LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	91	rBV	578141	642276	37.82%	6.654%
2	1.410	128	135	139	rBV	106626	131820	7.76%	1.366%
3	1.453	139	142	146	rVB	21494	25854	1.52%	0.268%
4	1.703	176	183	185	rBV2	54723	77278	4.55%	0.801%
5	1.733	185	188	197	rVB	170393	217414	12.80%	2.252%
6	1.965	221	226	231	rBV	27727	39211	2.31%	0.406%
7	2.050	236	240	247	rVB2	11951	17440	1.03%	0.181%
8	2.196	258	264	272	rVB	53249	91027	5.36%	0.943%
9	2.379	287	294	303	rBV	1090415	1698284	100.00%	17.593%
10	2.623	328	334	342	rVB	13209	24599	1.45%	0.255%
11	2.867	368	374	384	rVB3	12328	26693	1.57%	0.277%
12	3.074	400	408	418	rVB	16969	36832	2.17%	0.382%
13	3.708	503	512	521	rVB	57090	133560	7.86%	1.384%
14	4.611	650	660	673	rVB2	50539	138500	8.16%	1.435%
15	5.513	797	808	824	rBV2	73912	207027	12.19%	2.145%
16	5.678	824	835	846	rVV2	103081	289215	17.03%	2.996%
17	5.812	848	857	867	rVB	22330	61377	3.61%	0.636%
18	6.080	890	901	909	rBV	85073	211426	12.45%	2.190%
19	6.208	916	922	932	rVB2	27023	71146	4.19%	0.737%
20	6.403	941	954	968	rBV	612101	1605946	94.56%	16.637%
21	6.872	1021	1031	1043	rBV	184361	431610	25.41%	4.471%
22	7.269	1092	1096	1105	rVB3	12605	26156	1.54%	0.271%
23	7.762	1168	1177	1191	rBV	326458	621867	36.62%	6.442%
24	8.049	1219	1224	1231	rVB3	11563	20655	1.22%	0.214%
25	8.518	1293	1301	1309	rBV	61883	102097	6.01%	1.058%
26	8.726	1328	1335	1343	rBV	387469	629466	37.06%	6.521%
27	9.524	1459	1466	1472	rBV2	75122	111244	6.55%	1.152%
28	9.799	1506	1511	1517	rBV	12998	17566	1.03%	0.182%
29	10.043	1542	1551	1555	rBV4	7992	17666	1.04%	0.183%
30	10.122	1558	1564	1571	rVB	426395	570973	33.62%	5.915%
31	10.445	1612	1617	1623	rVB2	13825	19684	1.16%	0.204%
32	10.707	1656	1660	1666	rVB	18670	23225	1.37%	0.241%
33	11.085	1716	1722	1727	rBV	17896	25544	1.50%	0.265%
34	11.146	1727	1732	1741	rVV	392793	509659	30.01%	5.280%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

35	11.676	1815	1819	1825	rVB	19680	23984	1.41%	0.248%
36	12.085	1881	1886	1894	rBV	519899	633783	37.32%	6.566%
37	12.310	1920	1923	1927	rVB3	22118	25441	1.50%	0.264%
38	12.768	1994	1998	2004	rVB4	10863	17167	1.01%	0.178%
39	12.908	2014	2021	2026	rBV2	13732	20237	1.19%	0.210%
40	13.359	2090	2095	2100	rBV	46175	57966	3.41%	0.601%

