

# Phytochemical Analysis of Extracts from Waste of Technical Grape Varieties and Pomegranate Peel Processed in South Kazakhstan

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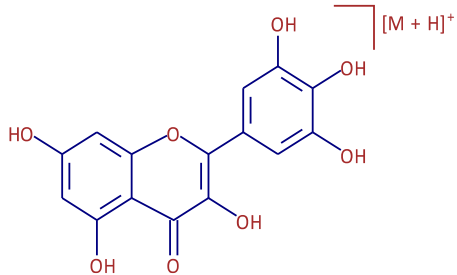
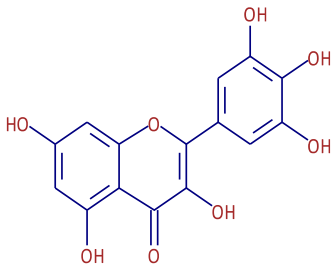
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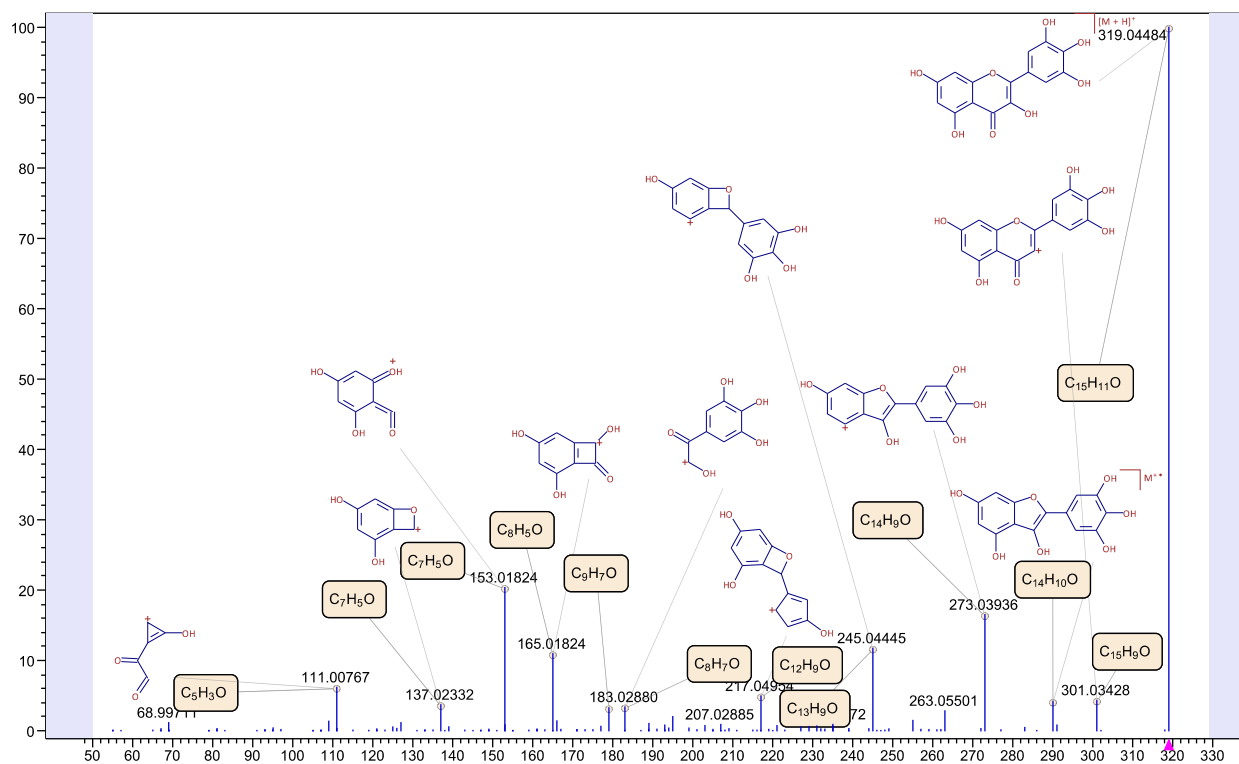
**Supplementary Figure S1:** The most remarkable examples of ion chromatogram mass spectra of aqueous-alcohol extraction of pomegranate peel obtained by tandem mass spectrometry in the positive mode. All compounds presented in the Supporting Information were tentatively identified using high-resolution LC-QTOF-MS/MS based on accurate mass measurements, molecular formula prediction, MS/MS fragmentation patterns, and comparison with spectral databases.

**Supplementary Figure S2:** The most remarkable examples of ion chromatogram mass spectra of aqueous-alcohol extraction of pomace mixture from two grape varieties (Saperavi and Cabernet Sauvignon) obtained by tandem mass spectrometry in the positive mode. All compounds presented in the Supporting Information were tentatively identified using high-resolution LC-QTOF-MS/MS based on accurate mass measurements, molecular formula prediction, MS/MS fragmentation patterns, and comparison with spectral databases.

