LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

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 : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.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	2.291	149	161	180	rBV	93205	151950	10.14%	1.537%
2	3.230	440	453	474	rBV	20413	50170	3.35%	0.507%
3	3.773	604	622	653	rBV	236265	615662	41.09%	6.227%
4	4.005	676	694	720	rBV	45516	131438	8.77%	1.329%
5	5.979	1286	1308	1339	rBV	415085	1313483	87.67%	13.284%
6	6.510	1456	1473	1487	rBV7	5159	15931	1.06%	0.161%
7	6.606	1487	1503	1524	rVB	11725	35037	2.34%	0.354%
8	6.799	1542	1563	1581	rBV3	10044	32002	2.14%	0.324%
9	7.149	1659	1672	1691	rBV3	5437	15771	1.05%	0.160%
10	7.564	1782	1801	1812	rBV2	98149	250201	16.70%	2.530%
11	7.641	1812	1825	1843	rVB	189466	453508	30.27%	4.587%
12	7.854	1878	1891	1904	rVB3	12398	29017	1.94%	0.293%
13	7.998	1914	1936	1960	rBV2	125939	328516	21.93%	3.322%
14	8.416	2054	2066	2082	rVB	22111	44584	2.98%	0.451%
15	8.564	2096	2112	2132	rBV2	429300	893116	59.61%	9.033%
16	8.764	2162	2174	2180	rBV2	10217	19938	1.33%	0.202%
17	8.815	2181	2190	2202	rVV3	27837	58721	3.92%	0.594%
18	8.886	2202	2212	2225	rVB6	9975	20086	1.34%	0.203%
19	9.300	2331	2341	2352	rVB	9740	18438	1.23%	0.186%
20	10.075	2566	2582	2595	rBV	473388	853324	56.96%	8.630%
21	10.140	2596	2602	2620	rVB2	16362	29574	1.97%	0.299%
22	10.333	2651	2662	2676	rVB2	25649	45128	3.01%	0.456%
23	10.619	2737	2751	2770	rVB	833910	1498159	100.00%	15.152%
24	10.780	2783	2801	2827	rBV	160199	374363	24.99%	3.786%
25	11.397	2980	2993	3012	rVB	439281	772326	51.55%	7.811%
26	11.654	3063	3073	3082	rVB2	14911	24626	1.64%	0.249%
27	11.989	3166	3177	3193	rVB	9229	17193	1.15%	0.174%
28	12.394	3291	3303	3321	rBV	356684	585612	39.09%	5.923%
29	12.908	3452	3463	3475	rVB	32894	49685	3.32%	0.502%
30	13.111	3513	3526	3542	rVV4	74611	166199	11.09%	1.681%
31	13.242	3559	3567	3583	rVB2	23600	41114	2.74%	0.416%
32	13.336	3583	3596	3617	rBV	429758	717820	47.91%	7.260%
33	13.442	3619	3629	3639	rBV2	95333	151452	10.11%	1.532%
34	13.506	3639	3649	3656	rBV3	42774	83538	5.58%	0.845%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

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 : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Title : SW846 8260

