720 | 548.1 | 0.0280 | 10.7508 |
| Ggttyyu       | 547.1322 | C18H31O12N3S2 | 548.1400 | 548.1 | 0.0400 | 10.7508 |
| Ggttyyu       | 547.0770 | C17H27O11N3S3 | 548.0848 | 548.1 | 0.0152 | 10.7508 |
| Ggggtyyy      | 547.1397 | C19H31O15N1S1 | 548.1475 | 548.1 | 0.0475 | 10.7508 |
| Ggggttyy      | 547.0845 | C18H27O14N1S2 | 548.0923 | 548.1 | 0.0077 | 10.7508 |
| GGGt yyyy-H2O | 547.1380 | C19H31O11N3S2 | 548.1458 | 548.1 | 0.0458 | 10.7508 |
| GGGtttyy-H2O  | 547.0828 | C18H27O10N3S3 | 548.0906 | 548.1 | 0.0094 | 10.7508 |
| GGGgt tyy-H2  | 547.1027 | C18H27O12N3S2 | 548.1105 | 548.1 | 0.0105 | 10.7508 |
| GGGgt tyy-H2  | 547.0475 | C17H23O11N3S3 | 548.0553 | 548.1 | 0.0447 | 10.7508 |
| gttld         | 547.1905 | C22H36O11S2   | 548.1983 | 548.2 | 0.0017 | 11.4419 |
| ttyyyun       | 547.2041 | C20H33O9N7S1  | 548.2119 | 548.2 | 0.0119 | 11.4419 |

|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| ttyyuyun     | 547.1489 | C19H29O8N7S2  | 548.1567 | 548.2 | 0.0433 | 11.4419 |
| ggyyyyn      | 547.2116 | C21H33O12N5   | 548.2194 | 548.2 | 0.0194 | 11.4419 |
| ggttyyyn     | 547.1564 | C20H29O11N5S1 | 548.1642 | 548.2 | 0.0358 | 11.4419 |
| Ggttyyyu     | 547.1874 | C19H35O13N3S1 | 548.1952 | 548.2 | 0.0048 | 11.4419 |
| Ggggyyyy     | 547.1949 | C20H35O16N1   | 548.2027 | 548.2 | 0.0027 | 11.4419 |
| GGggggdu-H2O | 547.2256 | C23H34O11N4   | 548.2334 | 548.2 | 0.0334 | 11.4419 |
| GGGtcccc-H2O | 547.1932 | C20H35O12N3S1 | 548.2010 | 548.2 | 0.0010 | 11.4419 |
| GGGGGGgn     | 547.1902 | C19H25O8N11   | 548.1980 | 548.2 | 0.0020 | 11.4419 |
| gyyld        | 547.3009 | C24H44O13     | 548.3087 | 548.3 | 0.0087 | 10.4682 |
| gtyld        | 547.2457 | C23H40O12S1   | 548.2535 | 548.3 | 0.0465 | 10.4682 |
| yyyyyun      | 547.2593 | C21H37O10N7   | 548.2671 | 548.3 | 0.0329 | 10.4682 |
| Ggggdun-H2O  | 547.2423 | C24H32O7N8    | 548.2501 | 548.3 | 0.0499 | 10.4682 |
| Gyyyyyu      | 547.2426 | C20H39O14N3   | 548.2504 | 548.3 | 0.0496 | 10.4682 |
| GGGyyyyy-H2O | 547.2484 | C21H39O13N3   | 548.2562 | 548.3 | 0.0438 | 10.4682 |
| gttttyn      | 563.0221 | C18H21O8N5S4  | 564.0299 | 564.0 | 0.0299 | 6.0104  |
| GGGtttly-H2  | 563.0236 | C17H23O10N3S4 | 564.0314 | 564.0 | 0.0314 | 6.0104  |
| gttyyyn      | 563.1325 | C20H29O10N5S2 | 564.1403 | 564.1 | 0.0403 | 6.9646  |
| gttyyyn      | 563.0773 | C19H25O9N5S3  | 564.0851 | 564.1 | 0.0149 | 6.9646  |
| Gttyyyu      | 563.1083 | C18H31O11N3S3 | 564.1161 | 564.1 | 0.0161 | 6.9646  |
| Gtttlyu      | 563.0531 | C17H27O10N3S4 | 564.0609 | 564.1 | 0.0391 | 6.9646  |
| Gggtttly     | 563.1158 | C19H31O14N1S2 | 564.1236 | 564.1 | 0.0236 | 6.9646  |
| Gggtttly     | 563.0606 | C18H27O13N1S3 | 564.0684 | 564.1 | 0.0316 | 6.9646  |
| GGGtcccc-H2  | 563.1340 | C19H31O12N3S2 | 564.1418 | 564.1 | 0.0418 | 6.9646  |
| GGGtttly-H2  | 563.0788 | C18H27O11N3S3 | 564.0866 | 564.1 | 0.0134 | 6.9646  |
| Glll-H2O     | 563.2400 | C20H33O16N1   | 564.2478 | 564.2 | 0.0478 | 7.5146  |
| ttyld        | 563.2218 | C23H40O11S2   | 564.2296 | 564.2 | 0.0296 | 7.5146  |
| tttdl        | 563.1666 | C22H36O10S3   | 564.1744 | 564.2 | 0.0256 | 7.5146  |
| GGGGAu-H2O   | 563.2244 | C20H27O8N11   | 564.2322 | 564.2 | 0.0322 | 7.5146  |
| gttyyyn      | 563.1877 | C21H33O11N5S1 | 564.1955 | 564.2 | 0.0045 | 7.5146  |
| Gggtdun-H2O  | 563.2184 | C24H32O6N8S1  | 564.2262 | 564.2 | 0.0262 | 7.5146  |
| Gggggdn-H2O  | 563.2259 | C25H32O90N6   | 564.2337 | 564.2 | 0.0337 | 7.5146  |
| GGGGlun-H2O  | 563.2253 | C20H27O8N11   | 564.2331 | 564.2 | 0.0331 | 7.5146  |
| ggggggdu     | 563.2034 | C23H34O14N2   | 564.2112 | 564.2 | 0.0112 | 7.5146  |

|              |          |               |          |       |        |         |
|--------------|----------|---------------|----------|-------|--------|---------|
| Gtyyyyyu     | 563.2187 | C20H39O13N3S1 | 564.2265 | 564.2 | 0.0265 | 7.5146  |
| Gt-yyyyu     | 563.1635 | C19H35O12N3S2 | 564.1713 | 564.2 | 0.0287 | 7.5146  |
| Gggyyyyy     | 563.2262 | C21H39O16N1   | 564.2340 | 564.2 | 0.0340 | 7.5146  |
| Gggt-yyyy    | 563.1710 | C20H35O15N1S1 | 564.1788 | 564.2 | 0.0212 | 7.5146  |
| GGgggtdu-H2O | 563.2017 | C23H34O10N4S1 | 564.2095 | 564.2 | 0.0095 | 7.5146  |
| GGgggggd-H2O | 563.2092 | C24H34O13N2   | 564.2170 | 564.2 | 0.0170 | 7.5146  |
| GGGGGglu-H2O | 563.2086 | C19H29O12N7   | 564.2164 | 564.2 | 0.0164 | 7.5146  |
| GGGGGGGyn    | 563.2215 | C20H29O8N11   | 564.2293 | 564.2 | 0.0293 | 7.5146  |
| GGGGGGGtn    | 563.1663 | C19H25O7N11S1 | 564.1741 | 564.2 | 0.0259 | 7.5146  |
| yyld         | 563.3322 | C25H48O13     | 564.3400 | 564.3 | 0.0400 | 7.2260  |
| tyld         | 563.2770 | C24H44O12S1   | 564.2848 | 564.3 | 0.0152 | 7.2260  |
| gyyyyyn      | 563.2429 | C22H37O12N5   | 564.2507 | 564.3 | 0.0493 | 7.2260  |
| Gggydun-H2O  | 563.2736 | C25H36O7N8    | 564.2814 | 564.3 | 0.0186 | 7.2260  |
| Gyyyyyu      | 563.2739 | C21H43O14N3   | 564.2817 | 564.3 | 0.0183 | 7.2260  |
| GGgggydu-H2O | 563.2569 | C24H38O11N4   | 564.2647 | 564.3 | 0.0353 | 7.2260  |
| ggttAu-H2O   | 591.1110 | C20H23O10N7S2 | 592.1188 | 592.1 | 0.0188 | 10.2494 |
| ggggtA-H2O   | 591.1185 | C21H23O13N5S1 | 592.1263 | 592.1 | 0.0263 | 10.2494 |
| ggttlun-H2O  | 591.1119 | C20H23O10N7S2 | 592.1197 | 592.1 | 0.0197 | 10.2494 |
| gggtlun-H2O  | 591.1194 | C21H23O13N5S1 | 592.1272 | 592.1 | 0.0272 | 10.2494 |
| Ggggtlu-H2O  | 591.0952 | C19H25O14N3S2 | 592.1030 | 592.1 | 0.0030 | 10.2494 |
| Ggggggtl-H2O | 591.1027 | C20H25O17N1S1 | 592.1105 | 592.1 | 0.0105 | 10.2494 |
| GGtttyun     | 591.1006 | C19H25O7N9S3  | 592.1084 | 592.1 | 0.0084 | 10.2494 |
| GGttttun     | 591.0454 | C18H21O6N9S4  | 592.0532 | 592.1 | 0.0468 | 10.2494 |
| GGggttyn     | 591.1081 | C20H25O10N7S2 | 592.1159 | 592.1 | 0.0159 | 10.2494 |
| GGggttn      | 591.0529 | C19H21O9N7S3  | 592.0607 | 592.1 | 0.0393 | 10.2494 |
| GGGGttyn-H2  | 591.1263 | C20H25O8N9S2  | 592.1341 | 592.1 | 0.0341 | 10.2494 |
| GGGGtttn-H2  | 591.0711 | C19H21O7N9S3  | 592.0789 | 592.1 | 0.0211 | 10.2494 |
| ggyyAu-H2O   | 591.2214 | C22H31O12N7   | 592.2292 | 592.2 | 0.0292 | 11.3204 |
| ggttAu-H2O   | 591.1662 | C21H27O11N7S1 | 592.1740 | 592.2 | 0.0260 | 11.3204 |
| ggggyA-H2O   | 591.1737 | C22H27O14N5   | 592.1815 | 592.2 | 0.0185 | 11.3204 |
| ggyylun-H2O  | 591.2223 | C22H31O12N7   | 592.2301 | 592.2 | 0.0301 | 11.3204 |
| ggtlun-H2O   | 591.1671 | C21H27O11N7S1 | 592.1749 | 592.2 | 0.0251 | 11.3204 |
| gggyln-H2O   | 591.1746 | C22H27O14N5   | 592.1824 | 592.2 | 0.0176 | 11.3204 |

|               |          |               |          |       |        |         |
|---------------|----------|---------------|----------|-------|--------|---------|
| Ggggyylu-H2O  | 591.2056 | C21H33O16N3   | 592.2134 | 592.2 | 0.0134 | 11.3204 |
| Ggggttylu-H2O | 591.1504 | C20H29O15N3S1 | 592.1582 | 592.2 | 0.0418 | 11.3204 |
| Ggggggyl-H2O  | 591.1579 | C21H29O18N1   | 592.1657 | 592.2 | 0.0343 | 11.3204 |
| GGttyyun      | 591.2110 | C21H33O9N9S1  | 592.2188 | 592.2 | 0.0188 | 11.3204 |
| GGttyyun      | 591.1558 | C20H29O8N9S2  | 592.1636 | 592.2 | 0.0364 | 11.3204 |
| GGggyyn       | 591.2185 | C22H33O12N7   | 592.2263 | 592.2 | 0.0263 | 11.3204 |
| GGggtyn       | 591.1633 | C21H29O11N7S1 | 592.1711 | 592.2 | 0.0289 | 11.3204 |
| GydA          | 591.3236 | C26H42O9N6    | 592.3314 | 592.3 | 0.0314 | 10.3858 |
| GtdA          | 591.2684 | C25H38O8N6S1  | 592.2762 | 592.3 | 0.0238 | 10.3858 |
| glldu-H2O     | 591.3116 | C25H42O13N2   | 592.3194 | 592.3 | 0.0194 | 10.3858 |
| Gyldn         | 591.3245 | C26H42O9N6    | 592.3323 | 592.3 | 0.0323 | 10.3858 |
| Gtldn         | 591.2693 | C25H38O8N6S1  | 592.2771 | 592.3 | 0.0229 | 10.3858 |
| GGyld         | 591.3078 | C25H44O13N2   | 592.3156 | 592.3 | 0.0156 | 10.3858 |
| GGtld         | 591.2526 | C24H40O12N2S1 | 592.2604 | 592.3 | 0.0396 | 10.3858 |
| GGyyyun       | 591.2662 | C22H37O10N9   | 592.2740 | 592.3 | 0.0260 | 10.3858 |
| gtttau-H2O    | 607.0871 | C20H23O90N7S3 | 608.0949 | 608.1 | 0.0051 | 5.7161  |
| ggttau-H2     | 607.1070 | C20H23O11N7S2 | 608.1148 | 608.1 | 0.0148 | 5.7161  |
| gggttA-H2O    | 607.0946 | C21H23O12N5S2 | 608.1024 | 608.1 | 0.0024 | 5.7161  |
| gttlun-H2O    | 607.0880 | C20H23O90N7S3 | 608.0958 | 608.1 | 0.0042 | 5.7161  |
| gttlun-H2     | 607.1079 | C20H23O11N7S2 | 608.1157 | 608.1 | 0.0157 | 5.7161  |
| gggtln-H2O    | 607.0955 | C21H23O12N5S2 | 608.1033 | 608.1 | 0.0033 | 5.7161  |
| Gggtylu-H2O   | 607.1265 | C20H29O14N3S2 | 608.1343 | 608.1 | 0.0343 | 5.7161  |
| Gggttlu-H2O   | 607.0713 | C19H25O13N3S3 | 608.0791 | 608.1 | 0.0209 | 5.7161  |
| Ggggtlu-H2    | 607.0912 | C19H25O15N3S2 | 608.0990 | 608.1 | 0.0010 | 5.7161  |
| Ggggttyl-H2O  | 607.1340 | C21H29O17N1S1 | 608.1418 | 608.1 | 0.0418 | 5.7161  |
| Ggggttl-H2O   | 607.0788 | C20H25O16N1S2 | 608.0866 | 608.1 | 0.0134 | 5.7161  |
| GGgtyyn       | 607.1394 | C21H29O10N7S2 | 608.1472 | 608.1 | 0.0472 | 5.7161  |
| GGgttytn      | 607.0842 | C20H25O9N7S3  | 608.0920 | 608.1 | 0.0080 | 5.7161  |
| GGgttn        | 607.0290 | C19H21O8N7S4  | 608.0368 | 608.1 | 0.0632 | 5.7161  |
| gtyyau-H2O    | 607.1975 | C22H31O11N7S1 | 608.2053 | 608.2 | 0.0053 | 6.5227  |
| gtyyau-H2O    | 607.1423 | C21H27O10N7S2 | 608.1501 | 608.2 | 0.0499 | 6.5227  |
| gggyyA-H2O    | 607.2050 | C23H31O14N5   | 608.2128 | 608.2 | 0.0128 | 6.5227  |
| gggytA-H2O    | 607.1498 | C22H27O13N5S1 | 608.1576 | 608.2 | 0.0424 | 6.5227  |

