LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074835.D
Acq On : 10 Oct 2022 16:36
Operator : JC\MD
Sample : N5042-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

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\82N100522W.M
Title : SW846 8260

Signal : TIC: VN074835.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	49	rBV	228973	409965	10.32%	1.470%
2	2.683	99	107	115	rBV	1510772	2794010	70.31%	10.018%
3	2.807	124	128	129	rBV2	66800	75061	1.89%	0.269%
4	2.842	130	134	137	rVV4	65832	145130	3.65%	0.520%
5	3.824	294	301	312	rBV2	91307	247728	6.23%	0.888%
6	4.312	372	384	400	rBV	468389	1365431	34.36%	4.896%
7	4.453	400	408	421	rVV	306161	870482	21.91%	3.121%
8	4.753	446	459	474	rBV	118116	399498	10.05%	1.432%
9	5.530	579	591	598	rBV4	18203	52742	1.33%	0.189%
10	6.753	786	799	812	rBV	1219389	3699874	93.11%	13.266%
11	7.236	874	881	882	rBV4	34710	52026	1.31%	0.187%
12	7.318	889	895	907	rVB2	29892	83803	2.11%	0.300%
13	7.447	910	917	923	rBV	38661	97477	2.45%	0.350%
14	8.177	1031	1041	1046	rBV	485812	1197237	30.13%	4.293%
15	8.236	1046	1051	1060	rVB	536572	1196404	30.11%	4.290%
16	8.588	1099	1111	1122	rBV2	587128	1371040	34.50%	4.916%
17	9.106	1188	1199	1210	rBV	831445	1710512	43.04%	6.133%
18	9.277	1223	1228	1235	rBV5	22106	52076	1.31%	0.187%
19	9.406	1243	1250	1257	rVB2	64349	131052	3.30%	0.470%
20	9.659	1287	1293	1302	rBV2	45854	98111	2.47%	0.352%
21	10.571	1439	1448	1462	rBV	2144460	3973795	100.00%	14.248%
22	10.806	1481	1488	1496	rBV2	171736	303232	7.63%	1.087%
23	10.953	1506	1513	1522	rBV5	35958	82070	2.07%	0.294%
24	11.065	1525	1532	1547	rBV	504856	889096	22.37%	3.188%
25	11.206	1549	1556	1563	rVV3	49159	91695	2.31%	0.329%
26	11.871	1655	1669	1681	rBV	1204592	2269237	57.11%	8.136%
27	12.853	1829	1836	1846	rVB	1207732	2088094	52.55%	7.487%
28	13.794	1986	1996	2004	rBV	1252489	2142747	53.92%	7.683%

