

SPME GCxGC ToF MS of 11 whiskies

Damien STEYER, PhD, CEO of Twistaroma



Implantation géographique



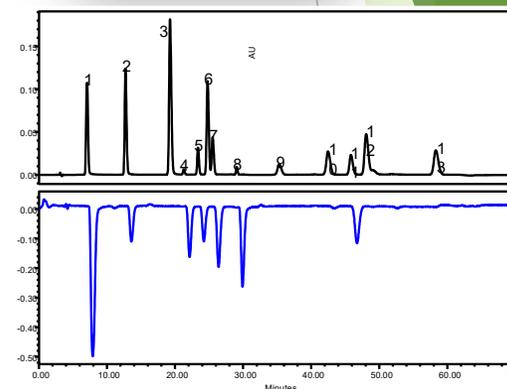
Localisée dans les locaux de
l'école Supérieure de
Biotechnologie de Strasbourg





Thèse

Présentée par
Céline LEITAO
 Pour obtenir le grade de
Docteur de l'Université de Strasbourg
 Spécialité
Chimie analytique
Etude de composés à intérêts technologique et fonctionnel dans la bière
 Soutenue le 28 mars 2011 devant la commission d'examen



Antioxydant screening



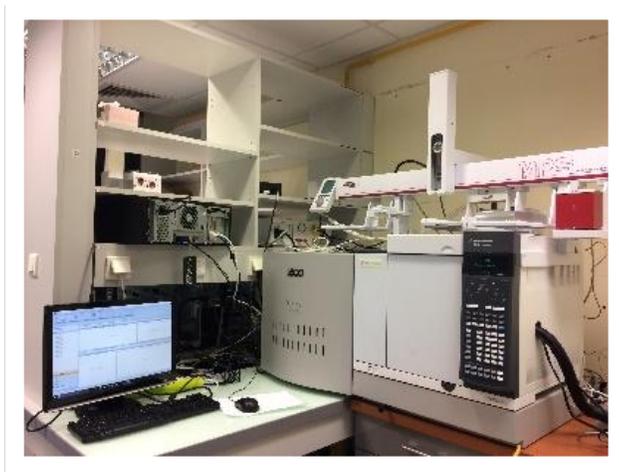
Thèse présentée pour obtenir le grade de
 Docteur de l'Université de STRASBOURG
 Discipline : Sciences du vivant
 ASPECTS MOLECULAIRES ET CELLULAIRES DE LA BIOLOGIE
 par
DAMIEN STEYER

Etude génétique du métabolisme des acides gras
 et des terpènes aromatiques chez la levure en
 conditions fermentaires

Small fermentations



UPLC/UV



GC/ToF-MS



GC/SCD/MS



4x MPS
workstations



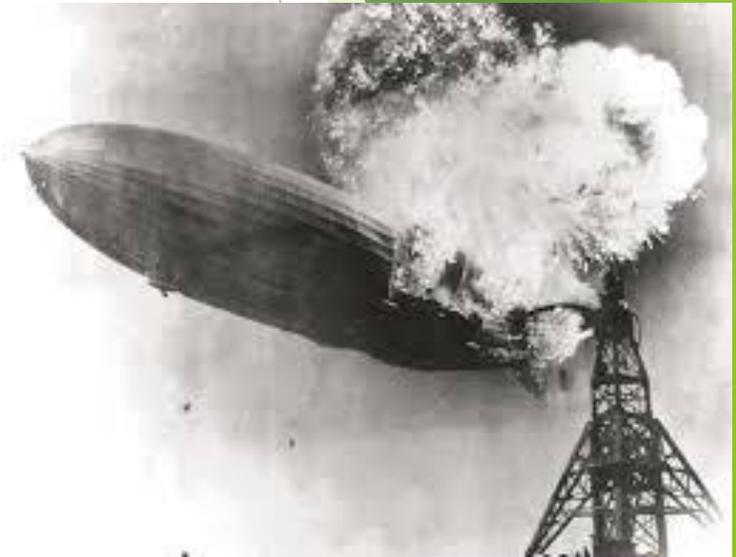
H₂ ? Comment on fait ?



H₂O



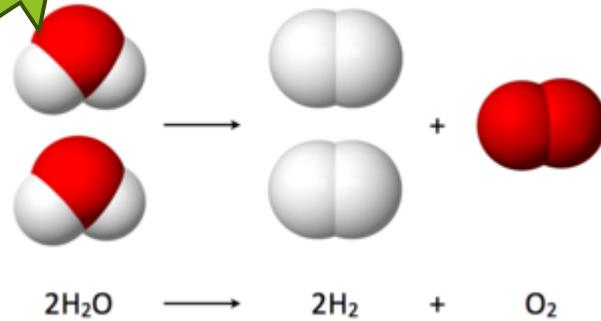
O₂



2H₂



e⁻





Codes Article	TVA	Désignation	Capacité	Emb./Qté	Prix unitaire (EUR) par 10 EMB	Montant H.T (EUR)
3340152	9	HELIUM 6.0 B50 SCIENTIFIQUE Lot: 171-25FI23 (1 EMB) CID: 25031101477712	9 M3	1 EMB	3.900,00 par 10 EMB	390,00
2210152	9	AZOTE 5.0 B50 INSTRUMENT Lot: 269-25FI06 (1 EMB) CID: 25031101917499	9,4 M3	1 EMB	880,00 par 10 EMB	88,00
		TRANSPORT FORFAIT ADR et énergie				40,00 13,00

GCxGC ? => 19/03/2025



Symposium Whisky : 11/06/2025

11 June, 2025

LECO Whisky Science Seminar – Hosted at SWRI

Aroma & Flavour Science in Whisky: Advanced Characterisation and Troubleshooting Approaches

11 June, 2025

LECO Europe invites you to attend a one-day technical seminar focused on aroma and flavour science in whisky production. This event will highlight the application of advanced analytical technologies—particularly comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry (GC×GC-TOFMS)—in the characterisation, quality control, and sensory understanding of whisky.

Facilitated by The Scotch Whisky Research Institute (SWRI) and hosted on their premises in Edinburgh, the seminar will feature a programme of expert-led presentations, technical case studies, and the opportunity to engage with peers from across the industry and research communities.

Event Location: The Scotch Whisky Research Institute The Robertson Trust Building, Research Ave N, Edinburgh EH14 4AP

[Register](#)



Dr. Damien Steyer

CEO – Twistaroma

Envoi des échantillons : 16/05/2025

De Christine Loeb-Stubbins 

Pour Damien Steyer , Hubert Latappy 

Sujet **Re: Invitation to present at SWRI event on June 11th in Edinburgh**

Répondre Répondre à tous Transférer Archiver Indésirable Supprimer Envoyer Plus Tard Autres

16/05/2025, 15:07

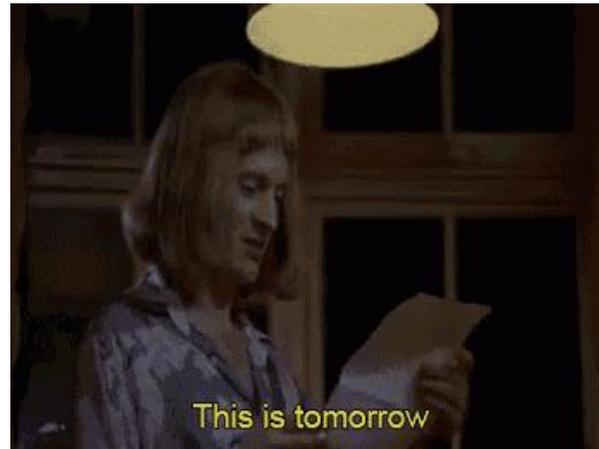
Hi Damien,

Apologies for the delay, it's been a crazy couple of weeks...

If it's not too late and you're still up for it, I have a suggestion for a few whiskys for you to test:
I'd like you to test a few very popular scotch whiskeys and compare them to some non-Scottish ones? What do you think?

The goal is to use GCxGC-TOFMS and PCA to explore the diversity within Scotch whiskies and compare them with a selection of non-Scottish whiskies from other regions (e.g. Ireland, USA, Japan, etc.).
The aim is to visualise both how broad the Scotch whisky category is in terms of aroma profiles, and how whiskies from other countries differ or overlap.

- Ship To
ILLKIRCH FR
- Label Created
United Kingdom
29/05/2025, 12:36
 - We Have Your Package
Derby, United Kingdom
29/05/2025, 15:26
 - Cleared Import Customs
29/05/2025, 20:21
 - On the Way
03/06/2025, 8:06
 - In Warehouse
Strasbourg, France
03/06/2025, 8:09
 - Out for Delivery
 - Delivery



Samples

16:18 1:08 74 16:18 1:12 74 16:18 1:10 74

Search or ask a question

- Eigashima Shuz Akashi White Oak Japanese Whisky, 50 cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £29.00
- Aberlour 12 Year Old Single Malt Scotch Whisky With Giftbox, 70 cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £33.97
- Monkey Shoulder Blended Malt Scotch Whisky, 70cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £24.50
- Old Pulteney 12 Years Old Single Malt Scotch Whisky, 70cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £23.78

Track shipment >

Buy it again >

Delivered
Delivery Estimate:
Sunday, 25 May 2025

- Amrut Indian Single Malt Whisky | 46 Percent | 70cl | Rich and
Qty: 1
Sold By: Amazon EU S.a.r.L. £47.45

Track shipment >

Buy it again >

Payment method

Mastercard/EuroCard ending in 1486

Dispatch to

Buy it again >

Home Person Cart Menu Add

16:18 1:05 74

Search or ask a question

Delivered
Delivery Estimate:
Monday, 26 May 2025

- Rittenhouse Straight Rye Whisky | Bottled-In-Bond | 70cl | 50% ABV |
Qty: 1
Sold By: Amazon EU S.a.r.L. £40.95
- Brenne Estate Cask Whisky, 70cl - 40% ABV French Single Malt Scotch
Qty: 1
Sold By: Amazon EU S.a.r.L. £55.68
- Powers Gold Label Distiller's Cut Irish Blended Malt Whiskey, 70cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £30.90
- Finlaggan Old Reserve Single Malt Scotch Whisky 70 cl
Qty: 1
Sold By: Amazon EU S.a.r.L. £34.52

Track shipment >

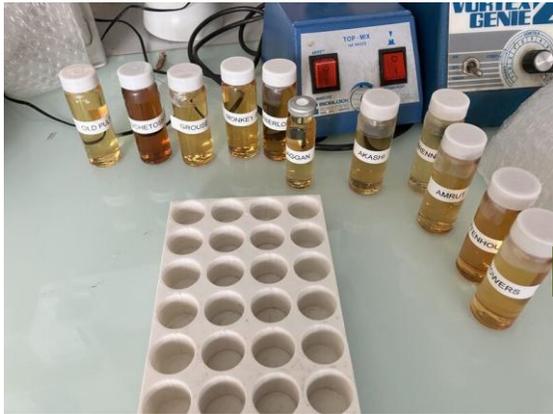
Buy it again >

Delivered
Delivery Estimate:

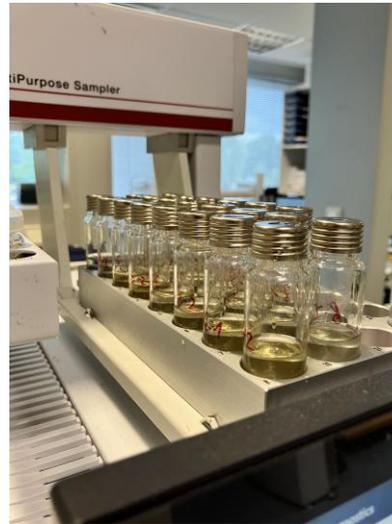
Home Person Cart Menu Add



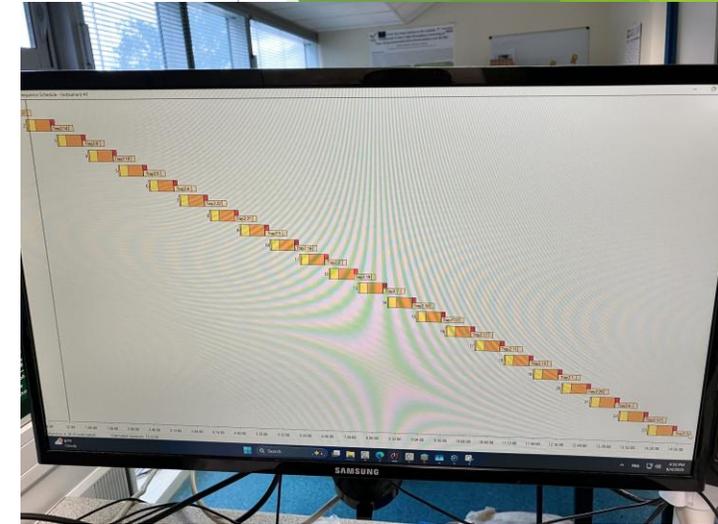
Sample	Whisky Name	Origin	Type / Maturation	Tasting Notes & Aromas
1	Old Pulteney 12 Years Old	Scotland	Ex-bourbon casks	Maritime, salty, vanilla, honey, citrus
2	Auchentoshan Three Wood	Scotland	Bourbon, Oloroso & Pedro Ximénez casks	Rich, toffee, dark fruit, chocolate, spice
3	The Famous Grouse Finest	Scotland	Ex-bourbon & sherry casks	Smooth, malty, light smoke, dried fruit, sweet grains
4	Monkey Shoulder	Scotland	Ex-bourbon casks	Creamy, vanilla, honey, malt, orange zest
5	Aberlour 12 Year Old	Scotland	Double cask (bourbon & sherry)	Rich, sherried, nutty, spice, dried fruits
6	Finlaggan Old Reserve	Scotland (Islay)	Ex-bourbon casks (undisclosed distillery)	Peaty, smoky, iodine, brine, earthy
7	Eigashima Shuzo Akashi	Japan	Shochu, bourbon & wine casks (varies)	Light, floral, apple, toffee, malt
8	Brenne Estate Cask	France	Cognac casks	Fruity, banana, tropical fruit, custard, light oak
9	Amrut Indian Single Malt	India	Bourbon casks	Tropical fruit, spice, oak, honey, intense due to climate aging
10	Rittenhouse Straight Rye	USA (Kentucky)	New charred oak barrels	Spicy, caramel, cinnamon, black pepper, bold finish
11	Powers Gold Label Cut (likely "Powers Gold Label")	Ireland	Bourbon casks	Spicy, honey, apple, cereal grain, vanilla



30 min



1 jour
11x3 +QCs
& blancs



1mL whisky
9mL NaCl 5M
+IS (1,4 dibromobenzene)

SPME CAR/DVB/PDMS
1cm
10 incubation 50°C
20 extraction 50°C
Injection port 250°C 5min



GCxGC/BTX

Carrier Gas : H₂

1st dimension : Rxi-5ms (30 m × 0.25 mm i.d. × 0.25 μm film thickness)

DB-Wax UI column (1.7 m × 0.25 mm i.d. × 0.25 μm film thickness)

Modulation : 2.3 sec

Hot pulse : 0.69 sec

Cool time : 0.46 sec

Acquired Samples

Name	Modified	Modified By	Version
TwGCGC-711	6/4/2025 4:54:45 PM	Twistaroma	3
TwGCGC-711 - Source and...	6/4/2025 5:20:15 PM	Twistaroma	2
TwGCGC-711 - Mass Calbr...	6/4/2025 5:21:15 PM	Twistaroma	3
TwGCGC-711 - Gain Optimi...	6/4/2025 5:24:30 PM	Twistaroma	2
TwGCGC-711 - Tune Valda...	6/4/2025 5:26:38 PM	Twistaroma	3
TwGCGC-712-7-2	6/7/2025 11:58:03 PM	Twistaroma	10
TwGCGC-713-4-2	6/8/2025 12:11:54 AM	Twistaroma	9
TwGCGC-714-9-2	6/8/2025 12:43:33 AM	Twistaroma	7
TwGCGC-715-3-1	6/8/2025 1:01:43 AM	Twistaroma	7
TwGCGC-716-2-2	6/8/2025 1:19:11 AM	Twistaroma	7
TwGCGC-717-11-2	6/8/2025 1:33:53 AM	Twistaroma	7
TwGCGC-718-11-1	6/8/2025 1:48:28 AM	Twistaroma	8
TwGCGC-719-5-1	6/8/2025 2:04:53 AM	Twistaroma	7
TwGCGC-720-8-2	6/8/2025 2:15:21 AM	Twistaroma	7
TwGCGC-721-1-2	6/8/2025 2:31:46 AM	Twistaroma	8
TwGCGC-722-10-1	6/8/2025 2:49:24 AM	Twistaroma	7
TwGCGC-723-4-1?	6/8/2025 3:05:52 AM	Twistaroma	8
TwGCGC-724-5-erreur	6/8/2025 3:17:45 AM	Twistaroma	7
TwGCGC-725-7-1	6/8/2025 3:32:34 AM	Twistaroma	7
TwGCGC-726-blanc	6/8/2025 3:42:15 AM	Twistaroma	6
TwGCGC-727-erreur	6/8/2025 3:59:34 AM	Twistaroma	7
TwGCGC-728-8-1	6/8/2025 4:15:46 AM	Twistaroma	6
TwGCGC-729-1-1	6/8/2025 4:32:29 AM	Twistaroma	5
TwGCGC-730-10-2	6/8/2025 4:50:15 AM	Twistaroma	5
TwGCGC-731-3-2	6/8/2025 5:03:57 AM	Twistaroma	4
TwGCGC-731-2 ?	6/8/2025 5:19:56 AM	Twistaroma	6
TwGCGC-732-6-2	6/8/2025 5:34:42 AM	Twistaroma	5
TwGCGC-733-2-1	6/8/2025 5:49:07 AM	Twistaroma	4
TwGCGC-734-9-1	6/8/2025 6:03:49 AM	Twistaroma	4
TwGCGC-735-4-1=duplicat	6/8/2025 6:17:01 AM	Twistaroma	5
TwGCGC-736-5-2	6/8/2025 6:30:36 AM	Twistaroma	4
TwGCGC-737-8-2-2	6/8/2025 6:44:26 AM	Twistaroma	4
TwGCGC-738	6/8/2025 6:44:27 AM	Twistaroma	4
New	6/8/2025 6:44:28 AM	Twistaroma	3
New:2	6/8/2025 6:45:08 AM	Twistaroma	5
TwGCGC-738 1	6/8/2025 6:58:34 AM	Twistaroma	6
TwGCGC-739 2	6/8/2025 7:12:22 AM	Twistaroma	5
TwGCGC-740 3	6/8/2025 7:24:10 AM	Twistaroma	5
TwGCGC-741 4	6/8/2025 7:36:52 AM	Twistaroma	5
TwGCGC-742 5	6/8/2025 7:49:29 AM	Twistaroma	5
TwGCGC-743 7	6/8/2025 8:01:12 AM	Twistaroma	6
TwGCGC-744 6	6/8/2025 8:16:47 AM	Twistaroma	7

Acquired Samples

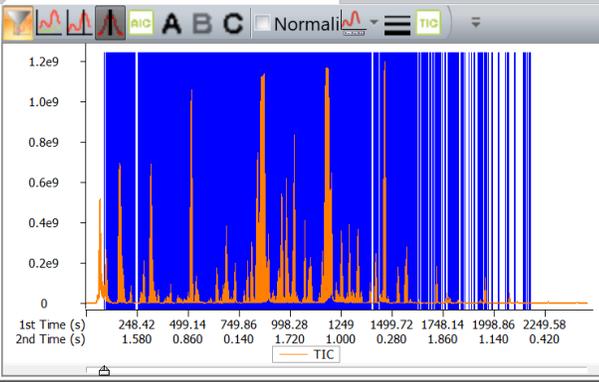
Libraries

References

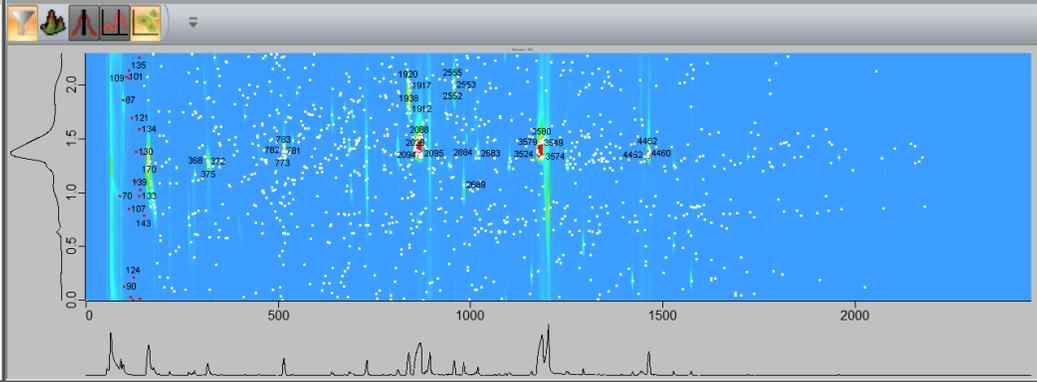
Quantitation

Acquisition Queue

Chromatogram - TwGCGC-729-1-1



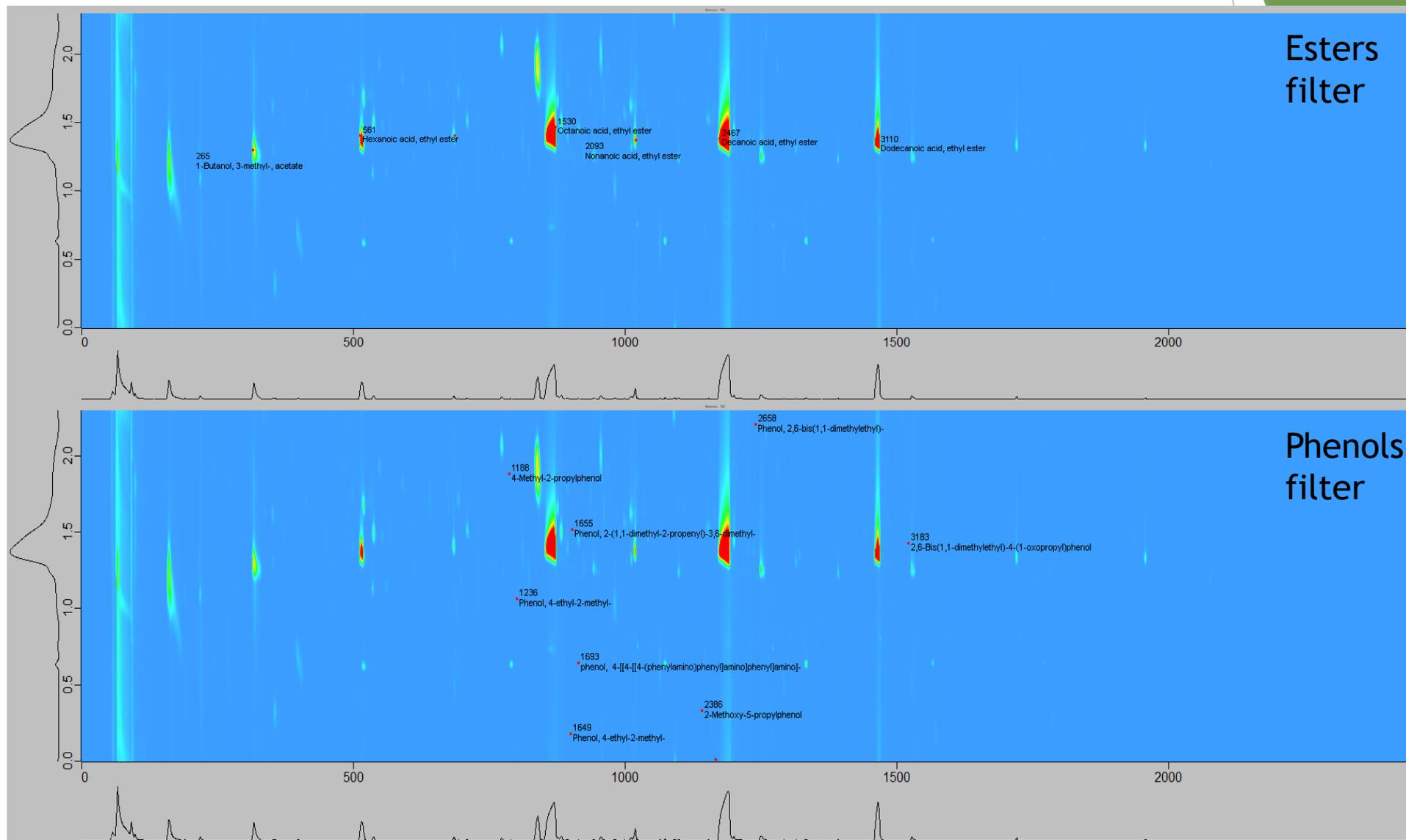
"TwGCGC-729-1-1"



