

SUPPORTING Table 1

**The chemodiversity of wines can reveal a metabo-geography
expression of cooperage oak wood**

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Supporting Table 1. Compilation of possible metabolites identified in the *Vitis vinifera* organism from the MassTrix database that can be associated with the exact masses and the corresponding formulas obtained from mass spectra. These masses, which correspond to PLS-DA score plots of Figure 2 discriminate red wines (a) from white wines (b); Chardonnay wines from Beaune (c) from Pinot noir wines from Mercurey (d) Syrah wines from Côte-Rotie (e) and Grenache wines from Gigondas (f); White wines aged in sessile oak (g) from white wines aged in pedunculate oak (h); Red wines aged in sessile oak (i) from red wines aged in pedunculate oak (j); Wines aged in barrels made of oaks from the forest of Darney (k) Citeaux (l) Tronçais (m) Bitche (n) Bertrange (o) Jupilles (p) Saint-Palais (q) Sud-Ouest (r) and Limousin (s) regardless of the oak species.

(a) red wines

mass	formula	name
166.02660867066	C ₈ H ₆ O ₄	4-Formylsalicylic acid
		4-Hydroxyphenylglyoxylate
		Phthalate
		Terephthalate
		3-Formylsalicylic acid
205.03750770751	C ₁₀ H ₇ NO ₄	Xanthurenic acid
		6-Hydroxykynurenate
218.05790879894	C ₁₂ H ₁₀ O ₄	2,2',3-Trihydroxydiphenylether
219.07428713905	C ₈ H ₁₃ NO ₆	O-Succinyl-L-homoserine
222.06742793578	C ₇ H ₁₄ N ₂ O ₄ S	L-Cystathionine
		Cystathionine
240.0633881022	C ₁₁ H ₁₂ O ₆	2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
244.07355886308	C ₁₄ H ₁₂ O ₄	3,3',4',5-Tetrahydroxystilbene (piceatannol)
258.08920892722	C ₁₅ H ₁₄ O ₄	Naphthyl-2-methyl-succinic acid
		2,2-Bis(4-hydroxyphenyl)-propanoic acid
266.15180918378	C ₁₅ H ₂₂ O ₄	Xanthoxic acid
272.06847348264	C ₁₅ H ₁₂ O ₅	Isosalipurpol
		Pinobanksin
		Butein
		Garbanzol
		Butin
		Naringenin
274.08412354678	C ₁₅ H ₁₄ O ₅	Afzelechin
		Apiforol
		(-)-Epiafzelechin
280.1310737392	C ₁₅ H ₂₀ O ₅	Phaseic acid
		8'-Hydroxyabscisate
284.12629908875	C ₁₀ H ₂₂ NO ₆ PR	1-(1-Alkenyl)-sn-glycero-3-phosphocholine
288.0633881022	C ₁₅ H ₁₂ O ₆	Fustin
		Dihydrokaempferol
		2',3,4,4',6'-Pentahydroxychalcone
		Eriodictyol
290.07903816634	C ₁₅ H ₁₄ O ₆	Luteoforol
		(-)-Epicatechin
		cis-3,4-Leucopelargonidin
		Fisetinidol-4beta-ol
		(+)-Catechin
290.12263431374	C ₁₀ H ₁₈ N ₄ O ₆	N-(L-Arginino)succinate
302.04265265762	C ₁₅ H ₁₀ O ₇	Tricetin
		Quercetin
306.0739527859	C ₁₅ H ₁₄ O ₇	(+)-Gallocatechin
		Leucocyanidin
		(-)-Epigallocatechin