Sum of corrected areas: 27889625

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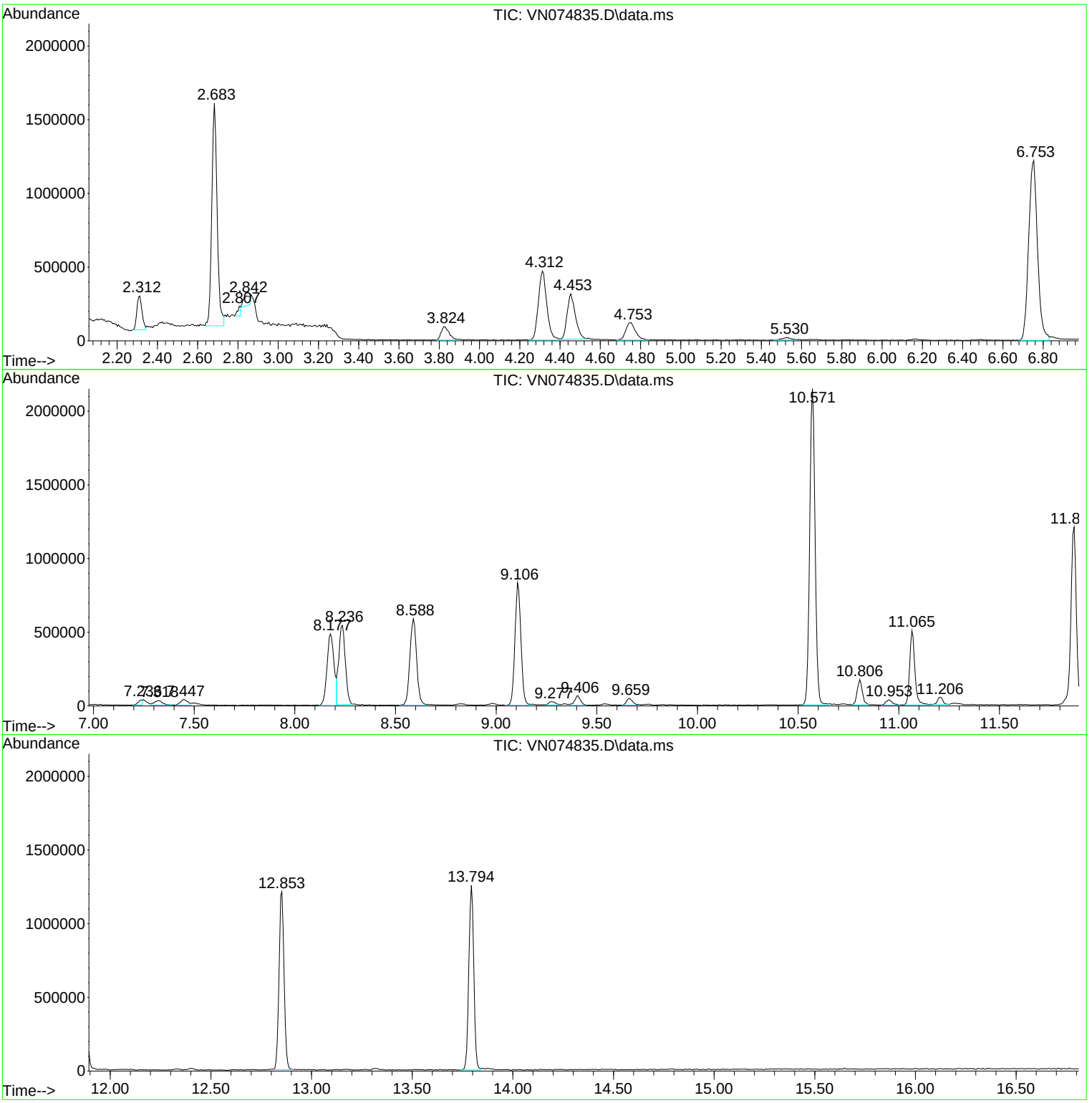
Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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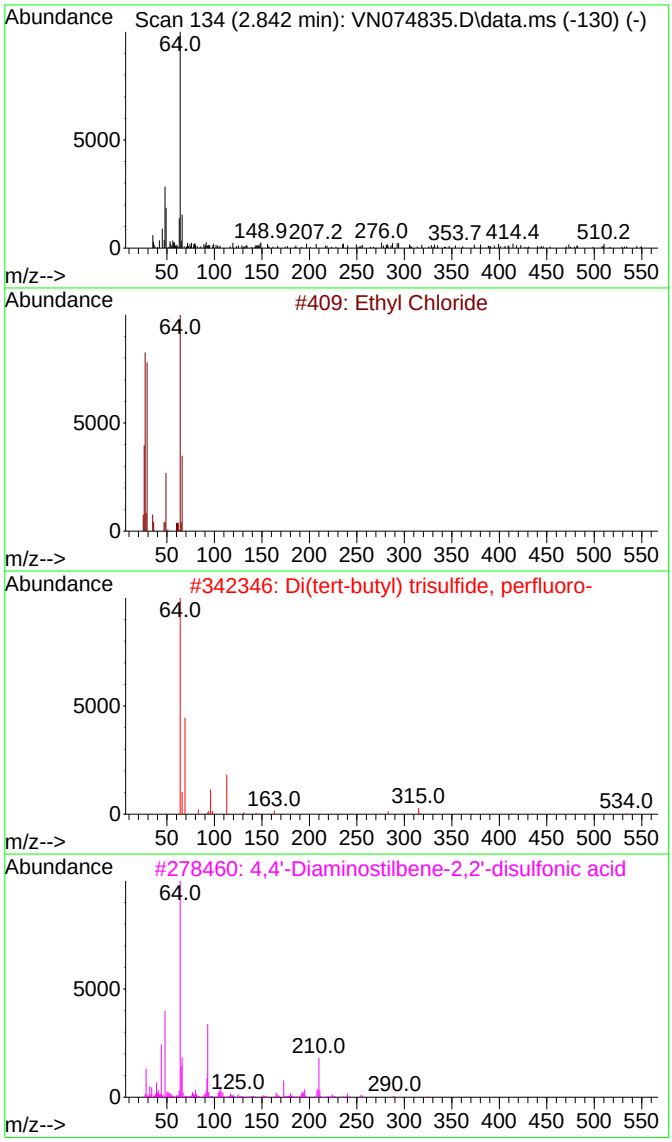
Quant Title : SW846 8260

