

Polyphenolic Profiling of Forestry Waste by UPLC-HDMS^E

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Supplementary information

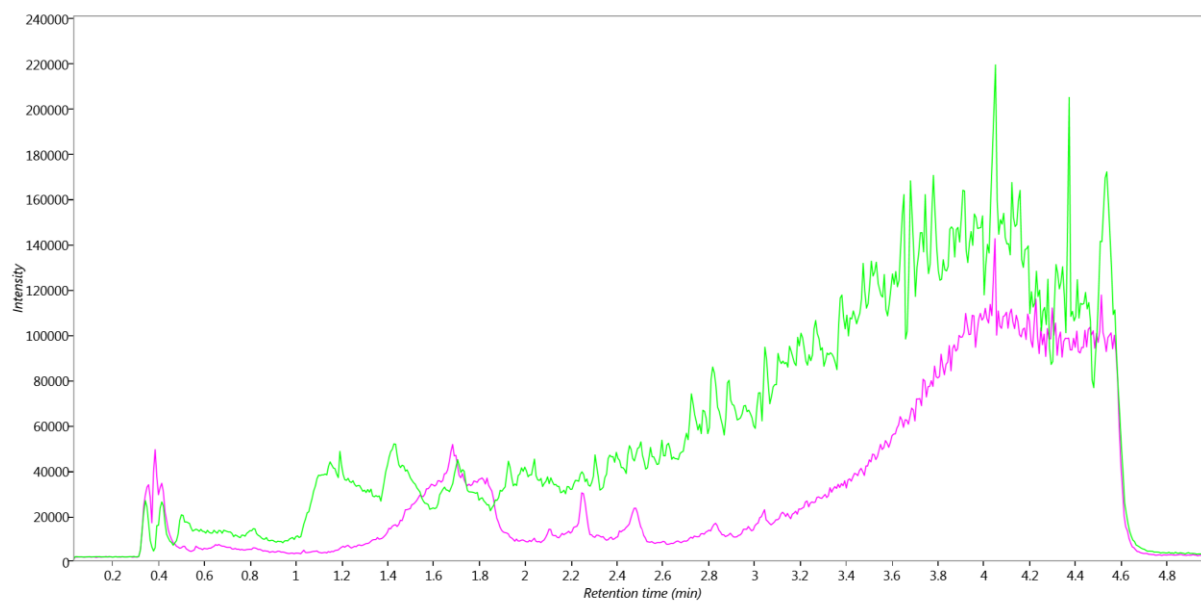


Figure S1. Total ion chromatogram of Lodge Pole Pine (green) and the alignment reference (magenta).

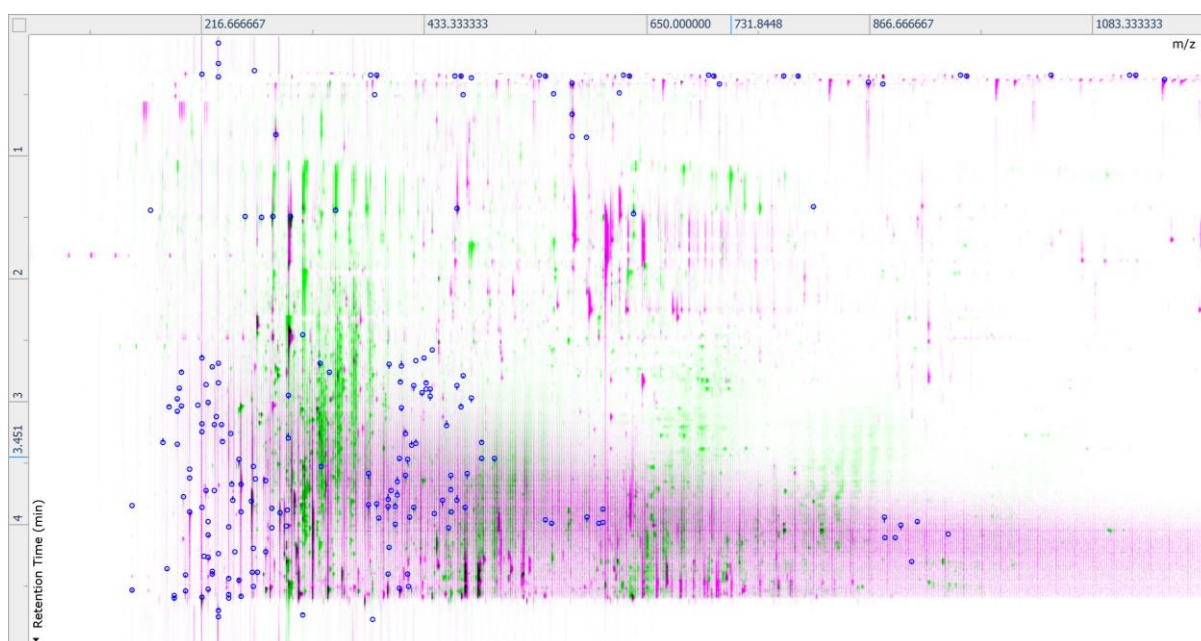


Figure S2. Ion intensity map of Lodge Pole Pine (green) and the alignment reference (magenta) used in vector editing.

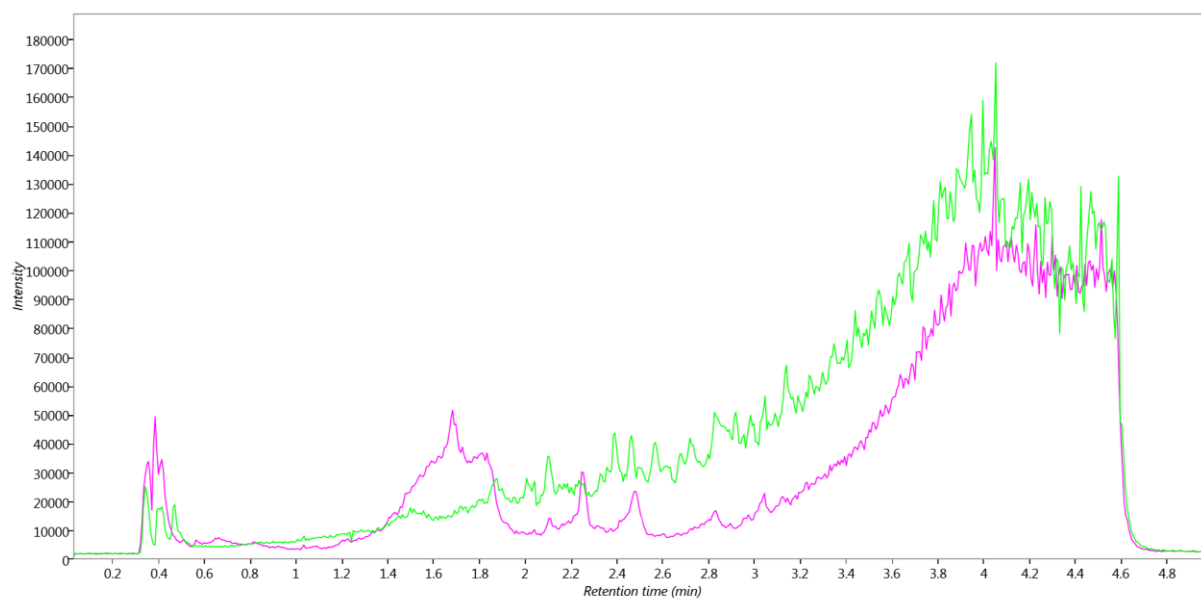


Figure S3. Total ion chromatogram of Oak (green) and the alignment reference (magenta).

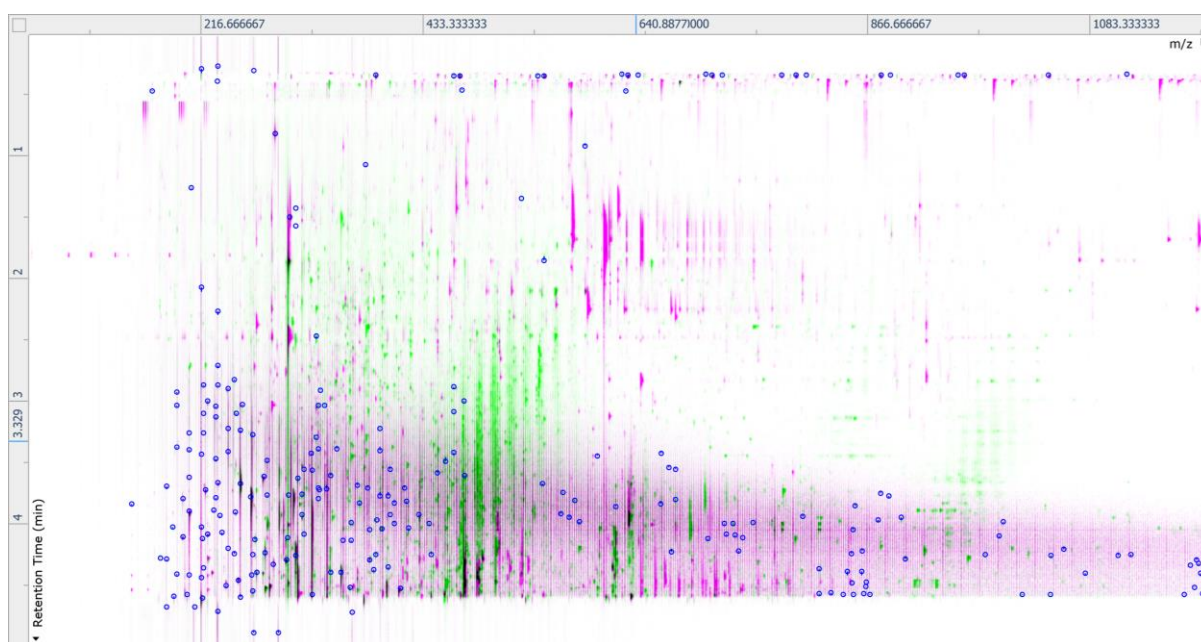


Figure S4. Ion intensity map of Oak (green) and the alignment reference (magenta) used in vector editing.

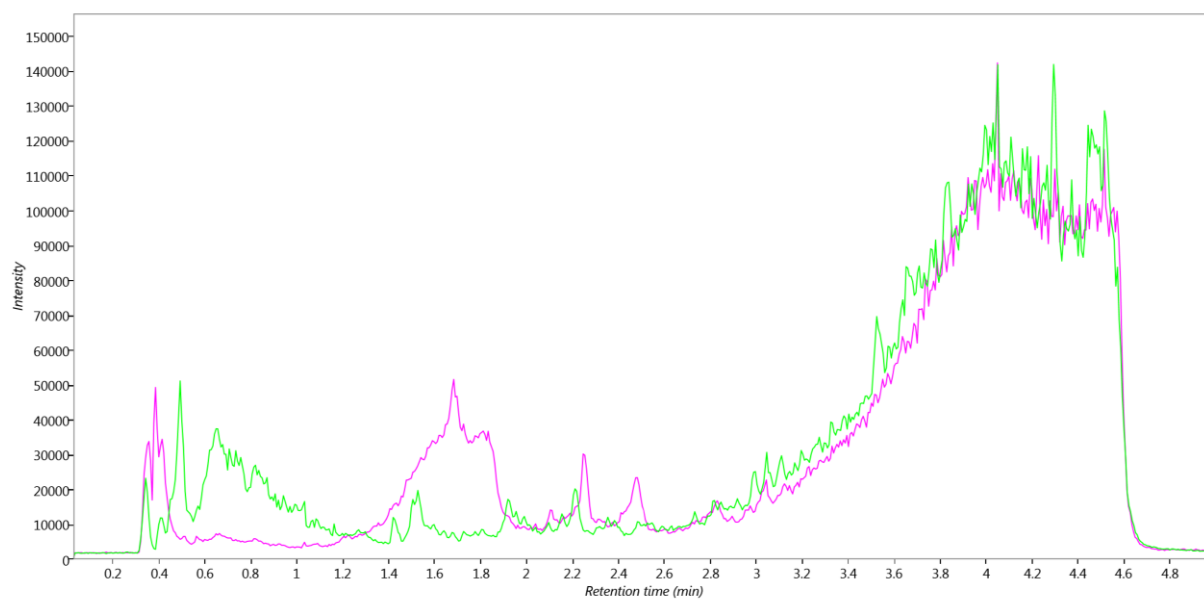


Figure S5. Total ion chromatogram of Scots Pine (green) and the alignment reference (magenta).

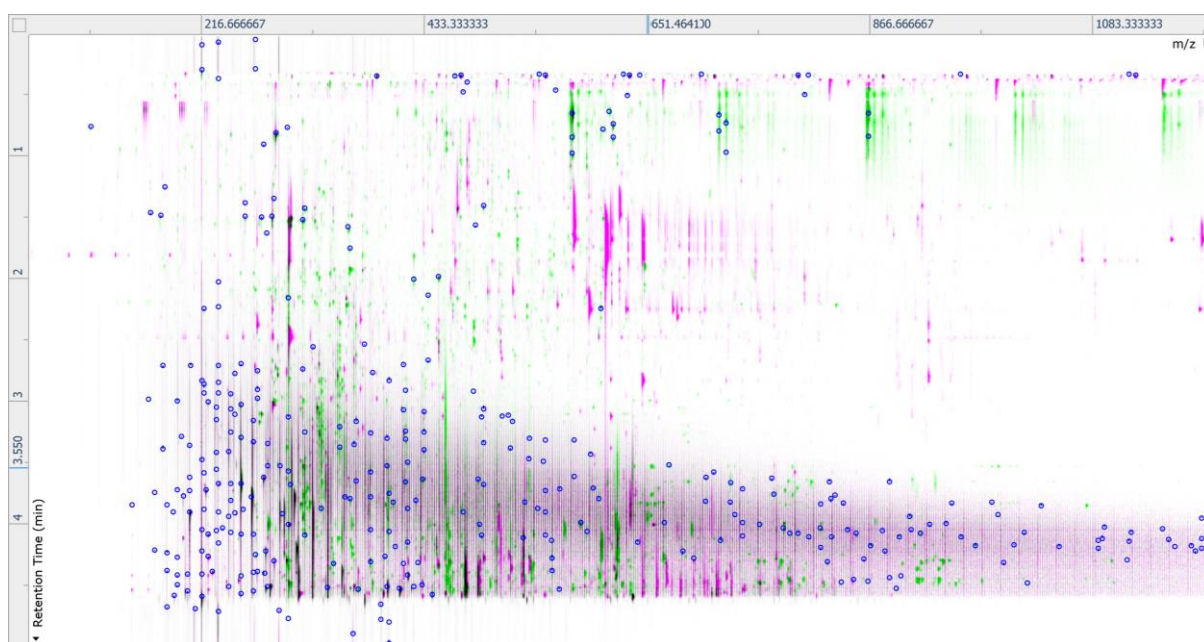


Figure S6. Ion intensity map of Scots Pine (green) and the alignment reference (magenta) used in vector editing.

