LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN060319\
Data File : VN055961.D
Acq On : 3 Jun 2019 15:05
Operator : JC/SP
Sample : K3125-25 5X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

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\82N052319W.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	2.307	153	166	195	rBV	1615257	2688565	39.37%	8.919%
2	3.285	453	470	506	rBV	432235	1132920	16.59%	3.758%
3	3.818	620	636	663	rBV	78422	207634	3.04%	0.689%
4	4.088	696	720	743	rBV	41867	124752	1.83%	0.414%
5	6.056	1311	1332	1360	rBV	238266	743590	10.89%	2.467%
6	6.648	1498	1516	1546	rBV	118401	348202	5.10%	1.155%
7	7.590	1790	1809	1820	rBV	199246	495497	7.26%	1.644%
8	7.664	1820	1832	1857	rVB	362545	863098	12.64%	2.863%
9	8.027	1925	1945	1965	rBV	215496	500986	7.34%	1.662%
10	8.593	2103	2121	2166	rBV2	3136411	6829605	100.00%	22.657%
11	8.841	2177	2198	2209	rBV	2778131	5600161	82.00%	18.578%
12	8.899	2210	2216	2252	rVB	393684	758455	11.11%	2.516%
13	10.088	2571	2586	2601	rBV	835277	1560252	22.85%	5.176%
14	10.349	2655	2667	2680	rBV	44536	76708	1.12%	0.254%
15	10.493	2699	2712	2737	rBV4	50528	101427	1.49%	0.336%
16	10.805	2788	2809	2818	rBV	1187891	3112980	45.58%	10.327%
17	11.406	2982	2996	3022	rBV	790242	1391956	20.38%	4.618%
18	11.541	3022	3038	3051	rBV	231518	381889	5.59%	1.267%
19	11.615	3052	3061	3072	rBV	43577	76880	1.13%	0.255%
20	12.027	3180	3189	3205	rVB	47600	81783	1.20%	0.271%
21	12.400	3280	3305	3334	rVB	614340	1073267	15.71%	3.561%
22	13.342	3585	3598	3613	rBV	668180	1132003	16.57%	3.755%
23	13.448	3622	3631	3643	rBV	49461	78617	1.15%	0.261%
24	14.892	4071	4080	4092	rBV2	138155	228619	3.35%	0.758%
25	15.130	4142	4154	4166	rBV	119607	224986	3.29%	0.746%
26	16.101	4446	4456	4465	rBV4	34256	72775	1.07%	0.241%
27	16.159	4466	4474	4489	rVV2	49121	102711	1.50%	0.341%
28	16.348	4522	4533	4545	rBV2	62365	153275	2.24%	0.508%

Sum of corrected areas: 30143593

LSC Report - Integrated Chromatogram

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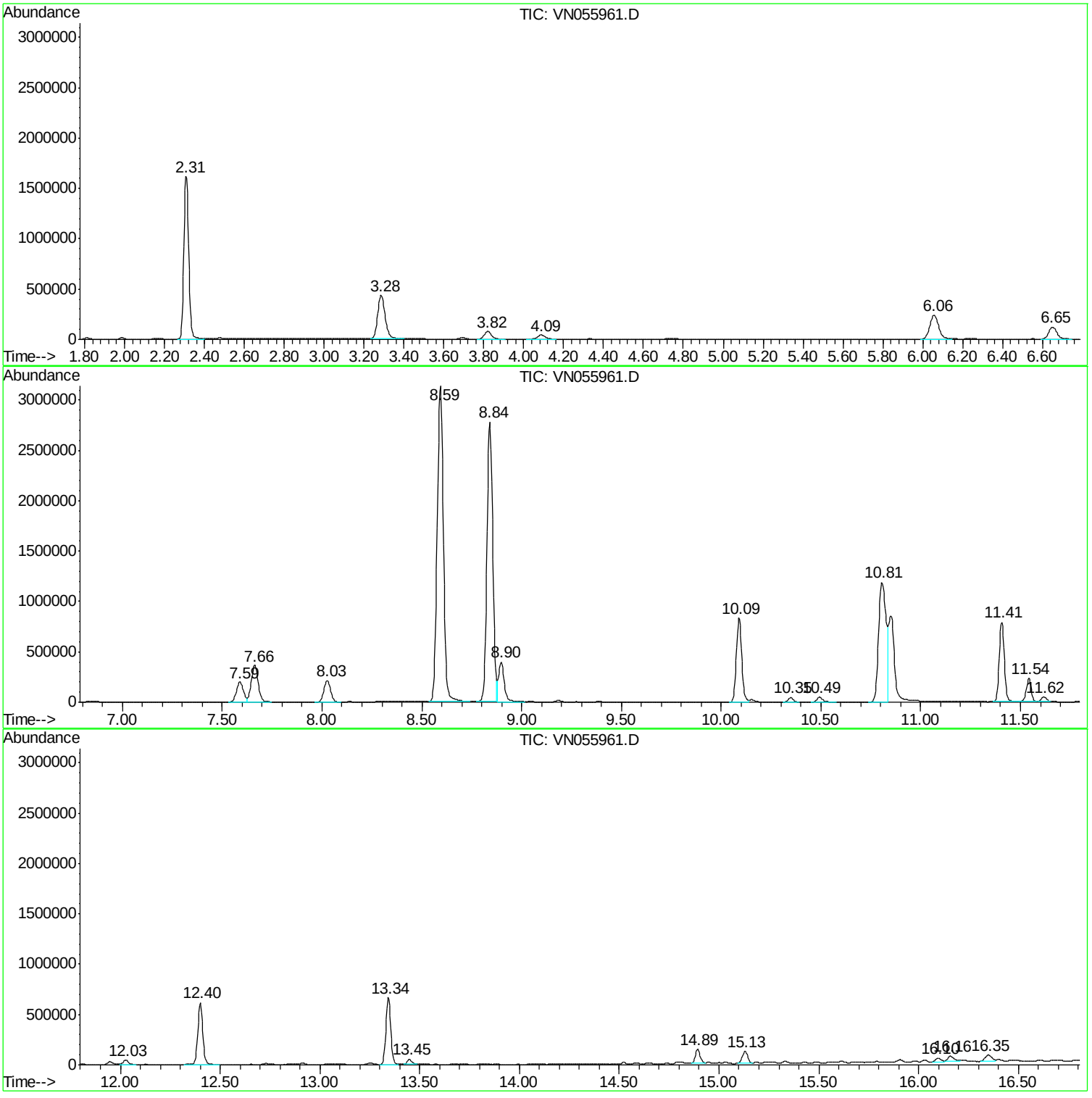
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Quant Title : SW846 8260

