Steric Systems Inc. NGS and Bourbon Pairs

Analysis of Volatiles in Spirits
By Immersion-TF-SPME-GC-TOFMS

Study for:
Brewing & Distilling Analytical Services (BDAS, LLC)

Commissioned by:
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I. Introduction:

GC-MS analysis of spirits was conducted by immersion TF-SPME-GC-TOFMS. Samples were extracted by TF-SPME followed by GC-TOFMS (Leco BT) analysis. TOFMS with peak deconvolution capability was necessary for detection of some important flavor and off-flavor compounds because of coelution problems. The goal of this study is to identify potential flavor and off-flavor chemicals in samples.

II. Description of Samples (two neutral grain spirits and two whiskeys):

82 CTRL MGP Neutral Grain Spirit Control 40%ABV 2g SW 5uL IS TF-SPME
83 Sample 474436 MGP Neutral Grain Spirit Processed 40%ABV 2g SW 5uL TF-SPME
84 Control 3 yr straight bourbon Control 44%ABV 2gm SW 5uL IS TF-SPME
85 Sample 474404 3 yr straight bourbon processed 44%ABV 2g SW 5uL IS TF-SPME

III. Analytical Methods:

Immersion Thin Film SPME (TF-SPME) GC-TOFMS: Two gms of spirits, 8 mLs distilled water, and 5 uL 2-undecanone internal standard (0.0267 ug/uL) were added to a 10 mL glass GC vial along with a PTFE micro-stirbar and fitted with a PDMS/DVB (on Carbon Mesh) TF-SPME device and capped. The sample was stirred 1hr at 900 rpm. The TF SPME membrane was removed, rinsed with DI water, dried with a lintless cloth, and then thermally desorbed at 250°C with the GERSTEL TDU into a glass baffled glass inlet liner while volatiles were cryotrapped at a temperature of -100°C. Cryotrapped chemicals were then released from the liner and into the GC capillary column by rapid heating of the liner to 260°C. Volatiles were separated with a 30m x 0.25 mm x 0.25 µg DB-5MS capillary column. (See Addendum for schematic diagram of analytical set up.)

Thermal desorption parameters used for TF-SPME: The PTV Solvent Vent mode was used at a flow of 60mL/ min. The GERSTEL TDU initial temperature was 40°C with a 0.4min delay time; the TDU was ramped at 60°C/min to 250°C with a 4min hold time. TDU transfer line temperature was 300°C. The GERSTEL CIS (cooled injection system) was fitted with a baffled liner. Cryo liquid nitrogen cooling of the CIS injector was used with an initial temperature of -100°C and an equilibration time of 0.5min. The CIS was then ramped to 260°C at 12 °C/s with a hold time of 3min. Injections was made in splitless mode.

Instrumentation:
GERSTEL MPS 2 robotic sampler with TDU option
Leco BT GC-TOFMS
GERSTEL TF-SPME PDMS/DVB on Carbon Mesh

IV. Results:

Notes: R.T. (s) is the retention time in seconds; CAS is the Chemical Abstract Services Number for the chemical; and ppb is the concentration in ug/L. Concentrations results are semiquantitative because they are based on the response factor of an internal standard (2-undecanone) added to each sample rather than response factors from pure standard chemicals for each analyte. Nonetheless, excellent sample-to-sample comparisons can be made.

A. Neutral grain spirits:

Chemical	CAS	R.T. (min)	S82 (ppb)	S83 (ppb)
Furan, 3-methyl-	930-27-8	3.957	0.14	0.00
Ethyl Acetate	141-78-6	4.012	12.30	0.00
1-Propanol, 2-methyl-	78-83-1	4.226	0.04	0.00
Acrolein	107-02-8	4.613	0.02	0.00
Acetoin	513-86-0	4.731	0.00	0.00
Acetic acid	64-19-7	4.876	26.74	0.63
Acetol	116-09-6	5.310	0.15	0.33
Ethane, 1,1-diethoxy-	105-57-7	5.370	1.23	0.08
1-Butanol, 3-methyl-	123-51-3	5.578	7.68	0.54
1-Butanol, 2-methyl-, (S)-	1565-80-6	5.632	5.15	0.27
Isopropyl pyruvate	NA	6.043	0.00	0.03
Toluene	108-88-3	6.075	0.94	0.56
Paraldehyde	123-63-7	6.298	0.39	0.00
Methacrylic acid, ethyl ester	97-63-2	6.309	0.00	0.04
Acetone	67-64-1	6.382	0.04	0.00
1-Octene	111-66-0	6.410	0.26	0.00
Pentanoic acid	109-52-4	6.429	0.00	0.01
Octane	111-65-9	6.564	0.39	0.01
Hexanal	66-25-1	6.581	0.00	0.38
2-Octanol, (R)-	5978-70-1	6.652	0.06	0.00
Propyl pyruvate	NA	7.063	0.00	0.01
Furfural	98-01-1	7.144	0.08	0.11
Pyridine, 2-methyl-	109-06-8	7.182	0.00	0.00
Butanoic acid, 3-methyl-	503-74-2	7.208	0.10	0.00
Butanoic acid, 2-methyl-, ethyl ester	7452-79-1	7.372	0.01	0.00
Butanoic acid, 3-methyl-, ethyl ester	108-64-5	7.455	0.01	0.00
Octane, 4-methyl-	2216-34-4	7.622	0.02	0.03
Ethylbenzene	100-41-4	7.646	0.19	0.07
1-Hexanol	111-27-3	7.720	0.03	0.00
Benzene, 1,3-dimethyl-	108-38-3	7.804	0.19	0.17
1-Butanol, 3-methyl-, acetate	123-92-2	7.838	0.83	0.13