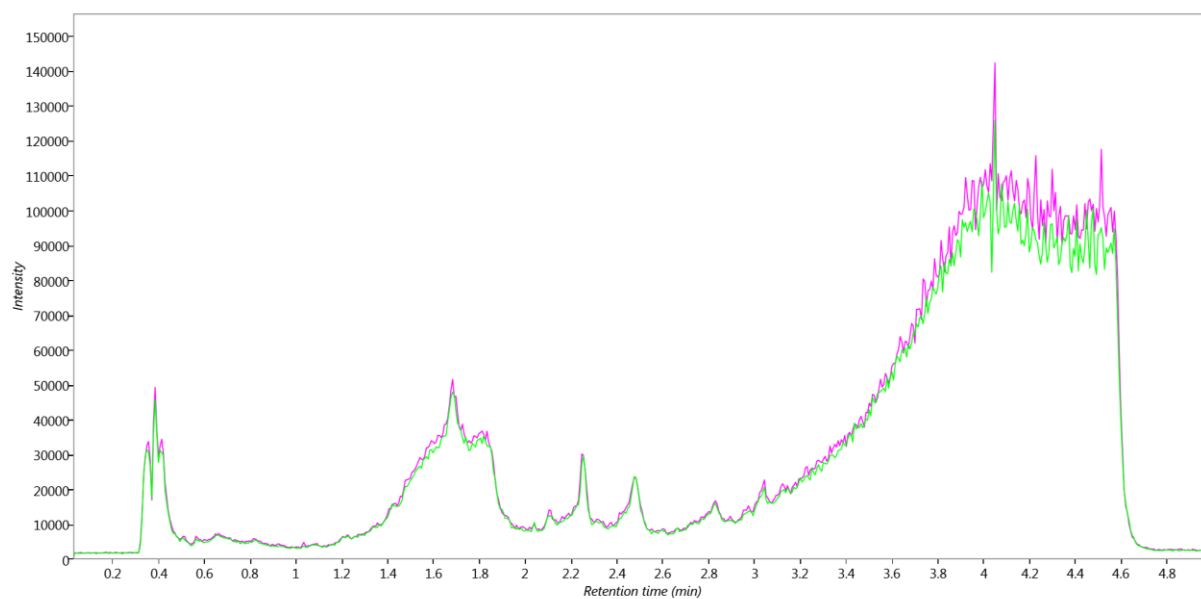


Figure S7. Total ion chromatogram of Pycnogenol (green) and the alignment reference (magenta).

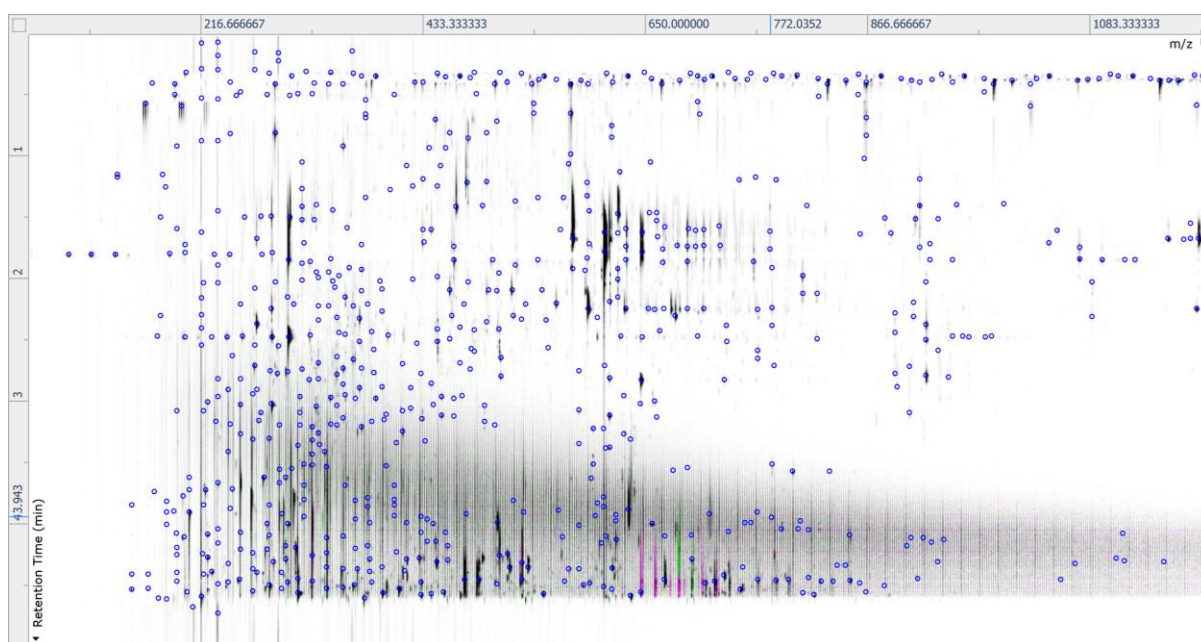
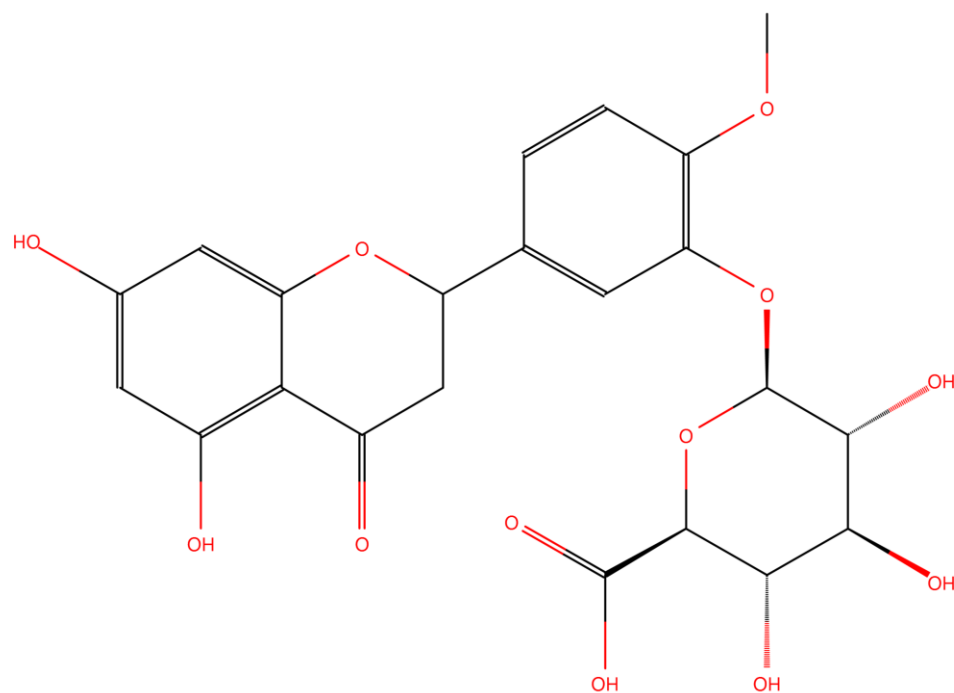
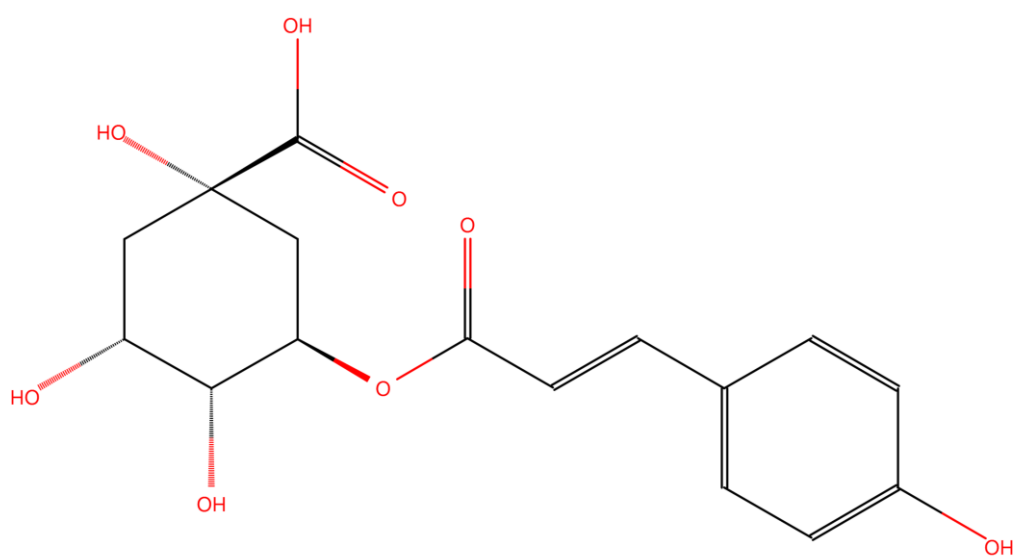
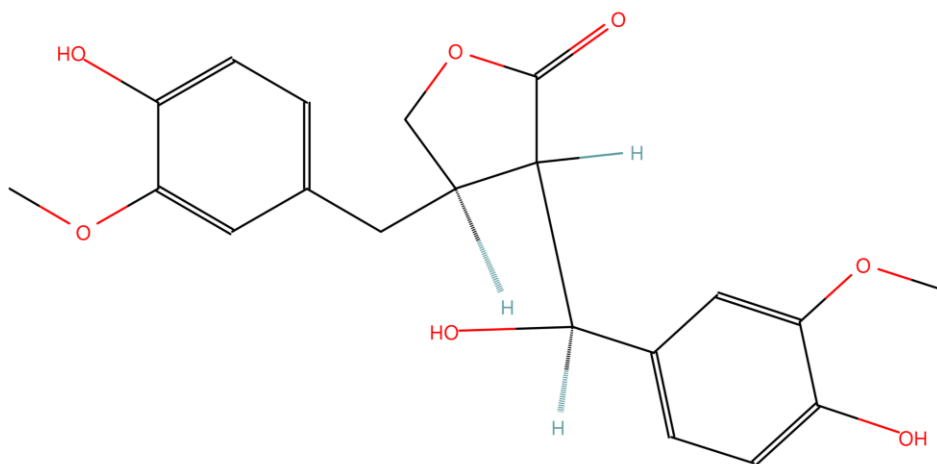


Figure S8. Ion intensity map of Pycnogenol (green) and the alignment reference (magenta) used in vector editing.

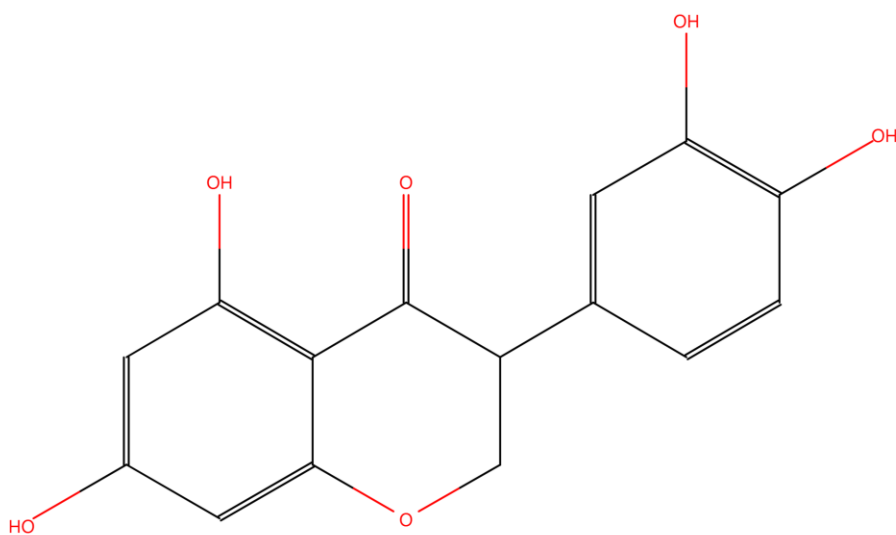


Isorhamnetin 3-glucoside - CSID32056973

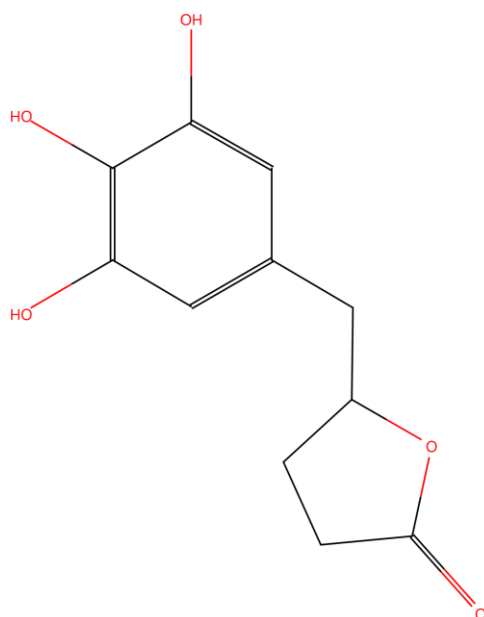
*trans*-5-O-(4-coumaroyl)-D-quinic acid - CSID4945466



