Analytical Results

W01061/21	W01062/21	W01063/21	W01064/21
UMHLANGA LAGOON CONTAMINATION: UMHL MOUTH A, B & C 16.07.2021	UMHLANGA LAGOON CONTAMINATION: UML TRIB 18.07.2021	UMHLANGA LAGOON CONTAMINATION: FISH 1	UMHLANGA LAGOON CONTAMINATION: FISH 2
Organics			

W01065/21	W01066/21	W01067/21
UMHLANGA LAGOON CONTAMINATION: CRAYFISH 1	UMHLANGA LAGOON CONTAMINATION: CRAYFISH 2	UMHLANGA LAGOON CONTAMINATION: UMHL MOUTH SEDIMENT A, B & C 16.07.2021
Organics		

ORGANIC FINGER PRINTING (GC-MS SCAN) *

The sample was analysed using a GC-MS coupled to an RTC PAL sampler System. The samples were analysed together with laboratory blanks for comparison purposes. The samples were analysed using a Solid Phase Micro Extraction technique, Liquid-Liquid Extraction and purge and trap.

GC-MS is a sensitive, reliable, and recommended technique for identifying unknown organic compounds. Samples are scanned down to levels of 0.1 ppb (µg/ℓ) against the National Institute of Standards and Technology (NIST) spectral library of reference compounds, including pesticides, volatile organic compounds, petroleum hydrocarbons and micropollutants. Only compounds with percentage match returns of greater than 80% are reported.

Table 1: Analytes detected with a Match Factor >80% for sample W01061/21.

Compound Name	Retention time (m)	Match Factor (%)
Azetidine, 1-nitroso	3.9888	83.8
Chlorobenzene	5.5395	90.9
Pyrolo[3,2-d] pyrimidin-2,4(1H,3H)- dione	5.9819	85
Ethanol, 2-butoxy	6.117	95.8
Benzene, (1-methylethyl)	6.3608	88
Pentane	6.6348	84.6
Benzeneacetaldehyde	6.6768	90
Benzene, 1-ethyl-2-methyl	6.7655	96.4
10-Ethyl-10H-acridin-9-one	6.8684	80.5
Benzene, 1-ethyl-4-methyl	6.9782	93.2
2-Octanol, (S)	7.1156	92.1
Acetic acid, hexyl ester	7.2561	93
Benzene, (1-methylpropyl)	7.3439	85.6
Benzeneethanamine, N-(2-phenylethyl)	7.344	84.2
Eucalyptol	7.6298	96.5
Indane	7.7135	98.2
Benzene, 1,2-diethyl	7.8562	88.9
Benzene, 1-methyl-4-propyl	7.857	88.2
Benzeneacetaldehyde, alpha -methyl	8.1107	93.8
Benzene, 1-ethyl-2,4-dimethyl	8.2535	97
1-Octanol	8.3498	91.1

Cyclopropane, pentyl	8.3541	86.5
4'-Methylpropiophenone	8.6768	80.9
Benzene, 1,2,4,5-tetramethyl	8.9155	97
Cyclobutanecarboxylic acid, 3-methylbutyl ester	9.3752	81.4
1H-Indene, 2,3-dihydro-4-methyl	9.3974	90
Camphor	9.5595	95.1
7-Methoxymethyl-2,7-dimethylcyclohepta-1,3,5-triene	9.6502	82.4
Pentafluoropropionic acid, pentyl ester	9.8876	80.4
Phenol, 2,4-dichloro	9.9523	95.4
Naphthalene	10.4634	97.8
Undecane, 3,7-dimethyl	12.6865	86.5
Naphthalene, 2-methyl	12.8105	90.8
1H-Indene-1-methanol, alpha-methyl-, acetate	13.0893	85.3
Eptam	13.691	98.6
2H-2,4a-Methanonaphthalene, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S)-	14.192	84.4
2,4,7,9-Tetramethyl-5-decyn-4,7-diol	14.2826	85.1
Carbonic acid, decyl vinyl ester	14.5631	84
Decyl isobutyl ether	14.5631	84.4
Tebuthiuron	15.3805	85
Heptasiloxane, hexadecamethyl	15.7373	90.4
Decane, 1-iodo	15.962	81.5
Cyclopentane, 1,1,3,3-tetramethyl	16.527	81.3
2-Decene, 7-methyl-, (Z)	16.5274	80.2
Trifluralin	16.61	98.5
1-Propanol, 2-(2-hydroxypropoxy)	16.8423	86.9
Dimethazone	17.171	84.7
Terbuthylazine	17.2734	80.2
Phosphorodithioic acid, S-[(tert-butylthio) methyl] O,Odiethyl ester	17.3041	95.3
Undecane, 4,6-dimethyl	17.3526	80.4
2-Ethylhexyl salicylate	17.4366	80.1
1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester	17.7611	83.9
Tonalid	17.8276	85.1
Acetamide, 2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6- methylphenyl)	17.9491	98.1
Spiroxamine	18.2289	86.6
Benthiocarb	18.3915	89.3
Metolachlor	18.466	91.5
Chlorpyrifos	18.4893	92.8
Pendimethalin	18.8366	95.9
Nonadecane	19.3852	87.7
Undecane, 3,8-dimethyl	19.3853	88.3
Triclopyr 2 butoxy ethyl ester	19.6584	85.9
Sulfurous acid, 2-ethylhexyl isohexyl ester	19.965	90.3
Propane, 1,1'- [ethylidenebis (oxy)] bis	21.8646	81