Peak Table - TwGCGC-729-1-1 Retention Index Table - whisk2 Hit Table - TwGCGC-729-1-1 Spectra

Peak #	Description	Group	2nd Dimensio	1st Dimensio	CAS	Name	Sample	Area	Probability	Similarity	FWHH (s)	Retention Inc	Lib. RI	Observed Ion	Type	Synonyms	Synonyms Lit	Base Mass	Concentra
750*			0.905	508.341	62338-07-2	1,3-Hexadiene, 3-ethyl-2,5-dimethyl-	TwGCGC-729-1-1	1098014	24.8	702	0.060	988.2	996 ± 0(1)	138.18	Unknown	1,3-Hexadien	1,3-Hexadien-	109.13	
141			1.359	149.512	110-80-5	Ethanol, 2-ethoxy-	TwGCGC-729-1-1	3048623	77.3	703	0.130	706.6	710 ± 8(10)	90.04	Unknown	Ethanol, 2-eth	Ethanol, 2-eth-	30.99	
421			1.467	347.328	16509-44-7	(Z)-Ethyl 2-methylbut-2-enoate	TwGCGC-729-1-1	707678	63.5	704	0.093	871.3	899 ± 0(1)	128.11	Unknown	(Z)-Ethyl 2-m	(Z)-Ethyl 2-m-	55.07	
662			0.905	480.738	629-08-3	Heptanonitrile	TwGCGC-729-1-1	1026392	71.6	704	0.139	968.6	985 ± 1(3)	96.05	Unknown	Heptanonitril	Heptanonitril-	82.09	
2350			0.098	920.074	96530-75-5	4-Fluoro-2-pyridone	TwGCGC-729-1-1	800841	5.4	704	0.107	1255.3	1278 ± 0(1)	113.09	Unknown	4-Fluoro-2-p	4-Fluoro-2-p-	113.09	
3574			1.340	1186.89	110-38-3	Decanoic acid, ethyl ester	TwGCGC-729-1-1	68133728	32.2	704	0.068	1421.1	1396 ± 2(69)	200.18	Unknown	Decanoic aci	Decanoic aci-	88.35	
4187			0.093	1357.11		(3aR,4S,7S,7aS)-3a,4,5,6,7,7a-Hexahydro-1H-4,7-methanoninden-6-yl pr	TwGCGC-729-1-1	2232415	39.4	704	0.113	1527.6	1522 ± 0(1)	206.19	Unknown	(3aR,4S,7S,7	(3aR,4S,7S,7	66.06	
781			1.392	515.241	123-66-0	Hexanoic acid, ethyl ester	TwGCGC-729-1-1	816415176	35.4	705	0.069	993.1	999 ± 3(153)	144.32	Unknown	Hexanoic acid	Hexanoic aci-	99.41	
860			0.941	538.243	62338-07-2	1,3-Hexadiene, 3-ethyl-2,5-dimethyl-	TwGCGC-729-1-1	601281	24.8	705	0.056	1008.8	996 ± 0(1)	138.18	Unknown	1,3-Hexadien	1,3-Hexadien-	109.13	
2788			1.018	1005.18	54889-48-4	Octane, 1,1-diethoxy-	TwGCGC-729-1-1	1526231	90.6	705	0.046	1308.2	1270 ± 0(1)	180.23	Unknown	Octane, 1,1-ε	Octane, 1,1-ε	85.08	
1223			0.007	121.91	116-09-6	2-Propanone, 1-hydroxy-	TwGCGC-729-1-1	8708190	81.9	706	0.173	682.4	666 ± 8(19)	74.09	Unknown	2-Propanone	2-Propanone-	43.06	
1188			1.558	664.753	2890-61-1	1-Methyl-1-cyclohexanecarboxylic acid chloride	TwGCGC-729-1-1	7425153	10.9	706	0.078	1093.2	1091 ± 0(1)	153.13	Unknown	1-Methyl-1-c	1-Methyl-1-c-	97.09	
3406			1.434	1143.19	122-84-9	2-Propanone, 1-(4-methoxyphenyl)-	TwGCGC-729-1-1	728975	48.2	706	0.148	1393.9	1384 ± 3(12)	164.17	Unknown	2-Propanone	2-Propanone-	121.11	
3939			1.353	1281.2	451-55-8	1-Methyl-4-(6-methylhept-5-en-2-yl)cyclohexa-1,3-diene	TwGCGC-729-1-1	1308499	10.8	707	0.088	1479.6	1480 ± 2(7)	204.23	Unknown	1-Methyl-4-(1-Methyl-4-(119.12	
4354			1.685	1426.11	73177-70-5	Bisabolatrien-7-ol,1,3,5-	TwGCGC-729-1-1	981021	9.5	707	0.074	1571.9	1601 ± 0(1)	203.22	Unknown	Bisabolatrien	Bisabolatrien-	145.14	
4717			0.208	1623.93	88034-74-6	Bergamotol, Z-α-trans-	TwGCGC-729-1-1	4760331	2.0	709	0.104	1703.5	1697 ± 7(13)	204.23	Unknown	Bergamotol	Bergamotol-	69.08	
5050			1.291	2164.47	111-06-8	Hexadecanoic acid, butyl ester	TwGCGC-729-1-1	1133873	64.4	710	0.052	2197.9	2175 ± 13(2)	312.38	Unknown	Hexadecanoic	Hexadecanoic-	56.07	
3880			1.466	1262.8	39701-09-2	1,4-Dimethoxy-2-methyl-5-(prop-1-en-2-yl)benzene	TwGCGC-729-1-1	5309155	15.1	711	0.071	1488.2	1443 ± 0(1)	192.21	Unknown	1,4-Dimetho	1,4-Dimetho-	192.21	
4370			1.524	1433.01	124-25-4	Tetradecanal	TwGCGC-729-1-1	432710	9.1	711	0.048	1576.3	1613 ± 2(11)	168.24	Unknown	Tetradecanal	Tetradecanal-	57.08	
4942			0.813	1890.95	6368-38-5	Benzenepropionic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl es	TwGCGC-729-1-1	362654	92.1	711	0.115	1912.5	1943 ± 0(1)	292.27	Unknown	Benzeneprop	Benzeneprop-	272.25	
3423			2.038	1147.79	80116-19-8	Shoal acetate	TwGCGC-729-1-1	1082677	3.6	712	0.070	1396.5	1419 ± 0(1)	192.20	Unknown	Shoal aceta	Shoal aceta-	93.09	
3563			1.481	1184.59	110-38-3	Decanoic acid, ethyl ester	TwGCGC-729-1-1	84507894	24.7	712	0.111	1419.6	1396 ± 2(69)	200.27	Unknown	Decanoic aci	Decanoic aci-	200.27	
4599			2.022	1543.42		Amberone (nonar 2)	TwGCGC-729-1-1	1008147	57.1	712	0.095	1649.3	1658 ± 0(1)	224.25	Unknown	Amberone (A	Amberone (A	191.23	
4854			1.286	1775.74	124-06-1	Tetradecanoic acid, ethyl ester	TwGCGC-729-1-1	4400286	9.3	712	0.057	1813.2	1794 ± 1(53)	270.21	Unknown	Tetradecanoic	Tetradecanoic-	101.08	
733			2.186	501.44	110-93-0	5-Hepten-2-one, 6-methyl-	TwGCGC-729-1-1	8494485	19.4	713	0.122	983.3	986 ± 2(22)	126.14	Unknown	5-Hepten-2-ε	5-Hepten-2-ε	43.04	
2670			1.585	977.578	118-61-6	Benzoic acid, 2-hydroxy-, ethyl ester	TwGCGC-729-1-1	6002239	87.5	713	0.071	1291.0	1270 ± 3(19)	166.11	Unknown	Benzoic acid	Benzoic aci-	120.04	
2725			0.316	991.379	7289-53-4	Methyl undecyl ester	TwGCGC-729-1-1	2307361	3.0	714	0.119	1299.6	1325 ± 0(1)	170.21	Unknown	Methyl undec	Methyl undec-	45.05	
623			1.401	462.337	81945-73-5	1H-Pyrazol-1-ol, Ac derivative	TwGCGC-729-1-1	597780	33.4	715	0.091	955.6	988 ± 0(1)	84.11	Unknown	1H-Pyrazol-1	1H-Pyrazol-1	84.11	
628			1.545	464.637	3420-59-5	Isomaltol	TwGCGC-729-1-1	247029	5.3	715	0.087	957.2	989 ± 4(5)	126.13	Unknown	Isomaltol	Isomaltol / E	111.11	
1978			0.982	948.768	1750-51-2	Naphthalene, decahydro-1,6-dimethyl-	TwGCGC-729-1-1	4671009	48.8	715	0.065	1211.0	1196 ± 0(1)	166.21	Unknown	Naphthalene	Naphthalene,	95.11	
2712			1.640	986.779	2855-19-8	Oxrane, decyl-	TwGCGC-729-1-1	6549777	3.4	715	0.181	1296.8	1307 ± 0(1)	175.18	Unknown	Oxrane, dec	Oxrane, dec-	57.07	
2819			0.609	1009.78	25564-22-1	2-Cyclopenten-1-one, 2-pentyl-	TwGCGC-729-1-1	2301202	83.0	715	0.146	1311.0	1288 ± 0(1)	152.17	Unknown	2-Cyclopente	2-Cyclopente-	96.08	
2866			1.041	1016.68	123-29-5	Nonanoic acid, ethyl ester	TwGCGC-729-1-1	78256293	0.9	715	0.052	1315.3	1296 ± 2(35)	172.19	Unknown	Nonanoic aci	Nonanoic aci-	88.08	
3905			1																

Results



Sync2D

Alignment name:

Alignment type:

Sample set (32 samples)

Databases:

Samples to compare:

Location	Name	Date	Class	Scale factor	Color
MainDatabase\Twistaroma\juin	TwGCGC-719-5-1	6/5/2025 12:35:18 AM	Aberfour 12 Year O	1	
MainDatabase\Twistaroma\juin	TwGCGC-736-5-2	6/5/2025 7:41:13 PM	Aberfour 12 Year O	1	
MainDatabase\Twistaroma\juin	TwGCGC-742-5	6/6/2025 1:10:40 AM	Aberfour 12 Year O	1	
MainDatabase\Twistaroma\juin	TwGCGC-714-9-2	6/4/2025 7:07:55 PM	Amrut Indian Sing	1	
MainDatabase\Twistaroma\juin	TwGCGC-734-9-1	6/5/2025 6:00:03 PM	Amrut Indian Sing	1	
MainDatabase\Twistaroma\juin	TwGCGC-746-9	6/6/2025 4:35:01 AM	Amrut Indian Sing	1	
MainDatabase\Twistaroma\juin	TwGCGC-716-2-2	6/4/2025 10:03:14 PM	Auchentoshan Th	1	
MainDatabase\Twistaroma\juin	TwGCGC-733-2-1	6/5/2025 5:09:43 PM	Auchentoshan Th	1	
MainDatabase\Twistaroma\juin	TwGCGC-739-2	6/5/2025 10:39:37 PM	Auchentoshan Th	1	
MainDatabase\Twistaroma\juin	TwGCGC-728-8-1	6/5/2025 10:26:00 AM	Brenne Estate Cas	1	
MainDatabase\Twistaroma\juin	TwGCGC-737-8-2-2	6/5/2025 8:32:15 PM	Brenne Estate Cas	1	
MainDatabase\Twistaroma\juin	TwGCGC-745-8	6/6/2025 3:43:59 AM	Brenne Estate Cas	1	
MainDatabase\Twistaroma\juin	TwGCGC-712-7-2	6/4/2025 5:27:43 PM	Eigashima Shuzo A	1	
MainDatabase\Twistaroma\juin	TwGCGC-725-7-1	6/5/2025 7:54:03 AM	Eigashima Shuzo A	1	
MainDatabase\Twistaroma\juin	TwGCGC-743-7	6/6/2025 2:01:44 AM	Eigashima Shuzo A	1	
MainDatabase\Twistaroma\juin	TwGCGC-749-7-4	6/6/2025 7:06:27 AM	Eigashima Shuzo A	1	
MainDatabase\Twistaroma\juin	TwGCGC-732-6-2	6/5/2025 4:19:28 PM	Finlaggan Old Res	1	
MainDatabase\Twistaroma\juin	TwGCGC-744-6	6/6/2025 2:52:49 AM	Finlaggan Old Res	1	
MainDatabase\Twistaroma\juin	TwGCGC-713-4-2	6/4/2025 6:17:40 PM	Monkey Shoulder	1	
MainDatabase\Twistaroma\juin	TwGCGC-741-4	6/6/2025 12:19:34 AM	Monkey Shoulder	1	

Rate: 200 spectra/sec Mass range: 29 : 401

Library search

Library Identity Search Mode

- Normal
- Quick

Library Search Mode

- Forward
- Reverse

Rank hits by

- Probability
- Similarity
- Reverse Similarity

Maximum number of hits:

Minimum mass to library search:

Maximum mass to library search:

Minimum molecular weight allowed:

Maximum molecular weight allowed:

Relative abundance threshold (0-998):

Minimum similarity for matches (0-999):

Minimum similarity before hit is assigned (0-999):

Retrieve retention indices

- Semi-standard non-polar
- Standard non-polar
- Polar

Filter hits that are at least units out of tolerance with computed retention index

Note: Use of this feature requires at least two landmarks with retention indices

Libraries to search:

- mainlib
- nist_ri

Alignment details

Semi-standard non-polar

Standard non-polar

Polar

Filter hits that are at least units out of tolerance with computed retention index

Note: Use of this feature requires at least two landmarks with retention indices

Libraries to search:

- mainlib
- nist_ri
- replib

Statistical processing

Landmarks (18)

Name	R.T. (sec)	R.I.	
Heptane	100	700	Remove
Octane	234.8	800	Remove
Nonane	379.7	900	Remove
Décane	532.4	1000	Remove
Undécane	690.5	1100	Remove
Dodécane	851.6	1200	Remove
Tridécane	1013.2	1300	Remove
Tétradécane	1172.9	1400	Remove
Pentadécane	1328.4	1500	Remove
Hexadécane	1477.1	1600	Remove
Heptadécane	1616.8	1700	Remove
Octadécane	1744.9	1800	Remove
Nonadécane	1859	1900	Remove
Eicosane	1956.8	2000	Remove
Heneicosane	2035.7	2100	Remove
Docosane	2093.5	2200	Remove
Tricosane	2127.7	2300	Remove
Tetracosane	2135.8	2400	Remove

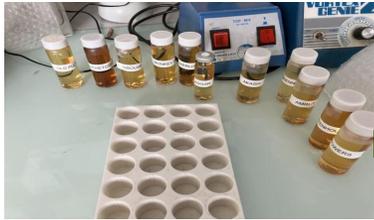
Add | Sort | Clear

Export | Import

Feature Filter

Alignment log

Copy to clipboard



30 min



1 day



1 day

ChromatOF.SYNC
LECO
EMPOWERING RESULTS

1mL whisky
9mL NaCl 5M
+IS (1,4
dibromobenzene)

SPME CAR/DVB/PDMS
1cm
10 incubation 50°C
20 extraction 50°C
Injection port 250°C
5min

Results

Id (2960)	Quality	Name	Formula	M.W.	Similarity	Reverse	Probability (%)	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	S/N	Loading (X)	Loading (Y)	p
19323	0.95	.tau.-Cadinol	C ₁₅ H ₂₆ O	222	815	821	7.65	5937-11-1	204	1638	1640	-2	1419.85	0.0004	-0.0003	0.000
9008	0.93	(-)-Aristolene	C ₁₅ H ₂₄	204	745	750	52.52	6831-16-9	148	1425	1447	-22	485.19	0.0001	-0.0000	0.000
5867	0.93	(+)-2-Phenylbutyronitrile	C ₁₀ H ₁₁ N	145	814	814	80.21	69350-73-8	145	1260	N.A.	N.A.	792.15	0.0002	0.0004	0.000
3647	0.93	(+)-2-Bornanone	C ₁₀ H ₁₆ O	152	845	845	68.19	464-49-3	152	1145	1144	1	1081.76	0.0002	-0.0000	0.000
11513	0.93	(1-Propoxy-pentyl)-cyclopropane	C ₁₁ H ₂₂ O	170	739	770	84.88	94883-97-3	113	1569	N.A.	N.A.	532.67	0.0001	0.0000	0.000
5095	0.96	(1-Propoxy-pentyl)-cyclopropane	C ₁₁ H ₂₂ O	170	764	764	93.86	94883-97-3	113	1223	N.A.	N.A.	2113.36	0.0007	-0.0009	0.018
6551	0.95	(1R,3S,4R,5S)-1-Isopropyl-4-methyl	C ₁₂ H ₂₀ O ₂	196	790	800	12.20	62181-91-3	136	1295	1281	14	1172.09	0.0004	-0.0001	0.000
9784	0.93	(1R,4R,4aS,8aR)-4,7-Dimethyl-1-(pr	C ₁₅ H ₂₄	204	782	791	44.69	92692-39-2	162	1465	1457	8	859.21	0.0001	-0.0001	0.000
1007	0.82	(1R)-2,6,6-Trimethylbicyclo[3.1.1]he	C ₁₀ H ₁₆	136	821	821	18.66	7785-70-8	93	913	932	-19	734.87	0.0001	-0.0002	0.009
11943	0.91	(1S,3aS,4S,5S,7aR,8R)-5-Isopropyl-1	C ₁₅ H ₂₆ O	222	774	807	4.17	21966-93-8	147	1600	N.A.	N.A.	632.74	0.0001	-0.0000	0.000
7676	0.94	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	772	772	37.63		87	1350	N.A.	N.A.	537.81	0.0001	0.0001	0.000
1091	0.80	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	772	772	37.63		87	924	N.A.	N.A.	113.36	0.0000	0.0000	0.000
844	0.81	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	786	786	95.26		87	885	N.A.	N.A.	478.77	0.0001	-0.0000	0.000
999	0.95	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	772	772	37.63		87	913	N.A.	N.A.	636.77	0.0000	-0.0000	0.000
9658	0.95	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	772	772	37.63		87	1457	N.A.	N.A.	1008.25	0.0000	-0.0001	0.003
7982	0.89	(2-Methyl[1,3]dioxolan-2-yl)thioac	C ₁₃ H ₂₀ O ₆ S	304	772	772	37.63		87	1369	N.A.	N.A.	234.64	0.0000	-0.0000	0.008
3380	0.96	(2R,4R)-4-Methyl-2-(2-methylprop	C ₁₀ H ₁₈ O	154	733	733	55.70	5258-11-7	139	1128	1127	1	2721.10	0.0009	0.0002	0.000
1529	0.94	(2R,5S)-2-Methyl-5-(prop-1-en-2-yl	C ₁₀ H ₁₆ O	152	715	719	30.85	54750-69-5	137	979	1007	-28	1592.78	0.0009	0.0012	0.000
870	0.83	(2S,6R,7S,8E)-(+)-2,7-Epoxy-4,8-me	C ₁₃ H ₂₀ O	192	797	797	66.45	108342-25-2	107	892	N.A.	N.A.	123.93	0.0000		0.000
5769	0.95	(2S,6R,7S,8E)-(+)-2,7-Epoxy-4,8-me	C ₁₃ H ₂₀ O	192	783	899	73.58	108342-25-2	122	1256	N.A.	N.A.	406.71	0.0000	0.0000	0.000

Data treatment

 Feature filter settings ✕

Show only features that satisfy the following conditions:

Simple Rules Advanced Rules

Similarity ▼ ✕

Greater than or equal (\geq) ▼

800

AND

Formula ▼ ✕

Does not contain ▼

Si

AND

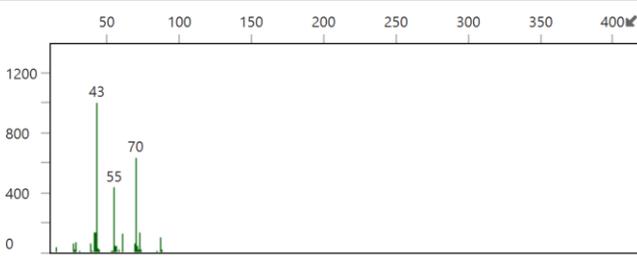
R.I. Δ ▼ ✕

Is not empty ▼

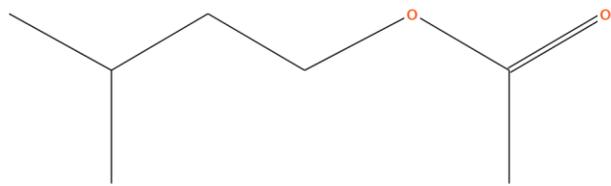
[Add rule](#) | [Remove all rules](#)

Filtering

Home » Alignments » whisky triPLICATE 4



43 55 70

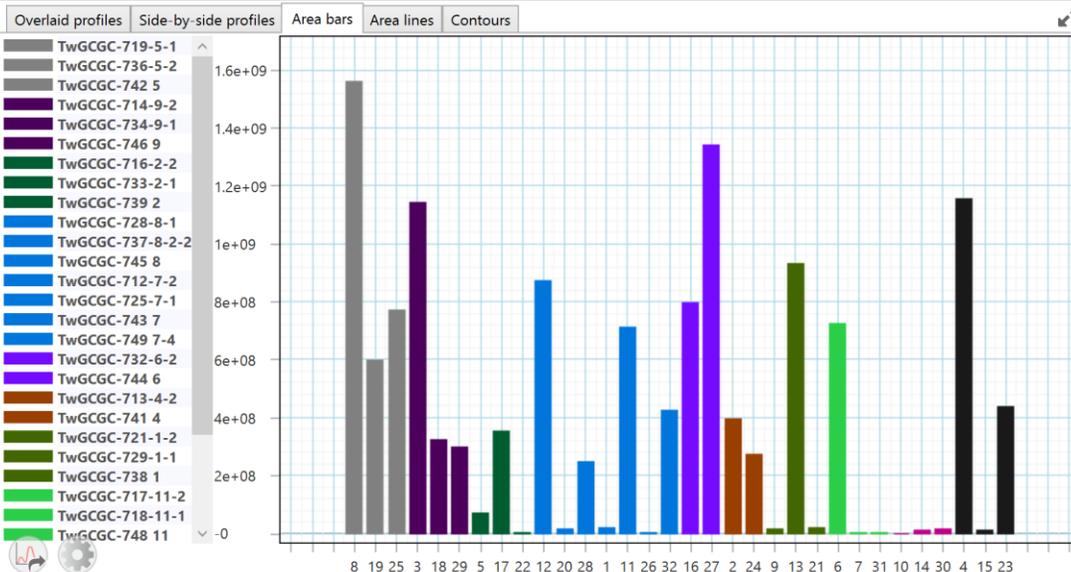


Feature: 1-Butanol, 3-methyl-, acetate

Library Hit: 823/823/73.64 1-Butanol, 3-methyl-, acetate Unassign

Overlaid profiles Side-by-side profiles Area bars Area lines Contours

- TwGCGC-719-5-1
- TwGCGC-736-5-2
- TwGCGC-742 5
- TwGCGC-714-9-2
- TwGCGC-734-9-1
- TwGCGC-746 9
- TwGCGC-716-2-2
- TwGCGC-733-2-1
- TwGCGC-739 2
- TwGCGC-728-8-1
- TwGCGC-737-8-2-2
- TwGCGC-745 8
- TwGCGC-712-7-2
- TwGCGC-725-7-1
- TwGCGC-743 7
- TwGCGC-749 7-4
- TwGCGC-732-6-2
- TwGCGC-744 6
- TwGCGC-713-4-2
- TwGCGC-741 4
- TwGCGC-721-1-2
- TwGCGC-729-1-1
- TwGCGC-738 1
- TwGCGC-717-11-2
- TwGCGC-718-11-1
- TwGCGC-748 11



Area bars Area lines Contours

8 19 25 3 18 29 5 17 22 12 20 28 1 11 26 32 16 27 2 24 9 13 21 6 7 31 10 14 30 4 15 23

Id (1018)	Name	Formula	M.W.	Similarity	Reverse	Probability (%)	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ
279	1-Butanol, 3-methyl-	C ₅ H ₁₂ O	88	818	828	56.59	123-51-3	70	750	736	14
315	1-Butanol, 3-methyl-	C ₅ H ₁₂ O	88	918	918	70.25	123-51-3	57	761	736	25
701	1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	130	837	841	86.92	123-92-2	70	857	876	-19
706	1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	130	823	823	73.64	123-92-2	70	858	876	-18
726	1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	130	836	836	79.11	123-92-2	70	861	876	-15
731	1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	130	917	925	90.31	123-92-2	87	863	876	-13
740	1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	130	918	925	89.19	123-92-2	43	864	876	-12
9369	1-Butanol, 3-methyl-, benzoate	C ₁₂ H ₁₆ O ₂	192	956	956	81.02	94-46-2	105	1442	1439	3
9397	1-Butanol, 3-methyl-, benzoate	C ₁₂ H ₁₆ O ₂	192	941	941	76.61	94-46-2	105	1443	1439	4
1322	1-Butanol, 3-methyl-, propanoate	C ₈ H ₁₆ O ₂	144	943	943	76.23	105-68-0	101	955	969	-14
1342	1-Butanol, 3-methyl-, propanoate	C ₈ H ₁₆ O ₂	144	842	851	65.40	105-68-0	87	958	969	-11
5877	1-Butanone, 1-phenyl-	C ₁₀ H ₁₂ O	148	902	918	68.99	495-40-9	105	1260	1260	0

Publication

Chemical class CAS

ELSEVIER

journal homepage: www.sciencedirect.com/journal/talanta-open



Comparison of head space solid phase micro extraction with conventional and comprehensive gas chromatography mass spectrometry for volatile profiling of Irish whiskey

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Table 2
Volatile congeners identified in Irish Whiskey samples.