4-Cyclopentene-1,3-dione	930-60-9	7.974	0.00	0.00
2-Heptanone	110-43-0	8.071	0.06	0.07
1-Nonene	124-11-8	8.102	0.09	0.05
Styrene	100-42-5	8.173	0.21	0.16
Furfuryl ethyl ether	6270-56-0	8.217	0.05	0.01
Nonane	111-84-2	8.247	0.06	0.04
Heptanal	111-71-7	8.291	0.00	0.13
2(5H)-Furanone	497-23-4	8.574	0.04	0.04
Anisole	100-66-3	8.578	0.00	0.00
Butyrolactone	96-48-0	8.596	0.04	0.03
Benzene, (1-methylethyl)-	98-82-8	8.709	0.06	0.02
3-Hepten-1-ol, (E)-	2108-05-6	8.735	0.00	0.04
α-Phellandrene	99-83-2	8.745	0.02	0.00
1,2-Cyclopentanedione	3008-40-0	8.782	0.02	0.00
2-Octene, 4-ethyl-	53966-52-2	8.979	0.01	0.00
Camphene	79-92-5	9.206	0.01	0.00
Benzene, propyl-	103-65-1	9.215	0.00	0.03
2-Furancarboxaldehyde, 5-methyl-	620-02-0	9.308	0.00	0.01
Benzaldehyde	100-52-7	9.383	0.00	0.09
Vinyl methacrylate	4245-37-8	9.395	0.00	0.01
Pentanoic acid	109-52-4	9.420	0.00	0.01
1-Octen-3-one	4312-99-6	9.538	0.02	0.00
Phenol	108-95-2	9.565	0.08	0.00
1-Octen-3-ol	3391-86-4	9.571	0.00	0.01
5-Hepten-2-one, 6-methyl-	110-93-0	9.653	0.12	0.13
β-Phellandrene	555-10-2	9.663	0.00	0.04
β-Pinene	127-91-3	9.664	0.10	0.00
Pyridine, 2,4,6-trimethyl-	108-75-8	9.829	0.00	0.00
Hexanoic acid, ethyl ester	123-66-0	9.852	0.11	0.03
Mesitylene	108-67-8	9.888	0.05	0.05
Benzofuran	271-89-6	9.951	0.01	0.00
Octanal	124-13-0	9.971	0.14	0.22
Furyl ethyl ketone	3194-15-8	10.051	0.01	0.00
Benzene, 1,3-dichloro-	541-73-1	10.113	0.08	0.06
1-Hexanol, 2-ethyl-	104-76-7	10.346	0.26	0.14
o-Cymene	527-84-4	10.381	2.76	0.71
Limonene	138-86-3	10.463	5.00	2.35
Eucalyptol	470-82-6	10.538	0.03	0.02
alpha-Ocimene	502-99-8	10.651	0.01	0.01
Benzeneacetaldehyde	122-78-1	10.691	0.05	0.02
Decane, 3,3,8-trimethyl-	62338-16-3	10.854	0.01	0.00
2-Octenal, (E)-	2548-87-0	10.849	0.00	0.02
γ-Terpinene	99-85-4	10.899	0.29	0.18
Acetophenone	98-86-2	11.041	0.11	0.06
p-Cresol	106-44-5	11.074	0.01	0.01