## Supplementary Figure S1

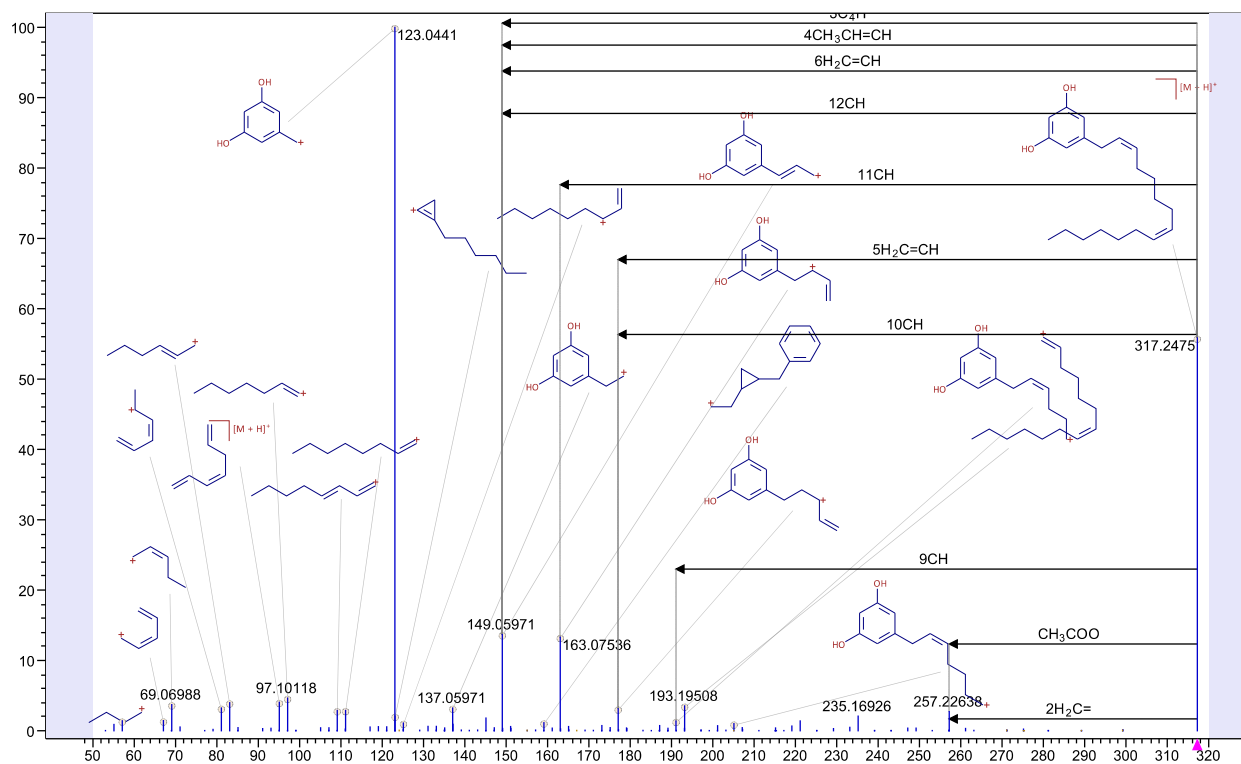
### Myricetin

| Precursor structure                                                                 | Compound structure                                                                    |
|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
|  |  |
| C <sub>15</sub> H <sub>11</sub> O <sup>+</sup> <sub>8</sub> m/z: 319.04484          | C <sub>15</sub> H <sub>10</sub> O <sub>8</sub> MM: 318.03757                          |



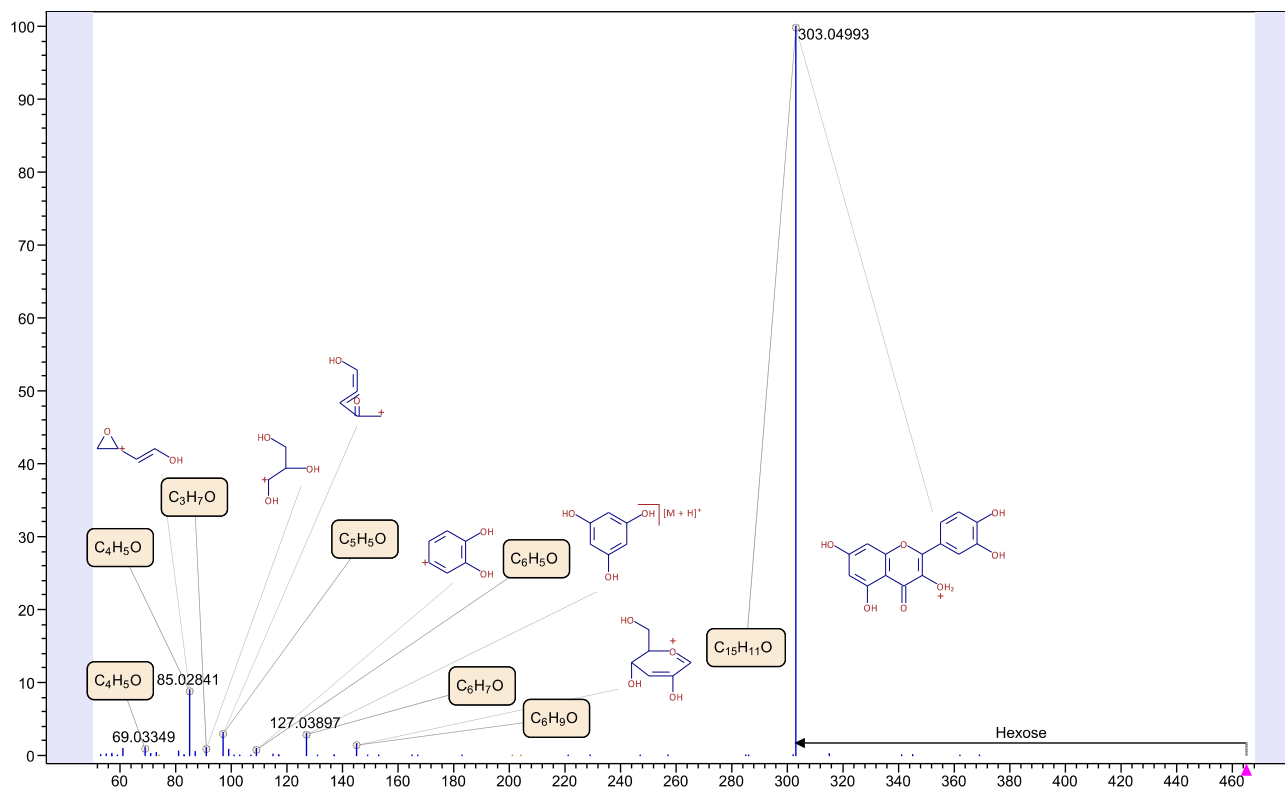
### 5 Z 8 Z 2 8 Pentadecadien 1 yl 1 3 benzenediol

| Precursor structure                | Compound structure              |
|------------------------------------|---------------------------------|
|                                    |                                 |
| $C_{21}H_{32}O^+_2$ m/z: 317.24751 | $C_{21}H_{32}O_2$ MM: 316.24023 |