Figure 1 Chromatogram for sample W01061/21

Figure 2 Chromatogram for sample W01061/21

Table 2: Analytes detected with a Match Factor >80% for sample W01062/21.

Compound Name	Retention time (m)	Match Factor (%)
1,3-Dioxol-2-one	3.9562	81.6
6-Fluoro-2-trifluoromethylbenzoic acid, 2-formyl-4,6- dichlorophenyl ester	5.2476	82.2
Benzene, chloro	5.5498	94.2
p-Xylene	5.7836	97.1
7-Oxabicyclo [4.2.1] nona-2,4-dien-8-one, 9-methyl	6.0337	84.3
Ethanol, 2-butoxy	6.1175	95.4
Benzene, (1-methylethyl)	6.3653	94.9
Butane, 1-(2-chloroethoxy)	6.3966	92
Benzene, propyl	6.6766	95
Benzene, 1-ethyl-2-methyl	6.7712	98.4
1-Propanol, 2-methyl	7.299	94.8
Toluene	7.307	88
Benzene, 1-methyl-3-propyl	7.3465	90.3
Benzeneacetaldehyde, alpha -methyl	7.3476	90.3
Fumaronitrile	7.4087	91.6
Ethene, chloro	7.456	91.3
Indane	7.7176	98
o-Cymene	7.9592	94.7
Benzene, 1,4-diethyl	8.0326	92.7
Benzene, 1-methyl-4-propyl	8.1112	97.3
Benzene, 4-ethyl-1,2-dimethyl	8.2789	97.5
Benzene, 1-ethyl-2,4-dimethyl	8.3887	98.3
Benzene, tert-butyl	8.5105	81
2-Pyrrolidinecarboxylic acid, 1,2-dimethyl-5-oxo-, methyl ester	8.5491	85.5
Benzene, 1-methyl-4-(1-methylpropyl)	8.6711	86.3
Carbonodithioic acid, S,S-diethyl ester	8.8284	80.3
Benzene, pentamethyl	8.8495	81.7
Benzene, 1,2,4,5-tetramethyl	8.9288	98.1
Disulfide, dimethyl	9.1031	94.9
Benzene, 1-methyl-2-(2-propenyl)	9.4053	96
Benzene, (1-methylbutyl)	9.5742	88.8
1,2-Dibutoxyethane	9.6601	86
Benzene, 1,2,3,5-tetramethyl	9.6673	88
4'-Methylpropiophenone	9.7593	83.7
Carbonic acid, octyl vinyl ester	9.9008	89.4
2,4,6-Trimethyl-1-nonene	9.9055	92.4
Benzene, 1-ethyl-4-(1-methylethyl)	9.942	89
Benzene, 1,4-diethyl-2-methyl	9.9422	90.7
Phenol, 2,4-dichloro	10.1031	94.6
Naphthalene	10.4792	98
Benzene, 1-ethyl-2,4,5-trimethyl	10.723	96.7
Ethylbenzene	10.8287	95.6
1-Heptanol, 2-propyl	10.863	97.8
trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]	11.2759	91
o-Xylene	11.3259	97.6