p-Ethylstyrene	3454-07-7	11.312	0.38	0.31
3-Undecene, (Z)-	821-97-6	11.338	0.15	0.04
Heptanoic acid, ethyl ester	106-30-9	11.391	0.00	0.00
Undecane	1120-21-4	11.465	0.15	0.08
7-Octen-2-ol, 2-methyl-6-methylene-	543-39-5	11.475	0.00	0.01
Linalool	78-70-6	11.474	0.03	0.00
Nonanal	124-19-6	11.552	0.62	0.98
Benzofuran, 2-methyl-	4265-25-2	11.720	0.02	0.00
Phenylethyl Alcohol	60-12-8	11.759	0.47	0.10
p-Cymene	99-87-6	11.864	0.04	0.01
Succinimide	123-56-8	11.929	0.00	0.01
1,4-Divinylbenzene	105-06-6	11.992	0.07	0.00
3-Methylheptyl acetate	72218-58-7	12.129	0.00	0.07
Acetic acid, 2-ethylhexyl ester	103-09-3	12.130	0.10	0.00
Benzene, 1-methyl-2-(1-methyl-2-propenyl)-	97664-19-2	12.146	0.01	0.00
ε-Caprolactone	502-44-3	12.193	0.02	0.02
2-Nonenal, (Z)-	60784-31-8	12.385	0.00	0.04
Butanedioic acid, diethyl ester	123-25-1	12.569	0.02	0.01
Benzoic acid, ethyl ester	93-89-0	12.588	0.05	0.05
Levomenthol	2216-51-5	12.721	0.03	0.03
Octanoic acid, ethyl ester	106-32-1	12.847	0.75	0.17
Undecane	1120-21-4	12.931	0.04	0.00
Naphthalene	91-20-3	12.943	4.43	1.56
Methyl salicylate	119-36-8	12.953	0.12	0.04
α-Terpineol	98-55-5	12.983	0.22	0.03
Decanal	112-31-2	13.036	0.13	0.13
O-Methylthymol	1076-56-8	13.385	0.05	0.01
Benzeneacetic acid, ethyl ester	101-97-3	13.573	0.01	0.01
(-)-Carvone	6485-40-1	13.673	0.06	0.02
Acetic acid, 2-phenylethyl ester	103-45-7	13.747	0.53	0.10
Nonanoic acid	112-05-0	13.823	0.08	0.03
2-Decenal, (Z)-	2497-25-8	13.832	0.00	0.04
p-Ethylacetophenone	937-30-4	13.897	0.01	0.01
1-Decanol	112-30-1	13.950	0.06	0.02
Ethyl salicylate	118-61-6	14.006	0.44	0.16
p-Cymen-7-ol	536-60-7	14.353	0.14	0.02
Undecanal	112-44-7	14.445	0.01	0.02
Naphthalene, 1-methyl-	90-12-0	14.493	0.56	0.16
2-Methoxy-4-vinylphenol	7786-61-0	14.551	0.00	0.00
Decanoic acid, methyl ester	110-42-9	14.604	0.01	0.00
Whiskey lactone	39212-23-2	14.680	0.00	0.04
trans-β-Ionone	79-77-6	15.021	0.05	0.07
Ionone	8013-90-9	15.176	0.00	0.06
n-Decanoic acid	334-48-5	15.177	2.00	0.09
1-Nonanol	143-08-8	15.261	0.00	0.01

Decanoic acid, ethyl ester	110-38-3	15.522	2.06	0.59
Tetradecane	629-59-4	15.613	0.02	0.02
Dodecanal	112-54-9	15.754	0.05	0.05
Naphthalene, 1-ethyl-	1127-76-0	15.764	0.02	0.01
Naphthalene, 1,7-dimethyl-	575-37-1	15.920	0.04	0.01
α-Ionone	127-41-3	16.001	0.84	0.73
Naphthalene, 1,8-dimethyl-	569-41-5	16.144	0.03	0.01
Octanoic acid, 3-methylbutyl ester	2035-99-6	16.177	0.00	0.01
5,9-Undecadien-2-one, 6,10-dimethyl-	3796-70-1	16.228	0.06	0.06
Dimethyl phthalate	131-11-3	16.281	0.11	0.13
Naphthalene, 1,3-dimethyl-	575-41-7	16.348	0.01	0.01
Cyclamal	103-95-7	16.485	0.09	0.12
1-Dodecanol	112-53-8	16.534	0.43	0.16
Ethyl (Z)-cinnamate	4610-69-9	16.543	0.01	0.01
α Isomethyl ionone	127-51-5	16.636	0.00	0.00
trans-β-Ionone	79-77-6	16.699	0.06	0.04
Cetene	629-73-2	16.751	0.03	0.02
2-Tridecanone	593-08-8	16.792	0.02	0.01
1-Dodecene	112-41-4	16.889	0.01	0.00
2,4-Di-tert-butylphenol	96-76-4	16.935	0.25	0.30
Tridecanal	10486-19-8	16.999	0.01	0.01
Dodecanoic acid, methyl ester	111-82-0	17.105	0.01	0.00
Naphthalene, 2-(1-methylethyl)-	2027-17-0	17.119	0.01	0.01
Calamenene	483-77-2	17.272	0.01	0.01
Dibenzofuran	132-64-9	17.320	0.02	0.00
Naphthalene, 1,6,7-trimethyl-	2245-38-7	17.435	0.01	0.00
Dodecanoic acid	143-07-7	17.669	8.20	1.55
1-Dodecanol	112-53-8	17.735	0.01	0.02
Dodecanoic acid, ethyl ester	106-33-2	17.918	0.50	0.15
Diethyl Phthalate	84-66-2	17.925	0.16	0.07
Tetradecanal	124-25-4	18.183	0.01	0.02
Benzophenone	119-61-9	18.538	0.10	0.05
Hexanoic acid, 2-phenylethyl ester	6290-37-5	18.556	0.03	0.00
Undecanoic acid	112-37-8	18.631	0.03	0.02
1-Tetradecene	1120-36-1	18.877	0.45	0.07
n-Hexyl salicylate	6259-76-3	18.988	0.01	0.00
2,3-Dihydrofarnesol	51411-24-6	19.003	0.15	0.02
β-Bisabolene	495-61-4	19.092	0.05	0.00
Benzoic acid, 2-ethylhexyl ester	5444-75-7	19.289	0.17	0.09
trans-Farnesol	106-28-5	19.323	0.22	0.05
Myristoleic acid	544-64-9	19.518	0.01	0.00
Tetradecanoic acid	544-63-8	19.736	0.47	0.25
Dodecanamide	1120-16-7	19.792	0.15	0.09
Benzyl Benzoate	120-51-4	20.003	0.00	0.02
Tetradecanoic acid, ethyl ester	124-06-1	20.082	0.09	0.04