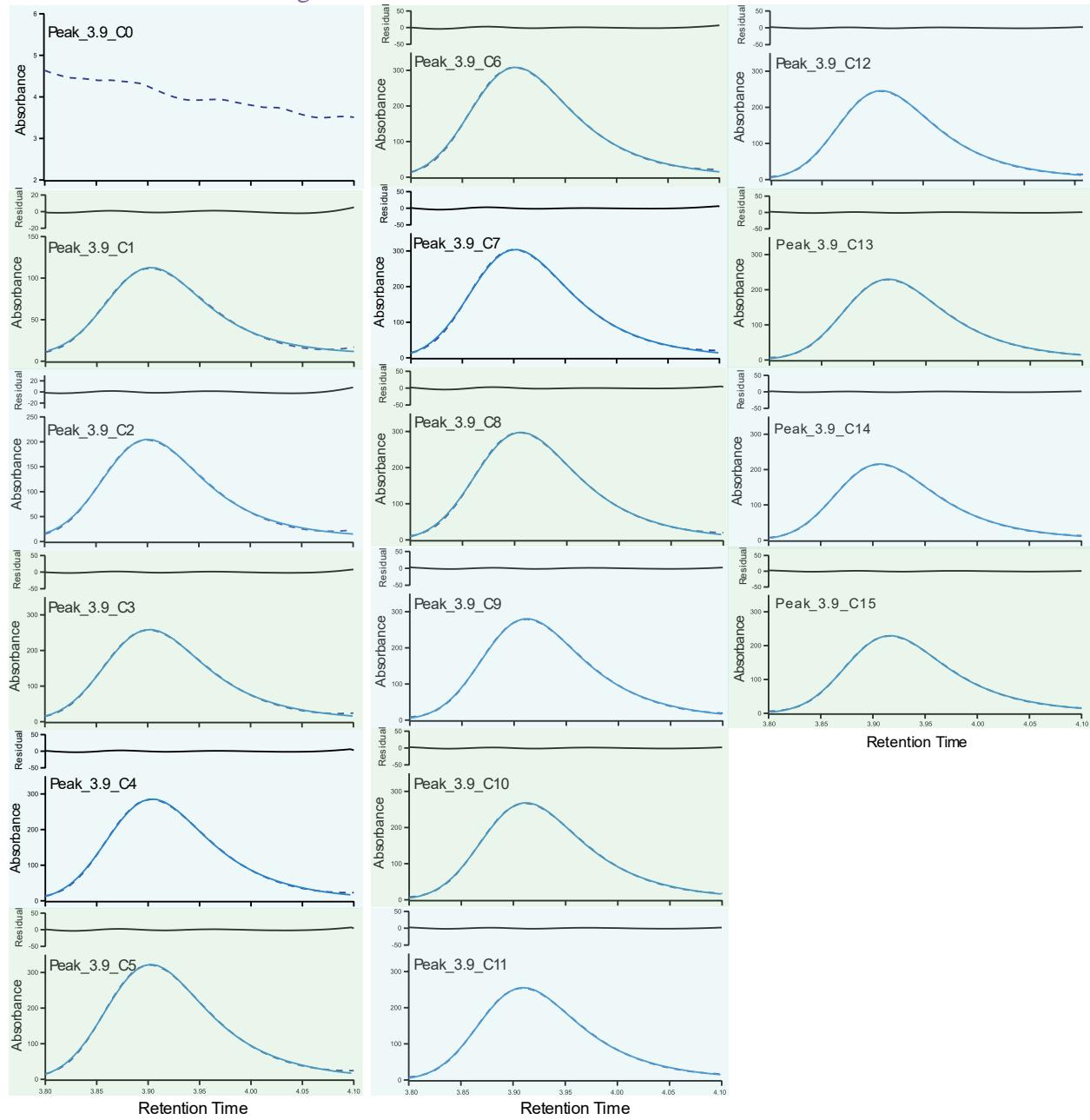
|              |          |               |          |       |        |        |
|--------------|----------|---------------|----------|-------|--------|--------|
| GGtld        | 607.2287 | C24H40O11N2S2 | 608.2365 | 608.2 | 0.0365 | 6.5227 |
| gtyylun-H2O  | 607.1984 | C22H31O11N7S1 | 608.2062 | 608.2 | 0.0062 | 6.5227 |
| gttylun-H2O  | 607.1432 | C21H27O10N7S2 | 608.1510 | 608.2 | 0.0490 | 6.5227 |
| gggyyln-H2O  | 607.2059 | C23H31O14N5   | 608.2137 | 608.2 | 0.0137 | 6.5227 |
| gggtyln-H2O  | 607.1507 | C22H27O13N5S1 | 608.1585 | 608.2 | 0.0415 | 6.5227 |
| Gggyyylu-H2O | 607.2369 | C22H37O16N3   | 608.2447 | 608.2 | 0.0447 | 6.5227 |
| Gggtyylu-H2O | 607.1817 | C21H33O15N3S1 | 608.1895 | 608.2 | 0.0105 | 6.5227 |
| Gggggyyl-H2O | 607.1892 | C22H33O18N1   | 608.1970 | 608.2 | 0.0030 | 6.5227 |
| GGgttyyn     | 607.1946 | C22H33O11N7S1 | 608.2024 | 608.2 | 0.0024 | 6.5227 |
| ylddu-H2O    | 607.3429 | C26H46O13N2   | 608.3507 | 608.3 | 0.0507 | 6.3013 |
| tlldu-H2O    | 607.2877 | C25H42O12N2S1 | 608.2955 | 608.3 | 0.0045 | 6.3013 |
| gllld-H2-H2O | 607.2952 | C26H40O15     | 608.3030 | 608.3 | 0.0030 | 6.3013 |
| gyyyAu-H2O   | 607.2527 | C23H35O12N7   | 608.2605 | 608.3 | 0.0395 | 6.3013 |
| GGyyl        | 607.3391 | C26H48O13N2   | 608.3469 | 608.3 | 0.0469 | 6.3013 |
| GGtyld       | 607.2839 | C25H44O12N2S1 | 608.2917 | 608.3 | 0.0083 | 6.3013 |
| gyyylun-H2O  | 607.2536 | C23H35O12N7   | 608.2614 | 608.3 | 0.0386 | 6.3013 |
| GGgyyyyn     | 607.2498 | C23H37O12N7   | 608.2576 | 608.3 | 0.0424 | 6.3013 |
| GGGggdun-H2O | 607.2805 | C26H36O7N10   | 608.2883 | 608.3 | 0.0117 | 6.3013 |
| tttttyyn-H2O | 635.0243 | C21H25O8N5S5  | 636.0321 | 636.0 | 0.0321 | 7.4150 |
| tttld-H2     | 635.1335 | C24H36O11S4   | 636.1413 | 636.1 | 0.0413 | 8.5714 |
| Gttll        | 635.1222 | C20H31O15N1S3 | 636.1300 | 636.1 | 0.0300 | 8.5714 |
| tttyyyyn-H2O | 635.1347 | C23H33O10N5S3 | 636.1425 | 636.1 | 0.0425 | 8.5714 |
| tttyyyyn-H2O | 635.0795 | C22H29O90N5S4 | 636.0873 | 636.1 | 0.0127 | 8.5714 |
| gttynyyn-H2  | 635.0994 | C22H29O11N5S3 | 636.1072 | 636.1 | 0.0072 | 8.5714 |
| gttynyyn-H2  | 635.0442 | C21H25O10N5S4 | 636.0520 | 636.1 | 0.0480 | 8.5714 |
| tttyld-H2    | 635.1887 | C25H40O12S3   | 636.1965 | 636.2 | 0.0035 | 9.2151 |
| Gtyyll       | 635.2326 | C22H39O17N1S1 | 636.2404 | 636.2 | 0.0404 | 9.2151 |
| Gtjylland    | 635.1774 | C21H35O16N1S2 | 636.1852 | 636.2 | 0.0148 | 9.2151 |
| GgtAun-H2O   | 635.1898 | C23H25O7N13S1 | 636.1976 | 636.2 | 0.0024 | 9.2151 |
| GgggAn-H2O   | 635.1973 | C24H25O10N11  | 636.2051 | 636.2 | 0.0051 | 9.2151 |
| gggggAu      | 635.1748 | C22H27O15N7   | 636.1826 | 636.2 | 0.0174 | 9.2151 |
| GGggyAu-H2O  | 635.2283 | C23H31O12N9   | 636.2361 | 636.2 | 0.0361 | 9.2151 |
| GGggtAu-H2O  | 635.1731 | C22H27O11N9S1 | 636.1809 | 636.2 | 0.0191 | 9.2151 |

|              |          |               |          |       |        |        |
|--------------|----------|---------------|----------|-------|--------|--------|
| GGggggA-H2O  | 635.1806 | C23H27O14N7   | 636.1884 | 636.2 | 0.0116 | 9.2151 |
| ttyyyyyn-H2O | 635.1899 | C24H37O11N5S2 | 636.1977 | 636.2 | 0.0023 | 9.2151 |
| gttyyyyyn-H2 | 635.1546 | C23H33O12N5S2 | 636.1624 | 636.2 | 0.0376 | 9.2151 |
| ggggglun     | 635.1757 | C22H27O15N7   | 636.1835 | 636.2 | 0.0165 | 9.2151 |
| GGgylun-H2O  | 635.2292 | C23H31O12N9   | 636.2370 | 636.2 | 0.0370 | 9.2151 |
| GGggtlun-H2O | 635.1740 | C22H27O11N9S1 | 636.1818 | 636.2 | 0.0182 | 9.2151 |
| GGgggln-H2O  | 635.1815 | C23H27O14N7   | 636.1893 | 636.2 | 0.0107 | 9.2151 |
| GGGdA        | 635.3305 | C27H42O9N8    | 636.3383 | 636.3 | 0.0383 | 8.7273 |
| ttyyld-H2    | 635.2439 | C26H44O13S2   | 636.2517 | 636.3 | 0.0483 | 8.7273 |
| Gyyyll       | 635.2878 | C23H43O18N1   | 636.2956 | 636.3 | 0.0044 | 8.7273 |
| GgyAun-H2O   | 635.2450 | C24H29O8N13   | 636.2528 | 636.3 | 0.0472 | 8.7273 |
| GGGldn       | 635.3314 | C27H42O9N8    | 636.3392 | 636.3 | 0.0392 | 8.7273 |
| GGGGgld      | 635.3147 | C26H44O13N4   | 636.3225 | 636.3 | 0.0225 | 8.7273 |
| yyyyyyyn-H2O | 635.3003 | C26H45O13N5   | 636.3081 | 636.3 | 0.0081 | 8.7273 |
| tyyyyyyn-H2O | 635.2451 | C25H41O12N5S1 | 636.2529 | 636.3 | 0.0471 | 8.7273 |
| tttyldu      | 679.2251 | C26H44O12N2S3 | 680.2329 | 680.2 | 0.0329 | 7.0645 |
| tttldu       | 679.1699 | C25H40O11N2S4 | 680.1777 | 680.2 | 0.0223 | 7.0645 |
| ggttyld      | 679.2326 | C27H44O15S2   | 680.2404 | 680.2 | 0.0404 | 7.0645 |
| ggttld       | 679.1774 | C26H40O14S3   | 680.1852 | 680.2 | 0.0148 | 7.0645 |
| GGGtyll      | 679.2395 | C23H39O17N3S1 | 680.2473 | 680.2 | 0.0473 | 7.0645 |
| GGGtll       | 679.1843 | C22H35O16N3S2 | 680.1921 | 680.2 | 0.0079 | 7.0645 |
| ttyyldu      | 679.2803 | C27H48O13N2S2 | 680.2881 | 680.3 | 0.0119 | 6.2752 |
| ggttyld      | 679.2878 | C28H48O16S1   | 680.2956 | 680.3 | 0.0044 | 6.2752 |

## Fraction 7 (retention time = 3.9 min)

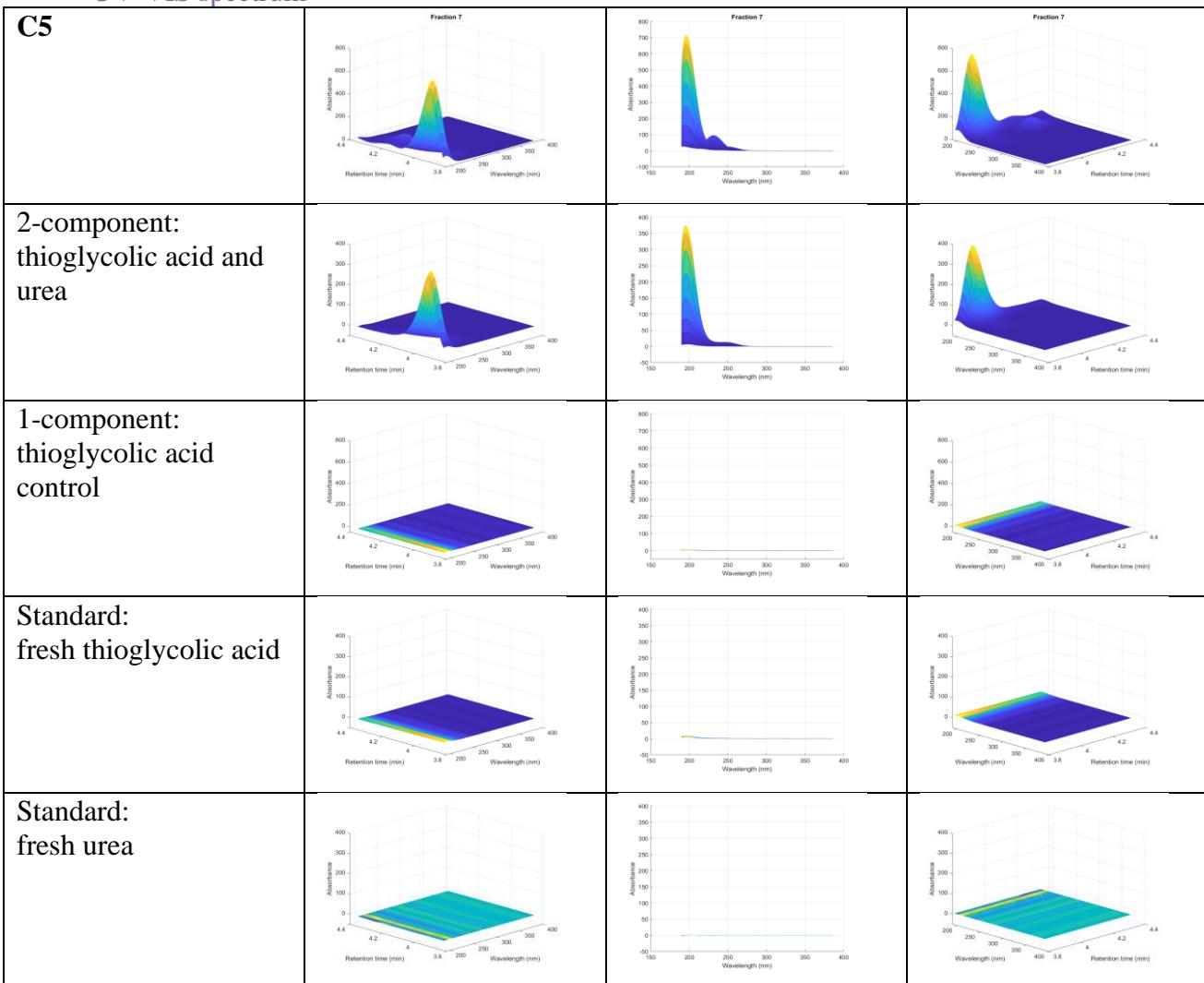
Fraction 7 is a product peak (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that this product is formed in cycle 1, reaches a maximum at cycle 5 and then decreases in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between this fraction of the 9-component system and a 2-component dry-down reaction involving thioglycolic acid and urea. MS analysis suggests that this fraction contains the heterodimer tu.

### HPLC Curve fitting



**Figure S17. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 7 which has a retention time of about 3.9 minutes.

### UV-VIS spectrum



**Figure S18. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 7 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula    | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3     | 91.0400           | 91.0              | 0.0400     | 95.5253  |
| t        | 91.9926      | C2H4O2S1   | 90.9848           | 91.0              | 0.0152     | 95.5253  |
| yu       | 134.0696     | C4H10O3N2  | 133.0618          | 133.1             | 0.0382     | 5.6846   |
| tu       | 134.0144     | C3H6O2N2S1 | 133.0066          | 133.0             | 0.0066     | 5.7950   |
| gl       | 244.0894     | C8H14O8    | 243.0816          | 243.1             | 0.0184     | 5.3376   |

|     |          |              |          |       |        |         |
|-----|----------|--------------|----------|-------|--------|---------|
| gg  | 134.0219 | C4H6O5       | 133.0141 | 133.0 | 0.0141 | 5.7950  |
| gyd | 305.1923 | C15H28O6     | 304.1845 | 304.5 | 0.3155 | 6.5354  |
| gtd | 305.1371 | C14H24O5S1   | 304.1293 | 304.5 | 0.3707 | 6.5354  |
| ggu | 176.0437 | C5H8O5N2     | 175.0359 | 175.0 | 0.0359 | 34.6257 |
| Gyd | 306.2087 | C15H29O5N1   | 305.2009 | 305.2 | 0.0009 | 8.3006  |
| Gtd | 306.1535 | C14H25O4N1S1 | 305.1457 | 305.1 | 0.0457 | 10.4599 |

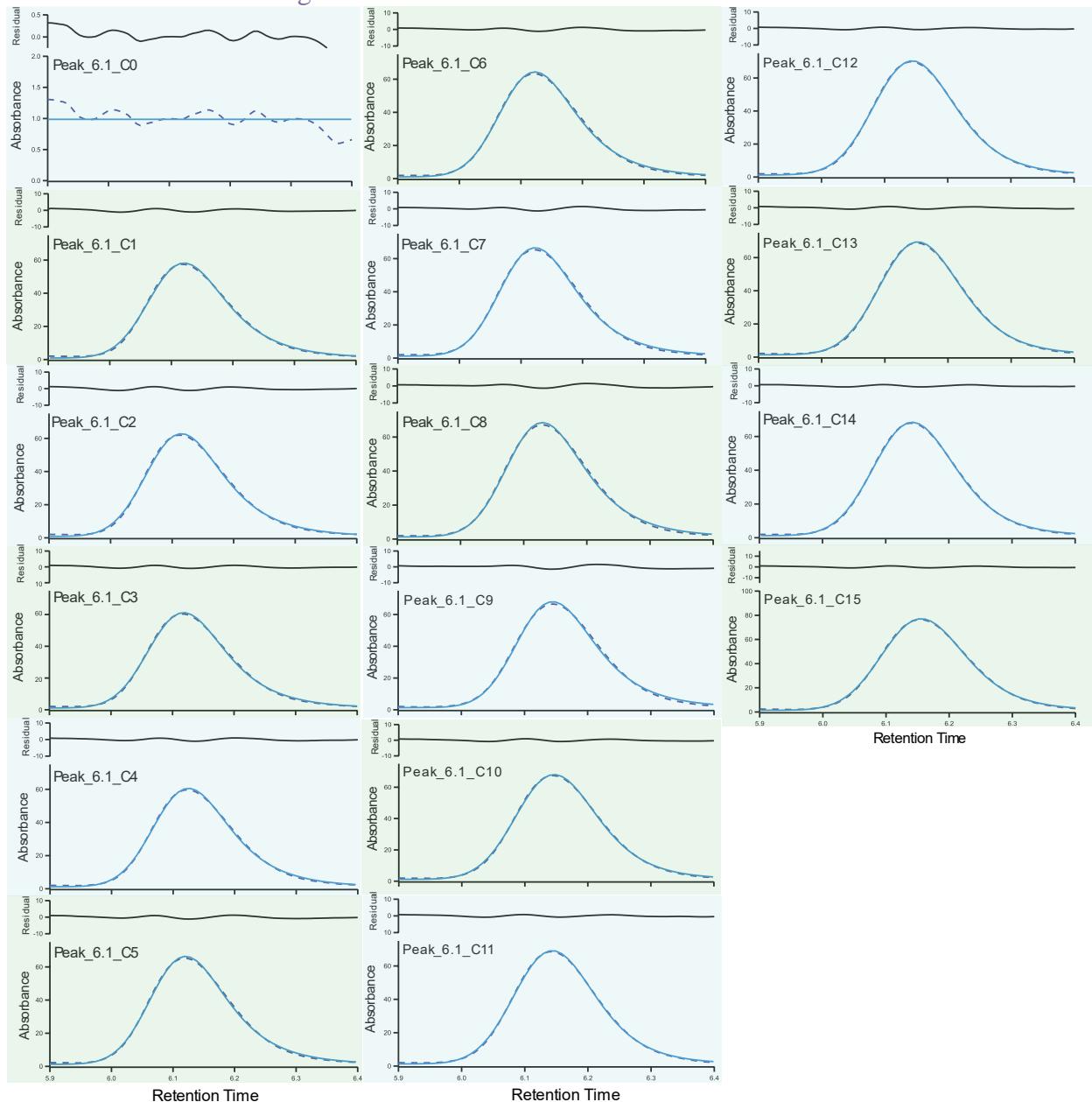
### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 23.0995  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 8.5621   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 11.0918  |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 11.0918  |
| yl-H2O   | 242.1091     | C9H16O7      | 243.1169          | 243.1             | 0.0169     | 5.1311   |
| tl-H2O   | 242.0539     | C8H12O6S1    | 243.0617          | 243.1             | 0.0383     | 5.1311   |
| ttyyy-H2 | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 6.5697   |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 6.5697   |
| GGGGgy   | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 6.5697   |
| GGGGgt   | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 6.5697   |
| GGGyn    | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 5.7961   |
| gtyl     | 392.1066     | C13H22O11S1  | 393.1144          | 393.1             | 0.0144     | 7.4065   |
| gttl     | 392.0514     | C12H18O10S2  | 393.0592          | 393.1             | 0.0408     | 7.4065   |
| gyyl     | 392.1618     | C14H26O12    | 393.1696          | 393.2             | 0.0304     | 7.4352   |
| GGGdu    | 392.2364     | C17H31O5N5   | 393.2442          | 393.2             | 0.0442     | 7.4352   |

### Fraction 8 (retention time = 6.1 min)

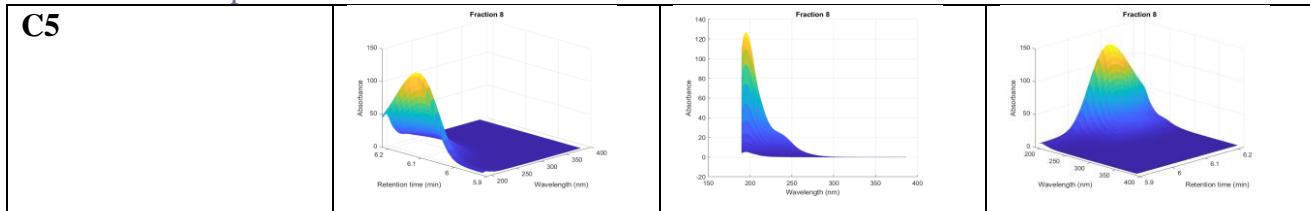
Fraction 8 is a new product peak (not found in the non-reacted mixture of MFP\_set 3). The HPLC curve fitting indicates that this product is formed in cycle 1 and slowly increases in abundance over cycles. Comparison of the 9-component system to a series of 2-component dry-down reactions indicates UV-Vis absorbance spectrum similarities between the 9-component system to a 2-component dry-down reaction involving thioglycolic acid and glycerol. Indeed, MS analysis suggests that this fraction contains the heterodimer ty.