Sum of corrected areas: 9652915

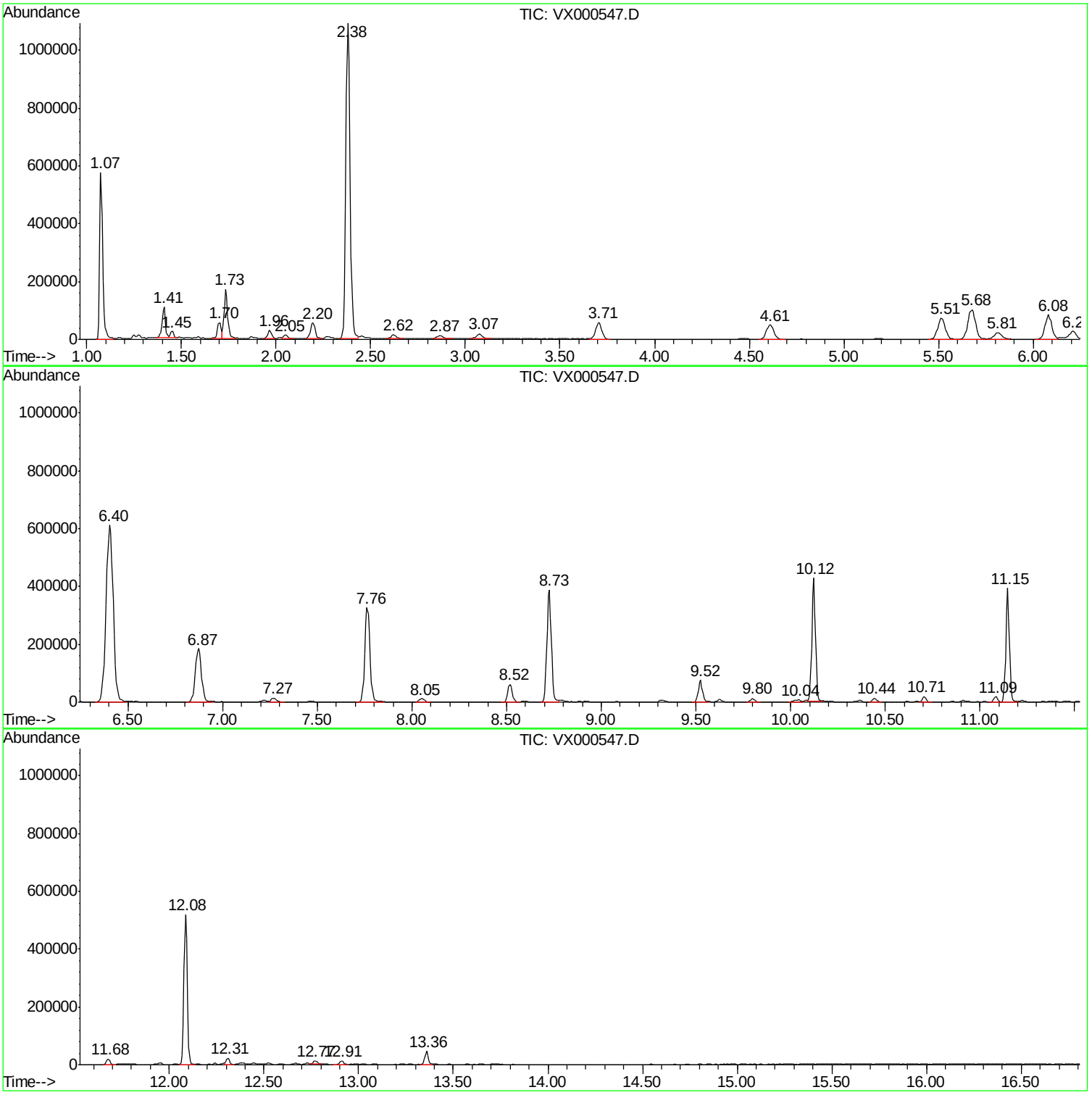
LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

