LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080837.D
Acq On : 31 Jan 2024 13:57
Operator : JC\MD
Sample : P1284-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

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\82N012924W.M
Title : SW846 8260

Signal : TIC: VN080837.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	28	rVB	83596	121250	2.93%	0.805%
2	2.659	110	120	137	rBV	2244474	4140409	100.00%	27.503%
3	3.783	299	311	330	rBV	471677	1261063	30.46%	8.377%
4	4.283	385	396	410	rBV	242191	706523	17.06%	4.693%
5	4.430	412	421	430	rVB2	14879	43027	1.04%	0.286%
6	7.224	886	896	907	rBV3	224406	614454	14.84%	4.081%
7	7.482	930	940	949	rBV	32950	85786	2.07%	0.570%
8	8.165	1046	1056	1061	rBV	89762	212600	5.13%	1.412%
9	8.224	1061	1066	1076	rVB2	145381	320296	7.74%	2.128%
10	8.577	1120	1126	1137	rVB	103784	233723	5.64%	1.552%
11	9.100	1207	1215	1228	rVB	277695	569751	13.76%	3.785%
12	9.265	1234	1243	1252	rBV3	90028	195559	4.72%	1.299%
13	9.653	1302	1309	1316	rBV2	25131	50991	1.23%	0.339%
14	10.565	1456	1464	1472	rBV	380187	723628	17.48%	4.807%
15	11.865	1672	1685	1693	rBV	449976	842541	20.35%	5.597%
16	12.423	1774	1780	1787	rVB	76932	120922	2.92%	0.803%
17	12.853	1844	1853	1859	rBV	288208	531220	12.83%	3.529%
18	13.247	1913	1920	1922	rBV3	38965	69657	1.68%	0.463%
19	13.270	1922	1924	1929	rVV3	36624	51870	1.25%	0.345%
20	13.335	1929	1935	1945	rVB	961819	1445010	34.90%	9.598%
21	13.688	1987	1995	2004	rVB2	143372	245892	5.94%	1.633%
22	13.794	2005	2013	2020	rBV	420337	692742	16.73%	4.602%
23	13.876	2020	2027	2036	rBV	817335	1299412	31.38%	8.631%
24	15.400	2280	2286	2292	rVV	150700	253805	6.13%	1.686%
25	15.823	2352	2358	2364	rBV2	38808	71150	1.72%	0.473%
26	15.941	2371	2378	2384	rBV3	46850	89987	2.17%	0.598%
27	16.123	2401	2409	2416	rBV2	30765	61395	1.48%	0.408%

