

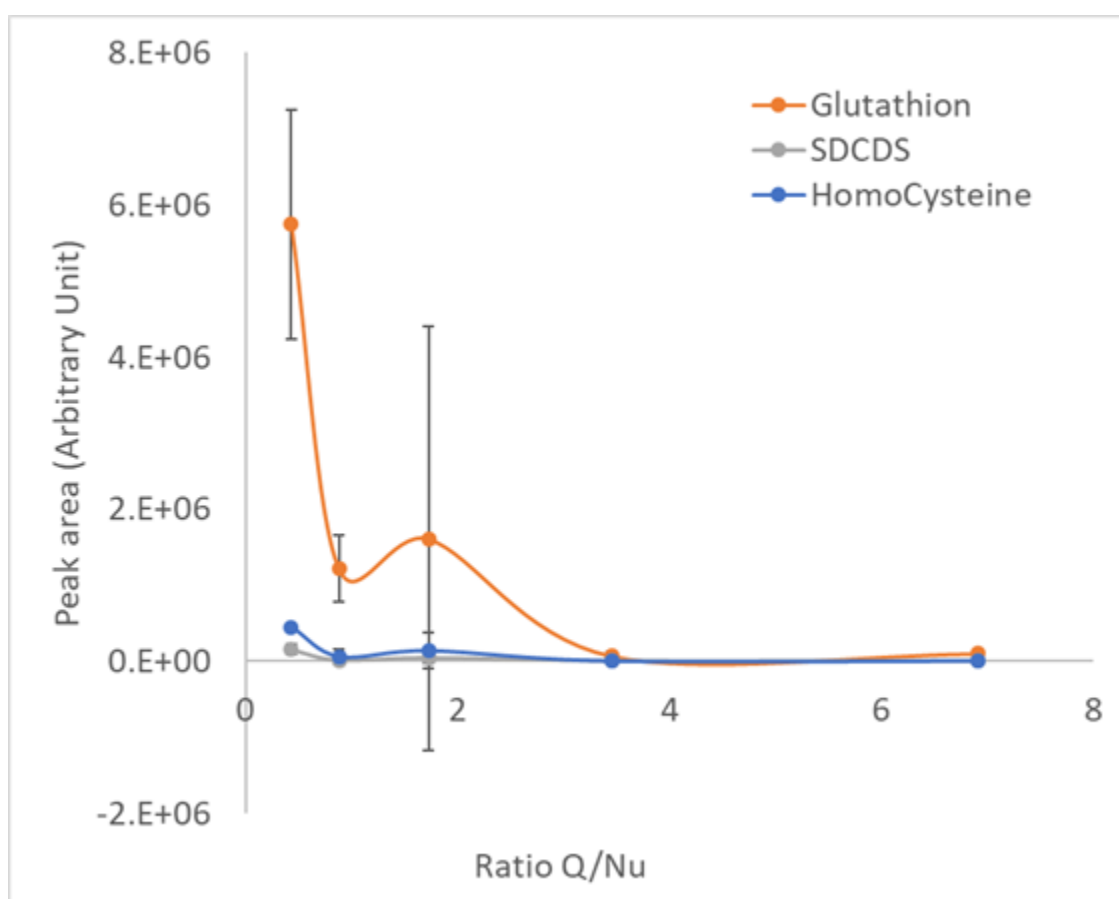
# Molecular characterization of white wines antioxidant metabolome by ultra high performance liquid chromatography high-resolution mass spectrometry

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