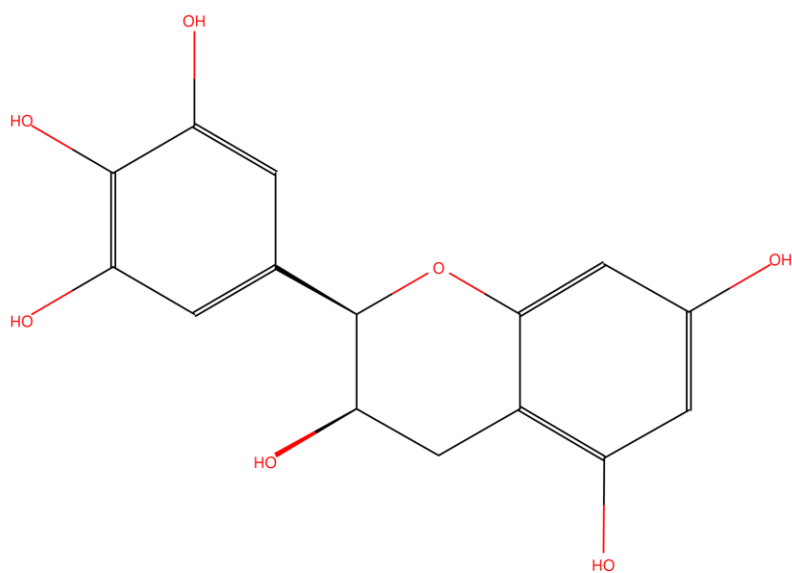
7-Hydroxymatairesinol - CSID59696173



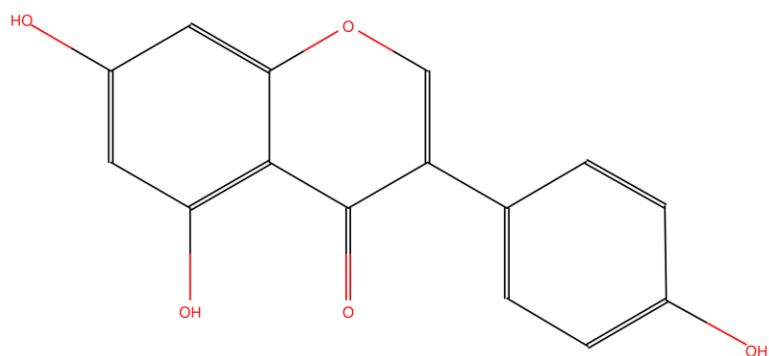
3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydro-4H-chromen-4-one - CSID35015212



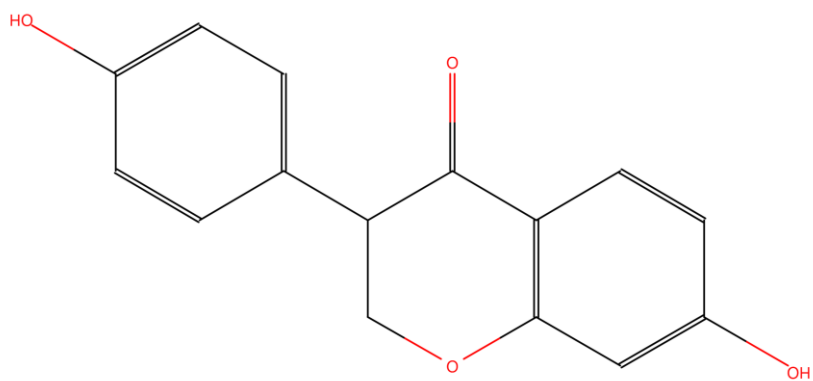
5-(3,4,5-Trihydroxybenzyl)dihydro-2(3H)-furanone - CSID23245203



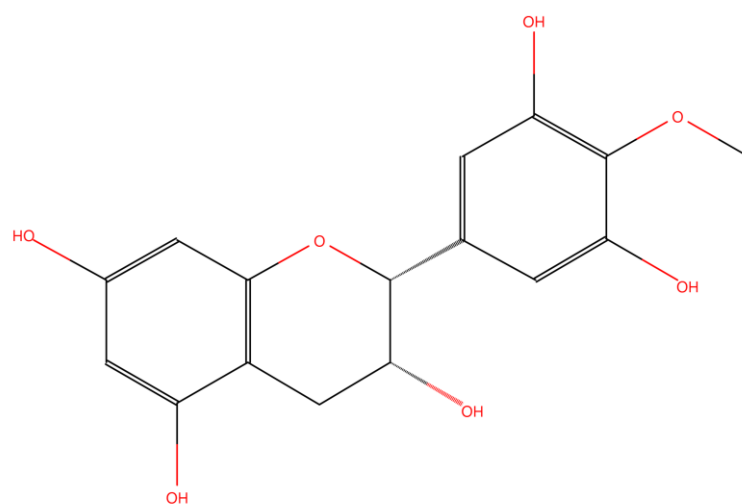
(-)-Epigallocatechin - CSID65231



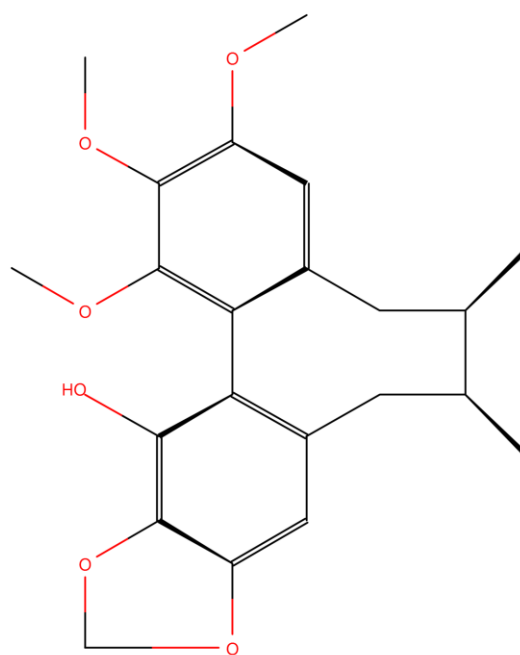
Genistein - CSID4444448



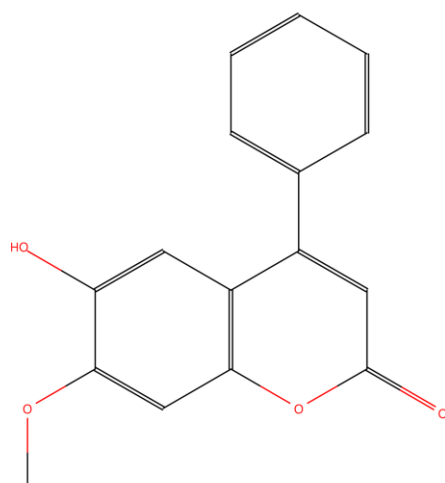
Dihydrodaidzein - CSID154076



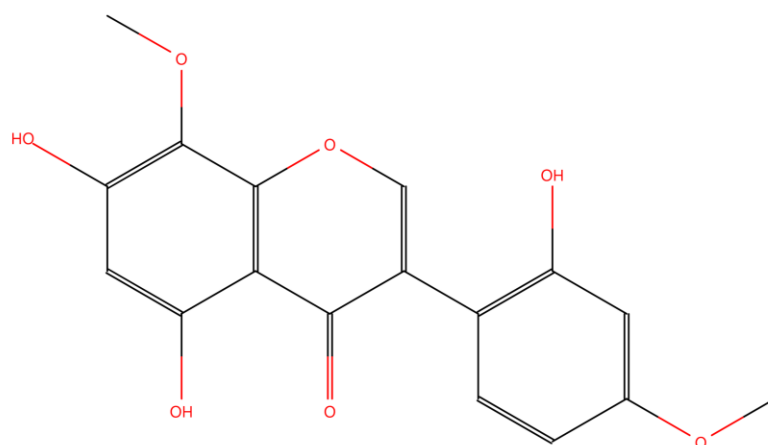
4'-Methylepigallocatechin - CSID154086



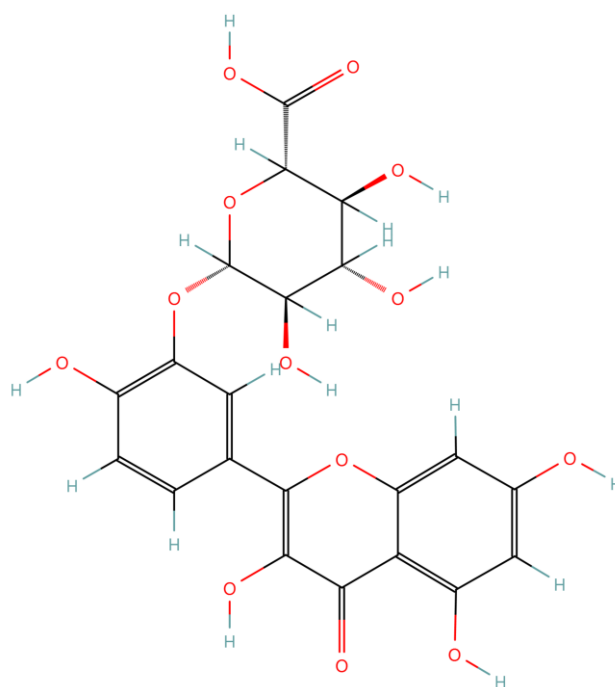
Gomisin M2 - CSID10278518



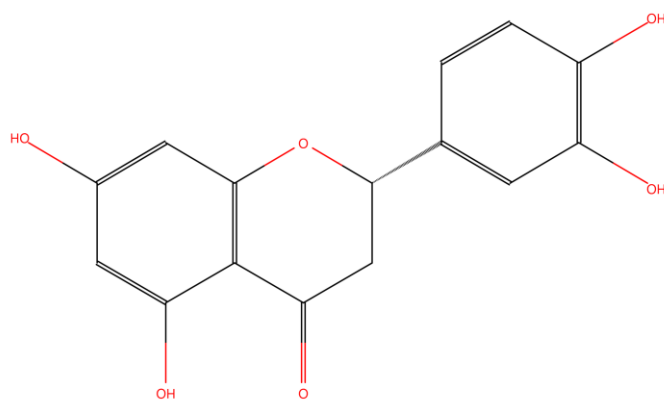
Dalbergin - CSID391108



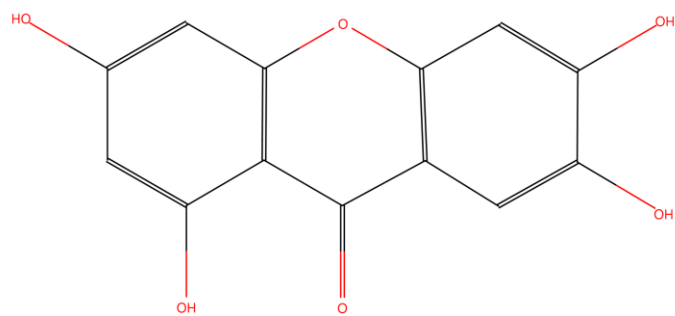
5,7-Dihydroxy-3-(2-hydroxy-4-methoxyphenyl)-8-methoxy-4H-chromen-4-one - CSID30777598