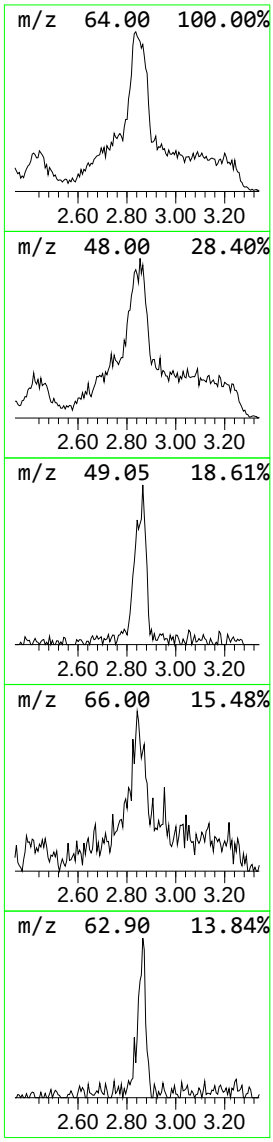
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethyl Chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.842	6.07 ug/l	145130	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Chloride	64	C2H5Cl	000075-00-3	86
2	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	83
3	4,4'-Diaminostilbene-2,2'-disulf...	370	C14H14N2O6S2	000081-11-8	43
4	2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	9
5	Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	9





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Operator : JC\MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

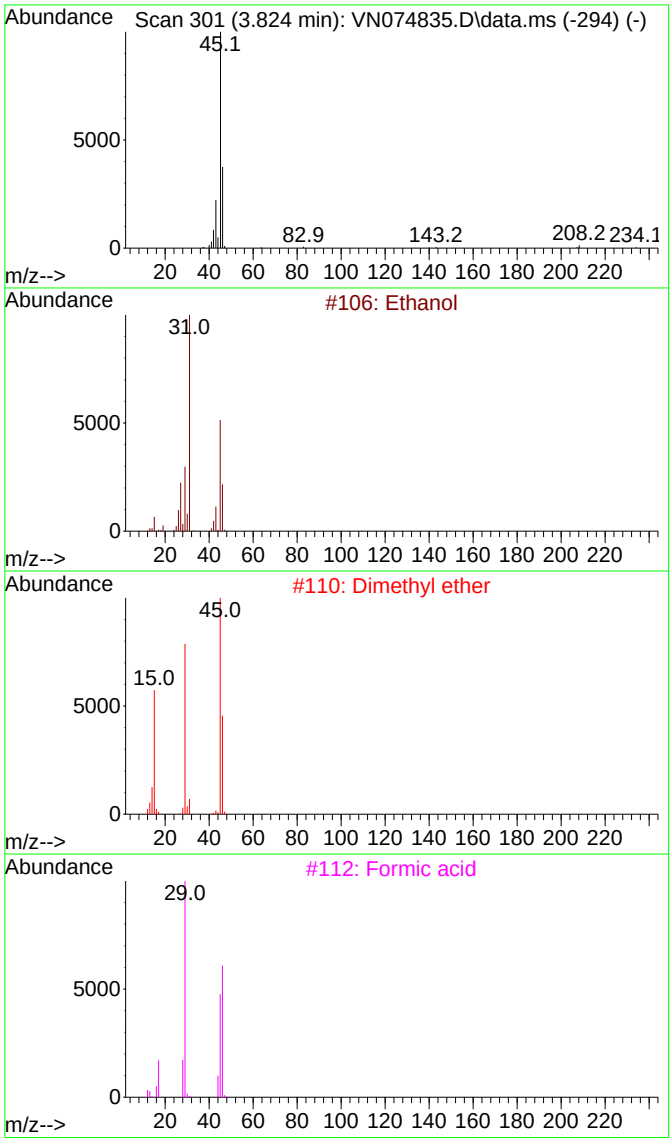
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