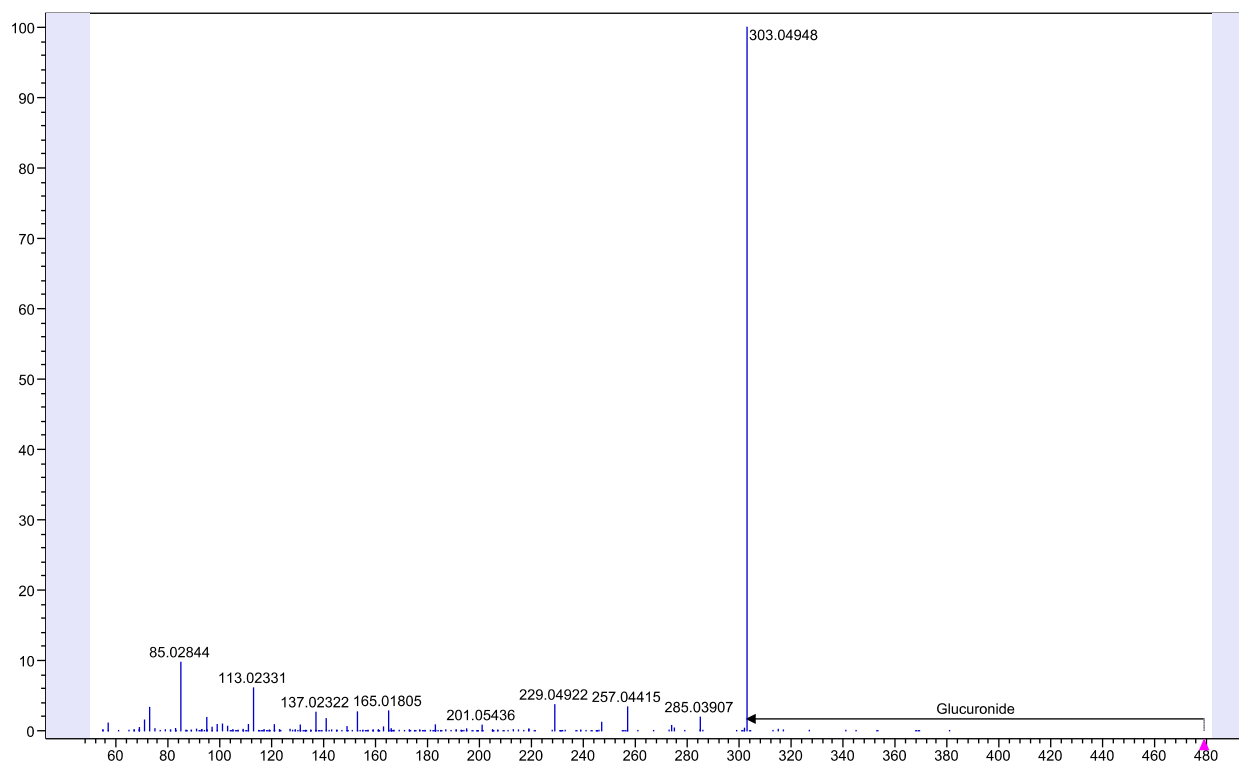
## Isoquercitrin

| Precursor structure                                             | Compound structure                                      |
|-----------------------------------------------------------------|---------------------------------------------------------|
|                                                                 |                                                         |
| $\text{C}_{21}\text{H}_{21}\text{O}^{+}_{12}$ $m/z$ : 465.10275 | $\text{C}_{21}\text{H}_{20}\text{O}_{12}$ MM: 464.09548 |



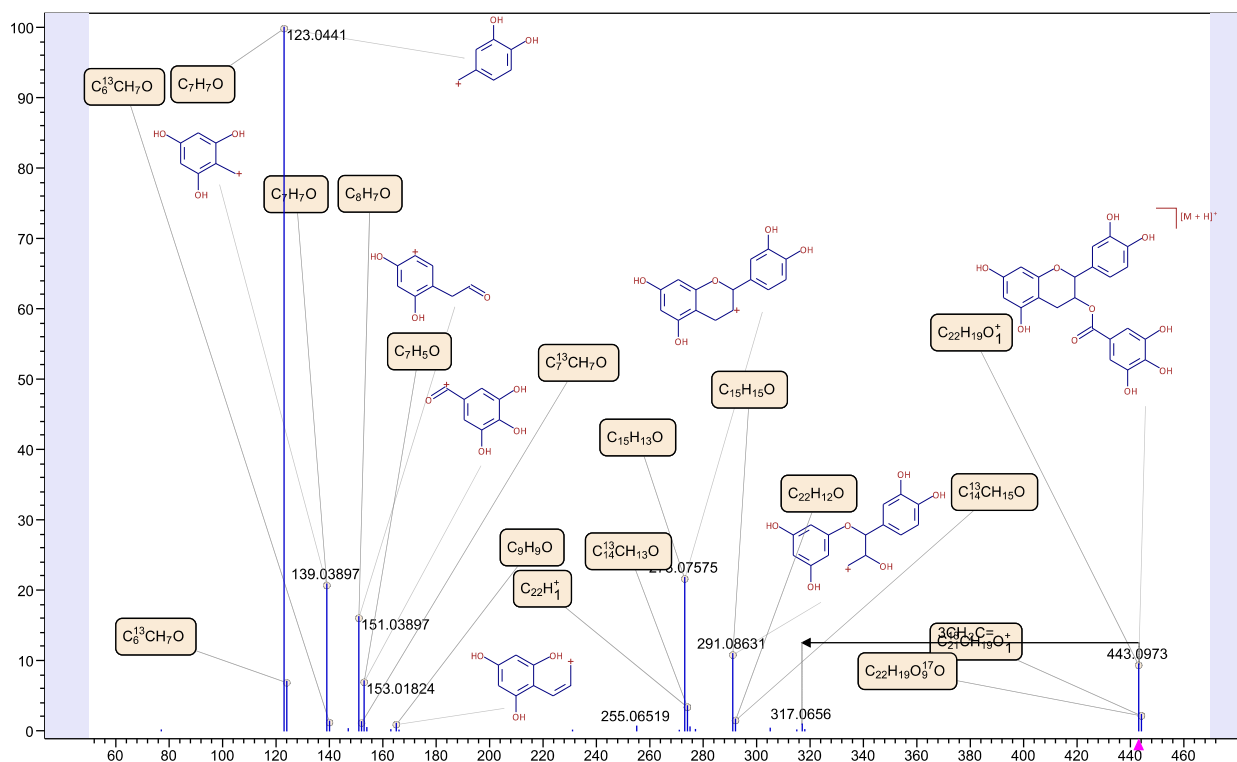
## Miquelianin

| Precursor structure | Compound structure                                            |
|---------------------|---------------------------------------------------------------|
|                     |                                                               |
|                     | C <sub>21</sub> H <sub>18</sub> O <sub>13</sub> MM: 478.07474 |