Sum of corrected areas: 9887682

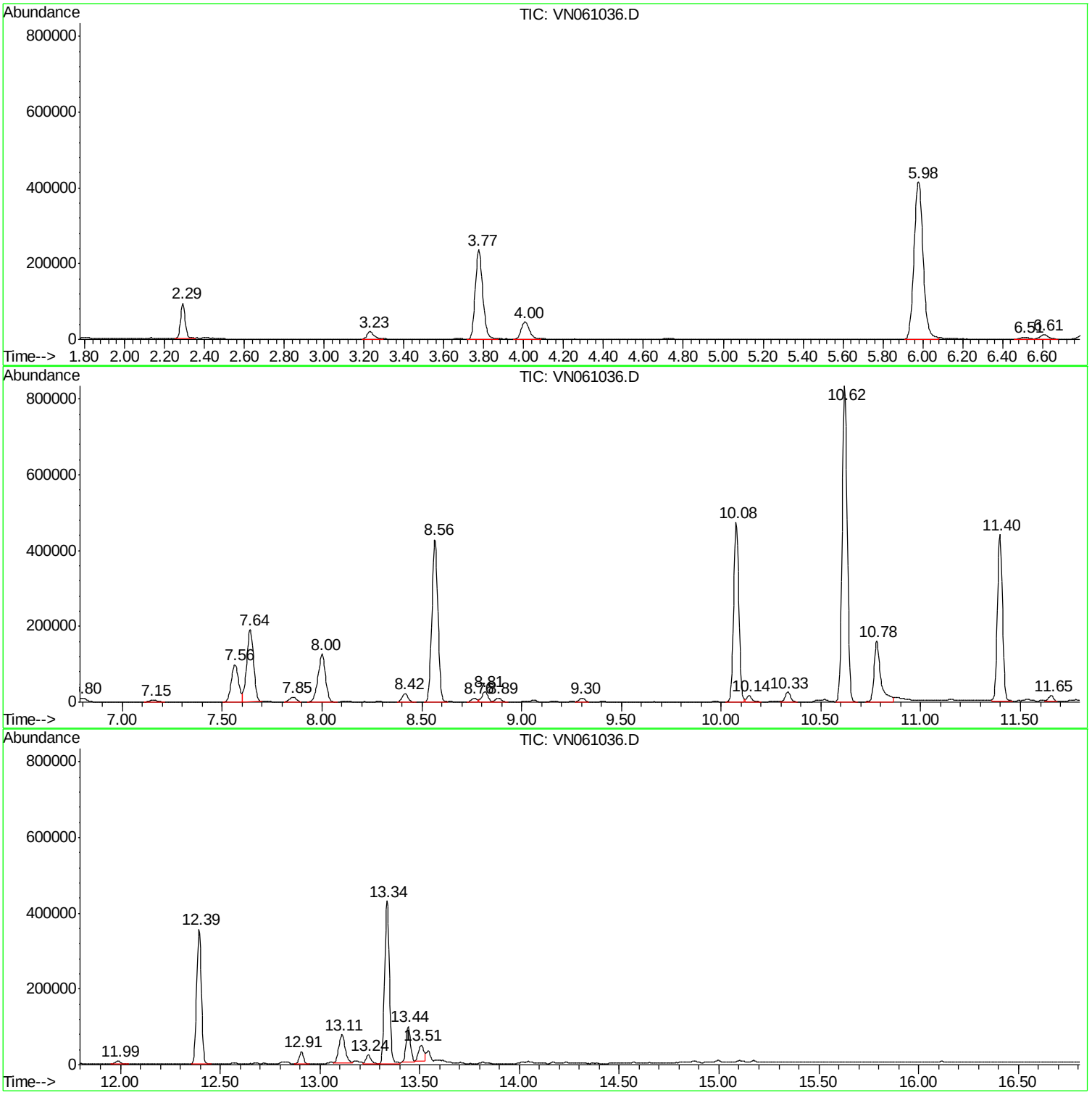
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

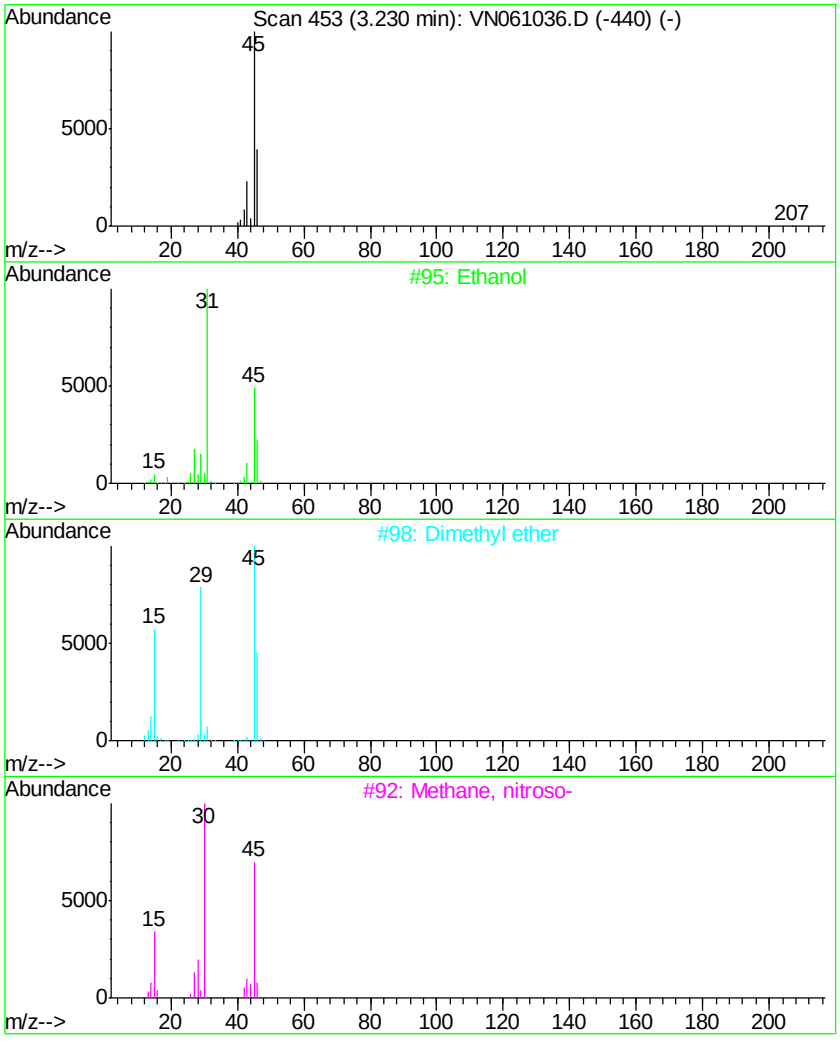
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

