LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 46 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	1.989	58	67	77	rBV	26711	37028	1.42%	0.239%
2	2.311	154	167	194	rBV	859096	1437122	55.15%	9.265%
3	3.285	455	470	503	rBV	163651	443552	17.02%	2.859%
4	3.822	621	637	660	rBV	31145	80668	3.10%	0.520%
5	4.089	707	720	743	rVB2	17725	47911	1.84%	0.309%
6	4.745	902	924	946	rBV	12892	46405	1.78%	0.299%
7	6.056	1312	1332	1361	rBV2	89084	291709	11.19%	1.881%
8	6.651	1500	1517	1541	rBV2	50034	151661	5.82%	0.978%
9	6.844	1560	1577	1598	rVB3	9376	27680	1.06%	0.178%
10	7.590	1791	1809	1820	rBV	199090	494331	18.97%	3.187%
11	7.664	1820	1832	1854	rVB	368447	876915	33.65%	5.653%
12	8.027	1927	1945	1966	rBV	210275	496460	19.05%	3.200%
13	8.590	2103	2120	2167	rVB3	1148931	2605907	100.00%	16.799%
14	8.841	2178	2198	2209	rBV	979896	1953271	74.96%	12.592%
15	8.899	2209	2216	2239	rVB	229708	449250	17.24%	2.896%
16	10.092	2572	2587	2600	rBV	835749	1561885	59.94%	10.069%
17	10.153	2601	2606	2627	rVB	44888	84100	3.23%	0.542%
18	10.493	2699	2712	2727	rBV4	17972	36291	1.39%	0.234%
19	10.825	2795	2815	2817	rBV	60720	139622	5.36%	0.900%
20	11.407	2982	2996	3021	rBV	772247	1391141	53.38%	8.968%
21	11.542	3021	3038	3050	rVB3	58230	113079	4.34%	0.729%
22	11.616	3050	3061	3074	rBV	51532	94900	3.64%	0.612%
23	11.947	3154	3164	3175	rBV	27159	46853	1.80%	0.302%
24	12.027	3180	3189	3201	rVB	20575	33785	1.30%	0.218%
25	12.400	3289	3305	3328	rVB	601365	1035430	39.73%	6.675%
26	13.040	3493	3504	3514	rBV	28833	46474	1.78%	0.300%
27	13.342	3585	3598	3616	rBV	639280	1065505	40.89%	6.869%
28	13.452	3621	3632	3644	rVV2	21989	36764	1.41%	0.237%
29	14.892	4070	4080	4093	rBV2	70100	119762	4.60%	0.772%
30	15.130	4142	4154	4165	rBV	81547	143645	5.51%	0.926%
31	16.159	4464	4474	4494	rVB3	27838	60312	2.31%	0.389%
32	16.349	4522	4533	4548	rBV	28028	62663	2.40%	0.404%

LSC Area Percent Report

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Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 46 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