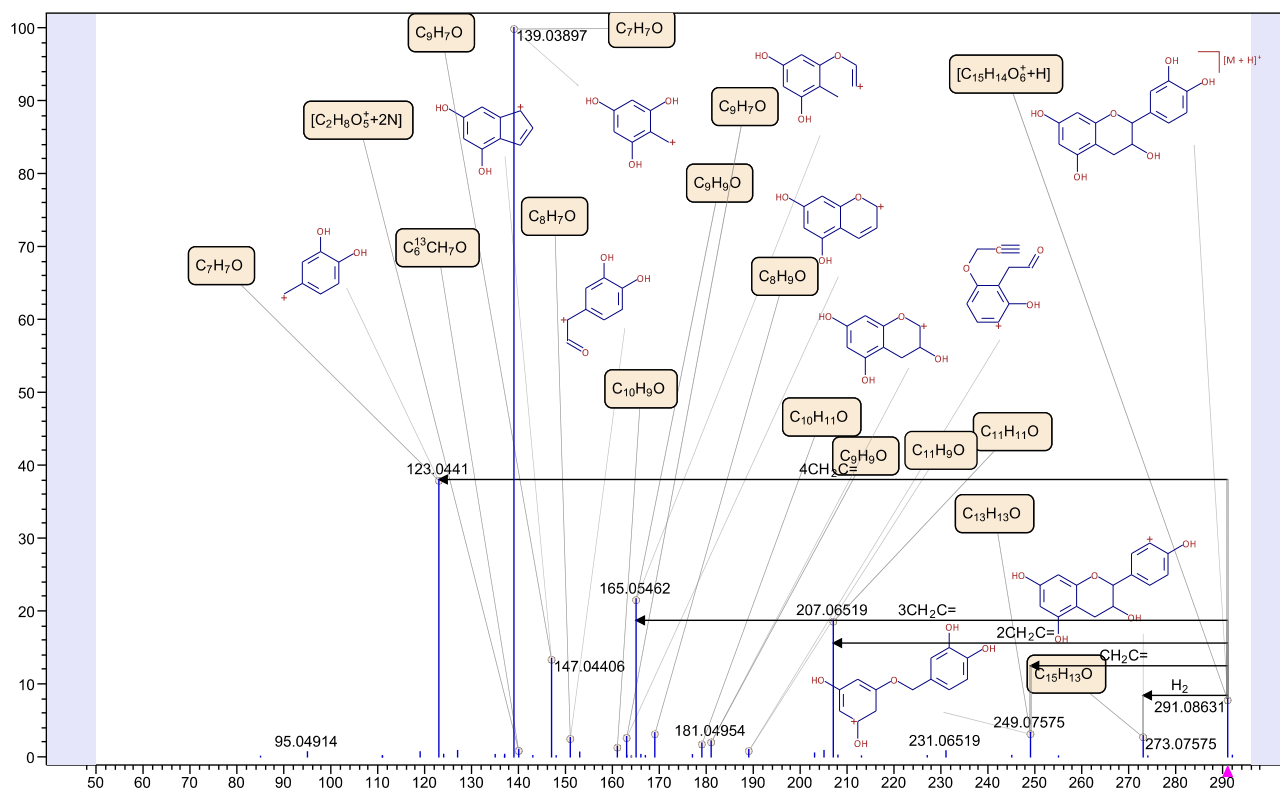


## Catechin gallate

| Precursor structure                                                         | Compound structure                                            |
|-----------------------------------------------------------------------------|---------------------------------------------------------------|
|                                                                             |                                                               |
| C <sub>22</sub> H <sub>19</sub> O <sub>10</sub> <sup>+</sup> m/z: 443.09727 | C <sub>22</sub> H <sub>18</sub> O <sub>10</sub> MM: 442.09000 |

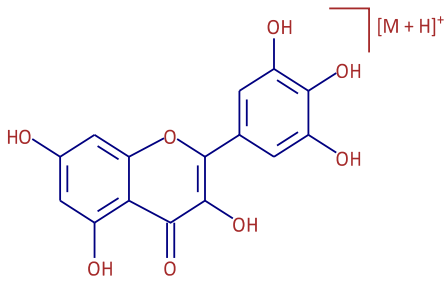
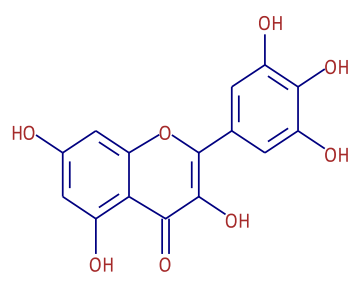