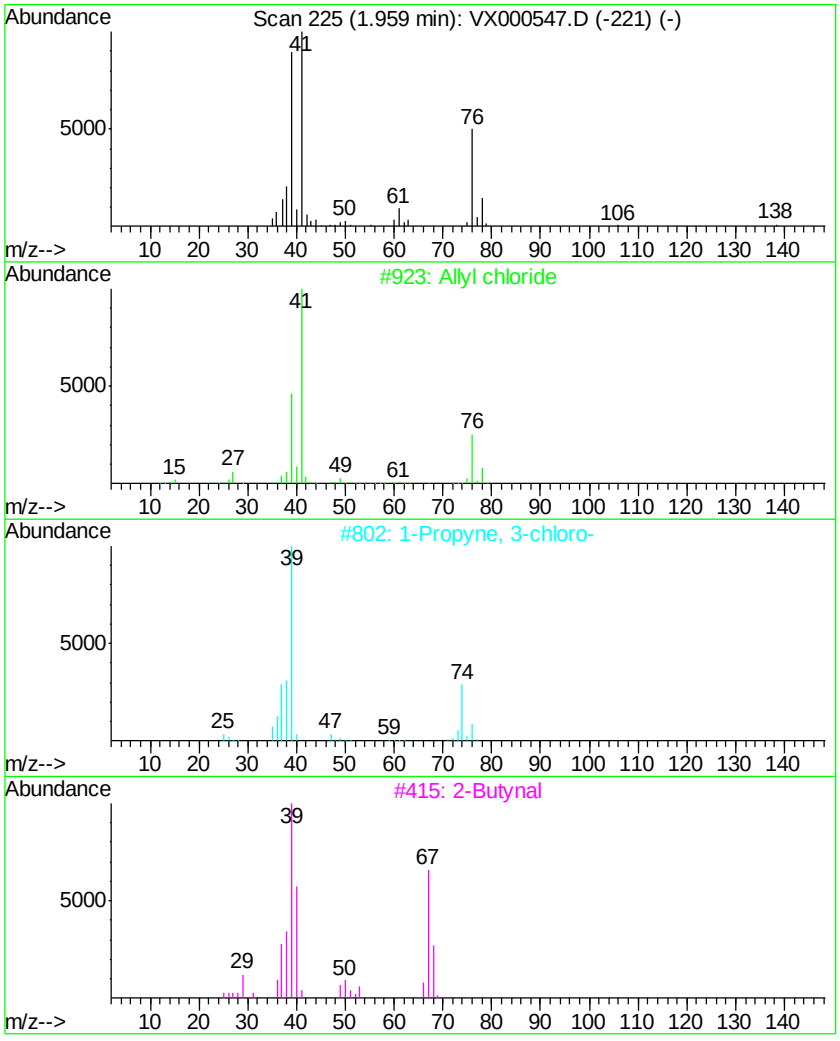
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

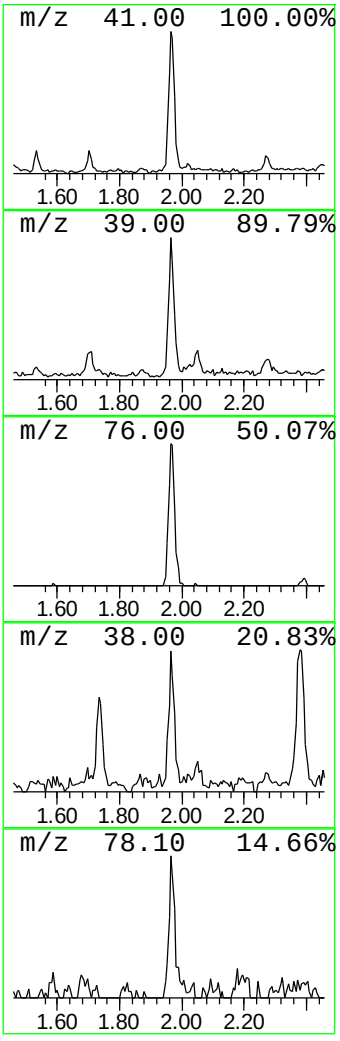
****

Peak Number 2 unknown1.96 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	6.78 ug/l	39211	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl chloride	76	C3H5Cl	000107-05-1	50
2	1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	40
3	2-Butynal	68	C4H4O	001119-19-3	40
4	3-Butenenitrile	67	C4H5N	000109-75-1	12
5	Methylacrylonitrile	67	C4H5N	000126-98-7	12