Number	Chemical class	Compound	CAS Number	Method		
				I	II	III
1	Ester	Ethyl acetate	141-78-6	+	+	+
2	Ester	Ethyl propanoate	105-37-3	+	nd	+
3	Ester	Ethyl butanoate	105-54-4	+	+	+
4	Ester	Ethyl pentanoate	539-82-2	nd	nd	+
5	Ester	Ethyl heptanoate	106-30-9	+	+	+
6	Ester	Ethyl hexanoate	123-66-0	+	+	+
7	Ester	Ethyl octanoate	106-32-1	+	+	+
8	Ester	Ethyl nonanoate	123-29-5	+	+	+
9	Ester	Ethyl decanoate	110-38-3	+	+	+
10	Ester	Ethyl dodecanoate	106-33-2	+	+	+
11	Ester	Ethyl undecanoate	627-00-7	+	+	+
12	Ester	Ethyl hexadecanoate	628-97-7	nd	+	+
13	Ester	Ethyl tetradecanoate	124-06-1	+	+	+
14	Ester	Ethyl octadecanoate	111-61-5	nd	+	+
15	Ester	Ethyl benzoate	93-89-0	+	+	+
16	Ester	3-Methylbutyl acetate	123-92-2	+	+	+
17	Ester	3-Methylbutyl hexanoate	2198-61-0	+	+	+
18	Ester	3-Methylbutyl decanoate	2306-91-4	+	+	+
19	Ester	3-Methylbutyl octanoate	2025-99-6	+	+	+
20	Ester	3-Methylbutyl dodecanoate	6309-51-9	+	+	+
21	Ester	2-Methylpropyl acetate	110-19-0	+	+	+
22	Ester	2-Methylpropyl hexanoate	105-79-3	+	+	+
23	Ester	2-Methylpropyl octanoate	5461-08-3	+	+	+
24	Ester	2-Methylpropyl decanoate	30673-38-2	+	+	+
25	Ester	2-Methylpropyl dodecanoate	37811-72-6	nd	+	+
26	Ester	2-Methylbutyl acetate	624-41-9	+	nd	nd
27	Ester	2-Methylbutyl octanoate	67121-39-5	+	nd	nd
28	Ester	Ethyl-2-methylbutanoate	1108-64-1	+	+	+
29	Ester	Ethyl-2-methylbutanoate	7452-79-1	+	+	+
30	Ester	Ethyl-2-methylpropanoate	97-62-1	nd	+	+
31	Ester	2-Phenylethyl hexanoate	6290-37-5	nd	+	+
32	Ester	2-Phenylethyl decanoate	61810-55-7	nd	+	+
33	Ester	Methyl octanoate	111-11-5	nd	+	+
34	Ester	Methyl decanoate	110-42-9	+	+	+
35	Ester	Methyl dodecanoate	111-82-0	nd	+	+
36	Ester	Propyl octanoate	624-13-5	nd	+	+

(continued on next page)

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Table 2 (continued)

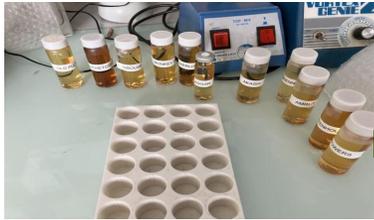
Number	Chemical class	Compound	CAS Number	Method		
				I	II	III
37	Ester	Propyl decanoate	30673-60-0	+	+	+
38	Ester	Propyl dodecanoate	3681-78-5	nd	+	+
39	Ester	Pentyl acetate	628-63-7	nd	nd	+
40	Ester	Hexyl acetate	142-92-7	+	+	+
41	Ester	Heptyl acetate	112-06-1	nd	+	+
42	Ester	Oxyl acetate	112-14-1	+	+	+
43	Ester	Decyl acetate	112-17-4	+	+	+
44	Ester	1-Tetradecyl acetate	638-59-5	+	+	+
45	Ester	Nonyl acetate	143-13-5	nd	+	+
46	Ester	Dodecyl acetate	112-66-3	nd	+	+
47	Ester	β-Phenylethyl acetate	103-45-7	+	+	+
48	Ester	(E,E)-Farnesyl acetate	4128-17-0	nd	+	+
49	Ester	(E)-2,3-Dihydrofarnesyl acetate	58130-58-8	nd	+	+
50	Ester	Phenethyl octanoate	5457-70-5	nd	+	+
51	Ester	Ethyl phenylacetate	101-97-3	+	+	+
52	Ester	Ethyl (Z)-4-decenoate	7367-84-2	+	+	+
53	Ester	Ethyl-2-furoate	614-99-3	nd	nd	+
54	Ester	Ethyl-3-nonenoate	91213-30-8	nd	+	+
55	Ester	Ethyl-7-octenoate	35194-38-8	nd	nd	+
56	Ester	Ethyl-9-decenoate	67233-91-4	nd	+	+
57	Ester	Ethyl-9-hexadecenoate	54546-22-4	nd	+	+
58	Ester	E,E-Ethyl Sorbate	2396-84-1	+	+	+
59	Ester	Ethyl Hydroxynamate	2021-28-5	nd	+	+
60	Benzene	Durene	95-92-2	+	+	+
61	Benzene	Induene	527-53-7	+	+	+
62	Benzene	Indane	496-11-7	nd	+	+
63	Benzene	Styrene	100-42-5	+	+	+
64	Benzene	p-o-dimethyl styrene	1195-32-0	nd	+	+
65	Benzene	o-Xylene	95-47-6	nd	+	+
66	Benzene	m-Xylene	108-38-3	nd	+	+
67	Benzene	2-Ethyl-p-xylene	1758-88-9	nd	+	+
68	Benzene	4-Ethyl-o-xylene	934-80-5	nd	+	+
69	Benzene	4-Ethyl-m-xylene	874-41-9	nd	+	+
70	Benzene	1,2-Dimethyl-2,3-dimethylbenzene	54340-1,2,3,4-	nd	+	+
71	Benzene	Tetramethylbenzene	488-23-3	nd	+	+
72	Benzene	(1,3-Methylphenyl)-1,3-dimethylbenzene	116669-49-9	nd	+	+
73	Benzene	1,2,3-Trimethylhemimellitene benzene	526-73-8	nd	+	+

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Table 2 (continued)

Number	Chemical class	Compound	CAS Number	Method		
				I	II	III
74	Benzene	p-Cymene	99-87-6	nd	+	+
75	Benzene	5-Methylindan	874-35-1	nd	+	+
76	Benzene	Pseudocumene	95-63-6	nd	+	+
77	Alcohol	1-Propanol	71-23-8	+	nd	nd
78	Alcohol	1-Pentanol	71-41-0	nd	+	+
79	Alcohol	1-Octanol	111-87-5	+	+	+
80	Alcohol	1-Decanol	112-30-1	nd	+	+
81	Alcohol	1-Dodecanol	112-53-8	+	+	+
82	Alcohol	1-Tetradecanol	112-72-1	+	+	+
83	Alcohol	2-Nonanol	628-99-9	+	+	+
84	Alcohol	2-Undecanol	1653-30-1	nd	+	+
85	Alcohol	Hexadecanol	36653-82-4	nd	+	+
86	Alcohol	Phenylethyl alcohol	60-12-8	+	+	+
87	Alcohol	2-Methyl propanol	78-83-1	+	+	+
88	Alcohol	2-Methyl butanol	137-32-6	+	+	+
89	Alcohol	3-Methyl butanol	123-51-3	+	+	+
90	Aldehyde	Heptanal	111-71-7	+	+	+
91	Aldehyde	Hexanal	66-25-1	+	nd	+
92	Aldehyde	Octanal	124-13-0	+	nd	nd
93	Aldehyde	Nonanal	124-19-6	+	+	+
94	Aldehyde	Dodecanal	112-54-9	nd	+	+
95	Aldehyde	Undecanal	112-44-7	+	+	+
96	Aldehyde	Pentadecanal	2765-11-9	nd	+	+
97	Aldehyde	Hexadecanal	629-80-1	nd	+	+
98	Aldehyde	Trans-2-Nonenal	18829-66-3	nd	+	+
99	Aldehyde	2-Methyl butanal	96-17-3	nd	+	+
100	Aldehyde	3-Methylbutanal	590-86-3	+	+	+
101	Aldehyde	Acetaldehyde	75-07-0	nd	+	+
102	Aldehyde	Benzaldehyde	100-52-7	+	+	+
103	Terpenoid	Trans-Nerolidol	40716-66-3	+	+	+
104	Terpenoid	Linalool	78-70-6	+	+	+
105	Terpenoid	(E)-β-Farnesene	18794-84-8	nd	+	+
106	Terpenoid	cis-α-Bisabolene	29837-07-8	nd	+	+
107	Terpenoid	Carvone	99-48-9	nd	+	+
108	Terpenoid	(-)-α-Bisabolol	23089-26-1	nd	+	+
109	Terpenoid	D-Limonene	5989-27-5	nd	+	+
110	Terpenoid	(S)-cis-Verbenol	1881-04-4	nd	+	+
111	Terpenoid	Trans,Trans-Farnesol	106-28-5	+	+	+
112	Terpenoid	Limetol	7392-19-0	nd	+	+
113	Terpenoid	β-Ocimene	13877-91-3	nd	+	+
114	Furan	Furfural	98-01-1	+	+	+
115	Furan	Furfuryl ethyl ether	6270-56-0	nd	+	+

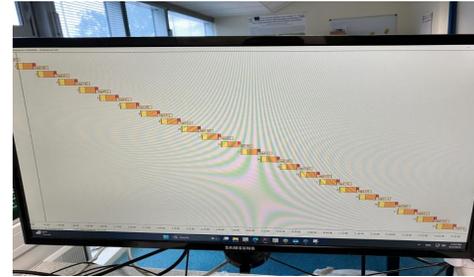
(continued on next page)



30 min



1 day



1 day

ChromatOF.SYNC
LECO
EMPOWERING RESULTS

1 day



1mL whisky
9mL NaCl 5M
+IS (1,4
dibromobenzene)

SPME CAR/DVB/PDMS
1cm
10 incubation 50°C
20 extraction 50°C
Injection port 250°C
5min

Pivot table

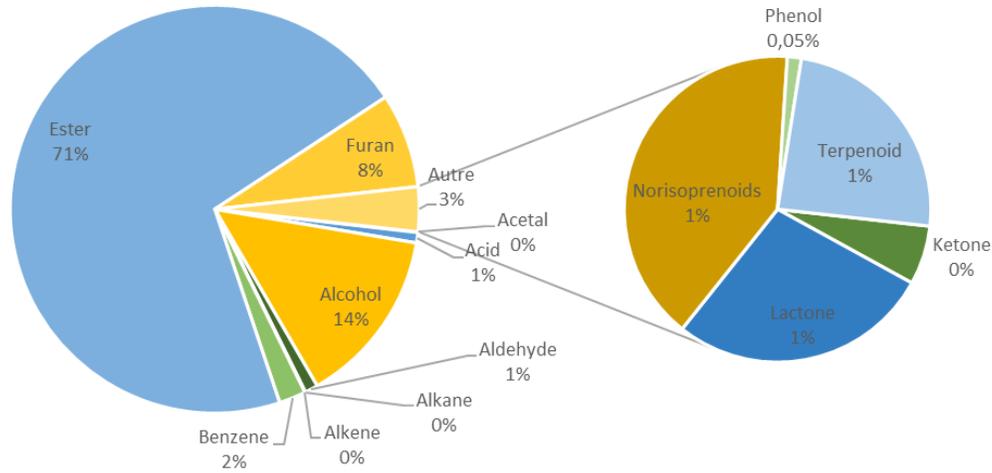
Famille	CAS	Étiquettes de lignes	TwGGCG-716-2-2	TwGGCG-733-2-1	TwGGCG-712-
Acetal	709364	Butane, 1,1-diethoxy-3-methyl-	21658262,41	20900544,99	1
Acetal	105-57-7	Ethane, 1,1-diethoxy-	2081668,213	1171468,224	1
Acetal	1741-41-9	Propane, 1,1-diethoxy-2-methyl-	1695535,008	1615450,991	9
Acid	143-07-7	Dodecanoic acid	1021214,878	733513,0838	4
Acid	334-48-5	n-Decanoic acid	448578,3584	211091,4425	2
Alcohol	137-32-6	1-Butanol, 2-methyl-	2816945965	30754370,69	5
Alcohol	123-51-3	1-Butanol, 3-methyl-	4894640225	6153753766	1
Alcohol	112-30-1	1-Decanol	555204155,9	515432822,7	3
Alcohol	112-53-8	1-Dodecanol	69189011,47	236435098,9	7
Alcohol	36653-82-4	1-Hexadecanol	2598031,482	2488021,144	1
Alcohol	111-87-5	1-Octanol	275678655,7	309083359,4	1
Alcohol	71-41-0	1-Pentanol	70164795,78	134458274	2
Alcohol	112-72-1	1-Tetradecanol	18719091,7	19657098,6	2
Alcohol	628-99-9	2-Nonanol	35144672,15	37909307,97	1
Alcohol	1653-30-1	2-Undecanol	1047238,015	651547,2342	2
Alcohol	60-12-8	Phenylethyl Alcohol	1547981742	619886979,6	1
Aldehyde	18829-56-6	2-Nonenal, (E)-	84082721,53	106414389,6	1
Aldehyde	100-52-7	Benzaldehyde	190748699,3	206210207,2	5
Aldehyde	112-54-9	Dodecanal	2165421,143	1549690,85	1
Aldehyde	111-71-7	Heptanal	1051706,432	23079139,57	5
Aldehyde	629-80-1	Hexadecanal	104484,6955	72793,9222	1
Aldehyde	66-25-1	Hexanal	22120529,16	21549475,72	1
Aldehyde	124-19-6	Nonanal	192706976,2	200891979,3	1



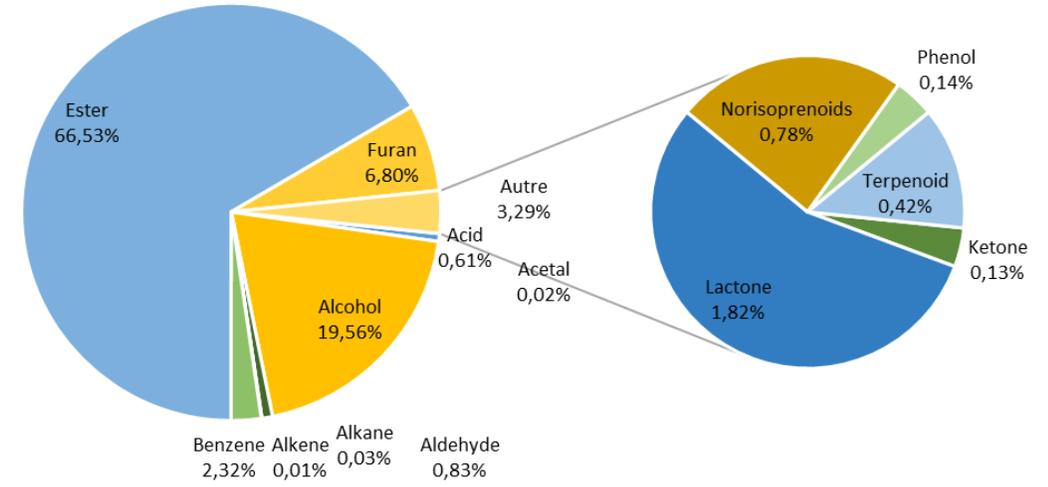
Étiquettes de lignes	Somme de Finlaggan Old Reserve	Somme de Aberlour 12 Year Old2	Somme de Old Pulteney 12 Years Old3	Somme de Auchentoshan Three Wood
Acetal	28193190,67	12107978,98	13576702,21	25435465,63
Acid	447622049,3	346472498,1	242608296,6	1469793,236
Alcohol	7574129304	11188723225	8619033419	10287313584
Aldehyde	561483619,2	472791029,4	453902067	572344966,2
Alkane	15195960,92	17889501,43	15857841,87	13460292,62
Alkene	8247735,327	2863934,399	3304584,232	3638141,555
Benzene	1145528694	1327461376	1610445025	1054907729
Ester	38316224983	38048868520	39172609011	34383474460
Furan	4052210281	3891647113	1757180131	2566944863
Ketone	119452284	75749493,88	93163282,63	34726754,54
Lactone	529760347,8	1040604330	348369797,2	357612678
Norisoprenoids	771807104,4	447476278,5	599915153,7	560364971,2
Phenol	28347125,37	78077791,62	127153659,8	28885389,54
Terpenoid	464480743,6	237724753,7	408015103,9	446328380,3
#N/A	1,95802E+11	1,52648E+11	1,52045E+11	1,35142E+11

Composition

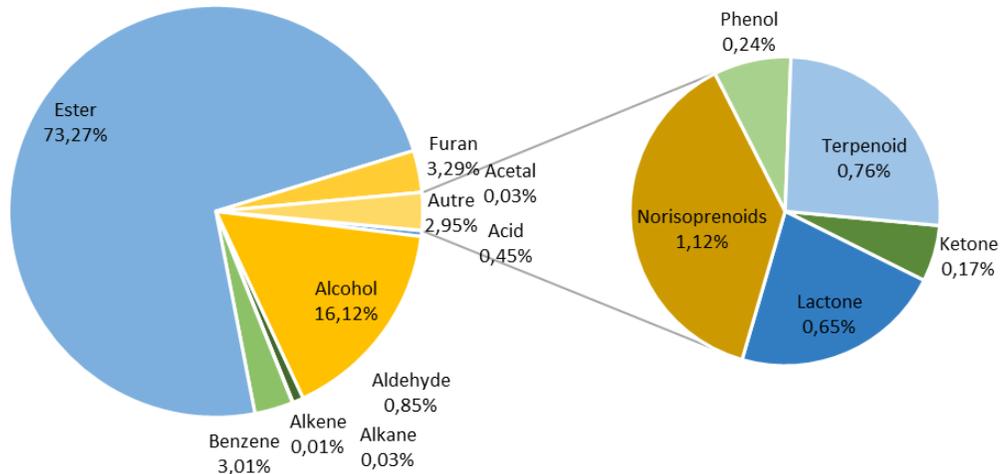
Finlaggan Old Reserve



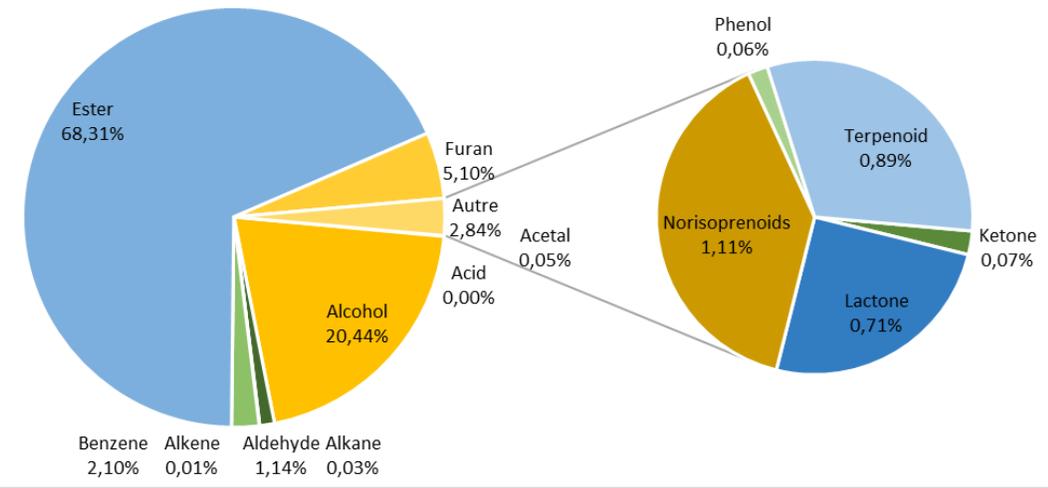
Aberlour 12 year old



Pulteney 12 Years Old



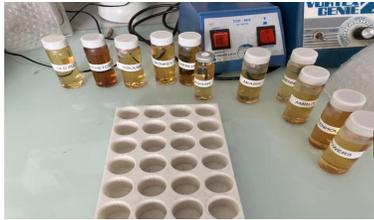
Auchentoshan Three Wood



Statistical analysis

Familie	CAS	Étiquettes de lignes	TwGGGC-716-2-2		TwGGGC-733-2-1		TwGGGC-712-
			Auchentoshan	Three Wood	Auchentoshan	Three Wood	Eigashima Sh
Acetal	709364	Butane, 1,1-diethoxy-3-methyl-		21658262,41		20900544,99	1
Acetal	105-57-7	Ethane, 1,1-diethoxy-		2081668,213		1171468,224	1
Acetal	1741-41-9	Propane, 1,1-diethoxy-2-methyl-		1695535,008		1615450,991	9
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Alcohol	123-51-3	1-Butanol, 3-methyl-		4894640225		6153753766	1
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Alcohol	112-53-8	1-Dodecanol		69189011,47		236435098,9	7
Alcohol	36653-82-4	1-Hexadecanol		2598031,482		2488021,144	11
Alcohol	111-87-5	1-Octanol		275678655,7		309083359,4	1
Alcohol	71-41-0	1-Pentanol		70164795,78		134458274	2
Alcohol	112-72-1	1-Tetradecanol		18719091,7		19657098,6	2
Alcohol	628-99-9	2-Nonanol		35144672,15		37909307,97	1
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Aldehyde	100-52-7	Benzaldehyde		190748699,3		206210207,2	5
Aldehyde	112-54-9	Dodecanal		2165421,143		1549690,85	1
Aldehyde	111-71-7	Heptanal		1051706,432		23079139,57	5
Aldehyde	629-80-1	Hexadecanal		104484,6955		72793,9222	:
Aldehyde	66-25-1	Hexanal		22120529,16		21549475,72	1
Aldehyde	124-19-6	Nonanal		192706976,2		200891979,3	!