Benzene, 2,4-dimethyl-1-(1-methylpropyl)	11.3523	89.9
Cyclohexanone, 4-(1,1-dimethylethyl)	11.47	96.3
Pentasiloxane, dodecamethyl	11.504	89.8
3,4-Dimethylcumene	11.6292	90.2
2,4-Dichloro-5-nitrobenzotrifluoride	11.8972	89.1
Benzenamine, N-ethyl-2-methyl	11.9118	93.4
Benzenamine, 2-ethyl-6-methyl	11.9118	94
1H-Indene, 2,3-dihydro-4,7-dimethyl	11.9646	88.3
Benzene, 1-ethyl-3-methyl	12.163	98
1H-Indene, 2,3-dihydro-1,6-dimethyl	12.2394	93.6
Benzene, 1,2,4-trimethyl	12.2581	97.9
Phenol, 4-chloro-2-methyl	12.4443	90.4
Oxirane, ethyl	12.5824	88,5
Decane, 6-ethyl-2-methyl	12.6888	90.1
Bicyclo [3.2.0] hepta-2,6-diene	12.7625	84.5
Naphthalene, 2-methyl	12.8138	98.3
Naphthalene, 1-methyl	13.0918	98
1-Pentanone, 1-(4-methylphenyl)	13.1168	85.5
Eptam	13.1954	83.7
Benzeneacetaldehyde, alpha-methyl	13.2438	92.6
Benzene, 1-methyl-2-propyl	13.4832	93.5
Benzene, 2-ethyl-1,4-dimethyl	13.5654	94.2
Acetamide, 2,2-dichloro-N,N-di-2-propenyl	13.7844	96
1,3,5-Cycloheptatriene, 3,7,7-trimethyl	13.7957	86
N,N-Diethylaniline	13.8801	86.5
Benzene, 2-ethyl-1,3-dimethyl	13.9636	96.6
Biphenyl	14.0152	91.1
1H-Indene, 2,3-dihydro-1,1,3-trimethyl	14.165	81
3-Methylbenzoic acid, 2,5-dichlorophenyl ester	14.1873	89
Benzene, 1,3-diethyl-5-methyl	14.2403	82.8
Hexane, 1-(hexyloxy)-5-methyl	14.2865	84.4
Naphthalene, 1,5-dimethyl	14.3197	95.3
D-Norleucine, N-propargyloxycarbonyl-, isohexyl ester	14.3374	83.5
1H-Indene, 2,3-dihydro-5-methyl	14.3953	93
Indan, 1-methyl	14.3953	93
Naphthalene, 1,3-dimethyl	14.4882	95.6
Naphthalene, 1,6-dimethyl	14.5275	94.6
Decane, 1,1'-oxybis	14.5685	82.1
Benzene, 1,1',1'',1'''-(1,2-ethanediylidene) tetrakis	14.5981	86.8
l-Alanine, N-(p-toluoyl)-, hexyl ester	14.7196	80.4
Acenaphthylene	14.8346	94.5
Naphthalene, 2-ethyl	14.8748	89.2
Octane, 1-chloro	14.8823	92.6
1,1'-Biphenyl, 4-methyl	15.1267	93.6
1-Dodecanamine, N,N-dimethyl	15.1675	96.6
Benzene, 1,1',1'',1'''-(1,2-ethanediylidene) tetrakis	15.2141	87
Succinic acid, 3-methylbut-2-en-1-yl diphenylmethyl ester	15.2142	87.9
Naphthalene, 2-(1-methylethyl)	15.3232	87.7
Tebuthiuron	15.3951	95
Benzene, 1-methyl-4-(phenylmethyl)	15.505	81
Naphthalene, 1,4,6-trimethyl	15.5216	85.2
Naphthalene, 1,6,7-trimethyl	15.5657	93
Phenol, 3,4,5-trichloro	15.611	80.3
Naphthalene, 2,3,6-trimethyl	15.8464	84.2
3,3'-Dimethylbiphenyl	16.1097	84.7
N,N-Dimethyldecanamide	16.2848	98.2

Trifluralin	16.5979	98.8
Benzene, 1,1'-(3-methyl-1-propene-1,3-diyl) bis	16.6673	86.9
Acetic acid, [(3,5,6-trichloro-2-pyridinyl) oxy]-, methyl ester	16.7931	92.8
Benzene, 1,1'-(2-methyl-1-propenylidene) bis	16.863	87
Atrazine	17.1011	98.9
Dimethazone	17.1712	94.6
Terbuthylazine	17.2763	90.5
Phosphorodithioic acid, S-[(tert-butylthio) methyl] O,Odiethyl ester	17.3041	94.9
Tetrachloroisophthalonitrile	17.6203	92.9
Benoxacor	17.7599	84.1
Acetamide, 2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6- methylphenyl)	17.9542	99.5
Ametryn	18.0363	80.7
Spiroxamine	18.2295	82.6
Benthiocarb	18.3928	92.6
Metolachlor	18.4716	98.7
Chlorpyrifos	18.4893	85.1
9,12-Octadecadienoic acid (Z,Z)-, methyl ester	18.8828	87.8
Octatriene, 1,3-trans-5-trans-	18.9211	82.6
Methyl stearate	19.0103	88.3
Acetic acid, (2,4-dichlorophenoxy)-, isooctyl ester	19.5757	88.3
Acetic acid, (2,4-dichlorophenoxy)-, 2-ethylhexyl ester	19.5758	88.2
Triclopyr 2 butoxy ethyl ester	19.6657	98

Figure 3: Chromatogram for sample W01062/21

Figure 4: Chromatogram for sample W01062/21

Table 3: Analytes detected with a Match Factor >80% for sample W01063/21.