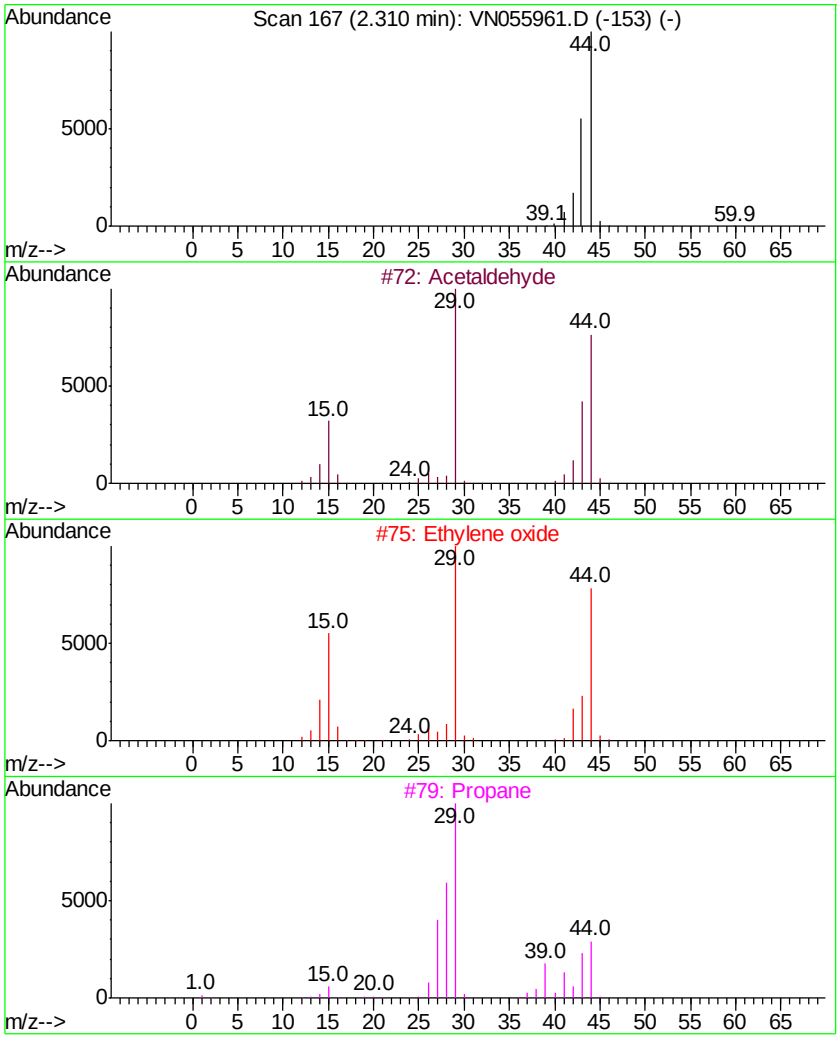
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

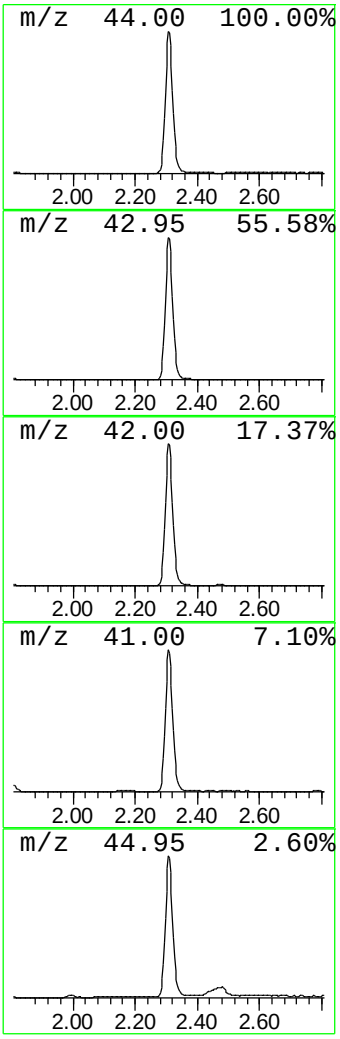
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	155.75 ug/l	2688570	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	Alanine	89	C3H7NO2	000056-41-7	4