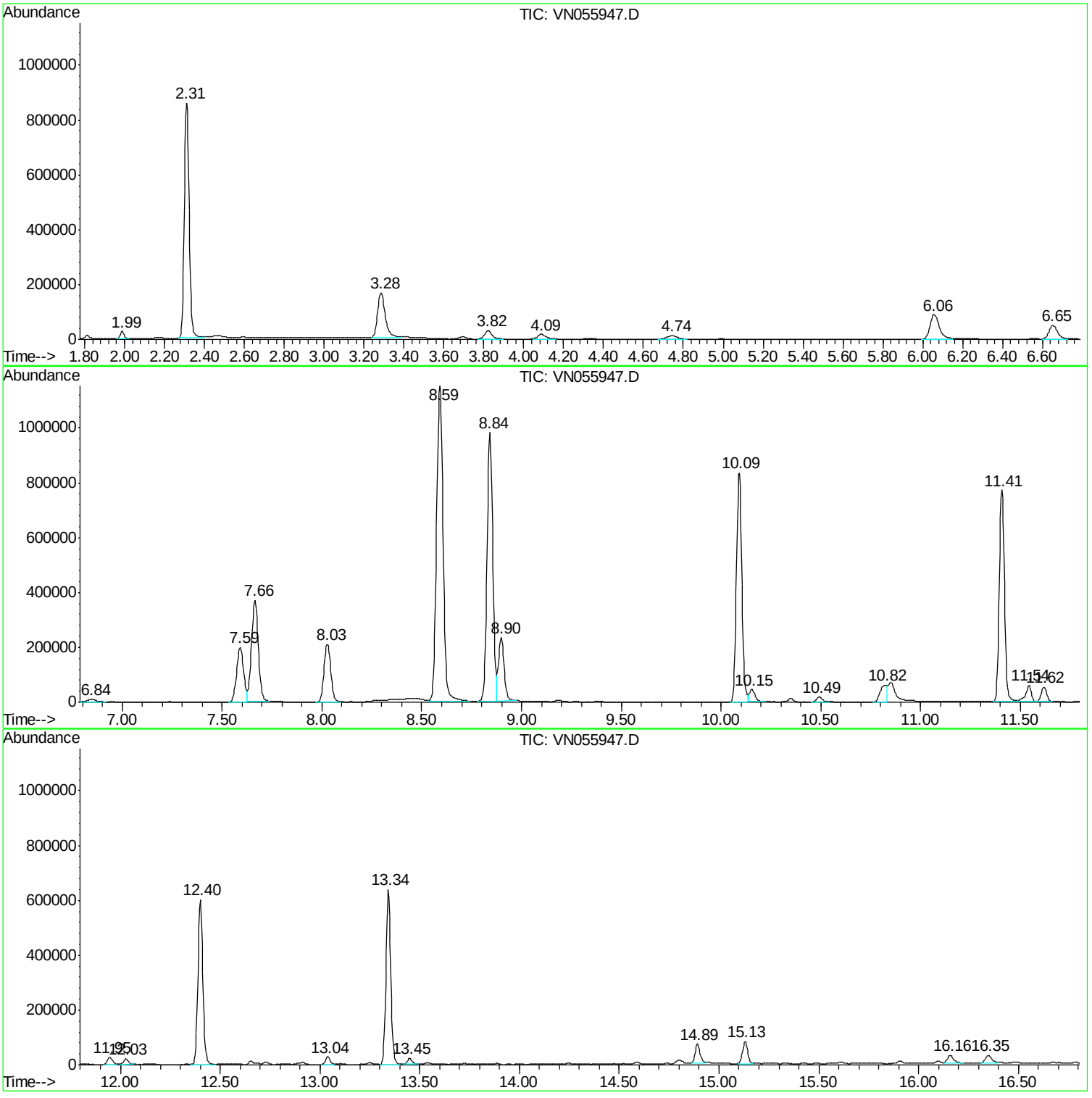
Sum of corrected areas: 15512081

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 46 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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

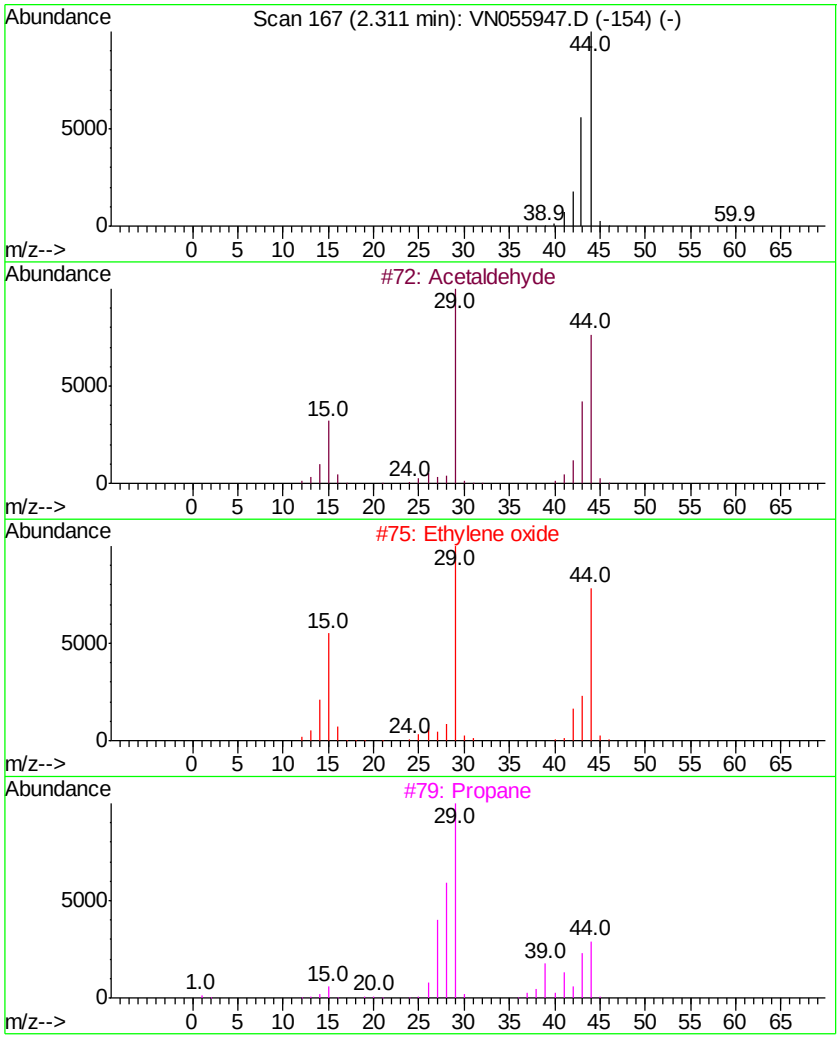
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