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

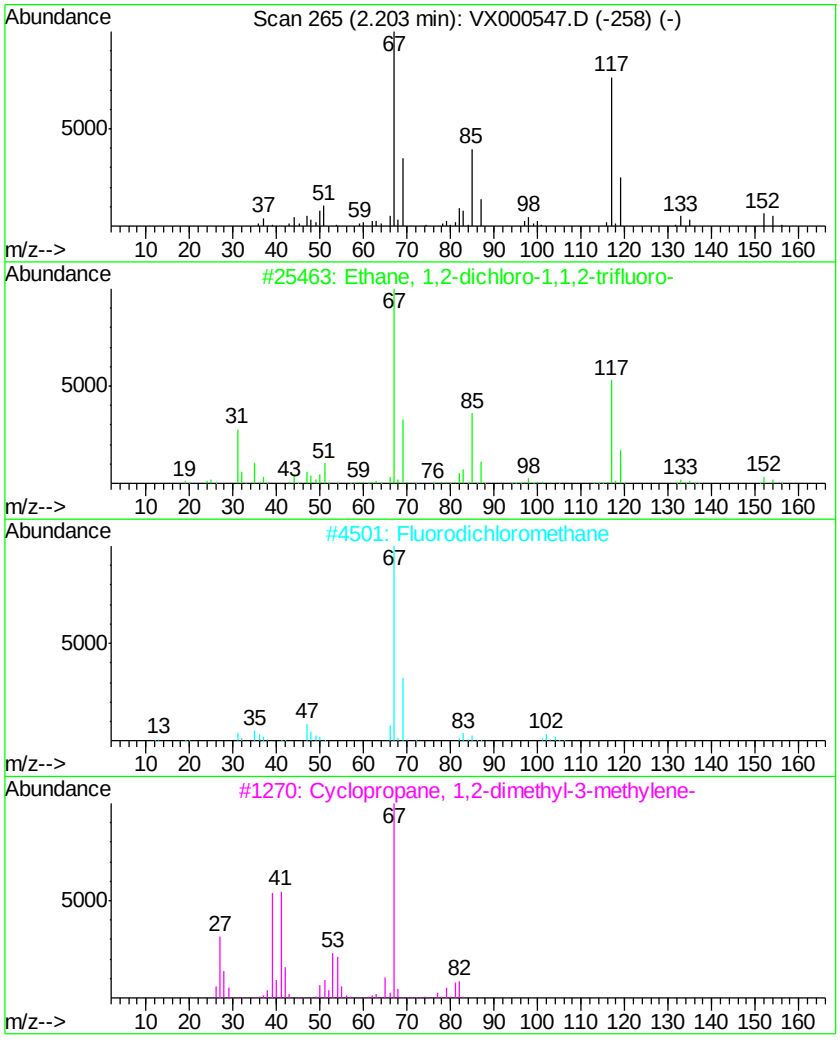
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

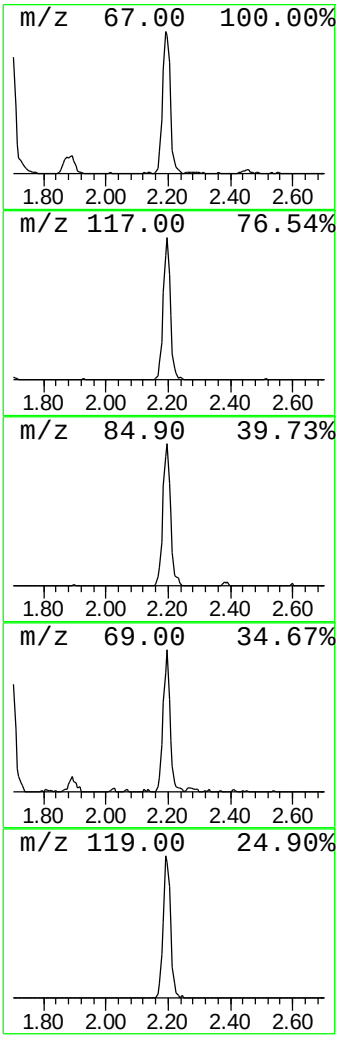
****

Peak Number 3 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	15.74 ug/l	91027	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	91
2	Fluorodichloromethane	102	CHCl2F	000075-43-4	12
3	Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	10
4	Chlorine dioxide	67	ClO2	010049-04-4	10
5	2-Pentyn-4-one	82	C5H6O	007299-55-0	9