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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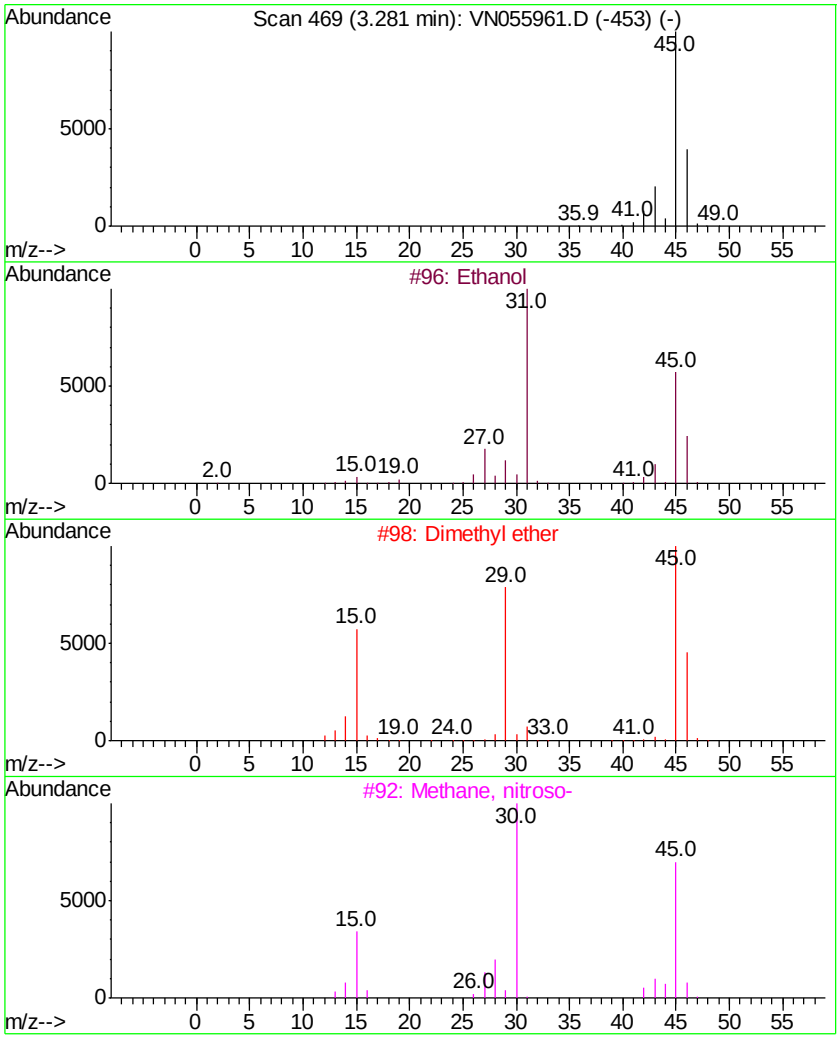
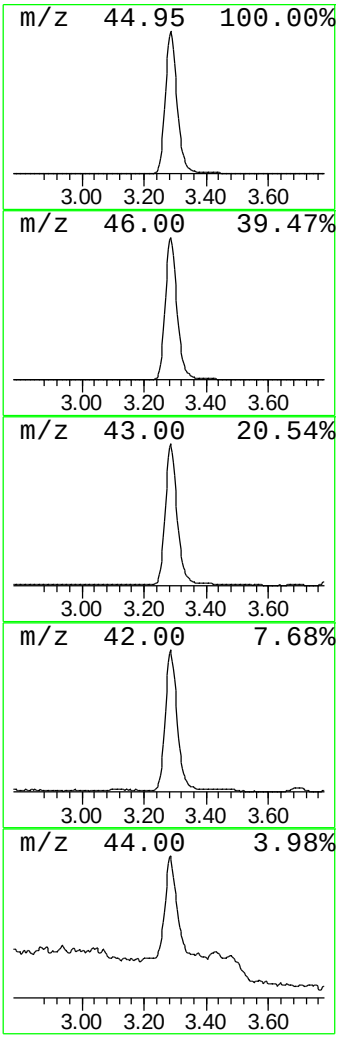
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	65.63 ug/l	1132920	Pentafluorobenzene	7.66

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	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





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Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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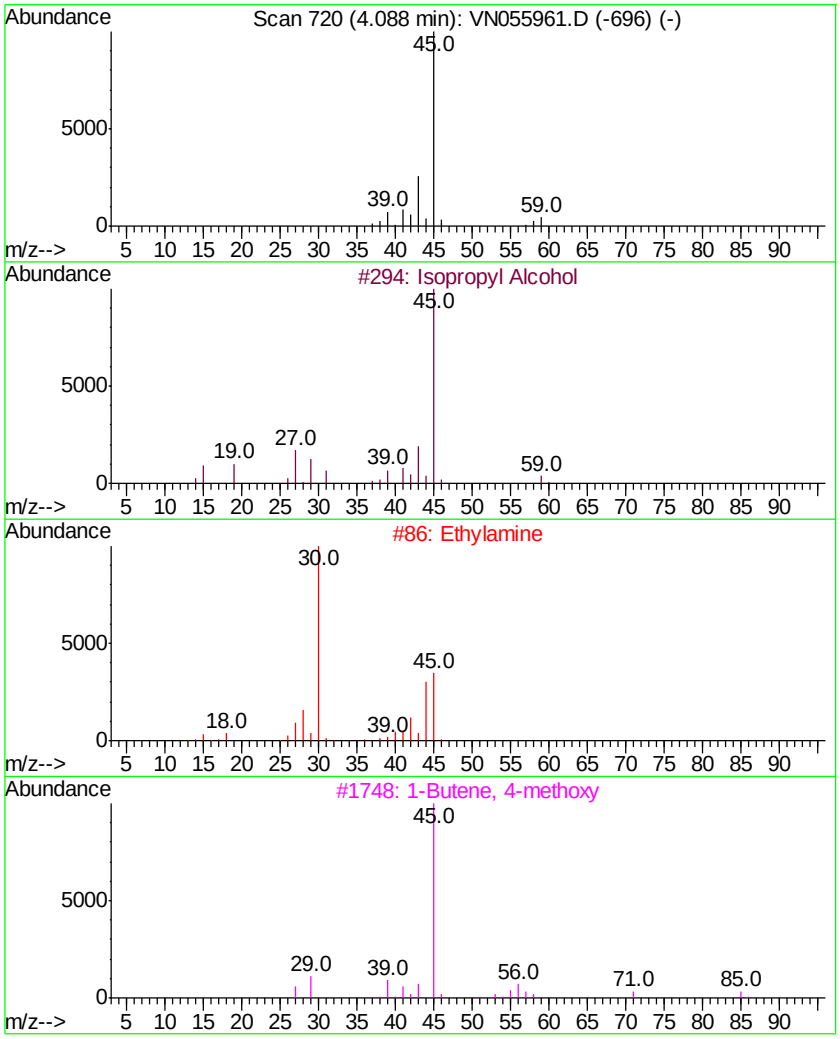
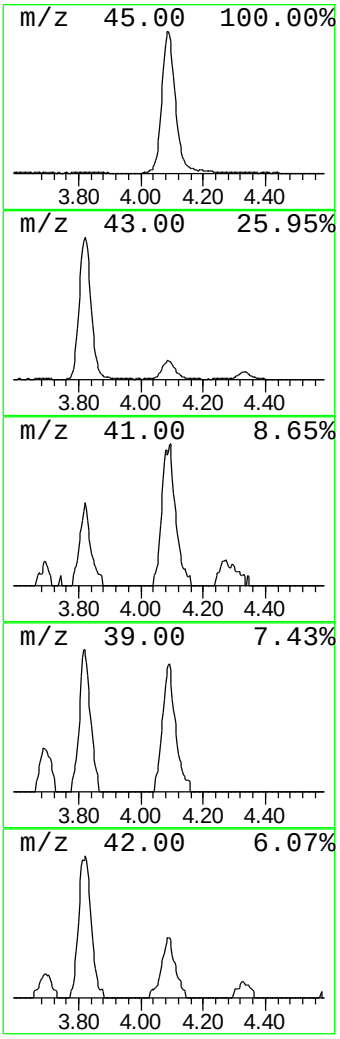
Peak Number 3 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	7.23 ug/l	124752	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2	Ethylamine	45	C2H7N	000075-04-7	5
3	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
4	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
5	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4





