

Table S6: GC-MS metabolites, with statistical and practical significance, for cellar ICVV. Numbers at the end of the acronyms represent sampling month. Values represent the area of the detected chromatographic peaks after applying variance stabilization. The metabolites can be grouped in the following chemical classes (1) benzene and substituted derivatives, (2) carbonyl compounds, (3) carboxylic acids and derivatives, (4) fatty acyls, (5) hydroxy acids and derivatives, (6) indoles and derivatives, (7) keto acids and derivatives, (8) lactones, (9) olefins, (10) oxolanes, (11) phenols, (12) phenylpropanoic acids, (13) phenol lipids, (14) saturated hydrocarbons, (15) stilbenes, (16) tetrahydrofurans, (17) thiolanes, (18) unsaturated hydrocarbons.

Compound	FML_0	BAO_3	BAO_9	BAO_12	BAN_3	BAN_9	BAN_12	BTO_12	BTN_12
2,4-di-tert-butylphenol ^{1D}	2,41E+06	3,08E+06	4,83E+05	1,64E+06	1,50E+06	4,56E+05	9,09E+05	5,62E+05	5,33E+05
2-hydroxy-3,4-dimethoxybenzoic acid ^{1U}	7,97E+05	1,24E+06	1,72E+06	7,66E+05	2,26E+06	2,49E+06	1,44E+06	5,91E+05	8,29E+05
2-phenethyl acetate ^{1D}	1,77E+06	1,07E+06	6,00E+05	3,33E+05	1,28E+06	5,62E+05	4,41E+05	3,63E+05	4,18E+05
4-nonylphenol ^{1U}	4,40E+05	4,30E+05	9,84E+05	5,85E+05	4,52E+05	9,89E+05	8,52E+05	5,39E+05	5,57E+05
benzyl alcohol ^{1U}	2,65E+05	1,49E+05	1,77E+06	9,84E+05	4,07E+05	1,59E+06	1,44E+06	1,10E+06	1,14E+06
dibutyl phthalate ^{1D}	1,44E+06	1,33E+06	2,23E+05	8,11E+05	1,26E+06	2,83E+05	4,18E+05	4,09E+05	5,38E+05
diphenylketone ^{1D}	1,22E+06	7,78E+05	2,54E+05	4,33E+05	7,68E+05	3,27E+05	3,01E+05	5,09E+05	6,44E+05
ethyl-4-hydroxybenzoate ^{1U}	1,79E+05	5,17E+05	7,79E+05	4,23E+05	2,67E+05	4,01E+05	3,70E+05	5,37E+05	3,98E+05
methyl,2-methoxy-2-phenylacetate ^{1D}	2,29E+05	9,65E+04	9,09E+04	1,17E+05	8,45E+04	1,91E+05	1,80E+05	2,57E+04	2,87E+04
2-isopropyl-5-methyl-2-hexenal ^{2D}	5,16E+05	5,38E+05	1,34E+05	3,17E+05	4,45E+05	1,43E+05	2,12E+05	3,73E+05	3,72E+05
ethyl 5-oxo-dl-proline ^{3U}	2,26E+06	4,94E+06	7,92E+06	5,94E+06	4,56E+06	6,39E+06	6,91E+06	5,25E+06	5,05E+06
hexadecyl trichloroacetate ^{3U}	2,87E+05	1,24E+05	2,55E+05	5,54E+05	1,88E+05	2,89E+05	2,74E+06	7,56E+05	7,89E+05
l,l-cyclo(leucylprolyl) ^{3U}	1,69E+05	2,66E+05	4,12E+05	2,41E+05	2,46E+05	4,33E+05	3,30E+05	2,78E+05	2,95E+05
methionol ^{3U}	3,07E+05	2,20E+06	4,68E+06	2,79E+06	7,48E+05	1,83E+06	1,58E+06	2,47E+06	3,84E+06
oxalic acid dibutyl ester ^{3U}	2,98E+05	1,70E+05	5,16E+05	5,78E+05	2,98E+05	7,47E+05	1,44E+06	1,19E+06	1,76E+06
1-dodecanol ^{4U}	4,29E+06	3,66E+05	4,84E+06	4,44E+06	3,25E+05	5,00E+06	4,35E+06	5,26E+06	4,58E+06
ethyl octanoate ^{4D}	4,34E+06	3,96E+06	4,47E+06	4,26E+06	3,58E+06	6,50E+05	4,31E+06	4,59E+06	4,33E+06
ethyl undecanoate ^{4D}	5,46E+05	4,44E+05	4,84E+05	3,48E+05	4,45E+05	4,63E+05	2,42E+05	3,35E+05	3,24E+05
palmitic acid ^{4U}	3,55E+06	3,97E+05	9,47E+06	3,07E+06	4,05E+06	4,08E+07	4,99E+06	4,78E+07	4,86E+07
stearic acid ^{4U}	9,74E+05	6,44E+04	5,27E+06	3,47E+06	6,31E+04	7,06E+06	2,38E+06	4,05E+07	4,09E+07
valeric acid ^{4D}	4,75E+06	3,83E+06	4,36E+06	9,93E+05	4,39E+06	2,06E+06	2,47E+06	7,72E+05	6,35E+05
diethyl malate ^{5U}	5,36E+05	5,35E+06	5,57E+06	5,55E+06	5,53E+06	5,09E+06	5,37E+06	7,76E+05	7,57E+05
ethyl-3-hydroxybutyrate ^{5D}	5,87E+06	3,26E+06	5,05E+06	5,68E+05	5,88E+06	9,96E+05	5,51E+06	5,56E+05	5,90E+05
d-tryptophan ^{6U}	9,49E+04	8,39E+04	2,58E+05	5,56E+05	5,21E+05	2,08E+05	2,04E+05	5,54E+05	5,47E+05
indole-3-methyl acetate ^{6D}	3,07E+05	2,21E+05	1,21E+05	1,34E+05	2,16E+05	1,31E+05	5,71E+04	1,09E+05	6,16E+04
tryptophol ^{6U}	2,30E+07	2,84E+07	1,04E+08	5,03E+07	4,10E+07	7,89E+07	8,59E+07	5,76E+07	5,74E+07
oxoglutaric acid ^{7U}	2,87E+05	2,33E+05	2,71E+05	1,42E+06	1,88E+05	2,17E+05	2,74E+06	7,17E+05	5,35E+05
5-ethoxyoxolan-2-one ^{8D}	8,96E+06	1,06E+05	2,52E+06	5,88E+05	3,39E+06	3,11E+06	1,08E+06	7,26E+04	6,52E+04
gamma-butyrolactone ^{8U}	1,44E+07	2,21E+07	3,81E+07	2,60E+07	2,11E+07	3,04E+07	3,49E+07	2,26E+07	2,15E+07
1-tetradecene ^{9D}	5,96E+05	9,18E+05	2,73E+05	3,71E+05	4,86E+05	3,49E+04	1,98E+05	8,38E+04	4,46E+04
succinic anhydride ^{10D}	2,05E+07	1,91E+06	3,48E+06	3,44E+06	7,02E+06	2,10E+06	9,74E+05	1,76E+06	1,05E+06
2-methoxy-4-vinylphenol ^{11D}	6,21E+05	5,57E+05	4,36E+05	2,26E+05	5,52E+05	2,76E+05	2,93E+05	2,83E+05	2,84E+05