Sum of corrected areas: 15054663

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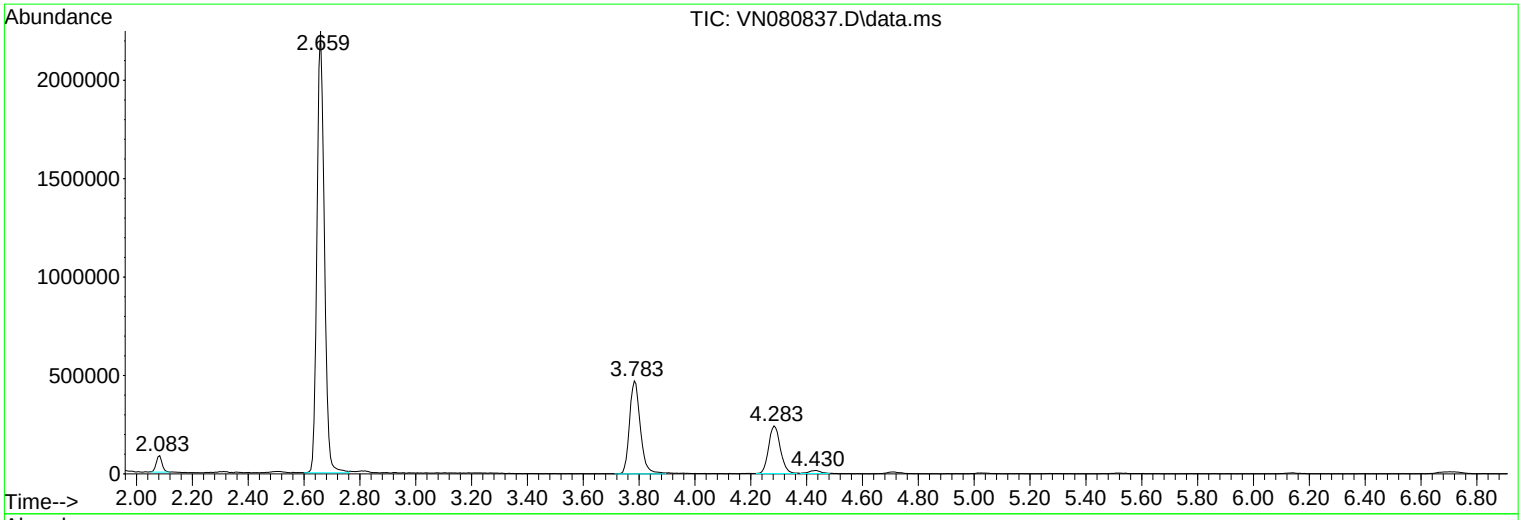
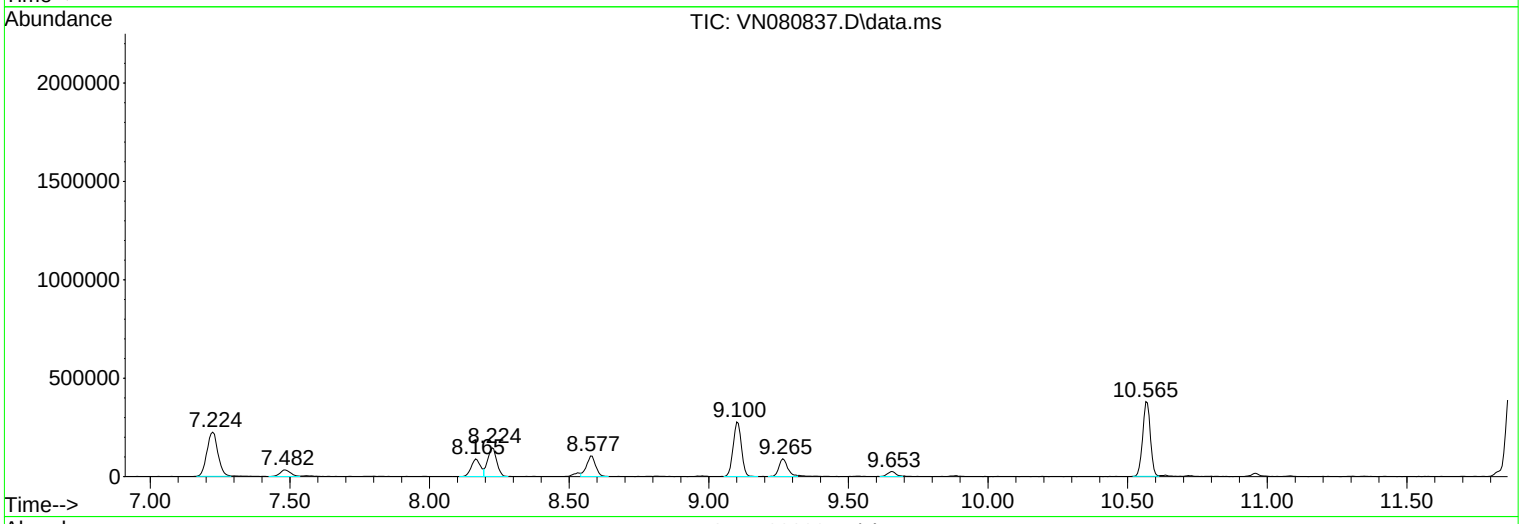
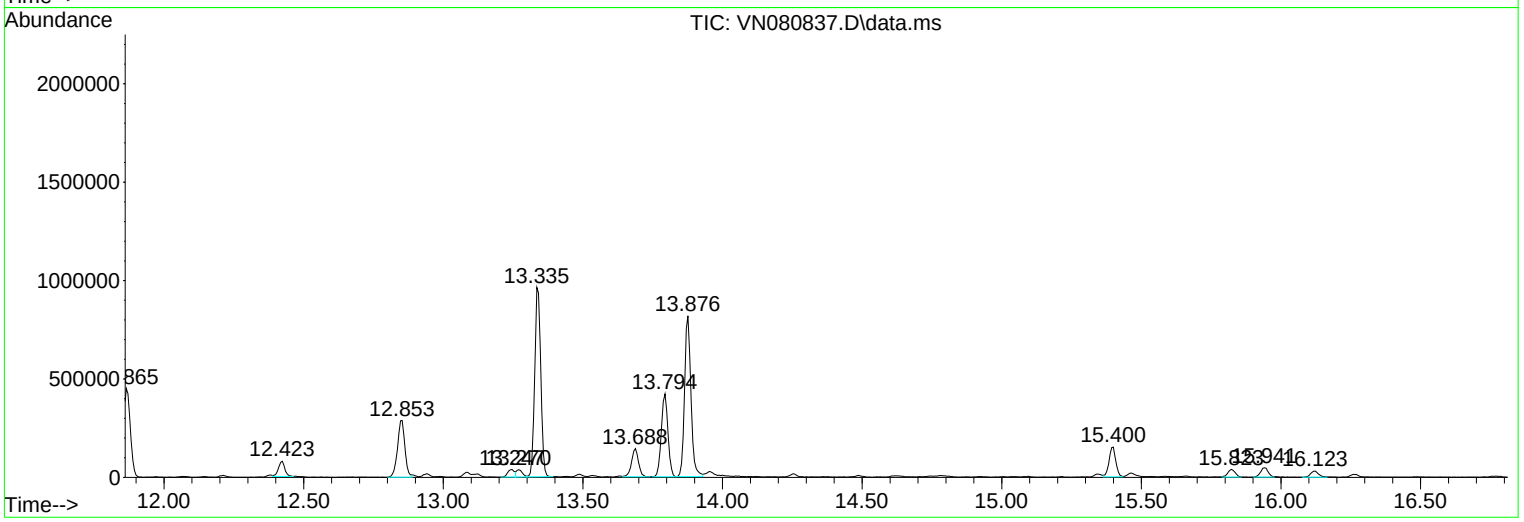
ClientSampleId :
1250