30 min



1 day



1 day

ChromatOF.SYNC
LECO
EMPOWERING RESULTS

1-5 days



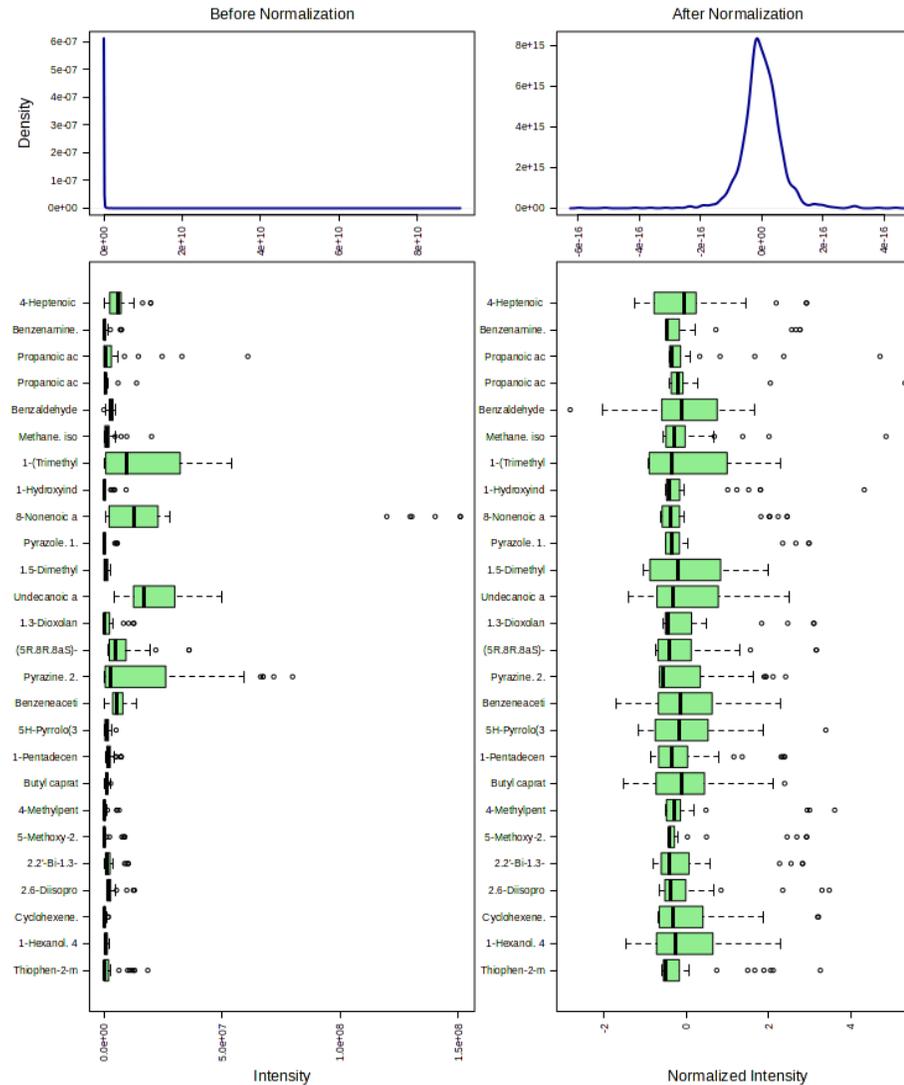
1 day



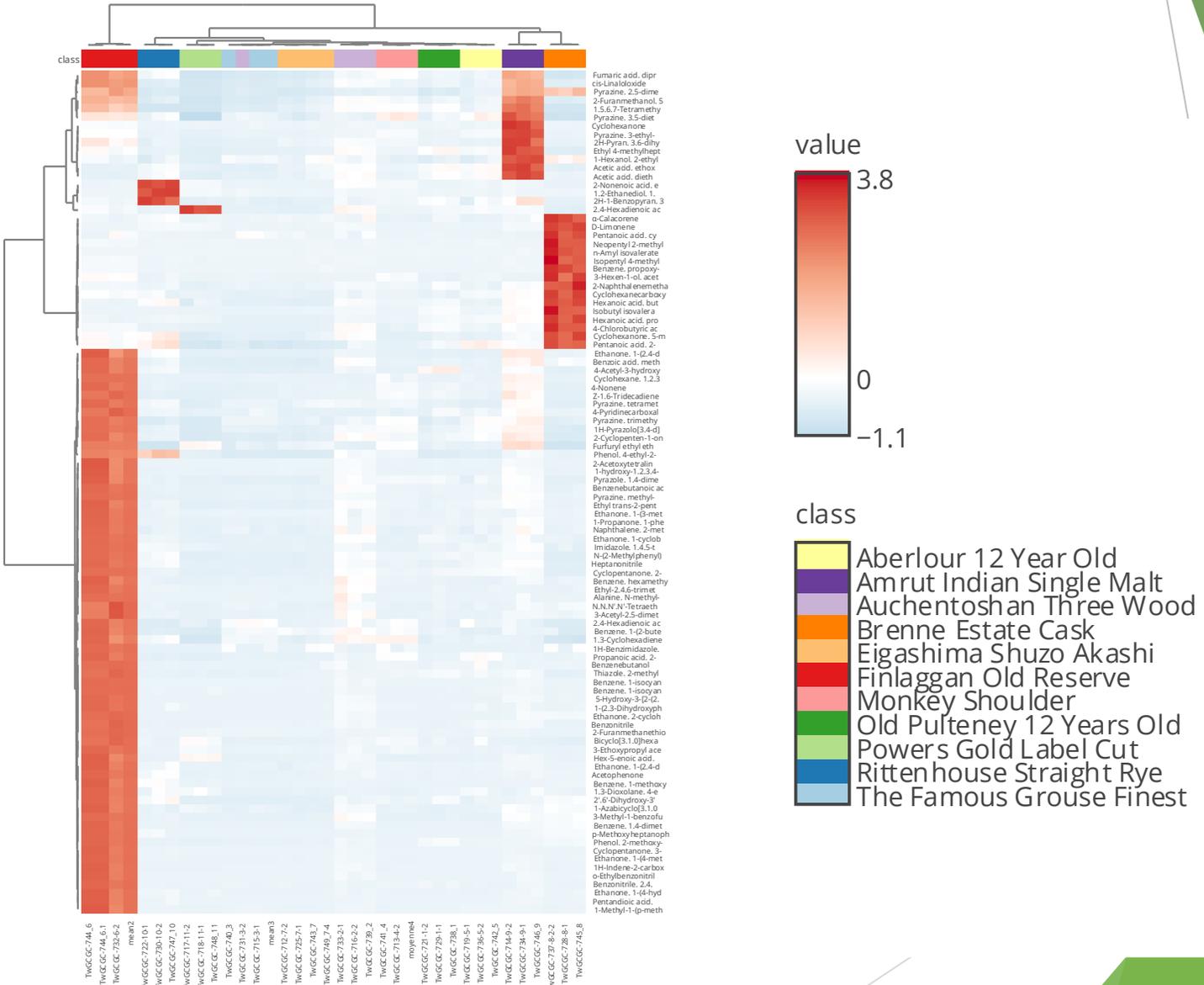
1mL whisky
9mL NaCl 5M
+IS (1,4
dibromobenzene)

SPME CAR/DVB/PDMS
1cm
10' incubation 50°C
20' extraction 50°C
Injection port 250°C 5min

Metaboanalyst=> normalization of the data

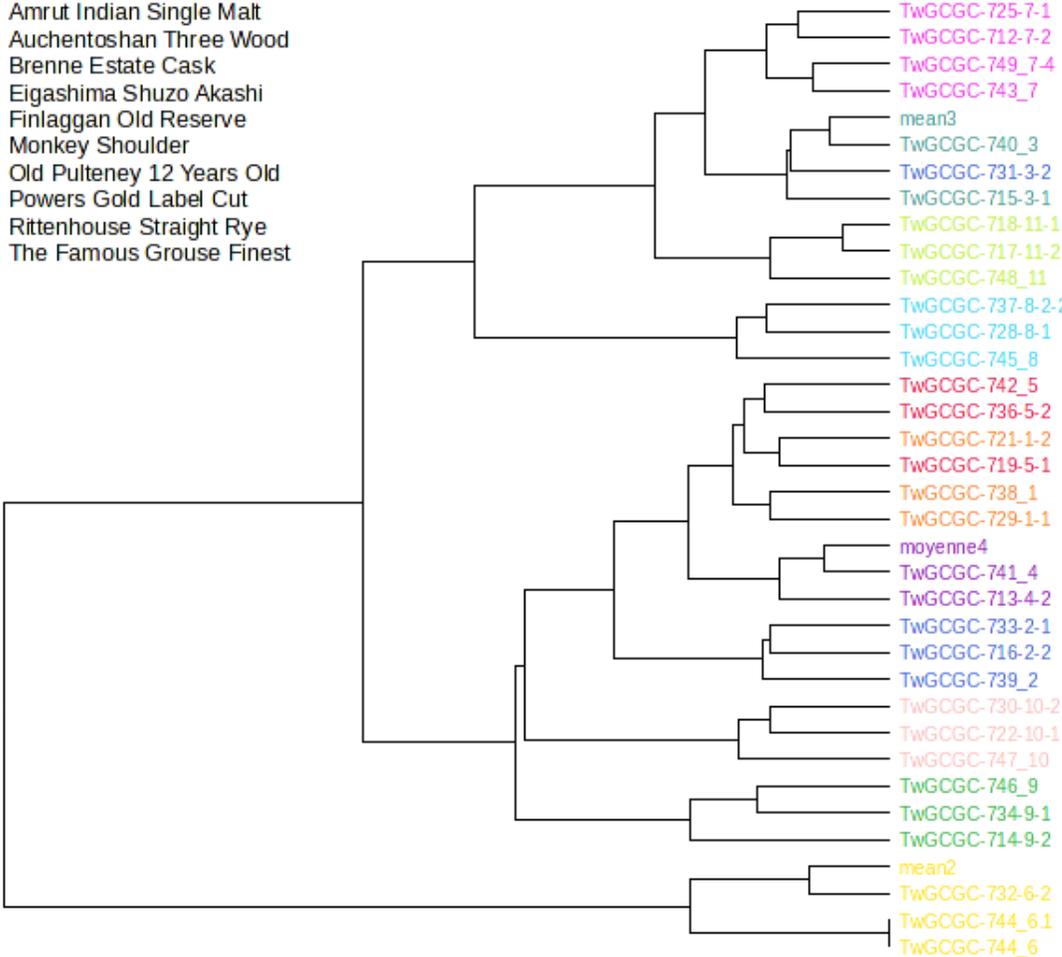


Heatmap



Dendrogram

- Aberlour 12 Year Old
- Amrut Indian Single Malt
- Auchentoshan Three Wood
- Brenne Estate Cask
- Eigashima Shuzo Akashi
- Finlaggan Old Reserve
- Monkey Shoulder
- Old Pulteney 12 Years Old
- Powers Gold Label Cut
- Rittenhouse Straight Rye
- The Famous Grouse Finest



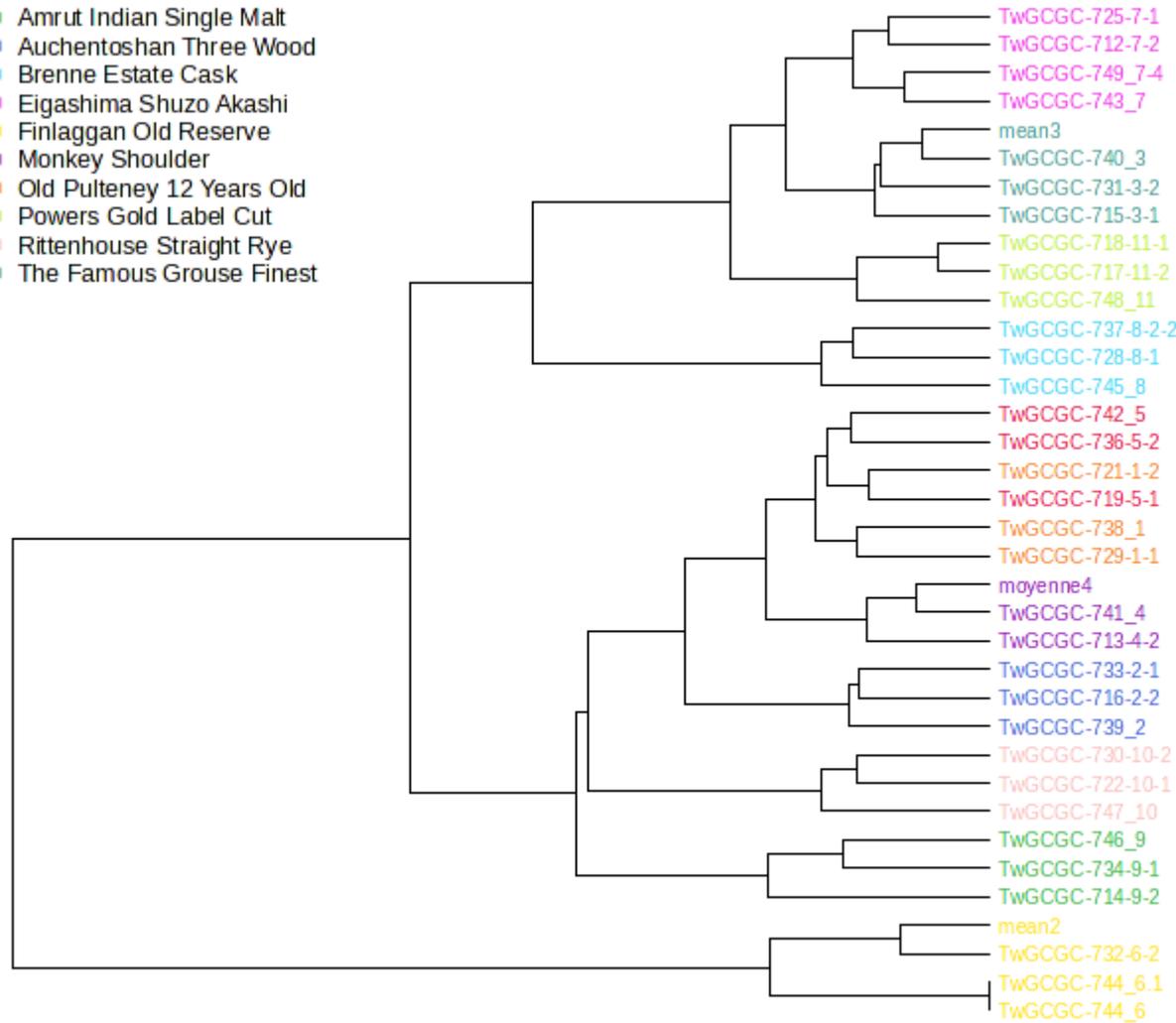
250 200 150 100 50 0



Excel spreadsheet showing a list of whisky samples and their corresponding numerical data. The spreadsheet is titled "Classeur1 - Excel" and has a search bar at the top. The data is organized into columns labeled R through Z. The first row of data (row 2) lists the following samples: TwGGCG-722-10-1, TwGGCG-725-7-1, TwGGCG-728-8-1, TwGGCG-730-10-2, TwGGCG-731-3-2, TwGGCG-729-1-1, TwGGCG-732-6-2, TwGGCG-744 6, and mean2. The cell containing "TwGGCG-731-3-2" is circled in green. The data consists of numerical values for each sample across multiple rows.

Sample	Whisky Name	Origin
1	Old Pulteney 12 Years Old	Scotland
2	Auchentoshan Three Wood	Scotland
3	The Famous Grouse Finest	Scotland
4	Monkey Shoulder	Scotland
5	Aberlour 12 Year Old	Scotland
6	Finlaggan Old Reserve	Scotland (Islay)
7	Eigashima Shuzo Akashi	Japan
8	Brenne Estate Cask	France
9	Amrut Indian Single Malt	India
10	Rittenhouse Straight Rye	USA (Kentucky)
11	Powers Gold Label Cut (likely "Powers Gold Label")	Ireland

- Aberlour 12 Year Old
- Amrut Indian Single Malt
- Auchentoshan Three Wood
- Brenne Estate Cask
- Eigashima Shuzo Akashi
- Finlaggan Old Reserve
- Monkey Shoulder
- Old Pulteney 12 Years Old
- Powers Gold Label Cut
- Rittenhouse Straight Rye
- The Famous Grouse Finest



Delivered
 Delivery Estimate:
 Monday, 26 May 2025



The Famous Grouse £14.97
 Finest | Scotch |
 Blended Whisky |
 Dried Fruit
 Qty: 1



Aberlour 12 Year £33.97
 Old Single Malt
 Scotch Whisky With
 Giftbox, 70 cl
 Qty: 1
 Sold By: Amazon EU S.a.r.L.

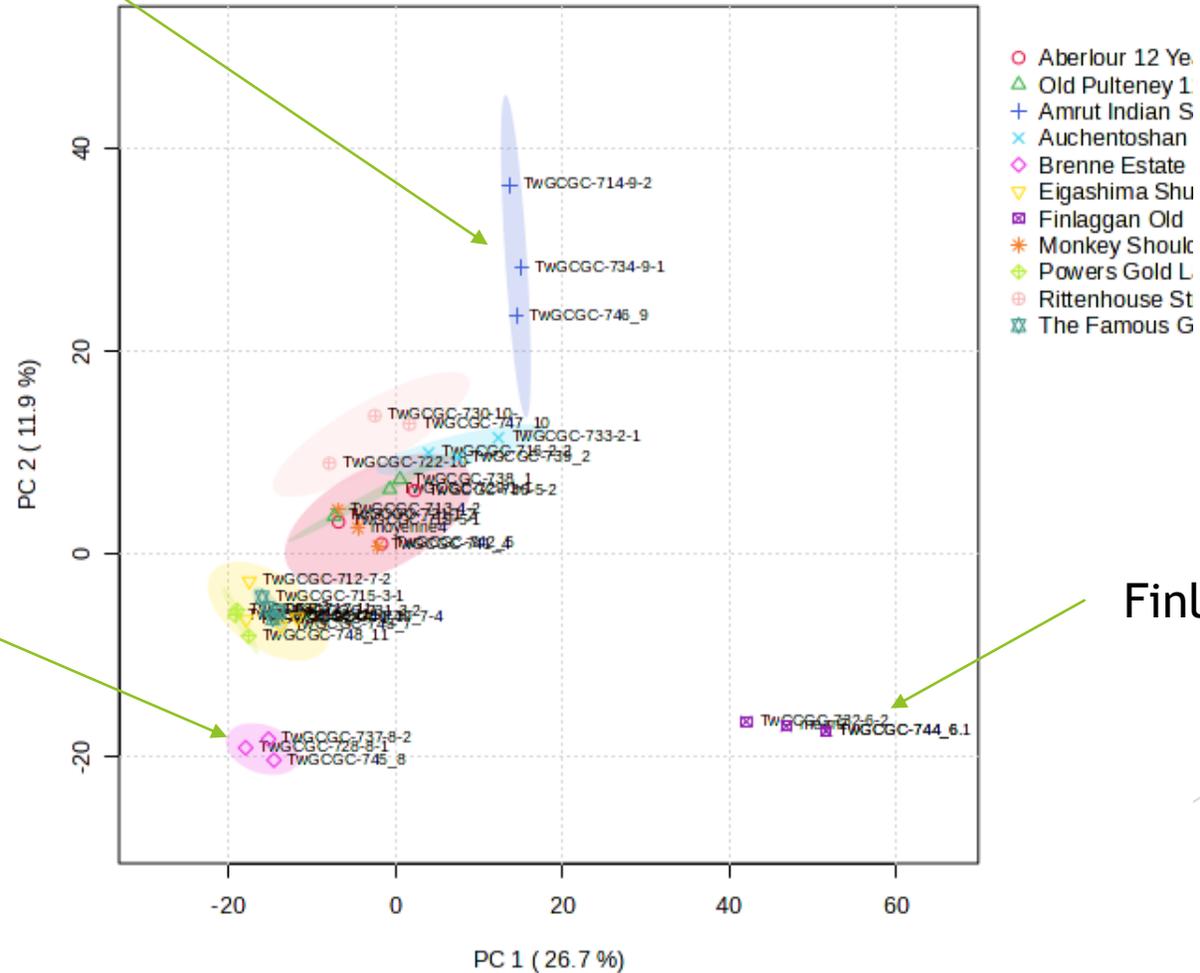


Old Pulteney 12 £23.78
 Years Old Single
 Malt Scotch Whisky,
 70cl
 Qty: 1
 Sold By: Amazon EU S.a.r.L.