316.05830272176	C16H12O7	3',4',5,7-Tetrahydroxy-3-methoxyflavone
318.03756727718	C15H10O8	Myricetin
320.05321734132	C15H12O8	Dihydromyricetin
320.08960285004	C16H16O7	4-Coumaroylshikimate
326.10016753374	C15H18O8	cis-beta-D-Glucosyl-2-hydroxycinnamate
		trans-beta-D-Glucosyl-2-hydroxycinnamate
332.05321734132	C16H12O8	Laricitrin
338.10016753374	C16H18O8	p-Coumaroyl quinic acid
344.08960285004	C18H16O7	3',5-Dihydroxy-3,4',7-trimethoxyflavone
344.13186158484	C12H24O11	Melibiitol
346.06886740546	C17H14O8	Syringetin
352.06417594784	C12H16O12	4-(4-Deoxy-alpha-D-gluc-4-enuronosyl)-D-galacturonate
356.11073221744	C16H20O9	Scopolin
360.0845174696	C18H16O8	Rosmarinate
422.08254204045	C12H23O14P	Maltose 6'-phosphate
		Lactose 6-phosphate
		alpha,alpha'-Trehalose 6-phosphate
		Sucrose 6-phosphate
448.10056145656	C21H20O11	Luteolin 7-O-beta-D-glucoside
		Kaempferol 3-O-glucoside
		Kaempferol 3-O-beta-D-galactoside
464.09547607612	C21H20O12	Quercetin 3-O-glucoside
580.17920570008	C27H32O14	Naringin

(b) white wines

mass	formula	name
160.07355886308	C7H12O4	6-Carboxyhexanoate
161.08406397711	C10H11NO	Indole-3-ethanol
165.04259308795	C8H7NO3	5-Pyridoxolactone
		Formylanthranilate
		4-Pyridoxolactone
165.99359428922	C4H6O5S	Thiodiacetic acid sulfoxide
167.05824315209	C8H9NO3	Isopyridoxal
		3-Methoxyanthranilate
		Pyridoxal
173.01466408695	C6H7NO3S	2-Aminobenzenesulfonate
179.05824315209	C9H9NO3	Hippurate
180.04562986208	C6H12O4S	5-Methylthio-D-ribose
180.07864424352	C10H12O3	Coniferyl alcohol
190.04773803806	C7H10O6	3-Dehydroquinate
		4-Hydroxy-2-oxo-heptanedioate
		2,4-Dihydroxyhept-2-enedioate
204.0422587348	C11H8O4	1,2-Dihydroxy-8-carboxynaphthalene
		Spirodilactone
		1,4-Dihydroxy-2-naphthoate

207.05315777165	C10H9NO4	4-(2-Aminophenyl)-2,4-dioxobutanoate
		2-Formaminobenzoylacetate
		1-Nitro-5,6-dihydroxy-dihydronaphthalene
207.05652889893	C7H13NO4S	S-(2-Hydroxyethyl)-N-acetyl-L-cysteine
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
217.05863707491	C8H11NO6	2-(Hydroxymethyl)-3-(acetamidomethylene)succinate...
278.12665706506	C14H18N2O4	alpha-Ribazole
300.03823598348	C14H8N2O6	Cinnavalinate
325.13140809235	C19H19NO4	(S)-Cheilanthifoline
334.05660207609	C11H15N2O8P	Nicotinamide D-ribonucleotide
335.07872089545	C11H17N3O7S	S-Formylglutathione
481.98926311559	C10H17N2O14P3	dTTP

(c) Chardonnay/Beaune

mass	formula	name
160.07355886308	C7H12O4	6-Carboxyhexanoate
161.08406397711	C10H11NO	Indole-3-ethanol
165.04259308795	C8H7NO3	5-Pyridoxolactone
		Formylanthranilate
		4-Pyridoxolactone
165.99359428922	C4H6O5S	Thiodiacetic acid sulfoxide
167.05824315209	C8H9NO3	Isopyridoxal
		3-Methoxyanthranilate
		Pyridoxal
173.01466408695	C6H7NO3S	2-Aminobenzenesulfonate
179.05824315209	C9H9NO3	Hippurate
180.04562986208	C6H12O4S	5-Methylthio-D-ribose
180.07864424352	C10H12O3	Coniferyl alcohol
190.04773803806	C7H10O6	3-Dehydroquinone
		4-Hydroxy-2-oxo-heptanedioate
		2,4-Dihydroxyhept-2-enedioate
197.06880783579	C9H11NO4	3,4-Dihydroxy-L-phenylalanine
		N-Hydroxy-L-tyrosine
204.0422587348	C11H8O4	1,2-Dihydroxy-8-carboxynaphthalene
		Spirodilactone
		1,4-Dihydroxy-2-naphthoate
207.05315777165	C10H9NO4	4-(2-Aminophenyl)-2,4-dioxobutanoate
		2-Formaminobenzoylacetate
		1-Nitro-5,6-dihydroxy-dihydronaphthalene
207.05652889893	C7H13NO4S	S-(2-Hydroxyethyl)-N-acetyl-L-cysteine
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
217.05863707491	C8H11NO6	2-(Hydroxymethyl)-3-(acetamidomethylene)succinate...
278.12665706506	C14H18N2O4	alpha-Ribazole
300.03823598348	C14H8N2O6	Cinnavalinate