Compound Name	Retention time (m)	Match Factor (%)
2-Propanone, 1-methoxy	2.8022	89.8
Methane, bromo	3.0179	84
2-Aminocyanoacetamide	3.0443	88.3
Propanamide, 2-hydroxy-N-methyl	3.0707	87
N-Dimethylaminomethyl-tert -butyl-isopropylphosphine	3.0827	86.2
Methylamine, N, N-dimethyl	3.1784	89.1
N-Nitrosodimethylamine	3.6986	81.2
4,6-Heptadiyn-3-one	3.8686	81.5
1,3-Difluoro-2-propanol	4.171	82.2
Hexanoic acid	4.928	81.2

n-Butyl ether	6.1425	90.6
2-Butanone	6.6883	96.5
3-Methylpyridazine	6.8803	88.8
Carbonic acid, dimethyl ester	6.92	92.3
Tetrahydrofuran	6.9859	83.5
Methyl propionate	7.0627	95.9
Arsenous acid, tris(trimethylsilyl) ester	7.6248	82.5
Heptane	7.8789	95.5
Methyl formate	8.0187	98.9
Methyl isobutyrate	8.0414	90.1
3-Pentanone	8.485	85.2
2-Pentene, 2,4-dimethyl	8.5251	84.9
Cyclopropane, 1,1,2,2-tetramethyl	8.5259	82.9
Butanoic acid, methyl ester	8.6875	98.4
Disulfide, dimethyl	9.1836	99.4
Propanoic acid	9.294	98.9
Toluene	9.4311	88.9
Borane, dimethoxy	9.456	83.4
Butanoic acid, 2-methyl-, methyl ester	9.5565	92.1
Acetonitrile, (dimethylamino)	9.6842	97.9
2-Propanone, 1-chloro	10.275	82.6
Formamide, N, N-dimethyl	10.5145	98.7
Ethylbenzene	10.8538	95.3
p-Xylene	10.9643	95.5
2,4-Dithiapentane	11.4344	83.6
Propanoic acid, propyl ester	11.6664	83.9
Tetrahydrofuran-D8	11.7084	86
Bicyclo [3.1.1] hept-2-ene, 3,6,6-trimethyl-	11.7124	96.3
Benzeneacetaldehyde	12.0958	88.3
Benzene, (1-methylethyl)	12.1715	89.3
Cyclooctane, methyl	12.2269	90.2
Decane	12.2844	95.9
1-Butanol, 2-methyl	12.5008	80.3
Dimethyl trisulfide	12.5431	99.2
3,6-Heptanedione	12.5748	82.5
Heptane, 4-ethyl	12.9611	89
1-Hexanone, 5-methyl-1-phenyl	13.0251	82.5
Benzene, 1-ethyl-4-methyl	13.0257	83
Decane, 3-methyl	13.1308	89.4
Benzene, 1-methyl-4-propyl	13.2446	90.5
Naphthalene, decahydro	13.392	86.5
Undecane	13.4414	96.8
Benzene, (1-methylpropyl)	13.4853	82.1
p-Toluic acid, 4-nitrophenyl ester	13.5669	85.2
1,3,8-p-Menthatriene	13.5693	86.5
Benzene, 1-ethyl-2,4-dimethyl	13.6699	88.1
Benzene, 4-ethenyl-1,2-dimethyl	13.7512	84.2
Benzoic acid, hydrazide	14.0242	83
Benzene, 1-ethyl-3,5-dimethyl	14.1158	93.4
1,2,4-Trithiolane	14.2623	83.6
Phosphinic acid, diethyl-, methyl ester	14.2757	83.9
Phenylethyl Alcohol	14.4765	93.7
3,4-Hexanedione, 2,2,5-trimethyl	14.5112	82.9
Benzene, 2,4-dimethyl-1-(1-methylethyl)	14.8831	80.1
1-Hexanol, 4-methyl	15.0599	87.9
Naphthalene	15.1786	89.7
2,6-Difluorobenzoic acid, 4-nitrophenyl ester	15.2049	90.2

Methenamine	15.6261	99.1
1,11-Dodecadiene	16.5018	86.9
Eptam	16.5571	85.3
1-Undecene, 9-methyl	16.6229	82.7
Indole	16.7542	98.1
3,4-Dihydroxyphenylglycol, 4TMS derivative	16.9305	82.7
Cyclononasiloxane, octadecamethyl	17.4305	86.4

Figure 5: Chromatogram for sample W01063/21

Figure 6: Chromatogram for sample W01063/21

Table 4: Analytes detected with a Match Factor >80% for sample W01064/21.