Library Search Compound Report

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Sample : K3125-25 5X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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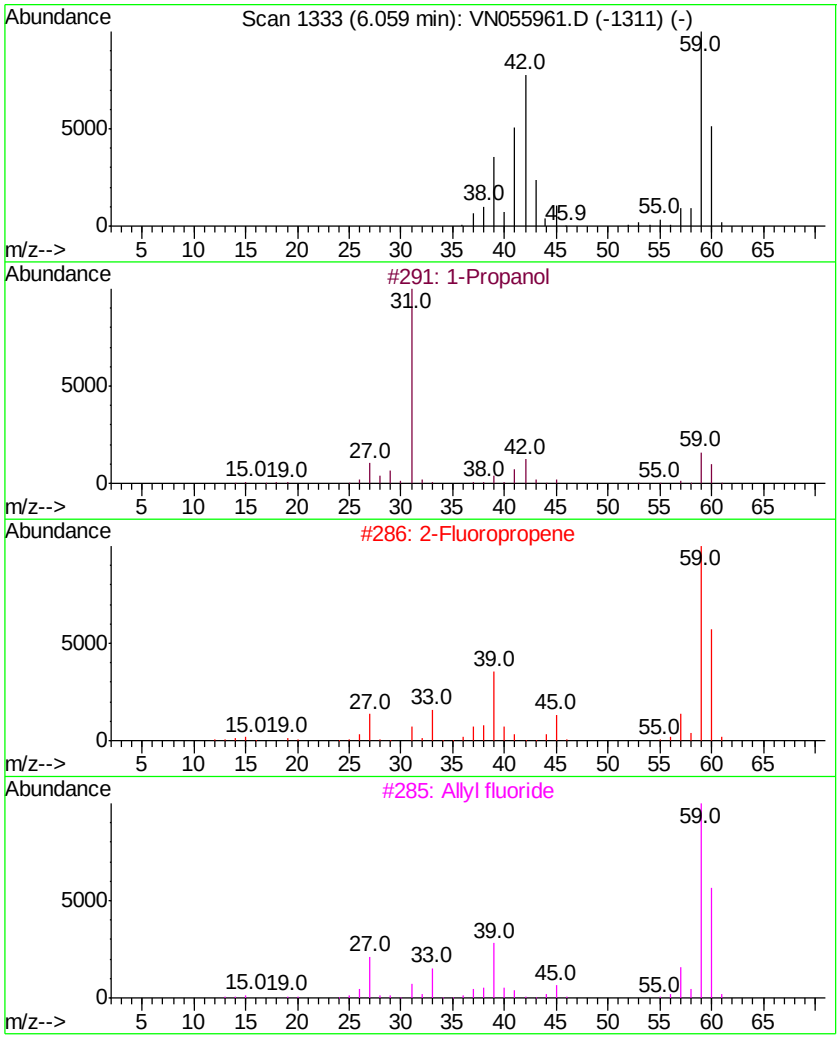
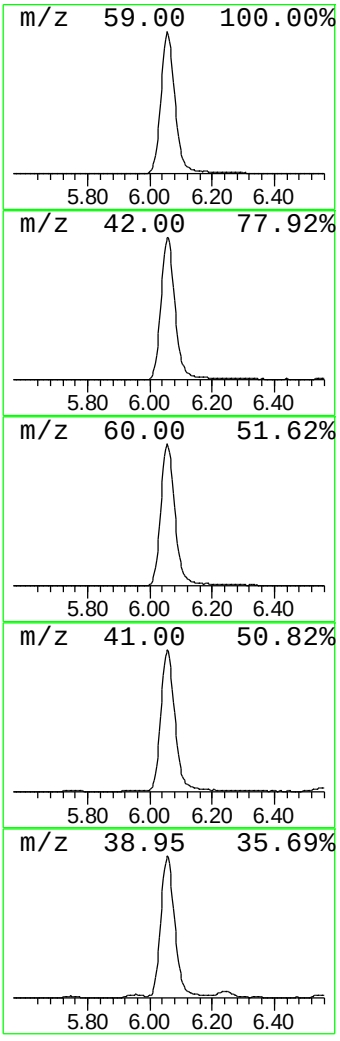
Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	43.08 ug/l	743590	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	72
2	2-Fluoropropene	60	C3H5F	001184-60-7	49
3	Allyl fluoride	60	C3H5F	000818-92-8	47
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	23
5	Cyclopropane	42	C3H6	000075-19-4	12





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Data File : VN055961.D
Acq On : 3 Jun 2019 15:05
Operator : JC/SP
Sample : K3125-25 5X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

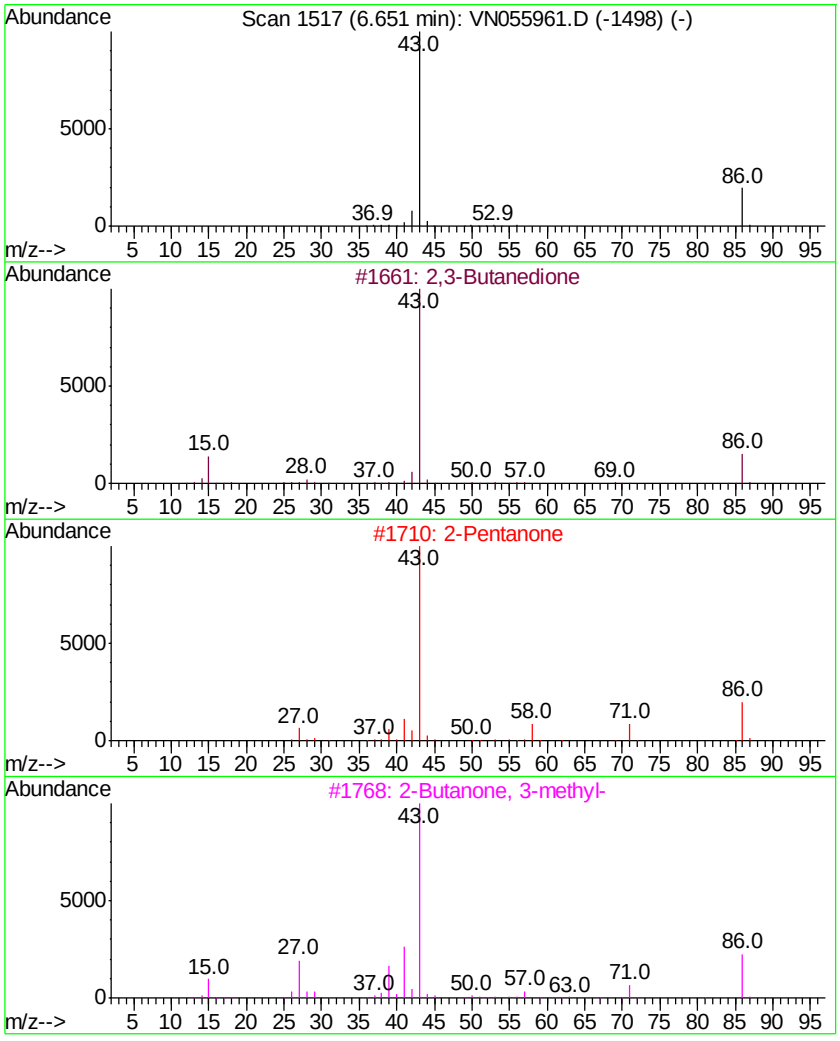
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