325.13140809235	C19H19NO4	(S)-Cheilanthifoline
334.05660207609	C11H15N2O8P	Nicotinamide D-ribonucleotide
335.07872089545	C11H17N3O7S	S-Formylglutathione
481.98926311559	C10H17N2O14P3	dTTP

(d) Pinot noir/Mercurey

mass	formula	name
160.08479225308	C6H12N2O3	N-gamma-Acetyldiaminobutyrate D-Alanyl-D-alanine
168.02834000608	C5H4N4O3	Urate
168.08987763352	C8H12N2O2	Pyridoxamine
190.01135252934	C6H6O7	Oxalosuccinate
190.06299417938	C11H10O3	1,2-Dihydroxy-7-hydroxymethylnaphthalene
190.09535693678	C7H14N2O4	LL-2,6-Diaminoheptanedioate meso-2,6-Diaminoheptanedioate
191.05824315209	C10H9NO3	5-Hydroxyindoleacetate
199.09569128993	C8H13N3O3	gamma-Glutamyl-beta-aminopropionitrile
204.08987763352	C11H12N2O2	L-Tryptophan Tryptophan
205.03750770751	C10H7NO4	Xanthurenic acid 6-Hydroxykynurenate
218.10552769766	C12H14N2O2	N-Acetylserotonin
220.08479225308	C11H12N2O3	5-Hydroxy-L-tryptophan
222.06742793578	C7H14N2O4S	L-Cystathionine Cystathionine
232.1211777618	C13H16N2O2	Melatonin
240.0633881022	C11H12O6	2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
245.14878949191	C9H19N5O3	beta-Alanyl-L-arginine
248.11609238136	C13H16N2O3	6-Hydroxymelatonin
250.15689456422	C15H22O3	Xanthoxin Abscisic alcohol
260.10485899136	C15H16O4	2,3-Bis(4-hydroxyphenyl)-1,2-propanediol
266.15180918378	C15H22O4	Xanthoxic acid
281.08993720319	C13H15NO6	4-Hydroxyphenylacetylglutamine
284.12629908875	C10H22NO6PR	1-(1-Alkenyl)-sn-glycero-3-phosphocholine
305.16270822063	C17H23NO4	(6S)-Hydroxyhyoscyamine
344.13186158484	C12H24O11	Melibiitol
354.0950821533	C16H18O9	Chlorogenate
360.0845174696	C18H16O8	Rosmarinate
422.08254204045	C12H23O14P	alpha, alpha'-Trehalose 6-phosphate Maltose 6'-phosphate Lactose 6-phosphate Sucrose 6-phosphate
614.14726755525	C20H31N4O16P	CMP-N-acetylneuraminat
838.15232277163	C24H41N8O17P3S	beta-Alanyl-CoA