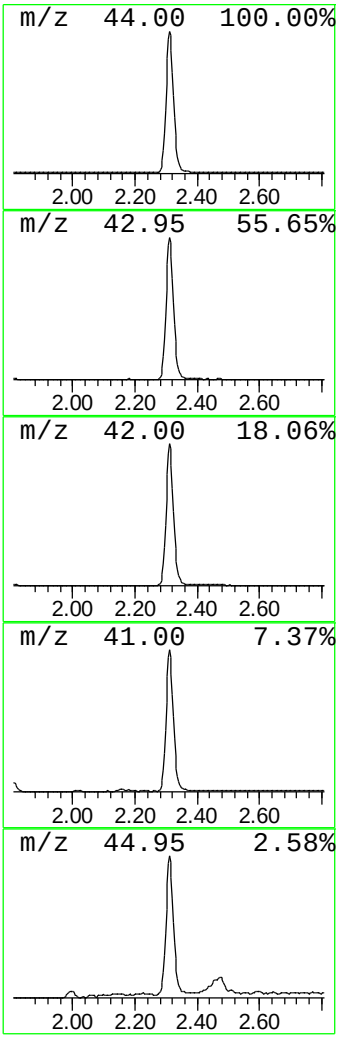
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	81.94 ug/l	1437120	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	Alanine	89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 46 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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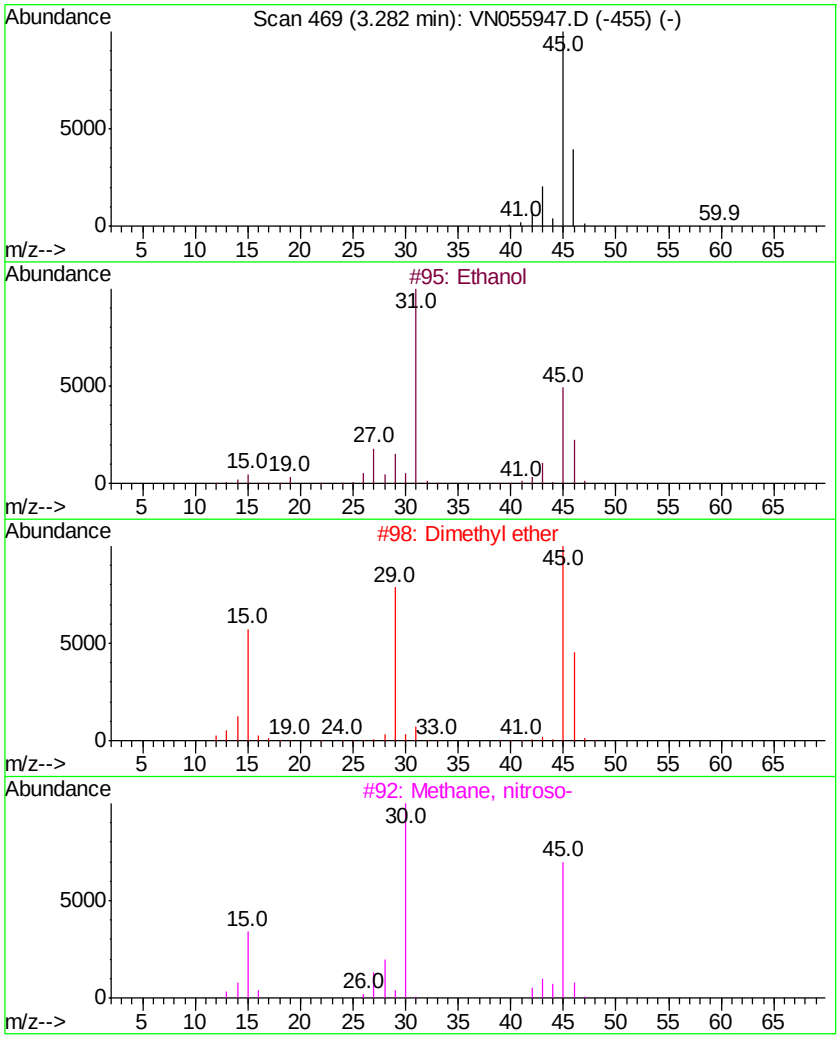
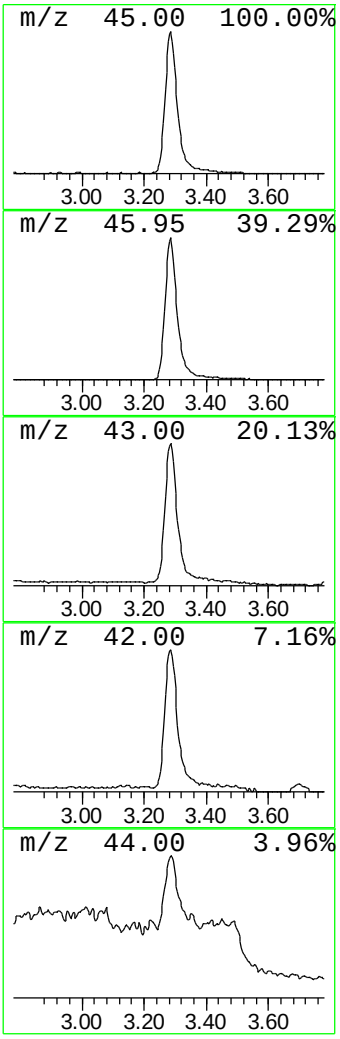
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	25.29 ug/l	443552	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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