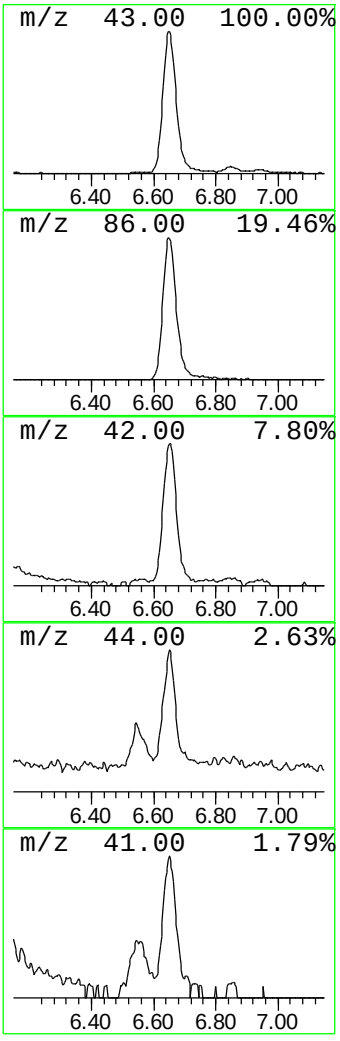
****

Peak Number 5 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	20.17 ug/l	348202	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	72
2	2-Pentanone	86	C5H10O	000107-87-9	72
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
4	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	7
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5





Library Search Compound Report

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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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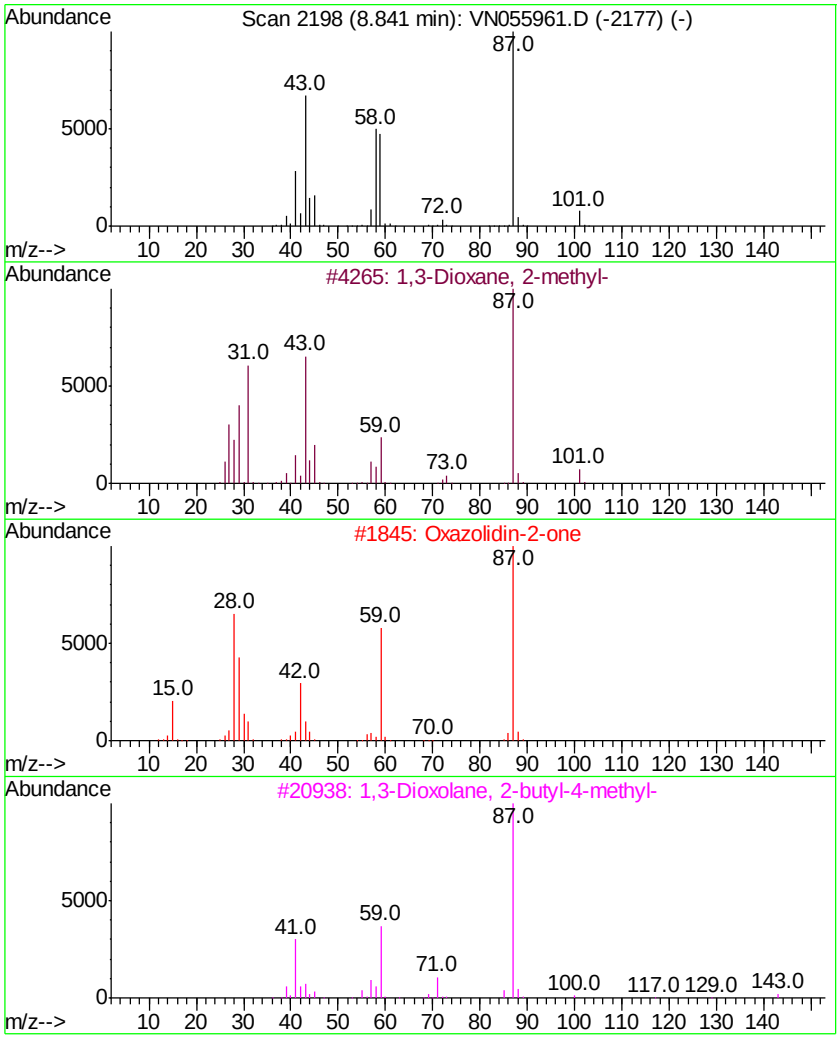
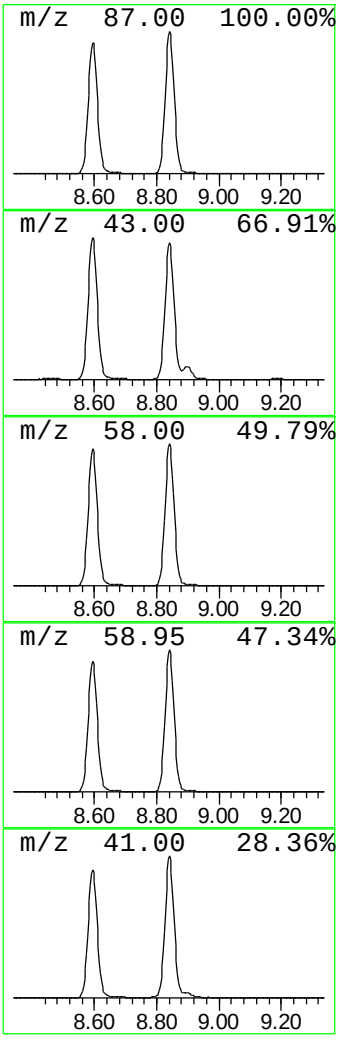
****