(e) Syrah/Côte Rotie

mass	formula	name
156.0422587348	C7H8O4	2-Hydroxy-6-keto-2,4-heptadienoate
		2-Hydroxy-5-methyl-cis,cis-muconic semialdehyde
		1,6-Dihydroxy-cis-2,4-cyclohexadiene-1-carboxylic acid
		4-Carboxymethyl-4-methylbut-2-en-1,4-olide
		3-Methyl-cis,cis-hexadienedioate
159.06841391297	C10H9NO	Indole-3-acetaldehyde
		N-Hydroxy-1-aminonaphthalene
180.0534921248	C8H8N2O3	Nicotinurate
219.05315777165	C11H9NO4	5-Hydroxyindolepyruvate
		8-Methoxykynurenate
219.11067264777	C9H17NO5	Pantothenate
242.05790879894	C14H10O4	cis-4-(1'-Hydroxynaphth-2'-yl)-2-oxobut-3-enoate
		2-Hydroxy-2H-benzo[h]chromene-2-carboxylate
250.06234255534	C8H14N2O5S	gamma-L-Glutamyl-L-cysteine
262.04536868609	C6H15O9P	Galactitol 1-phosphate
		Sorbitol 6-phosphate
		D-Mannitol 1-phosphate
267.09675391905	C10H13N5O4	Deoxyguanosine
		Adenosine
274.00898317737	C6H11O10P	6-Phospho-2-dehydro-D-gluconate
		1-Phospho-alpha-D-galacturonate
		D-Glucuronate 1-phosphate
274.12771969418	C10H18N4O5	N2-Succinyl-L-arginine
307.08380627589	C10H17N3O6S	Glutathione
309.985484458	C5H12O11P2	D-Ribose 1,5-bisphosphate
		D-Ribulose 1,5-bisphosphate
318.03756727718	C15H10O8	Myricetin
322.06886740546	C15H14O8	Leucodelphinidin
338.05151669565	C10H15N2O9P	1-(5-Phosphoribosyl)imidazole-4-acetate
338.10016753374	C16H18O8	p-Coumaroyl quinic acid
362.17293855118	C20H26O6	Gibberellin A19
		Gibberellin A36
370.07474063154	C12H18O13	Digalacturonate
464.09547607612	C21H20O12	Quercetin 3-O-glucoside

(f) Grenache/Gigondas

mass	formula	name
150.0528234185	C5H10O5	L-Ribulose
		D-Lyxose
		D-Xylose

		L-Lyxose
		L-Xylulose
		D-Ribose
		D-Ribulose
		D-Xylulose
		L-Arabinose
158.02152329022	C6H6O5	2-Maleylacetate
		3-Hydroxy-cis,cis-muconate
		(Z)-5-Oxohex-2-enedioate
		2-Hydroxymuconate
		4-Methylene-2-oxoglutarate
174.11167570722	C6H14N4O2	L-Arginine
180.0647255148	C7H8N4O2	Theophylline
		1,7-Dimethylxanthine
180.0647255148	C7H8N4O2	Theobromine
195.05315777165	C9H9NO4	Dopaquinone
		2-Carboxy-2,3-dihydro-5,6-dihydroxyindole
207.08954328037	C11H13NO3	N-Acetyl-D-phenylalanine
		N-Acetyl-L-phenylalanine
208.0888150044	C15H12O	1-Methoxyphenanthrene
210.12559443594	C12H18O3	(-)-Jasmonic acid
218.05790879894	C12H10O4	2,2',3-Trihydroxydiphenylether
240.0633881022	C11H12O6	2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
250.15689456422	C15H22O3	Xanthoxin
		Abscisic alcohol
258.01406855781	C6H11O9P	D-Glucono-1,5-lactone 6-phosphate
		2-Deoxy-5-keto-D-gluconic acid 6-phosphate
		2-Dehydro-3-deoxy-6-phospho-D-gluconate
		2-Dehydro-3-deoxy-D-galactonate 6-phosphate
276.02463324151	C6H13O10P	6-Phospho-D-gluconate
296.23514488492	C18H32O3	13(S)-HODE
		9(10)-EpOME
		9(S)-HODE
		12(13)-EpOME
300.0633881022	C16H12O6	5,7,4'-Trihydroxy-3'-methoxyflavone
		Kaempferide
318.03756727718	C15H10O8	Myricetin
325.10089580971	C11H19NO10	N-Glycoloyl-neuraminate
330.0739527859	C17H14O7	3',4',5'-Trihydroxy-3,7-dimethoxyflavone
344.13186158484	C12H24O11	Melibiotol
352.06417594784	C12H16O12	4-(4-Deoxy-alpha-D-gluc-4-enuronosyl)-D-galacturonate
354.0950821533	C16H18O9	Chlorogenate
356.11073221744	C16H20O9	Scopolin
388.13694696528	C17H24O10	Secologanin