Compound Name	Retention time (m)	Match Factor (%)
6-Hepten-3-one, 5-hydroxy-4-methyl	3.0347	92.2
Glyoxal	3.3178	88.2
Methylamine, N,N-dimethyl	3.6361	84.5
N-Dimethylaminomethyl-tert -butyl-isopropylphosphine	3.6361	89.3
Tetramethyl orthocarbonate	3.7223	80.1
2-Propynal	3.8007	87.1
2-Propanamine	4.1613	89.4
Glycine	5.1257	82.5
2-Propenal	5.1727	88.8
1,2-Ethanediol	5.267	85.9
Ethanol, 2-nitro	5.2671	85.9
1-Azabicyclo [3.1.0] hexane	5.3943	84.9
Ethanol, 2-butoxy	6.1325	91.2
Azetidine	6.4199	88.6
Isobutylene epoxide	6.8925	92.6
Carbonic acid, dimethyl ester	7.0974	91.6
Methyl propionate	7.2632	97.3
Propanamide, N-methyl	7.3072	82.4
Arsenous acid, tris(trimethylsilyl) ester	7.6236	81
Benzeneacetaldehyde	7.7768	89.5
Hexane, 2,2,5,5-tetramethyl	8.0344	88.9
Acetic acid	8.1177	99
Methyl isobutyrate	8.1857	90
1-Butanol, 2-methyl	8.4707	85.5
3-Pentanone	8.5818	89.6

2,4-Azetidinedione, 3,3-diethyl-1-methyl	8.6445	83.8
Butanoic acid, methyl ester	8.7782	99.3
1-Penten-1-one, 2-methyl	9.106	98.3
Disulfide, dimethyl	9.2607	83.1
Propanoic acid	9.328	83.4
t-Butyl nitrite	9.6183	87.4
Acetamide	9.6246	90.3
Butanoic acid, 2-methyl-, methyl ester	9.6247	81.4
Acetonitrile, (dimethylamino)	9.7178	97.6
L-Alanine, methyl ester	10.4243	81.5
Formamide, N,N-dimethyl	10.5564	96.9
Ethylbenzene	10.8888	80.6
p-Xylene	10.9883	95.4
Butanoic acid, 3-methyl	11.1421	95.3
Aminoguanidine	11.264	86.2
Propanediamide, 2-amino	11.2652	85.7
Benzeneethanol, alpha,.beta.-dimethyl	11.3583	84.3
2,4-Dithiapentane	11.46	81.7
Bicyclo [3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)	11.7266	83.5
Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)	11.7274	82.5
S-Methyl 3-methylbutanethioate	11.94	94.8
Cyclopropane, 1-hexyl-2-methyl	12.2357	92.5
1-Decene	12.2359	94.9
Decane	12.2931	98.4
4-Nonene, 2-methyl	12.5121	86.3
Dimethyl trisulfide	12.5617	97.9
Heptane, 4-ethyl	12.9663	89.7
Decane, 2-methyl	13.0489	89.8
Decane, 3-methyl	13.136	90.7
Phenol	13.2935	96
Undecane	13.4452	98.1
1-Hexanone, 5-methyl-1-phenyl	13.8785	88.1
Benzoic acid, hydrazide	14.0263	86.5
Benzene, 1,2,3,5-tetramethyl	14.1202	82.6
Phenylethyl Alcohol	14.4701	95.1
2-Phenylpropenal	14.8679	83.5
1-Octene, 6-methyl	15.0564	90
Methenamine	15.6336	96.8
Cyclohexanepropanol	15.7619	85.9
1,9-Decadiene	16.501	89.7
Eptam	16.5615	80.6
1-Undecanol	16.6226	92.5
Heptadecane	16.6658	94.5
Indole	16.7534	98.7
Methyl tetradecanoate	16.834	83
Tetradecanoic acid	17.0293	94
Cyclononasiloxane, octadecamethyl	17.4305	83.7
9-Hexadecenoic acid, methyl ester, (Z)	17.8973	84
Hexadecenoic acid, Z-11	18.0743	93.4
n-Hexadecanoic acid	18.1623	97.8
cis-Vaccenic acid	19.0795	92.6
Octadecanoic acid	19.18	93.7

Figure 7: Chromatogram for sample W01064/21

Figure 8: Chromatogram for sample W01064/21

Table 5: Analytes detected with a Match Factor >80% for sample W01065/21.