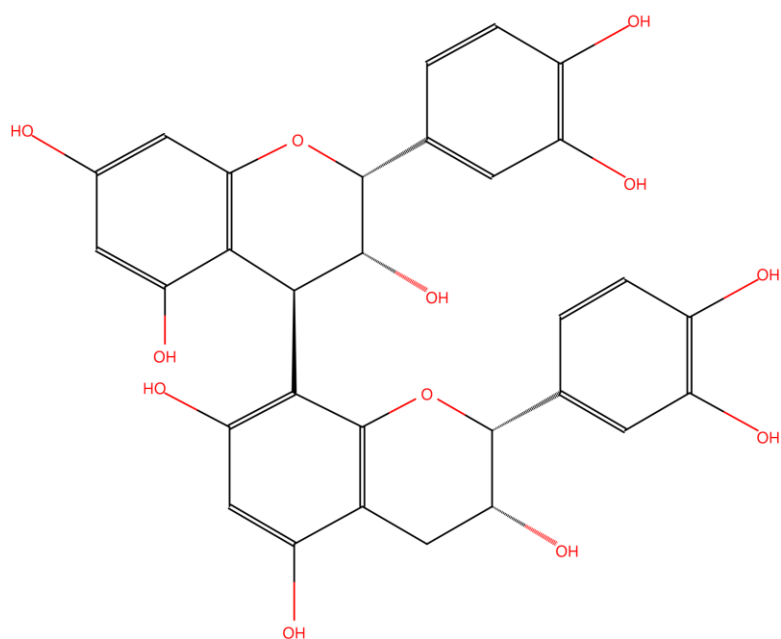
Quercetin-3'-Glucuronide - CSID9830649



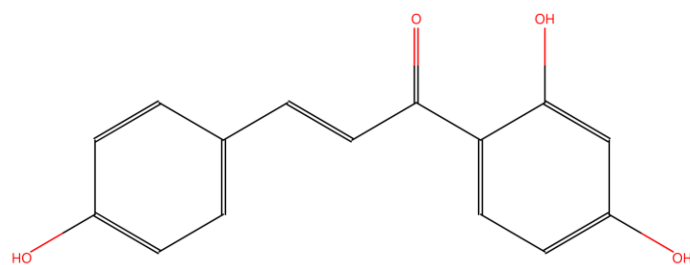
Eriodictyol - CSID389606



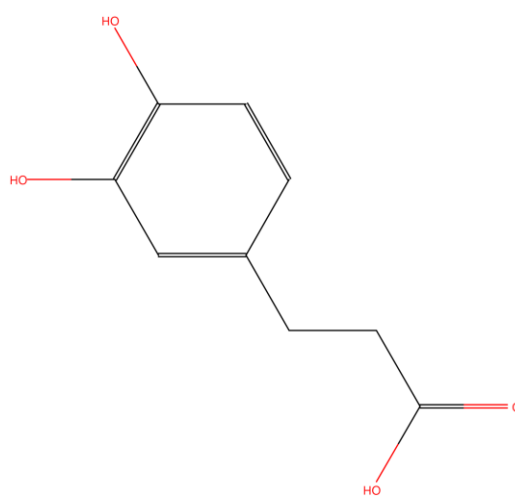
Norathyriol - CSID4444975



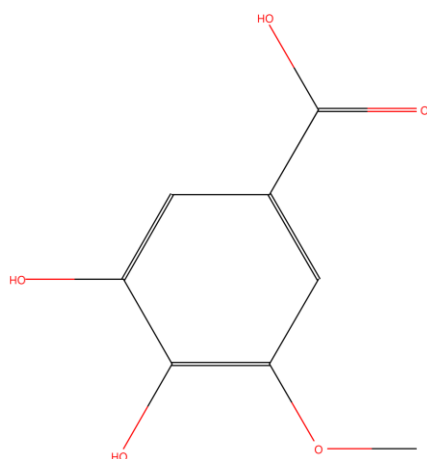
Procyanidin B2 - CSID109417



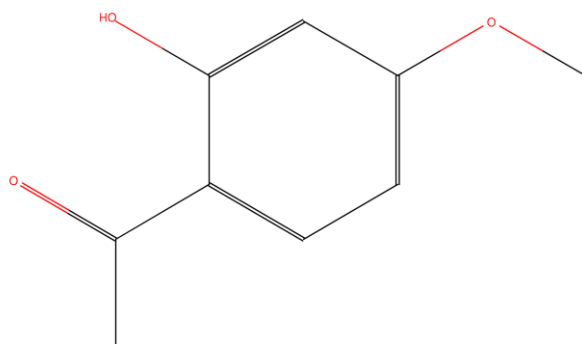
Isoliquiritigenin - CSID553829



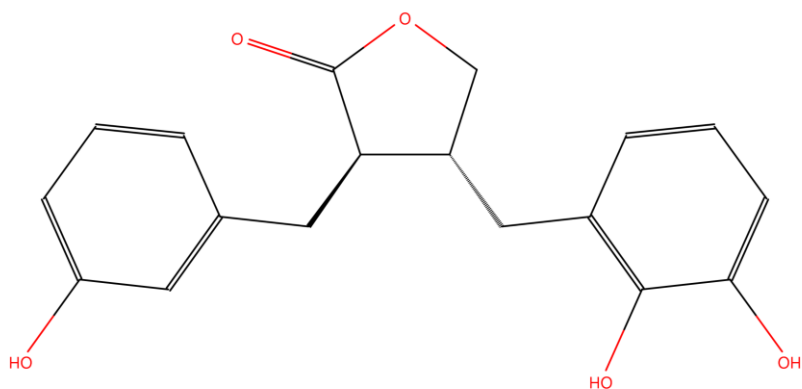
Dihydrocaffeic acid - CSID308986



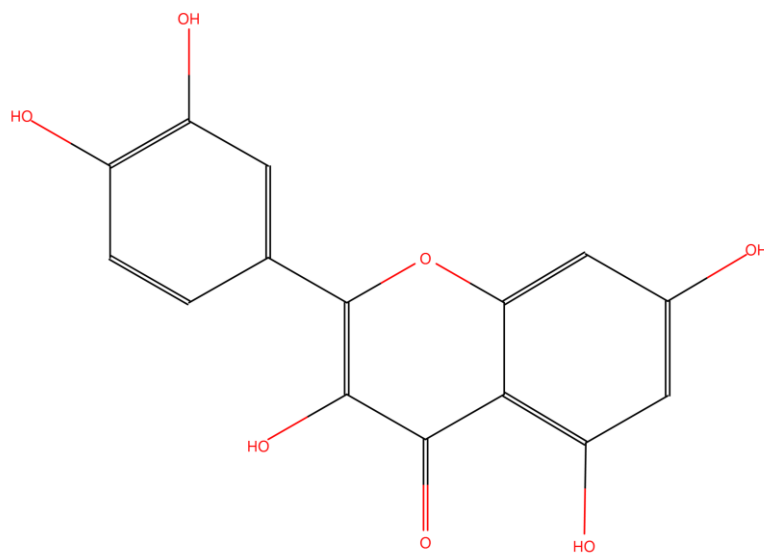
3,4-Dihydroxy-5-methoxybenzoic acid - CSID18679



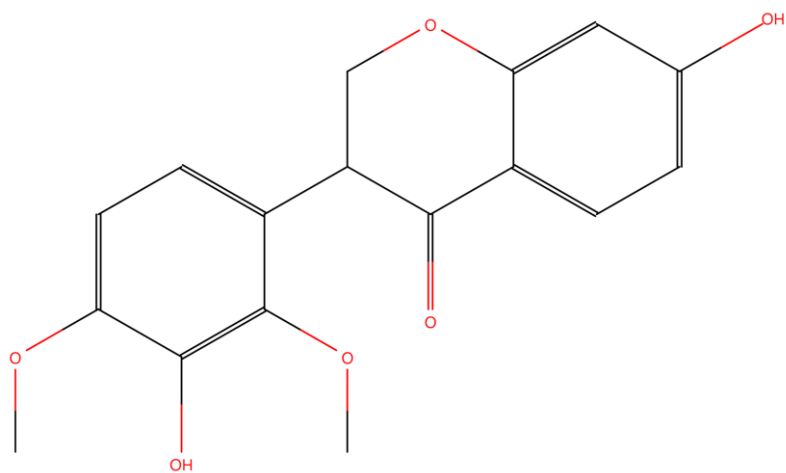
Paeonol - CSID10621



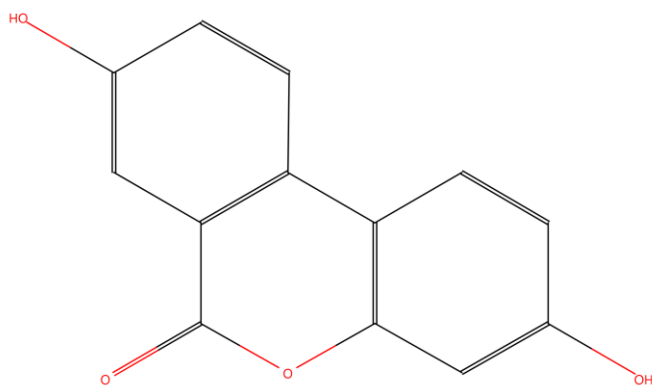
(3R,4R)-4-(2,3-Dihydroxybenzyl)-3-(3-hydroxybenzyl)dihydro-2(3H)-furanone - CSID30777587



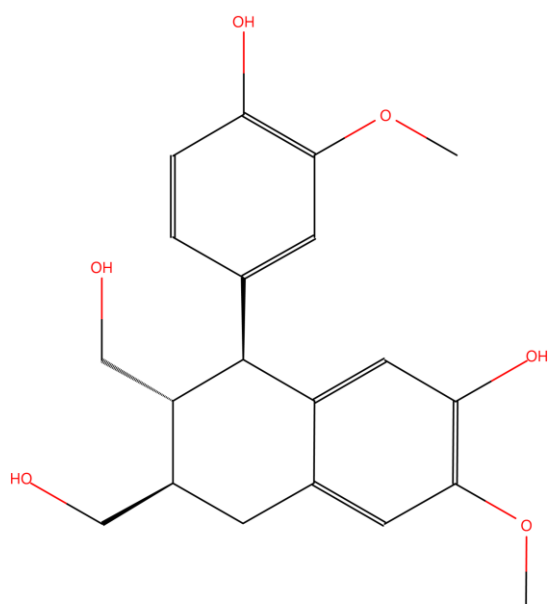
Quercetin - CSID4444051



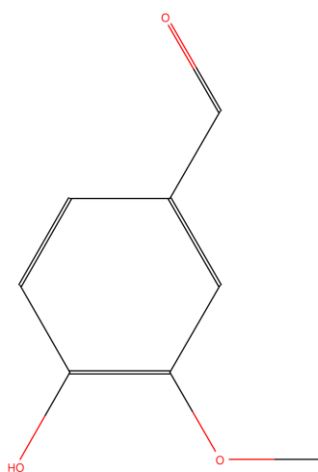
7-Hydroxy-3-(3-hydroxy-2,4-dimethoxyphenyl)-2,3-dihydro-4H-chromen-4-one - CSID24842912



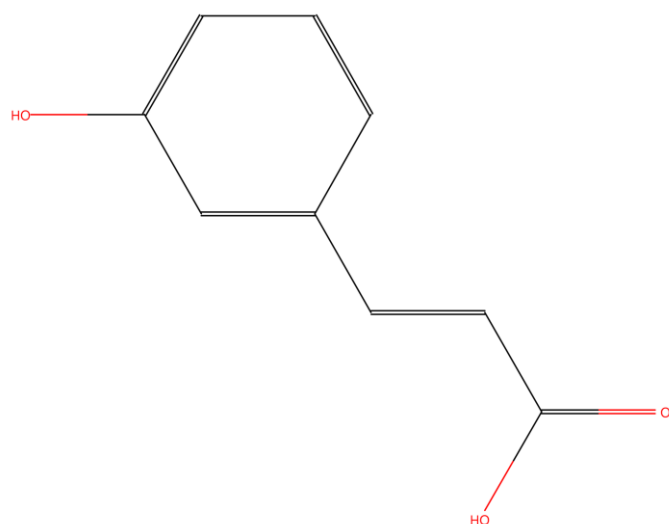
Urolithin A - CSID4589709



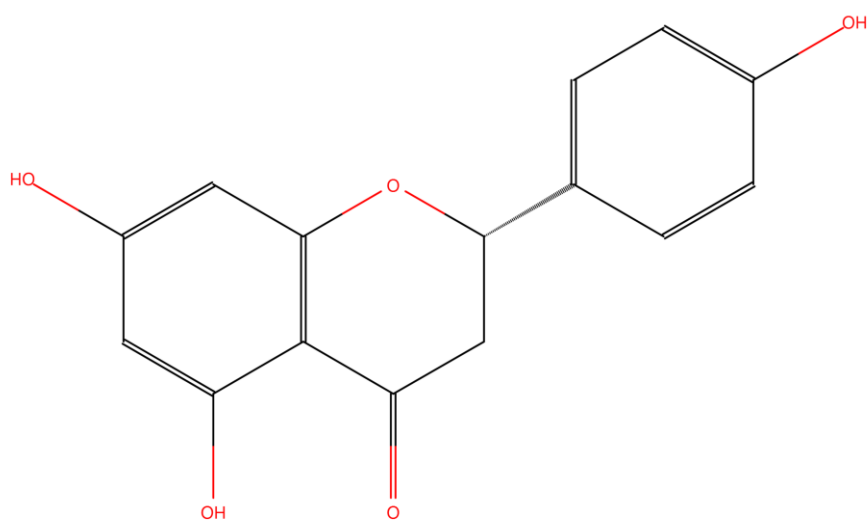
(+)-Isolariciresinol - CSID141054



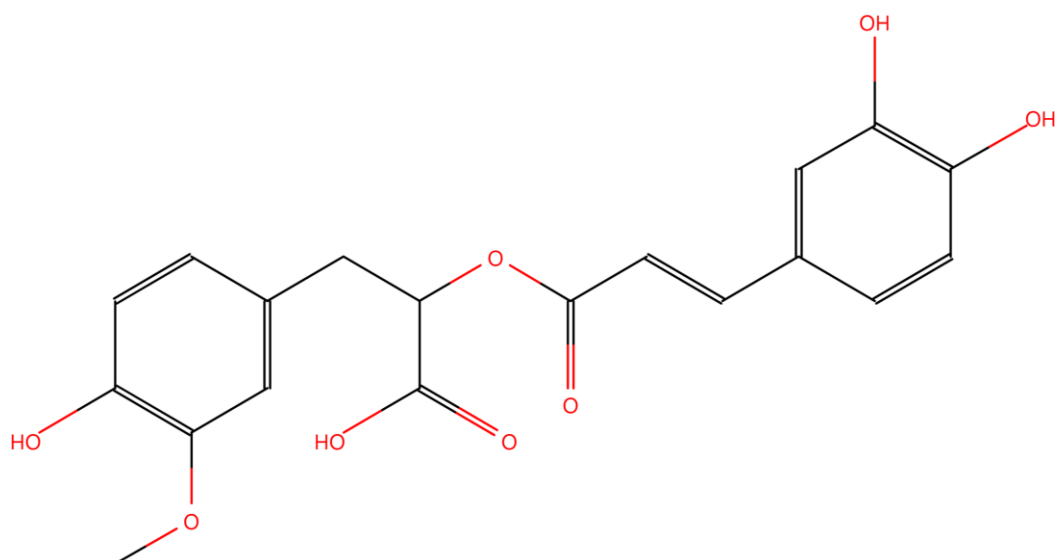
Vanillin - CSID13860434



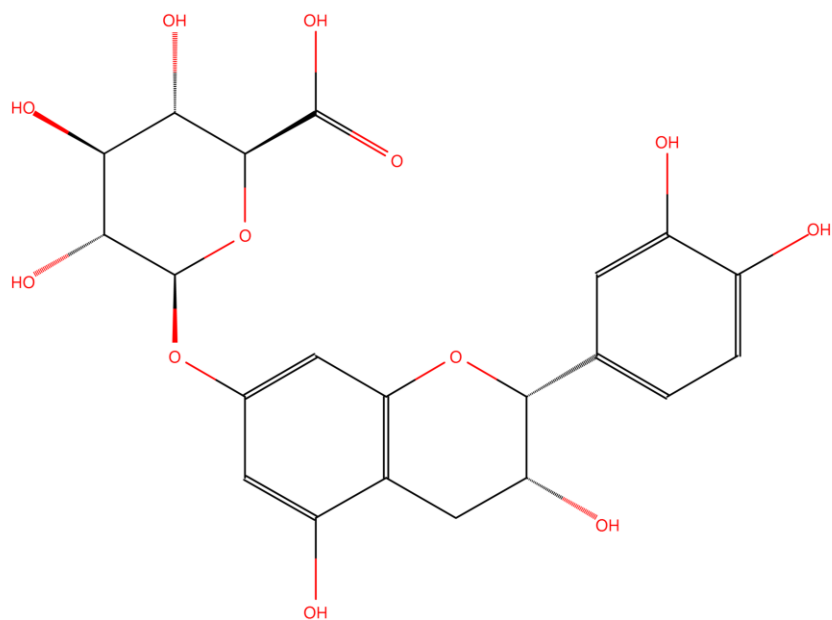
m-Coumaric acid - CSID553147



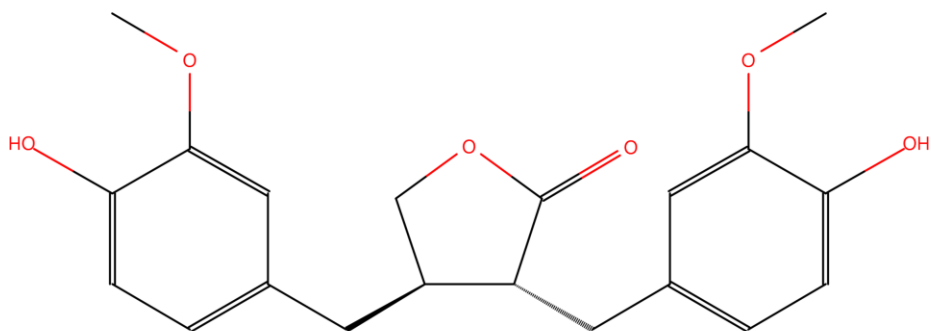
Naringenin - CSID388383



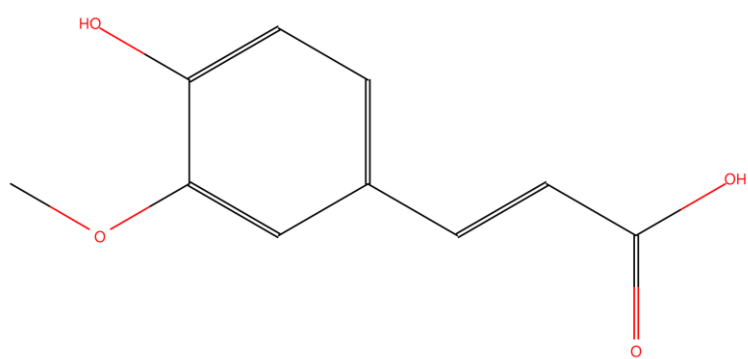
3-O-Methylrosmarinic acid - CSID35015215