Peak Number 6 unknown8.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	41.00 ug/l	5600160	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	49
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
3	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
4	Formamide, N-butyl-	101	C5H11NO	000871-71-6	10
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9





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Quant Title : SW846 8260

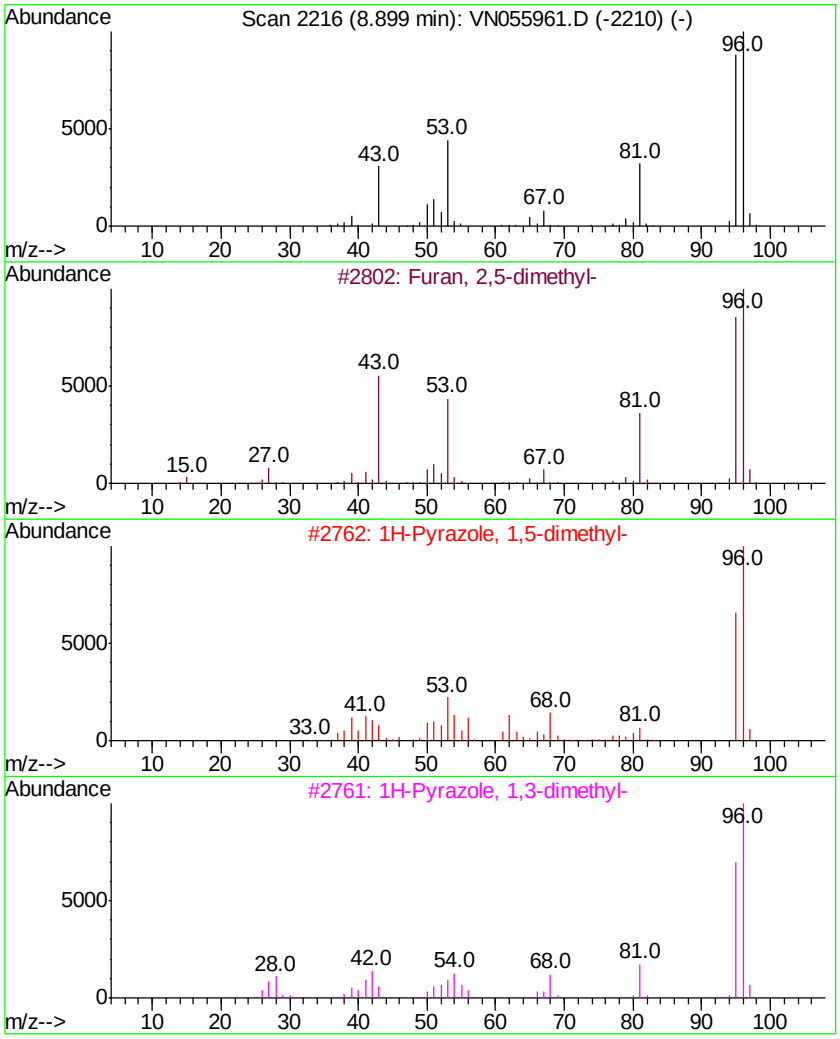
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

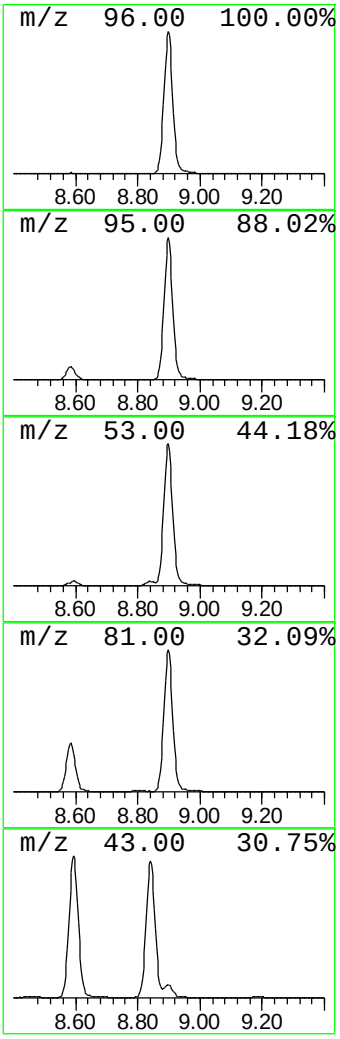
****

Peak Number 7 Furan, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	5.55 ug/l	758455	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	95
2	1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	000694-31-5	43
3	1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	38
4	Furfural	96	C5H4O2	000098-01-1	35
5	3,5-Dimethylpyrazole	96	C5H8N2	000067-51-6	35