Compound Name W1065	Retention time (m)	Match Factor (%)
Methylamine, N,N-dimethyl	2.9878	93.6
Hydrazinecarbothioamide	3.777	83.6
Pyridine	4.5545	88.2
Cyanic acid, ethyl ester	4.6854	82.1
Methane-d, trichloro	4.7082	81.9
2-Propanamine	4.9017	89.8
Ethanamine, N-methyl	4.9787	88.6
Pentane, 3-methyl	5.3357	88.6
Azetidine	5.3358	88.7
Ethanone, 1-oxiranyl	5.8363	89.9
Propanoic acid, 2-methylpropyl ester	6.1305	88.9
Ethene, ethoxy	6.4923	91.9
N,N-Dimethylglycine	6.7166	94.9
Methane, nitro	6.8037	93.5
1-Propene, 1-methoxy-2-methyl	6.8982	86.8
t-Butyl nitrite	6.96	80
Aziridine, 2-ethyl	7.2282	87.7
N-Dimethylaminomethyl-tert -butyl-isopropylphosphine	7.4952	86.8
Arsenous acid, tris(trimethylsilyl) ester	7.6246	80.4
Benzeneacetaldehyde	7.7742	89.9
Acetic acid	7.8594	97.8
Methyl isobutyrate	7.9488	90.1
Nonane, 3,7-dimethyl	8.0377	90.4
5-Methyloxazolidine	8.1497	81.7
Cyclopentanamine	8.15	80.3
2-Pentanone	8.3234	91.7
1-Methyl-2-phenylcyclopropane	8.3719	80.9
Oxalic acid, diallyl ester	8.4175	82.5
Cyclohexane, methyl	8.4196	82.1
Undecane	8.4737	96
Butanoic acid, methyl ester	8.6116	97.5
2,2-Dimethoxybutane	9.0485	85.1
Disulfide, dimethyl	9.1	96.1
Propanoic acid	9.2243	98.9
L-Homoserine lactone, N,N-dimethyl	9.259	96.1

Toluene	9.3597	94.9
2-Chloroethyl benzoate	9.479	84.9
Hydrazine, (2-methylpropyl)	9.5137	82.6
Methyl isovalerate	9.5414	96.2
Acetonitrile, (dimethylamino)	9.7128	93.5
3-Buten-2-one, 3-methyl	10.0746	81.8
Cyclopentanone, 3-methyl	10.7852	86.6
Ethylbenzene	10.8221	94.3
o-Xylene	10.9433	97.8
Nonane	10.9726	95.3
Butanoic acid, 3-methyl	11.145	96.2
Aminoguanidine	11.2669	84.3
p-Xylene	11.3205	96.2
Hexanoic acid, methyl ester	11.6125	80.8
(1R)-2,6,6-Trimethylbicyclo [3.1.1] hept-2-ene	11.6889	97.5
Alpha-Pinene	11.6889	97.4
Nonane, 4-methyl	11.8269	81.6
3,4-Hexanedione, 2,2,5-trimethyl	11.9264	83.6
Benzene, 1-ethyl-2-methyl	12.159	85.4
1-Decene	12.2102	98.3
2-Decene, (Z)	12.3483	91.1
Benzene, (1-methylethyl)	12.4416	81.4
2-Decene, (E)	12.4917	95.6
Dimethyl trisulfide	12.5423	91.8
Bicyclo [2.2.1]heptane, 7,7-dimethyl-2-methylene	12.6547	82.7
Heptane, 2,6-dimethyl	12.7095	87.6
Indole	12.7144	88
2,2,6,6-Tetramethylheptane	12.7721	87.1
Acetic acid, hydrazide	12.8276	83.5
Heptane, 4-ethyl	12.9498	92.6
Hexane, 2,3-dimethyl	12.9925	92.6
Decane, 2-methyl	13.0337	97.3
Decane, 3-methyl	13.1214	98
Benzene, 1,4-diethyl	13.2967	83.6
Phenol	13.3141	94
Benzene, 2-ethyl-1,3-dimethyl	13.6689	88.4
Benzene, 1-ethyl-2,4-dimethyl	13.6689	87.7
1-Propene, 3-propoxy	13.8326	92.1
1-Hexanone, 5-methyl-1-phenyl	13.896	87.2
Acetophenone	13.8985	83.6
Benzoic acid, hydrazide	14.0233	90.7
Benzene, 1,2,3,5-tetramethyl	14.1166	90.4
Undecane, 5,7-dimethyl	14.5067	90.7
2-Piperidinone	15.5908	93
Methenamine	15.6273	96.7
Benzenepropanoic acid, methyl ester	15.8615	85.5
Decane, 2,9-dimethyl	15.9624	87.3
2,4-Imidazolidinedione, 3-methyl	16.4306	94.1
3-Hexen-1-ol, formate, (Z)	16.497	82.9
Cyclooctane, 1,4-dimethyl-, trans	16.6228	87.9
Tetradecanoic acid	17.0305	86.1
Decane	17.2874	92.3
Phenol, 2,6-bis(1,1-dimethylethyl)	17.3397	92.2
Cyclononasiloxane, octadecamethyl	17.4331	87.8
1-Propene, 3-(1,1-dimethylethoxy)	17.8456	85.2
Hexadecenoic acid, Z-11	18.0739	84.6
n-Hexadecanoic acid	18.159	95.9
Cyclodecasiloxane, eicosamethyl	18.255	81
Undecane, 3,8-dimethyl	18.3633	90.5

Octadecanoic acid	19.1802	86.1
Undecane, 4,7-dimethyl	19.3846	89.5
Tetracosamethyl-cyclododecasiloxane	19.8111	82.8
Phthalic acid, di(2-propylpentyl) ester	21.9986	86.1
2-Propenoic acid, 2-methyl-, oxiranylmethyl ester	22.3474	82

Figure 9: Chromatogram for sample W01065/21

Figure 10: Chromatogram for sample W01065/21

Table 6: Analytes detected with a Match Factor >80% for sample W01066/21.