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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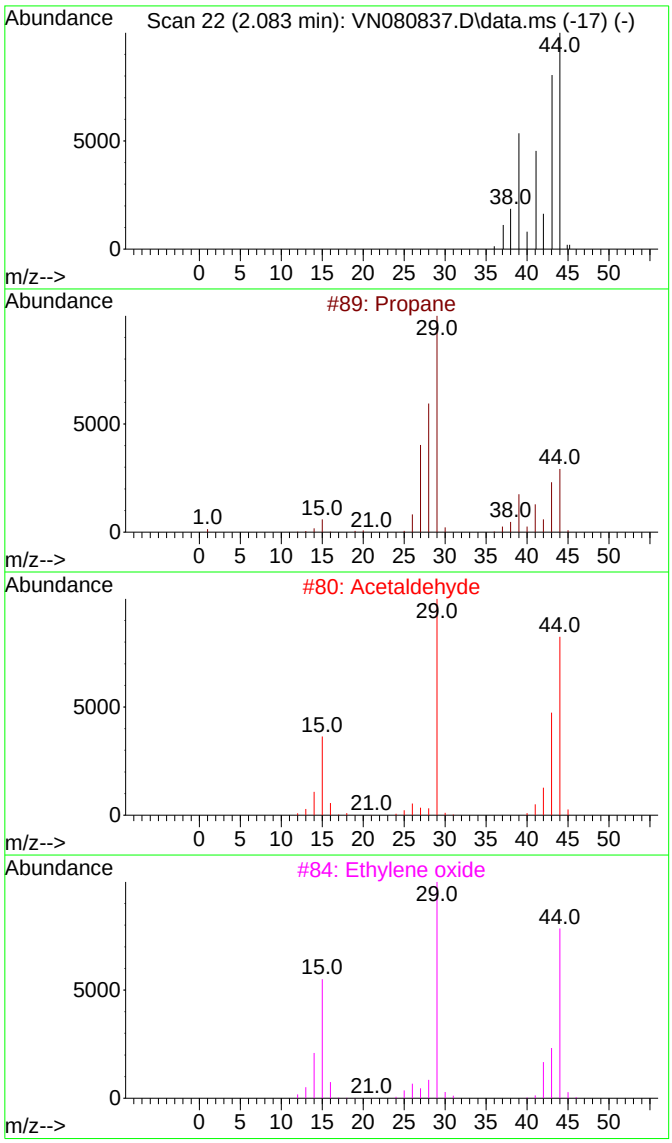
TIC Integration Parameters: LSCINT.P

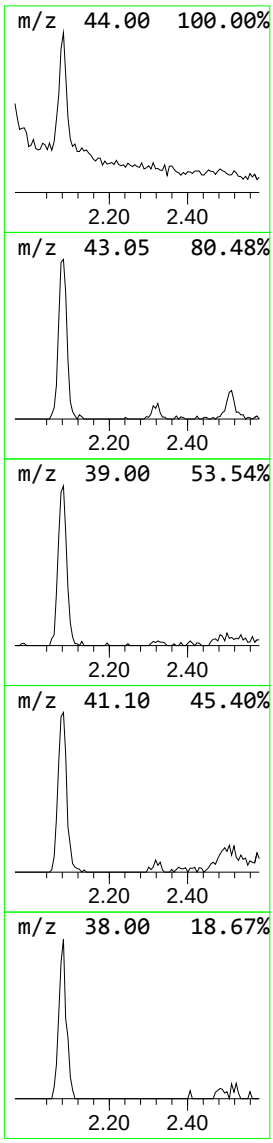
****

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	18.93 ug/l	121250	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Cyclopropene	40	C3H4	002781-85-3	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





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Data File : VN080837.D
Acq On : 31 Jan 2024 13:57
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

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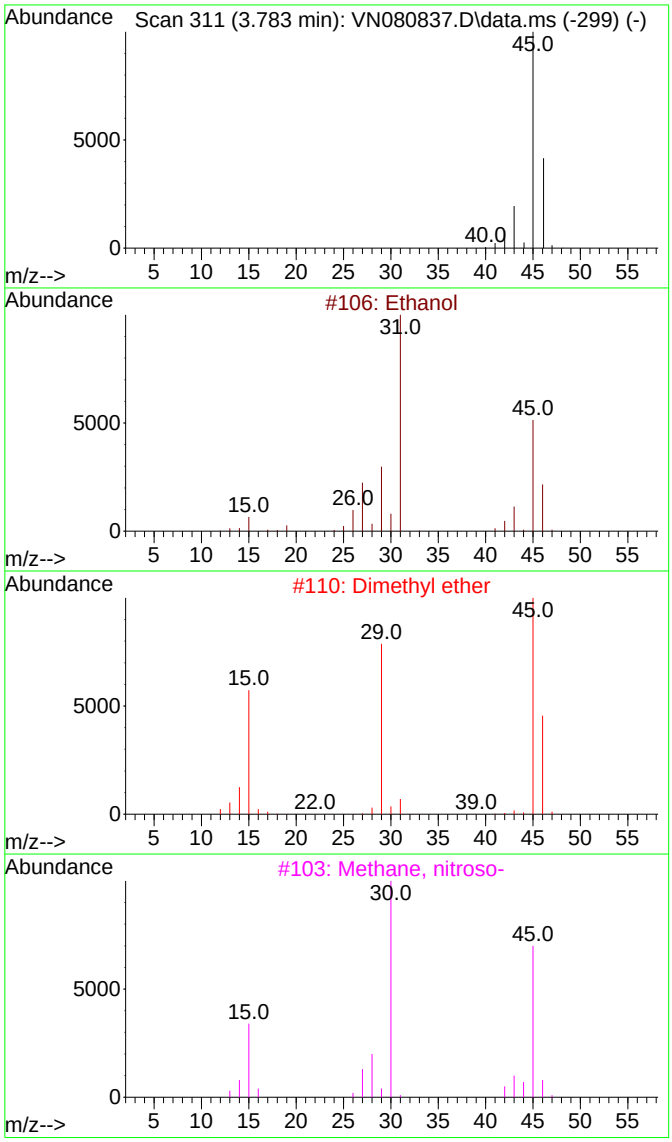
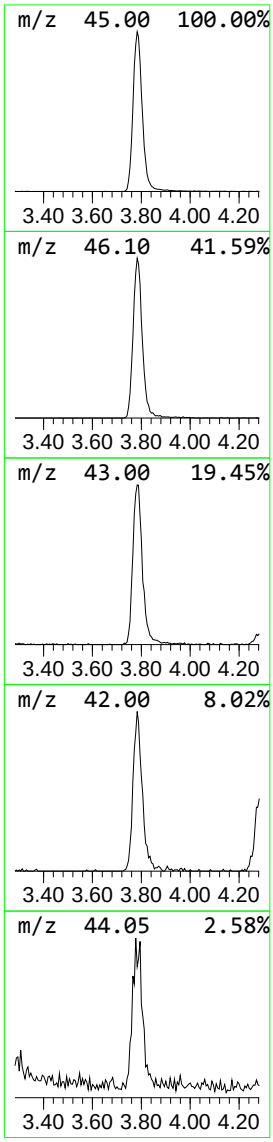
Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	196.86 ug/l	1261060	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	90
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	7
4	Formic acid	46	CH2O2	000064-18-6	4
5	L-Lactic acid	90	C3H6O3	000079-33-4	4