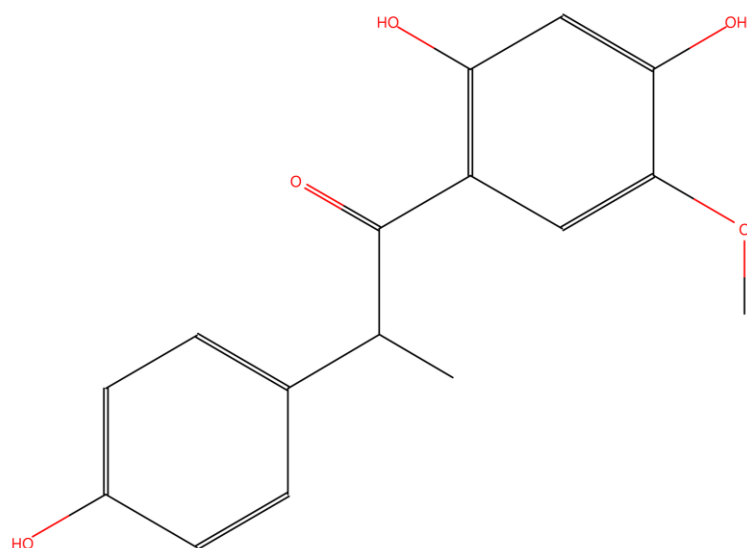
Epicatechin-glucuronide - CSID30777622



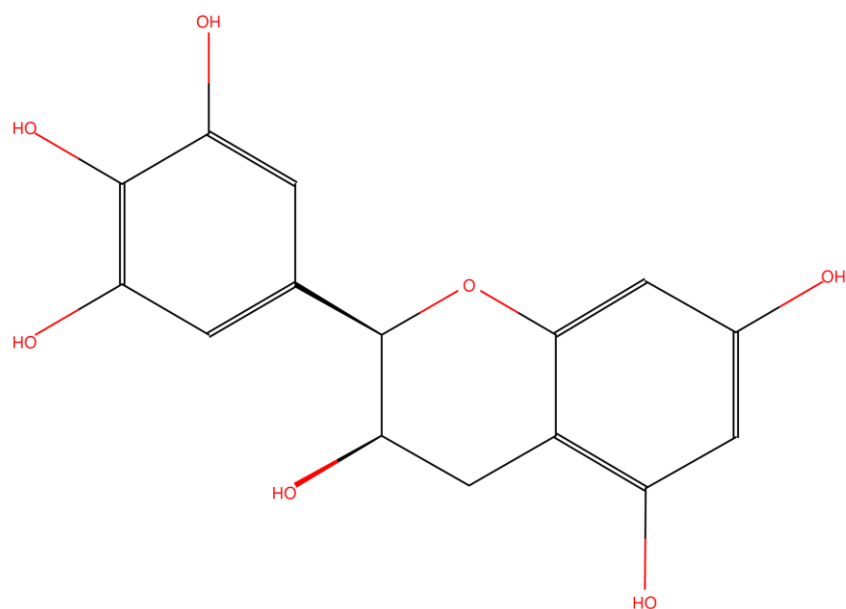
Matairesinol - CSID106491



Ferulic acid - CSID689

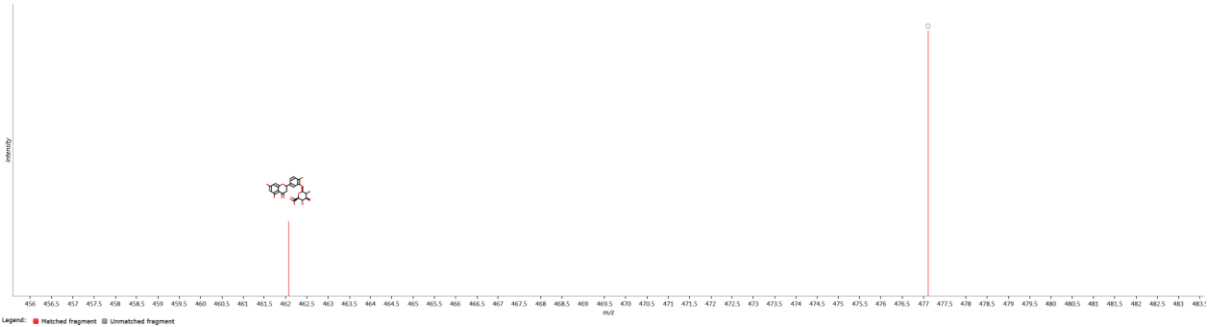


5'-Methoxy-O-desmethylangolensin - CSID28554480

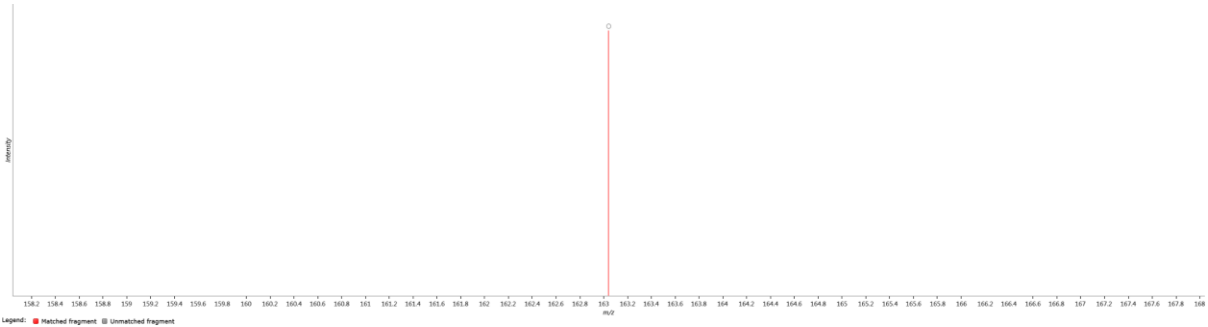


(-)-Epigallocatechin - CSID65231

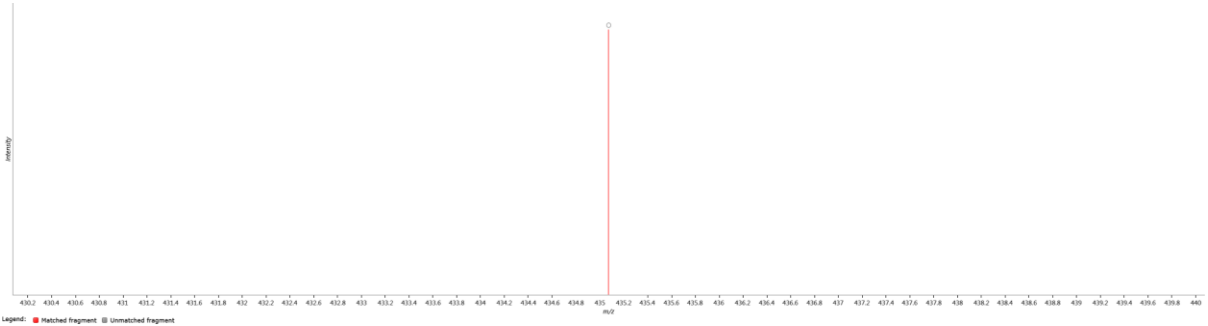
Figure S9. Molecular structures of identifications ordered from high to low score value.



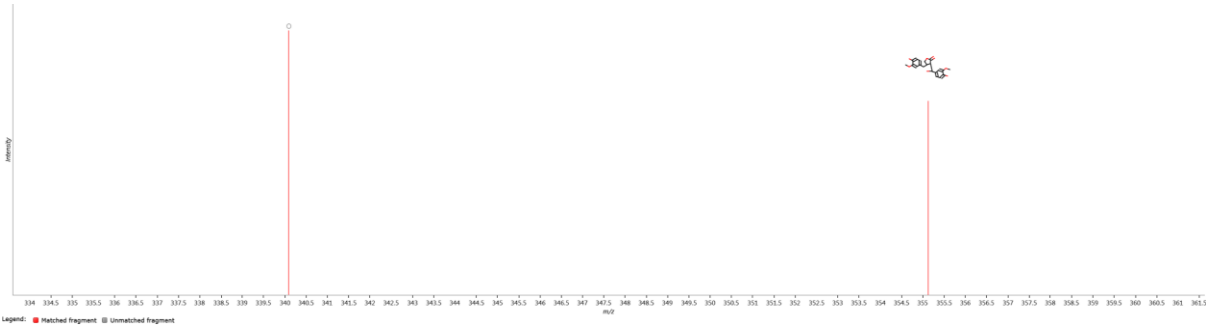
Isorhamnetin 3-glucoside fragmentation trace



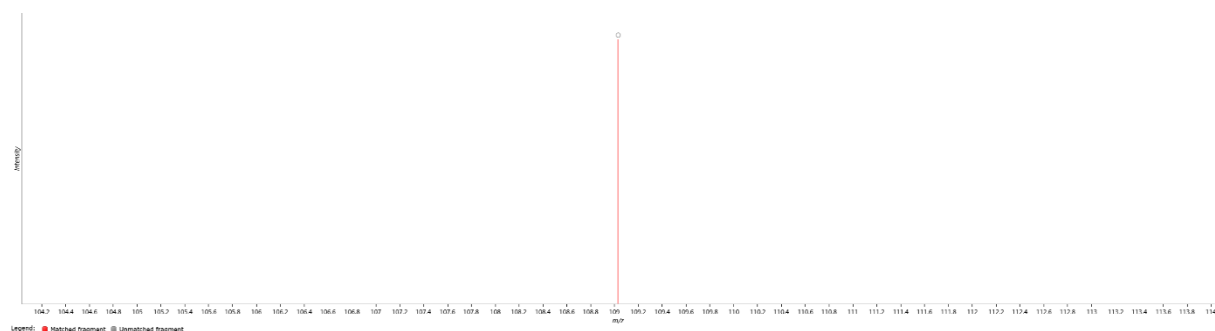
trans-5-*O*-(4-coumaroyl)-D-quinic acid fragmentation trace



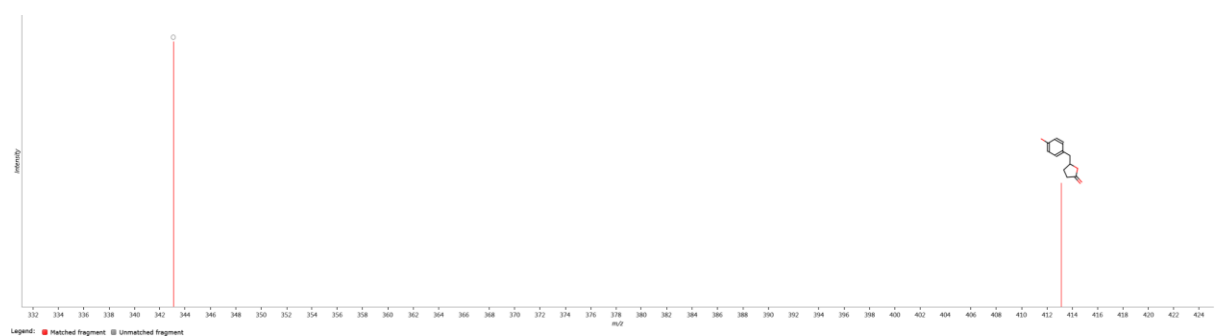
3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydro-4H-chromen-4-one fragmentation trace



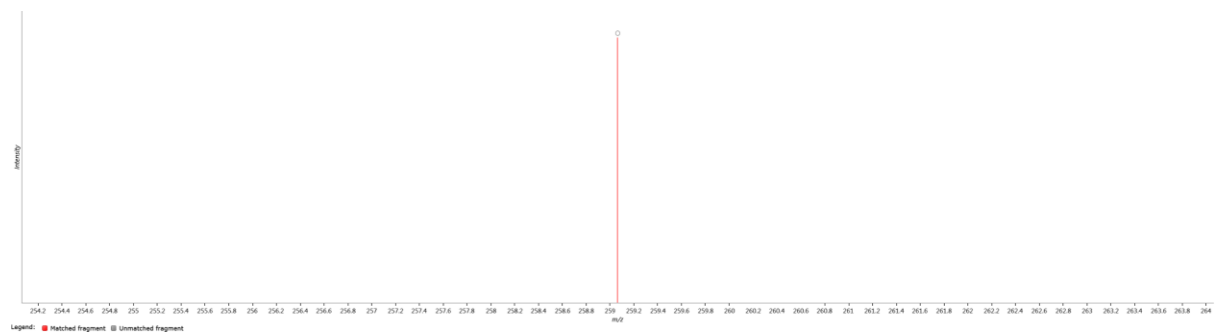
7-Hydroxymatairesinol fragmentation trace