Compound Name	Retention time (m)	Match Factor (%)
Ethanol, 2-methoxy-, acetate	2.7862	80.5
2-Imidazolidinone	3.0447	85.1
Hydrazinecarbothioamide	3.794	86.1
Ethylenimine, N-chloro	3.8377	83.4
1-Butanol	5.1804	91.7
Boric acid, trimethyl ester	5.7488	80.5
Ethanol, 2-butoxy	6.1367	94.2
N,N-Dimethyl-2-methoxyethylamine	6.64	90.9
Methyl propionate	6.8386	90
Decane	7.1186	85.2
N,N-Dimethylglycine	7.29	84.2
Butanal, 3-methyl	7.5699	91.7
Arsenous acid, tris(trimethylsilyl) ester	7.6245	81.3
Butanal, 2-methyl	7.7174	92.4
Benzeneacetaldehyde	7.7735	88.1
1,2,3-Trimethyldiaziridine	8.0358	85.7
3,4-Hexanedione, 2,2,5-trimethyl	8.0374	82.6
2,4-Azetidinedione, 3,3-diethyl-1-methyl	8.3487	84.9
1-Methyl-2-phenylcyclopropane	8.3824	80.8
Nonane, 3,7-dimethyl	8.4747	87.4
Butanoic acid, methyl ester	8.585	94.9
Furan, 2,5-dihydro-3,4-dimethyl	8.9431	86.4
6-Oxabicyclo [3.1.0] hexan-2-one	8.9431	85.4
Disulfide, dimethyl	9.0999	94.3
L-Homoserine lactone, N,N-dimethyl	9.2715	91.3
Methyl isovalerate	9.4966	84.3
Aluminum, triethyl	12.6984	84.9
Indole	12.7086	98.7
(S)-(+)-6-Methyl-1-octanol	15.0572	87.8
1,11-Dodecadiene	16.4977	83
Benzene, 1-isocyano-3-methyl	16.7567	85.5
Cyclononasiloxane, octadecamethyl	17.4336	85.7

9-Hexadecenoic acid, methyl ester, (Z)	17.8984	86.2
n-Hexadecanoic acid	18.1546	89.9
2-t-Butylamino-2-methyl-malononitrile	22.319	80.2
2-Butenoic acid, 3-hexenyl ester, (E, Z)	24.5081	80

Figure 11: Chromatogram for sample W01066/21

Figure 12: Chromatogram for sample W01066/21

Table 7: Analytes detected with a Match Factor >80% for sample W01067/21.

Compound Name	Retention time (m)	Match Factor (%)
Methane-d, trichloro	2.6626	82.4
Carbamic acid, ethyl-, methyl ester	3.6687	80.5
Acetic anhydride	4.6464	87.5
Ethanimidic acid, ethyl ester	4.6464	81.2
Ethanone, 1-oxiranyl	5.8527	95.9
2-Butanone	6.5631	96.2
Phenethylamine, N-benzyl-p-chloro	6.6791	80
Carbonic acid, dimethyl ester	6.7604	92
Benzene, (1-methylethyl)	6.7631	92.1
1-Butanol, 3-methoxy-, acetate	6.8888	90
Dimethyl trisulfide	6.9114	92.4
Methyl propionate	6.951	94.3
1-Hexanone, 5-methyl-1-phenyl	6.9788	80.9
Aziridine, 2,2-dimethyl	7.1963	92.5
Heptane	7.6846	95.8
Indane	7.7172	83.5
Acetic acid, methoxy	7.7707	83.9
Benzene, 1-methyl-3-propyl	7.86	92.2
Methyl isobutyrate	7.9426	96.3
o-Cymene	7.9578	92.2
Benzene, (1-methylpropyl)	8.1081	91.8
Benzene, 1-ethyl-2,4-dimethyl	8.2684	94.7
2-Pentanone	8.2914	91.2
Oxalic acid, allyl butyl ester	8.4211	90.8
Butanoic acid, methyl ester	8.6199	97
1,3,8-p-Menthatriene	8.7554	93.3
Benzene, tert-butyl	8.9166	82.5
Benzene, 1,2,4,5-tetramethyl	8.9168	95.4
Toluene	9.3614	93.4
2H-Pyran-2-one, tetrahydro-4,4,6-trimethyl	9.4371	87.4
Cyclopropane, 1,1,2,3-tetramethyl	9.4373	87.5
Butanoic acid, 2-methyl-, methyl ester	9.5268	91.2
p-Cymene	9.6601	84.2