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

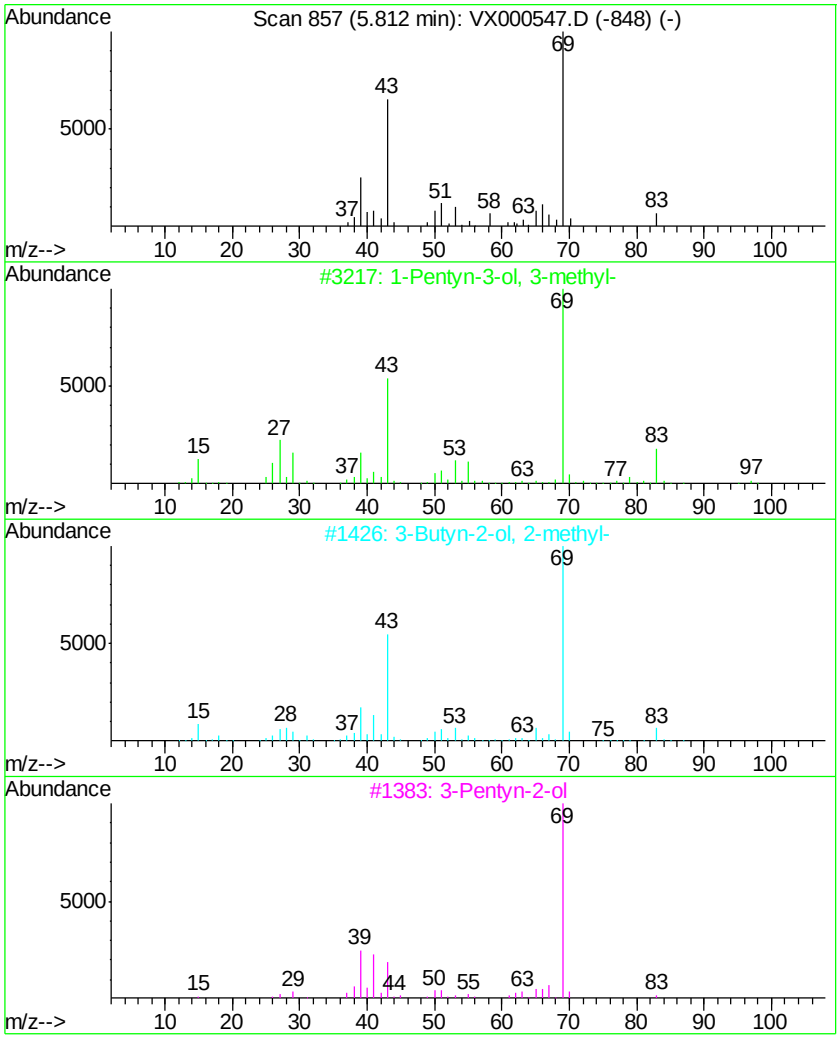
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

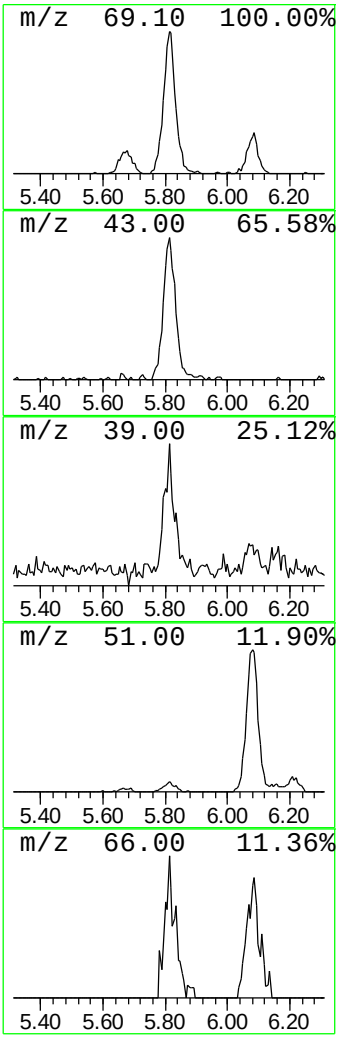
****

Peak Number 4 1-Pentyn-3-ol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.81	10.61 ug/l	61377	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentyn-3-ol, 3-methyl-	98	C6H10O	000077-75-8	64
2	3-Butyn-2-ol, 2-methyl-	84	C5H8O	000115-19-5	64
3	3-Pentyn-2-ol	84	C5H8O	027301-54-8	59
4	2-Butyne, 1-methoxy-	84	C5H8O	002768-41-4	38
5	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