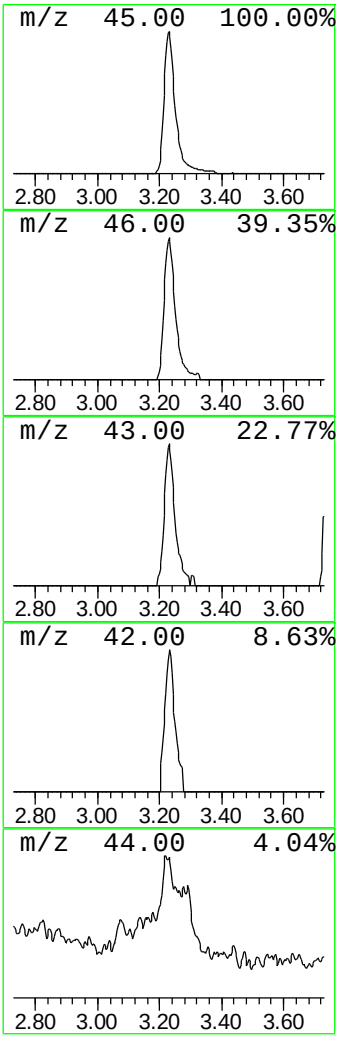
****

Peak Number 2 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	5.53 ug/l	50170	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	5
3	Methane, nitroso-	45	CH3NO	000865-40-7	3
4	Formic acid	46	CH2O2	000064-18-6	3
5	Nitrogen dioxide	46	NO2	010102-44-0	2





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

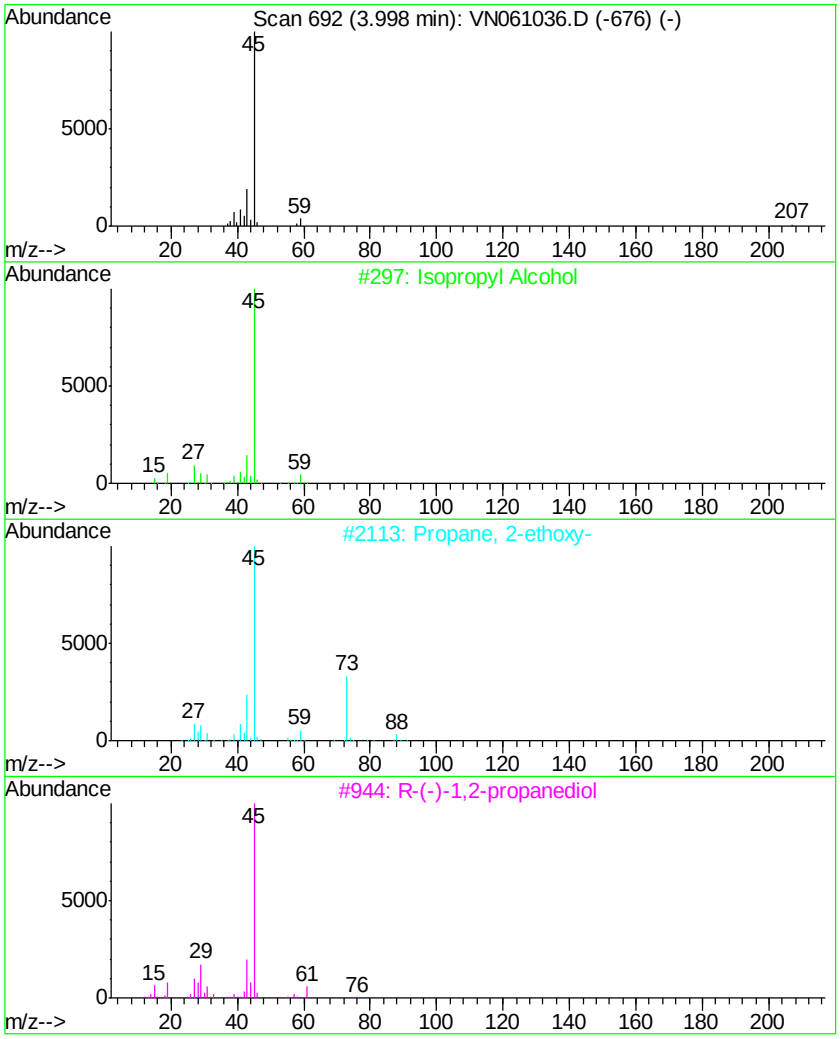
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