Cyclohexanone, 5-methyl-2-(1-methylethyl)-, trans	9.6755	94.1
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1.alpha,2.betau,5.alpha.)	10.0422	97.8
Benzene, 1-methyl-4-(1-methylpropyl)	10.0846	86.7
3-Buten-2-one, 3-methyl	10.0852	87.2
Cyclohexanol, 4-(1,1-dimethylethyl)-, cis	10.2003	88
Cyclohexanol, 2-(1,1-dimethylethyl)	10.2041	87.3
Naphthalene	10.4663	97.7
1H-1,2,4-Triazol-3-amine, 5-methyl	10.5904	80.1
Cyclobutanone, 2,3,3-trimethyl	10.7941	83.6
Ethylbenzene	10.8275	94
o-Xylene	10.9499	98
Nonane	10.974	97.1
Acetic acid, anhydride with formic acid	11.1704	91.6
Benzene, 1,3-dimethyl	11.3264	96
p-Xylene	11.3264	95.5
Cyclohexanone, 4-(1,1-dimethylethyl)	11.465	93.8
Pentasiloxane, dodecamethyl	11.4973	89
(1R)-2,6,6-Trimethylbicyclo [3.1.1] hept-2-ene	11.6917	97.9
2-Pyrrolidinone	11.7667	81.7
Butane, 2,2-dimethyl	11.8312	85.4
2,2-Dimethyl-propyl 2,2-dimethyl-propanesulfinyl sulfone	11.9284	82.7
Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate, trans	11.9822	84.6
3-Hexen-1-ol, propanoate, (Z)	12.1191	84.9
1-Butanol	12.1456	89.7
1-Decene	12.2128	99.2
Decane	12.2694	98.8
cis-4-Decene	12.3503	93.5
trans-3-Decene	12.4943	97.7
Benzene, pentamethyl	12.5322	81
Benzene, 1,3-dichloro-2-methoxy	12.626	97.2
Cyclohexene, 4-methylene-1-(1-methylethyl)	12.6594	89.7
Decane, 2,9-dimethyl	12.7104	87
o-tert-Butyl cyclohexyl acetate 2	12.7212	88.5
Undecane, 3,7-dimethyl	12.7731	85.6
Silane, 1,3-butadiynyltrimethyl	12.7747	81.6
Naphthalene, 2-methyl	12.8132	90.4
Heptane, 2,2,4-trimethyl	12.8952	81.5
Heptane, 4-ethyl	12.9515	90.3
Octane, 3-ethyl	12.9936	84.3
Decane, 2-methyl	13.0349	97.2
Decane, 3-methyl	13.1224	98.5
4-tert-Butylcyclohexyl acetate	13.3175	81.3
Undecane	13.4359	99.5
Eptam	13.6466	97.8
Benzoic acid, hydrazide	14.0221	86.8
Hexasiloxane, tetradecamethyl	14.1948	91.9
Naphthalene, 1,2-dimethyl	14.3021	83
Naphthalene, 1,3-dimethyl	14.4795	83
Dodecane	14.5091	93.7
2,5-cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-4- hydroxy-4-methyl-	14.921	88.5
4H-Inden-4-one, 1,2,3,5,6,7-hexahydro-1,1,2,3,3- pentamethyl	15.3078	83.5
3,4-Hexanedione, 2,2,5-trimethyl	15.5054	85.8
Nonane, 3,7-dimethyl	15.5054	85.3
2-Piperidinone	15.5883	93.6
Methenamine	15.6241	95.1
Heptasiloxane, hexadecamethyl	15.7383	88.7
Benzoic acid, 2-hydroxy-, pentyl ester	15.8712	90.7
2,4-Imidazolidinedione, 5-methyl	16.4264	97.8
2-Butanone, 3-methyl	16.4355	82.6
Cycloheptane, methyl	16.5266	86.9

Trifluralin	16.5864	96.8
2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)-propionaldehyde	16.6238	80.6
m-Aminophenylacetylene	16.7594	90.5
1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7- hexamethyl-, trans-	16.8356	80.4
Benzene, (1-butyloctyl)	16.9468	85.4
Benzene, (1-propylnonyl)	17.0283	80.5
Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8- tetramethyl-1H-3a,7-methanoazulen-5-yl)	17.3343	83.9
Phenol, 2,6-bis(1,1-dimethylethyl)	17.34	91.8
Undecane, 3,5-dimethyl	17.3495	83.6
Cyclononasiloxane, octadecamethyl	17.4328	80.6
2-Ethylhexyl salicylate	17.4395	96.5
Benzene, (1-pentyloctyl)	17.5031	81.9
Metolachlor	18.4651	87.7
Chlorpyrifos	18.49	85.8

Figure 13: Chromatogram for sample W01067/21

Figure 14: Chromatogram for sample W01067/21

Refer to the “Notes” section at the end of this report for further explanations.

Where a deviation has been noted, the validity of the results may be affected. Results should be u

Specific Observations

None