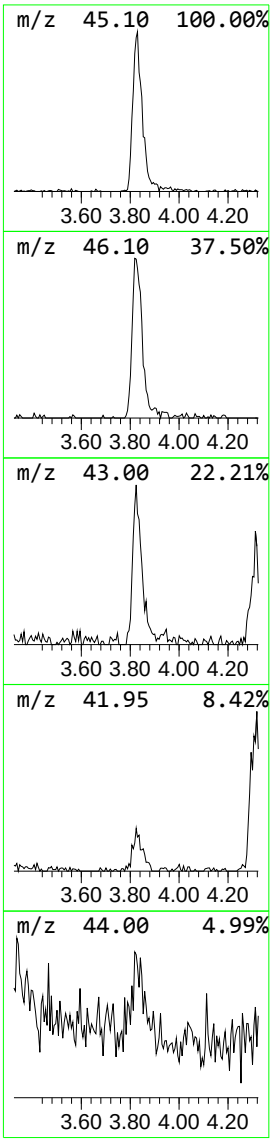
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.824	10.35 ug/l	247728	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	56
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Formic acid	46	CH2O2	000064-18-6	4
4	Methane, nitroso-	45	CH3NO	000865-40-7	4
5	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4





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Data File : VN074835.D
Acq On : 10 Oct 2022 16:36
Operator : JC\MD
Sample : N5042-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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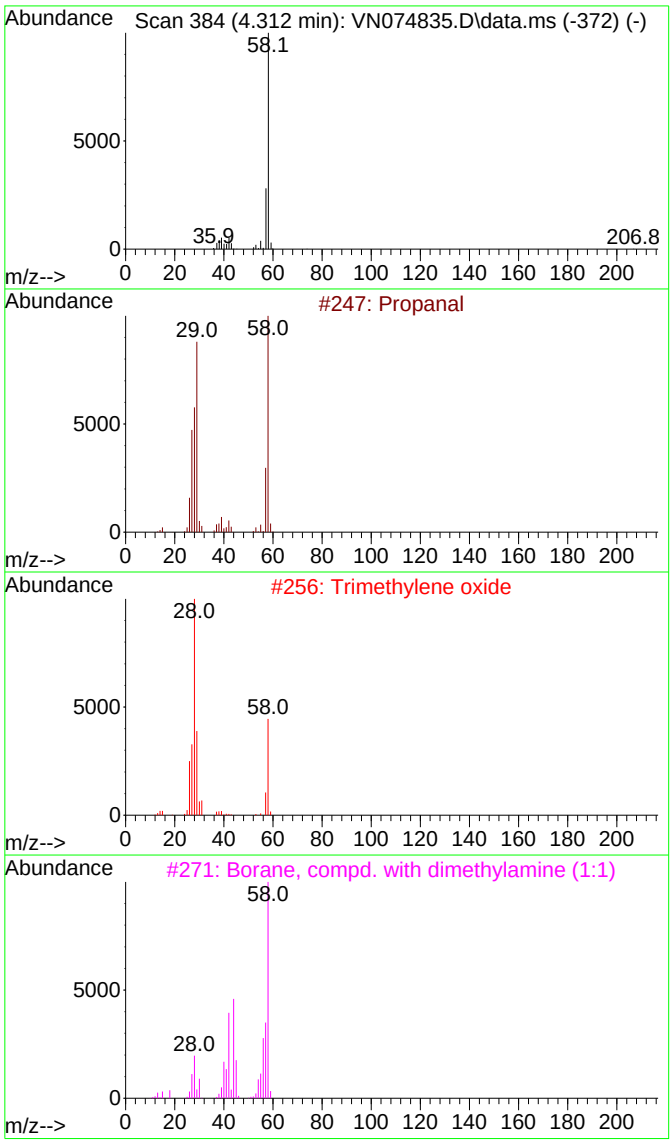
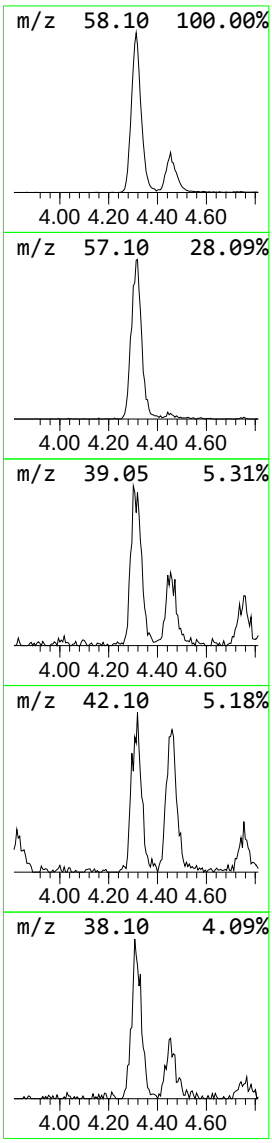
Peak Number 5 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	57.06 ug/l	1365430	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Propylene oxide	58	C3H6O	000075-56-9	7