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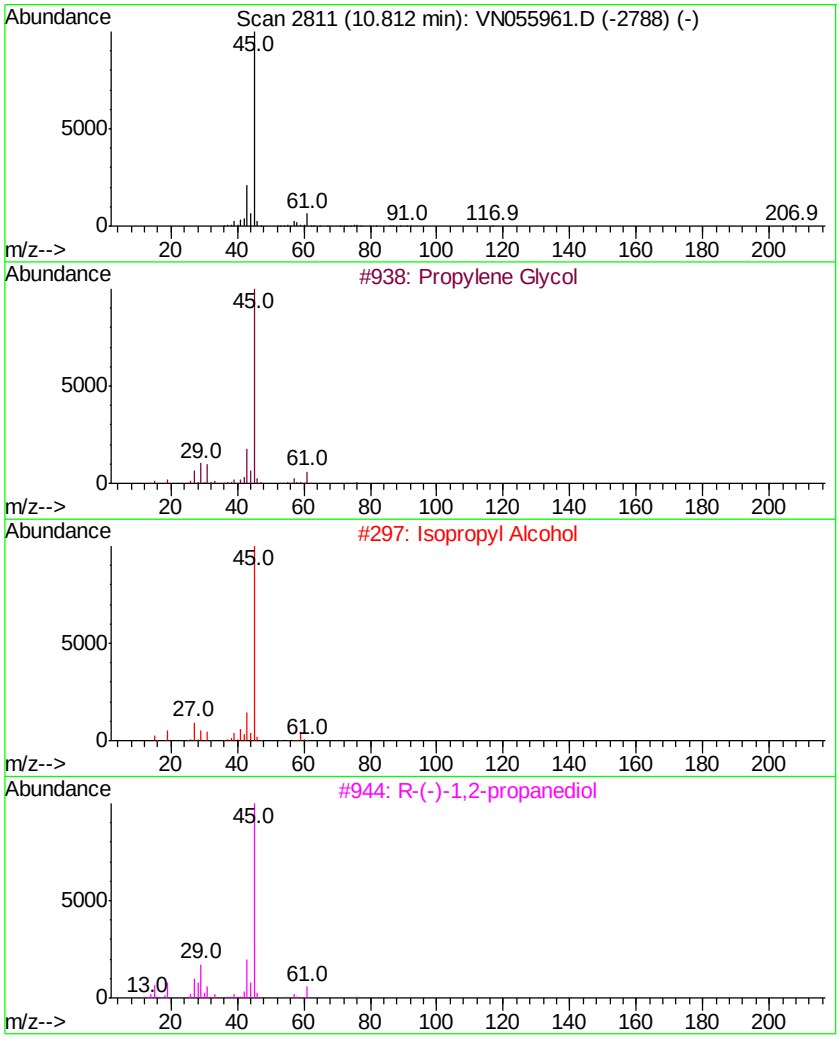
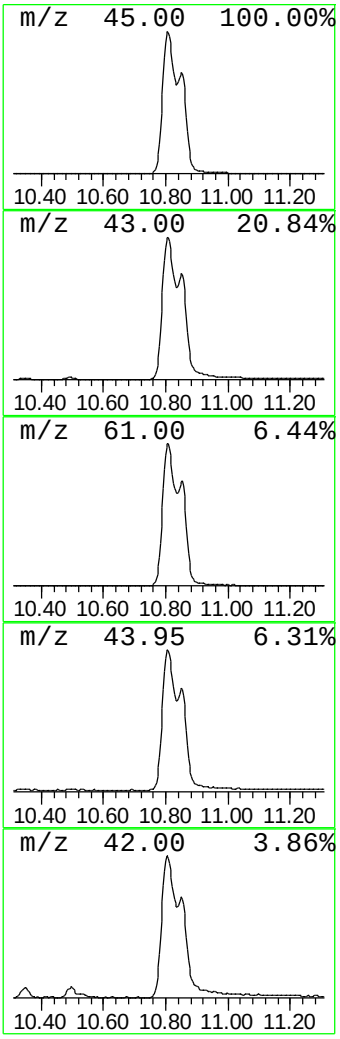
Peak Number 8 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	111.82 ug/l	3112980	Chlorobenzene-d5	11.41

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	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	2-Butanol	74	C4H10O	000078-92-2	9





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Quant Title : SW846 8260

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

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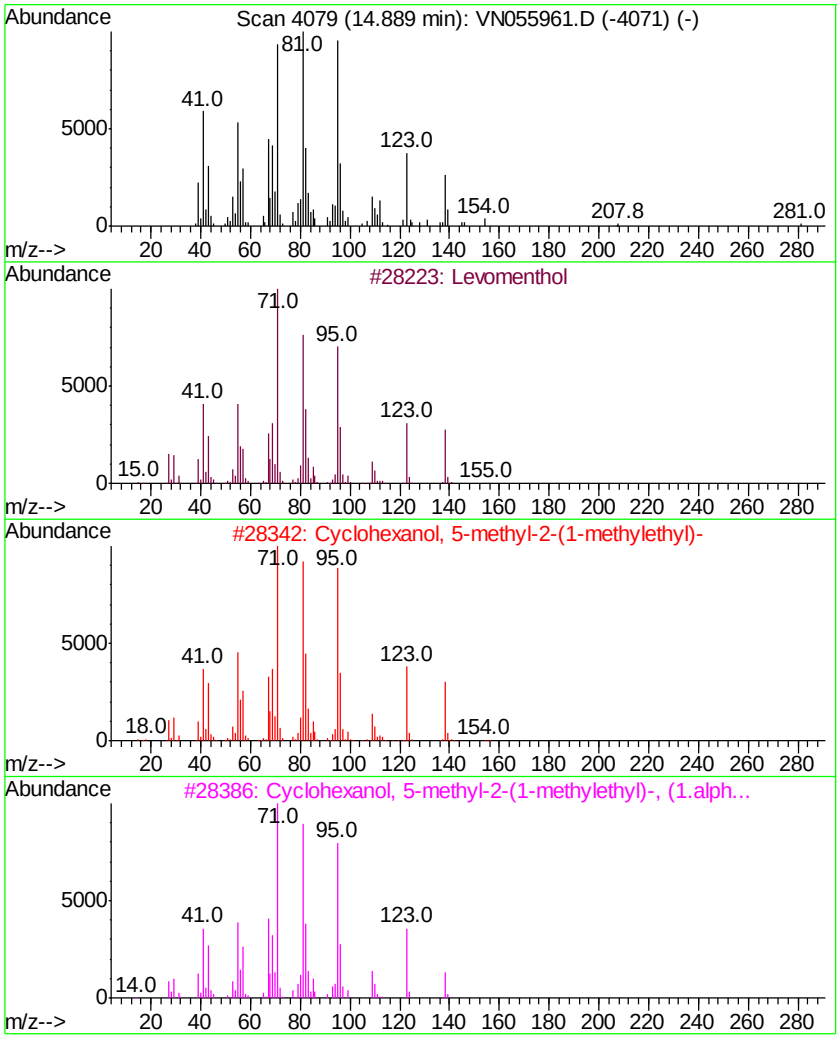
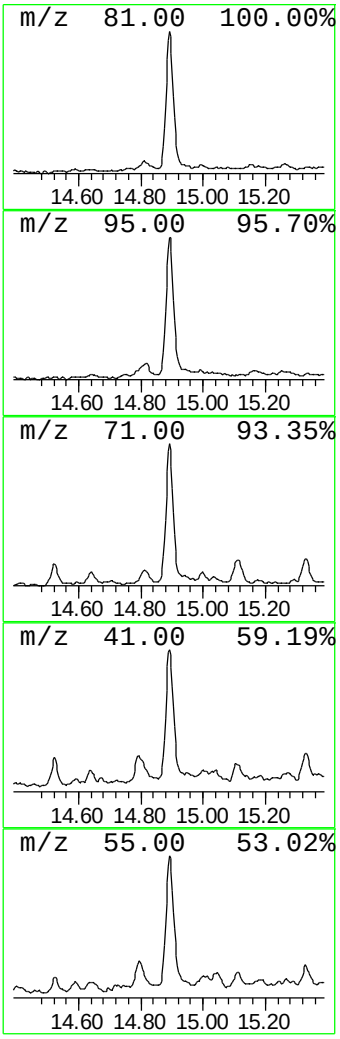
Peak Number 9 Levomenthol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	10.10 ug/l	228619	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levomenthol	156	C10H20O	002216-51-5	87
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	87
4	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	86
5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	86