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Data File : VN080837.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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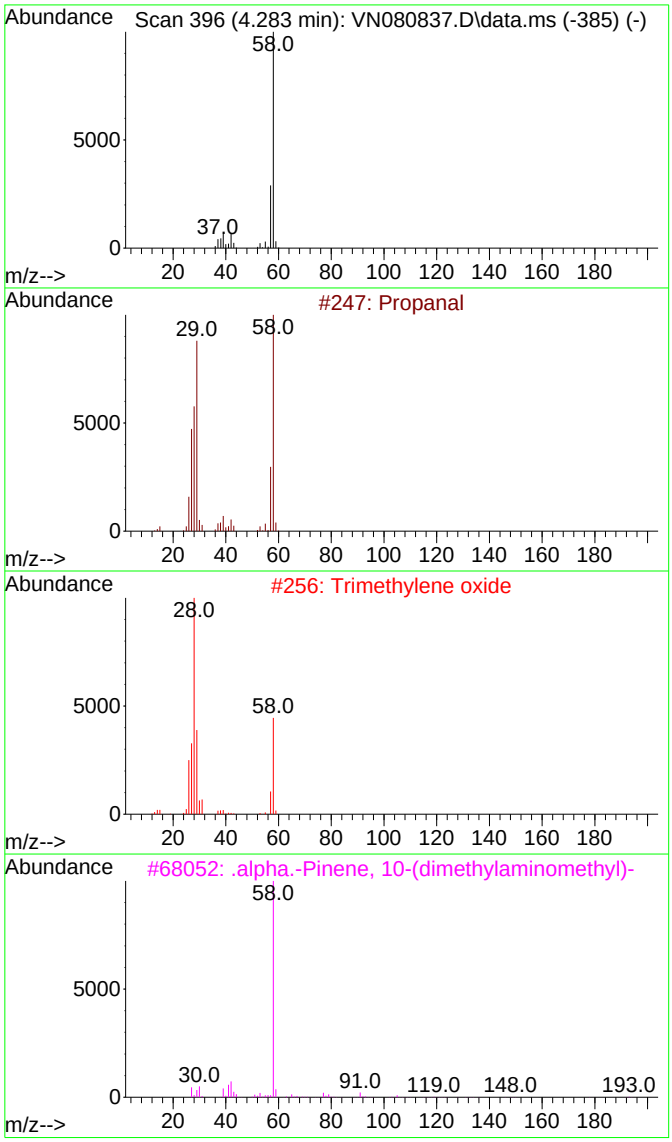
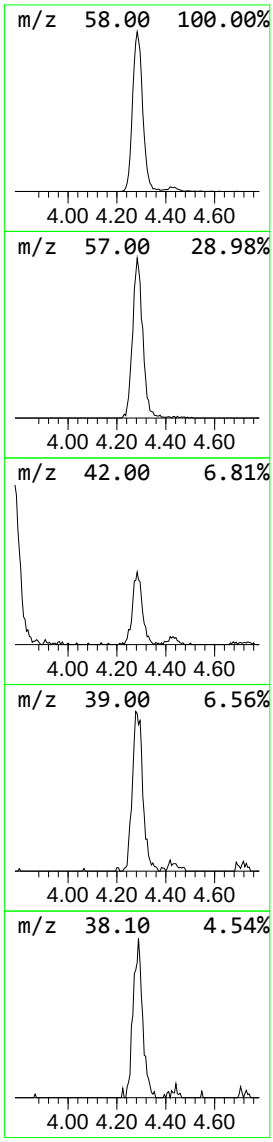
****

Peak Number 4 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	110.29 ug/l	706523	Pentafluorobenzene	8.224

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	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	7