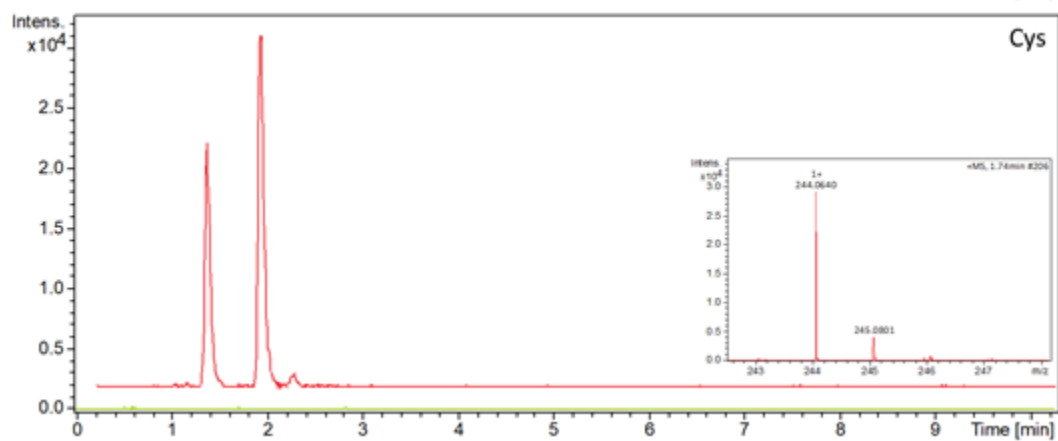
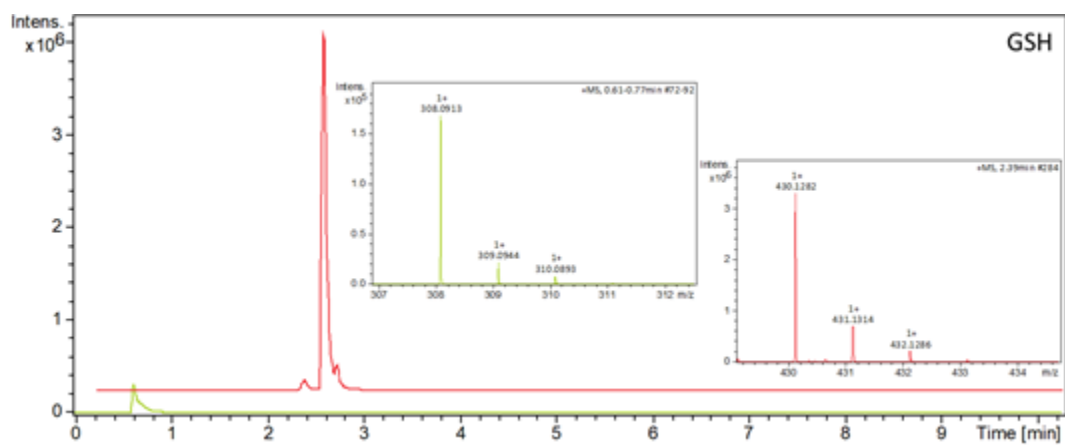
Université de Bourgogne Franche-Comté, AgroSup Dijon, PAM UMR A 02.102, Institut Universitaire de la Vigne et du Vin, Jules Guyot, Rue Claude Ladrey, BP 27877, 21078 Dijon Cedex, France