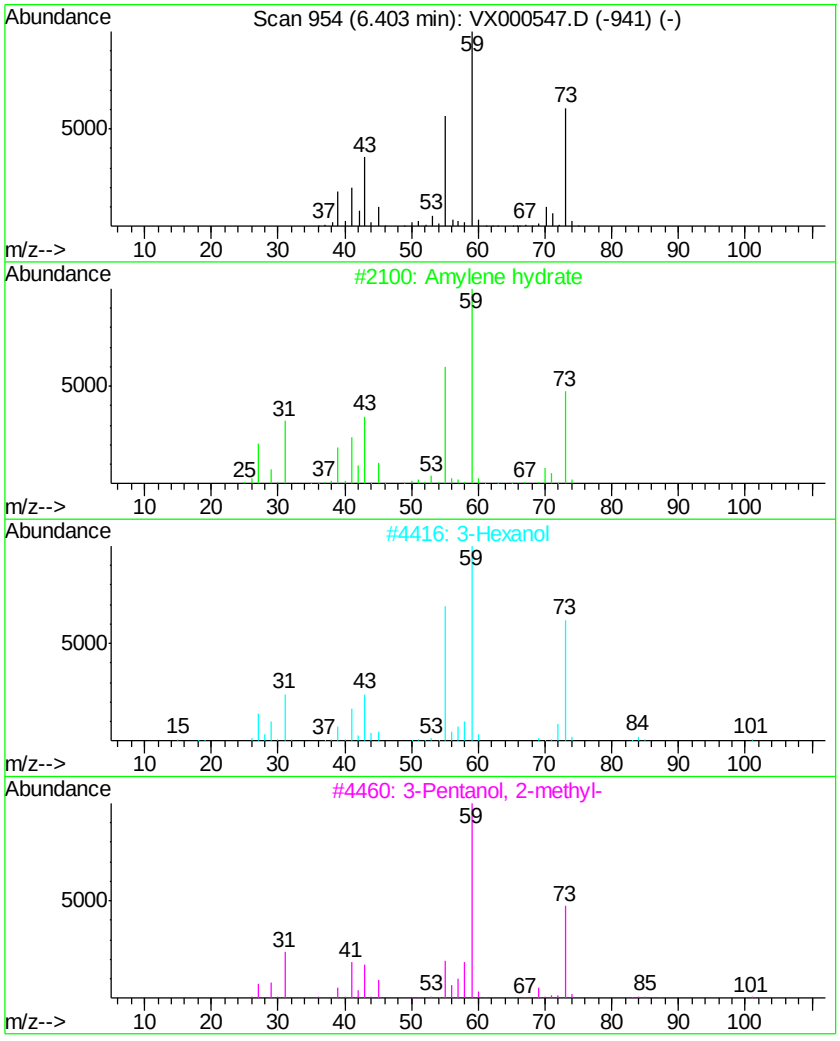
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

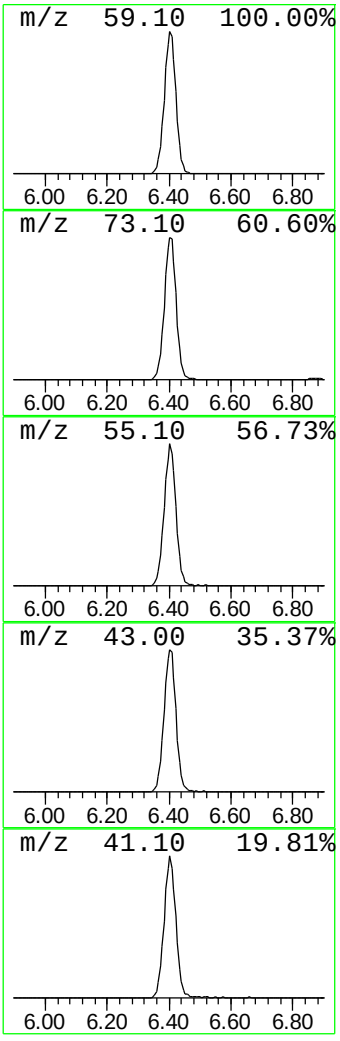
****

Peak Number 5 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	186.04 ug/l	1605950	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	3-Hexanol	102	C6H14O	000623-37-0	45
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