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

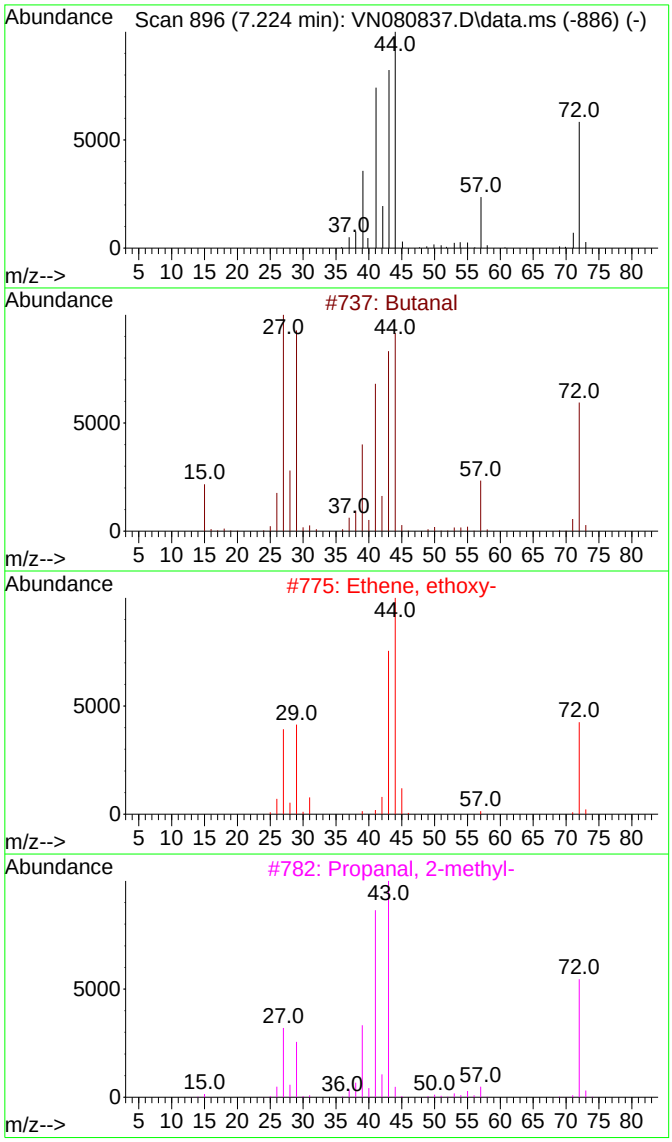
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

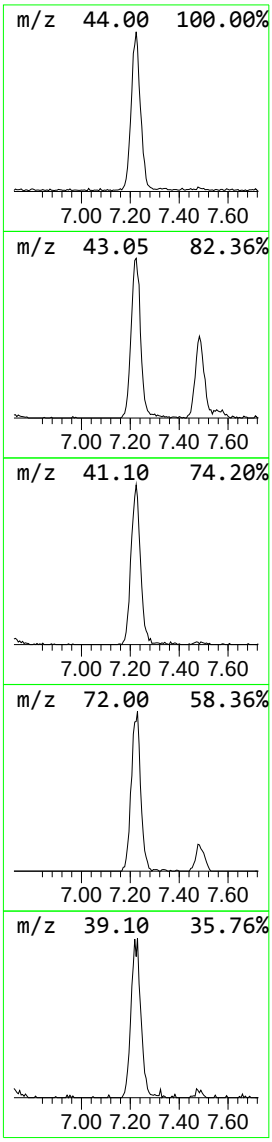
****

Peak Number 5 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	95.92 ug/l	614454	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	59
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	27
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Acq On : 31 Jan 2024 13:57
Operator : JC\MD
Sample : P1284-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

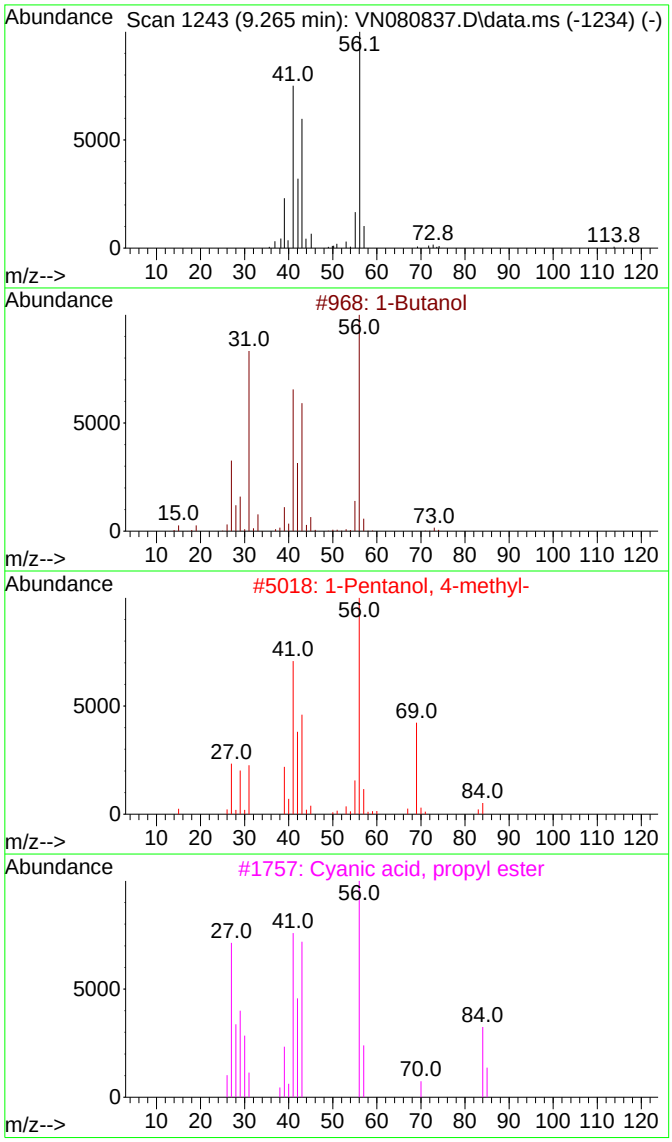
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