PCA

Amrut Indian Single Malt

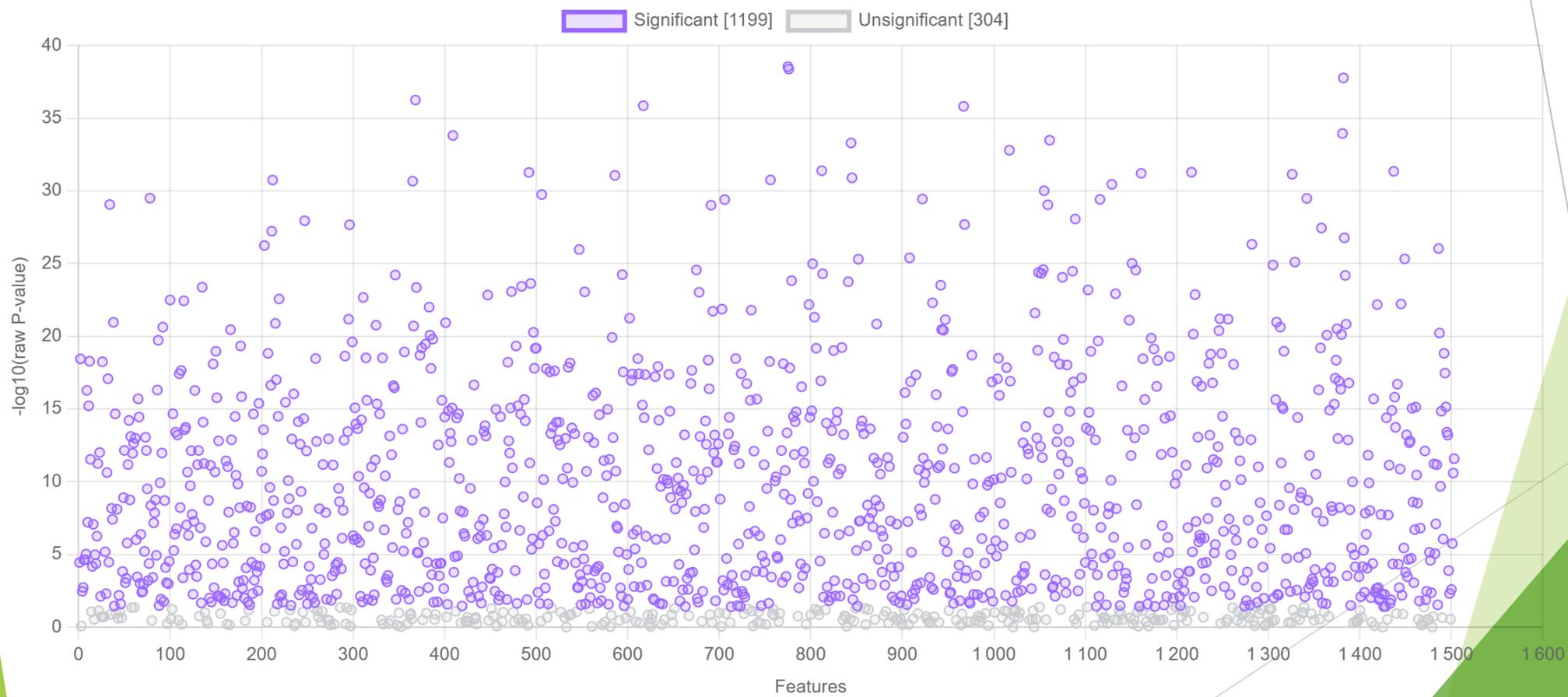
Scores Plot



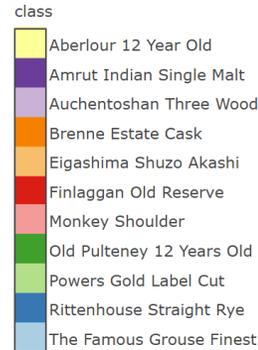
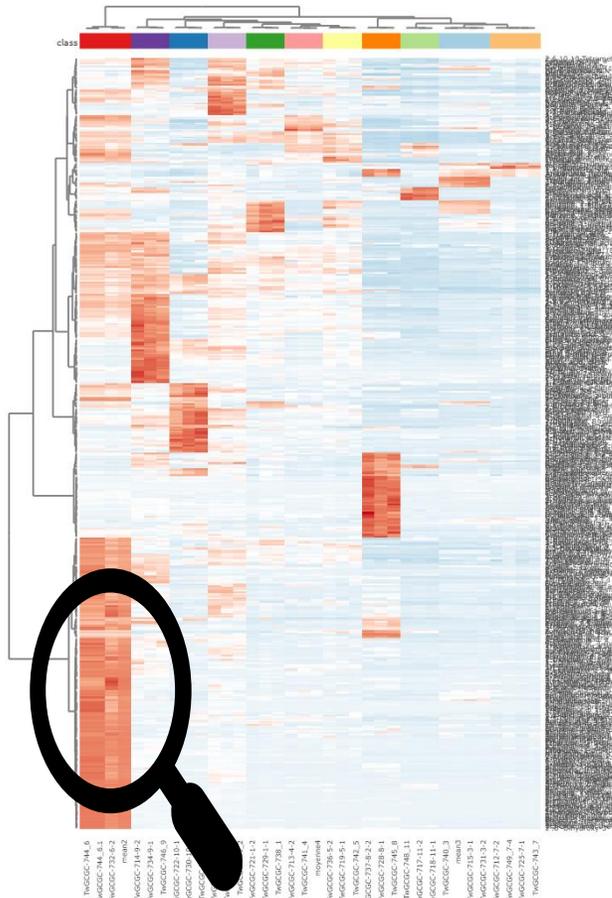
Brenne Estate Cask

Finlaggan Old Reserve

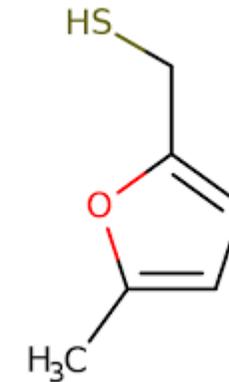
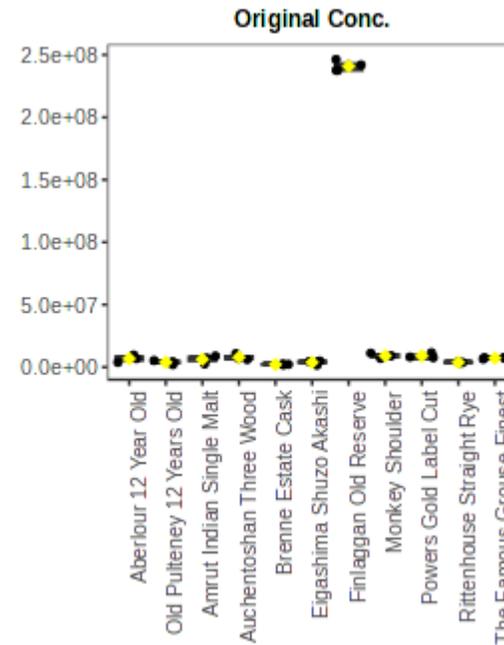
ANOVA



Finlaggan old reserve

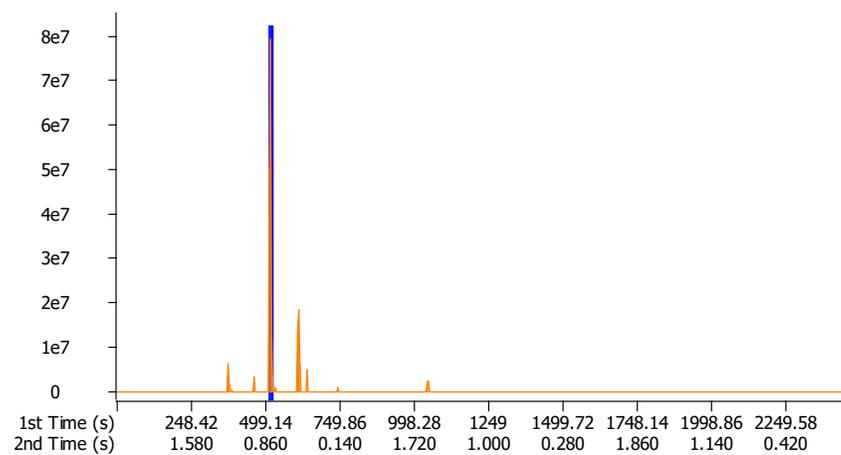
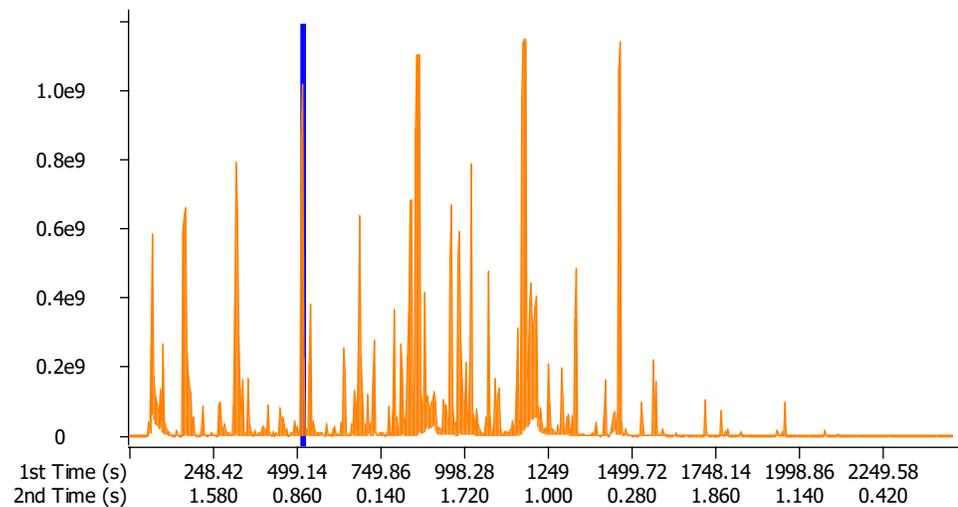
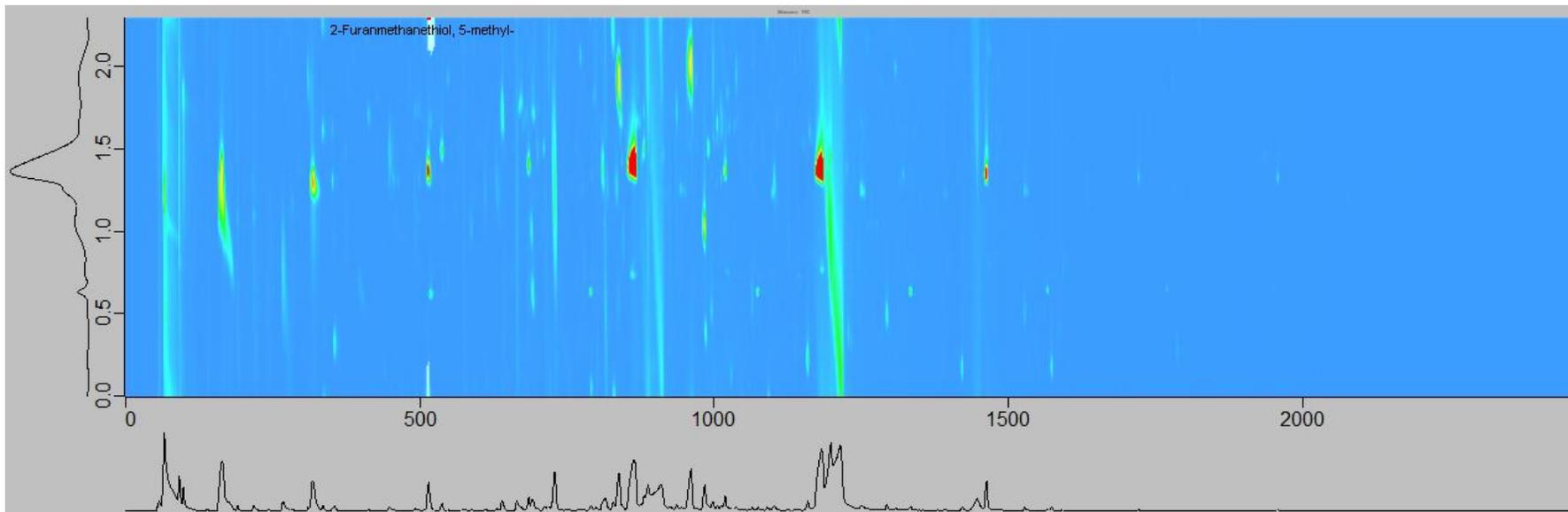


2-Furanmethanethiol, 5-methyl-



The *trans*-2-nonenal, as any other aliphatic aldehydes, could interact with tannins and sulfur dioxide. L. Blanchard and T. Tominaga have respectively identified furfuryl-thiol and 5-methyl-2-furamethanethiol (coffee-like smell compounds with very low odor thresholds: 0.4 ng/L and 50 ng/L) as products of transformation of furfural and 5-methylfurfural, respectively, in wine medium.^{3,21,22}

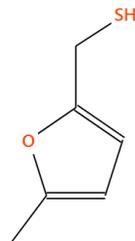
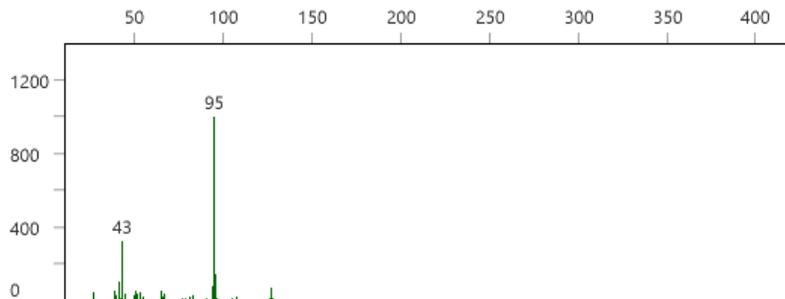
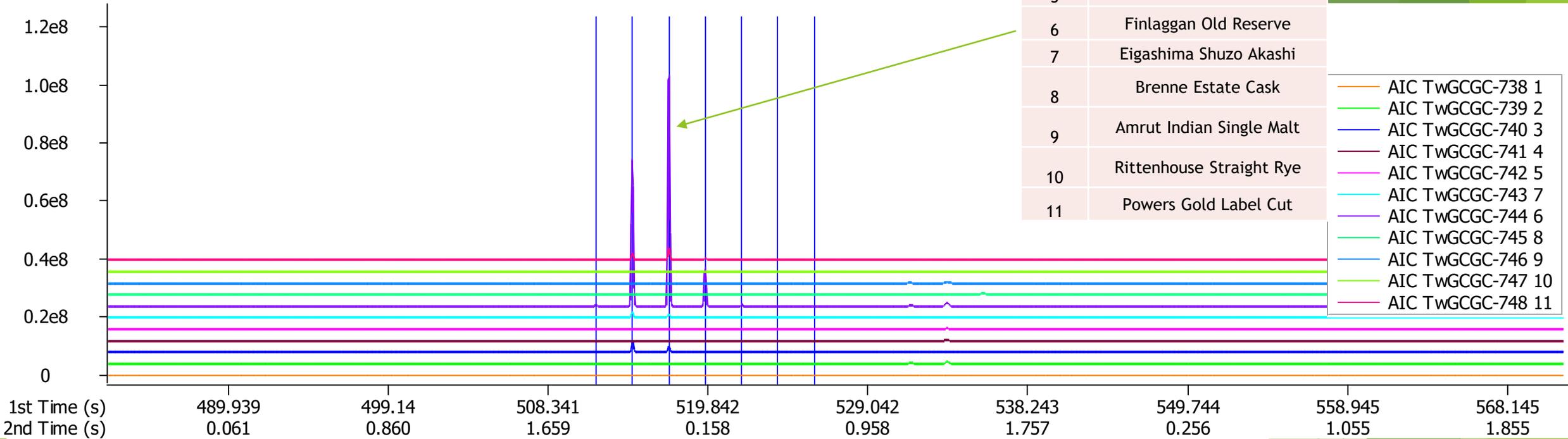
GCxGC



AIC (m/z=95.06)

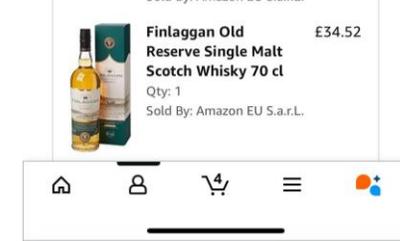
Sample	Whisky Name
1	Old Pulteney 12 Years Old
2	Auchentoshan Three Wood
3	The Famous Grouse Finest
4	Monkey Shoulder
5	Aberlour 12 Year Old
6	Finlaggan Old Reserve
7	Eigashima Shuzo Akashi
8	Brenne Estate Cask
9	Amrut Indian Single Malt
10	Rittenhouse Straight Rye
11	Powers Gold Label Cut

—	AIC TwGCGC-738 1
—	AIC TwGCGC-739 2
—	AIC TwGCGC-740 3
—	AIC TwGCGC-741 4
—	AIC TwGCGC-742 5
—	AIC TwGCGC-743 7
—	AIC TwGCGC-744 6
—	AIC TwGCGC-745 8
—	AIC TwGCGC-746 9
—	AIC TwGCGC-747 10
—	AIC TwGCGC-748 11

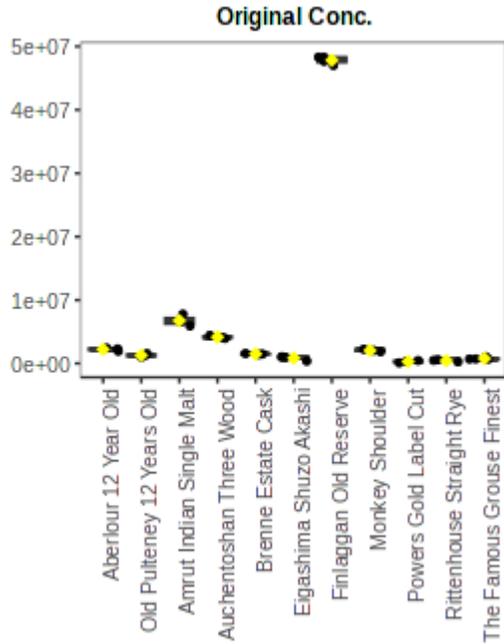


Coffee-like
Perception threshold : 50ng/L

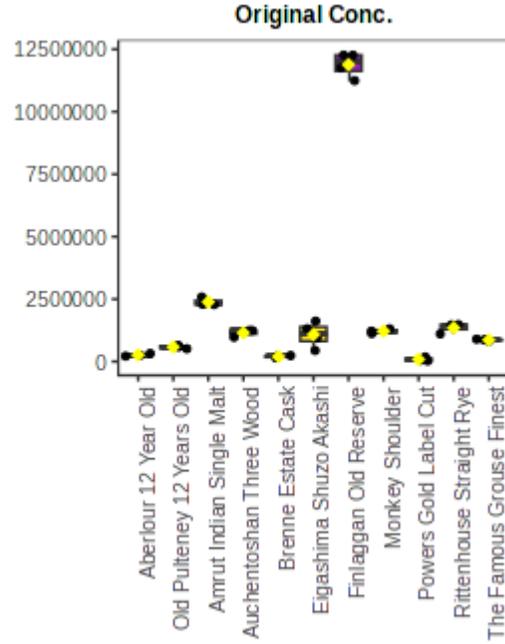
Finlaggan old reserve



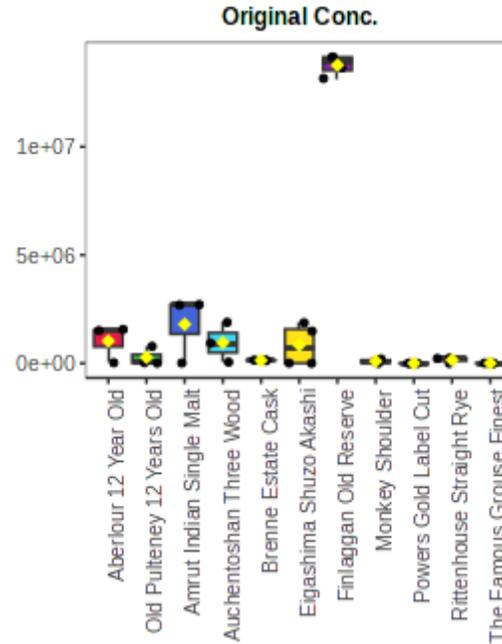
Pyrazine. methyl-



Pyrazine. tetramethyl-



Pyrazine. 2.5-diethyl-



“Peaty, smoky, iodine, brine, earthy”

Journal of The Institute of Brewing

Research article | Free Access

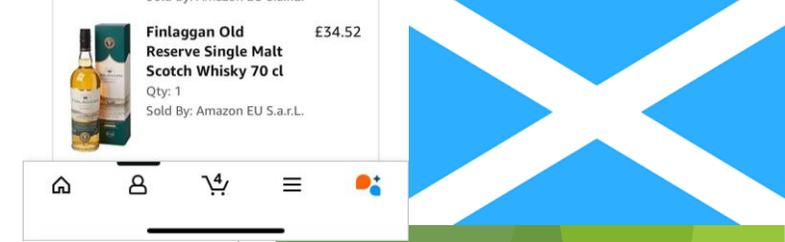
Origins of the perceived nutty character of new-make malt whisky spirit

Emily Boothroyd, Robert S. T. Linforth, Frances Jack, David J. Cook

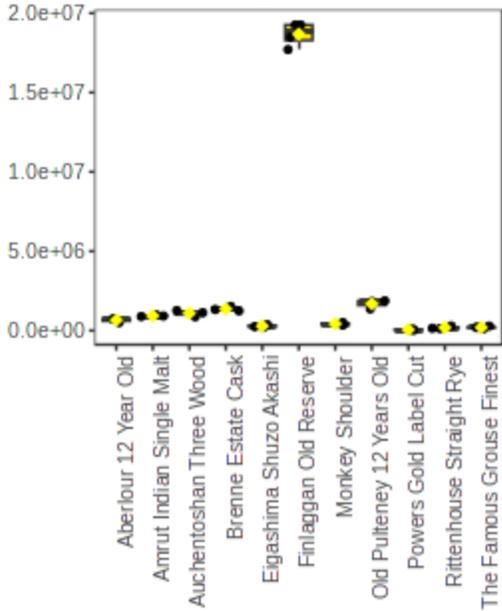
First published: 02 December 2013 | <https://doi.org/10.1002/jib.103> | Citations: 33

Molecule	Odor Threshold (water)	Aromatic Description
2-Methylpyrazine	60 000 - 105 000 ppb	Nutty, cocoa, green, roasted, chocolate, meaty
2,3,5,6-Tetramethylpyrazine	~10 ppm	Musty, fermented soybean, coffee/chocolate-like, heated-lard notes
2,5-Diethylpyrazine	Not explicitly reported ¹	Likely nutty, roasted, buttery—common pyrazinic profile; no precise threshold found

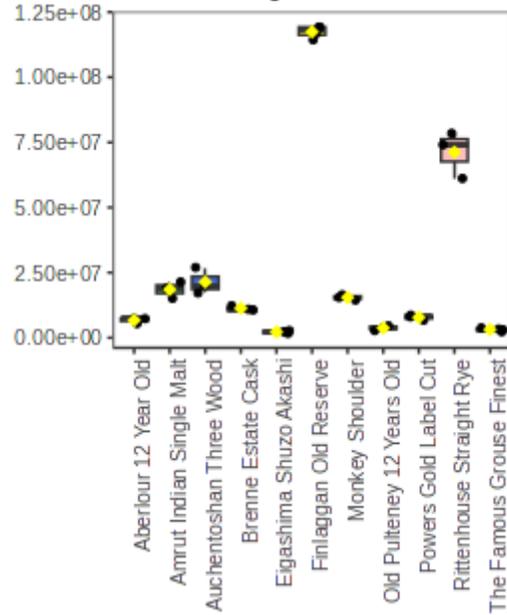
Finlaggan old reserve



o-Guaiacol
Original Conc.



4-Ethylguaiacol
Original Conc.



Molecule	Odor Threshold (water)	Aromatic Description
Guaiacol	0.48 ppb	Sweet, smoky, vanilla-like, medicinal, bacon/ham nuances
4-Ethylguaiacol (4-EG)	<u>~ 50 ppb</u>	Spicy, clove-like, smoky, woody, sweet-vanilla nuances

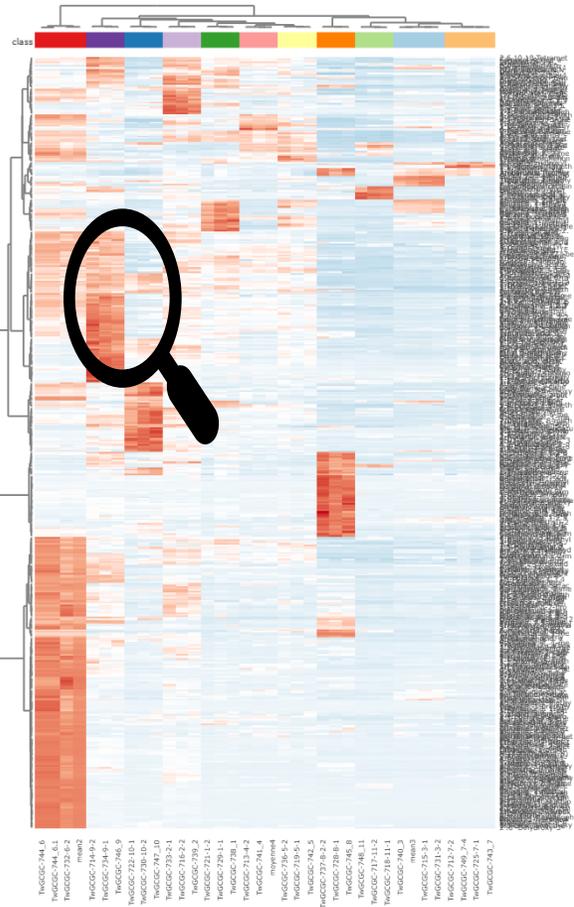
“Peaty, smoky, iodine, brine, earthy”

Amrut Indian Single Malt

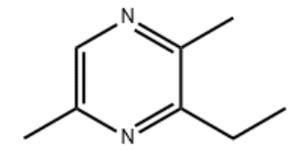
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 Delivery Estimate:
 Sunday, 25 May 2025



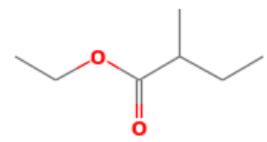
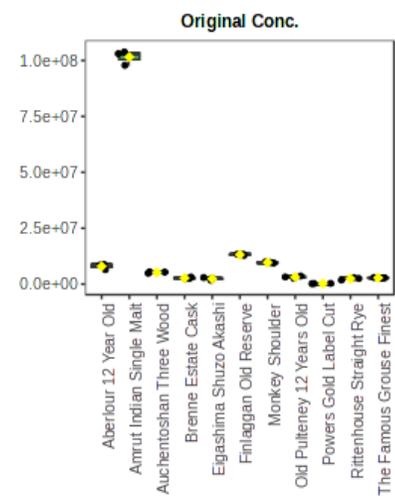
Amrut Indian Single Malt Whisky | 46 Percent | 70cl | Rich and £47.45
 Qty: 1
 Sold By: Amazon EU S.a.r.L.