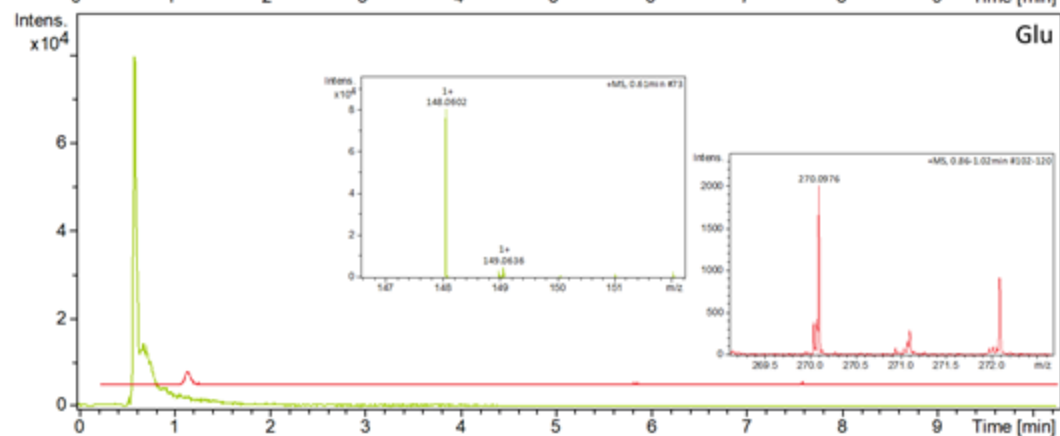
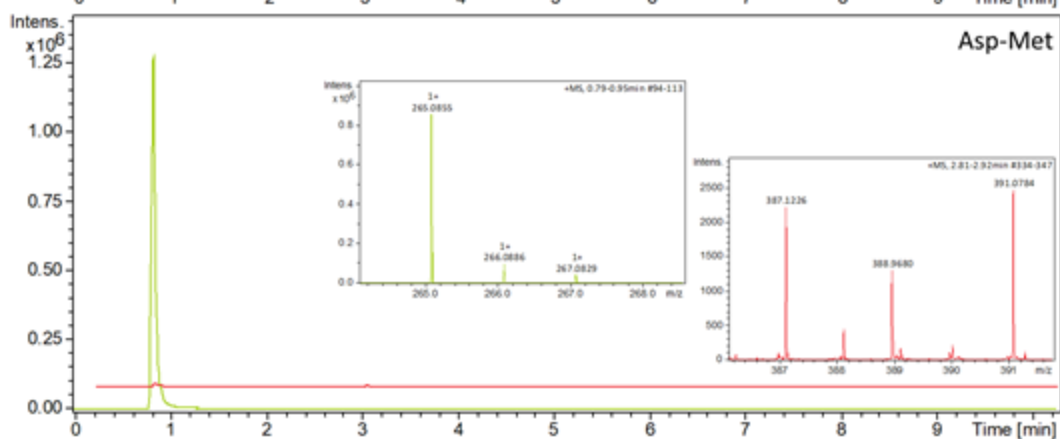
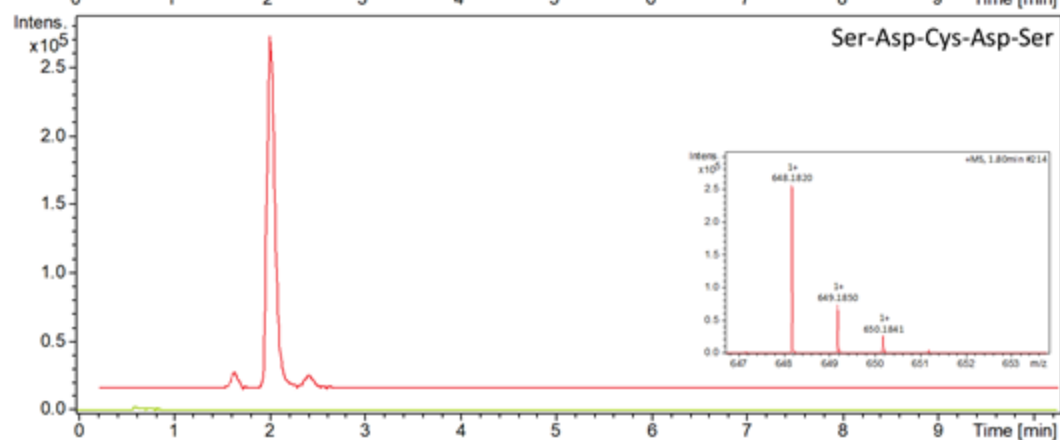
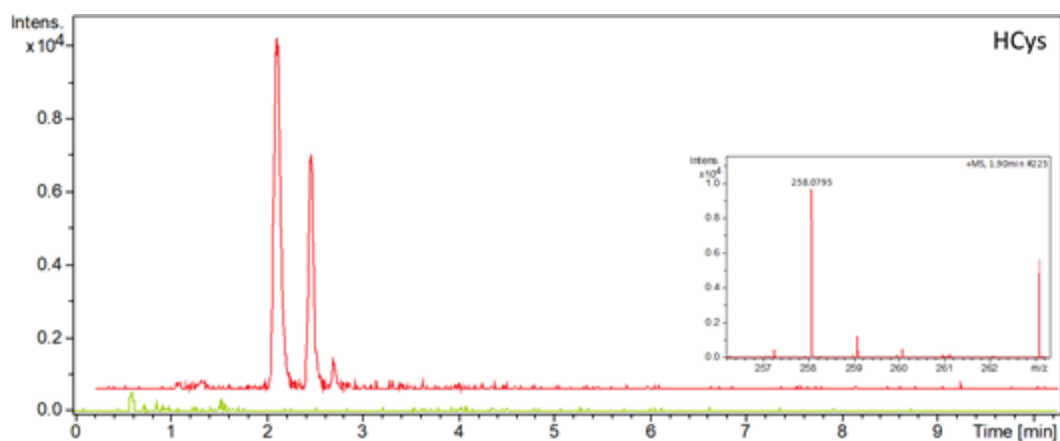
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## Supplementary Data