Bis(2-ethylhexyl) phthalate	117-81-7	20.214	1.03	0.00
2-Ethylhexyl salicylate	118-60-5	20.303	0.000	0.003
Isopropyl myristate	110-27-0	20.391	0.01	0.00
Octanoic acid, 2-phenylethyl ester	5457-70-5	20.717	0.40	0.00
Pentadecanoic acid	1002-84-2	20.731	0.07	0.03
Diisobutyl phthalate	84-69-5	20.821	0.12	0.06
1-Hexadecanol	36653-82-4	20.993	0.09	0.05
γ-Tetradecalactone	2721-23-5	21.153	0.03	0.02
Homosalate	118-56-9	21.198	0.01	0.01
Hexadecanoic acid, methyl ester	112-39-0	21.409	0.01	0.01
n-Hexadecanoic acid	57-10-3	21.730	0.19	0.19
Dibutyl phthalate	84-74-2	21.753	0.65	0.84
Hexadecanoic acid, ethyl ester	628-97-7	22.055	0.11	0.18
γ-Dodecalactone	2305-05-7	22.172	0.02	0.01
Isopropyl palmitate	142-91-6	22.328	0.06	0.05
Oxybenzone	131-57-7	22.599	0.01	0.00
Didecan-2-yl phthalate	28029-89-2	23.088	15.16	0.00
δ-Tetradecalactone	2721-22-4	23.455	0.06	0.05
Tributyl acetylcitrate	77-90-7	24.484	0.03	0.03
Benzyl butyl phthalate	85-68-7	25.866	0.03	0.02
9-Octadecenamide, (Z)-	301-02-0	25.995	0.15	0.21
Triethylene glycol di(2-ethylhexoate)	94-28-0	27.553	0.88	0.61
2-Undecanone (IS)	112-12-9	14.290	66.75	66.75

B. Whiskeys:

Chemical	CAS	R.T. (min)	S84 (ppb)	S85 (ppb)
Ethyl Acetate	141-78-6	4.016	292.86	93.15
1-Propanol, 2-methyl-	78-83-1	4.259	0.00	15.36
Pentanal	110-62-3	4.522	0.00	2.87
Acetic acid	64-19-7	4.679	1.55	9.61
Acetoin	513-86-0	5.018	0.00	3.54
Acetol	116-09-6	5.180	0.44	0.00
Propanoic acid, ethyl ester	105-37-3	5.189	0.00	2.53
n-Propyl acetate	109-60-4	5.229	0.00	0.17
Ethane, 1,1-diethoxy-	105-57-7	5.416	29.44	3.86
Vinyl acetate	108-05-4	5.507	0.00	1.43
1-Pentene	109-67-1	5.513	0.00	0.86
1-Butanol, 3-methyl-	123-51-3	5.822	186.49	212.85
1-Butanol, 2-methyl-	137-32-6	5.889	26.96	33.54
2,5-Furandione, dihydro-3-methyl-	4100-80-5	5.892	0.00	130.97
Propanoic acid, 2-methyl-, ethyl ester	97-62-1	6.053	0.73	4.35

