LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073732.D
Acq On : 04 Aug 2022 13:27
Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

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\82N072822W.M
Title : SW846 8260

Signal : TIC: VN073732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.004	15	20	26	rBV2	56974	84061	1.60%	0.256%
2	2.551	105	113	127	rBV	694710	1247577	23.79%	3.793%
3	2.704	133	139	152	rVB5	20057	77772	1.48%	0.236%
4	3.634	285	297	324	rBV	952671	2443995	46.61%	7.429%
5	4.081	363	373	389	rBV	714214	1941302	37.02%	5.901%
6	4.222	389	397	415	rVB	134385	395593	7.54%	1.203%
7	6.510	772	786	809	rBV	1728809	5243909	100.00%	15.941%
8	6.986	856	867	877	rBV2	47554	138646	2.64%	0.421%
9	7.251	901	912	920	rBV4	18361	66269	1.26%	0.201%
10	7.957	1021	1032	1036	rBV	289111	692820	13.21%	2.106%
11	8.016	1036	1042	1056	rVB	506634	1161452	22.15%	3.531%
12	8.369	1093	1102	1115	rBV	290000	689845	13.16%	2.097%
13	8.910	1183	1194	1212	rBV2	1272500	2724054	51.95%	8.281%
14	9.092	1218	1225	1229	rBV2	71255	145293	2.77%	0.442%
15	9.151	1229	1235	1241	rVV	424575	841103	16.04%	2.557%
16	9.210	1241	1245	1256	rVB	74565	137730	2.63%	0.419%
17	9.475	1282	1290	1299	rBV2	27411	59959	1.14%	0.182%
18	9.563	1299	1305	1316	rVB	37863	73195	1.40%	0.223%
19	10.380	1436	1444	1453	rBV	1027284	1875227	35.76%	5.700%
20	10.627	1478	1486	1502	rBV	2077730	3488277	66.52%	10.604%
21	10.769	1502	1510	1526	rVV	1549162	2790010	53.20%	8.481%
22	10.898	1526	1532	1543	rVB2	28466	60021	1.14%	0.182%
23	11.033	1547	1555	1561	rBV	35719	60065	1.15%	0.183%
24	11.686	1649	1666	1679	rBV	1084547	2048093	39.06%	6.226%
25	11.810	1681	1687	1692	rVB3	30890	52696	1.00%	0.160%
26	11.927	1703	1707	1715	rVB	38888	63799	1.22%	0.194%
27	12.233	1752	1759	1771	rVB5	58189	115692	2.21%	0.352%
28	12.627	1821	1826	1828	rBV	52211	77401	1.48%	0.235%
29	12.674	1828	1834	1845	rVB	839289	1425579	27.19%	4.334%
30	13.151	1904	1915	1928	rVB3	79626	159950	3.05%	0.486%
31	13.380	1947	1954	1962	rBV3	99594	201818	3.85%	0.614%
32	13.615	1987	1994	2004	rBV	1046351	1735756	33.10%	5.277%
33	13.715	2005	2011	2016	rVV	72611	132485	2.53%	0.403%
34	13.774	2016	2021	2025	rVV2	112457	223362	4.26%	0.679%
35	13.815	2025	2028	2032	rVV2	57403	91974	1.75%	0.280%
36	13.851	2032	2034	2044	rVB5	25539	54477	1.04%	0.166%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

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\82N072822W.M
Title : SW846 8260