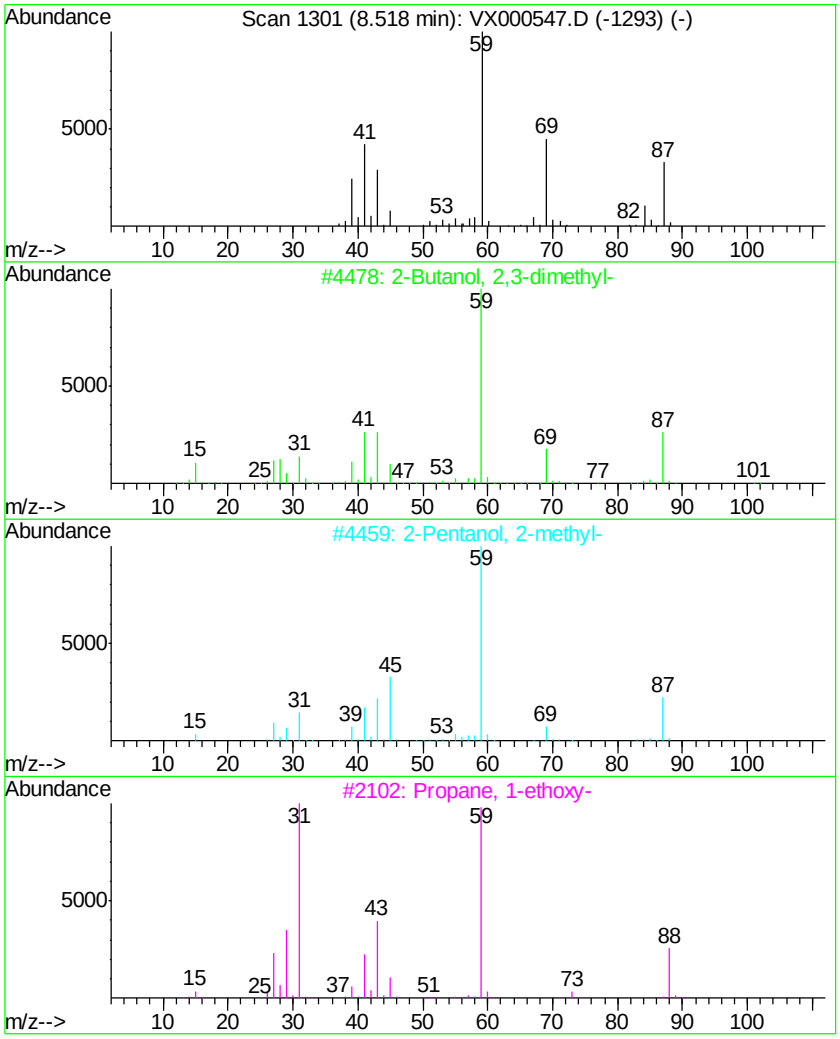
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

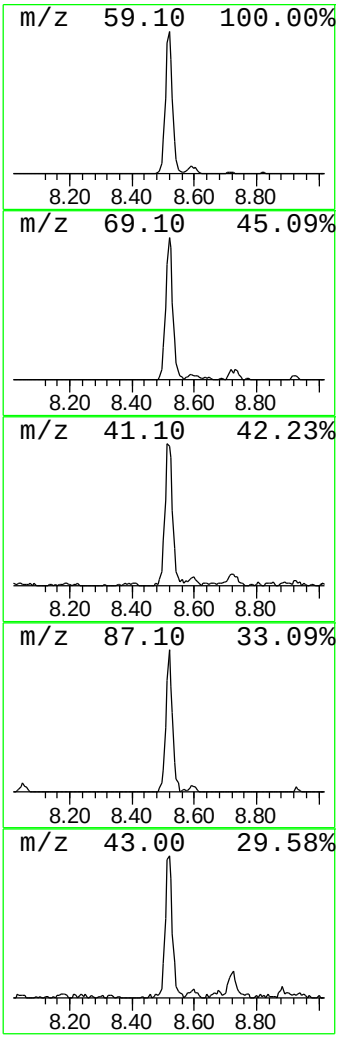
****

Peak Number 6 2-Butanol, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	8.94 ug/l	102097	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	49
4	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	40
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	38





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Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
Operator : JC/MD
Sample : J2127-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

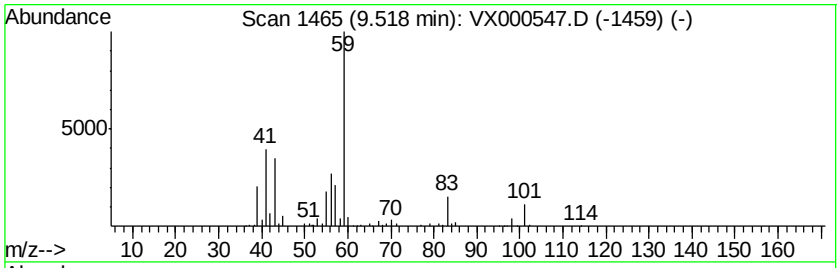
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