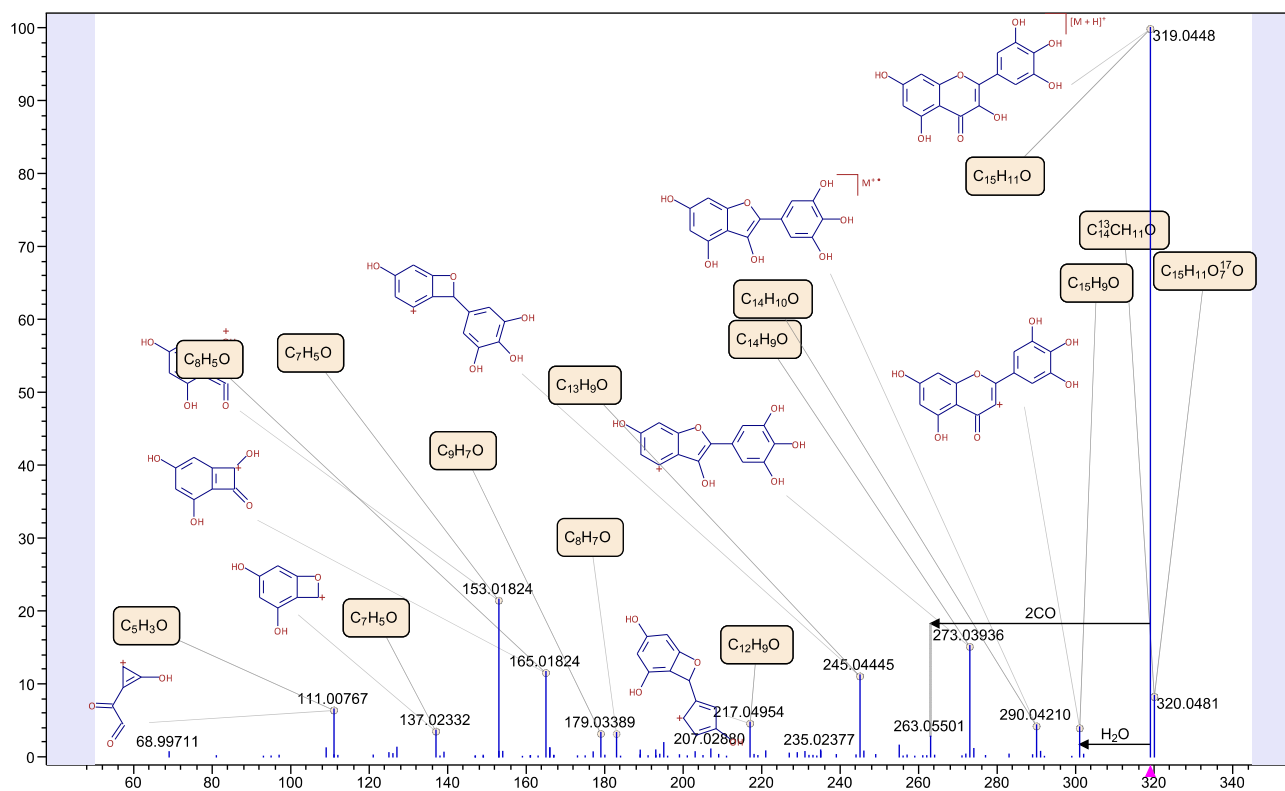
## Catechin



## Supplementary Figure S2

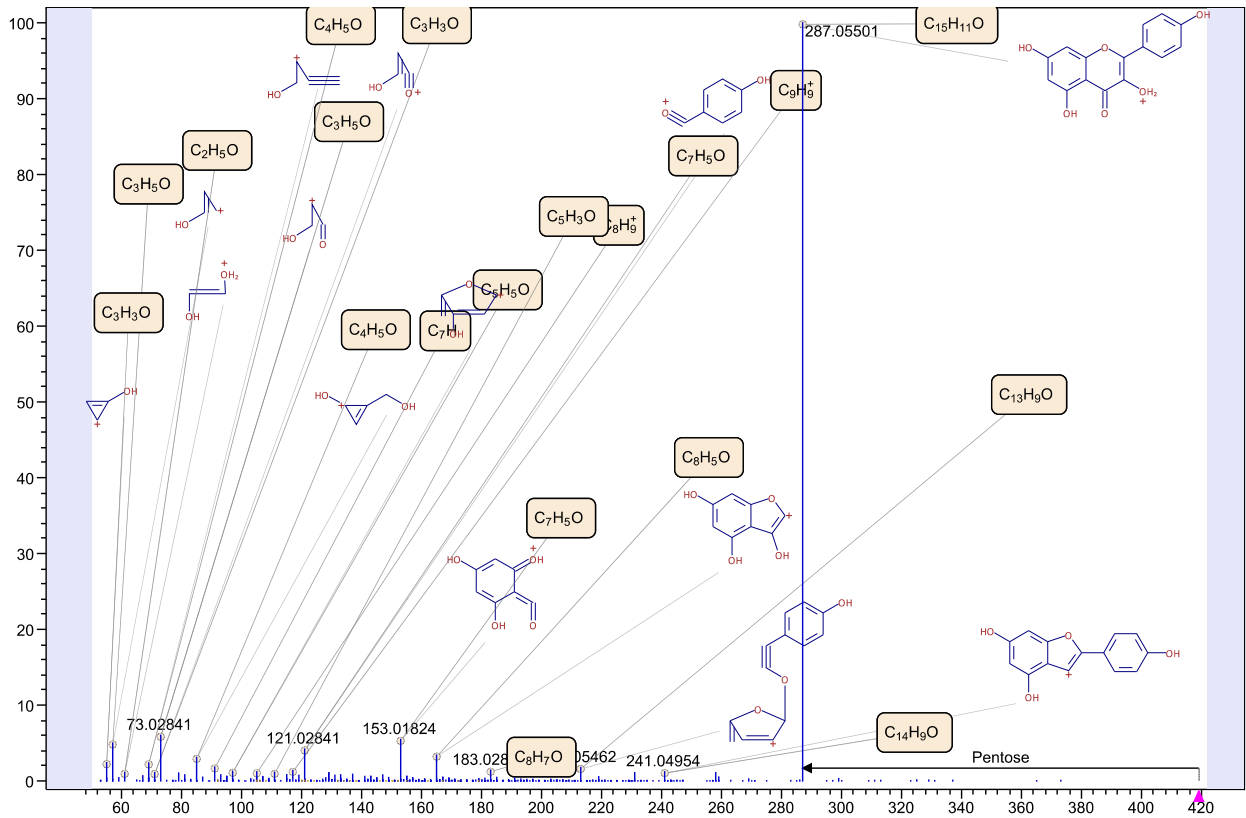
### Myricetin

| Precursor structure                                                               | Compound structure                                                                 |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| C15H11O8 <sup>+</sup> m/z: 319.04484                                              | C15H10O8MM: 318.03757                                                              |

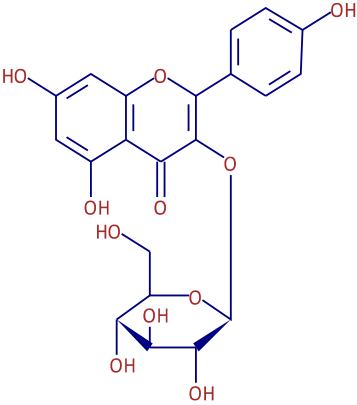


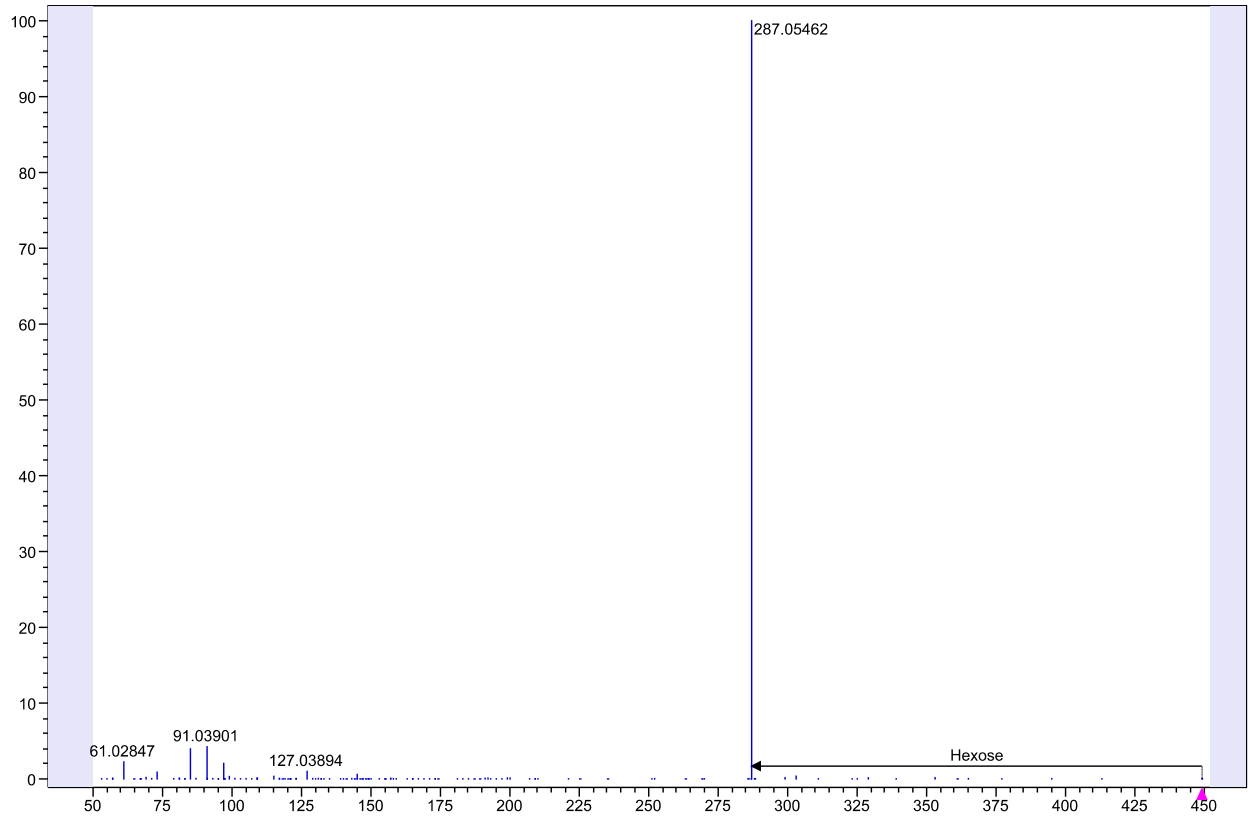
Kaempferol 3-O-beta-D-xylofuranoside

| Precursor structure | Compound structure    |
|---------------------|-----------------------|
|                     |                       |
|                     | C20H18O10MM: 418,0899 |

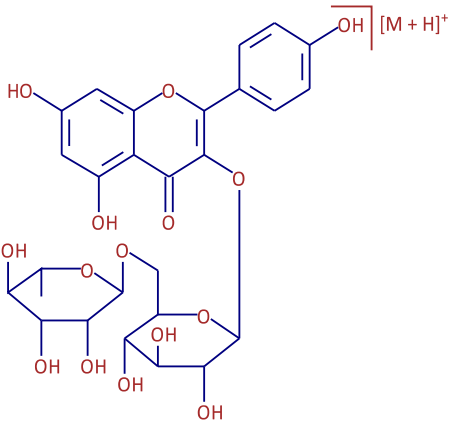
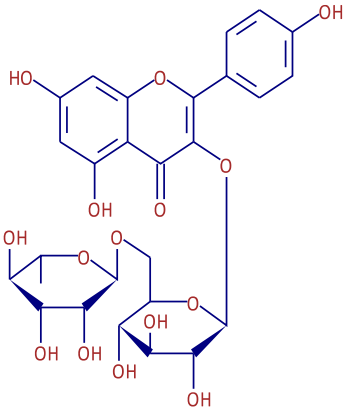