Acetic acid, butyl ester	123-86-4	6.089	0.70	0.00
Isobutyl acetate	110-19-0	6.155	18.44	9.26
1-Butanol, 3-methyl-, formate	110-45-2	6.433	0.55	0.00
Butanoic acid, ethyl ester	105-54-4	6.589	11.20	13.86
Hexanal	66-25-1	6.622	0.00	4.87
Propanoic acid, 2-hydroxy-, ethyl ester, (L)-	687-47-8	6.853	1.23	0.00
Hexanoic acid, 3-methyl-2-butenyl ester	76649-22-4	6.940	0.89	1.17
Furfural	98-01-1	7.186	0.00	19.09
1-Pentanol, 4-methyl-	626-89-1	7.282	0.00	0.81
2-Butenoic acid, ethyl ester, (E)-	623-70-1	7.348	0.00	0.20
Butanoic acid, 2-methyl-, ethyl ester	7452-79-1	7.401	2.01	3.09
1-Pentanol, 3-methyl-	589-35-5	7.436	0.00	1.30
Butanoic acid, 3-methyl-, ethyl ester	108-64-5	7.474	4.79	4.79
Butane, 1,1-diethoxy-	3658-95-5	7.524	0.00	0.41
Ethylbenzene	100-41-4	7.656	0.58	0.51
1-Butanol, 3-methyl-, acetate	123-92-2	7.896	84.93	93.37
4-Cyclopentene-1,3-dione	930-60-9	8.032	0.00	0.01
2-Heptanone	110-43-0	8.097	1.80	2.62
2-n-Butyl furan	4466-24-4	8.131	0.07	0.21
Butanoic acid, 3-methyl-, 2-phenylethyl ester	140-26-1	8.200	0.25	0.00
o-Xylene	95-47-6	8.212	3.34	3.04
Furfuryl ethyl ether	6270-56-0	8.238	2.81	3.75
Pentanoic acid, ethyl ester	539-82-2	8.253	1.86	2.17
Heptanal	111-71-7	8.310	1.76	2.35
2-Acetylfuran	1192-62-7	8.463	0.19	0.30
Anisole	100-66-3	8.590	0.02	0.03
2(5H)-Furanone	497-23-4	8.612	0.00	0.04
3-Hexanone, 2,5-dimethyl-	1888-57-9	8.659	1.12	0.51
Cumene	98-82-8	8.724	0.00	0.08
Pentanoic acid, 2-methyl-, ethyl ester	39255-32-8	8.870	0.02	0.00
Ethyl tiglate	5837-78-5	8.896	0.69	0.87
α-Pinene, (-)-	7785-26-4	8.908	0.03	0.02
Butane, 1,1-diethoxy-3-methyl-	3842-03-3	9.081	2.47	0.31
Butanoic acid, 2-methylpropyl ester	539-90-2	9.172	0.07	0.06
2-Heptenal, (E)-	18829-55-5	9.244	0.17	0.27
2-Furancarboxaldehyde, 5-methyl-	620-02-0	9.324	1.55	2.77
Pentanoic acid, 4-methyl-, ethyl ester	25415-67-2	9.327	0.32	0.00
Benzaldehyde	100-52-7	9.400	2.66	4.03
Acetaldehyde ethyl isoamyl acetal	NA	9.406	9.55	0.00
Benzene, 1,2,3-trimethyl-	526-73-8	9.478	2.15	2.15
3-Furancarboxylic acid, methyl ester	13129-23-2	9.512	0.07	0.00
2-Acetyl-5-methylfuran	1193-79-9	9.530	0.01	0.08
1-Octen-3-one	4312-99-6	9.556	0.21	0.36
1-Octen-3-ol	3391-86-4	9.612	1.49	2.64
5-Hepten-2-one, 6-methyl-	110-93-0	9.675	0.78	1.01

2-Octanone	111-13-7	9.768	0.00	1.72
Furan, 2-pentyl-	3777-69-3	9.774	1.67	3.80
Pentane, 1,1-diethoxy-	3658-79-5	9.785	0.29	0.00
Furan, 2-ethyl-5-methyl-	1703-52-2	9.850	0.26	0.00
Ethyl 3-furoate	614-98-2	9.859	0.12	0.34
Hexanoic acid, ethyl ester	123-66-0	9.885	15.42	32.50
2-Octanol, (R)-	5978-70-1	9.945	1.01	1.34
Benzofuran	271-89-6	9.965	0.10	0.13
Octanal	124-13-0	10.000	0.42	0.50
2-Thiophenecarboxaldehyde	98-03-3	10.057	0.08	0.11
Acetic acid, hexyl ester	142-92-7	10.077	1.32	1.37
Butanoic acid, 3-methylbutyl ester	106-27-4	10.097	0.31	0.36
Propanoic acid, 2-methyl-, 2-methylbutyl ester	2445-69-4	10.149	0.12	0.00
Benzeneacetaldehyde, α-methyl-	93-53-8	10.157	0.14	0.00
2-Acetyl-5-methylfuran	1193-79-9	10.167	0.01	0.00
α-Phellandrene	99-83-2	10.236	0.01	0.02
3-Ethyl-4-methylpentan-1-ol	38514-13-5	10.268	0.00	0.42
o-Cymene	527-84-4	10.300	0.35	0.32
1-Hexanol, 2-ethyl-	104-76-7	10.366	0.00	0.88
Limonene	138-86-3	10.468	0.81	0.49
3-Octen-2-one	1669-44-9	10.525	0.40	0.58
Furan, 2-pentyl-	3777-69-3	10.609	0.07	0.15
Benzeneacetaldehyde	122-78-1	10.699	0.21	0.57
2-Furancarboxylic acid, ethyl ester	614-99-3	10.729	2.49	3.90
1,3-Benzodioxole	274-09-9	10.737	0.09	0.17
Benzene, 1-methyl-3-propyl-	1074-43-7	10.789	1.24	1.16
Pentanoic acid, 2-hydroxy-4-methyl-, ethyl ester	10348-47-7	10.808	0.82	1.48
2-Octenal, (E)-	2548-87-0	10.863	1.17	1.43
Diethyl malonate	105-53-3	10.910	0.00	0.57
Propanoic acid, 2-hydroxy-, ethyl ester	97-64-3	10.998	0.16	0.00
Propane, 1,1,3-triethoxy-	7789-92-6	11.004	0.00	0.76
1-Octanol	111-87-5	11.018	2.85	3.95
Acetophenone	98-86-2	11.051	0.34	0.49
Hydroxymethyl 2-hydroxy-2-methylpropionate	NA	11.061	0.02	0.03
Heptanoic acid	111-14-8	11.090	0.10	0.00
Benzaldehyde, 3-methyl-	620-23-5	11.118	0.18	0.17
Benzene, 2-ethyl-1,4-dimethyl-	1758-88-9	11.177	1.19	1.14
Benzene, 1-ethyl-2,4-dimethyl-	874-41-9	11.225	1.18	0.00
Hexane, 1,1-diethoxy-	3658-93-3	11.262	1.76	0.13
p-Cymene	99-87-6	11.321	1.98	1.92
2-Cyclopenten-1-one, 3,4,5-trimethyl-	55683-21-1	11.330	0.36	0.00
1H-Pyrrole-2-carboxaldehyde	1003-29-8	11.345	0.03	0.00
Heptanoic acid, ethyl ester	106-30-9	11.402	4.63	4.64
2,4-Hexadienoic acid, ethyl ester, (2E,4E)-	2396-84-1	11.449	0.06	0.08
Benzene, 4-ethenyl-1,2-dimethyl-	27831-13-6	11.476	0.22	0.34