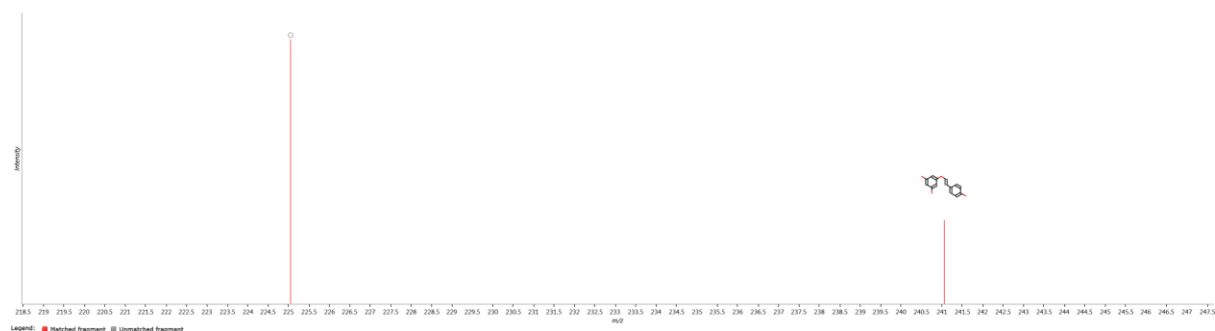
3-(3,4-Dihydroxyphenyl)-2-methoxypropanoic acid fragmentation trace



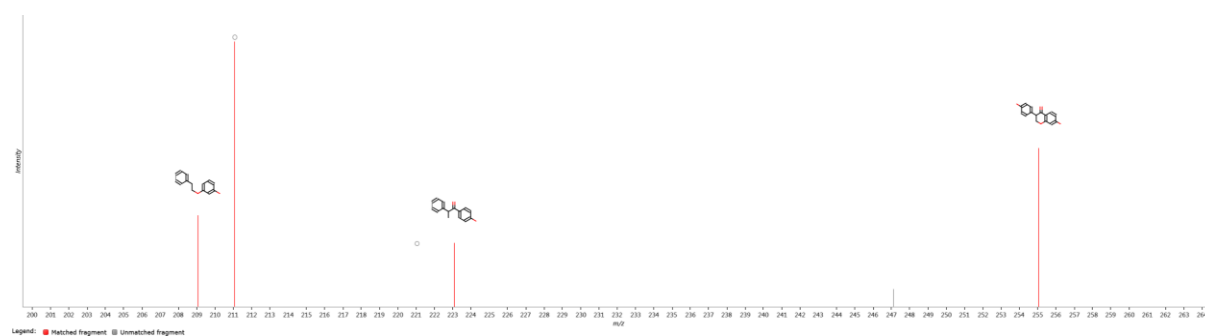
5-(3,4,5-Trihydroxybenzyl)dihydro-2(3H)-furanone fragmentation trace



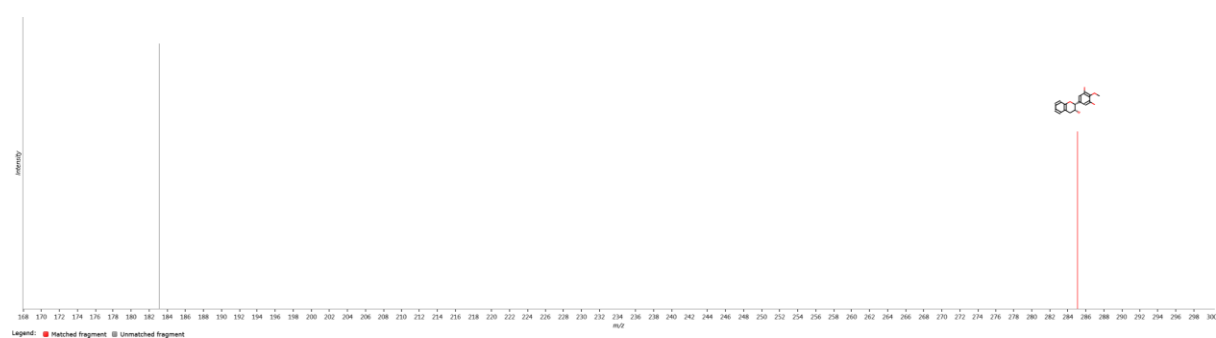
(-)-Epigallocatechin fragmentation trace



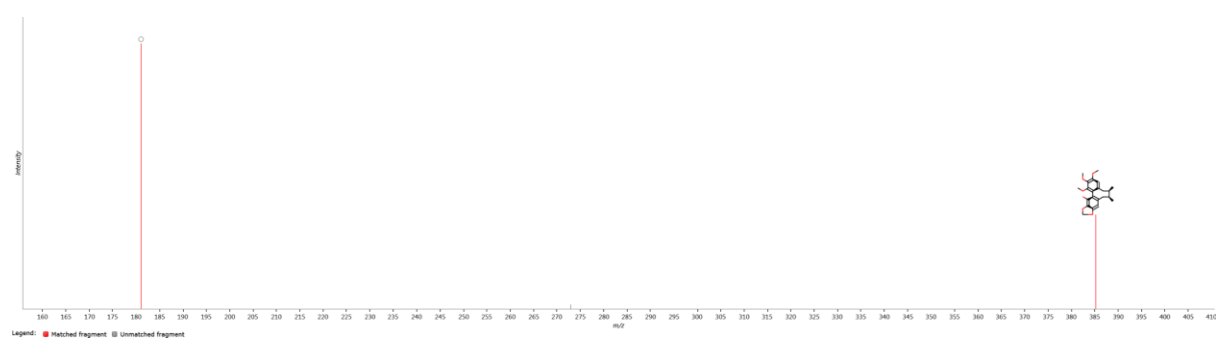
Genistein fragmentation trace



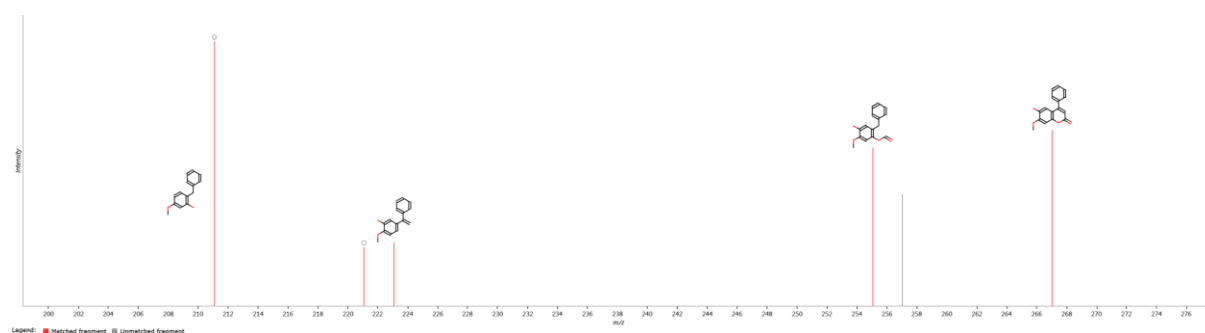
Dihydrodaidzein fragmentation trace



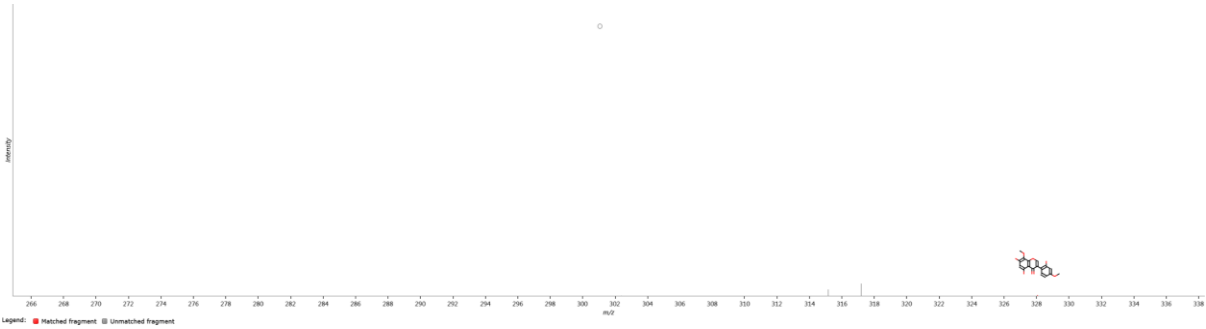
4'-Methylepigallocatechin ragmentation trace



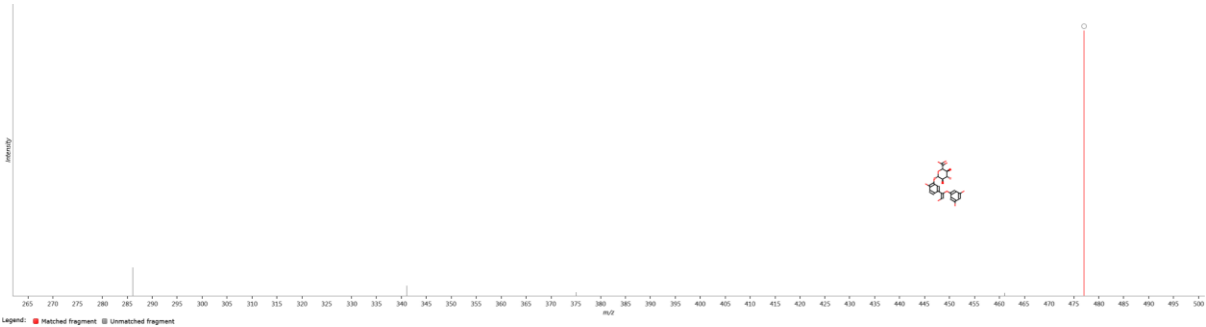
Gomisin M2 fragmentation trace



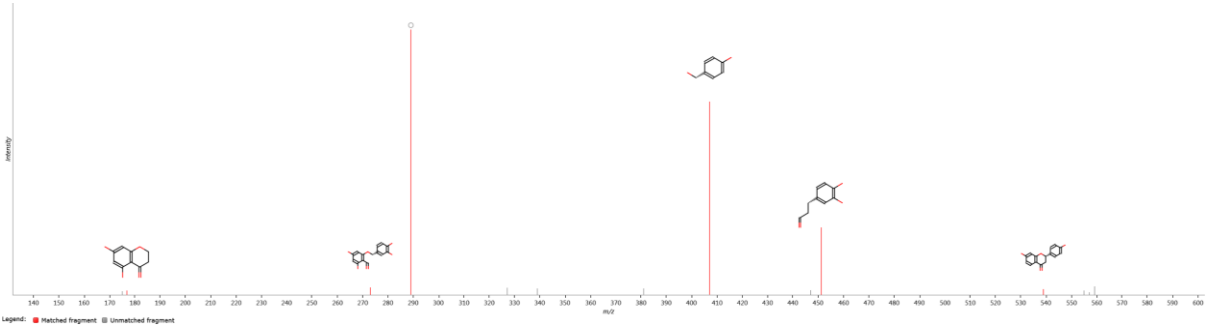
Dalbergin fragmentation trace



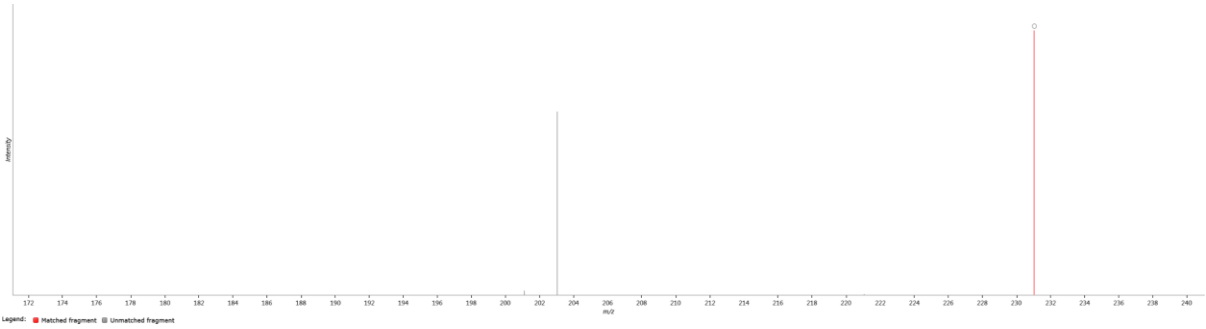
5,7-Dihydroxy-3-(2-hydroxy-4-methoxyphenyl)-8-methoxy-4H-chromen-4-one fragmentation trace



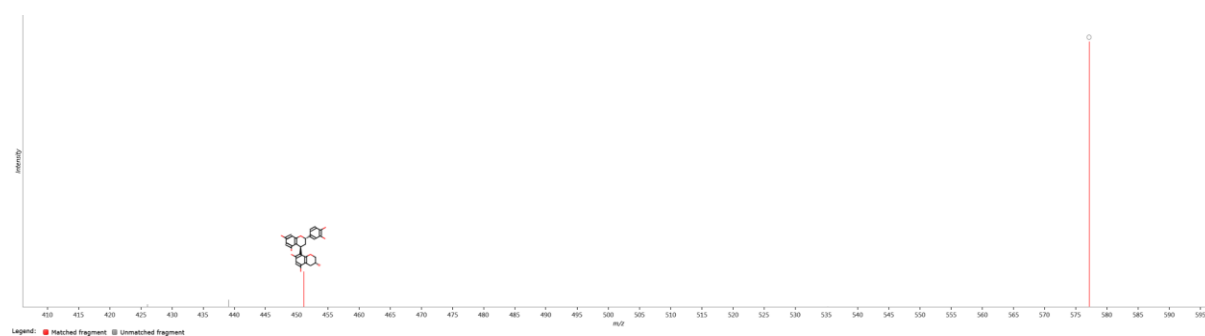
Quercetin-3'-glucuronide fragmentation trace