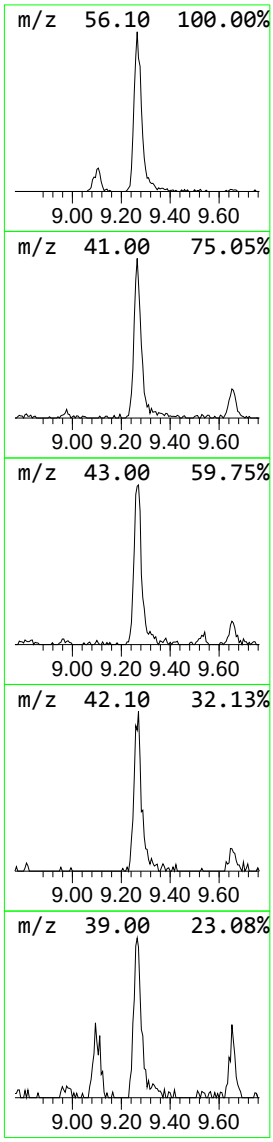
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	17.16 ug/l	195559	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64
3	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	50
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	45
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	39





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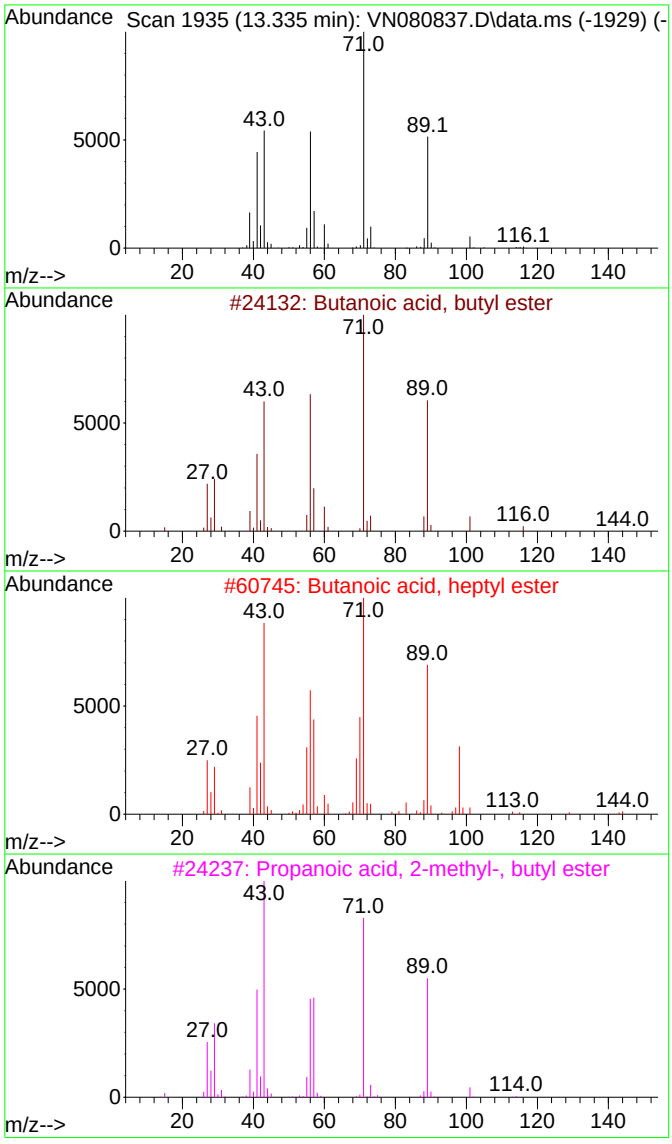
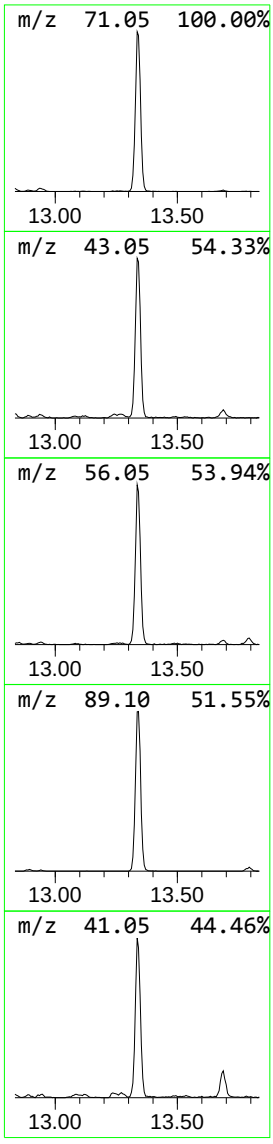
****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	104.30 ug/l	1445010	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59