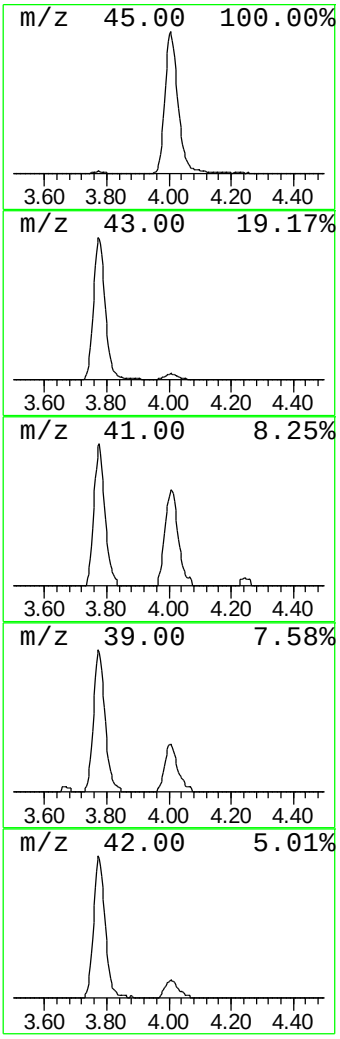
****

Peak Number 3 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	14.49 ug/l	131438	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

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

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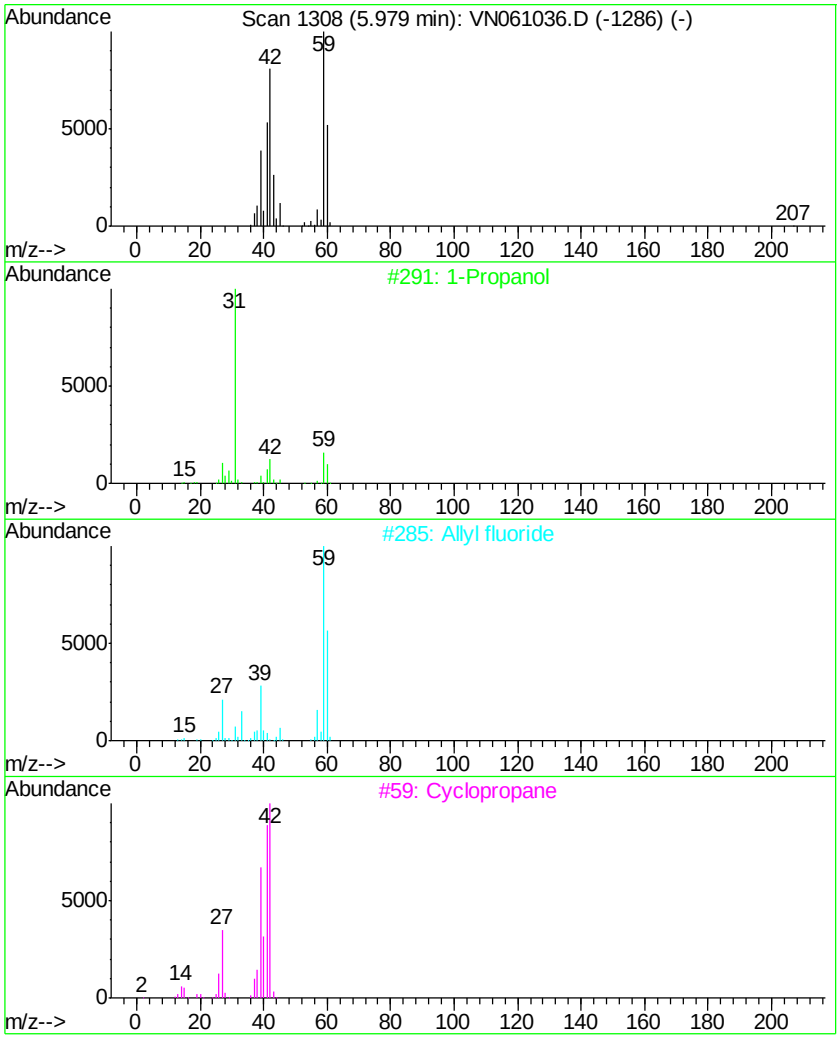
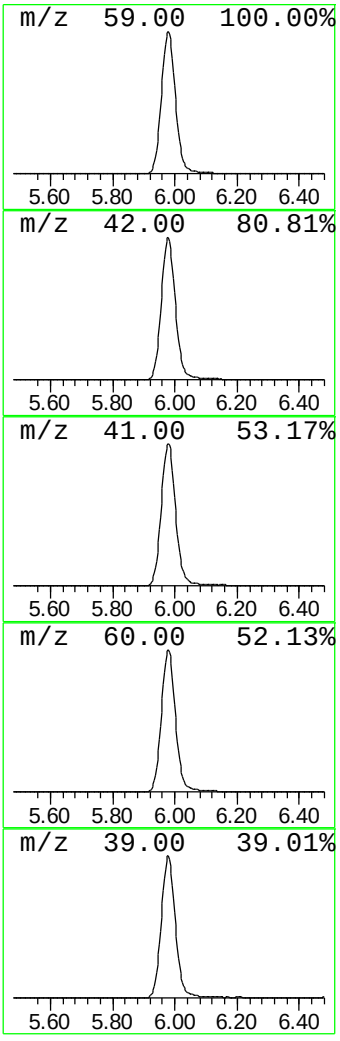
Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.98	144.81 ug/l	1313480	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	Allyl fluoride	60	C3H5F	000818-92-8	32
3	Cyclopropane	42	C3H6	000075-19-4	32
4	2-Fluoropropene	60	C3H5F	001184-60-7	25
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