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

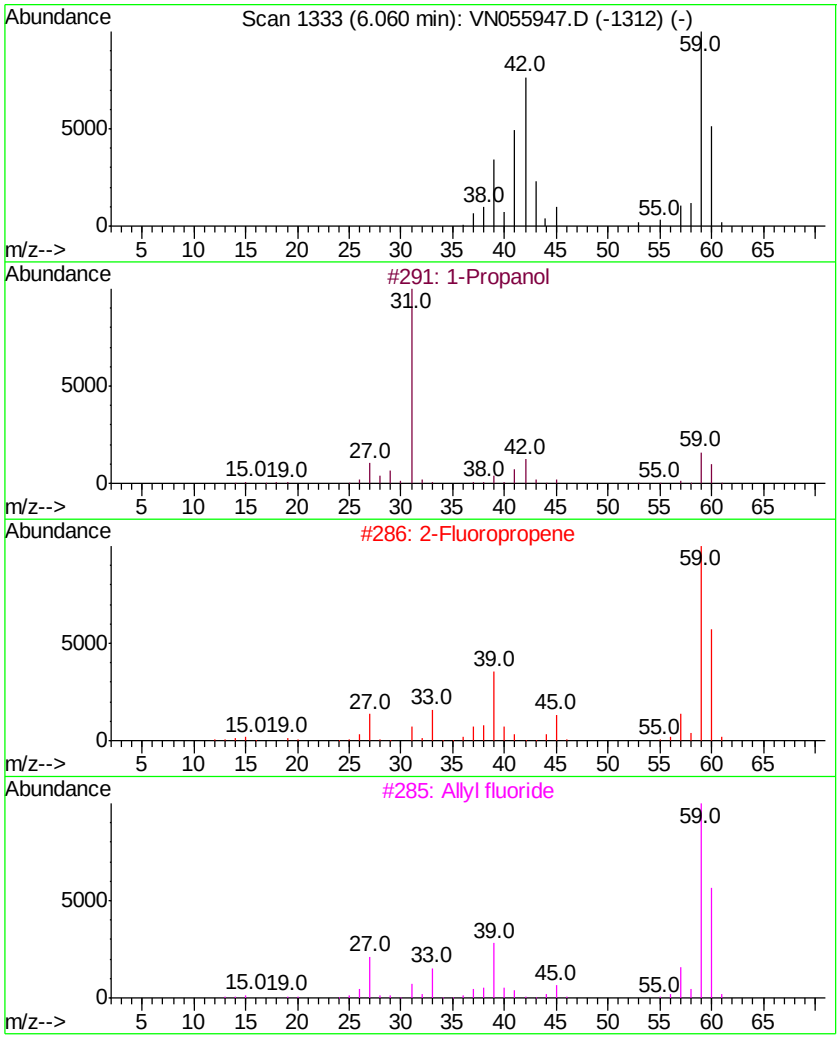
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