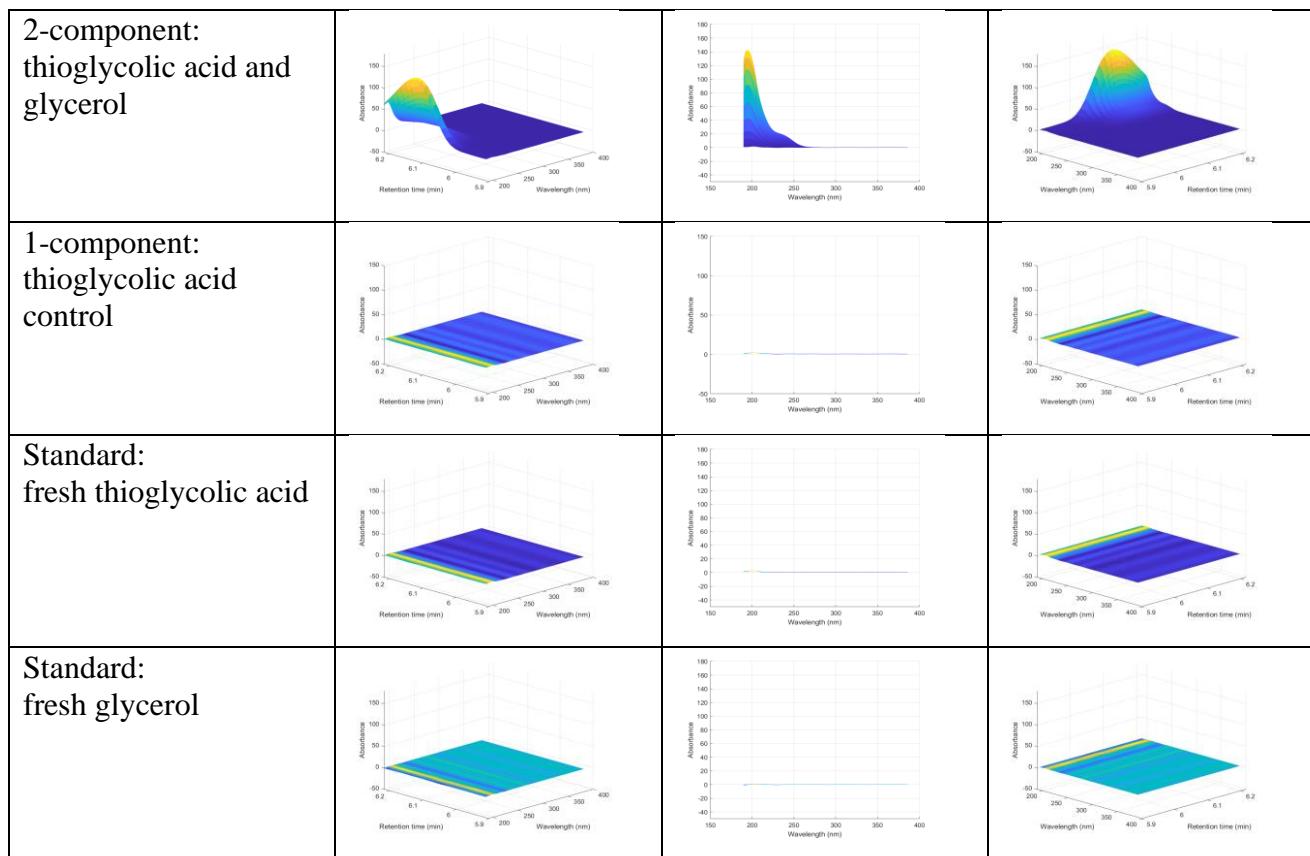
### HPLC Curve fitting



**Figure S19. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 8 which has a retention time of about 6.1 minutes.

### UV-VIS spectrum





**Figure S20. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 8 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3       | 91.0400           | 91.0              | 0.0400     | 83.6464  |
| t        | 91.9926      | C2H4O2S1     | 90.9848           | 91.0              | 0.0152     | 83.6464  |
| yy       | 166.0845     | C6H14O5      | 165.0767          | 165.1             | 0.0233     | 15.2167  |
| ty       | 166.0293     | C5H10O4S1    | 165.0215          | 165.0             | 0.0215     | 15.1511  |
| tt       | 165.9741     | C4H6O3S2     | 164.9663          | 165.0             | 0.0337     | 15.1511  |
| ggu      | 176.0437     | C5H8O5N2     | 175.0359          | 175.0             | 0.0359     | 30.2499  |
| Gtd      | 306.1535     | C14H25O4N1S1 | 305.1457          | 305.1             | 0.0457     | 8.1942   |

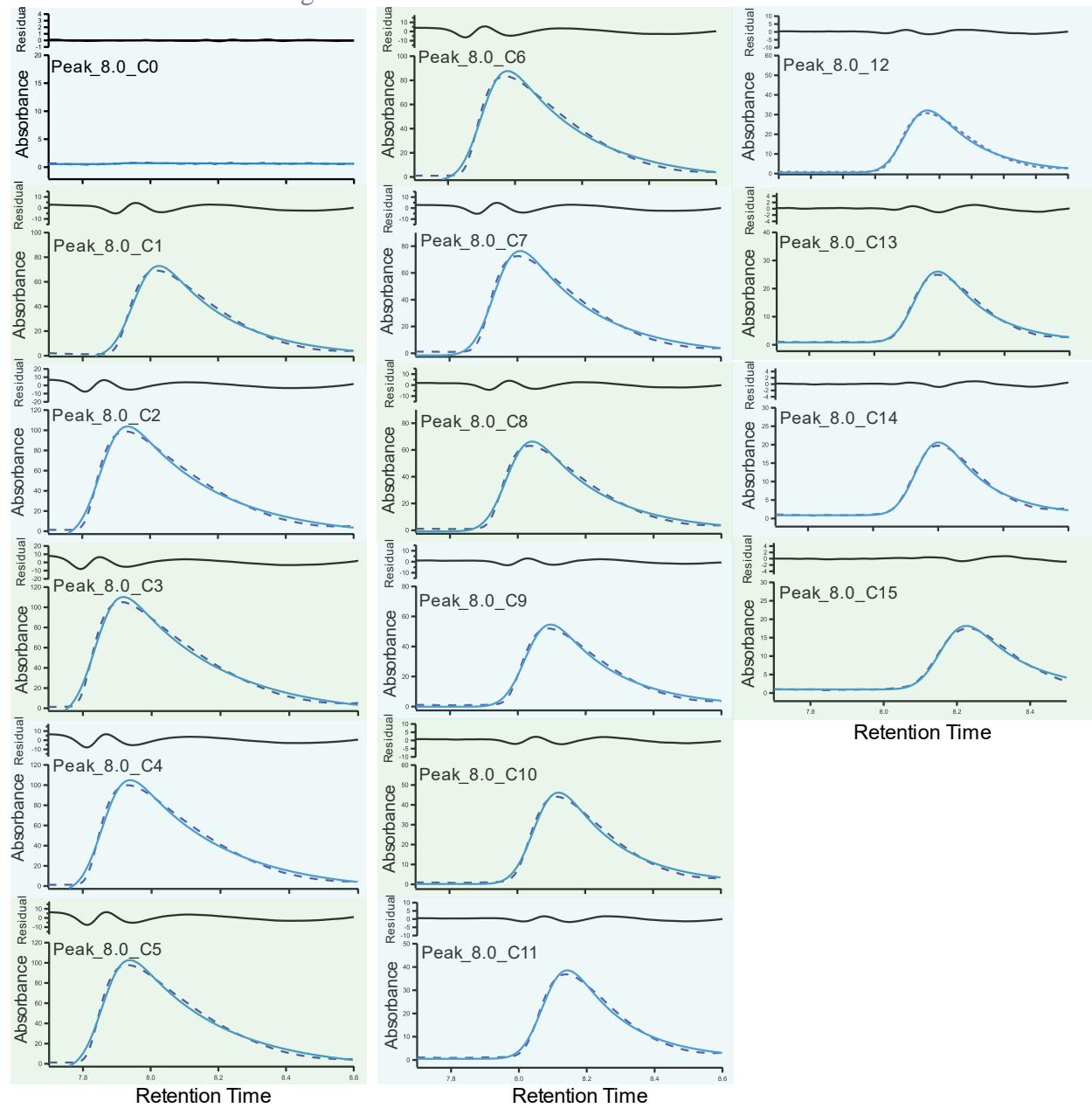
**HPLC MS – positive mode**

| Sequence | Neutral Mass | Formula       | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|---------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5       | 167.0913          | 167.1             | 0.0087     | 28.9903  |
| gyu-H2O  | 174.0634     | C6H10O4N2     | 175.0712          | 175.1             | 0.0288     | 10.1347  |
| yn-H2O   | 191.0801     | C8H9O1N5      | 192.0879          | 192.1             | 0.0121     | 12.1337  |
| Ggy-H2O  | 191.0634     | C7H11O5N1     | 192.0712          | 192.1             | 0.0288     | 12.1337  |
| Gyn-H2O  | 250.1019     | C10H12O2N6    | 251.1097          | 251.1             | 0.0097     | 5.0942   |
| ggyu     | 250.0794     | C8H14O7N2     | 251.0872          | 251.1             | 0.0128     | 5.0942   |
| GGgy-H2O | 250.0852     | C9H14O6N2     | 251.0930          | 251.1             | 0.0070     | 5.0942   |
| Gtyl-H2O | 375.1124     | C13H21O90N1S1 | 376.1202          | 376.1             | 0.0202     | 5.5348   |
| Gttl-H2O | 375.0572     | C12H17O8N1S2  | 376.0650          | 376.1             | 0.0350     | 5.5348   |
| Gyyl-H2O | 375.1676     | C14H25O10N1   | 376.1754          | 376.2             | 0.0246     | 5.1424   |
| ttyyy-H2 | 386.0686     | C13H22O9S2    | 387.0764          | 387.1             | 0.0236     | 6.7931   |
| GGGtn    | 386.1009     | C13H16O4N8S1  | 387.1087          | 387.1             | 0.0087     | 6.7931   |
| GGGGgy   | 386.1394     | C13H22O9N4    | 387.1472          | 387.1             | 0.0472     | 6.7931   |
| GGGGgt   | 386.0842     | C12H18O8N4S1  | 387.0920          | 387.1             | 0.0080     | 6.7931   |
| GGGyn    | 386.1561     | C14H20O5N8    | 387.1639          | 387.2             | 0.0361     | 5.6852   |
| gtyl     | 392.1066     | C13H22O11S1   | 393.1144          | 393.1             | 0.0144     | 17.3040  |
| gttl     | 392.0514     | C12H18O10S2   | 393.0592          | 393.1             | 0.0408     | 17.3040  |
| gyyl     | 392.1618     | C14H26O12     | 393.1696          | 393.2             | 0.0304     | 17.9074  |
| GGGdu    | 392.2364     | C17H31O5N5    | 393.2442          | 393.2             | 0.0442     | 17.9074  |
| Gyyl     | 393.1782     | C14H27O11N1   | 394.1860          | 394.2             | 0.0140     | 5.0824   |

## Fraction 9 (retention time = 8.0 min)

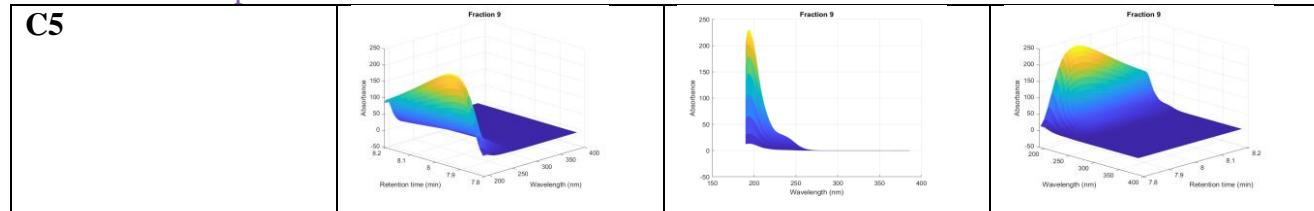
Fraction 9 is a product peak (not found in the non-reacted mixture of MFP\_set 3). HPLC curve fitting indicates that this product is formed in cycle 1, reaches a maximum in cycle 3, and then slowly decreases in abundance over cycles. Comparison of the 9-component system to a series of 2-component dry-down reactions indicates UV-Vis absorbance spectrum similarities between the 9-component system and a 2-component dry-down reaction involving thioglycolic acid and glycolic acid. MS analysis suggests that this fraction contains the heterodimer of thioglycolic acid.

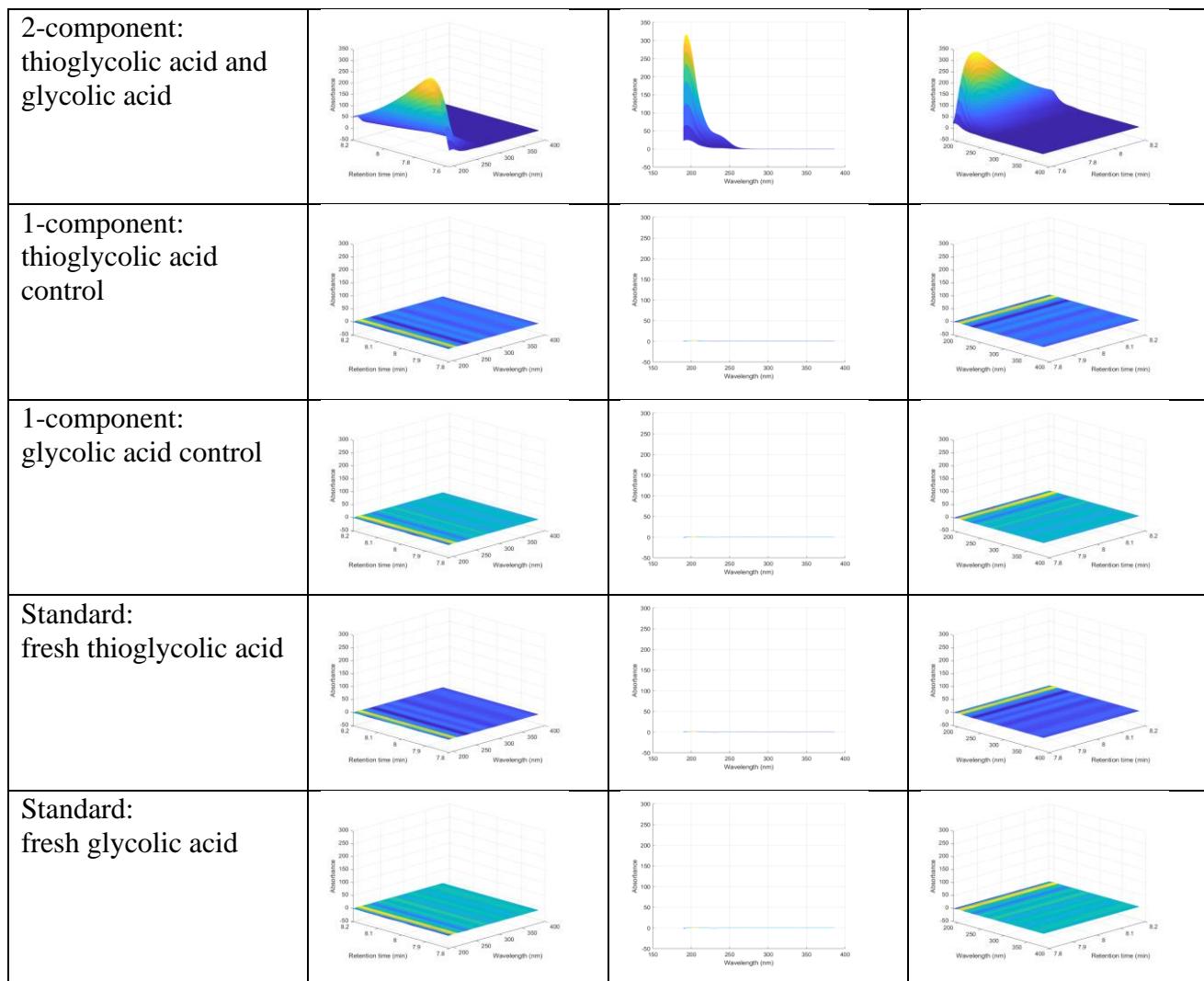
### HPLC Curve fitting



**Figure S21. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 9 which has a retention time of about 8.0 minutes.

### UV-VIS spectrum





**Figure S22. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 9 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula  | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|----------|-------------------|-------------------|------------|----------|
| t        | 91.9926      | C2H4O2S1 | 90.9848           | 91.0              | 0.0152     | 70.8018  |
| y        | 92.0478      | C3H8O3   | 91.0400           | 91.0              | 0.0400     | 70.8018  |
| gt       | 149.9980     | C4H6O4S1 | 148.9902          | 149.0             | 0.0098     | 80.8003  |
| gy       | 150.0532     | C5H10O5  | 149.0454          | 149.0             | 0.0454     | 80.8003  |
| ggu      | 176.0437     | C5H8O5N2 | 175.0359          | 175.0             | 0.0359     | 18.5163  |

|          |          |               |          |       |        |         |
|----------|----------|---------------|----------|-------|--------|---------|
| lu       | 228.1058 | C7H14O6N2     | 227.0980 | 227.1 | 0.0020 | 6.9568  |
| gggu     | 234.0491 | C7H10O7N2     | 233.0413 | 233.0 | 0.0413 | 10.0080 |
| Gtd      | 306.1535 | C14H25O4N1S1  | 305.1457 | 305.0 | 0.1457 | 5.2113  |
| gttyu-H2 | 338.0234 | C10H14O7N2S2  | 337.0156 | 337.0 | 0.0156 | 8.8038  |
| gggtt-H2 | 337.9757 | C10H10O9S2    | 336.9679 | 337.0 | 0.0321 | 8.8038  |
| gttu-H2  | 337.9682 | C9H10O6N2S3   | 336.9604 | 337.0 | 0.0396 | 8.8038  |
| Ggtd     | 364.1589 | C16H27O6N1S1  | 363.1511 | 363.0 | 0.1511 | 5.7333  |
| tdn      | 364.1756 | C17H25O2N5S1  | 363.1678 | 363.0 | 0.1678 | 5.7333  |
| Ggyd     | 364.2141 | C17H31O7N1    | 363.2063 | 363.0 | 0.2063 | 5.7333  |
| ydn      | 364.2308 | C18H29O3N5    | 363.2230 | 363.0 | 0.2230 | 5.7333  |
| gttttu   | 487.9458 | C13H16O8N2S5  | 486.9380 | 486.9 | 0.0380 | 7.1076  |
| gggttt   | 487.9533 | C14H16O11S4   | 486.9455 | 486.9 | 0.0455 | 7.1076  |
| gggtty   | 488.0085 | C15H20O12S3   | 487.0007 | 487.0 | 0.0007 | 6.6409  |
| gtttxyu  | 488.0010 | C14H20O9N2S4  | 486.9932 | 487.0 | 0.0068 | 6.6409  |
| gtttxyu  | 488.0562 | C15H24O10N2S3 | 487.0484 | 487.0 | 0.0484 | 6.6409  |
| gggttyy  | 488.0637 | C16H24O13S2   | 487.0559 | 487.1 | 0.0441 | 5.1554  |