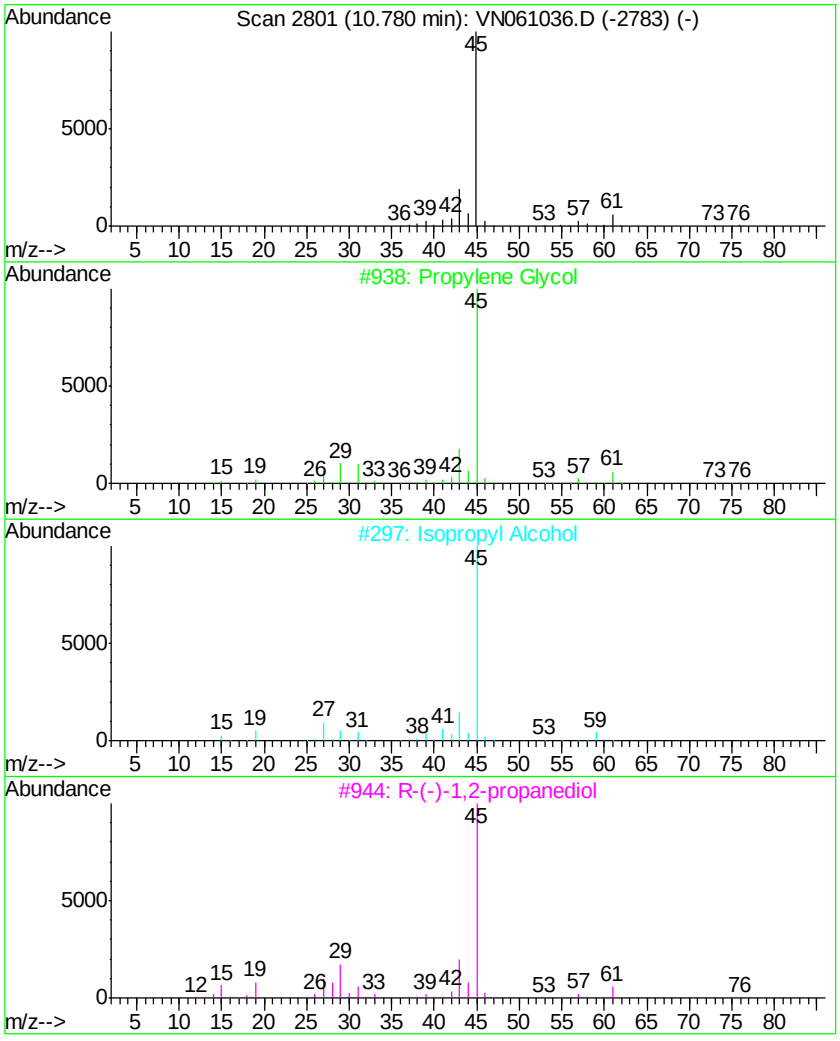
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

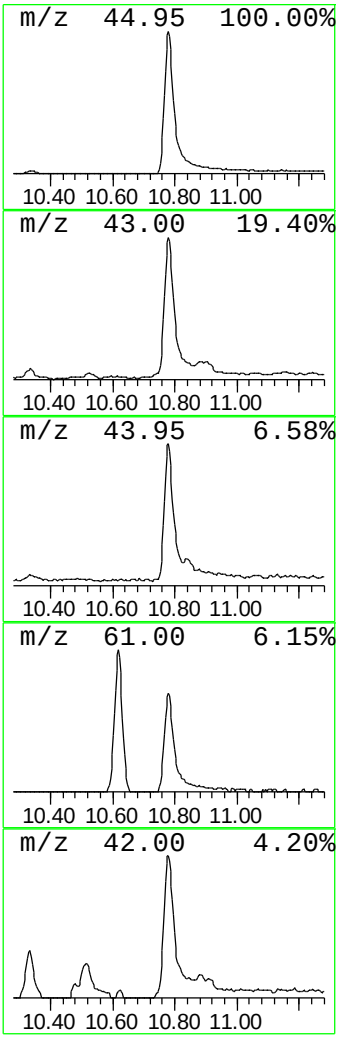
****

Peak Number 5 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	24.24 ug/l	374363	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	2-Butanol	74	C4H10O	000078-92-2	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