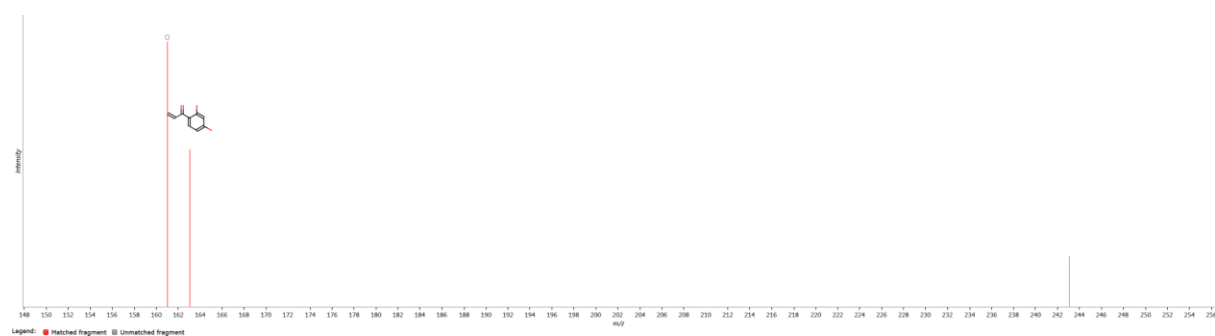
Eriodictyol fragmentation trace



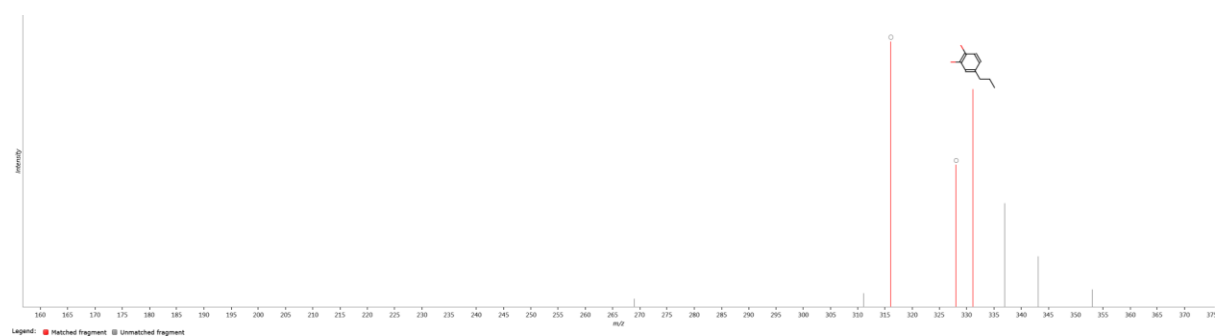
Norathyriol fragmentation trace



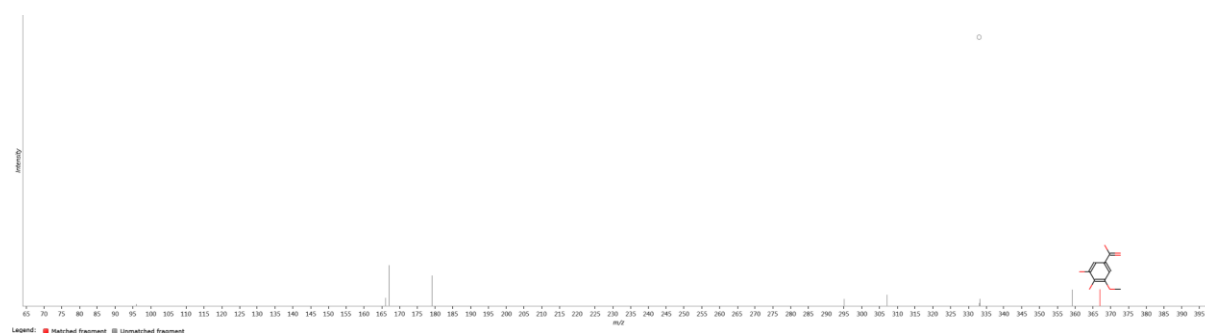
Procyanidin B1, B2, B3 or B4 fragmentation trace



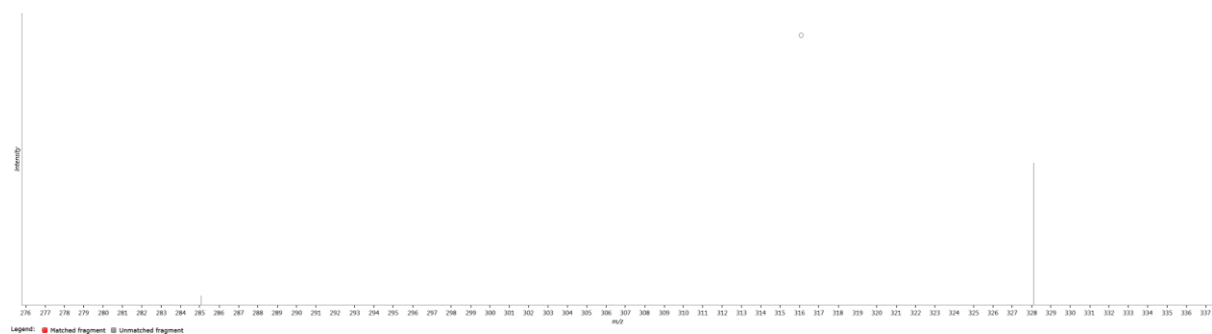
Isoliquiritigenin fragmentation trace



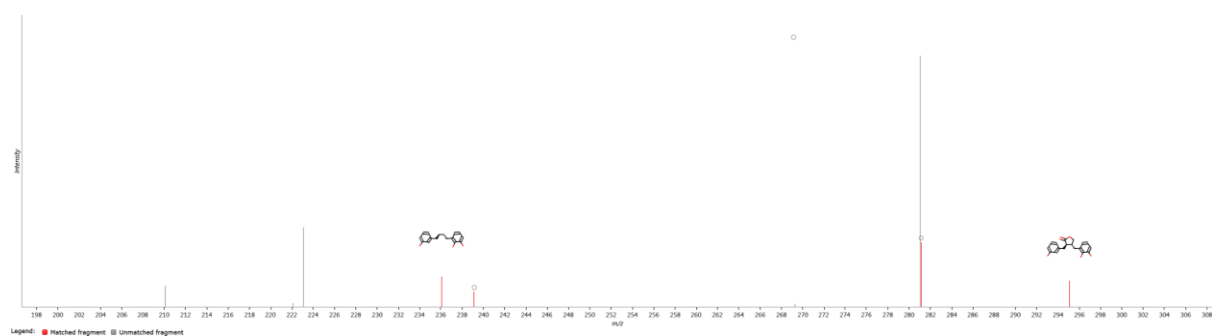
Dihydrocaffeic acid fragmentation trace



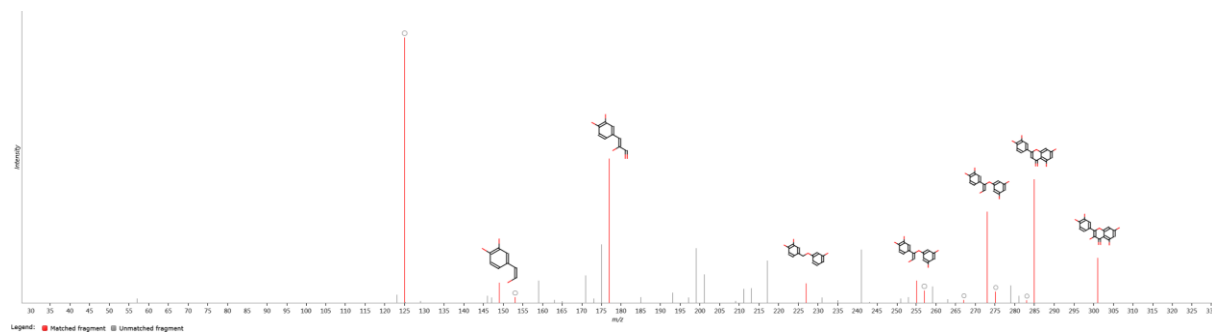
3,4-Dihydroxy-5-methoxybenzoic acid fragmentation trace



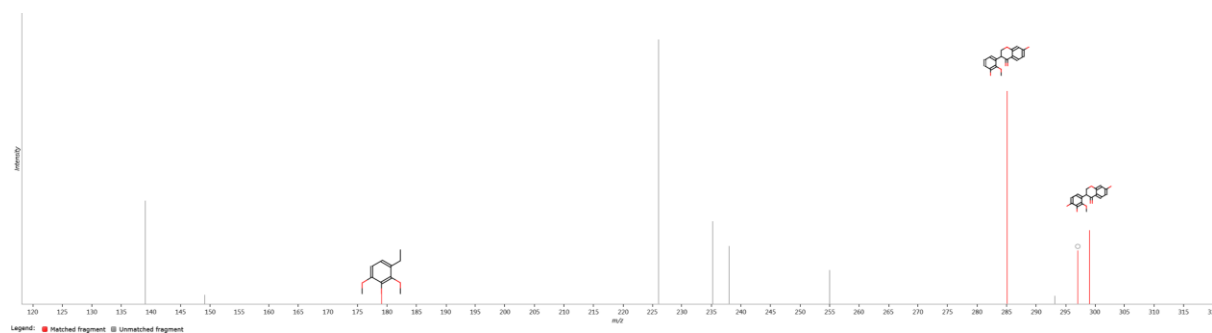
Paeonol fragmentation trace



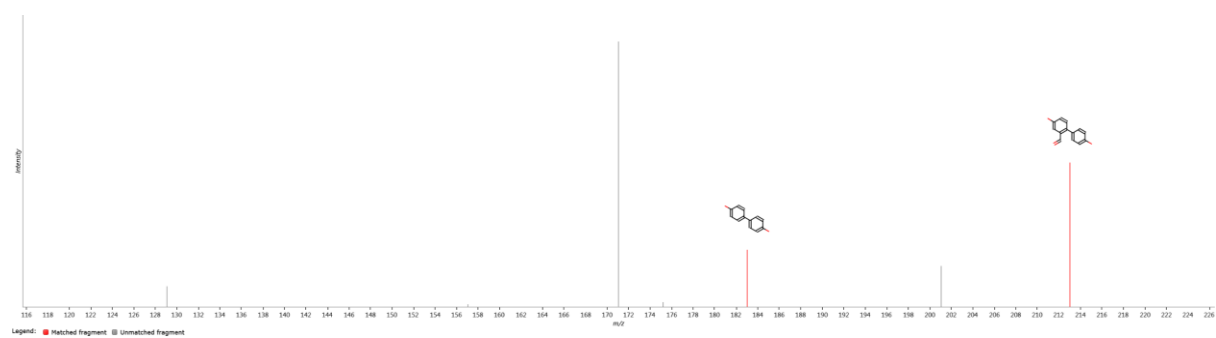
(3R,4R)-4-(2,3-Dihydroxybenzyl)-3-(3-hydroxybenzyl)dihydro-2(3H)-furanone fragmentation trace



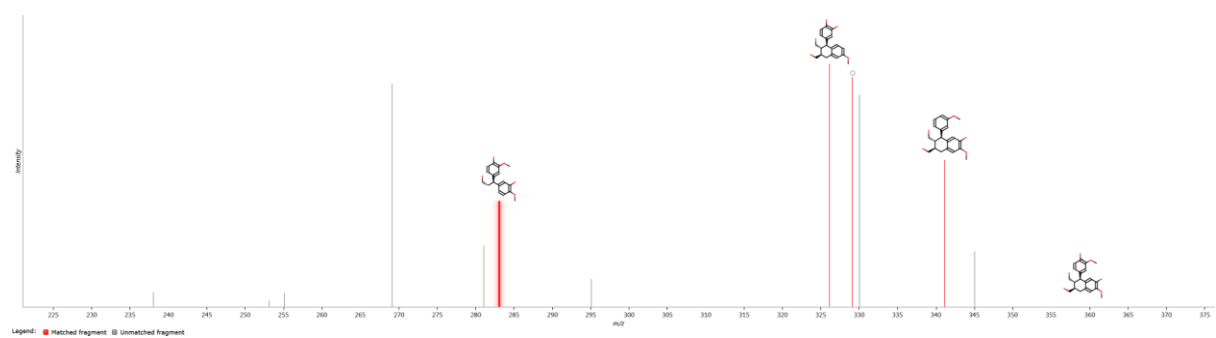
Quercetin fragmentation trace



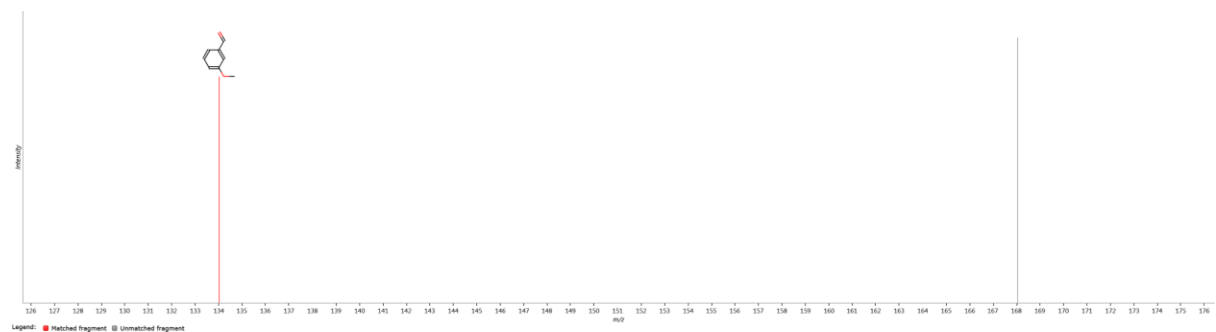
7-Hydroxy-3-(3-hydroxy-2,4-dimethoxyphenyl)-2,3-dihydro-4H-chromen-4-one fragmentation trace