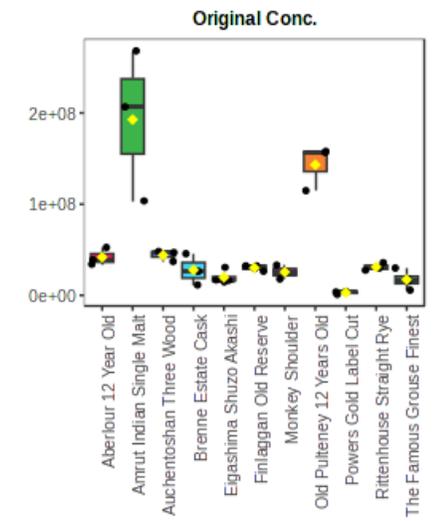
- class
- Aberlour 12 Year Old
 - Amrut Indian Single Malt
 - Auchentoshan Three Wood
 - Brenne Estate Cask
 - Eigashima Shuzo Akashi
 - Monkey Shoulder
 - Old Pulteney 12 Years Old
 - Powers Gold Label Cut
 - Rittenhouse Straight Rye
 - The Famous Grouse Finest



Pyrazine. 3-ethyl-2,5-dimethyl-



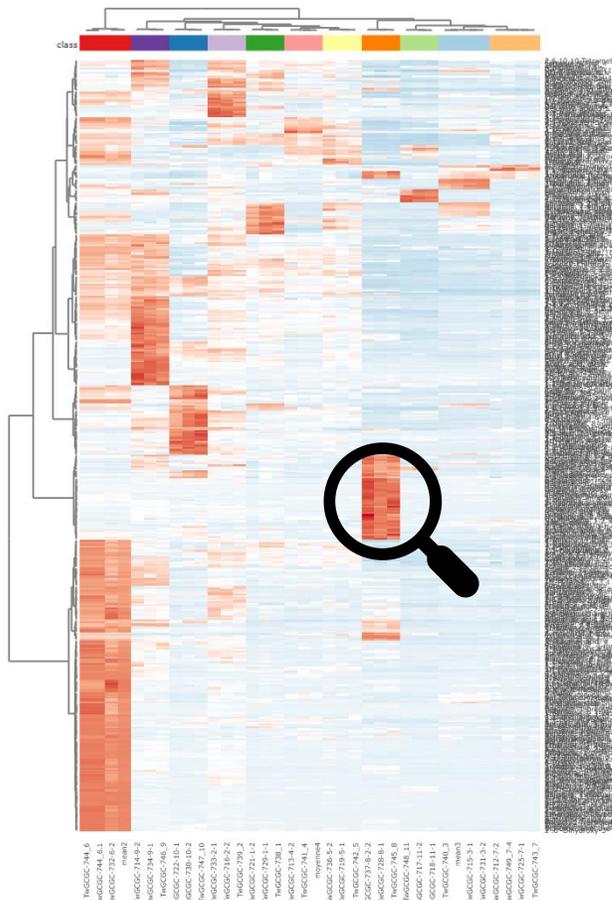
Butanoic acid. 2-methyl-. ethyl ester



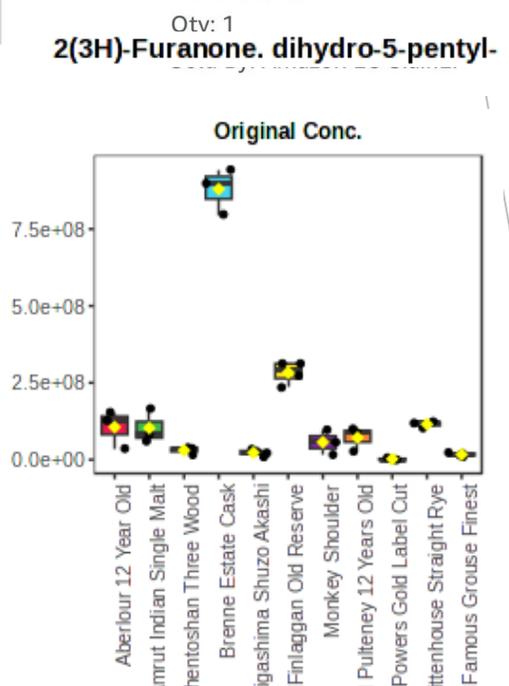
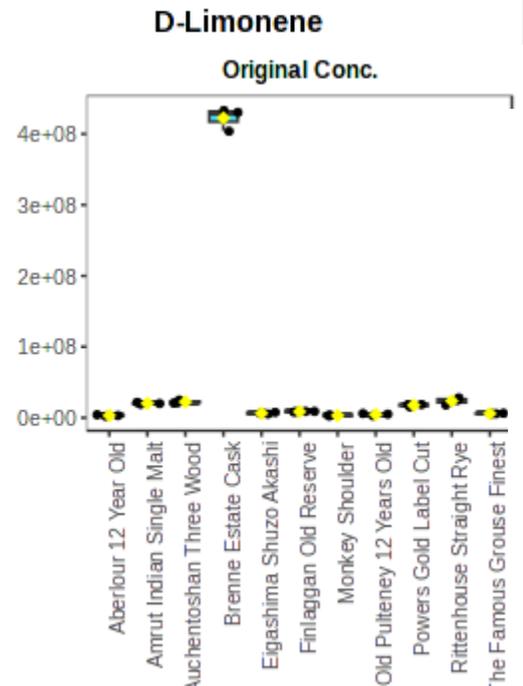
Molecule	Odor Threshold (water)	Aromatic Description
3-Ethyl-2,5-dimethylpyrazine	0.04 µg/L	Toasted nut, roasted, nutty
2-Methyl-ethyl butanoate	0.5 µg/L	Fruity, green, apple peel, pineapple, strawberry, tropical

“Tropical fruit, spice, oak, honey, intense due to climate aging”

Brenne Estate Cask



Fruity, banana, tropical fruit, custard, light oak

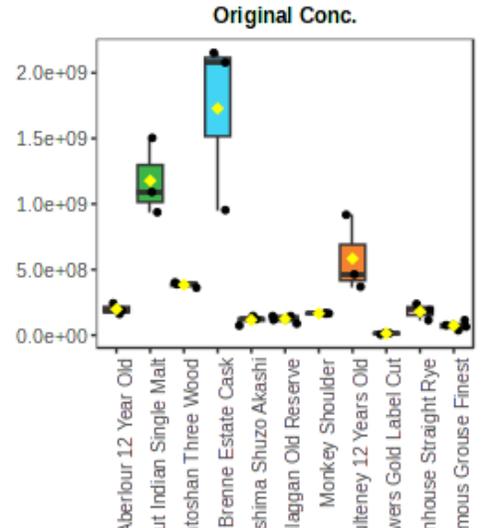


Common Name	Odor Threshold (water)	Description
γ-Nonalactone	ppb - 30 ppb (water);	Creamy, coconut-like, sweet, buttery, waxy; imparts “ tropical ” lactonic nuances
Limonene	~38 ppb (absolute); ~200 ppb (R-enantiomer)	Fresh citrus (orange/lemon zest), fruity, tangerine, subtle green/herbal notes
Ethyl isovalerate	Not precisely defined; branched butanoate esters have very low thresholds (estimated in tens ppb)	Fruity —green apple/pineapple, with subtle berry note (“myrtille”)

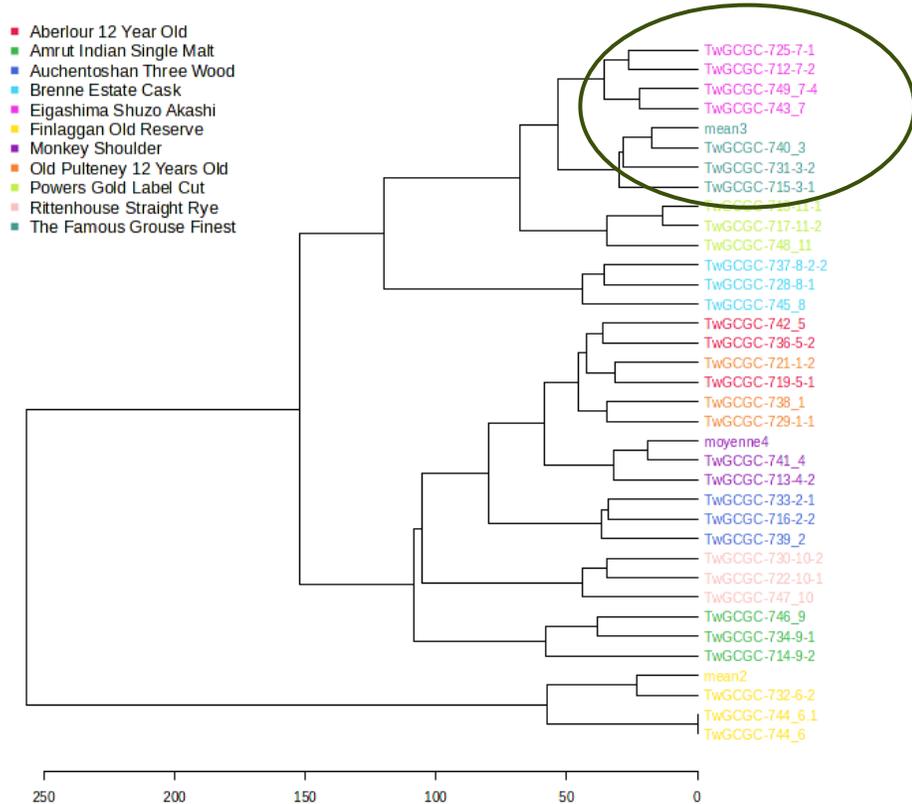
 Brenne Estate Cask Whisky, 70cl - 40% ABV French Single Malt Scotch
Otv: 1
2(3H)-Furanone. dihydro-5-pentyl-

£55.68

Butanoic acid. 3-methyl-. ethyl ester

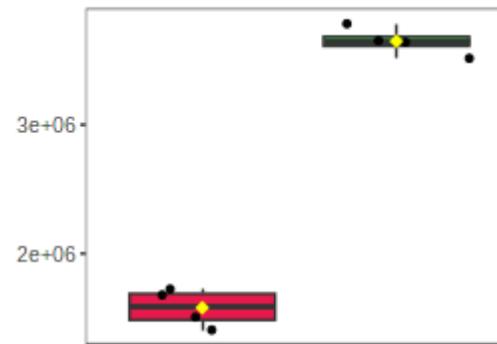


2 whiskies very close ?



(E)- β -Farnesene

Original Conc.



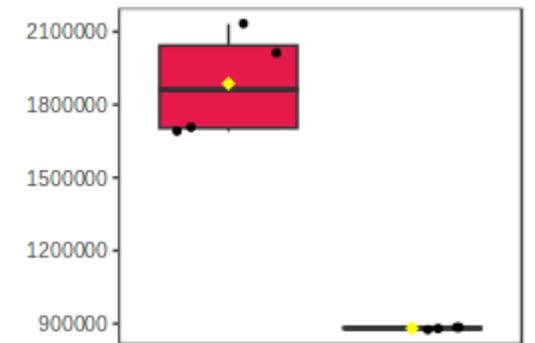
Eigashima Shuzo Akashi

The Famous Grouse Finest



Farnesol isomer a

Original Conc.

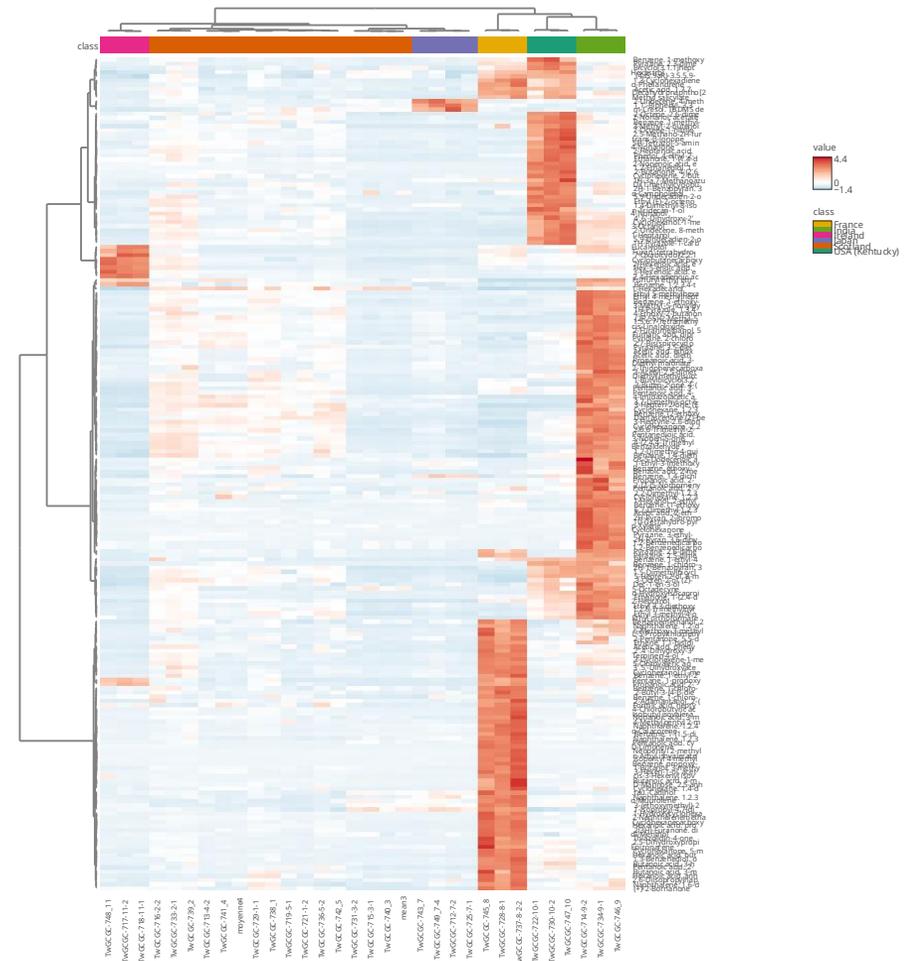
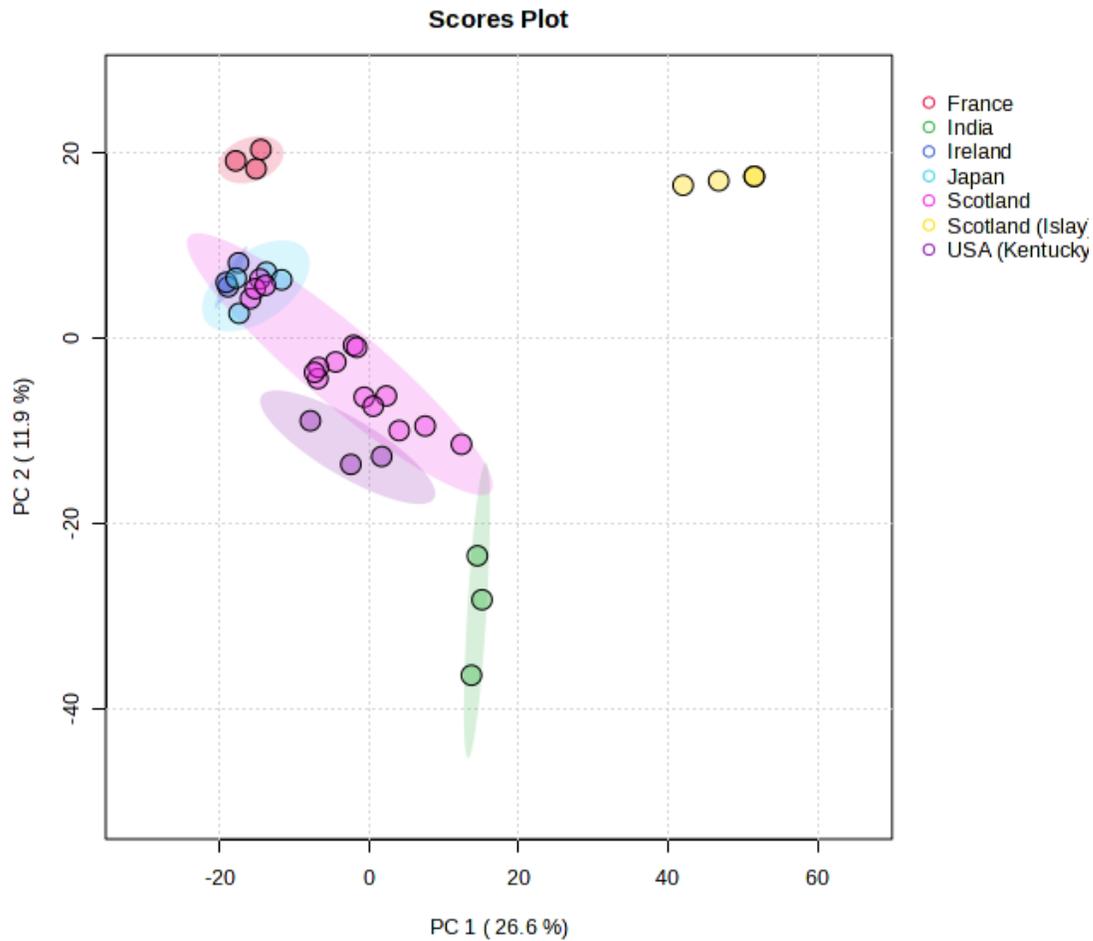


Eigashima Shuzo Akashi

The Famous Grouse Finest

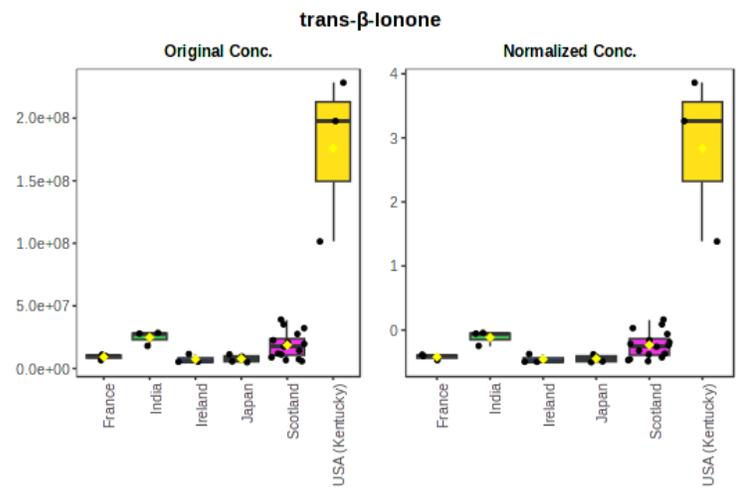


VOCs signature by country ?





USA ? (Rittenhouse Straight Rye)



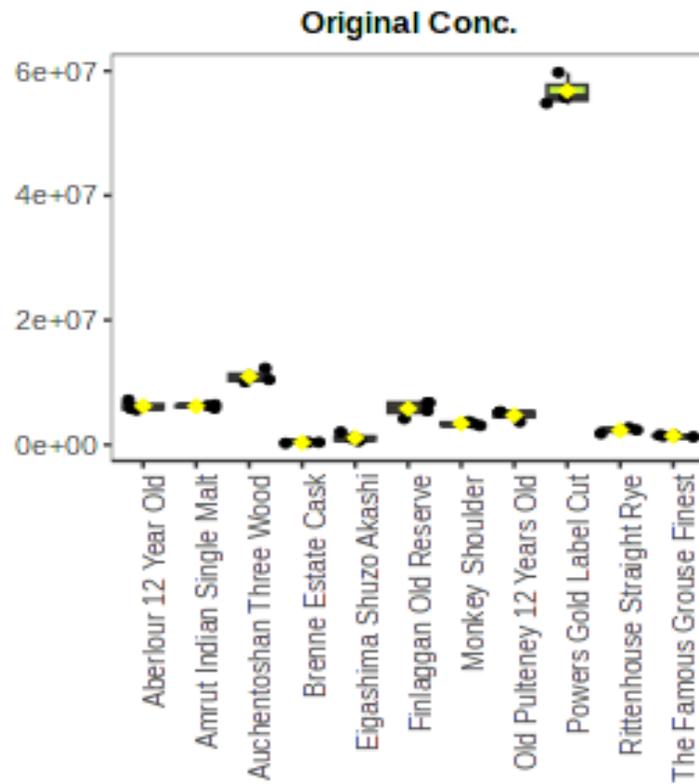
Common Name	Odor Threshold (water)	Aromatic Description
β -Ionone	~30 ng/L (~0.03 μ g/L) in water	Floral-violet, woody-sweet, fruity-raspberry, green; warm floral and subtle fruity nuances

“Spicy, caramel, cinnamon, black pepper, bold finish”

Ireland (Powers Gold Label Cut)