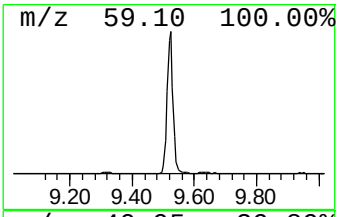
****

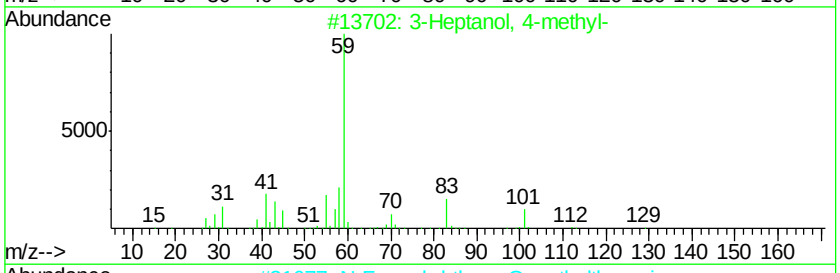
Peak Number 7 3-Heptanol, 4-methyl- Concentration Rank 5

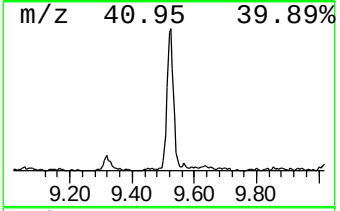
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	9.74 ug/l	111244	Chlorobenzene-d5	10.12

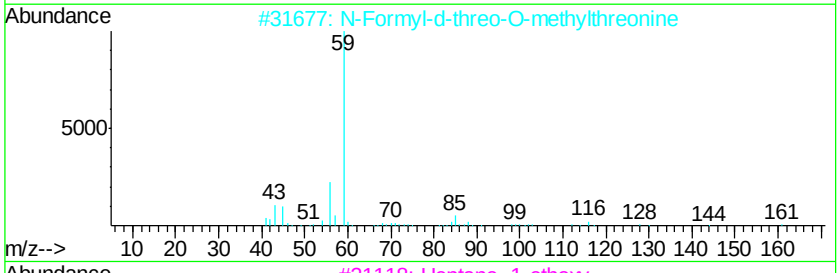
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	59
2	N-Formyl-d-threo-O-methylthreonine	161	C6H11NO4	1000214-69-5	38
3	Heptane, 1-ethoxy-	144	C9H20O	001969-43-3	38
4	Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	38
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	36

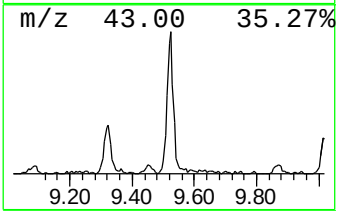


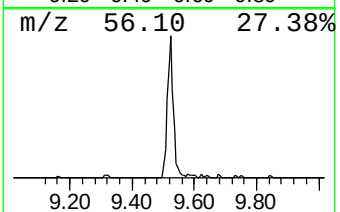


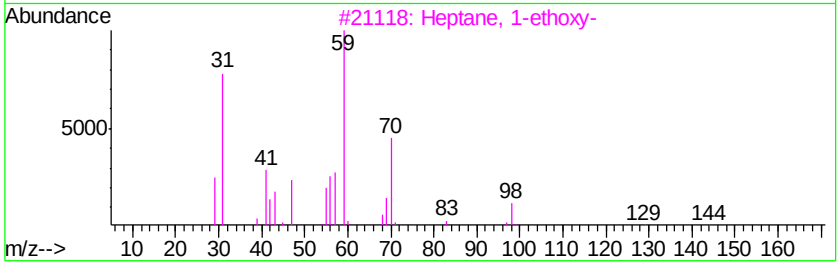


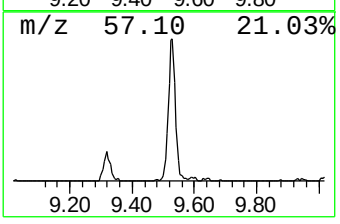












Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000547.D
Acq On : 30 Mar 2018 06:52
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Sample : J2127-01
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ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.96	1.96	6.8	ug/l	39211	1	5.68	289215	50.0
Ethane, 1,2-dichl...	2.20	15.7	ug/l	91027	1	5.68	289215	50.0
1-Pentyn-3-ol, 3-...	5.81	10.6	ug/l	61377	1	5.68	289215	50.0
Amylene hydrate	6.40	186.0	ug/l	1605950	2	6.87	431610	50.0
2-Butanol, 2,3-di...	8.52	8.9	ug/l	102097	3	10.12	570973	50.0
3-Heptanol, 4-met...	9.52	9.7	ug/l	111244	3	10.12	570973	50.0