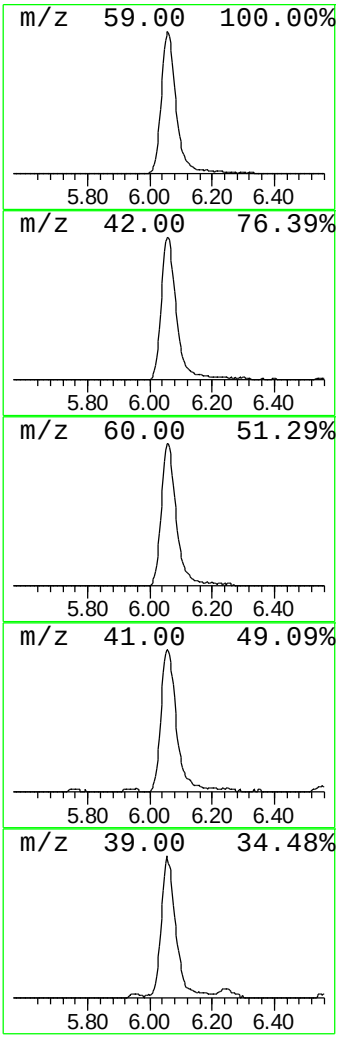
****

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	16.63 ug/l	291709	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	1,2-Butanediol	90	C4H10O2	000584-03-2	17
5	Cyclopropane	42	C3H6	000075-19-4	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
Sample : K3125-25 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 46 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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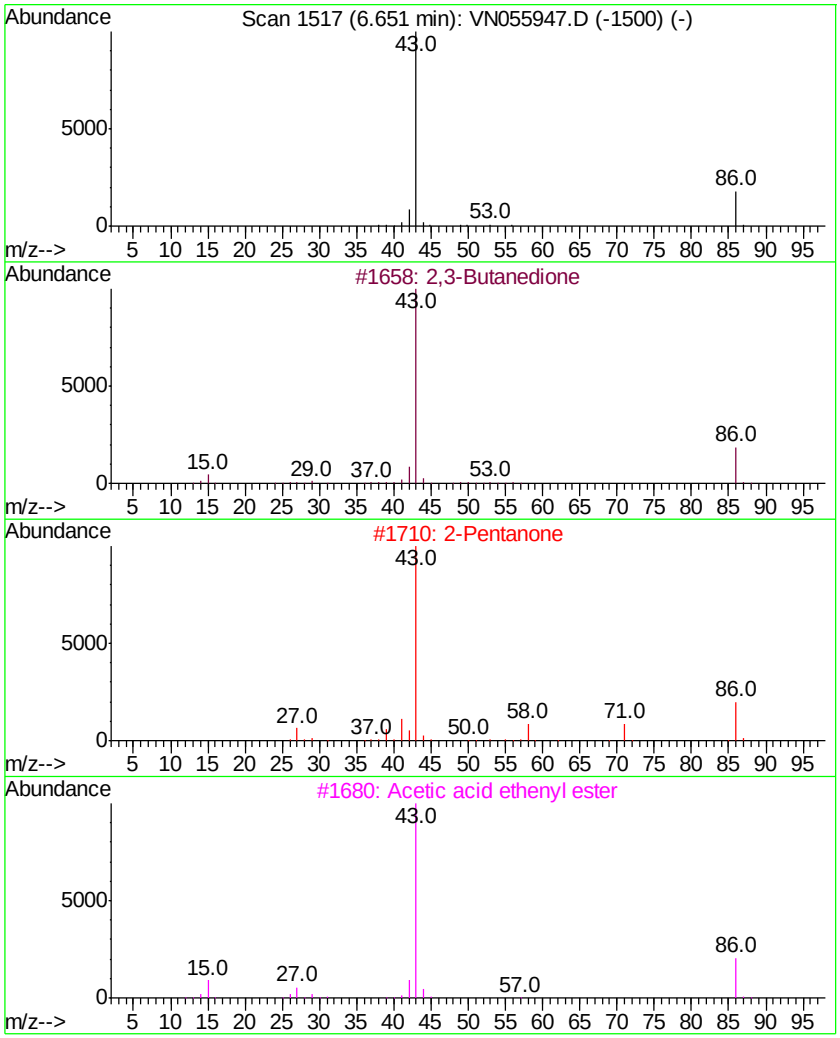
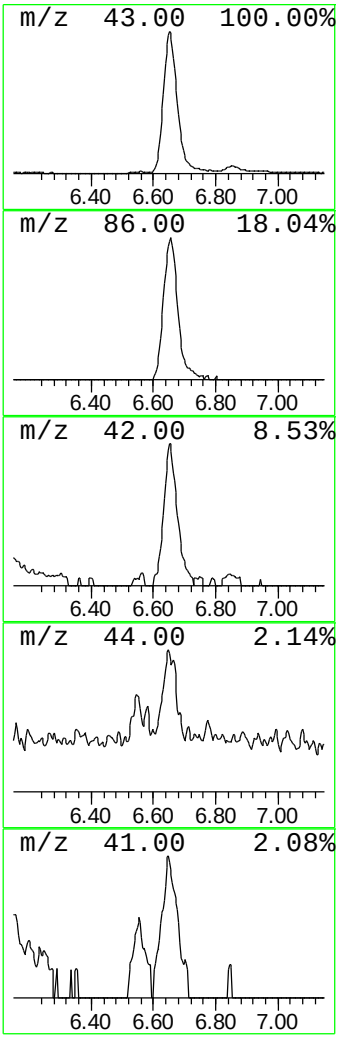
Peak Number 4 2,3-Butanedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	8.65 ug/l	151661	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	90
2	2-Pentanone	86	C5H10O	000107-87-9	56
3	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	45
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	7





Library Search Compound Report

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

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

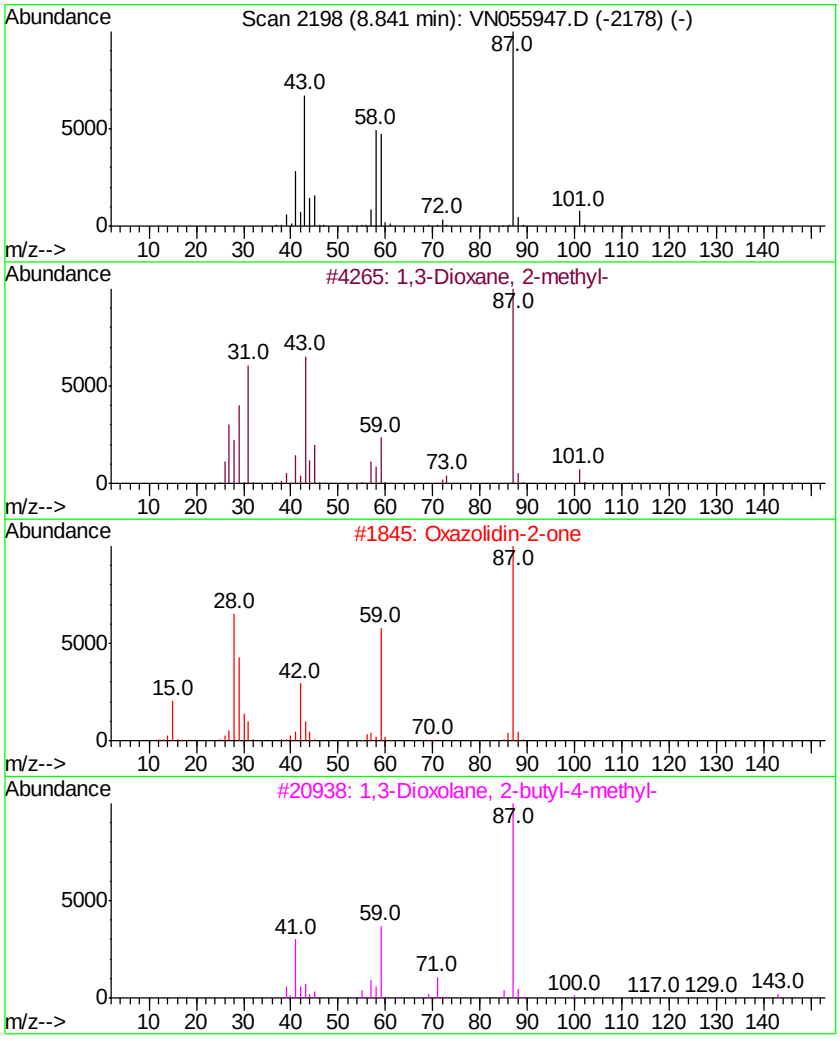
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