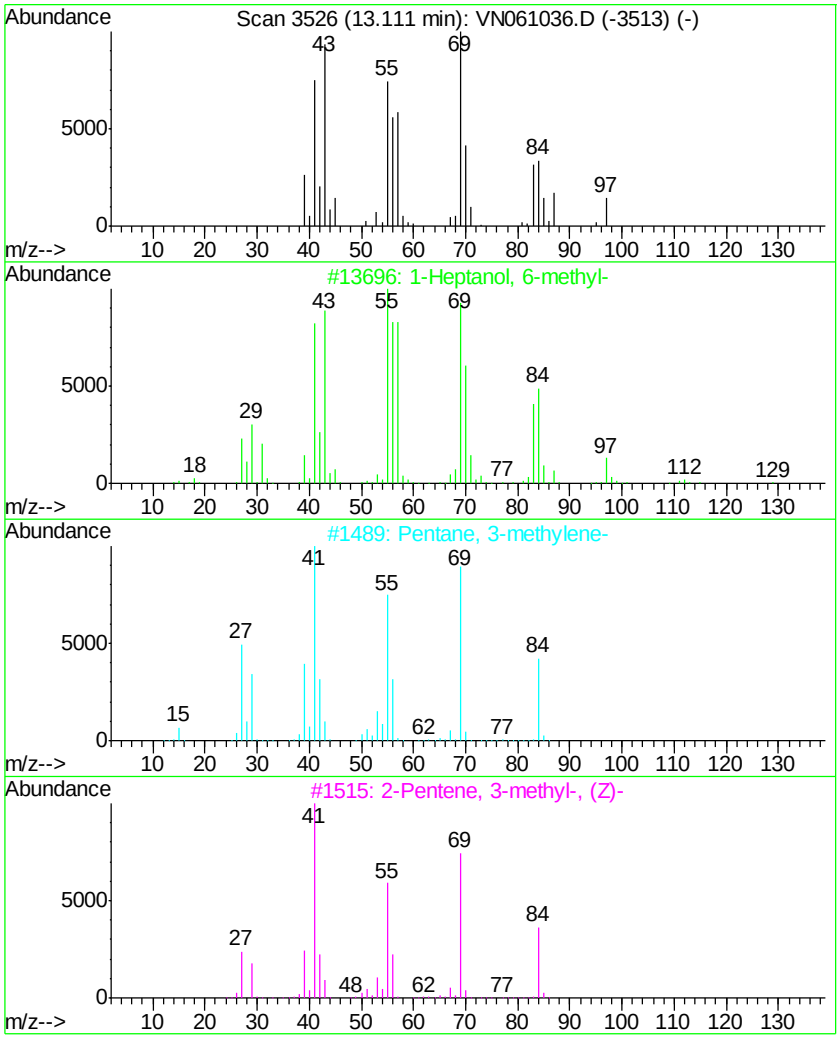
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

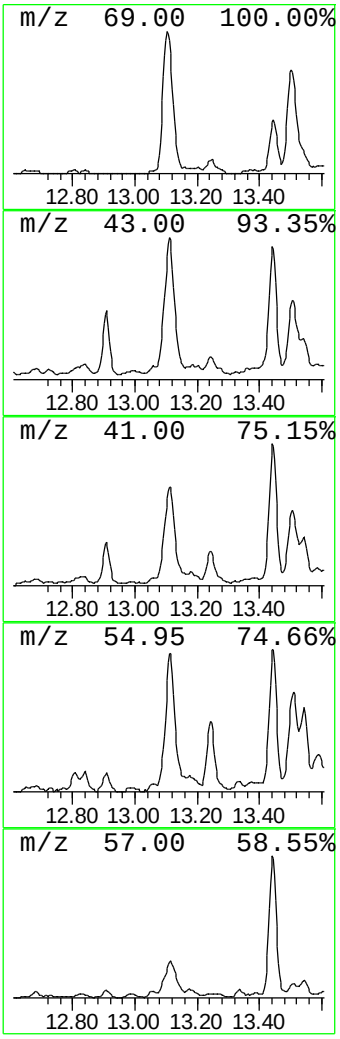
****

Peak Number 6 1-Heptanol, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	11.58 ug/l	166199	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	53
2	Pentane, 3-methylene-	84	C6H12	000760-21-4	47
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	47
4	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	43
5	Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