Nonanal	124-19-6	11.563	1.90	1.91
1-Penten-3-one, 4-methyl-	1606-47-9	11.598	0.06	1.91
Acetic acid, heptyl ester	112-06-1	11.604	0.22	0.22
Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	11.631	0.36	0.35
trans-Rose oxide	876-18-6	11.677	0.02	0.00
Levoglucosenone	37112-31-5	11.716	0.04	0.00
Benzofuran, 2-methyl-	4265-25-2	11.727	0.08	0.09
Phenylethyl Alcohol	60-12-8	11.822	36.58	60.78
2(3H)-Furanone, dihydro-5-methyl-	108-29-2	11.911	0.02	0.00
α-Campholenal	4501-58-0	11.990	0.04	0.00
Benzene, 1,3-diethenyl-	108-57-6	12.001	0.12	0.14
3-Nonen-2-one	14309-57-0	12.054	0.18	0.26
2-Heptenoic acid, ethyl ester, (E)-	54340-72-6	12.155	0.17	0.19
trans-2-Nonenal	18829-56-6	12.401	2.37	2.56
trans-2-Pinanol	4948-29-2	12.453	0.86	0.78
1-Nonanol	143-08-8	12.586	5.61	8.26
Benzoic acid, ethyl ester	93-89-0	12.602	6.13	6.79
Butanedioic acid, diethyl ester	123-25-1	12.631	13.77	22.15
Heptane, 1,1-diethoxy-	688-82-4	12.698	0.31	0.00
Octanoic acid	124-07-2	12.719	6.72	7.59
Octanoic acid, ethyl ester	106-32-1	12.898	12.38	80.72
Methyl salicylate	119-36-8	12.980	0.52	0.55
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-	619-01-2	13.072	0.83	0.92
3-Nonenoic acid, ethyl ester	91213-30-8	13.157	1.58	1.73
2,4-Nonadienal, (E,E)-	5910-87-2	13.232	0.36	0.00
Citronellol	106-22-9	13.331	0.89	1.17
Isophthalaldehyde	626-19-7	13.346	0.03	0.00
β-Cyclocitral	432-25-7	13.371	0.14	0.15
Isothymol methyl ether	31574-44-4	13.399	0.26	0.25
2-Octenoic acid, ethyl ester	2351-90-8	13.583	0.68	0.70
Benzeneacetic acid, ethyl ester	101-97-3	13.594	10.88	12.56
Geraniol	106-24-1	13.683	0.49	0.52
Acetic acid, 2-phenylethyl ester	103-45-7	13.796	30.10	46.14
Butanedioic acid, hydroxy-, diethyl ester	7554-12-3	13.834	0.08	0.16
1-Decanol	112-30-1	13.978	3.49	3.91
Pentanedioic acid, diethyl ester	818-38-2	14.006	0.77	0.80
Ethyl salicylate	118-61-6	14.021	0.24	0.30
Geranyl vinyl ether	NA	14.067	0.99	1.04
Nonanoic acid, ethyl ester	123-29-5	14.271	6.23	0.00
t-Whiskylactone	39638-67-0	14.352	13.01	16.48
Undecanal	112-44-7	14.454	0.06	0.07
Naphthalene, 1-methyl-	90-12-0	14.506	0.49	0.37
2-Furancarboxylic acid, 2-methylbutyl ester	NA	14.518	0.05	0.04
Benzoic acid, 3,4-dimethyl-, methyl ester	38404-42-1	14.572	0.12	0.13
2-Methoxy-4-vinylphenol	7786-61-0	14.589	0.57	0.00