**Figure 1.** Peak area of tested sulfur compounds in native form for different quantity of 4MeQ, explain as ratio of quinone and total nucleophilic compounds in mol. Met, Glu and Asp-Met were not plot here, because the corresponding derivatized compounds was not detected. No trace of Cys in native from has been detected. .





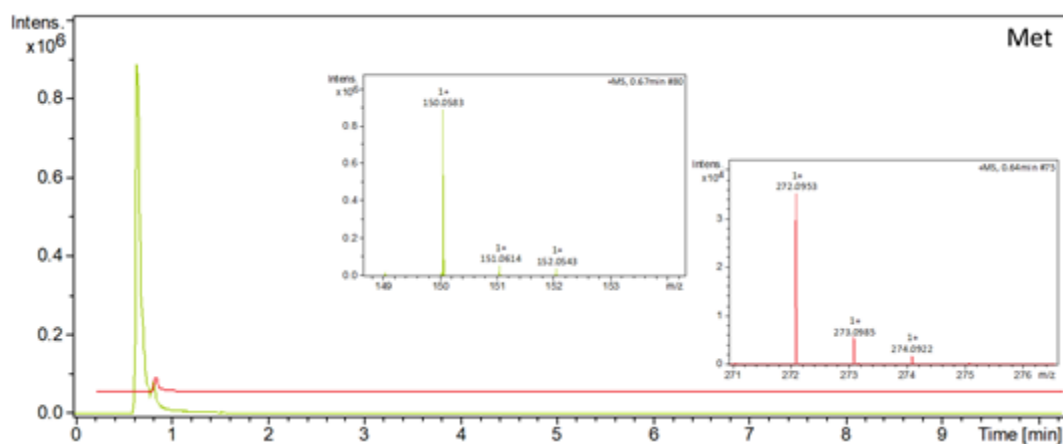
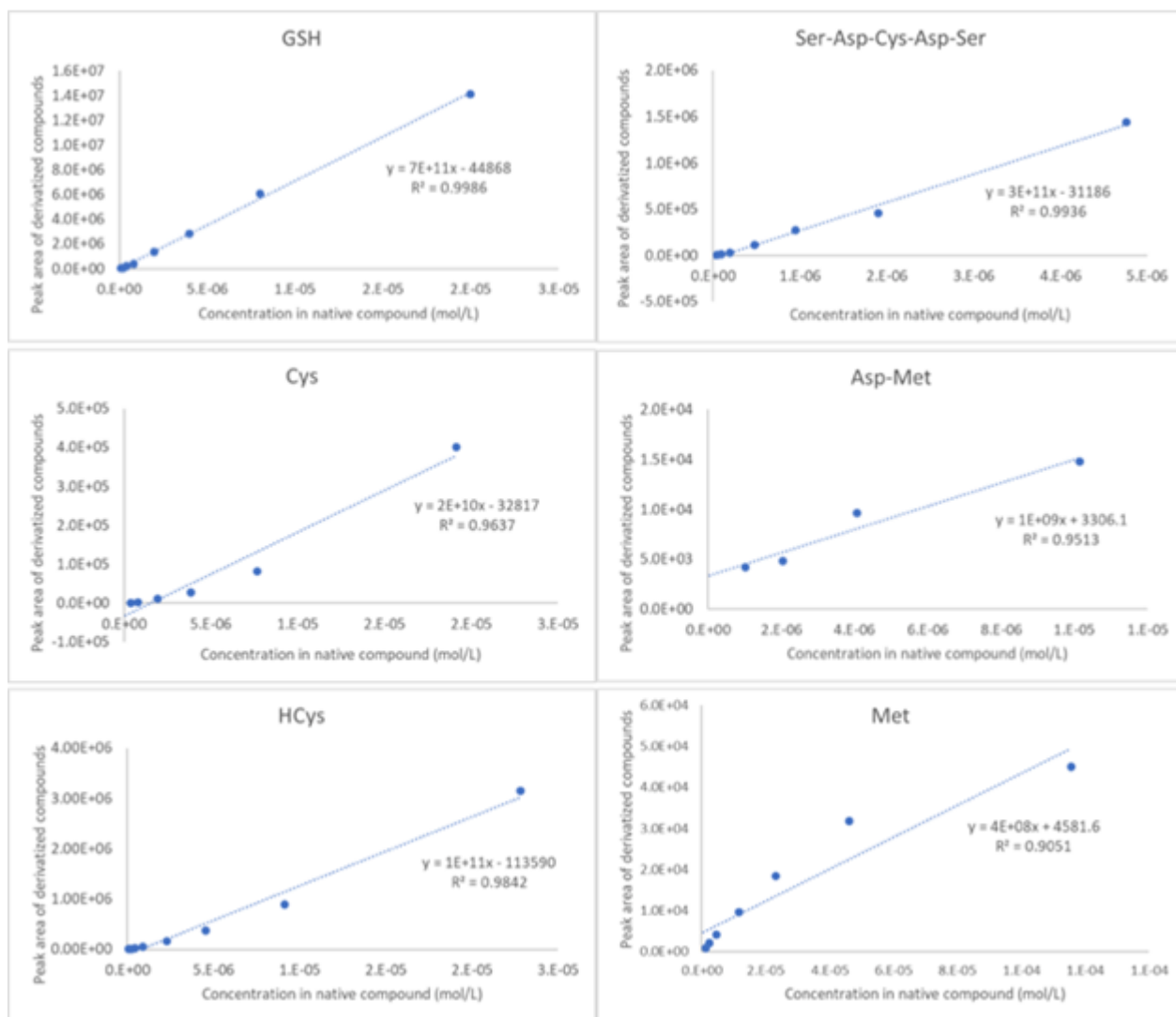
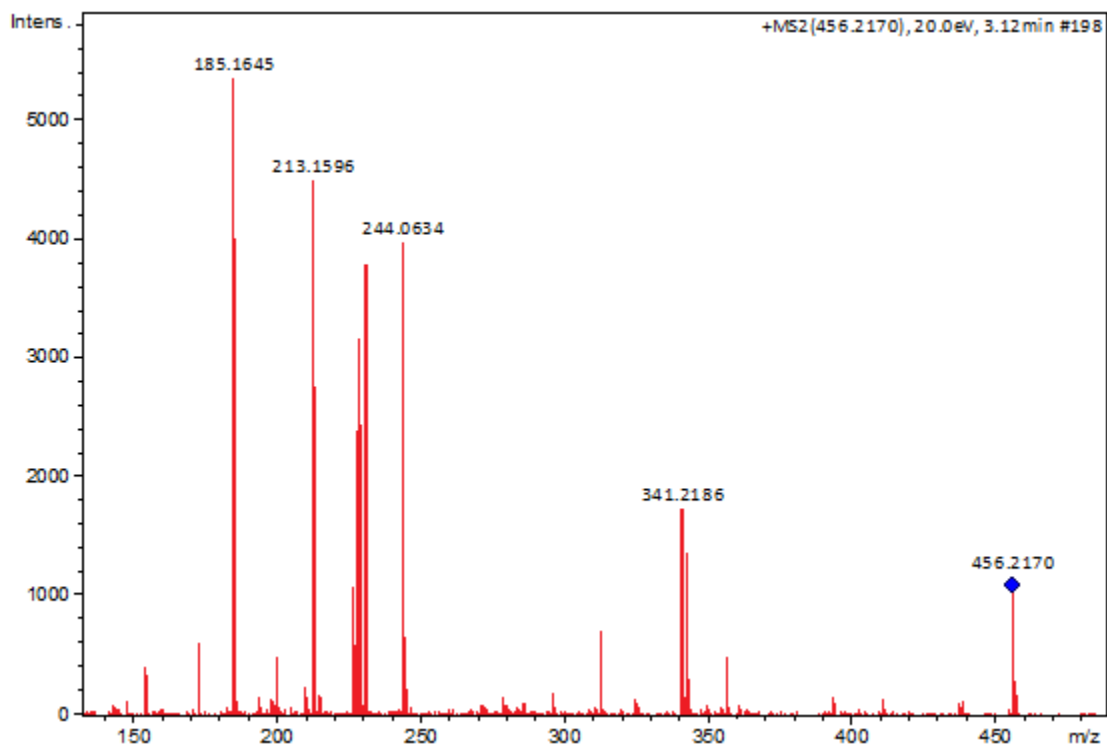


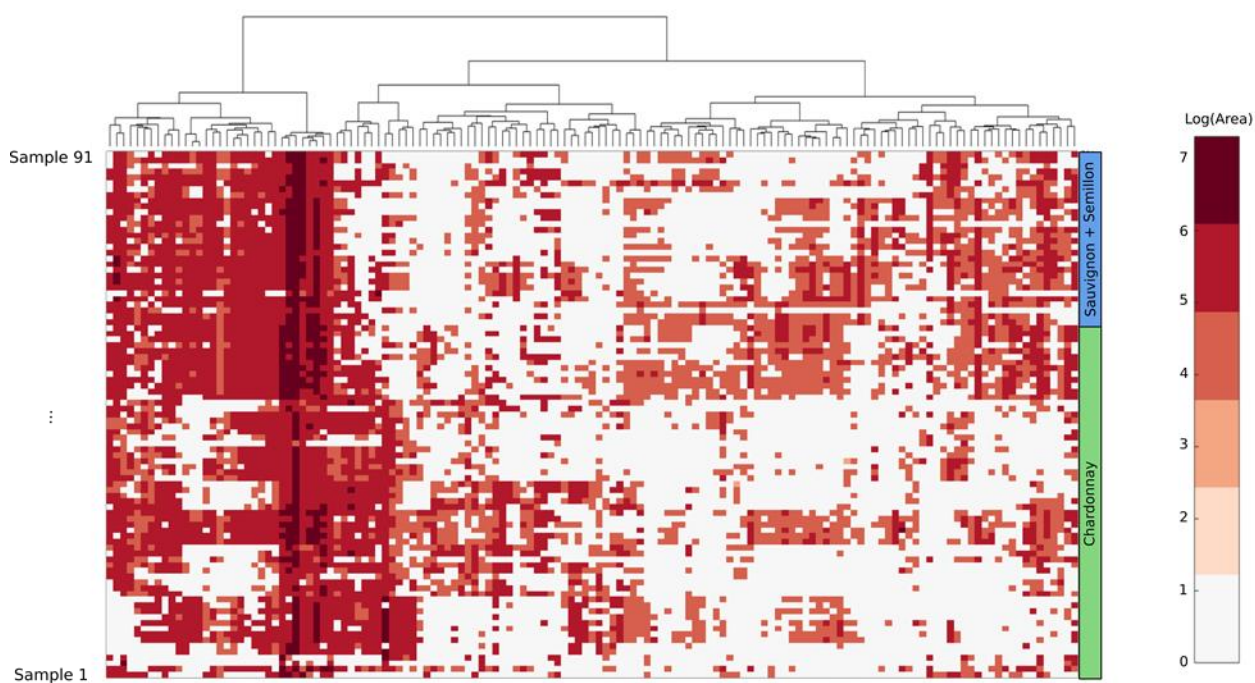
Figure S1 Visualization of the extract ions chromatograms and mass spectrum obtained for standard compounds (GSH, Cys, HCys and Ser-Asp-Cys-Asp-Ser, Asp-Met, Met and Glu) without (green line) and with derivatization (red line) using 4MeQ.