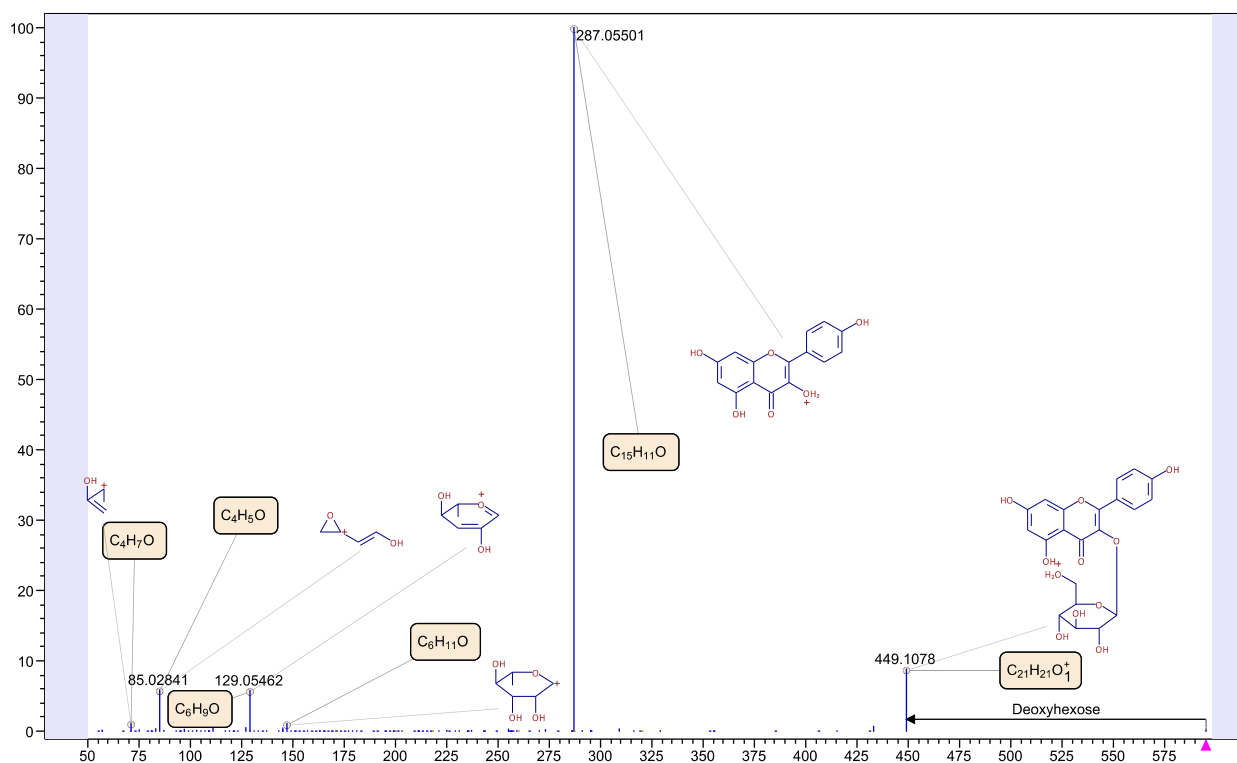
Kaempferol-3-O-galactoside

| Precursor structure | Compound structure                                                                  |
|---------------------|-------------------------------------------------------------------------------------|
|                     |  |
|                     | C21H20O11 MM: 448.1006                                                              |

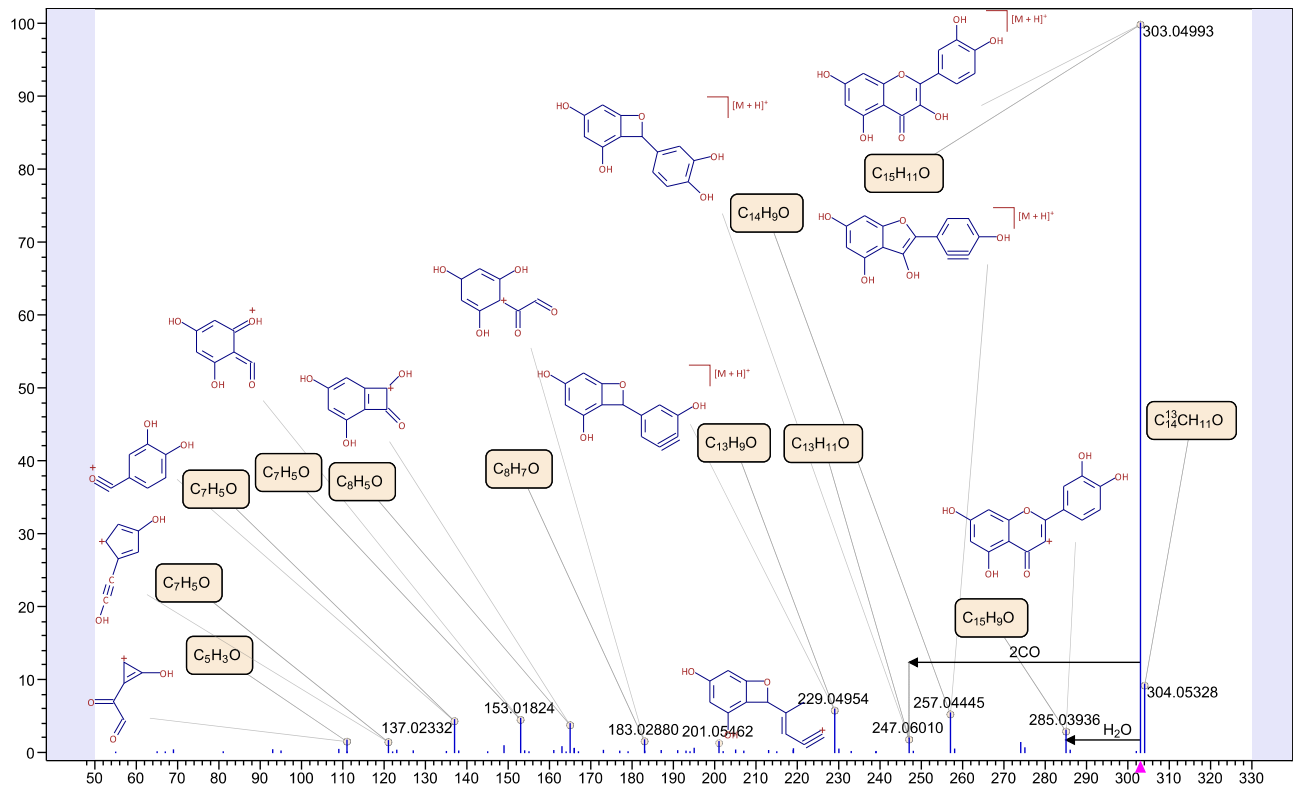


# Kaempferol 3-O-beta-glucopyranoside-7-O-alpha-rhamnopyranoside

| Precursor structure                                                               | Compound structure                                                                  |
|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|  |  |
| C <sub>27</sub> H <sub>31</sub> O <sub>15</sub> <sup>+</sup> m/z: 595.16575       | C <sub>27</sub> H <sub>30</sub> O <sub>15</sub> MM: 594.15847                       |