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TIC Library : C:\DATABASE\NIST11.L
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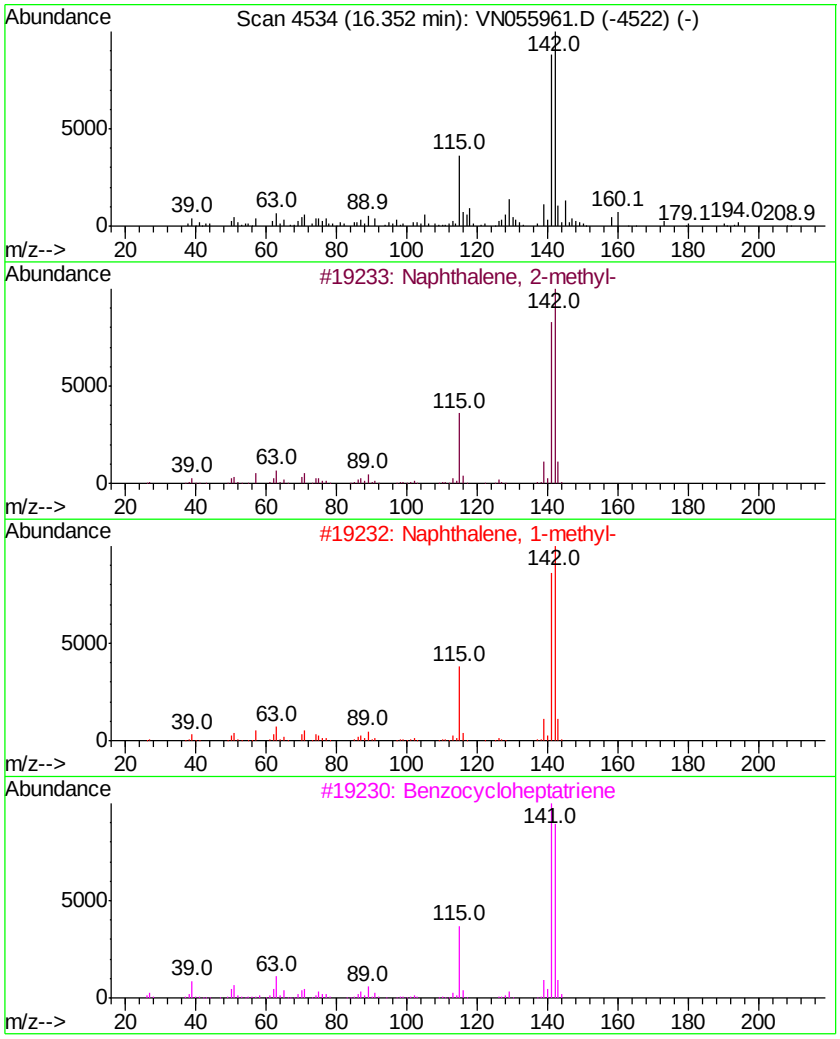
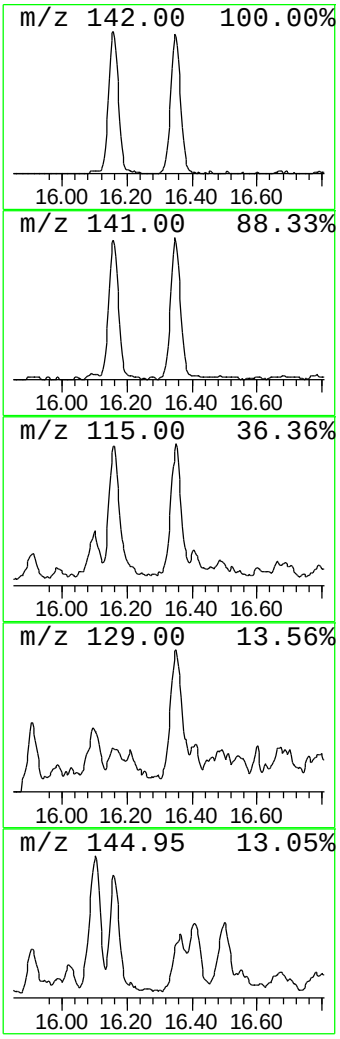
Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	6.77 ug/l	153275	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3	Benzocycloheptatriene	142	C11H10	000264-09-5	87
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	83
5	Spiro(9-methylenetricyclo[6.2.1....	184	C13H12O	033929-47-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN060319\
Data File : VN055961.D
Acq On : 3 Jun 2019 15:05
Operator : JC/SP
Sample : K3125-25 5X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.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
Acetaldehyde	2.31	155.8	ug/l	2688570	1	7.66	863098	50.0
Ethanol	3.28	65.6	ug/l	1132920	1	7.66	863098	50.0
Isopropyl Alcohol	4.09	7.2	ug/l	124752	1	7.66	863098	50.0
1-Propanol	6.06	43.1	ug/l	743590	1	7.66	863098	50.0
2,3-Butanedione	6.65	20.2	ug/l	348202	1	7.66	863098	50.0
unknown8.84	8.84	41.0	ug/l	5600160	2	8.58	6829610	50.0
Furan, 2,5-dimethyl-	8.90	5.5	ug/l	758455	2	8.58	6829610	50.0
Propylene Glycol	10.81	111.8	ug/l	3112980	3	11.41	1391960	50.0
Levomenthol	14.89	10.1	ug/l	228619	4	13.34	1132000	50.0
Naphthalene, 2-me...	16.35	6.8	ug/l	153275	4	13.34	1132000	50.0