homovanillic acid ^{11U}	1,17E+05	2,53E+05	4,91E+05	2,10E+05	2,08E+05	4,61E+05	3,56E+05	1,88E+05	1,92E+05
tyrosol ^{11U}	7,44E+06	9,68E+06	3,49E+07	2,63E+07	1,44E+07	3,24E+07	1,99E+07	2,36E+07	2,29E+07
methyl,3-(4-hydroxyphenyl) propanoate ^{12U}	3,74E+05	7,97E+05	1,67E+06	1,00E+06	8,38E+05	1,59E+06	1,60E+06	9,25E+05	8,23E+05
phenol, 2-(2h-benzotriazol-2-yl)-4,6-bis (1,1-dimethylpropyl) ^{12D}	1,292E+06	9,90E+05	1,47E+06	7,85E+05	1,32E+06	1,55E+06	7,18E+05	3,66E+05	6,47E+05
borneol ^{13D}	5,85E+05	4,72E+05	4,56E+05	2,47E+05	4,96E+05	5,48E+05	4,35E+05	2,74E+05	2,77E+05
carvacrol ^{13D}	4,01E+05	3,72E+05	1,33E+05	1,95E+05	2,15E+05	1,45E+05	1,87E+05	1,71E+05	2,25E+05
2,10-dimethylundecane ^{14U}	8,45E+04	1,64E+05	7,69E+05	3,97E+05	4,74E+04	4,75E+05	3,99E+05	5,80E+04	5,65E+04
2,7,10-trimethyldodecane ^{14D}	1,77E+06	9,45E+05	2,14E+05	7,17E+05	1,40E+06	6,14E+05	7,81E+05	1,50E+06	1,20E+06
3,8-dimethylundecane ^{14U}	2,22E+05	2,89E+05	1,11E+05	3,50E+05	2,13E+05	1,02E+05	1,81E+05	3,46E+05	3,18E+05
isoheptane ^{14D}	2,47E+06	2,10E+06	8,16E+05	1,69E+06	1,86E+06	6,71E+05	1,14E+06	2,19E+06	1,87E+06
1,2-diphenylcyclobutane ^{15D}	3,34E+05	3,46E+05	2,73E+05	1,78E+05	1,90E+05	3,18E+05	1,03E+05	1,23E+05	8,95E+04
7,9-di-tert-butyl-1-oxaspiro[4,5]deca-6,9-diene-2,8-dione ^{16D}	2,02E+06	1,91E+06	5,92E+05	7,06E+05	1,54E+06	6,20E+05	1,01E+06	4,00E+05	3,85E+05
2-methyltetrahydrothiophen-3-one ^{17U}	3,98E+06	3,89E+06	3,69E+07	1,73E+07	5,17E+06	2,73E+07	2,30E+07	1,78E+07	1,78E+07
4,6,8-trimethylnon-1-ene ^{18D}	1,06E+06	7,24E+05	5,81E+05	7,27E+05	9,73E+05	4,53E+05	7,95E+05	1,48E+06	1,66E+06
5-eicosene ^{18U}	2,74E+05	1,41E+05	3,08E+05	5,90E+05	1,74E+05	3,22E+05	4,30E+05	7,64E+05	7,92E+05
6-tridecene ^{18U}	1,85E+05	5,70E+05	2,05E+06	2,60E+05	1,01E+05	2,13E+06	7,00E+05	8,03E+06	7,02E+06