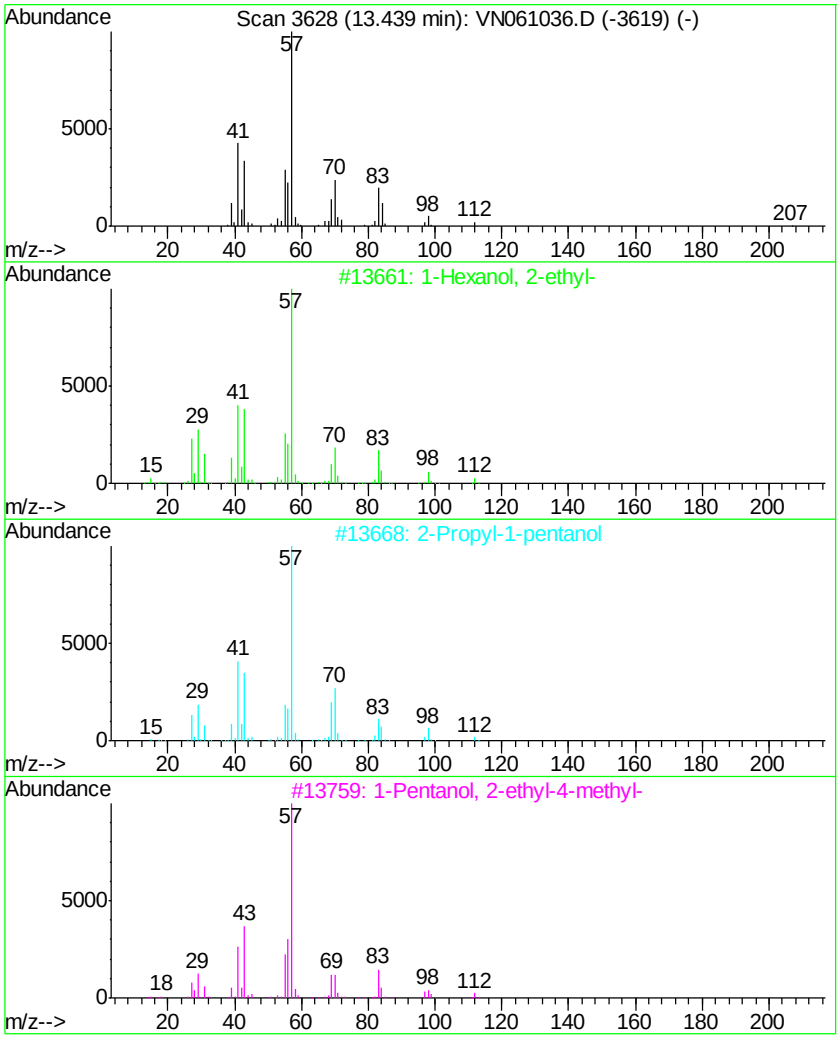
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

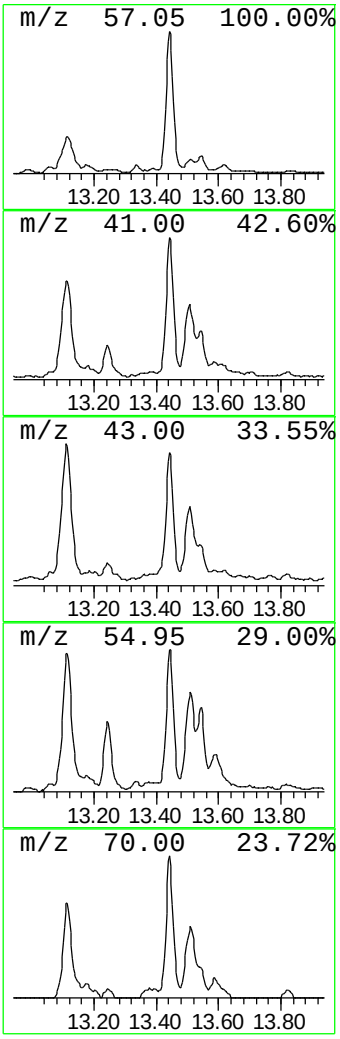
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	10.55 ug/l	151452	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.M
Quant Title : SW846 8260