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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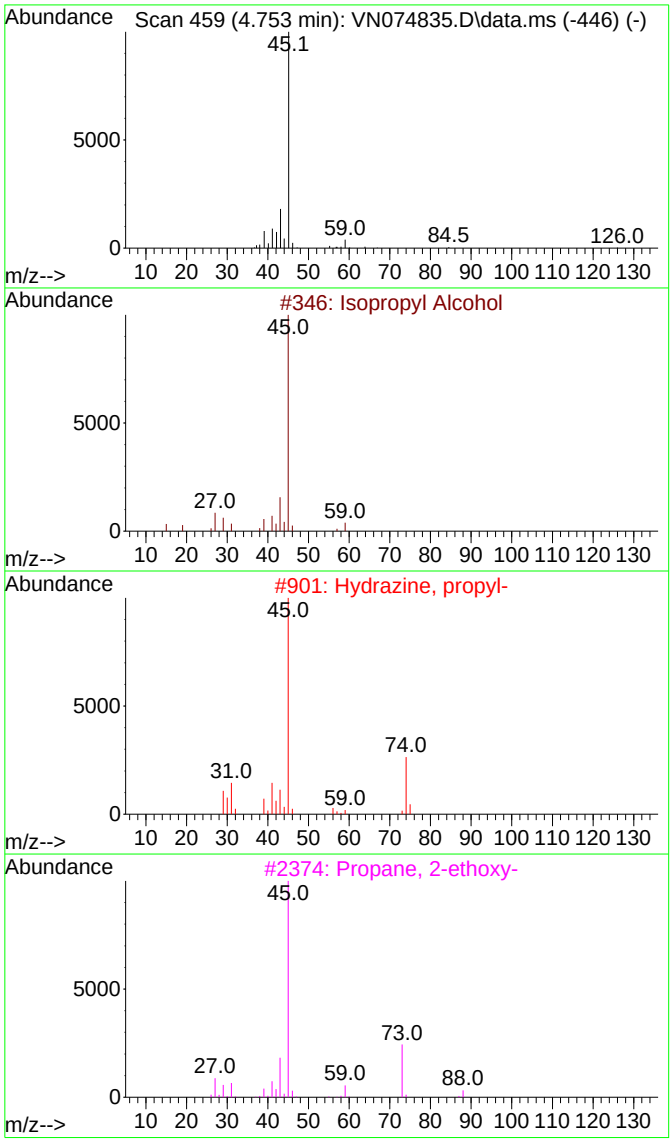
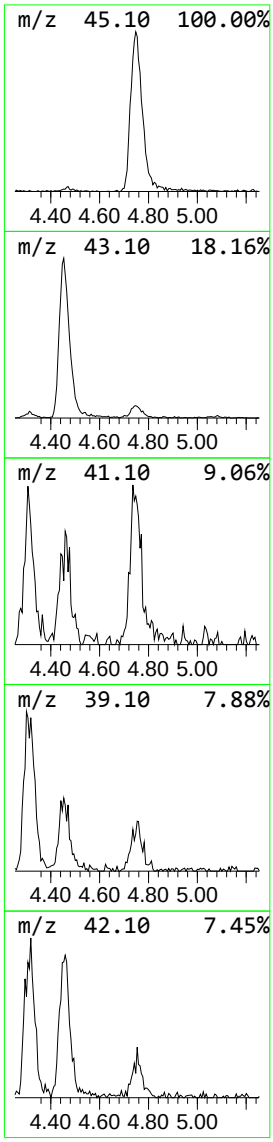
Peak Number 6 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.753	16.70 ug/l	399498	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2	Hydrazine, propyl-	74	C3H10N2	005039-61-2	9
3	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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Operator : JC\MD
Sample : N5042-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0614