422.08254204045	C12H23O14P	alpha,alpha'-Trehalose 6-phosphate
		Maltose 6'-phosphate
		Lactose 6-phosphate
		Sucrose 6-phosphate
462.07982601198	C21H18O12	Luteolin 7-O-glucuronide
490.12132759089	C16H23N6O10P	L-2-Aminoadipate adenylate
566.05502056976	C15H24N2O17P2	UDP-D-galactose
		UDP-glucose

(g) White/sessile

mass	formula	name
212.03208797392	C9H8O6	3-(2-Carboxyethyl)-cis,cis-muconate
		2-Hydroxy-6-keptononatrienedioate
276.13213636832	C11H20N2O6	N6-(L-1,3-Dicarboxypropyl)-L-lysine
278.12665706506	C14H18N2O4	alpha-Ribazole
280.24023026536	C18H32O2	9-cis,11-trans-Octadecadienoate
		Linoleate
282.0950821533	C10H17O9R	sn-3-D-Galactosyl-sn-2-acylglycerol
346.17802393162	C20H26O5	Gibberellin A24
427.02941495855	C10H15N5O10P2	Adenosine 3',5'-bisphosphate
		dGDP
		ADP

(h) White/pedunculate

mass	formula	name
161.08406397711	C10H11NO	Indole-3-ethanol
286.10525291418	C13H18O7	Salicin
286.10556364417	C9H20NO7PR	1-Acyl-sn-glycero-3-phosphocholine
		2-Acyl-sn-glycero-3-phosphocholine

(i) Red/sessile

mass	formula	name
161.08406397711	C10H11NO	Indole-3-ethanol
162.10044231722	C6H14N2O3	N6-Hydroxy-L-lysine
		Procollagen 5-hydroxy-L-lysine
179.05824315209	C9H9NO3	Hippurate
208.0888150044	C15H12O	1-Methoxyphenanthrene
265.11230718287	C12H17N4OS	Thiamin
316.20384475664	C20H28O3	15-Deoxy-delta-12,14-PGJ2
		Gibberellin A12 aldehyde
338.24570956862	C20H34O4	5,6-DHET
		14,15-DHET
		8,9-DHET
		Aphidicolin
		11,12-DHET
362.17293855118	C20H26O6	Gibberellin A19

	Gibberellin A36
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(j) Red/pedunculate

mass	formula	name
236.07970687264	C ₁₁ H ₁₂ N ₂ O ₄	L-Formylkynurenine
506.98622981623	C ₁₀ H ₁₅ N ₅ O ₁₃ P ₂ S	3'-Phosphoadenylyl sulfate

(k) Darney

mass	formula	name
223.04807239121	C ₁₀ H ₉ NO ₅	4-(2-Amino-5-hydroxyphenyl)-2,4-dioxobutanoate 7,8-Dihydro-7,8-dihydroxykynurenate
256.07355886308	C ₁₅ H ₁₂ O ₄	4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate Liquiritigenin Pinocembrin Isoliquiritigenin
267.09675391905	C ₁₀ H ₁₃ N ₅ O ₄	Deoxyguanosine Adenosine
282.2558803295	C ₁₈ H ₃₄ O ₂	(9Z)-Octadecenoic acid
320.05321734132	C ₁₅ H ₁₂ O ₈	Dihydromyricetin
425.04496822237	C ₁₂ H ₁₉ N ₄ O ₇ P ₂ S	Thiamin diphosphate

(l) Citeaux

mass	formula	name
172.04840674436	C ₆ H ₈ N ₂ O ₄	Hydantoin-5-propionate
173.01466408695	C ₆ H ₇ NO ₃ S	2-Aminobenzenesulfonate
190.05897142806	C ₆ H ₁₀ N ₂ O ₅	N-Carbamyl-L-glutamate
195.05315777165	C ₉ H ₉ NO ₄	2-Carboxy-2,3-dihydro-5,6-dihydroxyindole Dopaquinone
212.03208797392	C ₉ H ₈ O ₆	3-(2-Carboxyethenyl)-cis,cis-muconate 2-Hydroxy-6-ketononatrienedioate
248.14124450008	C ₁₅ H ₂₀ O ₃	Abscisic aldehyde
256.07355886308	C ₁₅ H ₁₂ O ₄	Liquiritigenin Pinocembrin Isoliquiritigenin
320.05321734132	C ₁₅ H ₁₂ O ₈	Dihydromyricetin
344.13186158484	C ₁₂ H ₂₄ O ₁₁	Melibiitol
425.04496822237	C ₁₂ H ₁₉ N ₄ O ₇ P ₂ S	Thiamin diphosphate