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TIC Library : C:\Database\NIST20.L
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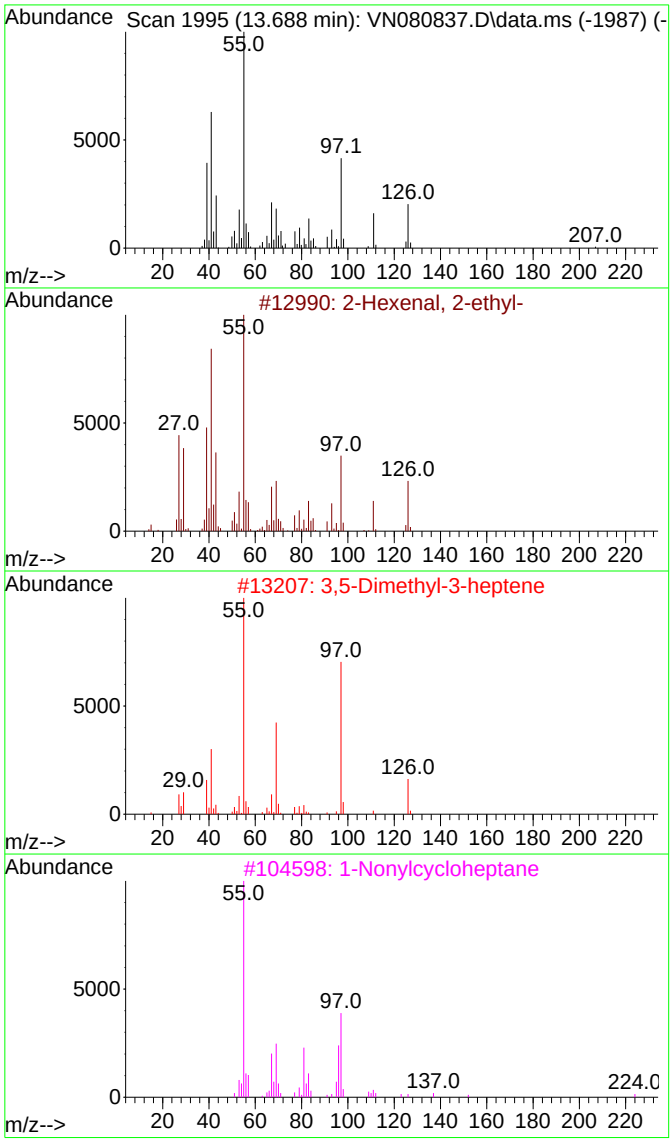
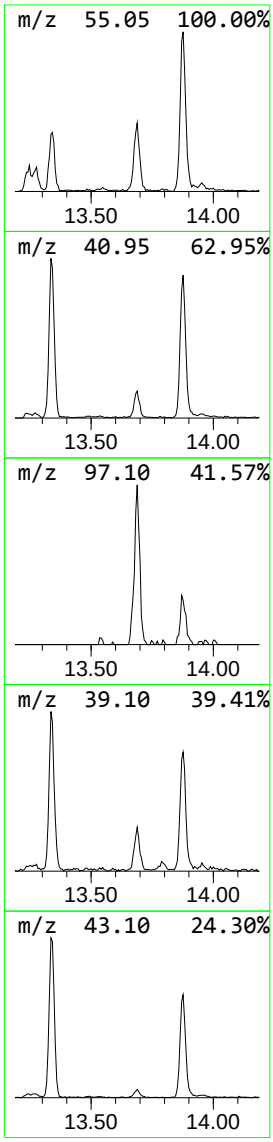
****
Peak Number 8 2-Hexenal, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	17.75 ug/l	245892	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	53
2	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	43
3	1-Nonylcycloheptane	224	C16H32	1000371-47-7	38
4	2-n-Butylacrolein	112	C7H12O	001070-66-2	38
5	3-Hepten-2-one, 5-methyl-	126	C8H14O	005090-16-4	35





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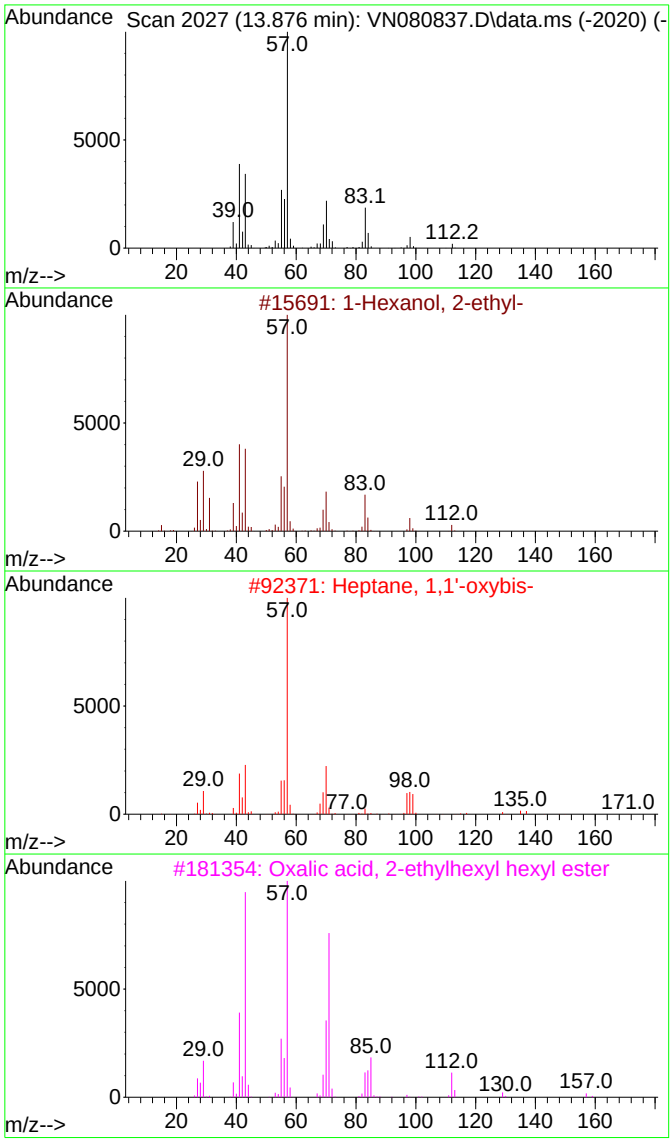
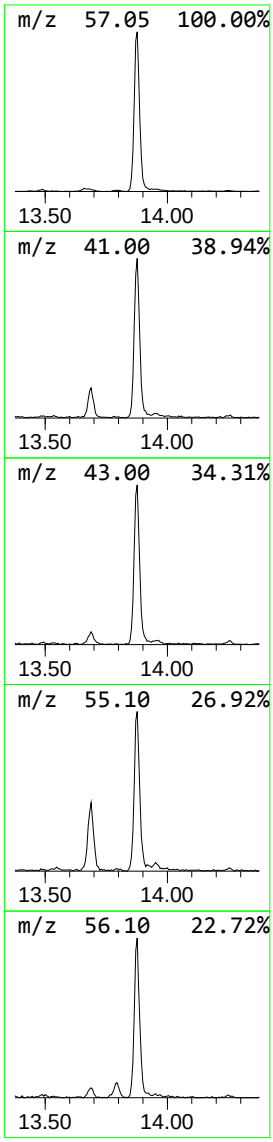
****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	93.79 ug/l	1299410	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	53