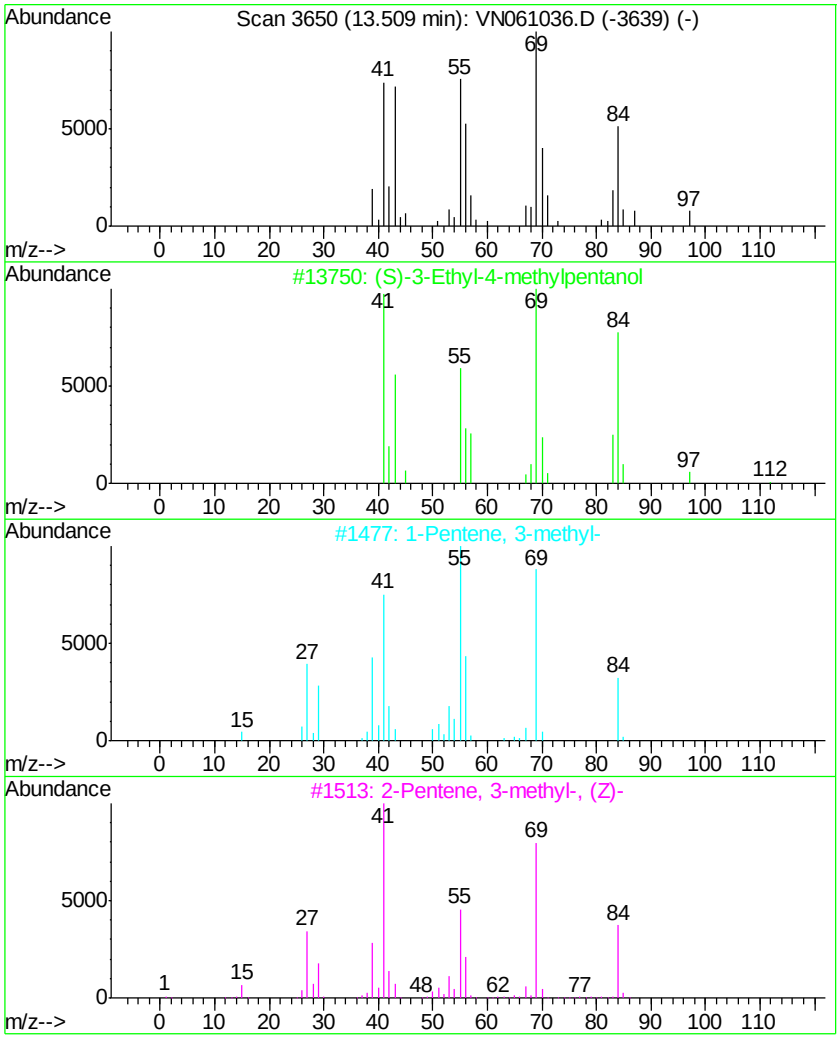
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

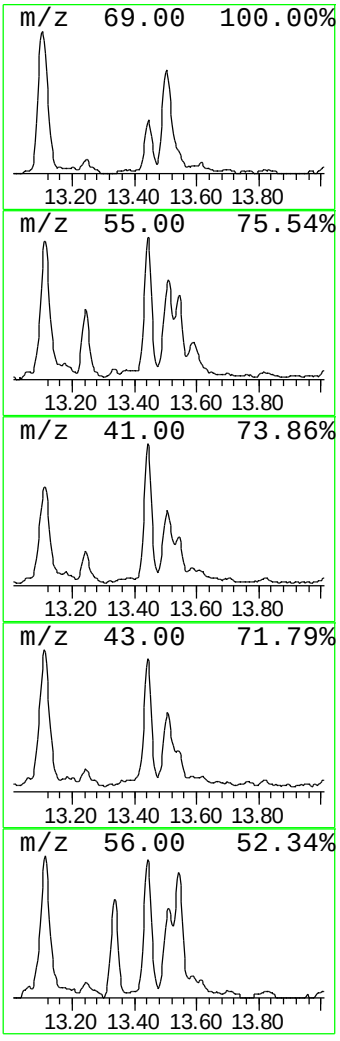
****

Peak Number 8 (S)-3-Ethyl-4-methylpentanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	5.82 ug/l	83538	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	72
2	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	59
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	50
4	2-Pentene, 2-methyl-	84	C6H12	000625-27-4	50
5	dl-Ornithine	132	C5H12N2O2	000616-07-9	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN041620\
Data File : VN061036.D
Acq On : 17 Apr 2020 00:38
Operator : JC/MD
Sample : L2299-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40862

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N041620W.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
Ethanol	3.23	5.5	ug/l	50170	1	7.64	453508	50.0
Isopropyl Alcohol	4.00	14.5	ug/l	131438	1	7.64	453508	50.0
1-Propanol	5.98	144.8	ug/l	1313480	1	7.64	453508	50.0
Propylene Glycol	10.78	24.2	ug/l	374363	3	11.40	772326	50.0
1-Heptanol, 6-met...	13.11	11.6	ug/l	166199	4	13.34	717820	50.0
1-Hexanol, 2-ethyl-	13.44	10.6	ug/l	151452	4	13.34	717820	50.0
(S)-3-Ethyl-4-met...	13.51	5.8	ug/l	83538	4	13.34	717820	50.0