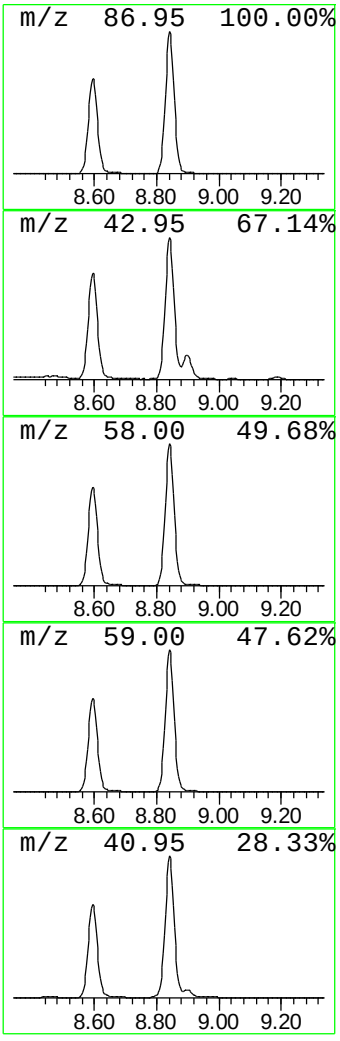
****

Peak Number 5 unknown8.84 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	37.48 ug/l	1953270	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	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	23
5	Formamide, N-butyl-	101	C5H11NO	000871-71-6	10





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ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

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

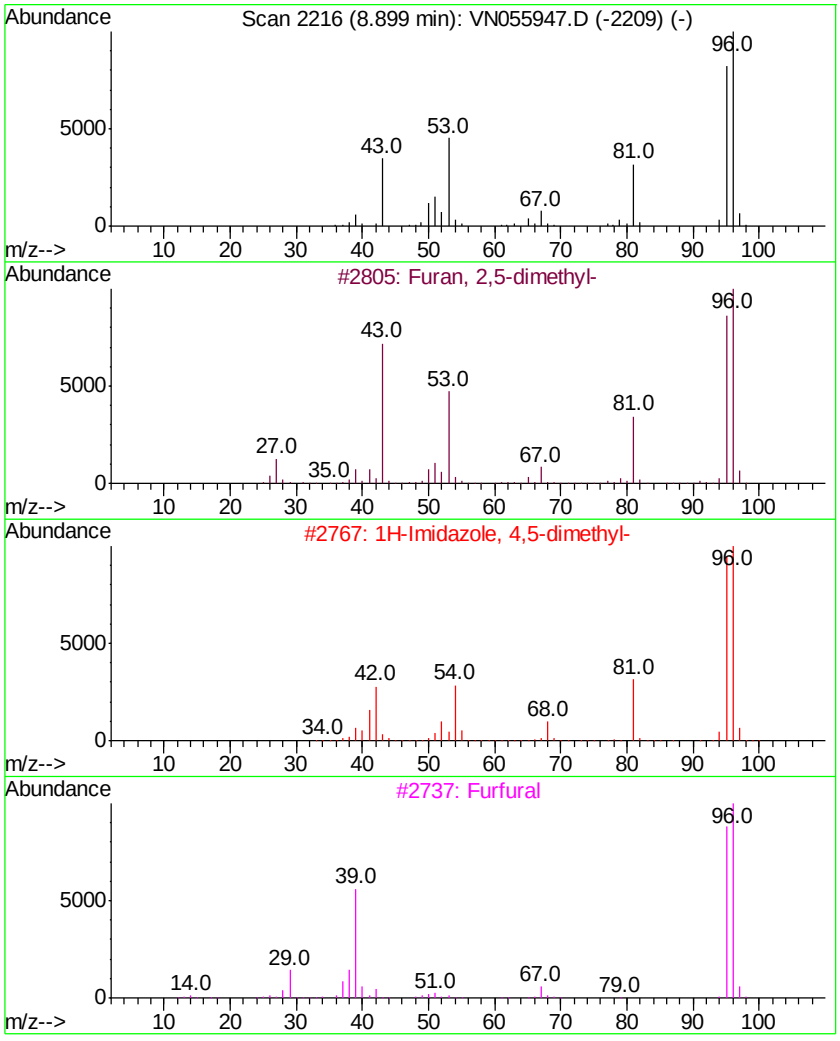
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