### HPLC MS – positive mode

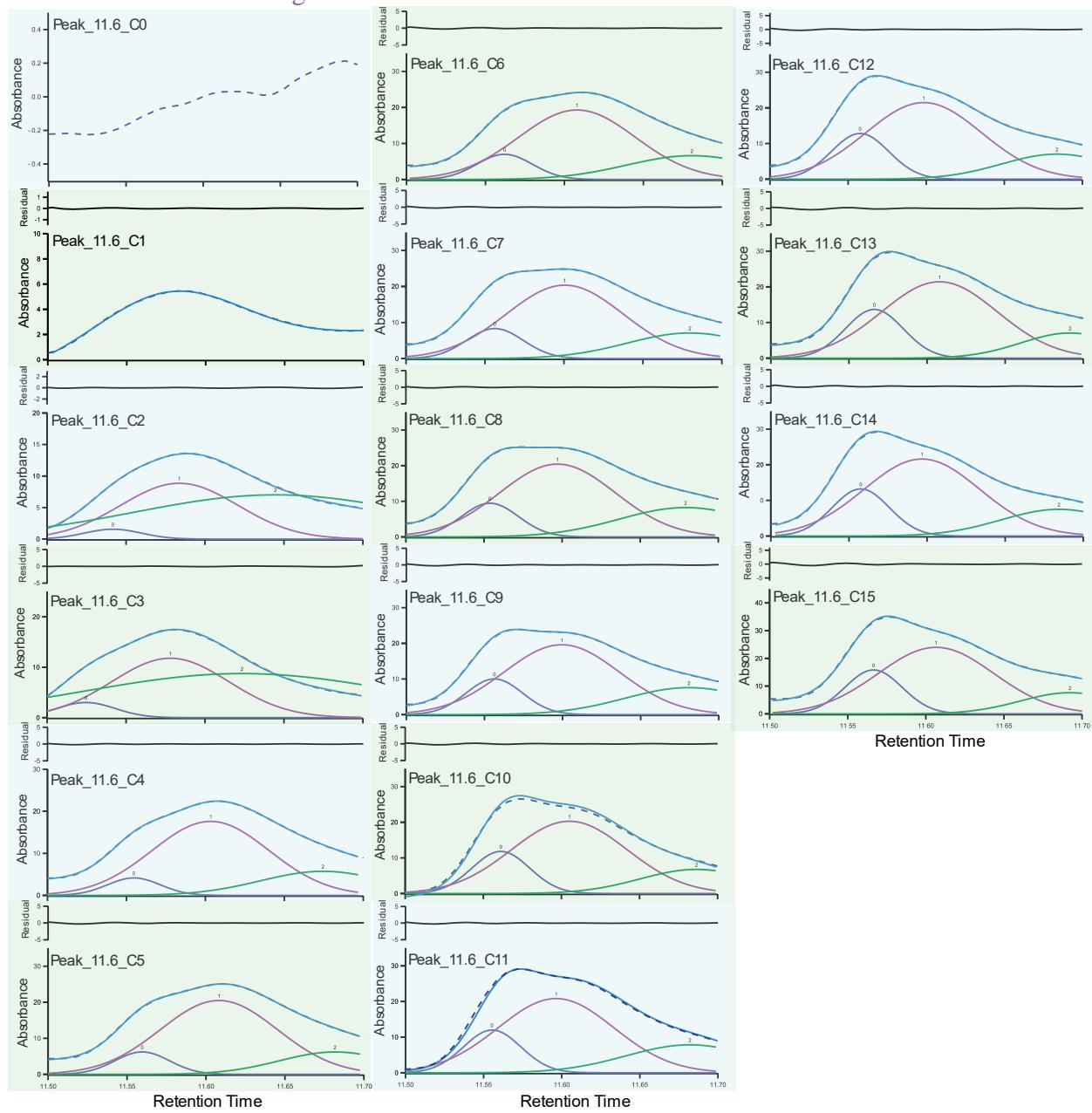
| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 23.0610  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 7.4159   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 9.7334   |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 9.7334   |
| td-H2O   | 229.1201     | C12H20O2S1   | 230.1279          | 230.1             | 0.0279     | 6.7673   |
| yd-H2O   | 229.1753     | C13H24O3     | 230.1831          | 230.2             | 0.0169     | 5.8013   |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 8.1473   |
| GGGGgy   | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 8.1473   |
| GGGGgt   | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 8.1473   |
| GGGyn    | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 7.3721   |

## Fraction 10 (retention time = 11.6 and 11.9 min)

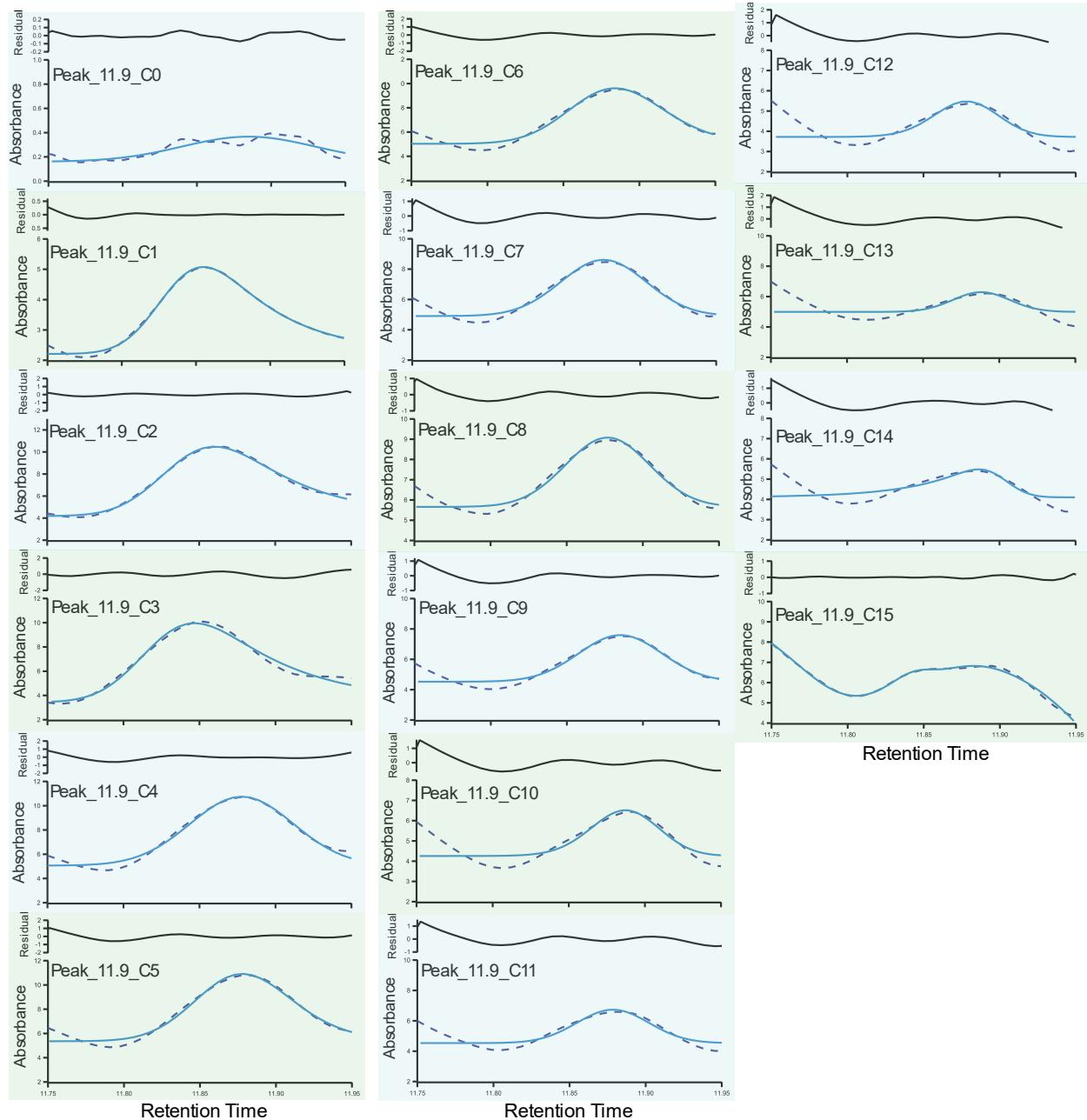
Fraction 10 contains product peaks (not found in the non-reacted mixture of MFP\_set 3). The HPLC peaks appear to contain a variety products. Comparison of the 9-component system to a series of 2-component dry-down reactions indicates that these peaks are not a result of any of the possible 2-component mixtures, suggesting at least a tertiary component source (such as Gtd, which is consistent with the MS analysis).

|    |                 |  |   |
|----|-----------------|--|---|
| 10 | 11.2723-11.9790 | peak_11.6a,<br>peak_11.6b,<br>peak_11.6c,<br>peak_11.9 | Group D<br>Group C<br>Others<br>Group B |
|----|-----------------|--|---|

### HPLC curve fitting



**Figure S23. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 10 which has a retention time of about 11.6 minutes.



**Figure S24. Curve fitting.** Curve fitting of HPLC data for cycle0 through 15 of fraction 10 which has a retention time of about 11.9 minutes.

### UV-VIS spectrum

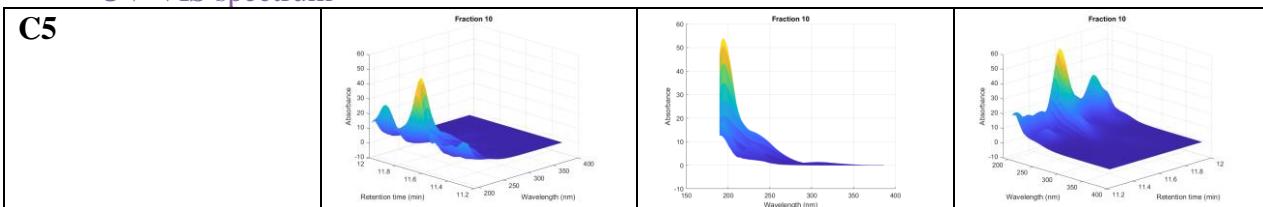


Figure S25. UV-Vis absorbance. UV-vis absorbance spectra of fraction 10.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| ggu      | 176.0437     | C5H8O5N2     | 175.0359          | 175.0             | 0.0359     | 25.8490  |
| Gtd      | 306.1535     | C14H25O4N1S1 | 305.1457          | 305.1             | 0.0457     | 9.2879   |

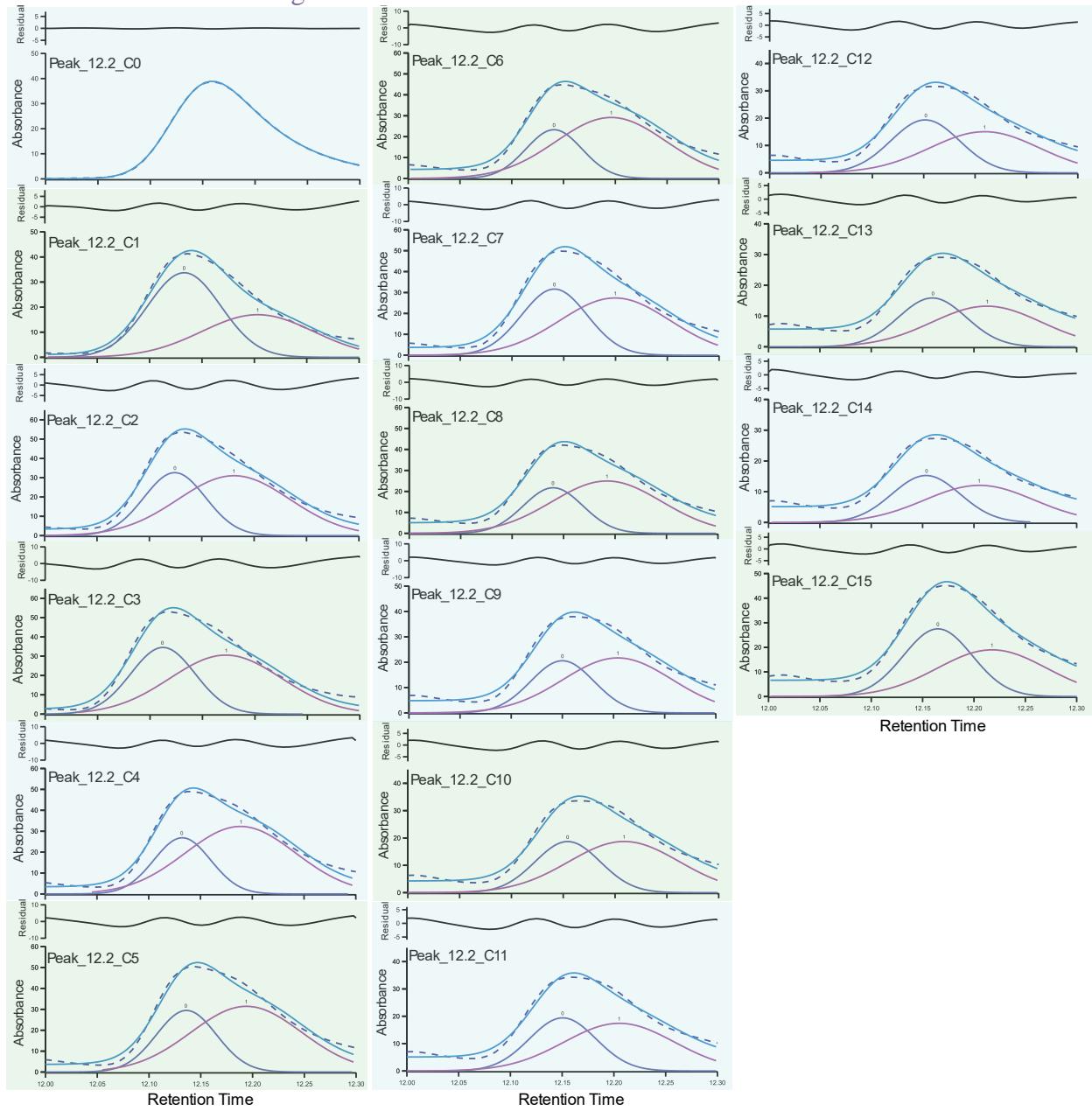
#### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 28.0419  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 9.6303   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 9.2050   |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 9.2050   |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 6.2604   |
| GGGGgy   | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 6.2604   |
| GGGGgt   | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 6.2604   |
| GGGyn    | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 5.8260   |

## Fraction 11(retention time = 12.2 min)

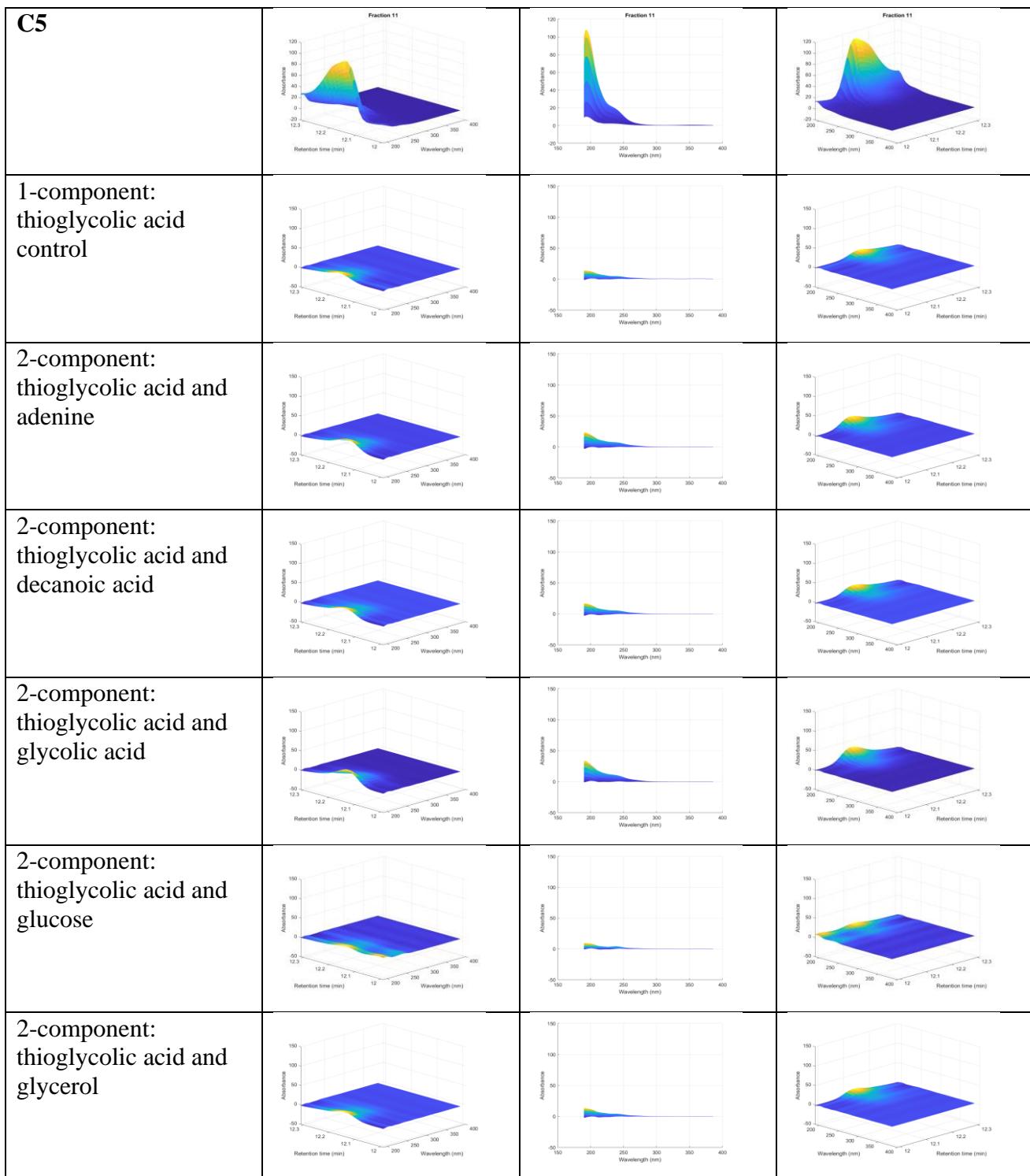
Fraction 11 is a collection of two product peaks, one of which is found in fresh MFP\_set 3. The HPLC curve fitting suggests that there are two product peaks in this region: the first initial peak is an oxidized dimer form of tg (tg-S-S-tg), already found in the fresh stock, which reaches a maxima in cycle 3 and then slowly decreases in abundance in subsequent cycles. The second product peak is not found in the fresh sample and a comparison of the 9-component system to a series of 2-component dry-down reactions indicates UV-Vis absorbance spectrum similarities between the 9-component system and a 2-component dry-down reaction involving thioglycolic acid and glycerol. MS analysis suggests that this fraction contains the heterodimer ty.