(m) Tronçais

mass	formula	name
163.06332853253	C ₉ H ₉ NO ₂	3-Methyldioxyindole
219.05315777165	C ₁₁ H ₉ NO ₄	5-Hydroxyindolepyruvate 8-Methoxykynurenate

223.04807239121	C10H9NO5	4-(2-Amino-5-hydroxyphenyl)-2,4-dioxobutanoate
		7,8-Dihydro-7,8-dihydroxykynurenate
		4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate
256.07355886308	C15H12O4	Liquiritigenin
		Pinocembrin
		Isoliquiritigenin
267.09675391905	C10H13N5O4	Deoxyguanosine
		Adenosine
282.2558803295	C18H34O2	(9Z)-Octadecenoic acid
289.07976644231	C11H15NO8	N-Succinyl-2-L-amino-6-oxoheptanedioate
320.05321734132	C15H12O8	Dihydromyricetin
364.18858861532	C20H28O6	Gibberellin A37 open lactone
		Gibberellin A44 diacid
425.04496822237	C12H19N4O7P2S	Thiamin diphosphate

(n) Bitche

mass	formula	name
160.08479225308	C6H12N2O3	N-gamma-Acetyldiaminobutyrate
		D-Alanyl-D-alanine
163.06332853253	C9H9NO2	3-Methyldioxyindole
174.0640568085	C6H10N2O4	N-Formimino-L-glutamate
174.06807955982	C11H10O2	1,2-Dihydroxy-8-methylnaphthalene
175.04807239121	C6H9NO5	N-Acetyl-L-aspartate
		N-Formyl-L-glutamate
178.1106130781	C10H14N2O	(S)-6-Hydroxynicotine
		(R)-6-Hydroxynicotine
179.05824315209	C9H9NO3	Hippurate
202.06299417938	C12H10O3	2,2',3-Trihydroxybiphenyl
219.11067264777	C9H17NO5	Pantothenate
252.08987763352	C15H12N2O2	Oxcarbazepine
		Carbamazepine-10,11-epoxide
265.11230718287	C12H17N4OS	Thiamin
267.09675391905	C10H13N5O4	Deoxyguanosine
		Adenosine
280.1310737392	C15H20O5	Phaseic acid
		8'-Hydroxyabscisate
288.0633881022	C15H12O6	Eriodictyol
		Fustin
		Dihydrokaempferol
		2',3,4,4',6'-Pentahydroxychalcone
312.23005950448	C18H32O4	9(S)-HPODE
		(9Z,12Z)-(11S)-11-Hydroperoxyoctadeca-9,12-dienoic acid<...

		(9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid<...
		(7S,8S)-DiHODE
		8(R)-HPODE
		9,10-Epoxy-13-hydroxy-11-octadecenoate
		9,10-12,13-Diepoxyoctadecanoate
		12,13-Epoxy-9-hydroxy-10-octadecenoate
325.13140809235	C19H19NO4	(S)-Cheilanthifoline
330.21949482078	C21H30O3	11beta-Hydroxyprogesterone
		11alpha-Hydroxyprogesterone
		17alpha-Hydroxyprogesterone
		11-Deoxycorticosterone
338.24570956862	C20H34O4	14,15-DHET
		8,9-DHET
		5,6-DHET
		Aphidicolin
		11,12-DHET
339.9960491417	C6H14O12P2	beta-D-Fructose 2,6-bisphosphate
		D-myo-Inositol 3,4-bisphosphate
		alpha-D-Glucose 1,6-bisphosphate
		beta-D-Fructose 1,6-bisphosphate
		1D-myo-Inositol 1,4-bisphosphate
		D-Fructose 1,6-bisphosphate
		D-myo-Inositol 1,3-bisphosphate
		D-Tagatose 1,6-bisphosphate
565.07100498705	C15H25N3O16P2	CDP-glucose