Decanoic acid, methyl ester	110-42-9	14.622	0.09	0.11
2,4-Decadienal	2363-88-4	14.639	0.62	0.67
Naphthalene, 2-methyl-	91-57-6	14.727	0.22	0.18
cis-Whiskey lactone	55013-32-6	14.802	54.52	72.31
2-Nonenoic acid, ethyl ester	17463-01-3	14.928	0.60	0.53
Syringol	91-10-1	15.022	0.22	0.50
Benzenepropanoic acid, ethyl ester	2021-28-5	15.039	3.91	4.24
Eugenol	97-53-0	15.128	3.08	4.00
trans-β-Ionone	79-77-6	15.197	0.03	0.03
γ-Nonalactone	104-61-0	15.220	2.30	2.99
p-Propylguaiacol	2785-87-7	15.251	0.41	0.52
Ethyl trans-4-decenoate	76649-16-6	15.361	0.47	0.45
Damascenone	23726-93-4	15.486	9.36	9.45
n-Decanoic acid	334-48-5	15.572	4.89	51.98
Decanoic acid, ethyl ester	110-38-3	15.625	93.58	83.78
Nonanoic acid, 2-phenylethyl ester	57943-67-6	15.643	0.00	0.09
Vanillin	121-33-5	15.785	3.14	6.11
Guaiacol acetate	613-70-7	15.917	0.05	0.00
Butanedioic acid, ethyl 3-methylbutyl ester	28024-16-0	15.953	1.47	2.12
α-Ionone	127-41-3	16.040	2.14	2.24
Dihydro-β-ionone	17283-81-7	16.173	0.92	0.82
Octanoic acid, 3-methylbutyl ester	2035-99-6	16.200	0.00	1.43
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	3879-26-3	16.253	6.22	6.17
5,9-Undecadien-2-ol, 6,10-dimethyl-	53837-34-6	16.302	2.36	2.95
Vanillyl ethyl ether	13184-86-6	16.419	0.20	0.30
Ethyl cinnamate	103-36-6	16.560	0.30	0.00
Diethyl pimelate	2050-20-6	16.616	0.11	0.14
trans-β-Ionone	79-77-6	16.716	0.74	0.76
Undecanoic acid, ethyl ester	627-90-7	16.757	0.26	0.21
2-Tridecanone	593-08-8	16.804	0.77	0.71
10,11-Epoxycalamenene	143785-42-6	16.875	0.06	0.06
Nonanoic acid, 9-oxo-, ethyl ester	3433-16-7	16.908	1.52	1.82
2,4-Di-tert-butylphenol	96-76-4	16.962	1.22	1.12
Butylated Hydroxytoluene	128-37-0	16.967	1.35	1.01
Undecanal	112-44-7	17.009	0.08	0.00
Heptane, 1,1-diethoxy-	688-82-4	17.052	0.05	0.00
Dodecanoic acid, methyl ester	111-82-0	17.112	0.03	0.03
5-tert-Butylpyrogallol	20481-17-8	17.120	0.10	0.13
Dibenzofuran	132-64-9	17.332	0.04	0.04
n-Capric acid isobutyl ester	30673-38-2	17.365	0.15	0.12
3,5-Di-tert-butyl-2-hydroxybenzaldehyde	37942-07-7	17.539	0.02	0.00
4-Vinylsyringol	28343-22-8	17.617	0.00	0.83
Nerolidol	7212-44-4	17.625	5.85	0.00
Dodecanoic acid	143-07-7	17.769	17.69	13.75
Diethyl suberate	2050-23-9	17.822	0.79	0.69