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MSVOA_N
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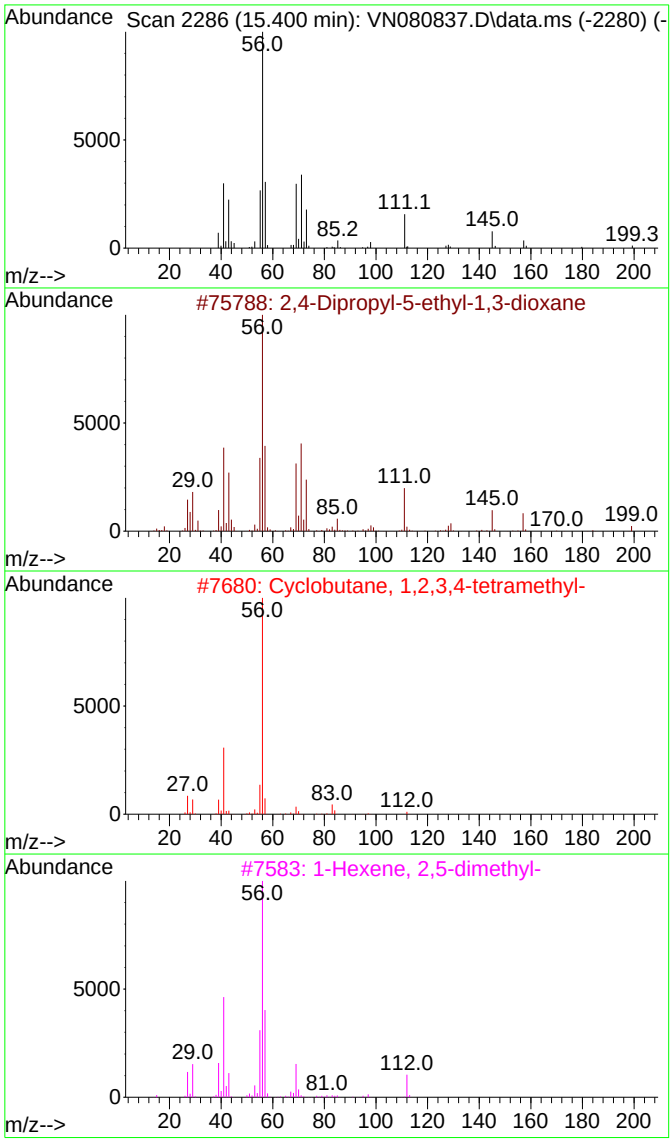
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

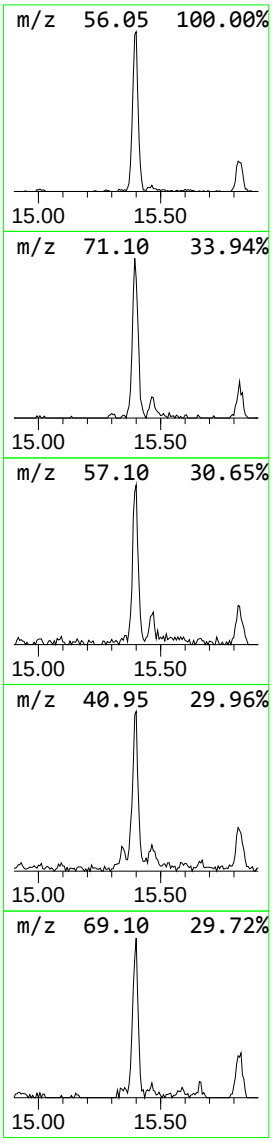
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.400	18.32 ug/l	253805	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	50
2	Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	43
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	25
4	1-Decene, 2-methyl-	154	C11H22	013151-27-4	25
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080837.D
Acq On : 31 Jan 2024 13:57
Operator : JC\MD
Sample : P1284-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1250

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	2.083	18.9	ug/l	121250	1	8.224	320296	50.0
Ethanol	3.783	196.9	ug/l	1261060	1	8.224	320296	50.0
Propanal	4.283	110.3	ug/l	706523	1	8.224	320296	50.0
Butanal	7.224	95.9	ug/l	614454	1	8.224	320296	50.0
1-Butanol	9.265	17.2	ug/l	195559	2	9.100	569751	50.0
Butanoic acid, ...	13.335	104.3	ug/l	1445010	4	13.794	692742	50.0
2-Hexenal, 2-et...	13.688	17.8	ug/l	245892	4	13.794	692742	50.0
1-Hexanol, 2-et...	13.876	93.8	ug/l	1299410	4	13.794	692742	50.0
2,4-Dipropyl-5-...	15.400	18.3	ug/l	253805	4	13.794	692742	50.0