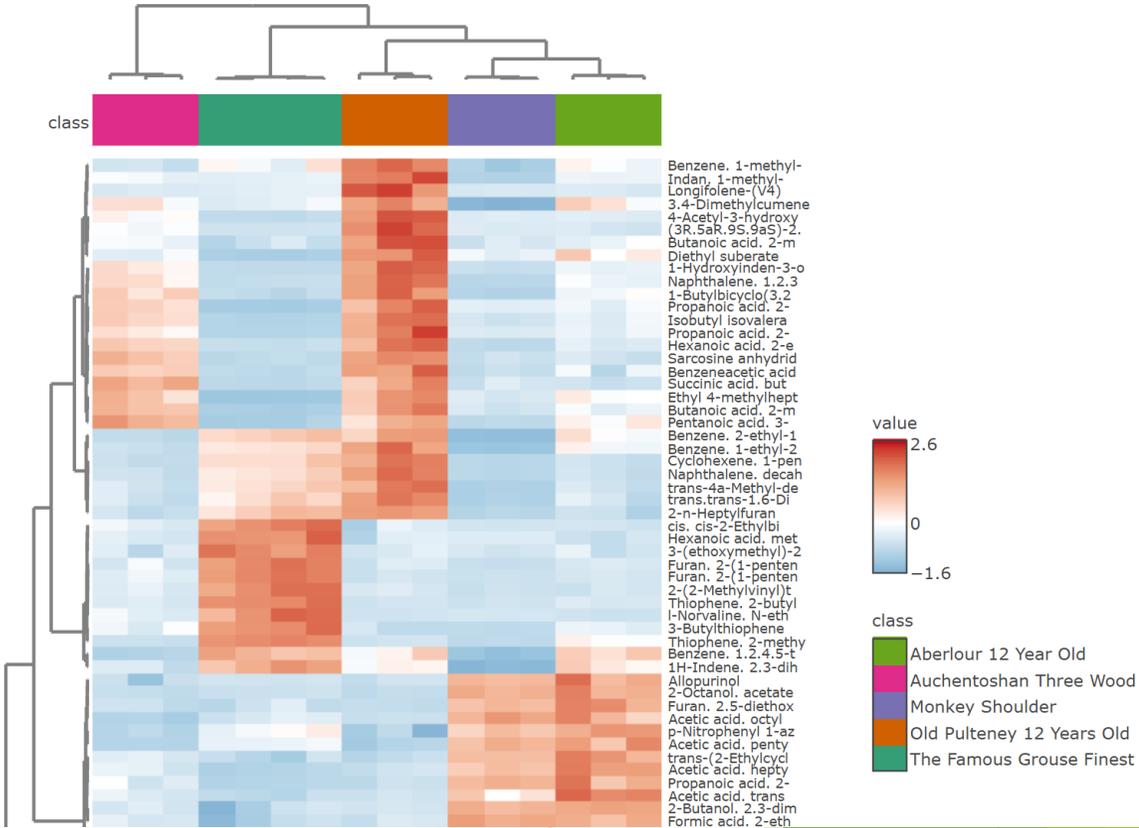
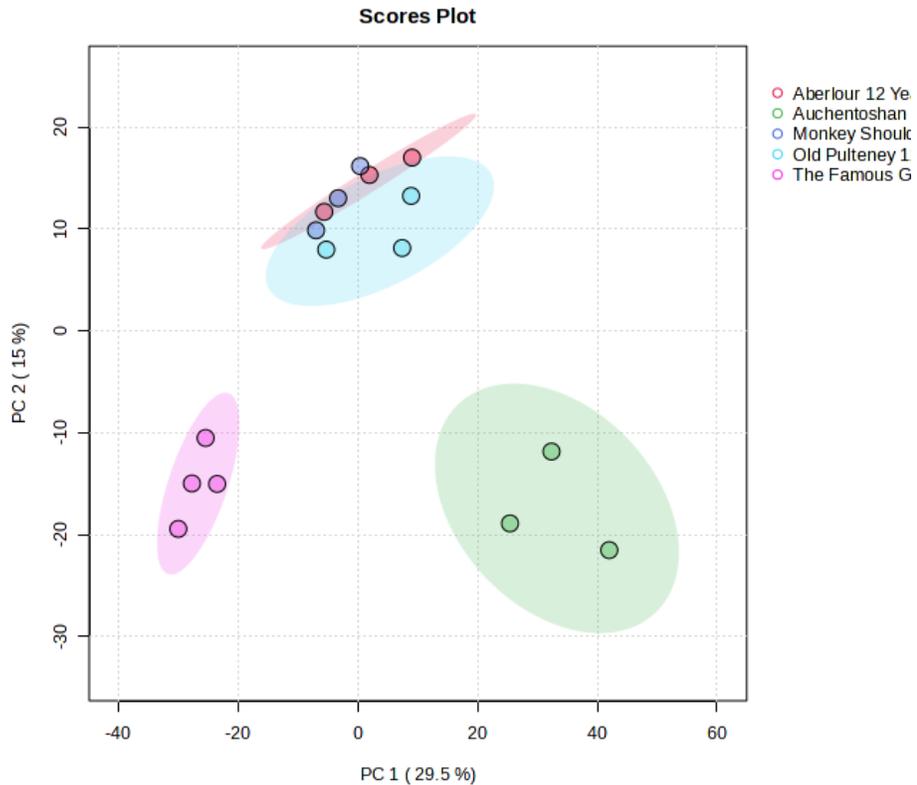
Ethyl sorbate



Common Name	Odor Threshold (water)	Aromatic Description
Ethyl sorbate	Detection threshold: ~100 ppb	Fruity, green, pineapple, passion-fruit, papaya, slightly tropical; ethereal/fresh nuances

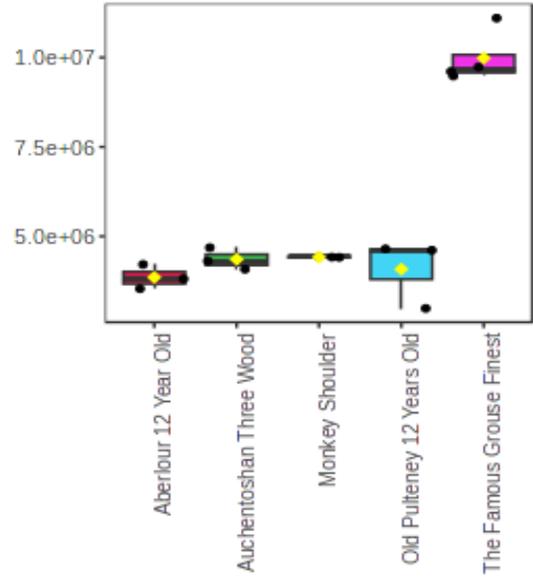
Spicy, honey, apple, cereal grain, vanilla

Difference between scotish wiskies

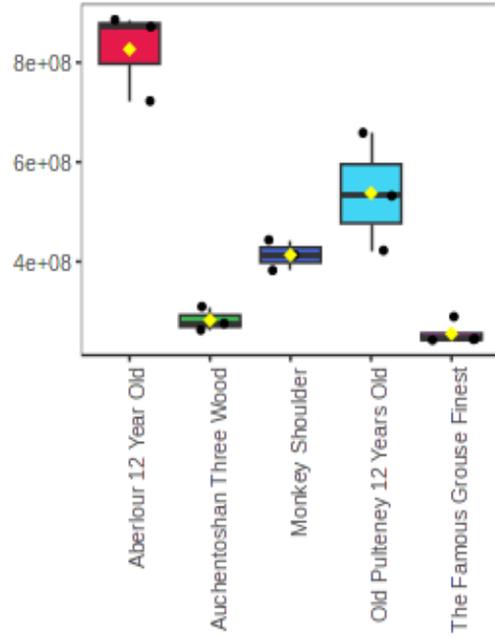




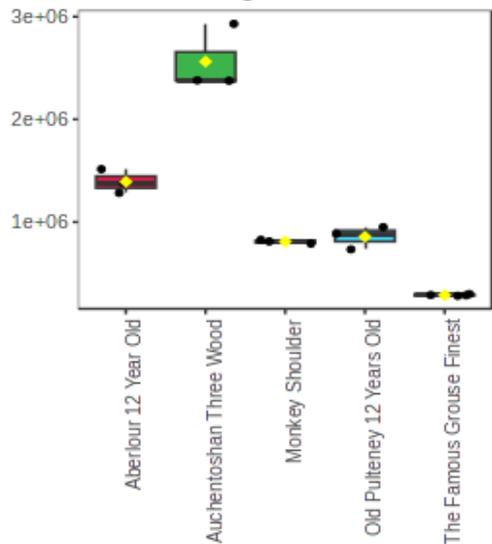
Hexanoic acid. methyl ester



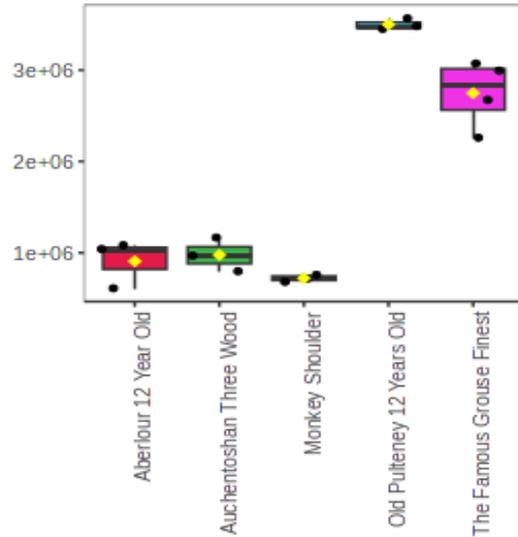
1-Octanol



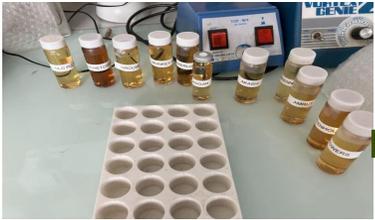
Cyclohexanol. 1-methyl-4-(1-methylethyl)-. cis-



2-n-Heptylfuran



Common Name	Odor Threshold (water)	Aromatic Description
Methyl hexanoate	~10-87 ppb	Fruity, sweet, exotic—pineapple, melon, apple, grape, papaya; ether-like
cis-Menthol	~60-500 ppb (variable)	Minty, herbal, slightly camphoraceous, cooling, green, resinous
1-Octanol (n-Octanol)	~2.7 ppb	Waxy, green, citrusy, aldehydic, floral; mild mushroom and orange peel nuance
2-Heptylfuran	Not well defined (~ppm range)	Woody, nutty, roasted, fatty, coffee-like, slightly fruity and tropical



30 min

1mL whisky
9mL NaCl 5M
+IS (1,4
dibromobenzene)



1 day



ChromaTOF.SYNC

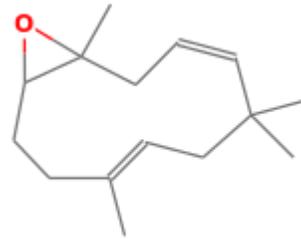
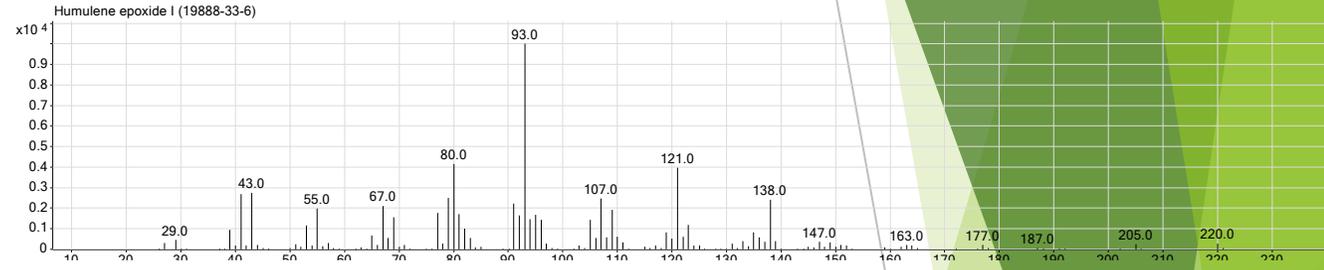
LECO
EMPOWERING RESULTS

1-5 days

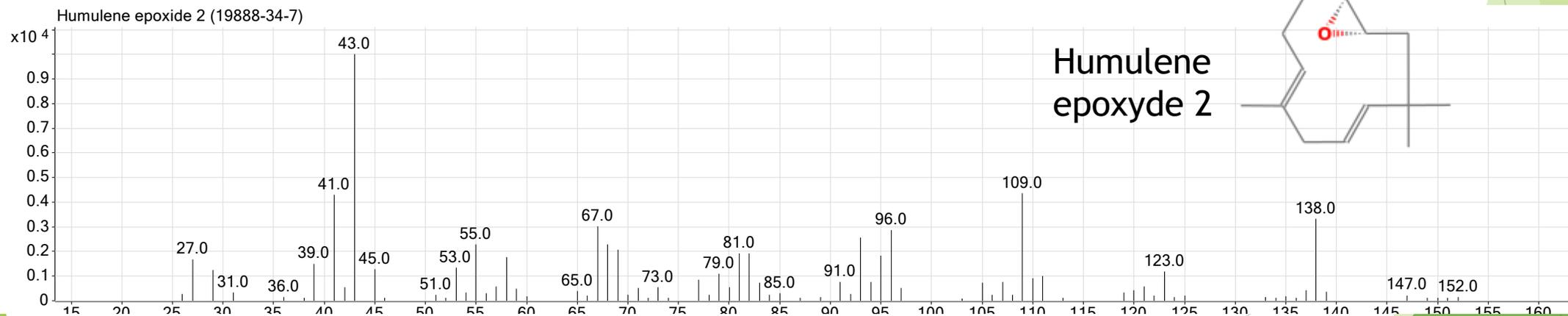
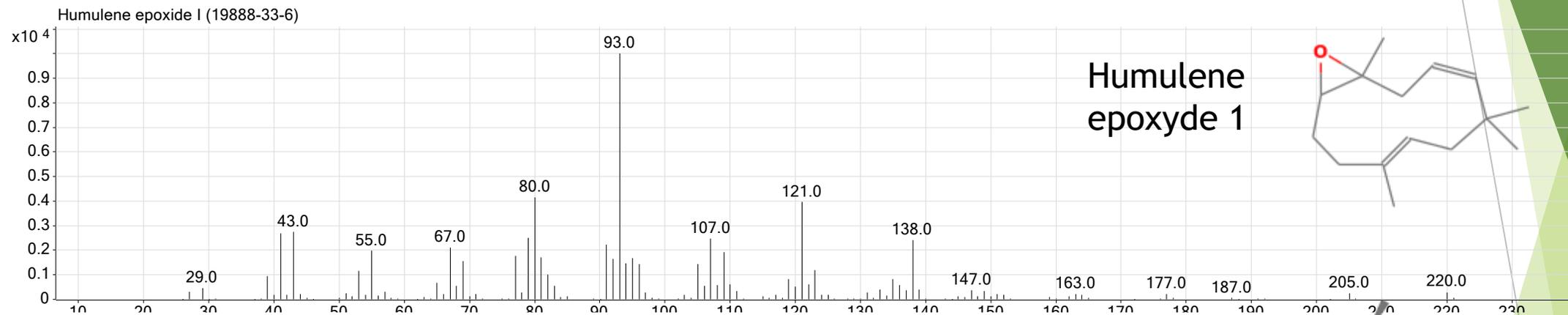




Humulene epoxyde 2



Humulene epoxyde 1

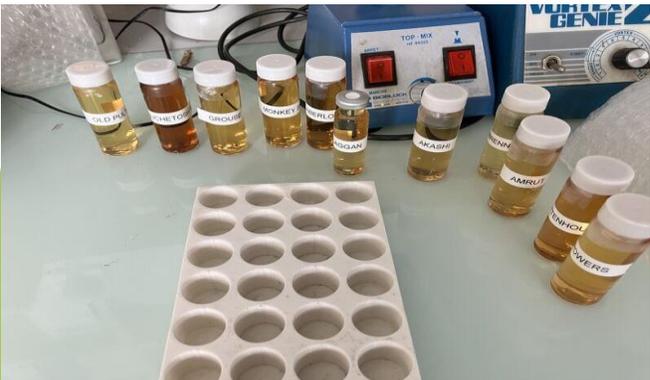


Et la suite ?



Name	Formula	CAS	odeurs	1	2	3	4	5	6	7	8	9	10
Dodecanoic acid, ethyl ester	C ₁₄ H ₂₈ O	106-33-2		431886304.00	79742432.00	89693296.00	92492408.00	213751936.00	100923352.00	92198632.00	50974572.00	301125472.00	275
Furfural	C ₅ H ₄ O ₂	98-01-1	alkane	407745472.00	859544896.00	2915311360.00	569738112.00	1397342720.00	248933072.00	243356864.00	1949571200.00	1152511360.00	1303
Phenylethyl Alcohol	C ₈ H ₁₀ O	60-12-8	rose	405523552.00	2100498816.00	301128256.00	478009568.00	661864704.00	53493744.00	50263852.00	17537.45	289593088.00	765
Dodecanoic acid, ethyl ester	C ₁₄ H ₂₈ O	106-33-2	fruit	397867680.00	283916064.00	489532128.00	272119872.00	378003040.00	293179584.00	277817856.00	267521312.00	280140768.00	319
Decanoic acid, ethyl ester	C ₁₂ H ₂₄ O	110-38-3		391151904.00	1391523456.00	1526173696.00	1687006208.00	439681056.00	2758151680.00	633585472.00	1926622208.00	1668277120.00	640
1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	123-92-2	banana	390771968.00	447611968.00	611997632.00	1298734848.00	331105024.00	627833024.00	374096256.00	683455936.00	314819264.00	1148
Benzaldehyde	C ₇ H ₆ O	100-52-7	almond	389622592.00	845146176.00	2707379200.00	295489824.00	1143635840.00	89065080.00	76034944.00	708347264.00	430895008.00	153
Decanoic acid, ethyl ester	C ₁₂ H ₂₄ O	110-38-3		386977504.00	408022528.00	288143744.00	576209088.00	536598944.00	807542592.00	117899152.00	309398976.00	679157696.00	493
Decanoic acid, ethyl ester	C ₁₂ H ₂₄ O	110-38-3		377752736.00	485379104.00	444090400.00	592743424.00	451878080.00	985408768.00	988393088.00	389766048.00	508560320.00	334
Octanoic acid, ethyl ester	C ₁₀ H ₂₀ O	106-32-1		375146048.00	460335744.00	338643936.00	259671472.00	309495648.00	324022624.00	176443952.00	331387200.00	325894464.00	266
Ethylbenzene	C ₈ H ₁₀	100-41-4	gas	352116000.00	123940760.00	449958944.00	628353152.00	49359132.00	35362288.00	40893080.00	36432224.00	74874488.00	476
Heptanoic acid, ethyl ester	C ₉ H ₁₈ O ₂	106-30-9	fruit	316535584.00	652060736.00	1092108288.00	275505376.00	770083008.00	526925248.00	483915968.00	704950592.00	567208192.00	1111
Dodecanoic acid, ethyl ester	C ₁₄ H ₂₈ O	106-33-2	fruit	308742816.00	563847744.00	69672656.00	70448416.00	62256704.00	65983492.00	75176160.00	46248000.00	49002432.00	51
Octanoic acid, 3-methylbutyl ester	C ₁₃ H ₂₆ O	2035-99-6	fruit	308654176.00	737231296.00	522908608.00	395532960.00	458984416.00	706891072.00	717103872.00	418307552.00	295133536.00	246
Furfural	C ₅ H ₄ O ₂	98-01-1	alkane	307032960.00	740764096.00	6953299968.00	460331776.00	65944600.00	84674728.00	62778512.00	1138405632.00	733468992.00	970
Dodecanoic acid, ethyl ester	C ₁₄ H ₂₈ O	106-33-2	fruit	305241152.00	426782656.00	422337952.00	636835520.00	755504384.00	827807232.00	922049408.00	534105792.00	199527680.00	238
2-Methylbutyl octanoate	C ₁₃ H ₂₆ O	67121-39-5	unknown	300846208.00	444098432.00	634819968.00	391941248.00	554409664.00	615854720.00	423036.47	354034336.00	380335584.00	196
Decanoic acid, ethyl ester	C ₁₂ H ₂₄ O	110-38-3	fruit	283778176.00	291862624.00	381871424.00	631587392.00	2179936256.00	686035456.00	668119744.00	2004460544.00	582500096.00	1460
Octanoic acid, ethyl ester	C ₁₀ H ₂₀ O	106-32-1		281583968.00	299548896.00	259492272.00	418908512.00	365824000.00	282621120.00	294040768.00	310911712.00	301681472.00	319
Decanoic acid, ethyl ester	C ₁₂ H ₂₄ O	110-38-3		270566400.00	308995488.00	442158272.00	422923008.00	413712448.00	705212160.00	294282496.00	647379072.00	523535712.00	319
1-Butanol, 3-methyl-, acetate	C ₇ H ₁₄ O ₂	123-92-2	banana	266855440.00	501299168.00	208321296.00	679869824.00	284395552.00	592241152.00	594663104.00	512235328.00	1006214656.00	537
Dodecanoic acid, ethyl ester	C ₁₄ H ₂₈ O	106-33-2	fruit	266216752.00	292764096.00	595729088.00	391193120.00	389789152.00	928265088.00	897612608.00	352494592.00	616690880.00	384
Octanoic acid, ethyl ester	C ₁₀ H ₂₀ O	106-32-1	fruit	262101728.00	118929408.00	20790814.00	208555952.00	345100160.00	178744224.00	47902408.00	167935696.00	134122936.00	155
Benzoic acid, ethyl ester	C ₉ H ₁₀ O ₂	93-89-0	fruit	259761232.00	553951872.00	670061760.00	223550912.00	470709920.00	35719356.00	30602988.00	289195104.00	355716992.00	137
1-Butanol, 3-methyl-	C ₈ H ₁₂ O	123-51-3		254717584.00	1729243008.00	2072393856.00	148443728.00	2114851200.00	220763744.00	248859872.00	1817317376.00	1508960000.00	2184

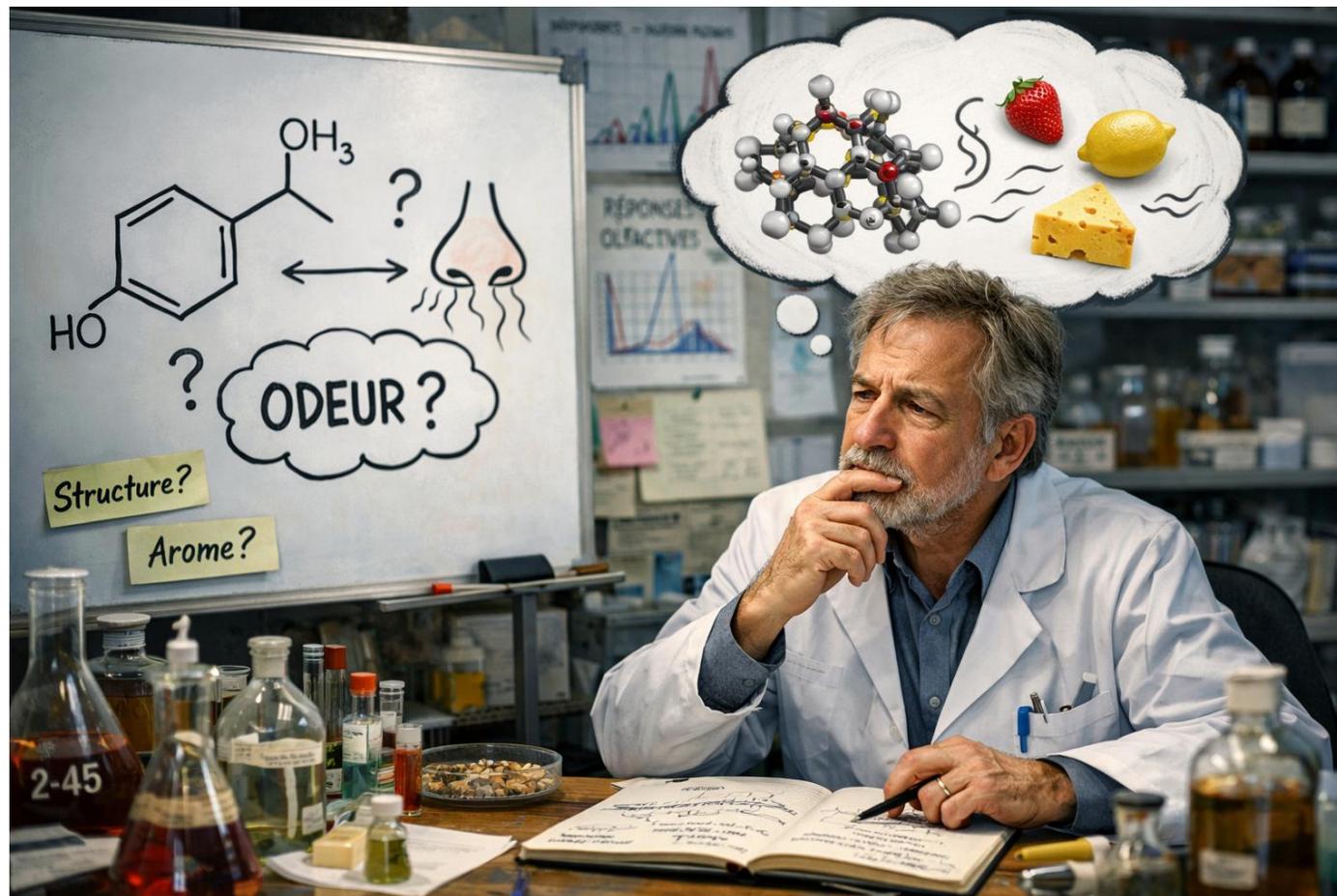
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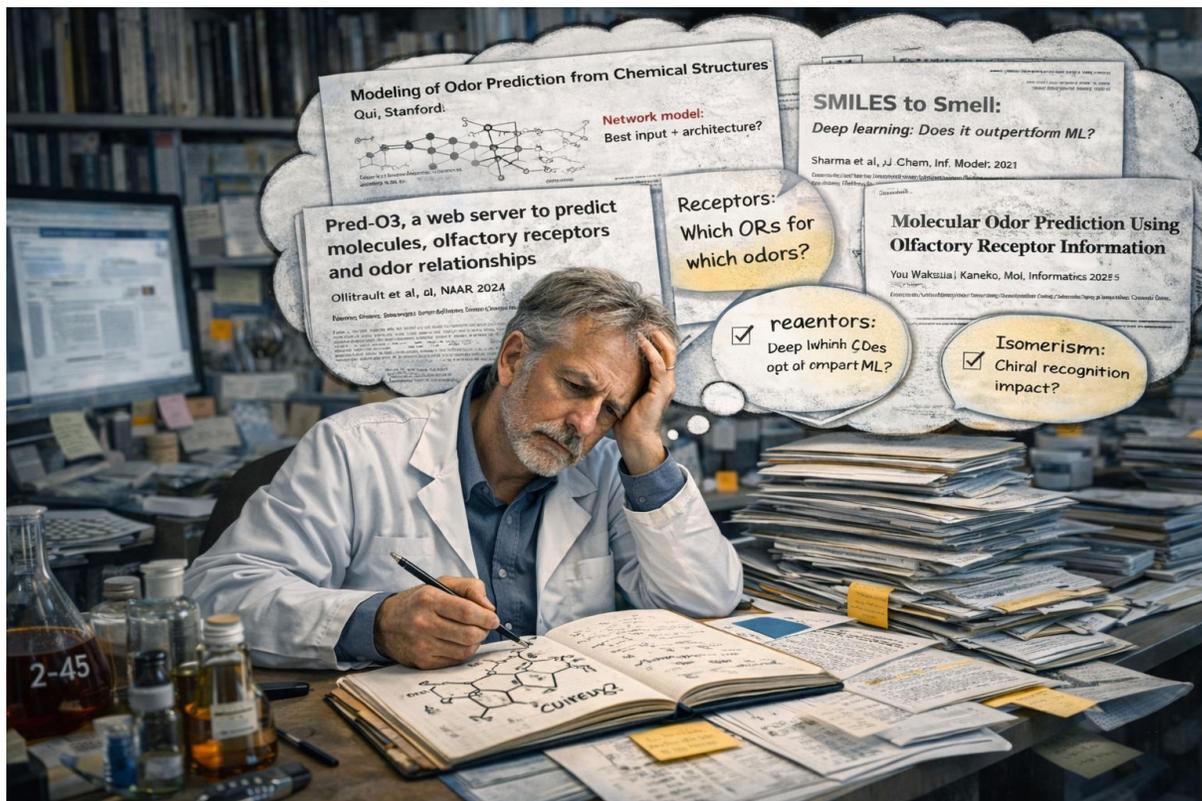




...Le travail
**c'est bien mais
mais j'en ferais
pas mon métier !**

Et si ??