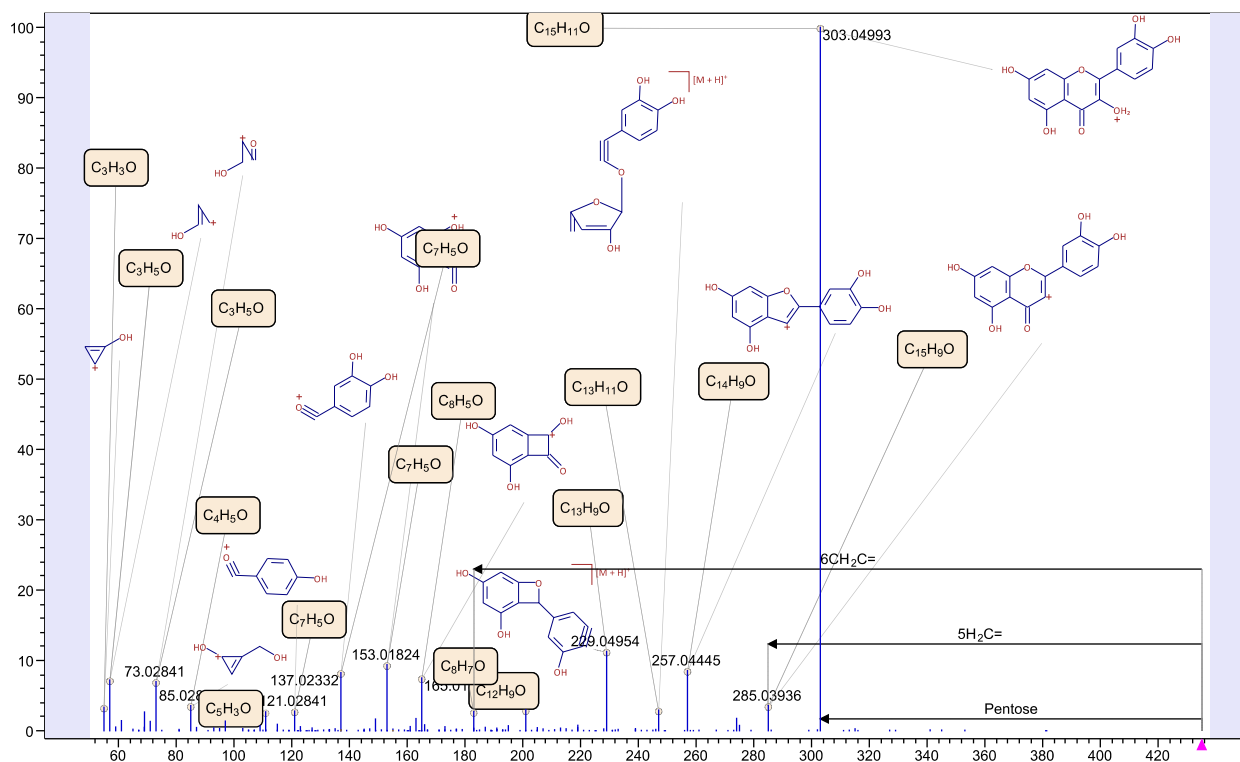


Quercetin

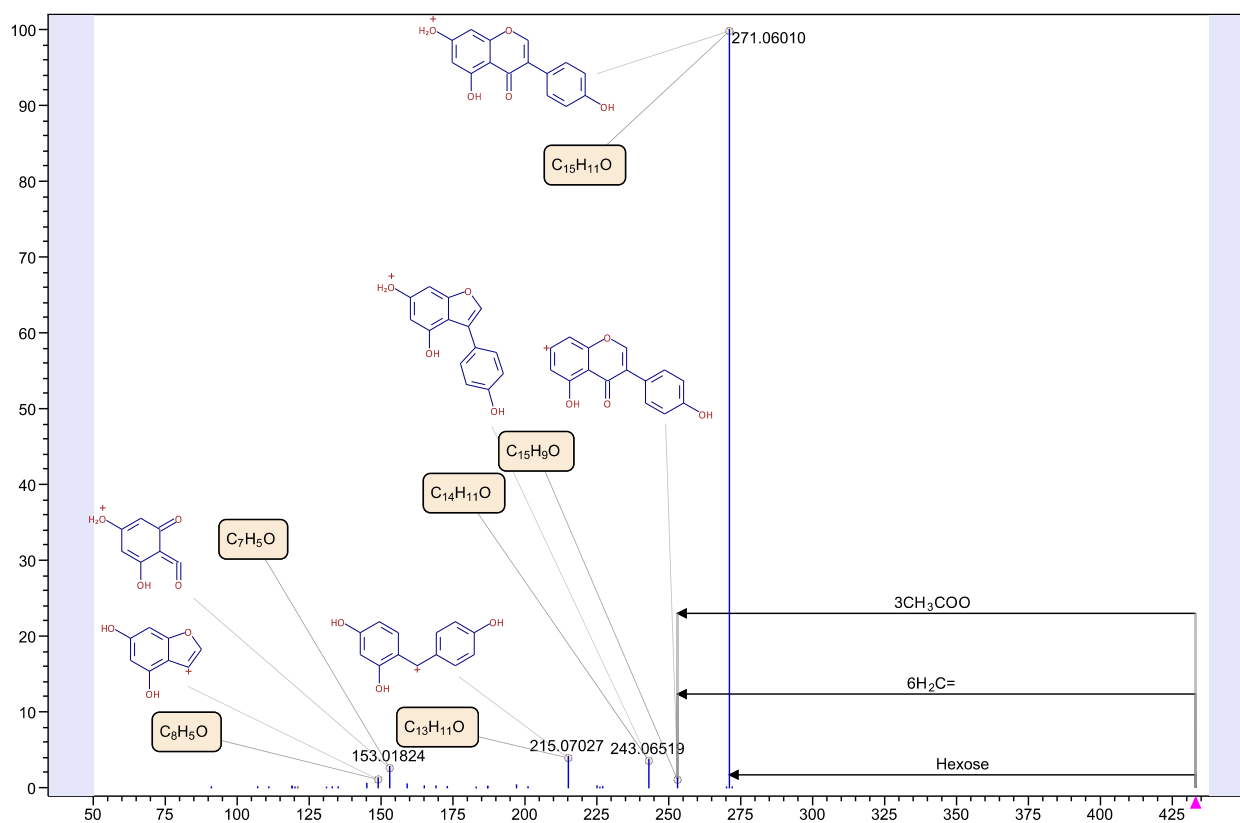


Quercetin-3-O- $\alpha$ -L-arabinoside

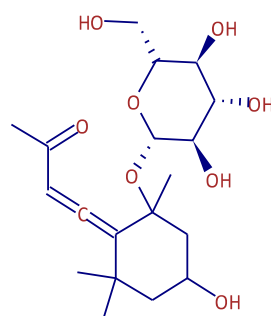
| Precursor structure | Compound structure                                            |
|---------------------|---------------------------------------------------------------|
|                     |                                                               |
|                     | C <sub>20</sub> H <sub>18</sub> O <sub>11</sub> MM: 434.08491 |