**Figure 3.** Representation of the area of derivatized compounds against the concentration of the native compounds (GSH, Cys, HCys and Ser-Aps-Cys-Asp-Ser, Asp-Met and Met). Glu have not been plotted because, it was not detected under our experimental conditions (pH 3).



**Figure 4.** Mass spectra obtain by fragmentation of unknown adduct  $C_{14}H_{27}N_3O_4S + 4MeQ$  (456.2156  $m/z$ ) at 20 eV. The blue square indicates the molecular ion.



**Figure 5.** Representative heatmap visualizing the intensities of the 141 derivatized compounds detected in the 91 white wines analyzed (Table S1). Missing values are shown in gray.



Table 1. Overview of global wine sample set.

| Sample | Winery | Grape variety | Vintage | Aging <sup>a</sup> |
|--------|--------|---------------|---------|--------------------|
| 1      | CN     | Chardonnay    | 2017    | After AF           |
| 2      | CN     | Chardonnay    | 2017    | After AF           |
| 3      | CN     | Chardonnay    | 2017    | After AF           |
| 4      | CN     | Chardonnay    | 2017    | After AF           |
| 5      | Lf     | Chardonnay    | 2017    | After AF           |
| 6      | Lf     | Chardonnay    | 2017    | After AF           |
| 7      | Lf     | Chardonnay    | 2017    | After AF           |
| 8      | Lf     | Chardonnay    | 2017    | After AF           |
| 9      | Lf     | Chardonnay    | 2017    | After AF           |
| 10     | Lf     | Chardonnay    | 2017    | After AF           |
| 11     | Lf     | Chardonnay    | 2017    | After AF           |
| 12     | Lf     | Chardonnay    | 2017    | After AF           |
| 13     | Lf     | Chardonnay    | 2017    | After AF           |
| 14     | Lf     | Chardonnay    | 2017    | After AF           |
| 15     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 16     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 17     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 18     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 19     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 20     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 21     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 22     | P      | Chardonnay    | 2016    | 1 years in barrel  |
| 23     | P      | Chardonnay    | 2017    | After AF           |
| 24     | P      | Chardonnay    | 2017    | After AF           |
| 25     | P      | Chardonnay    | 2017    | After AF           |
| 26     | P      | Chardonnay    | 2017    | After AF           |
| 27     | P      | Chardonnay    | 2017    | After AF           |
| 28     | P      | Chardonnay    | 2017    | After AF           |
| 29     | P      | Chardonnay    | 2017    | After AF           |
| 30     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 31     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 32     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 33     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 34     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 35     | Lf     | Chardonnay    | 2016    | 1 years in barrel  |
| 36     | B      | Chardonnay    | 2017    | After AF           |