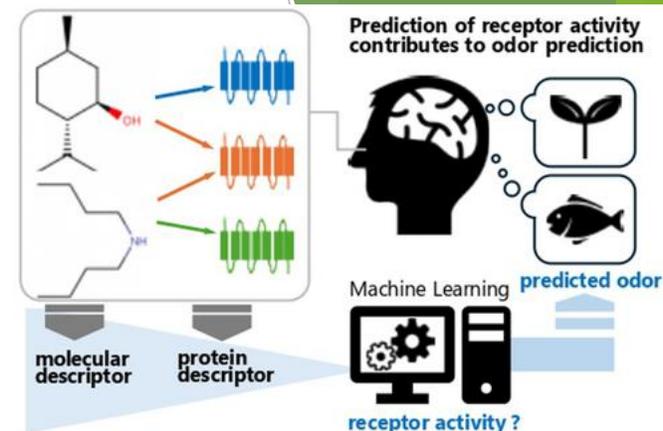
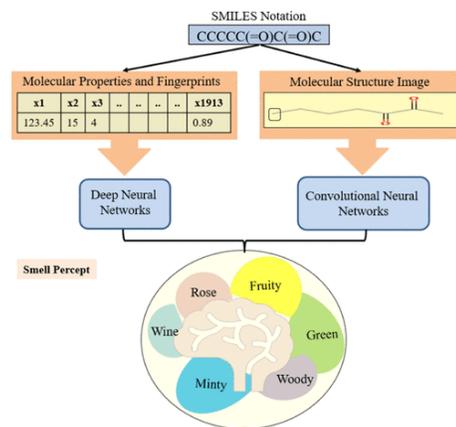
• **Qiu, C. (2020)** – *Modeling of Odor Prediction from Chemical Structures*. Stanford University (CS229/CS230 project).

• **Sharma, A. et al. (2021)** – *SMILES to Smell: Decoding the Structure–Odor Relationship Using Deep Neural Networks*. *J. Chem. Inf. Model.* 61, 676–688.

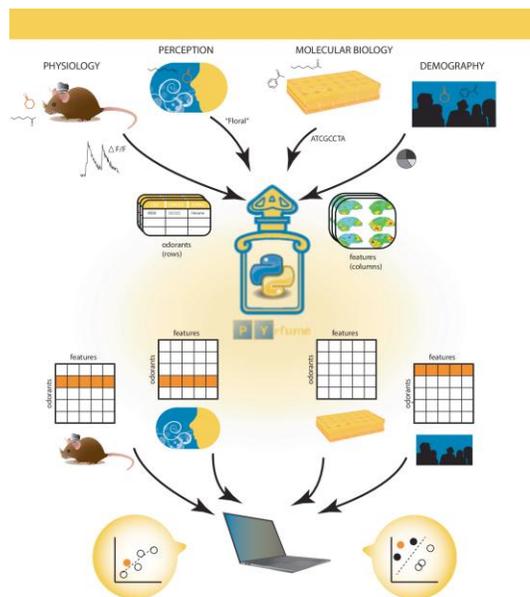
• **Ollitrault, G. et al. (2024)** – *Pred-O3: a web server to predict molecules, olfactory receptors and odor relationships*. *Nucleic Acids Research*, 52(W1), W507–W512.

• **Wakutsu, Y.; Kaneko, H. (2025)** – *Molecular Odor Prediction Using Olfactory Receptor Information*. *Molecular Informatics*, 44:e202400274.

Collecte de données



Molecular Odor Prediction Using Olfactory Receptor Information



SMILES to Smell: Decoding the Structure-Odor Relationship of Chemical Compounds Using the Deep Neural Network Approach



Pyrfume: A window to the world's olfactory data

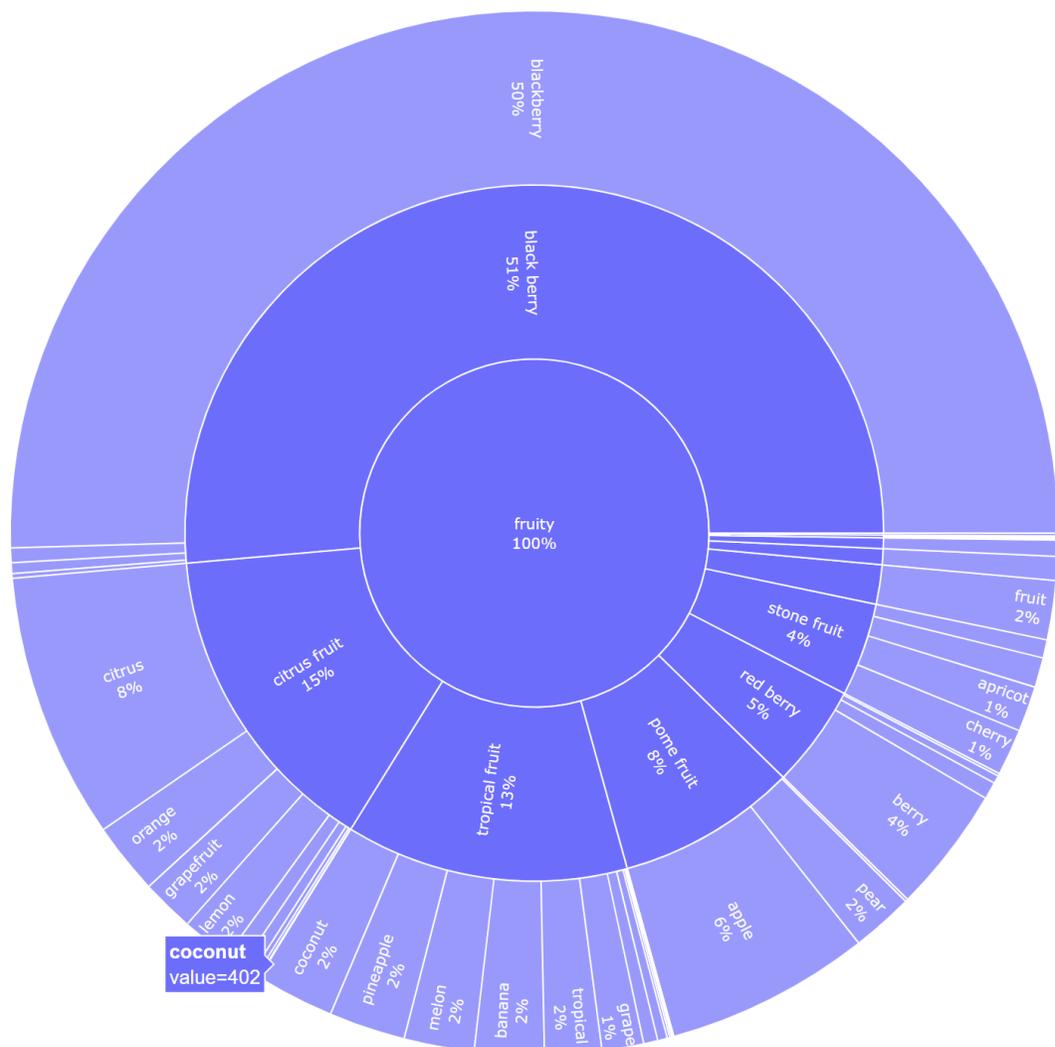
Pred-O3, a web server to predict molecules, olfactory receptors and odor relationships

Données

11 052 molécules
772 labels => 300 labels normalisés

A	B	C	D
CAS	NOM	ODEURS_EN	SOURCES
15111-56-5	Ethyl 3-cyclohexenecarboxylate	balsamic floral fresh fruity herbal musty sweet woody ylang	41598_2024_70696_MOESM1_ESMV2 ComplementN
3681-82-1	3-Hexen-1-ol, acetate, (E)-	apple banana banana unripe banana cortex dry floral fresh fruity green hyacinth narcissus no	41598_2024_70696_MOESM1_ESMV2 ComplementN
7492-45-7	CID 73555259	apricot citrus clean dairy fatty floral fruity fruity aroma green herbal nasturtium oily peach	41598_2024_70696_MOESM1_ESMV2 pyrfume_cand
4698-08-2	2,6-Octadienoic acid, 3,7-dimethyl-, (E)- 1,4,4-Trimethyltricyclo[5.3.1.02,6]undecan-11-ol	acidic citrus dry feet floral flowery fresh fruity grass greasy green herbaceous herbal lemon	41598_2024_70696_MOESM1_ESMV2 ComplementN
	Menthadien carboxaldehyde	balsamic earthy moss mossy resinous spicy woody	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
1195-92-2	Limonene 1,2-Epoxyde	fatty herbal spicy	41598_2024_70696_MOESM1_ESMV2
536-60-7	p-Cymen-7-ol	green	41598_2024_70696_MOESM1_ESMV2
20662-84-4	Oxazole, trimethyl-	aromatic caraway cinnamon cumin floral herb herbaceous herbal leather leathery musk oily p	41598_2024_70696_MOESM1_ESMV2 ComplementN
72203-97-5	Isoneral	bee beefy body boiled chocolate fish food fruity green meat mustard nut nut skin nutty roast	41598_2024_70696_MOESM1_ESMV2 ComplementN
138-22-7	Butyl lactate	green	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
75587-05-2	Ethyl 5-Hydroxyoctanoate	apple apple skin appleskin burnt butter buttery caramel cheese cheesy chemical creamy dairy	41598_2024_70696_MOESM1_ESMV2 ComplementN
72214-23-4	1,1,5-Trimethyl-4,6-heptadienyl acetate (isomer 1)	apple fatty fruity pineapple sweet tropicalfruit	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
2110-18-1	2-(3-Phenylpropyl)pyridine	bergamot citrus cologne ethereal floral fresh fruity green lavender lemon	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
43219-68-7	Ethanone, 1-(1,4-dimethyl-3-cyclohexen-1-yl)-	bellpepper cortex earthy fresh green herbaceous herbal metallic nasturtium pea pepper pepp	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
87-69-4	(R,R)-Tartaric acid	camphoraceous fresh fruity herbaceous herbal mint minty	41598_2024_70696_MOESM1_ESMV2 ComplementN
62488-24-8	3-Methylbutyl tetradecanoate	acid caramel mild odorless tart	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
68990-37-4	Propanoic acid	fatty fragrant fruity mouthfeel oily waxy	41598_2024_70696_MOESM1_ESMV2 ComplementN
	(3Z,6Z)-dodeca-3,6-dienal	acidic cheese cheesy dairy disagreeable fatty fruity milk pungent rancid silage sour soy spice	41598_2024_70696_MOESM1_ESMV2 ComplementN
1117-59-5	Hexyl n-valerate	citrus fatty herbal	41598_2024_70696_MOESM1_ESMV2
	Pentadeca-2,4,6-trienal	apple brandy fruity green musk oily sweet unripe vegetative	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
2094-69-1	Propanoic acid, 2,2-dimethyl-, phenylmethyl ester	fatty	41598_2024_70696_MOESM1_ESMV2
120-51-4	Benzyl Benzoate	apple chamomile floral herbaceous herbal	41598_2024_70696_MOESM1_ESMV2 ComplementN
16630-55-0	3-(Methylthio)propyl acetate	almond aromatic balsam balsamic berry bitter cheese cherry faint fatty floral fruity herb her	41598_2024_70696_MOESM1_ESMV2 ComplementN
75-18-3	Dimethyl sulfide	alliaceous asparagus cabbage cheese cheesy earthy ester fatty fruit fruity green herbaceous h	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
124-76-5	Npc152989	asparagus berry cabbage chemical cooked corn creamy diacetyl earthy fishy fruity gasoline gr	41598_2024_70696_MOESM1_ESMV2 ComplementN
562-74-3	Terpinen-4-ol	balsamic camphor camphoraceous camphoreous herbal resinous woody	41598_2024_70696_MOESM1_ESMV2 pyrfume_cand
108793-59-5	3,5-Octadien-2-one	balsamic citrus cooling earth earthy floral fresh grapefruit green herbaceous herbal lemon li	41598_2024_70696_MOESM1_ESMV2 ComplementN
40010-99-9	2(3H)-Furanone, 3-acetyl-5-butylidihydro-	earthy fat fatty fruit fruity green hay herbaceous metallic mushroom pungent pungent herbac	41598_2024_70696_MOESM1_ESMV2 Table_S1_Prec
625-84-3	1H-Pyrrole, 2,5-dimethyl-	floral fruity jasmin whiteflower	41598_2024_70696_MOESM1_ESMV2
		animal animalic burnt earthy green nutrid	41598_2024_70696_MOESM1_ESMV2 ComplementN

Regroupement



Drill-down (L3 → top molécules)

Clique un secteur L3 (feuille) pour afficher les 20 molécules où ce L3 est le plus cité.
Note: si les labels L3 sont cachés, c'est normal (trop de feuilles). Clique/hover.

L3: coconut

INCHIKEY	Nom	SMILES	score
HLZKNKRTKFSKGZ-UHFFFAOYSA-N	1-Tetradecanol	nan	12.00
IAFYUQIAOWKSB-UHFFFAOYSA-N	Ethyl Undecanoate	nan	10.00
ILJDYMFZBMWGGZ-UHFFFAOYSA-N	2,3-Dihydroxypropyl 5-Hydroxydecanoate	nan	8.00
RGZSQWQPBWRIAQ-CABCVRRESA-N	Levomenol	nan	8.00
NEDIAPMIWNCQJNW-UHFFFAOYSA-N	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-	CCCCC1CC=CC(=O)O1	7.00
WNZQDUSMALZDQF-UHFFFAOYSA-N	1(3H)-Isobenzofuranone	O=C1OCC2CCCCC21	7.00
NGSXTBFUMNXJDK-UHFFFAOYSA-N	2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-7-methyl-	CC1=CC2=CC(=O)CCC2CC1	7.00
MAUFTTLGOUBZNA-UHFFFAOYSA-N	2H-Pyran-2-one, 6-pentyl-	CCCCC1CCCC(=O)O1	7.00
XPTXKXKPKWKNYKB-UHFFFAOYSA-N	2H-Pyran-2-one, 6-heptyl-5,6-dihydro-	CCCCCCC1CC=CC(=O)O1	7.00
VMUXSMXIQBNGMZ-UHFFFAOYSA-N	Hydrocoumarin	c1ccc2c(c1)CCC(=O)O2	6.00
PSQMUBJRXIGVIT-UHFFFAOYSA-N	Pentyl Heptanoate	nan	6.00
OALYTRUKMRCXNH-UHFFFAOYSA-N	2(3H)-Furanone, dihydro-5-pentyl-	CCCC[C@H]1CCC(=O)O1	6.00
IPBFYZQJXZJBFQ-UHFFFAOYSA-N	2(3H)-Furanone, 5-butylidihydro-	CCCC1CCC(=O)O1	6.00
ZIJOACABGITYIL-	2-(Trans-2-Pentenvl)Cvclopentanone	nan	6.00

Entraînement et validation modèle

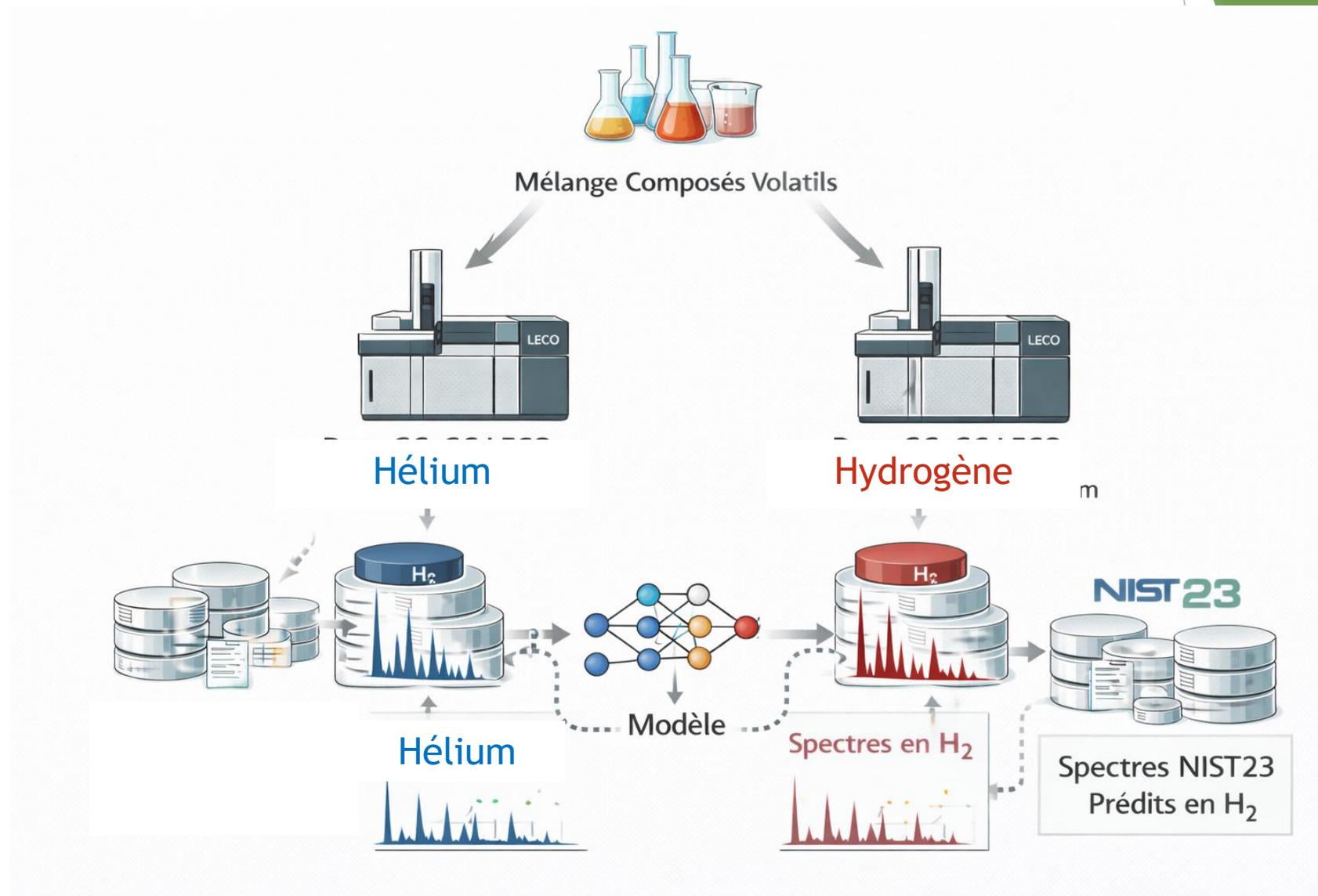
```
Anaconda Prompt - conda ac x + v
01. banana 0.8979
02. fermented 0.8696
03. fruit 0.8266
04. apple 0.7428
05. ether 0.6887
06. cognac 0.6170
07. brandy 0.5284
08. apricot 0.4714
09. green 0.4472
10. fatty 0.4185

CAS/SMILES/NAME (topk=10)> myrcene
Resolving NAME via CACTUS: myrcene
Resolved SMILES: CC(C)=CCCC(=C)C=C
[CACTUS] CAS: 123-35-3
2153-31-3
[CACTUS] IUPAC: 7-methyl-3-methylideneocta-1,6-diene
[CACTUS] Names (first 5): 7-methyl-3-methylideneocta-1,6-diene, 7-methyl-3-methylene-octa-1,6-diene, 7-Methyl-3-methylen
eocta-1,6-diene, 7-methyl-3-methylidene-octa-1,6-diene, 123-35-3

[DB] Compound NOT found in internal DB.

Top predictions:
01. plastic 0.8843
02. pepper 0.8706
03. balsamic 0.7004
04. spicy 0.6564
05. woody 0.5710
06. herbal 0.5440
07. citrus 0.5193
```

A venir....





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Acknowledgements

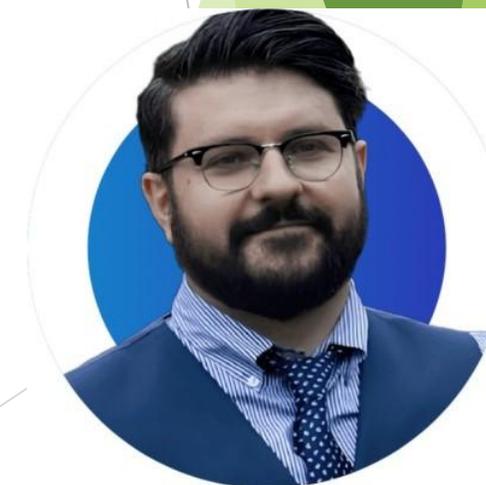
My sincere thanks to the entire **LECO** team for their valuable collaboration. I am particularly grateful to **Christine Loeb-Stubbins**, **Hubert Latappy**, and **Ryan Sutherill** for their hospitality, professionalism, and confidence in our work.

Thank you for your attention.



Hubert Latappy
Separation Science
Specialist

[Send email](#)



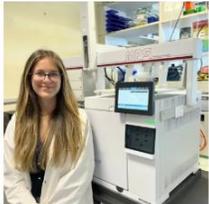
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Merci pour votre attention