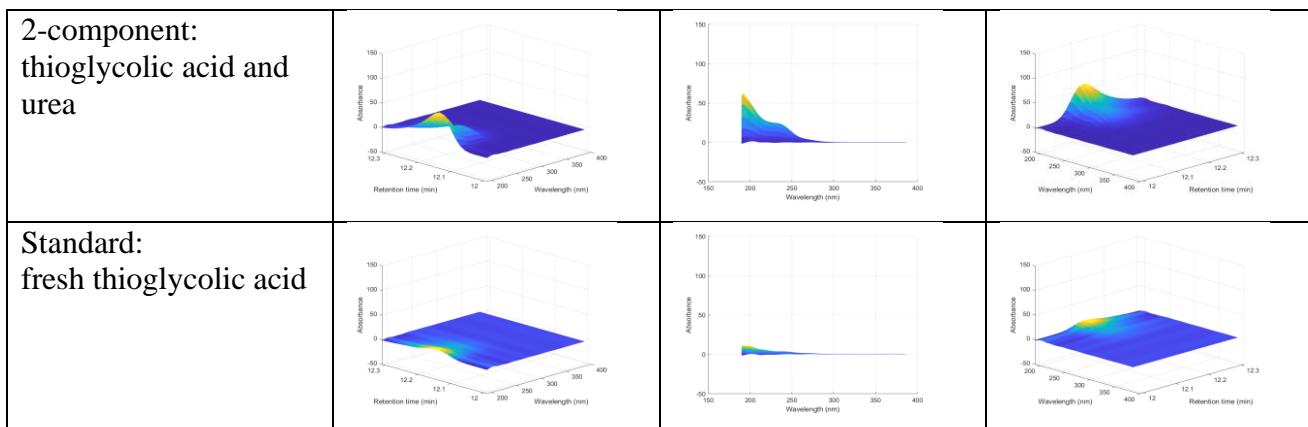
### HPLC curve fitting



**Figure S26. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 11 which has a retention time of about 12.2 minutes.

### UV-VIS spectrum

**C5**



**Figure S27. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 11 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3    | 91.0400           | 91.0              | 0.0400     | 63.3512  |
| t        | 91.9926      | C2H4O2S1  | 90.9848           | 91.0              | 0.0152     | 63.3512  |
| gyy      | 224.0899     | C8H16O7   | 223.0821          | 223.1             | 0.0179     | 13.2730  |
| gty      | 224.0347     | C7H12O6S1 | 223.0269          | 223.0             | 0.0269     | 13.4294  |
| gtt      | 223.9795     | C6H8O5S2  | 222.9717          | 223.0             | 0.0283     | 13.4294  |
| ggu      | 176.0437     | C5H8O5N2  | 175.0359          | 175.0             | 0.0359     | 19.5541  |

#### HPLC MS – positive mode

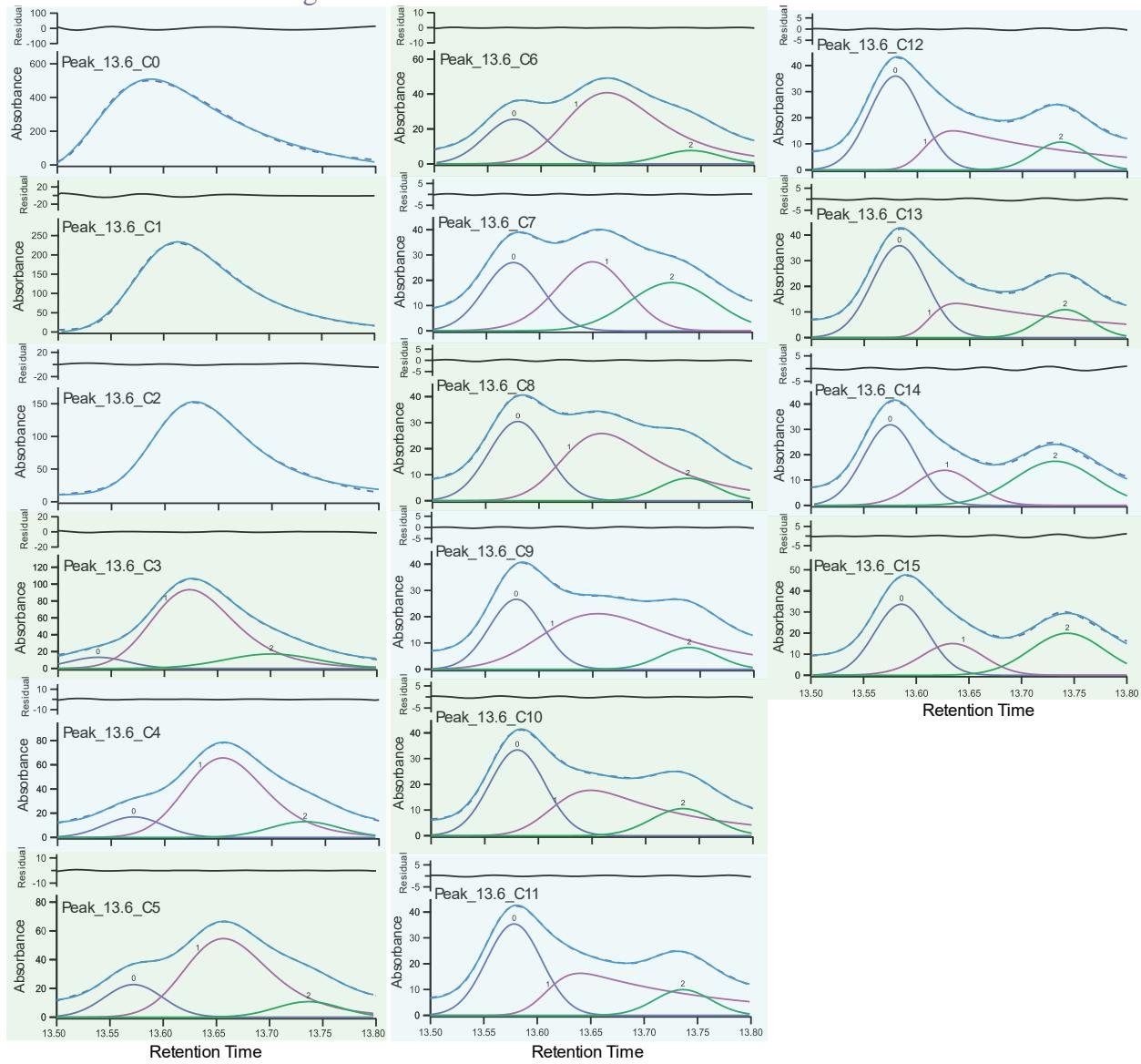
| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 30.5419  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 9.2500   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 10.2523  |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 10.2523  |
| ttyy-H2  | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 6.4523   |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 6.4523   |
| GGGGgy   | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 6.4523   |
| GGGGgt   | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 6.4523   |
| GGGyn    | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 5.3962   |

|       |          |             |          |       |        |        |
|-------|----------|-------------|----------|-------|--------|--------|
| gtyl  | 392.1066 | C13H22O11S1 | 393.1144 | 393.1 | 0.0144 | 8.8830 |
| gttl  | 392.0514 | C12H18O10S2 | 393.0592 | 393.1 | 0.0408 | 8.8830 |
| gyyl  | 392.1618 | C14H26O12   | 393.1696 | 393.2 | 0.0304 | 9.3011 |
| GGGdu | 392.2364 | C17H31O5N5  | 393.2442 | 393.2 | 0.0442 | 9.3011 |

## Fraction 12 (retention time = 13.6 min)

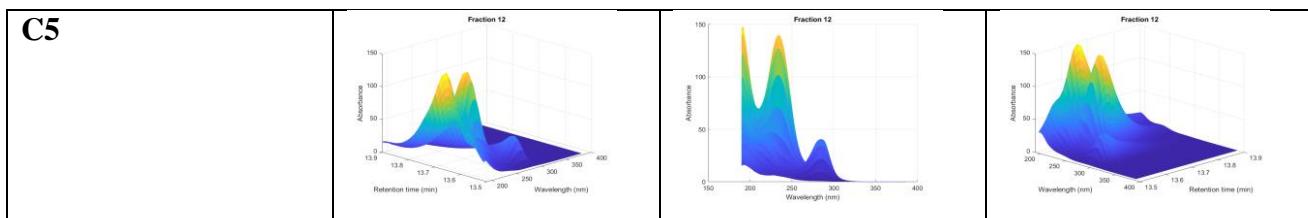
Fraction 12 is a collection of three main product peaks (two of which are not found in the fresh mixture of MFP\_set 3). LCMS analysis indicates that the first molecule located in this region is a thioester-linked homodimer of thioglycolic acid  $[(t)_2]$ . HPLC curve fitting indicates that  $(tg)_2$  is gradually being consumed over cycles. Another product in this region is found in cycle 1, reaches a maximum at cycle 6 and then decreases in subsequent cycles. A second product in this region is formed in cycle 8, reaches a maximum at cycle 12 and then decreases in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and the dry-down reaction involving thioglycolic acid and glucose. A corresponding mass was not identified in our MS analysis, possibly due to insufficient ionizable groups in the case of a co-oligomer between thioglycolic acid and glucose.

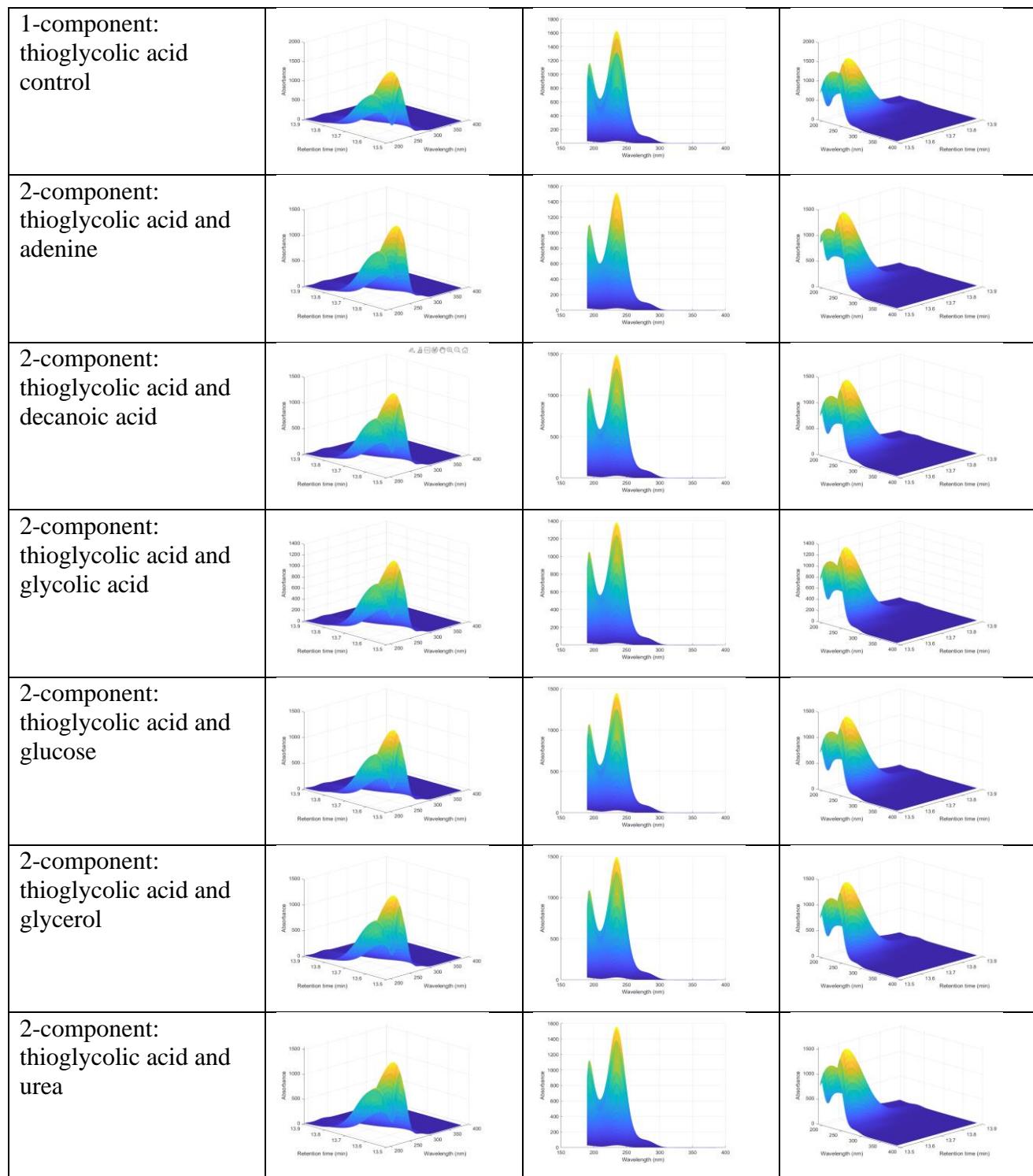
### HPLC curve fitting

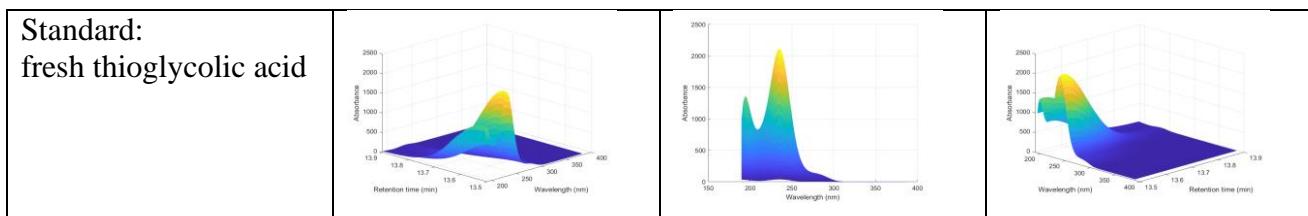


**Figure S28. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 12 which has a retention time of about 13.6 minutes.

### UV-VIS spectrum







**Figure S29. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 12 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula       | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|---------------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3        | 91.0400           | 91.0              | 0.0400     | 69.0775  |
| t        | 91.9926      | C2H4O2S1      | 90.9848           | 91.0              | 0.0152     | 69.0775  |
| yy       | 166.0845     | C6H14O5       | 165.0767          | 165.1             | 0.0233     | 7.9219   |
| ty       | 166.0293     | C5H10O4S1     | 165.0215          | 165.0             | 0.0215     | 7.9398   |
| tt       | 165.9741     | C4H6O3S2      | 164.9663          | 165.0             | 0.0337     | 7.9398   |
| ggu      | 176.0437     | C5H8O5N2      | 175.0359          | 175.0             | 0.0359     | 18.3293  |
| Gyd      | 306.2087     | C15H29O5N1    | 305.2009          | 305.1             | 0.1009     | 5.8485   |
| Gtd      | 306.1535     | C14H25O4N1S1  | 305.1457          | 305.1             | 0.0457     | 5.8485   |
| GGyyyy   | 432.2015     | C16H32O11N2   | 431.1937          | 431.2             | 0.0063     | 7.2561   |
| GGtyyy   | 432.1463     | C15H28O10N2S1 | 431.1385          | 431.1             | 0.0385     | 7.3027   |
| GGttyy   | 432.0911     | C14H24O9N2S2  | 431.0833          | 431.1             | 0.0167     | 7.3027   |
| GGttty   | 432.0359     | C13H20O8N2S3  | 431.0281          | 431.0             | 0.0281     | 6.7493   |
| GGtttt   | 431.9807     | C12H16O7N2S4  | 430.9729          | 431.0             | 0.0271     | 6.7493   |

#### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 32.9982  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 10.5979  |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 10.9537  |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 10.9537  |
| ttyyy-H2 | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 33.4232  |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 33.4232  |

|            |          |              |          |       |        |         |
|------------|----------|--------------|----------|-------|--------|---------|
| GGGGgy     | 386.1394 | C13H22O9N4   | 387.1472 | 387.1 | 0.0472 | 33.4232 |
| GGGGgt     | 386.0842 | C12H18O8N4S1 | 387.0920 | 387.1 | 0.0080 | 33.4232 |
| GAu-H2O    | 386.1590 | C14H18O5N8   | 387.1668 | 387.2 | 0.0332 | 30.6395 |
| Glun-H2O   | 386.1599 | C14H18O5N8   | 387.1677 | 387.2 | 0.0323 | 30.6395 |
| GGglu-H2O  | 386.1432 | C13H20O90N4  | 387.1510 | 387.2 | 0.0490 | 30.6395 |
| GGGyn      | 386.1561 | C14H20O5N8   | 387.1639 | 387.2 | 0.0361 | 30.6395 |
| GGGGGt     | 387.1006 | C12H19O7N5S1 | 388.1084 | 388.1 | 0.0084 | 8.4538  |
| ggydu-H2O  | 387.2079 | C18H30O7N2   | 388.2157 | 388.2 | 0.0157 | 7.4008  |
| ggtdu-H2O  | 387.1527 | C17H26O6N2S1 | 388.1605 | 388.2 | 0.0395 | 7.4008  |
| gggd-H2O   | 387.1602 | C18H26O9     | 388.1680 | 388.2 | 0.0320 | 7.4008  |
| GGGlu-H2O  | 387.1596 | C13H21O8N5   | 388.1674 | 388.2 | 0.0326 | 7.4008  |
| GGGGGy     | 387.1558 | C13H23O8N5   | 388.1636 | 388.2 | 0.0364 | 7.4008  |
| gtyl       | 392.1066 | C13H22O11S1  | 393.1144 | 393.1 | 0.0144 | 8.0143  |
| gttl       | 392.0514 | C12H18O10S2  | 393.0592 | 393.1 | 0.0408 | 8.0143  |
| Ggggun-H2O | 392.1032 | C14H14O6N8   | 393.1110 | 393.1 | 0.0110 | 8.0143  |
| GGgggu-H2O | 392.0865 | C13H16O10N4  | 393.0943 | 393.1 | 0.0057 | 8.0143  |
| gyyl       | 392.1618 | C14H26O12    | 393.1696 | 393.2 | 0.0304 | 8.5363  |
| GGGdu      | 392.2364 | C17H31O5N5   | 393.2442 | 393.2 | 0.0442 | 8.5363  |
| gttdu-H2O  | 403.1288 | C17H26O5N2S2 | 404.1366 | 404.1 | 0.0366 | 9.8236  |
| ggtd-H2O   | 403.1363 | C18H26O8S1   | 404.1441 | 404.1 | 0.0441 | 9.8236  |
| Ggglu      | 403.1374 | C13H21O11N3  | 404.1452 | 404.1 | 0.0452 | 9.8236  |
| gAu        | 403.1532 | C14H19O7N7   | 404.1610 | 404.2 | 0.0390 | 9.4708  |
| GGA-H2O    | 403.1590 | C15H19O6N7   | 404.1668 | 404.2 | 0.0332 | 9.4708  |
| glun       | 403.1541 | C14H19O7N7   | 404.1619 | 404.2 | 0.0381 | 9.4708  |
| GGln-H2O   | 403.1599 | C15H19O6N7   | 404.1677 | 404.2 | 0.0323 | 9.4708  |
| gyydu-H2O  | 403.2392 | C19H34O7N2   | 404.2470 | 404.2 | 0.0470 | 9.4708  |
| gtydu-H2O  | 403.1840 | C18H30O6N2S1 | 404.1918 | 404.2 | 0.0082 | 9.4708  |
| ggyyd-H2O  | 403.1915 | C19H30O9     | 404.1993 | 404.2 | 0.0007 | 9.4708  |
| GGGgl-H2O  | 403.1432 | C14H21O10N3  | 404.1510 | 404.2 | 0.0490 | 9.4708  |
| tyyl       | 408.1379 | C14H26O11S1  | 409.1457 | 409.1 | 0.0457 | 8.5415  |
| ttyl       | 408.0827 | C13H22O10S2  | 409.0905 | 409.1 | 0.0095 | 8.5415  |
| Gggyun-H2O | 408.1345 | C15H18O6N8   | 409.1423 | 409.1 | 0.0423 | 8.5415  |
| Gggtun-H2O | 408.0793 | C14H14O5N8S1 | 409.0871 | 409.1 | 0.0129 | 8.5415  |

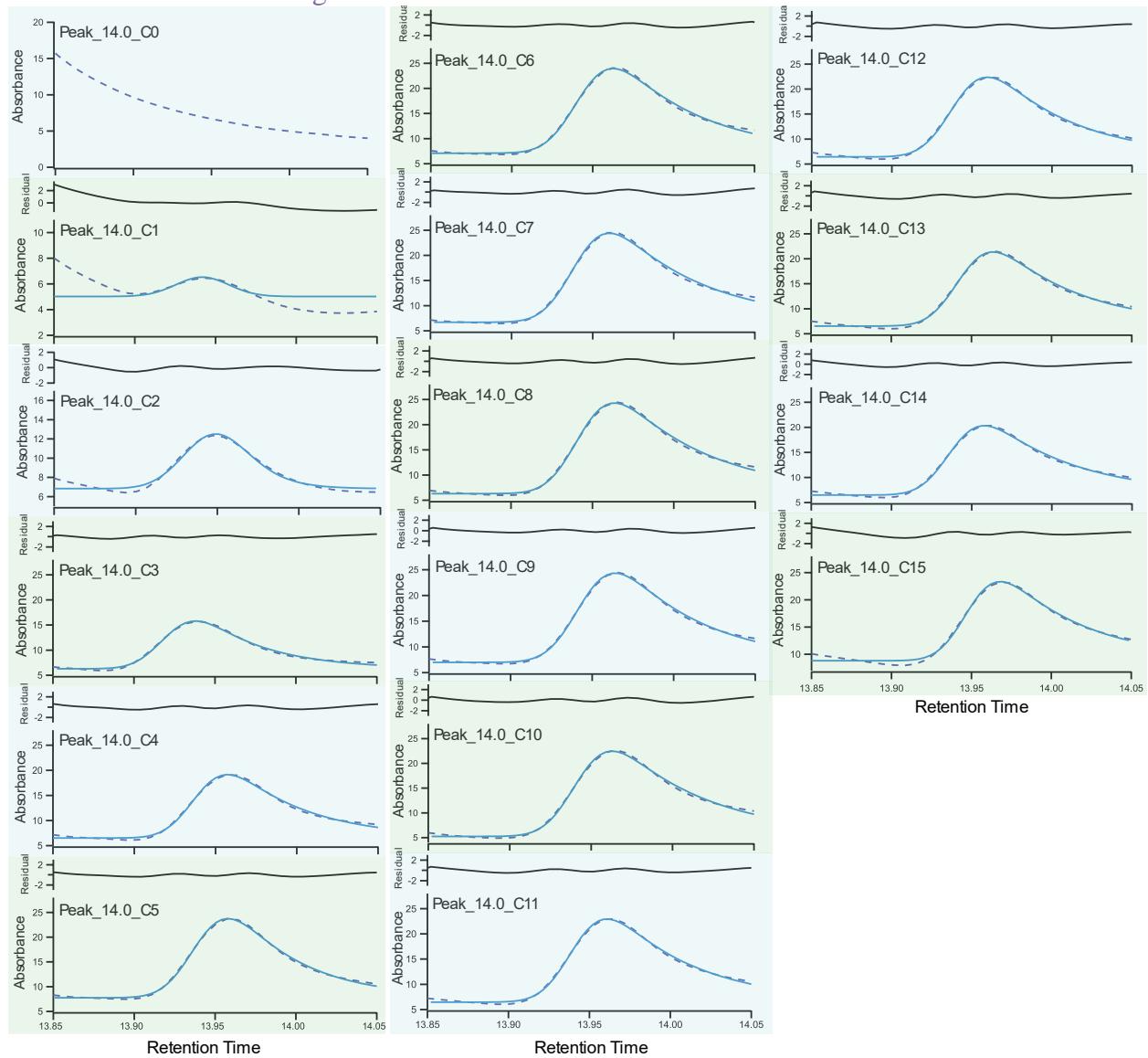
|             |          |               |          |       |        |        |
|-------------|----------|---------------|----------|-------|--------|--------|
| Ggggn-H2O   | 408.0868 | C15H14O8N6    | 409.0946 | 409.1 | 0.0054 | 8.5415 |
| gggggu      | 408.0643 | C13H16O13N2   | 409.0721 | 409.1 | 0.0279 | 8.5415 |
| GGgggyu-H2O | 408.1178 | C14H20O10N4   | 409.1256 | 409.1 | 0.0256 | 8.5415 |
| GGgggtu-H2O | 408.0626 | C13H16O90N4S1 | 409.0704 | 409.1 | 0.0296 | 8.5415 |
| GGggggg-H2O | 408.0701 | C14H16O12N2   | 409.0779 | 409.1 | 0.0221 | 8.5415 |
| yyyl        | 408.1931 | C15H30O12     | 409.2009 | 409.2 | 0.0009 | 7.5374 |
| GGdn        | 408.2367 | C19H29O3N7    | 409.2445 | 409.2 | 0.0445 | 7.5374 |
| GGGgd       | 408.2200 | C18H31O7N3    | 409.2278 | 409.2 | 0.0278 | 7.5374 |
| ttytn       | 431.0352 | C14H17O5N5S3  | 432.0430 | 432.0 | 0.0430 | 8.8956 |
| ttytn       | 431.0904 | C15H21O6N5S2  | 432.0982 | 432.1 | 0.0018 | 9.0255 |
| Ggtyyy      | 431.1289 | C15H27O11N1S1 | 432.1367 | 432.1 | 0.0367 | 9.0255 |
| Ggttyy      | 431.0737 | C14H23O10N1S2 | 432.0815 | 432.1 | 0.0185 | 9.0255 |
| yyyyn       | 431.2008 | C17H29O8N5    | 432.2086 | 432.2 | 0.0086 | 8.1603 |
| ttyyn       | 431.1456 | C16H25O7N5S1  | 432.1534 | 432.2 | 0.0466 | 8.1603 |
| Ggdun-H2O   | 431.2315 | C20H28O3N8    | 432.2393 | 432.2 | 0.0393 | 8.1603 |
| Ggyyyy      | 431.1841 | C16H31O12N1   | 432.1919 | 432.2 | 0.0081 | 8.1603 |
| GGggdu-H2O  | 431.2148 | C19H30O7N4    | 432.2226 | 432.2 | 0.0226 | 8.1603 |
| GGGGGGG     | 431.1627 | C14H23O8N7    | 432.1705 | 432.2 | 0.0295 | 8.1603 |
| Gtyyy       | 447.1050 | C15H27O10N1S2 | 448.1128 | 448.1 | 0.0128 | 5.9988 |
| Gtttyy      | 447.0498 | C14H23O9N1S3  | 448.0576 | 448.1 | 0.0424 | 5.9988 |
| Gtdun-H2O   | 447.2076 | C20H28O2N8S1  | 448.2154 | 448.2 | 0.0154 | 5.6502 |
| Gggdn-H2O   | 447.2151 | C21H28O5N6    | 448.2229 | 448.2 | 0.0229 | 5.6502 |
| ggggdu      | 447.1926 | C19H30O10N2   | 448.2004 | 448.2 | 0.0004 | 5.6502 |
| Gyyyyy      | 447.2154 | C17H35O12N1   | 448.2232 | 448.2 | 0.0232 | 5.6502 |
| Gtyyy       | 447.1602 | C16H31O11N1S1 | 448.1680 | 448.2 | 0.0320 | 5.6502 |
| GGgydu-H2O  | 447.2461 | C20H34O7N4    | 448.2539 | 448.2 | 0.0539 | 5.6502 |
| GGgtdu-H2O  | 447.1909 | C19H30O6N4S1  | 448.1987 | 448.2 | 0.0013 | 5.6502 |
| GGgggd-H2O  | 447.1984 | C20H30O90N2   | 448.2062 | 448.2 | 0.0062 | 5.6502 |
| tttdn       | 512.1376 | C21H29O4N5S3  | 513.1454 | 513.1 | 0.0454 | 6.5266 |
| Ggttd       | 512.1209 | C20H31O8N1S3  | 513.1287 | 513.1 | 0.0287 | 6.5266 |
| gllu        | 512.1885 | C17H28O15N2   | 513.1963 | 513.2 | 0.0037 | 5.6012 |
| Ggttyd      | 512.1761 | C21H35O9N1S2  | 513.1839 | 513.2 | 0.0161 | 5.6012 |



### Fraction 13 (retention time = 14 min)

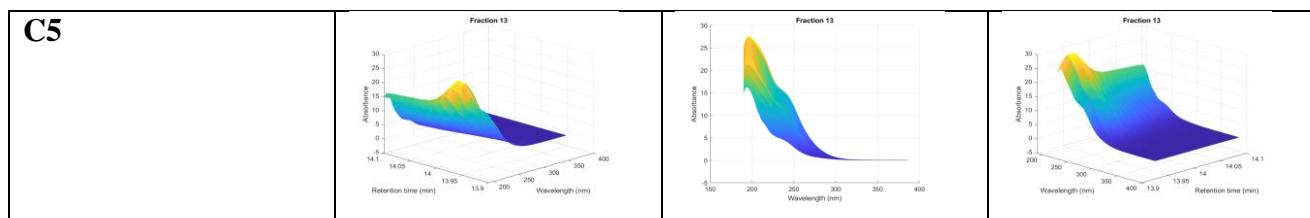
Fraction 13 is a product peak (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that a first product in this region is formed in cycle 1, reaches a maximum at cycle 7 and then decreases in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and the dry-down reaction involving thioglycolic acid and glucose. A corresponding mass was not identified in our MS analysis, possibly due to insufficient ionizable groups in the case of a co-oligomer between thioglycolic acid and glucose.

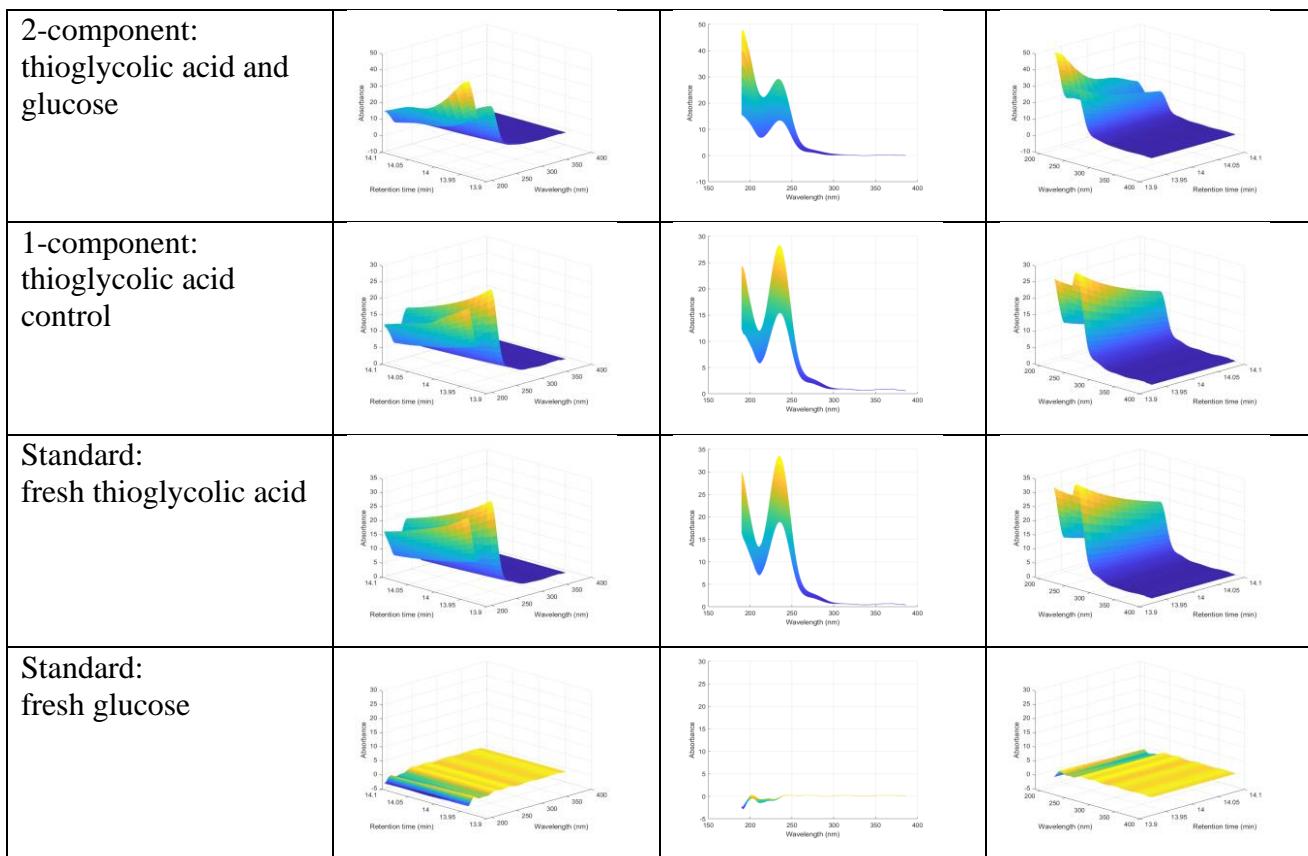
### HPLC Curve fitting



**Figure S30. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 13 which has a retention time of about 14.0 minutes.

### UV-VIS spectrum





**Figure S31. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 13 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula  | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|----------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3   | 91.0400           | 91.0              | 0.0400     | 34.7419  |
| t        | 91.9926      | C2H4O2S1 | 90.9848           | 91.0              | 0.0152     | 34.7419  |
| ggu      | 176.0437     | C5H8O5N2 | 175.0359          | 175.0             | 0.0359     | 18.1698  |

#### HPLC MS – positive mode

| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5   | 167.0913          | 167.1             | 0.0087     | 29.0915  |
| gyu-H2O  | 174.0634     | C6H10O4N2 | 175.0712          | 175.1             | 0.0288     | 10.0684  |
| yn-H2O   | 191.0801     | C8H9O1N5  | 192.0879          | 192.1             | 0.0121     | 10.1441  |

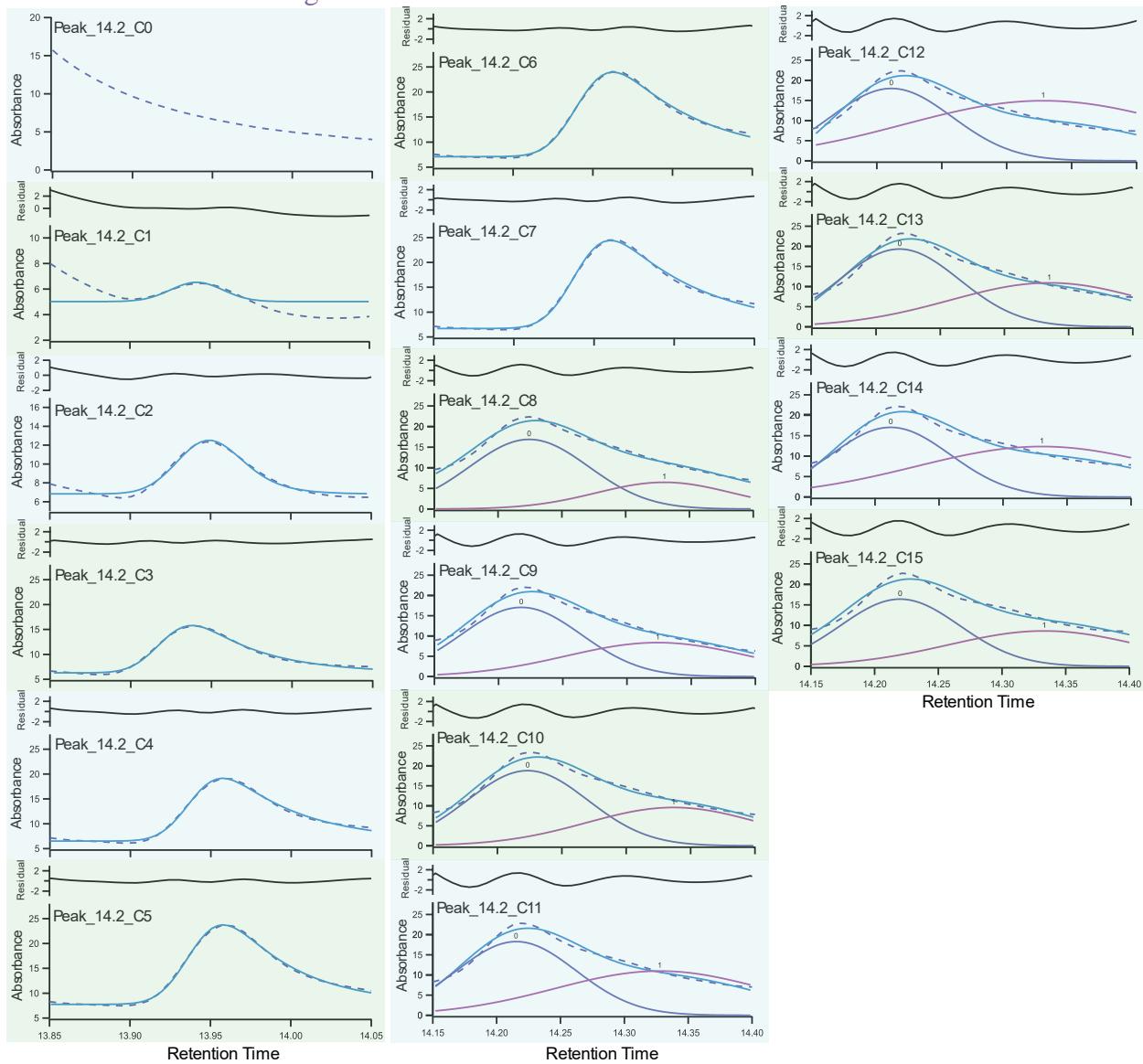
|         |          |              |          |       |        |         |
|---------|----------|--------------|----------|-------|--------|---------|
| Ggy-H2O | 191.0634 | C7H11O5N1    | 192.0712 | 192.1 | 0.0288 | 10.1441 |
| GGGtn   | 386.1009 | C13H16O4N8S1 | 387.1087 | 387.1 | 0.0087 | 9.9220  |
| GGGGgy  | 386.1394 | C13H22O9N4   | 387.1472 | 387.1 | 0.0472 | 9.9220  |
| GGGGgt  | 386.0842 | C12H18O8N4S1 | 387.0920 | 387.1 | 0.0080 | 9.9220  |
| GGGyn   | 386.1561 | C14H20O5N8   | 387.1639 | 387.2 | 0.0361 | 9.1142  |

### Fraction 14 (retention time = 14.2 min)

Fraction 15 is a collection of two main product peaks (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that a first product in this region is formed in cycle 1, reaches a maximum at cycle 6 and then decreases in subsequent cycles. A second product in this region is formed in cycle 8, reaches a maximum at cycle 12 and then decreases in subsequent cycles.