| 37     | B      | Chardonnay    | 2017    | After AF           |
| 38     | B      | Chardonnay    | 2017    | After AF           |
| 39     | B      | Chardonnay    | 2017    | After AF           |
| 40     | B      | Chardonnay    | 2017    | After AF           |
| 41     | B      | Chardonnay    | 2017    | After AF           |
| 42     | B      | Chardonnay    | 2017    | After AF           |
| 43     | B      | Chardonnay    | 2017    | After AF           |
| 44     | B      | Chardonnay    | 2017    | After AF           |
| 45     | B      | Chardonnay    | 2017    | After AF           |
| 46     | B      | Chardonnay    | 2017    | After AF           |
| 47     | B      | Chardonnay    | 2017    | After AF           |
| 48     | Lf     | Chardonnay    | 2016    | After AF           |
| 49     | P      | Chardonnay    | 2016    | After AF           |
| 50     | Lf     | Chardonnay    | 2017    | After AF           |
| 51     | Lf     | Chardonnay    | 2017    | After AF           |
| 52     | Lf     | Chardonnay    | 2017    | After AF           |
| 53     | Lf     | Chardonnay    | 2017    | After AF           |
| 54     | Lf     | Chardonnay    | 2017    | After AF           |
| 55     | Lf     | Chardonnay    | 2017    | After AF           |
| 56     | Lf     | Chardonnay    | 2017    | After AF           |
| 57     | P      | Chardonnay    | 2017    | After AF           |
| 58     | P      | Chardonnay    | 2017    | After AF           |
| 59     | P      | Chardonnay    | 2017    | After AF           |
| 60     | P      | Chardonnay    | 2017    | After AF           |

|    |     |            |      |          |
|----|-----|------------|------|----------|
| 61 | P   | Chardonnay | 2017 | After AF |
| 62 | P   | Chardonnay | 2017 | After AF |
| 63 | Ltm | Sémillon   | 2017 | After AF |
| 64 | Ltm | Sémillon   | 2017 | After AF |
| 65 | Ltm | Sémillon   | 2017 | After AF |
| 66 | Ltm | Sémillon   | 2017 | After AF |
| 67 | Y   | Sauvignon  | 2017 | After AF |
| 68 | Y   | Sauvignon  | 2017 | After AF |
| 69 | Y   | Sauvignon  | 2017 | After AF |
| 70 | Y   | Sauvignon  | 2017 | After AF |
| 71 | Y   | Sauvignon  | 2017 | After AF |
| 72 | Y   | Sauvignon  | 2017 | After AF |
| 73 | Y   | Sauvignon  | 2017 | After AF |
| 74 | Y   | Sauvignon  | 2017 | After AF |
| 75 | Shl | Sauvignon  | 2017 | After AF |
| 76 | Shl | Sauvignon  | 2017 | After AF |
| 77 | Shl | Sauvignon  | 2017 | After AF |
| 78 | Shl | Sauvignon  | 2017 | After AF |
| 79 | Shl | Sauvignon  | 2017 | After AF |
| 80 | Shl | Sauvignon  | 2017 | After AF |
| 81 | Shl | Sauvignon  | 2017 | After AF |
| 82 | Shl | Sauvignon  | 2017 | After AF |
| 83 | Shl | Sauvignon  | 2017 | After AF |
| 84 | Shl | Sauvignon  | 2017 | After AF |
| 85 | L   | Sémillon   | 2017 | After AF |
| 86 | L   | Sémillon   | 2017 | After AF |
| 87 | M   | Sauvignon  | 2017 | After AF |
| 88 | M   | Sauvignon  | 2017 | After AF |
| 89 | M   | Sauvignon  | 2017 | After AF |
| 90 | M   | Sauvignon  | 2017 | After AF |
| 91 | M   | Sauvignon  | 2017 | After AF |
| 92 | M   | Sauvignon  | 2017 | After AF |

<sup>a</sup> After AF: analysis just after alcoholic fermentation.