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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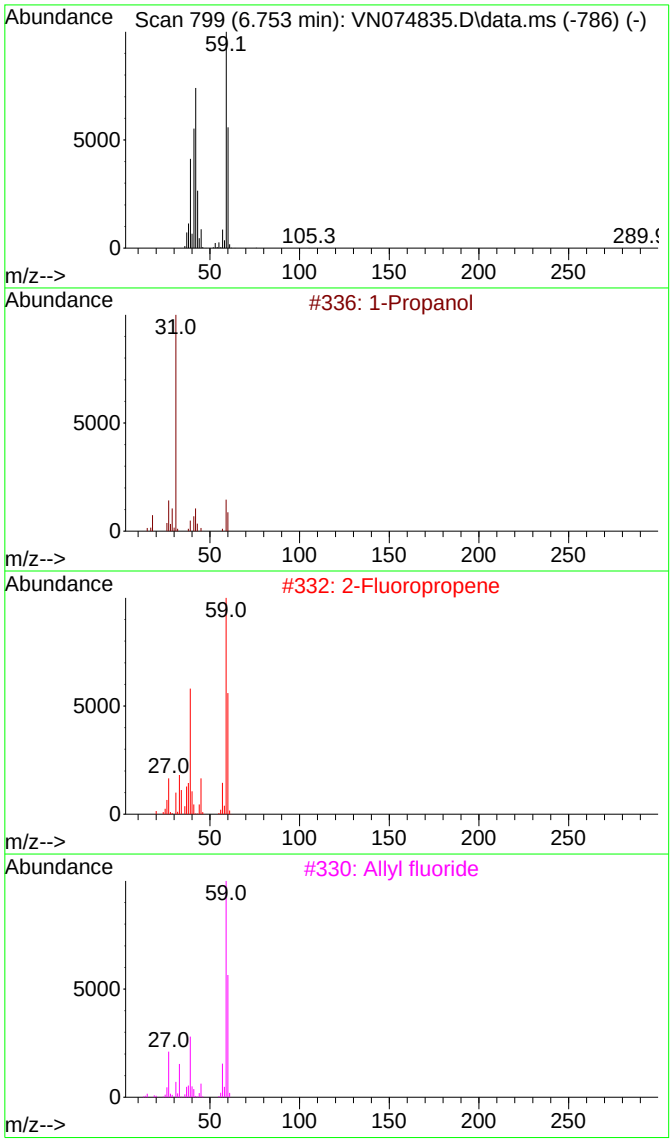
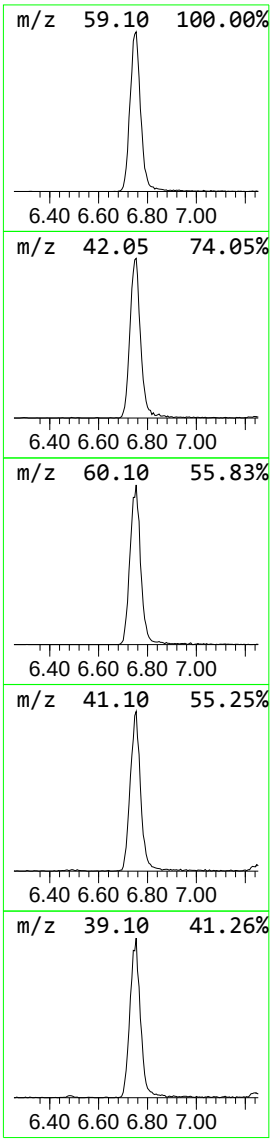
Peak Number 7 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.753	154.63 ug/l	3699870	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	35
4	Cyclopropane	42	C3H6	000075-19-4	32
5	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17