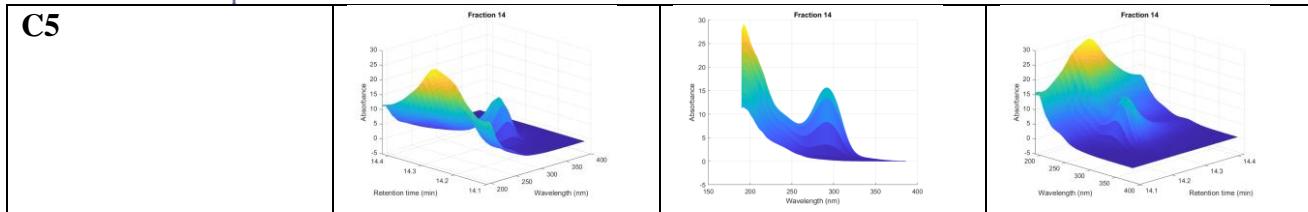
Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and the dry-down reaction involving thioglycolic acid and glucose. A corresponding mass was not identified in our MS analysis, possibly due to insufficient ionizable groups in the case of a co-oligomer between thioglycolic acid and glucose.

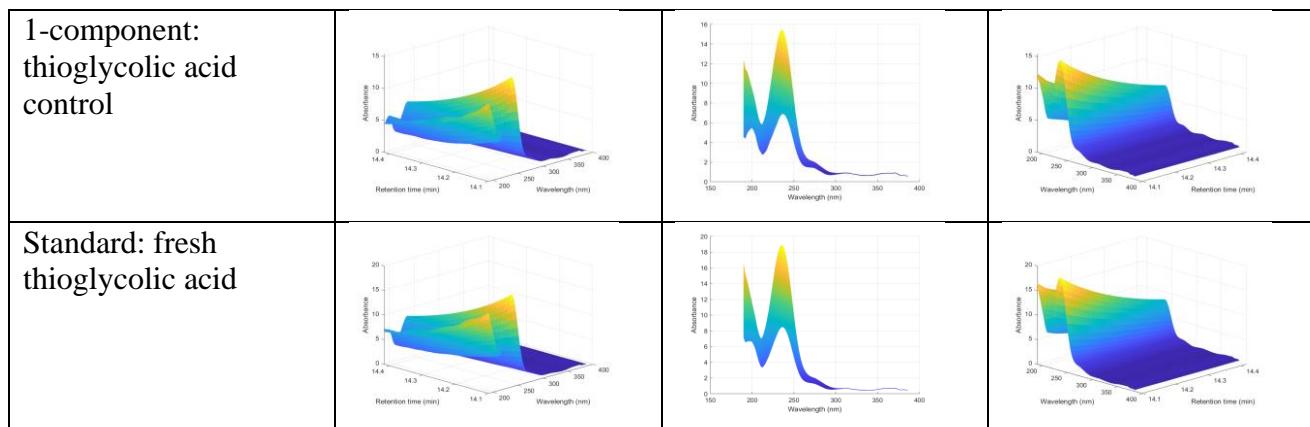
### HPLC curve fitting



**Figure S32. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 14 which has a retention time of about 14.2 minutes.

### UV-VIS spectrum





**Figure S33.** UV-Vis absorbance. UV-vis absorbance spectra of fraction 14 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula  | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|----------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3   | 91.0400           | 91.0              | 0.0400     | 64.4745  |
| t        | 91.9926      | C2H4O2S1 | 90.9848           | 91.0              | 0.0152     | 64.4745  |
| ggu      | 176.0437     | C5H8O5N2 | 175.0359          | 175.0             | 0.0359     | 19.9450  |

#### HPLC MS – positive mode

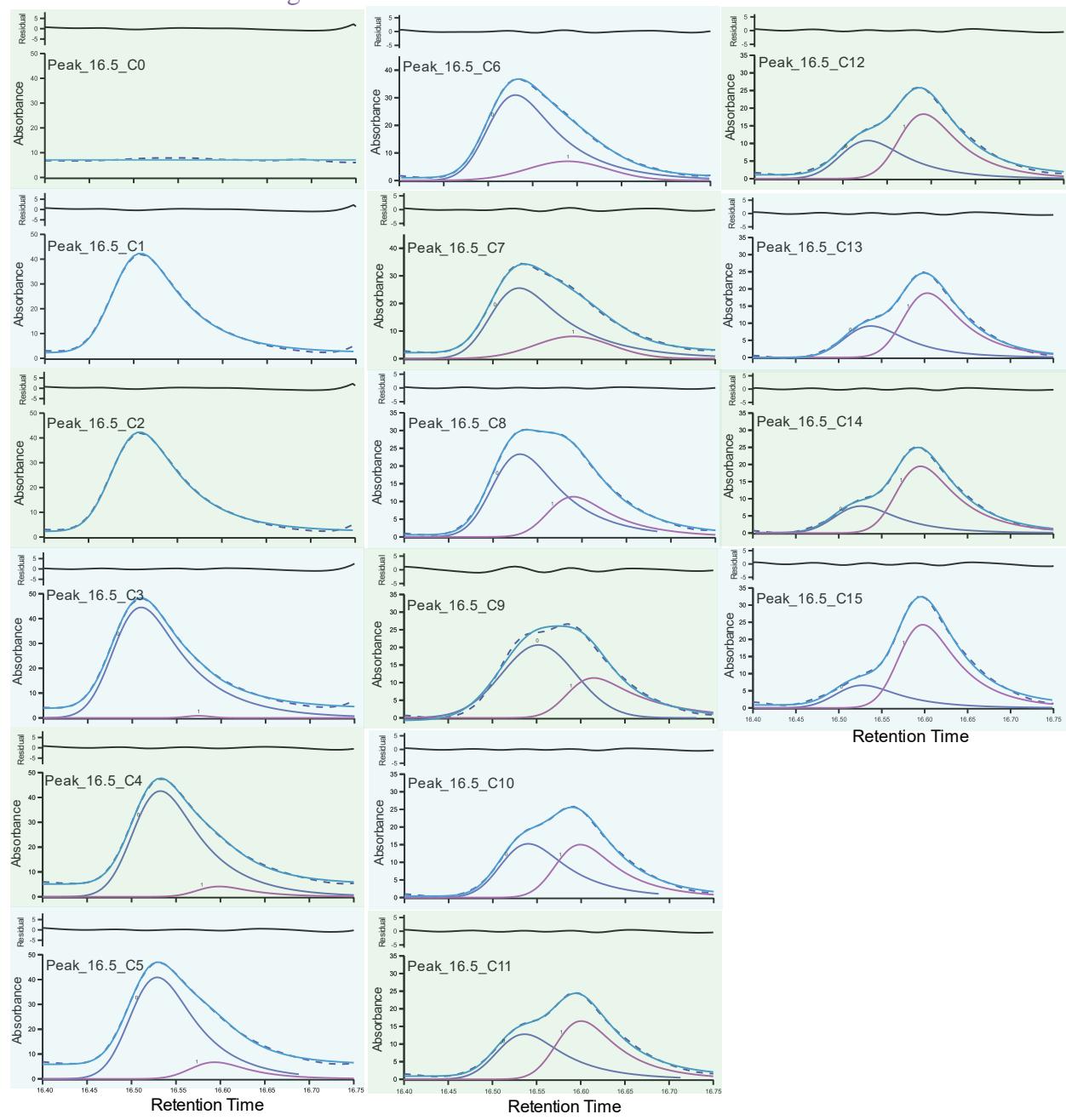
| Sequence | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy       | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 39.2655  |
| gyu-H2O  | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 9.7801   |
| yn-H2O   | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 8.2218   |
| Ggy-H2O  | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 8.2218   |
| Ggn-H2O  | 234.0706     | C9H8O2N6     | 235.0784          | 235.1             | 0.0216     | 5.9880   |
| GGyu-H2O | 234.1016     | C8H14O4N4    | 235.1094          | 235.1             | 0.0094     | 5.9880   |
| Gtyy     | 299.0868     | C10H19O7N1S1 | 300.0946          | 300.1             | 0.0054     | 5.6812   |
| ttyy-H2  | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 12.7052  |
| GGGtn    | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 12.7052  |
| GGGGgy   | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 12.7052  |
| GGGGgt   | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 12.7052  |
| GGGyn    | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 11.2794  |

|       |          |             |          |       |        |        |
|-------|----------|-------------|----------|-------|--------|--------|
| gtyl  | 392.1066 | C13H22O11S1 | 393.1144 | 393.1 | 0.0144 | 7.7163 |
| gttl  | 392.0514 | C12H18O10S2 | 393.0592 | 393.1 | 0.0408 | 7.7163 |
| gyyl  | 392.1618 | C14H26O12   | 393.1696 | 393.2 | 0.0304 | 8.9951 |
| GGGdu | 392.2364 | C17H31O5N5  | 393.2442 | 393.2 | 0.0442 | 8.9951 |

### Fraction 15 (retention time = 16.5 min)

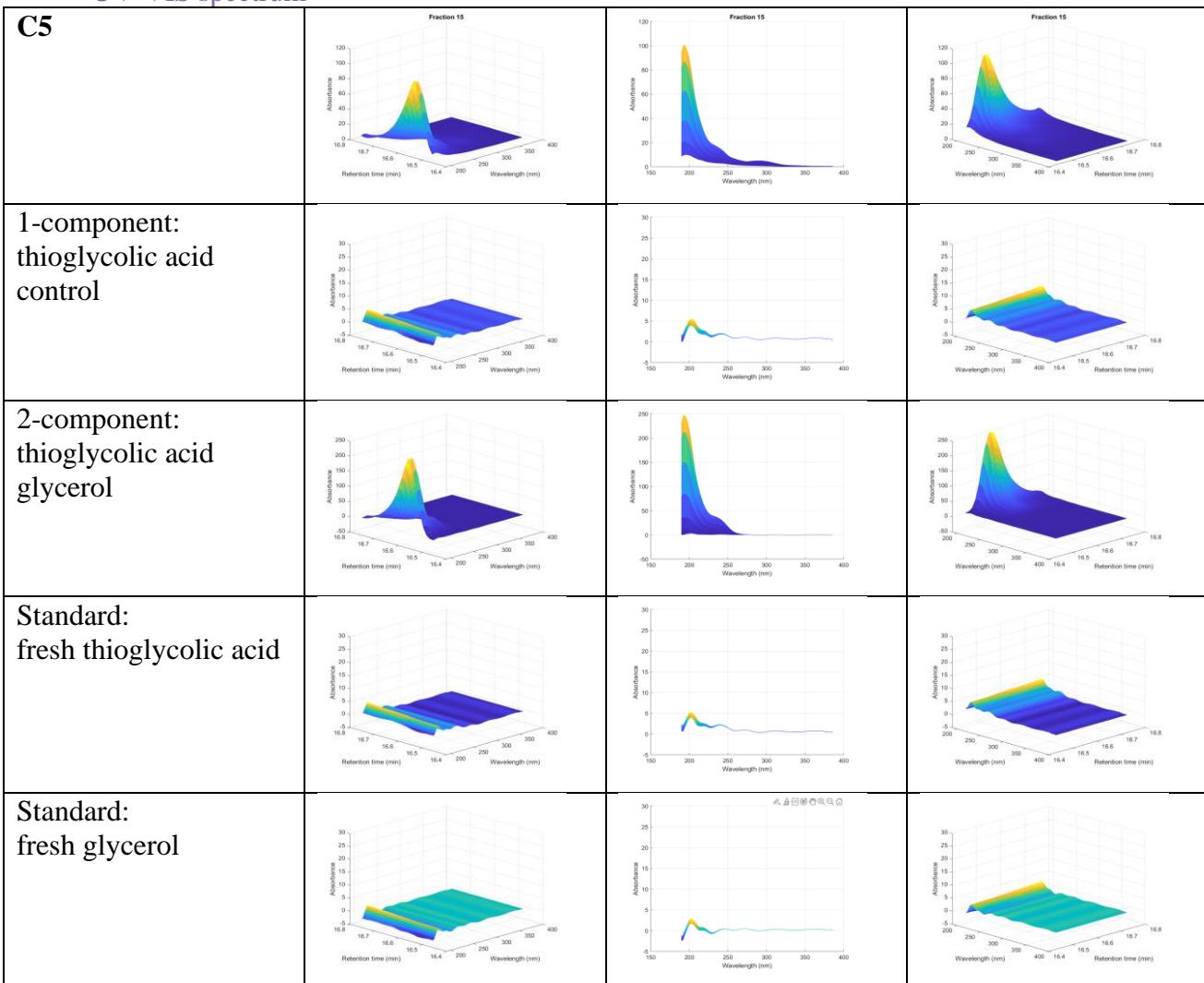
Fraction 15 is a collection of two main product peaks (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that a first product in this region is formed in cycle 1, reaches a maximum at cycle 3 and then decreases in subsequent cycles. A second product in this region is formed in cycle 3 and gradually increases in its abundance in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-down reactions indicates UV-Vis absorbance spectrum similarities between the 9-component system and the binary dry-down reaction involving thioglycolic acid and glycerol. MS analysis confirms the existence of co-oligomers of thioglycolic acid and glycerol, such as tyy and tty. The UV-Vis spectra for the two peaks is indicative of an ester linkage.

### HPLC curve fitting



**Figure S34. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 15 which has a retention time of about 16.5 minutes.

### UV-VIS spectrum



**Figure S35. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 15 and relevant fresh, control, and 2 building-block dry-downs.

### HPLC MS

#### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula   | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|-----------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3    | 91.0400           | 91.0              | 0.0400     | 53.9873  |
| t        | 91.9926      | C2H4O2S1  | 90.9848           | 91.0              | 0.0152     | 53.9873  |
| yyy      | 240.1212     | C9H20O7   | 239.1134          | 239.1             | 0.0134     | 10.6882  |
| tyy      | 240.0660     | C8H16O6S1 | 239.0582          | 239.1             | 0.0418     | 10.6882  |
| tty      | 240.0108     | C7H12O5S2 | 239.0030          | 239.0             | 0.0030     | 11.4554  |

|     |          |          |          |       |        |         |
|-----|----------|----------|----------|-------|--------|---------|
| ttt | 239.9556 | C6H8O4S3 | 238.9478 | 238.9 | 0.0478 | 11.3541 |
| ggu | 176.0437 | C5H8O5N2 | 175.0359 | 175.0 | 0.0359 | 11.8821 |