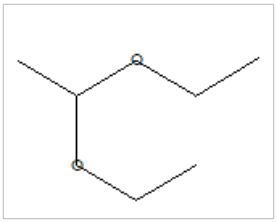
Naphthalene, 1,6,7-trimethyl-	2245-38-7	17.856	0.06	0.06
Butyrovanillone	64142-23-0	17.918	4.24	0.00
Ethyl vanillate	617-05-0	17.921	0.00	5.99
Diethyl Phthalate	84-66-2	17.946	0.00	0.17
Dodecanoic acid, ethyl ester	106-33-2	17.966	35.13	28.45
Methoxyeugenol	6627-88-9	18.044	0.17	0.21
Benzaldehyde, 3,4,5-trimethoxy-	86-81-7	18.056	0.11	0.14
Undecanoic acid, ethyl ester	627-90-7	18.092	0.13	0.12
Homosyringaldehyde	87345-52-6	18.115	0.22	0.25
Isoeugenol acetate (E)	5912-87-8	18.145	0.03	0.03
Nerolidol	142-50-7	18.271	0.08	0.06
Juniperol	465-24-7	18.367	0.24	0.24
Rosifoliol	63891-61-2	18.438	0.05	0.00
Megastigmatrienone	38818-55-2	18.445	0.00	0.07
Ethyl homovanillate	60563-13-5	18.480	0.49	0.75
Pentadecanoic acid, 3-methylbutyl ester	2306-91-4	18.515	0.89	0.70
Hexanoic acid, 2-phenylethyl ester	6290-37-5	18.569	3.73	3.80
γ-Eudesmole	1209-71-8	18.599	0.20	0.19
Syringaldehyde	134-96-3	18.720	2.34	0.00
1-Tetradecene	1120-36-1	18.890	0.76	0.75
Diethyl azelate	624-17-9	18.937	2.75	3.12
2,3-Dihydrofarnesol	51411-24-6	19.021	0.44	0.46
2-n-Octylfuran	4179-38-8	19.060	0.78	1.14
α-Bisabolol	515-69-5	19.115	0.77	0.41
Ethylhexyl benzoate	5444-75-7	19.295	0.09	0.00
trans-Farnesol	106-28-5	19.337	1.09	1.12
Acetosyringone	2478-38-8	19.484	0.09	0.18
Coniferaldehyde	458-36-6	19.582	0.41	0.91
Tetradecanoic acid	544-63-8	19.819	3.74	2.88
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	19.855	0.13	0.14
m-Eugenol	501-19-9	19.898	0.00	0.05
Decanedioic acid, diethyl ester	110-40-7	19.993	0.22	0.26
Tetradecanoic acid, ethyl ester	124-06-1	20.095	4.23	3.63
Hexadecanal	629-80-1	20.380	0.06	0.01
Acetyl syringic acid, ethyl ester	NA	20.520	0.95	1.37
Octanoic acid, 2-phenylethyl ester	5457-70-5	20.726	1.77	1.56
Pentadecanoic acid	1002-84-2	20.767	0.20	0.17
Hexyl vanillate	84375-71-3	20.784	0.05	0.00
1-Hexadecanol	36653-82-4	21.001	0.43	0.00
Benzyl salicylate	118-58-1	21.079	0.17	0.21
Pentadecanoic acid, ethyl ester	41114-00-5	21.095	0.12	0.13
2-Hexadecanone	18787-63-8	21.201	0.05	0.05
Ethyl (E)-ferulate	28028-62-8	21.415	0.21	0.27
δ-Undecalactone	710-04-3	21.467	0.02	0.03
Diethyl azelate	624-17-9	21.502	0.00	0.01

Dibutyl phthalate	84-74-2	21.757	0.73	1.21
Sinapinaldehyde	87345-53-7	22.006	0.22	0.11
γ-Dodecalactone	2305-05-7	22.183	0.02	0.03
Isopropyl palmitate	142-91-6	22.333	0.06	0.13
Butylsyringone	69271-91-6	22.409	0.06	0.07
Oxybenzone	131-57-7	22.606	0.01	0.01
Dodecanoic acid, 2-phenylethyl ester	6309-54-2	22.706	0.99	0.88
Oleic Acid	112-80-1	23.403	0.17	0.11
Linoleic acid ethyl ester	544-35-4	23.636	0.24	0.27
Hexadecanamide	629-54-9	23.829	0.14	0.19
Tributyl acetylcitrate	77-90-7	24.492	0.57	0.65
Parsol MCX	5466-77-3	25.480	0.07	0.07
Ethyl linolenate	1191-41-9	25.899	0.28	0.37
2-Undecanone (IS)	112-12-9	14.310	66.75	66.75

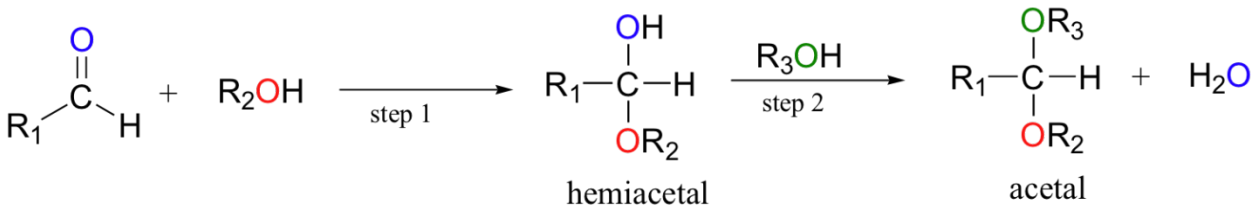
V. Appendix:

A. Acetal formation:

Acetal (shown below) can form from the reaction of the acetaldehyde with ethanol (in the case of 1,1-diethoxy ethane) or from acetaldehyde with other alcohols. These chemicals, especially 1,1-diethoxy ethane (aka acetal), can contribute off-flavors.



1,1-diethoxy ethane (acetal)



Acetals are formed by the stepwise addition of two alcohol molecules to an aldehyde in an acid-catalyzed reaction. An example of an acetal with potential off- flavor contribution is 1,1-diethoxyethane (simply called acetal). Acetal forms from the reaction of acetaldehyde (R1 = H) and ethanol (R2 = CH_3-CH_2-) to form 1,1-diethoxy ethane (acetal).

B. Schematic diagram of TF-SPME-GC-TOFMS with Gerstel TDU/CIS.