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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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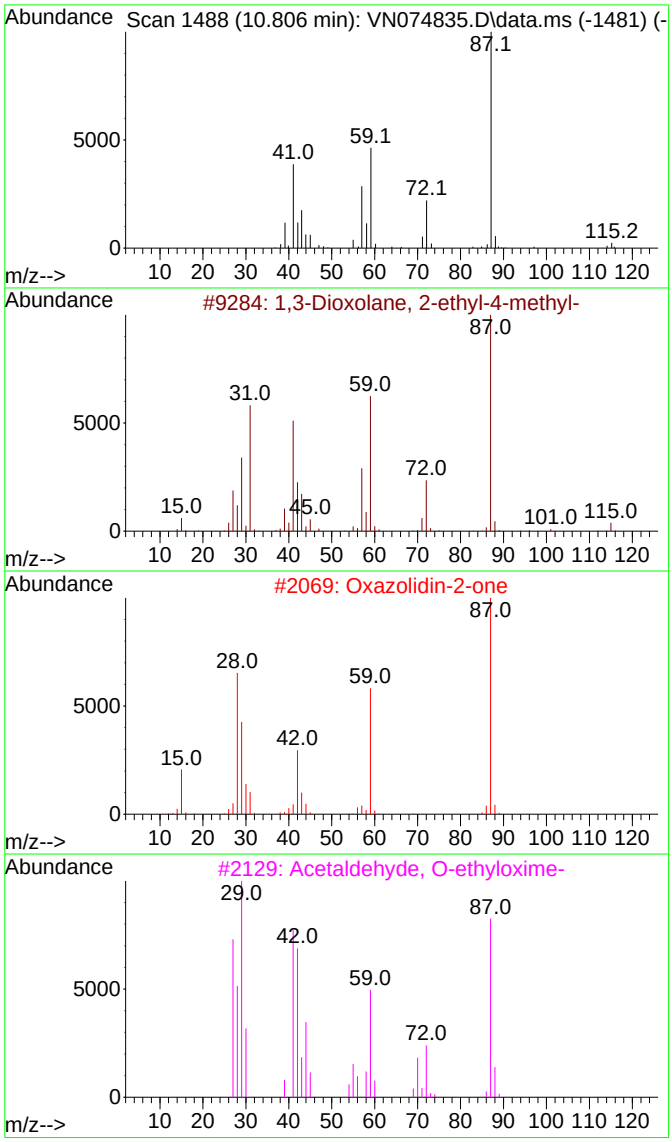
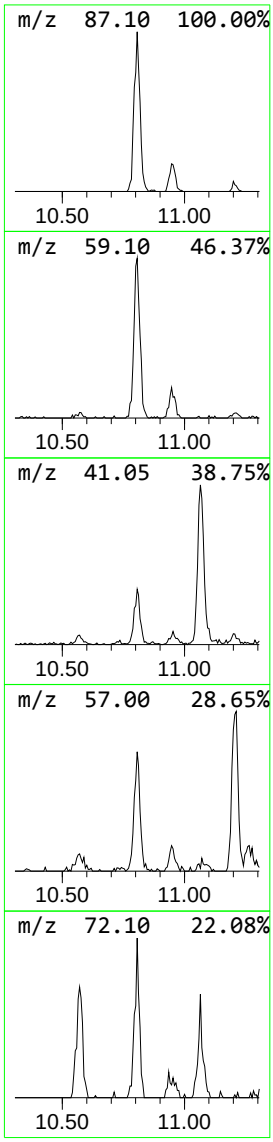
****
Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.806	6.68 ug/l	303232	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	74
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	59
3	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	56
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	50
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50