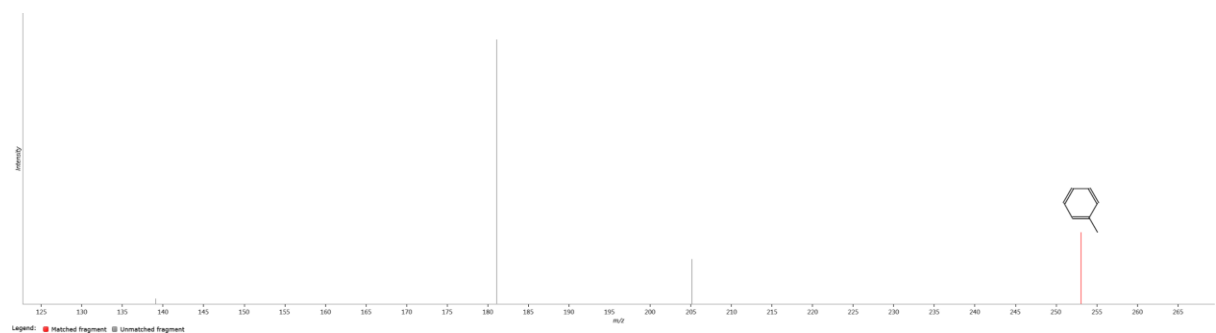
Urolithin A fragmentation trace



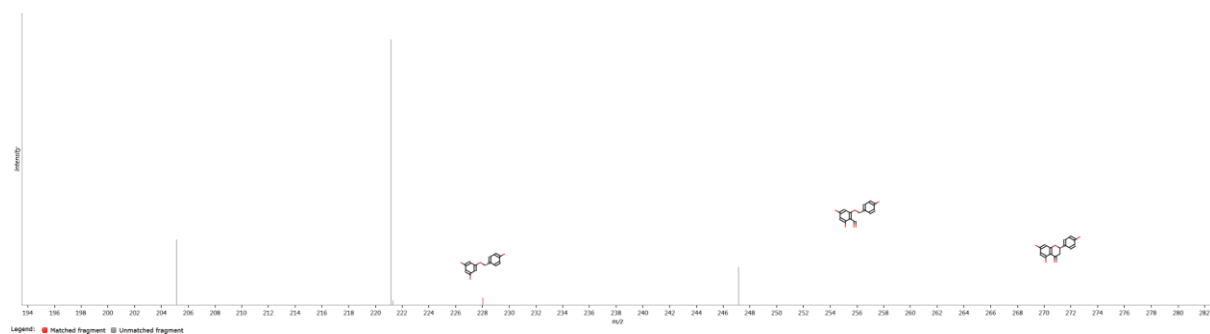
(+)–Isolariciresinol fragmentation trace



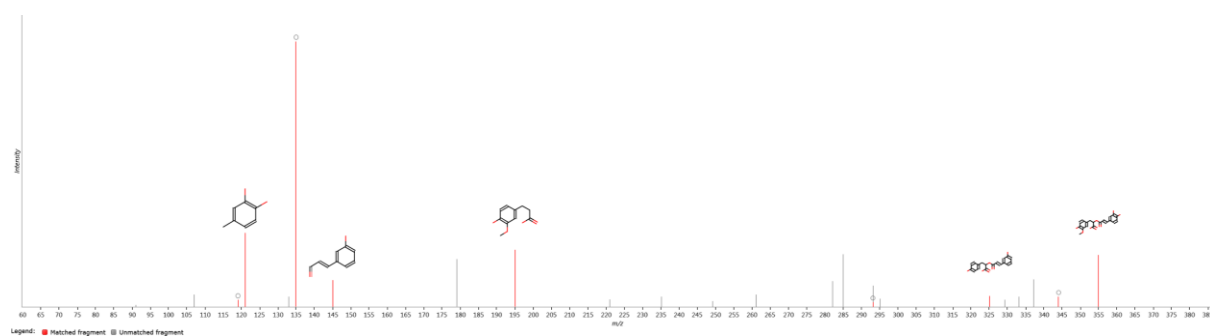
Vanillin fragmentation trace



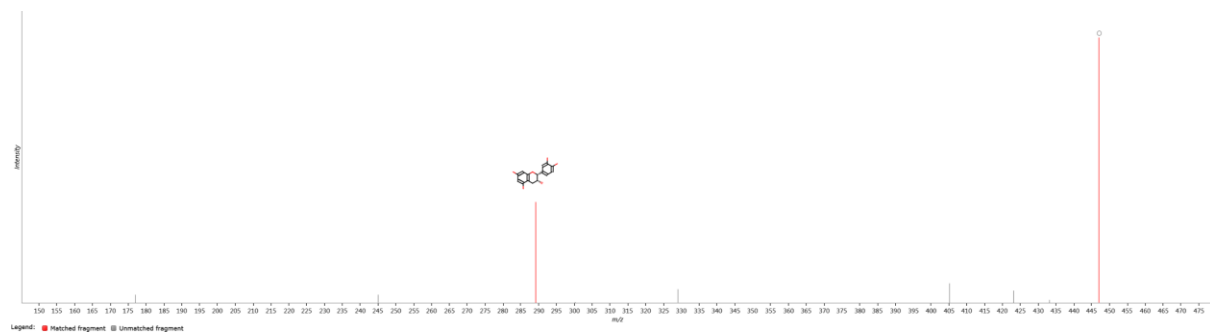
Meta or para-coumaric acid fragmentation trace



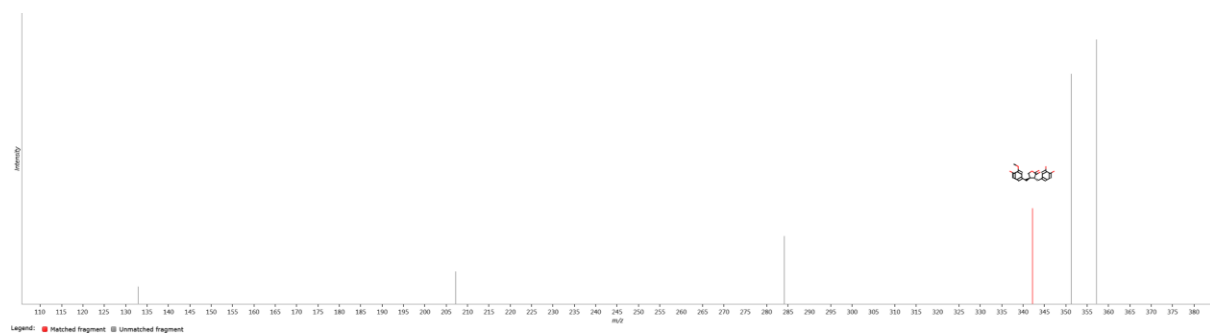
Naringenin fragmentation trace



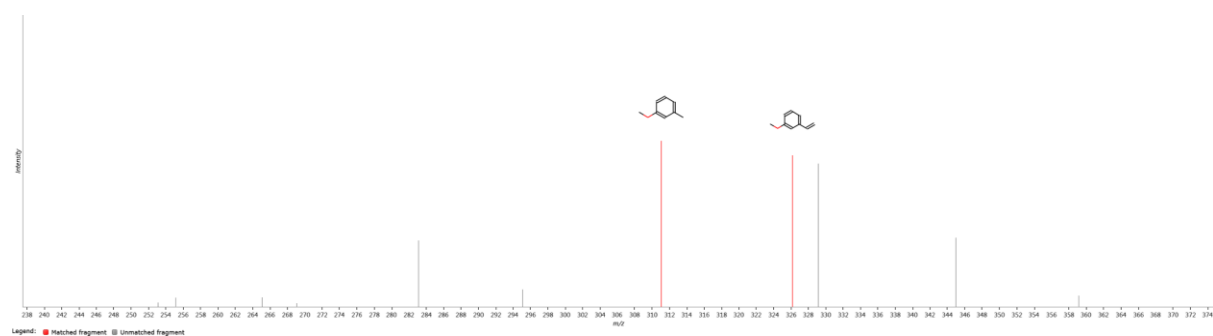
3-O-Methylrosmarinic acid fragmentation trace



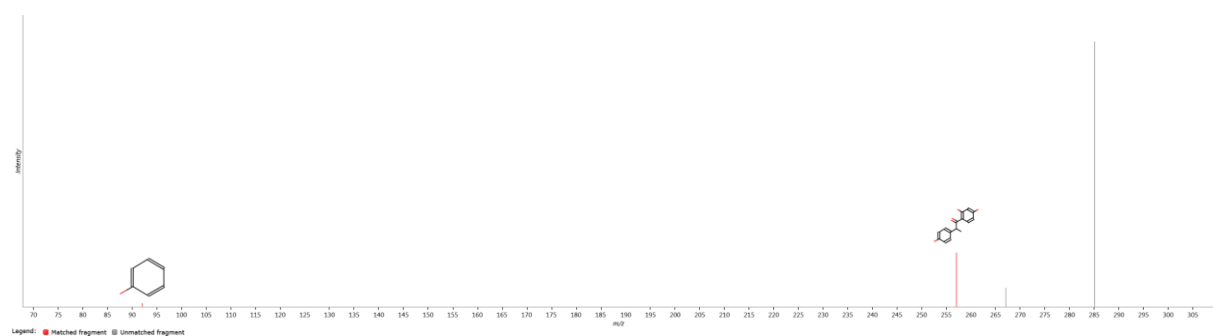
3' or 7-epicatechin-glucuronide fragmentation trace



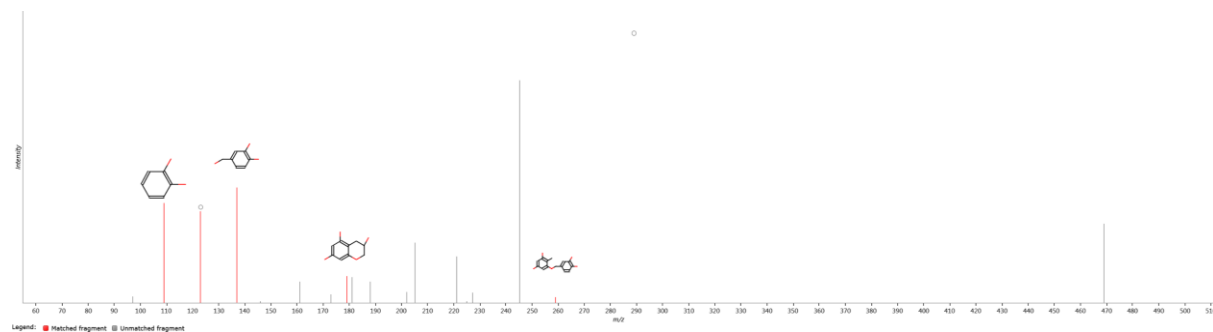
Matairesinol fragmentation trace



Ferulic acid fragmentation trace



5'-Methoxy-O-desmethylangolensin fragmentation trace



(-)-Epicatechin fragmentation trace

Figure S10. Mass spectra of identifications ordered from high to low score value.

Loadings Bi Plot Comp[1] vs. Comp[2] colored by Condition

- Blanks
- Lodge Pole Pine
- Oak
- Pyrogenol
- Scots Pine
- X variables

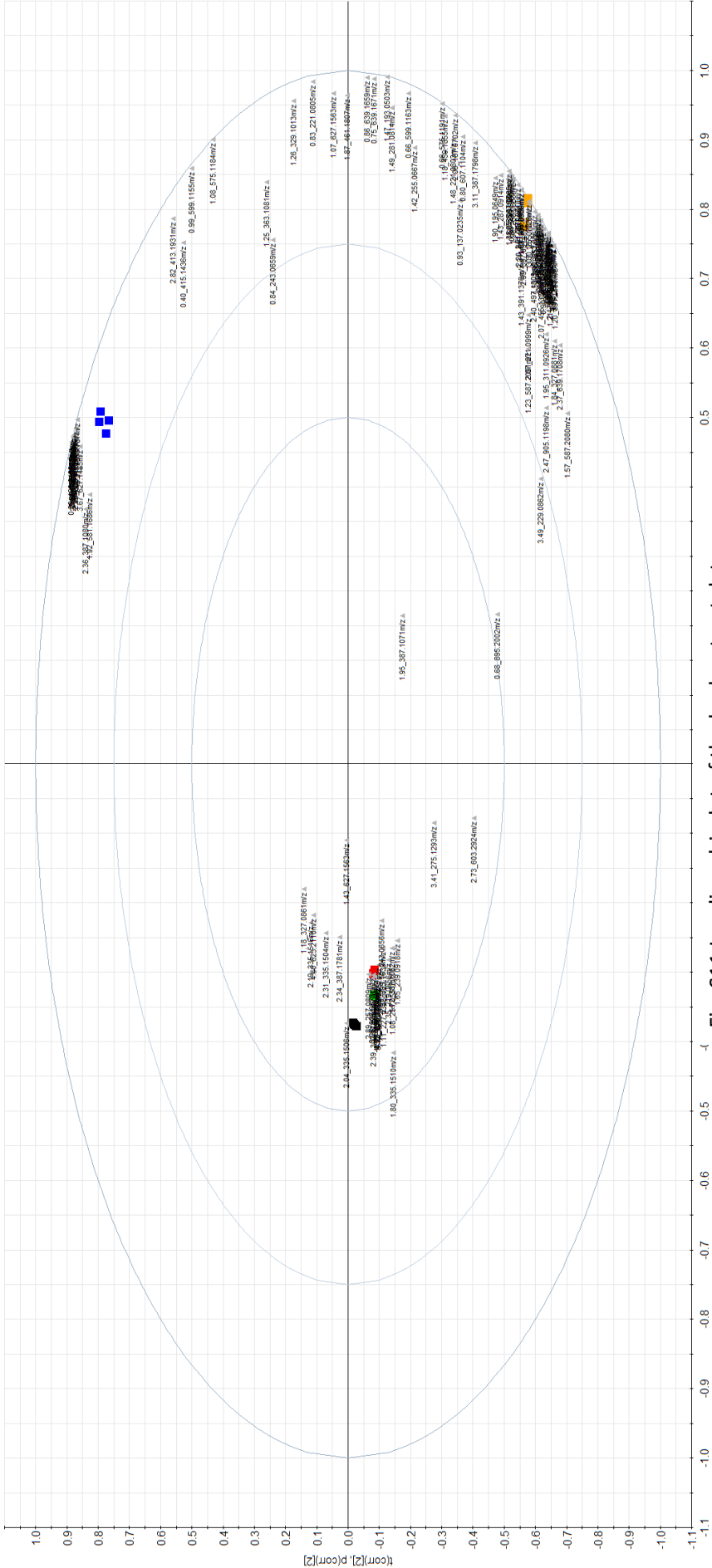


Fig. S11 Loadings bi-plot of the bark extract data.

Figure S11: Bark extracts 2019 after filtering with some (Data up (M1 PCA)) - 2020-10-30 12:36:42 (UTC+0)