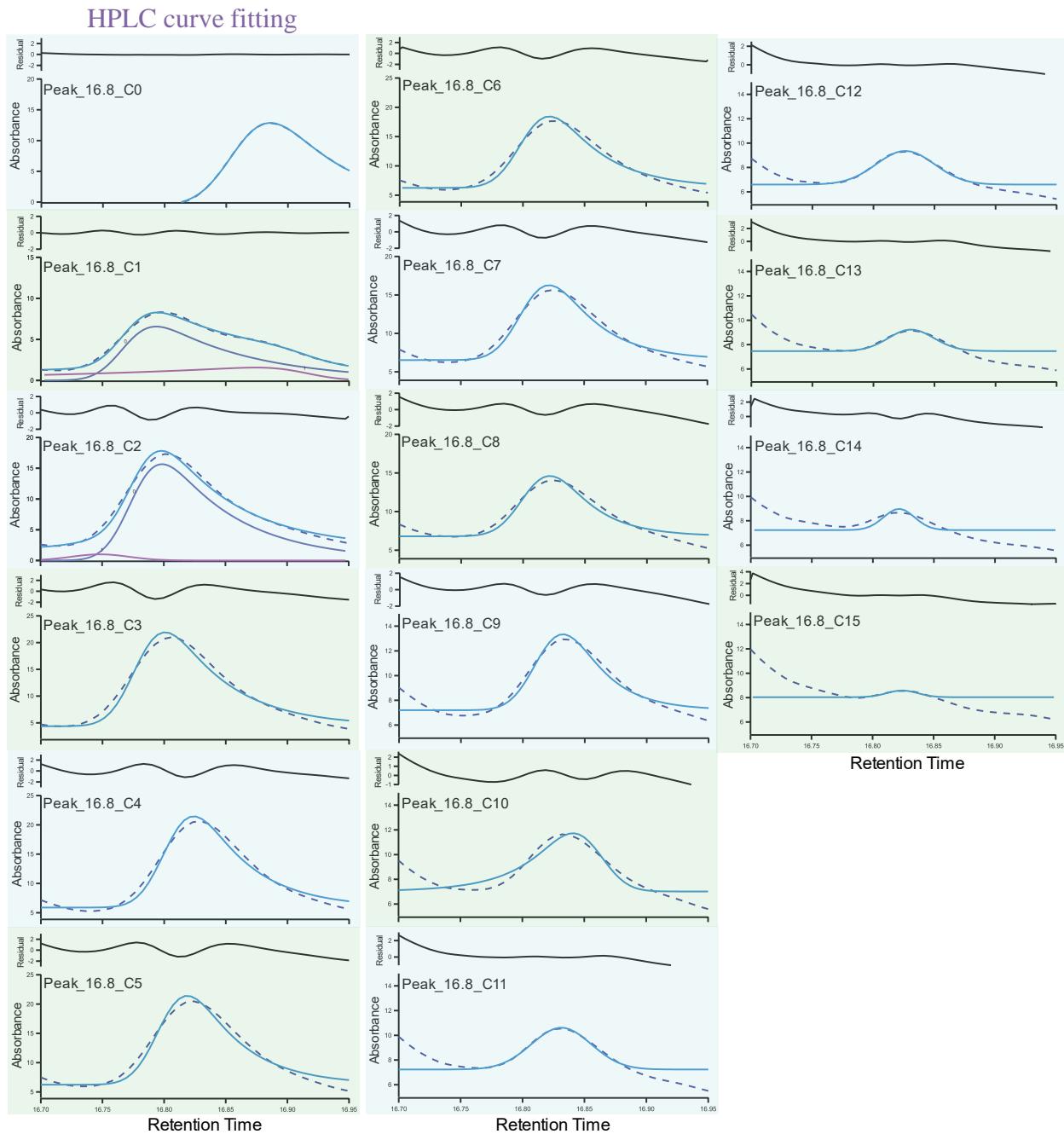
### HPLC MS – positive mode

| Sequence  | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|-----------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy        | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 30.1143  |
| gyu-H2O   | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 12.4961  |
| yn-H2O    | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 8.7561   |
| Ggy-H2O   | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 8.7561   |
| Ggn-H2O   | 234.0706     | C9H8O2N6     | 235.0784          | 235.1             | 0.0216     | 5.5656   |
| GGyu-H2O  | 234.1016     | C8H14O4N4    | 235.1094          | 235.1             | 0.0094     | 5.5656   |
| ttyyy-H2  | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 14.1802  |
| GGGtn     | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 14.1802  |
| GGGGgy    | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 14.1802  |
| GGGGgt    | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 14.1802  |
| GAu-H2O   | 386.1590     | C14H18O5N8   | 387.1668          | 387.2             | 0.0332     | 12.3927  |
| Glun-H2O  | 386.1599     | C14H18O5N8   | 387.1677          | 387.2             | 0.0323     | 12.3927  |
| GGglu-H2O | 386.1432     | C13H20O90N4  | 387.1510          | 387.2             | 0.0490     | 12.3927  |
| GGGyn     | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 12.3927  |
| gtyl      | 392.1066     | C13H22O11S1  | 393.1144          | 393.1             | 0.0144     | 7.5993   |
| gttl      | 392.0514     | C12H18O10S2  | 393.0592          | 393.1             | 0.0408     | 7.5993   |
| gyyl      | 392.1618     | C14H26O12    | 393.1696          | 393.2             | 0.0304     | 7.9076   |
| GGGdu     | 392.2364     | C17H31O5N5   | 393.2442          | 393.2             | 0.0442     | 7.9076   |
| ttyl      | 408.0827     | C13H22O10S2  | 409.0905          | 409.1             | 0.0095     | 5.2758   |
| ggggggu   | 408.0643     | C13H16O13N2  | 409.0721          | 409.1             | 0.0279     | 5.2758   |

### Fraction 16 (retention time = 16.8 min)

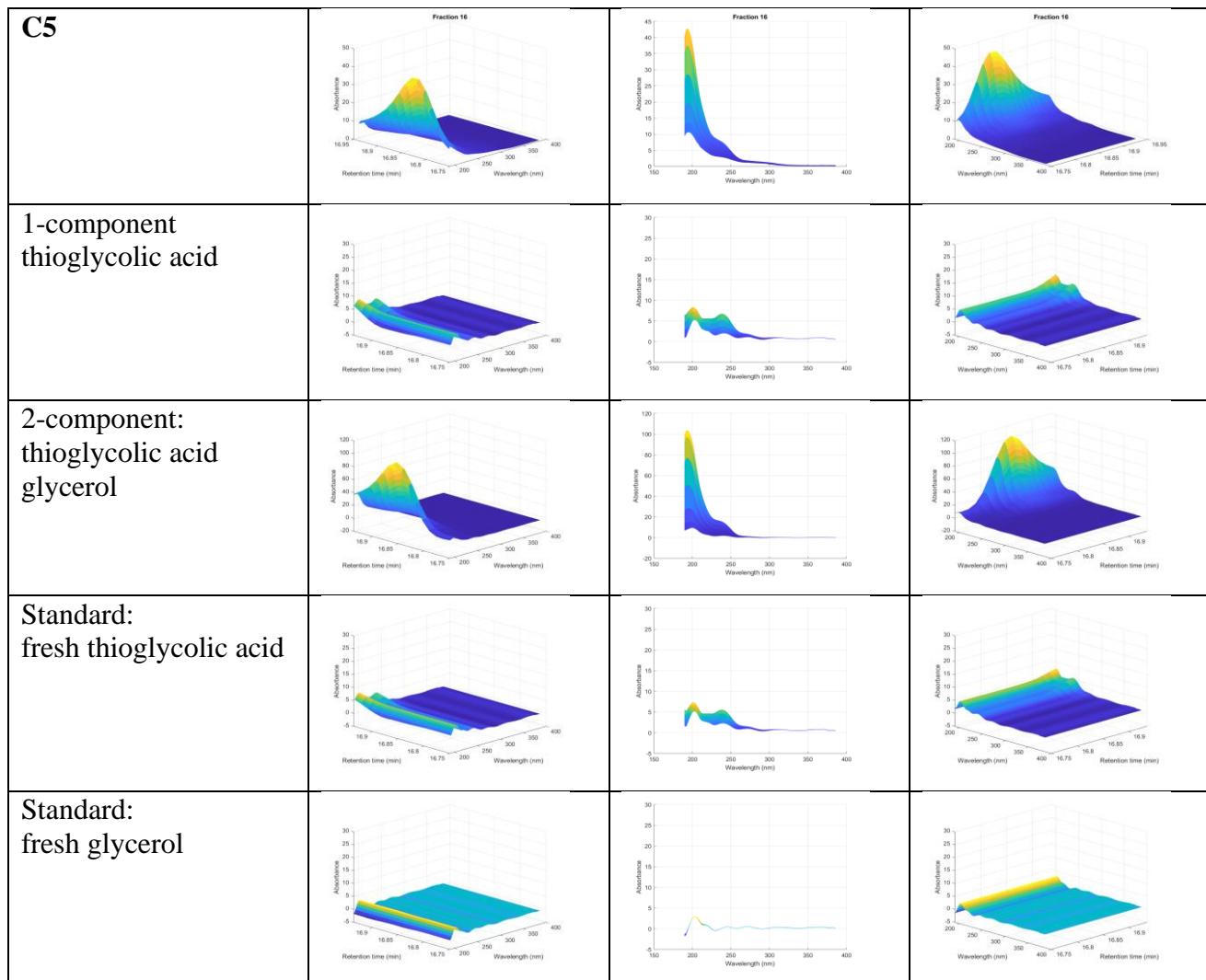
Fraction 16 is a product peak (not found in the fresh mixture of MFP\_set 3). HPLC curve fitting indicates that this product is formed in cycle 1, reaches a maximum at cycle 3 and then decreases in subsequent cycles. Comparison of the 9-component system to a series of 2-component dry-downs indicates UV-Vis absorbance spectrum similarities between the 9-component system and the binary dry-down reaction involving thioglycolic acid and glycerol. MS analysis confirms the existence of co-oligomers of thioglycolic acid and glycerol, such as tyy and tty. The UV-Vis

spectra is indicative of an ester linkage. Fraction 16 is an oligomer of thioglycolic acid and glycerol



**Figure S36. Curve fitting.** Curve fitting of HPLC data for cycle 0 through 15 of fraction 16 which has a retention time of about 16.8 minutes.

## UV-VIS spectrum



**Figure S37. UV-Vis absorbance.** UV-vis absorbance spectra of fraction 16 and relevant fresh, control, and 2 building-block dry-downs.

## HPLC MS

### HPLC MS – negative mode

| Sequence | Neutral Mass | Formula | Deprotonated Mass | Experimental Mass | Difference | Relative |
|----------|--------------|---------|-------------------|-------------------|------------|----------|
| y        | 92.0478      | C3H8O3  | 91.0400           | 91.0              | 0.0400     | 52.1070  |

|     |          |           |          |       |        |         |
|-----|----------|-----------|----------|-------|--------|---------|
| t   | 91.9926  | C2H4O2S1  | 90.9848  | 91.0  | 0.0152 | 52.1070 |
| yyy | 240.1212 | C9H20O7   | 239.1134 | 239.1 | 0.0134 | 9.2037  |
| tyy | 240.0660 | C8H16O6S1 | 239.0582 | 239.1 | 0.0418 | 9.2037  |
| tty | 240.0108 | C7H12O5S2 | 239.0030 | 239.0 | 0.0030 | 9.3052  |
| ttt | 239.9556 | C6H8O4S3  | 238.9478 | 238.9 | 0.0478 | 8.8454  |
| ggu | 176.0437 | C5H8O5N2  | 175.0359 | 175.0 | 0.0359 | 13.8957 |

### HPLC MS – positive mode

| Sequence    | Neutral Mass | Formula      | Deprotonated Mass | Experimental Mass | Difference | Relative |
|-------------|--------------|--------------|-------------------|-------------------|------------|----------|
| yy          | 166.0835     | C6H14O5      | 167.0913          | 167.1             | 0.0087     | 36.3406  |
| gyu-H2O     | 174.0634     | C6H10O4N2    | 175.0712          | 175.1             | 0.0288     | 11.9843  |
| yn-H2O      | 191.0801     | C8H9O1N5     | 192.0879          | 192.1             | 0.0121     | 8.0112   |
| Ggy-H2O     | 191.0634     | C7H11O5N1    | 192.0712          | 192.1             | 0.0288     | 8.0112   |
| ttyyy-H2    | 386.0686     | C13H22O9S2   | 387.0764          | 387.1             | 0.0236     | 23.3049  |
| GGGtn       | 386.1009     | C13H16O4N8S1 | 387.1087          | 387.1             | 0.0087     | 23.3049  |
| GGGGgy      | 386.1394     | C13H22O9N4   | 387.1472          | 387.1             | 0.0472     | 23.3049  |
| GGGGgt      | 386.0842     | C12H18O8N4S1 | 387.0920          | 387.1             | 0.0080     | 23.3049  |
| GAu-H2O     | 386.1590     | C14H18O5N8   | 387.1668          | 387.2             | 0.0332     | 22.0889  |
| Glun-H2O    | 386.1599     | C14H18O5N8   | 387.1677          | 387.2             | 0.0323     | 22.0889  |
| GGglu-H2O   | 386.1432     | C13H20O90N4  | 387.1510          | 387.2             | 0.0490     | 22.0889  |
| GGGyn       | 386.1561     | C14H20O5N8   | 387.1639          | 387.2             | 0.0361     | 22.0889  |
| GGGGGt      | 387.1006     | C12H19O7N5S1 | 388.1084          | 388.1             | 0.0084     | 5.6833   |
| ggydu-H2O   | 387.2079     | C18H30O7N2   | 388.2157          | 388.2             | 0.0157     | 5.5379   |
| ggtdu-H2O   | 387.1527     | C17H26O6N2S1 | 388.1605          | 388.2             | 0.0395     | 5.5379   |
| gggd-H2O    | 387.1602     | C18H26O9     | 388.1680          | 388.2             | 0.0320     | 5.5379   |
| GGGlu-H2O   | 387.1596     | C13H21O8N5   | 388.1674          | 388.2             | 0.0326     | 5.5379   |
| GGGGGy      | 387.1558     | C13H23O8N5   | 388.1636          | 388.2             | 0.0364     | 5.5379   |
| gtyl        | 392.1066     | C13H22O11S1  | 393.1144          | 393.1             | 0.0144     | 8.9733   |
| gttl        | 392.0514     | C12H18O10S2  | 393.0592          | 393.1             | 0.0408     | 8.9733   |
| Ggggun-H2O  | 392.1032     | C14H14O6N8   | 393.1110          | 393.1             | 0.0110     | 8.9733   |
| GGggggu-H2O | 392.0865     | C13H16O10N4  | 393.0943          | 393.1             | 0.0057     | 8.9733   |
| gyyl        | 392.1618     | C14H26O12    | 393.1696          | 393.2             | 0.0304     | 8.8733   |
| GGGdu       | 392.2364     | C17H31O5N5   | 393.2442          | 393.2             | 0.0442     | 8.8733   |

|             |          |               |          |       |        |         |
|-------------|----------|---------------|----------|-------|--------|---------|
| gttdu-H2O   | 403.1288 | C17H26O5N2S2  | 404.1366 | 404.1 | 0.0366 | 6.5871  |
| gggtd-H2O   | 403.1363 | C18H26O8S1    | 404.1441 | 404.1 | 0.0441 | 6.5871  |
| Ggglu       | 403.1374 | C13H21O11N3   | 404.1452 | 404.1 | 0.0452 | 6.5871  |
| gAu         | 403.1532 | C14H19O7N7    | 404.1610 | 404.2 | 0.0390 | 6.4325  |
| GGA-H2O     | 403.1590 | C15H19O6N7    | 404.1668 | 404.2 | 0.0332 | 6.4325  |
| glun        | 403.1541 | C14H19O7N7    | 404.1619 | 404.2 | 0.0381 | 6.4325  |
| GGln-H2O    | 403.1599 | C15H19O6N7    | 404.1677 | 404.2 | 0.0323 | 6.4325  |
| gyydu-H2O   | 403.2392 | C19H34O7N2    | 404.2470 | 404.2 | 0.0470 | 6.4325  |
| gtydu-H2O   | 403.1840 | C18H30O6N2S1  | 404.1918 | 404.2 | 0.0082 | 6.4325  |
| gggyd-H2O   | 403.1915 | C19H30O9      | 404.1993 | 404.2 | 0.0007 | 6.4325  |
| GGGgl-H2O   | 403.1432 | C14H21O10N3   | 404.1510 | 404.2 | 0.0490 | 6.4325  |
| ttyl        | 408.1379 | C14H26O11S1   | 409.1457 | 409.1 | 0.0457 | 10.4987 |
| ttyl        | 408.0827 | C13H22O10S2   | 409.0905 | 409.1 | 0.0095 | 10.4987 |
| Gggyun-H2O  | 408.1345 | C15H18O6N8    | 409.1423 | 409.1 | 0.0423 | 10.4987 |
| Gggtun-H2O  | 408.0793 | C14H14O5N8S1  | 409.0871 | 409.1 | 0.0129 | 10.4987 |
| Ggggn-H2O   | 408.0868 | C15H14O8N6    | 409.0946 | 409.1 | 0.0054 | 10.4987 |
| gggggu      | 408.0643 | C13H16O13N2   | 409.0721 | 409.1 | 0.0279 | 10.4987 |
| GGgggyu-H2O | 408.1178 | C14H20O10N4   | 409.1256 | 409.1 | 0.0256 | 10.4987 |
| GGgggtu-H2O | 408.0626 | C13H16O90N4S1 | 409.0704 | 409.1 | 0.0296 | 10.4987 |
| GGggggg-H2O | 408.0701 | C14H16O12N2   | 409.0779 | 409.1 | 0.0221 | 10.4987 |
| yyyl        | 408.1931 | C15H30O12     | 409.2009 | 409.2 | 0.0009 | 9.8873  |
| GGdn        | 408.2367 | C19H29O3N7    | 409.2445 | 409.2 | 0.0445 | 9.8873  |
| GGGgd       | 408.2200 | C18H31O7N3    | 409.2278 | 409.2 | 0.0278 | 9.8873  |
| gggggtu     | 424.0404 | C13H16O12N2S1 | 425.0482 | 425.0 | 0.0482 | 5.2163  |
| GGggtu-H2O  | 424.0387 | C13H16O8N4S2  | 425.0465 | 425.0 | 0.0465 | 5.2163  |
| Ggtyun-H2O  | 424.1106 | C15H18O5N8S1  | 425.1184 | 425.1 | 0.0184 | 5.0726  |
| Gttun-H2O   | 424.0554 | C14H14O4N8S2  | 425.0632 | 425.1 | 0.0368 | 5.0726  |
| Gggyn-H2O   | 424.1181 | C16H18O8N6    | 425.1259 | 425.1 | 0.0259 | 5.0726  |
| Gggtn-H2O   | 424.0629 | C15H14O7N6S1  | 425.0707 | 425.1 | 0.0293 | 5.0726  |
| gggggyu     | 424.0956 | C14H20O13N2   | 425.1034 | 425.1 | 0.0034 | 5.0726  |
| ggggggg     | 424.0479 | C14H16O15     | 425.0557 | 425.1 | 0.0443 | 5.0726  |
| GGgggyu-H2O | 424.1491 | C15H24O10N4   | 425.1569 | 425.1 | 0.0569 | 5.0726  |
| GGggtu-H2O  | 424.0939 | C14H20O90N4S1 | 425.1017 | 425.1 | 0.0017 | 5.0726  |

|            |          |               |          |       |        |        |
|------------|----------|---------------|----------|-------|--------|--------|
| GGgggy-H2O | 424.1014 | C15H20O12N2   | 425.1092 | 425.1 | 0.0092 | 5.0726 |
| GGgggt-H2O | 424.0462 | C14H16O11N2S1 | 425.0540 | 425.1 | 0.0460 | 5.0726 |
| ttyyn      | 431.0904 | C15H21O6N5S2  | 432.0982 | 432.1 | 0.0018 | 5.9099 |
| tttyn      | 431.0352 | C14H17O5N5S3  | 432.0430 | 432.1 | 0.0570 | 5.9099 |
| Ggtyyy     | 431.1289 | C15H27O11N1S1 | 432.1367 | 432.1 | 0.0367 | 5.9099 |
| Ggttyy     | 431.0737 | C14H23O10N1S2 | 432.0815 | 432.1 | 0.0185 | 5.9099 |
| yyyn       | 431.2008 | C17H29O8N5    | 432.2086 | 432.2 | 0.0086 | 6.0905 |
| ttyyn      | 431.1456 | C16H25O7N5S1  | 432.1534 | 432.2 | 0.0466 | 6.0905 |
| Ggdun-H2O  | 431.2315 | C20H28O3N8    | 432.2393 | 432.2 | 0.0393 | 6.0905 |
| Ggyyyy     | 431.1841 | C16H31O12N1   | 432.1919 | 432.2 | 0.0081 | 6.0905 |
| GGggdu-H2O | 431.2148 | C19H30O7N4    | 432.2226 | 432.2 | 0.0226 | 6.0905 |
| GGGGGGG    | 431.1627 | C14H23O8N7    | 432.1705 | 432.2 | 0.0295 | 6.0905 |