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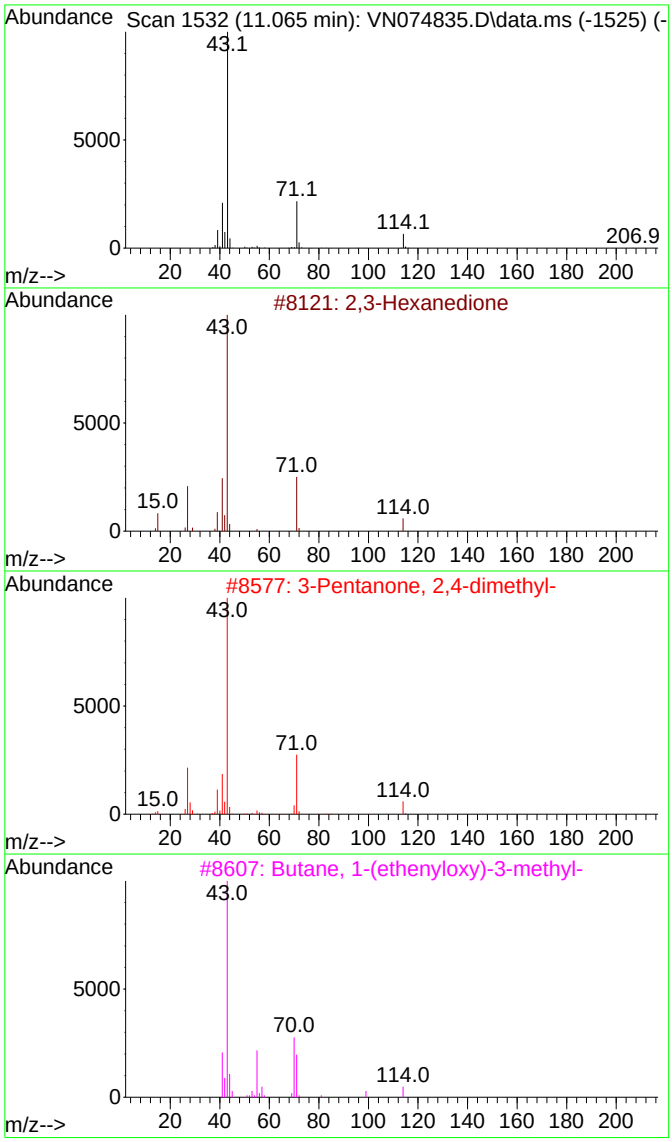
Quant Title : SW846 8260

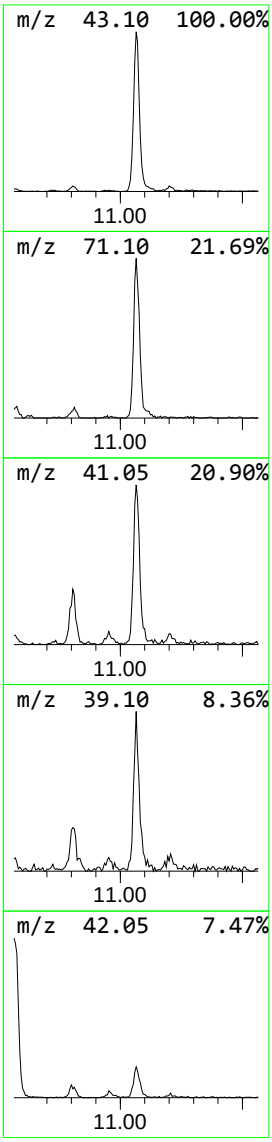
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2,3-Hexanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.065	19.59 ug/l	889096	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Hexanedione	114	C6H10O2	003848-24-6	90
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	72
3	Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	39
4	4-Heptanone	114	C7H14O	000123-19-3	9
5	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	9





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethyl Chloride	2.842	6.1	ug/l	145130	1	8.236	1196400	50.0
Ethanol	3.824	10.4	ug/l	247728	1	8.236	1196400	50.0
Propanal	4.312	57.1	ug/l	1365430	1	8.236	1196400	50.0
Isopropyl Alcohol	4.753	16.7	ug/l	399498	1	8.236	1196400	50.0
1-Propanol	6.753	154.6	ug/l	3699870	1	8.236	1196400	50.0
1,3-Dioxolane, ...	10.806	6.7	ug/l	303232	3	11.871	2269240	50.0
2,3-Hexanedione	11.065	19.6	ug/l	889096	3	11.871	2269240	50.0