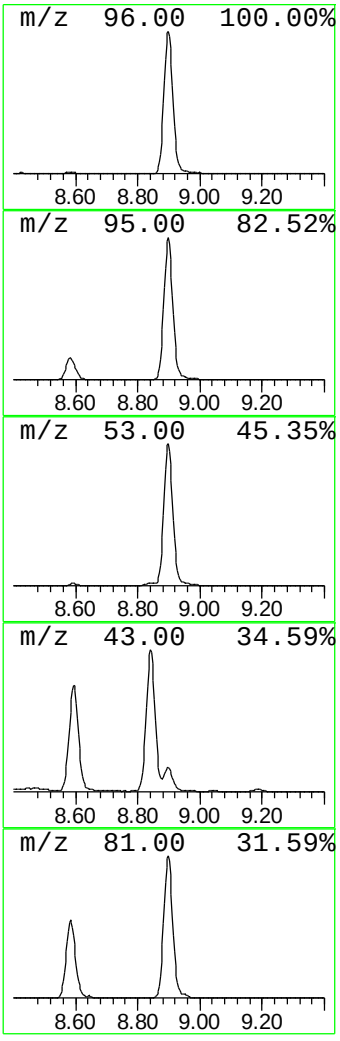
****

Peak Number 6 Furan, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	8.62 ug/l	449250	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	94
2	1H-Imidazole, 4,5-dimethyl-	96	C5H8N2	002302-39-8	43
3	Furfural	96	C5H4O2	000098-01-1	43
4	1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	000694-31-5	43
5	1H-Imidazole, 1,5-dimethyl-	96	C5H8N2	010447-93-5	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN053119\
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Sample : K3125-25 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 13899

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

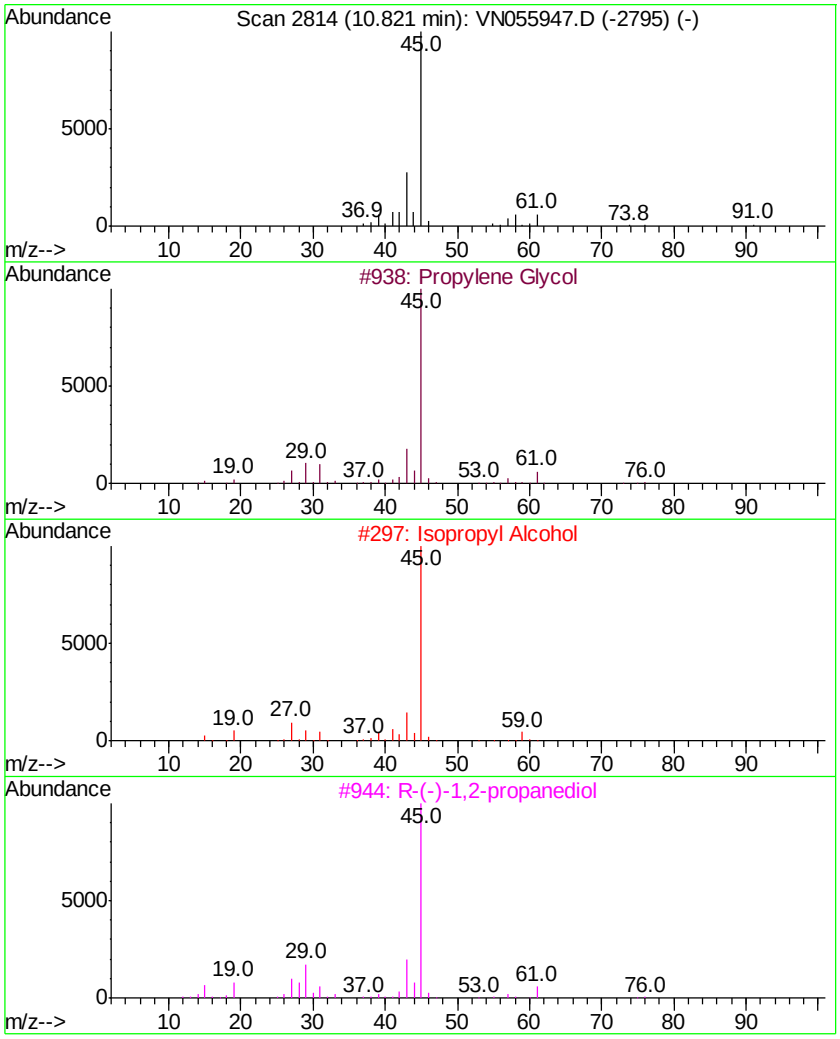
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

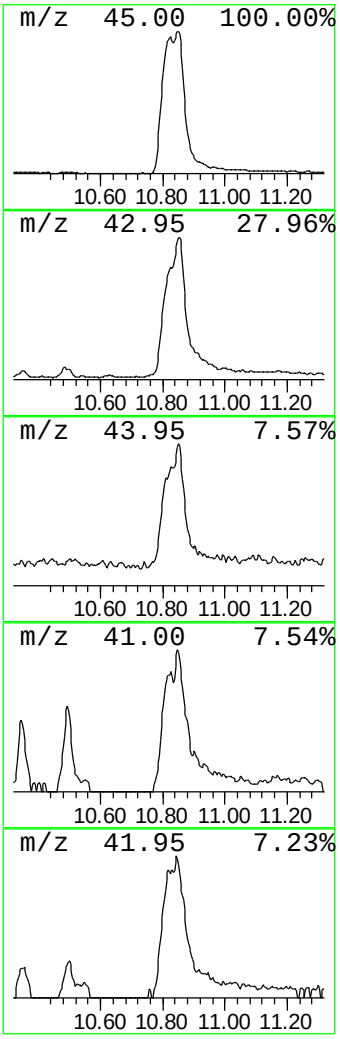
****

Peak Number 7 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	5.02 ug/l	139622	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5	2-Propanol, 1-hydrazino-	90	C3H10N2O	018501-20-7	9