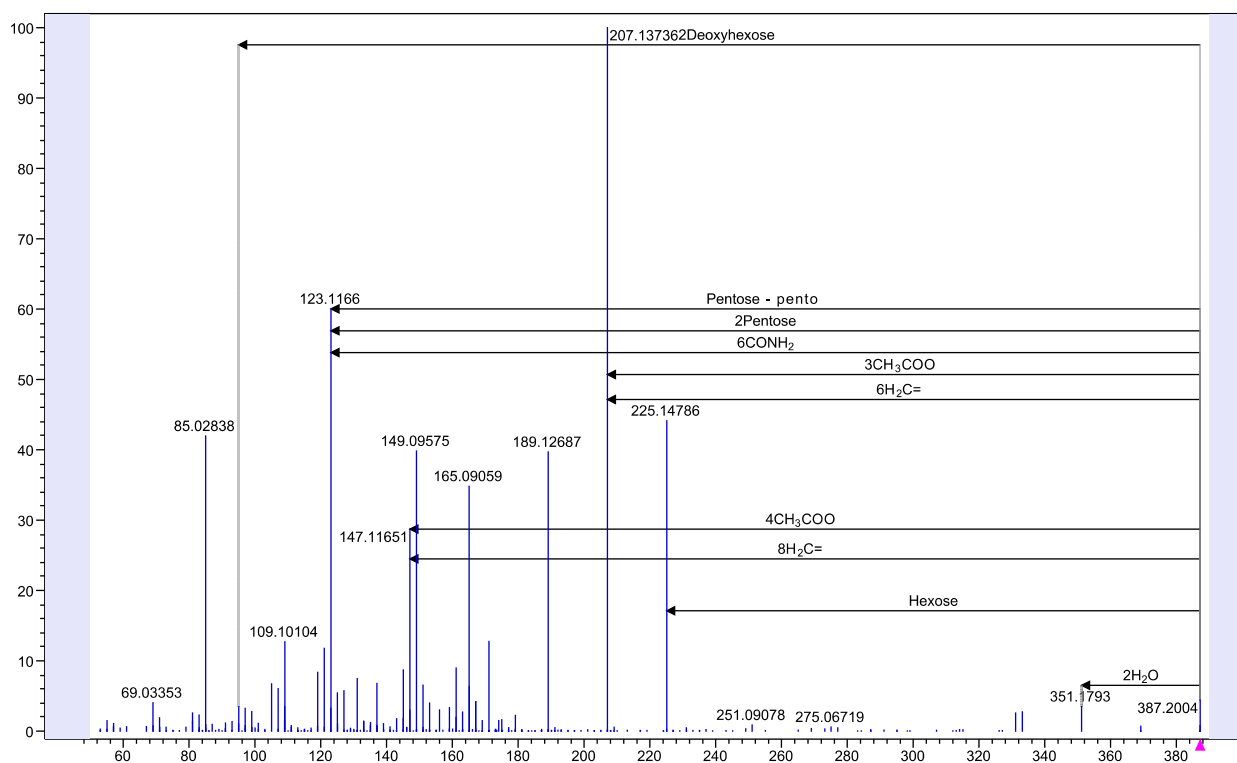


## Genistin

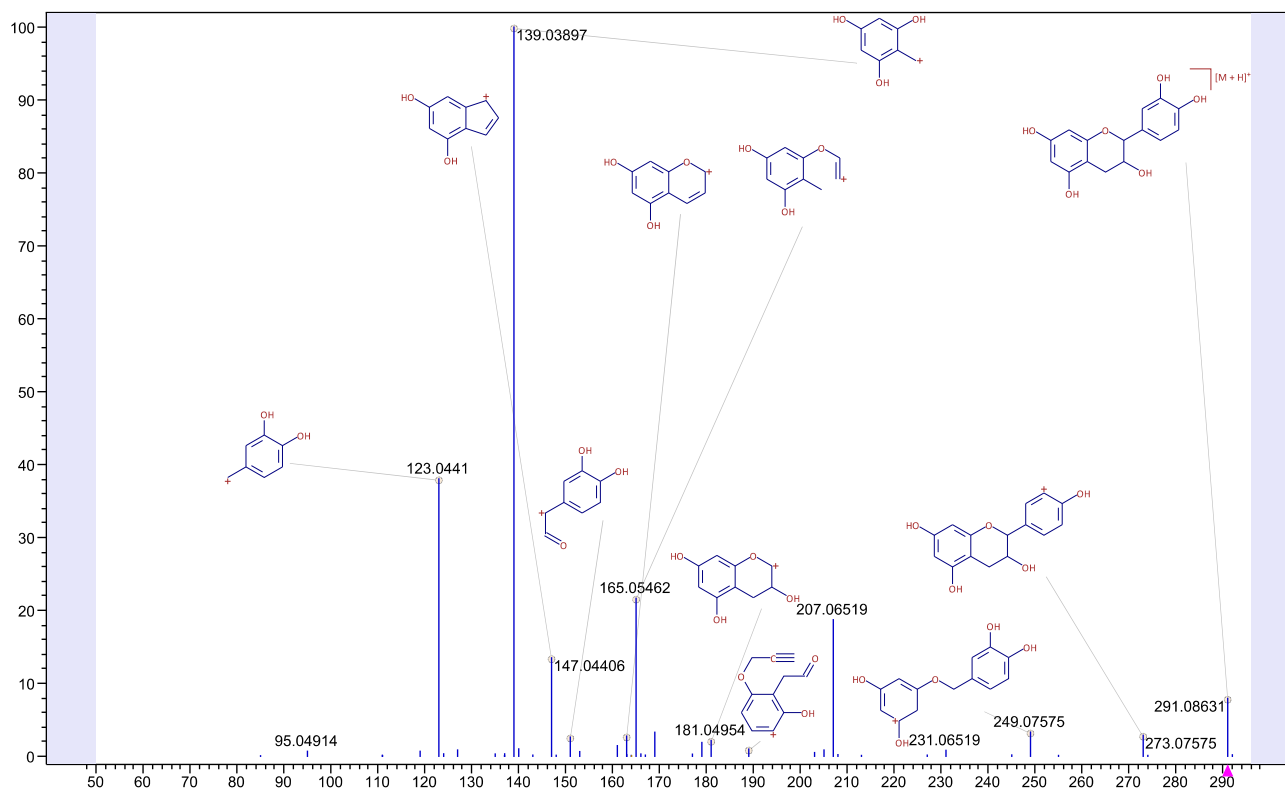


# Megastigmane glycoside

| Precursor structure                 | Compound structure                                                                  |
|-------------------------------------|-------------------------------------------------------------------------------------|
|                                     |  |
| C19H31O8 <sup>+</sup> m/z: 387.1931 | C19H30O8 MM: 386.1941                                                               |



## Catechin



## Epigallocatechin