(o) Bertrange

mass	formula	name
150.01643790978	C4H6O6	meso-Tartaric acid
		(R,R)-Tartaric acid
177.04596421523	C6H11NO3S	N-Formyl-L-methionine
197.03242232707	C8H7NO5	3-Hydroxy-2-methylpyridine-4,5-dicarboxylate
197.10519334451	C10H15NO3	L-Metanephine
208.0888150044	C15H12O	1-Methoxyphenanthrene
210.06807955982	C14H10O2	Phenanthrene-3,4-diol
212.08372962396	C14H12O2	Pinosylvin
		(+)-cis-3,4-Dihydrophenanthrene-3,4-diol
		trans-9(S),10(S)-Dihydrodiolphenanthrene
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
226.09535693678	C10H14N2O4	Porphobilinogen
245.14878949191	C9H19N5O3	beta-Alanyl-L-arginine
248.11609238136	C13H16N2O3	6-Hydroxymelatonin
302.04265265762	C15H10O7	Tricetin
		Quercetin

352.06417594784	C12H16O12	4-(4-Deoxy-alpha-D-gluc-4-enuronosyl)-D-galacturonate
547.06044030335	C15H23N3O15P2	CDP-4-dehydro-6-deoxy-D-glucose

(p) Jupilles

mass	formula	name
197.10519334451	C10H15NO3	L-Metanephrine
210.06807955982	C14H10O2	Phenanthrene-3,4-diol
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
245.14878949191	C9H19N5O3	beta-Alanyl-L-arginine
248.11609238136	C13H16N2O3	6-Hydroxymelatonin
302.04265265762	C15H10O7	Quercetin
		Tricetin
547.06044030335	C15H23N3O15P2	CDP-4-dehydro-6-deoxy-D-glucose

(q) Saint-Palais

mass	formula	name
177.04596421523	C6H11NO3S	N-Formyl-L-methionine
180.07864424352	C10H12O3	Coniferyl alcohol
192.07864424352	C11H12O3	cis-1,2-Dihydroxy-1,2-dihydro-7-hydroxymethylnaphthalene...
197.03242232707	C8H7NO5	3-Hydroxy-2-methylpyridine-4,5-dicarboxylate
197.10519334451	C10H15NO3	L-Metanephrine
208.0888150044	C15H12O	1-Methoxyphenanthrene
210.06807955982	C14H10O2	Phenanthrene-3,4-diol
212.08372962396	C14H12O2	Pinosylvin
		(+)-cis-3,4-Dihydrophenanthrene-3,4-diol
		trans-9(S),10(S)-Dihydrodiolphenanthrene
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
226.09535693678	C10H14N2O4	Porphobilinogen
248.11609238136	C13H16N2O3	6-Hydroxymelatonin
250.04773803806	C12H10O6	2-Hydroxy-6-oxo-6-(2-hydroxyphenoxy)-hexa-2,4-dienoate
302.04265265762	C15H10O7	Tricetin
		Quercetin
352.06417594784	C12H16O12	4-(4-Deoxy-alpha-D-gluc-4-enuronosyl)-D-galacturonate
434.12129690114	C21H22O10	Naringenin 7-O-beta-D-glucoside
547.06044030335	C15H23N3O15P2	CDP-4-dehydro-6-deoxy-D-glucose

(r) Sud-Ouest

mass	formula	name
214.04773803806	C9H10O6	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
547.06044030335	C15H23N3O15P2	CDP-4-dehydro-6-deoxy-D-glucose

(s) Limousin

mass	formula	name
180.0647255148	C7H8N4O2	Theophylline
		1,7-Dimethylxanthine
		Theobromine
195.05315777165	C9H9NO4	2-Carboxy-2,3-dihydro-5,6-dihydroxyindole
		Dopaquinone
245.14878949191	C9H19N5O3	beta-Alanyl-L-arginine
248.14124450008	C15H20O3	Abscisic aldehyde
278.12665706506	C14H18N2O4	alpha-Ribazole
355.15523462397	C14H23N6O3S	S-Adenosylmethioninamine