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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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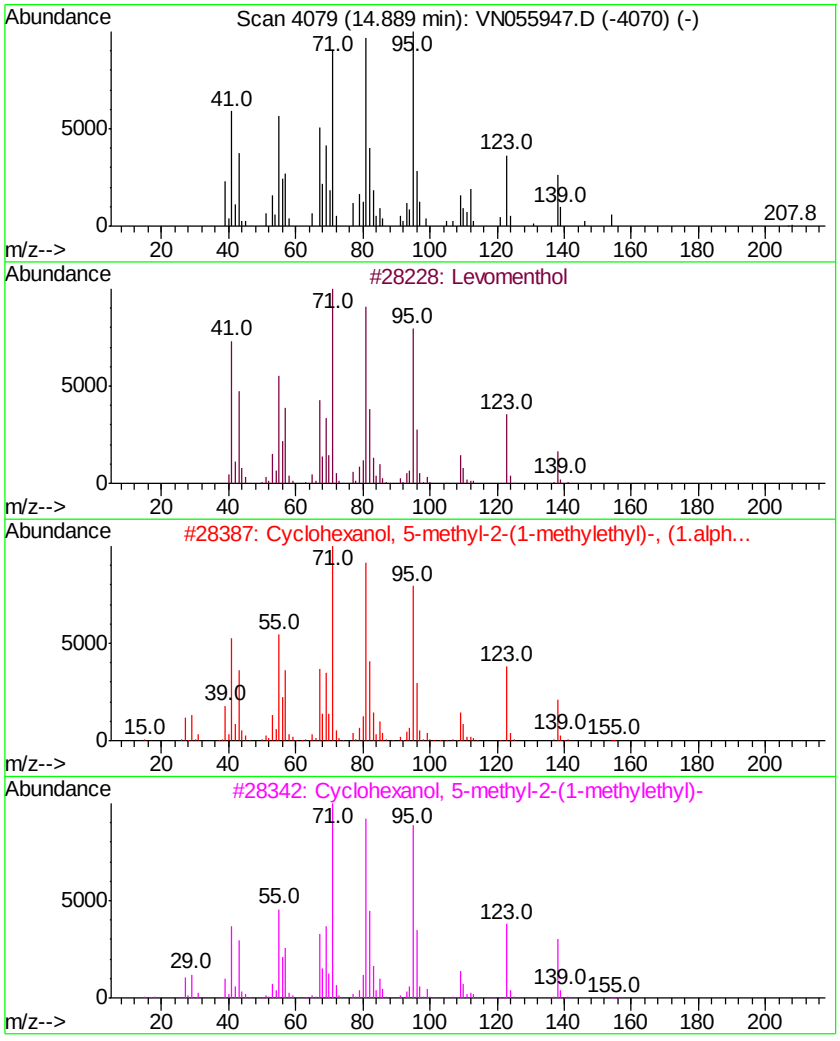
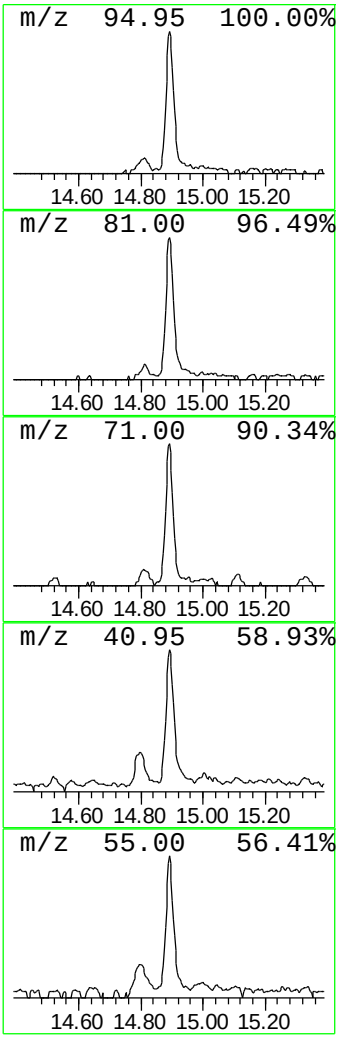
Peak Number 8 Levomenthol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	5.62 ug/l	119762	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levomenthol	156	C10H20O	002216-51-5	90
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	87
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87
4	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	86
5	L-Menthyl chloroformate	218	C11H19ClO2	014602-86-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN053119\
Data File : VN055947.D
Acq On : 1 Jun 2019 4:31
Operator : JC/SP
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ALS Vial : 46 Sample Multiplier: 1

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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	81.9	ug/l	1437120	1	7.66	876915	50.0
Ethanol	3.28	25.3	ug/l	443552	1	7.66	876915	50.0
1-Propanol	6.06	16.6	ug/l	291709	1	7.66	876915	50.0
2,3-Butanedione	6.65	8.7	ug/l	151661	1	7.66	876915	50.0
unknown8.84	8.84	37.5	ug/l	1953270	2	8.58	2605910	50.0
Furan, 2,5-dimethyl-	8.90	8.6	ug/l	449250	2	8.58	2605910	50.0
Propylene Glycol	10.82	5.0	ug/l	139622	3	11.41	1391140	50.0
Levomenthol	14.89	5.6	ug/l	119762	4	13.34	1065510	50.0