37	16.356	2453	2460	2468	rVB7	32066	74602	1.42%	0.227%

Sum of corrected areas: 32895859

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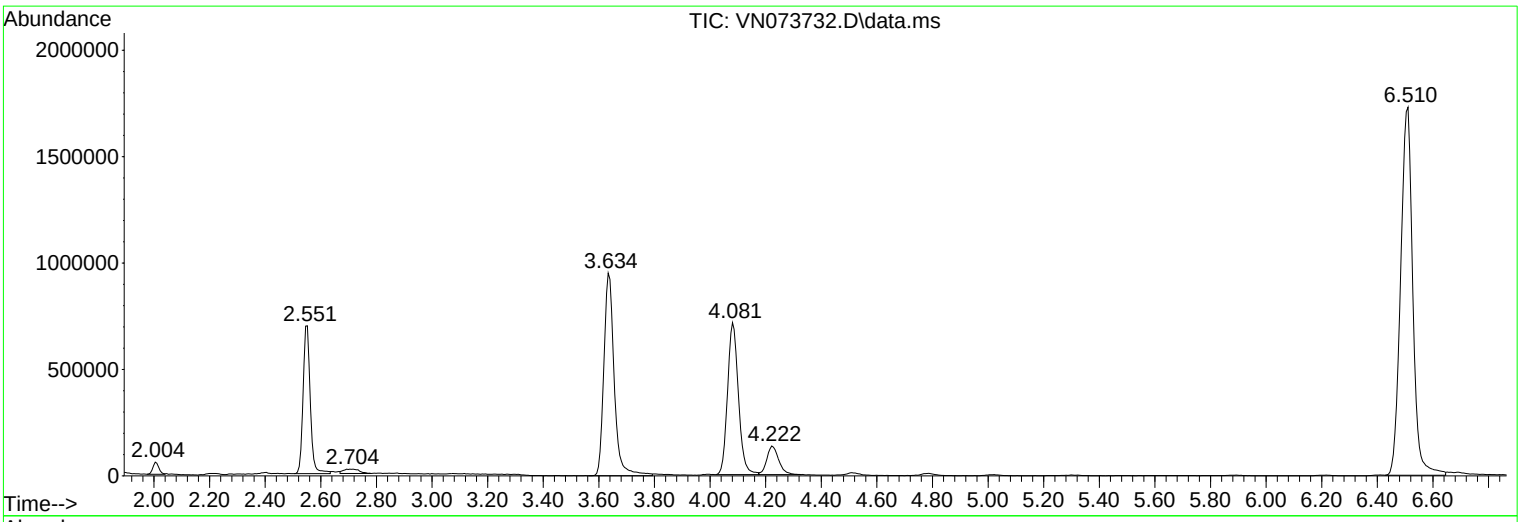
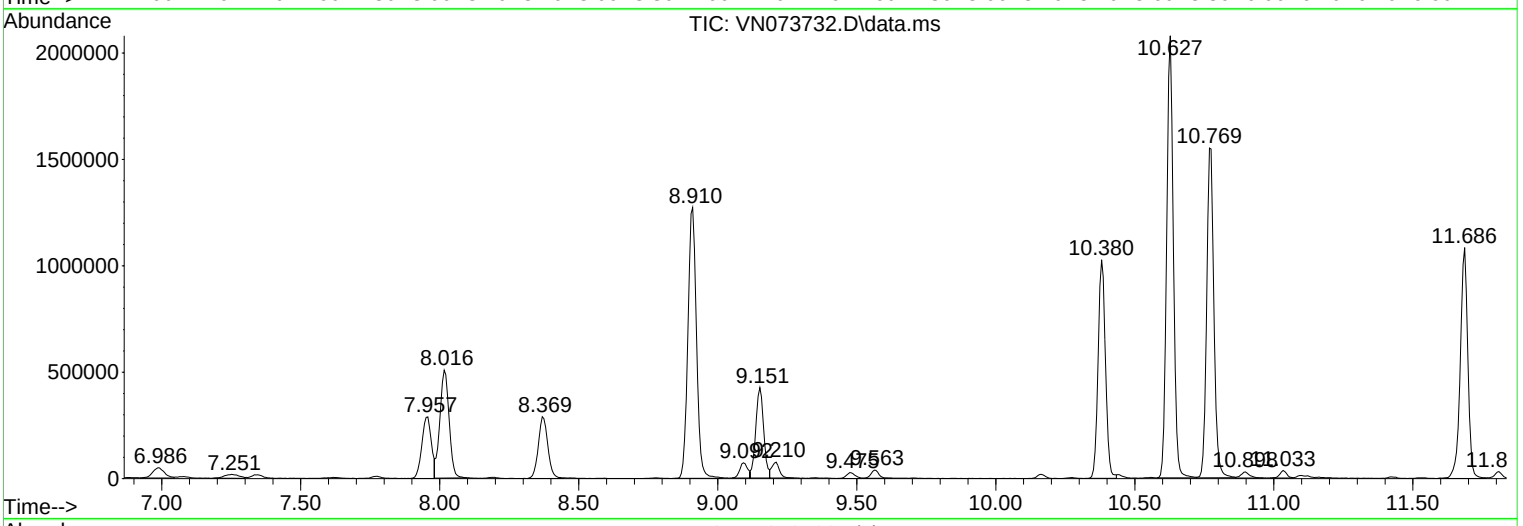
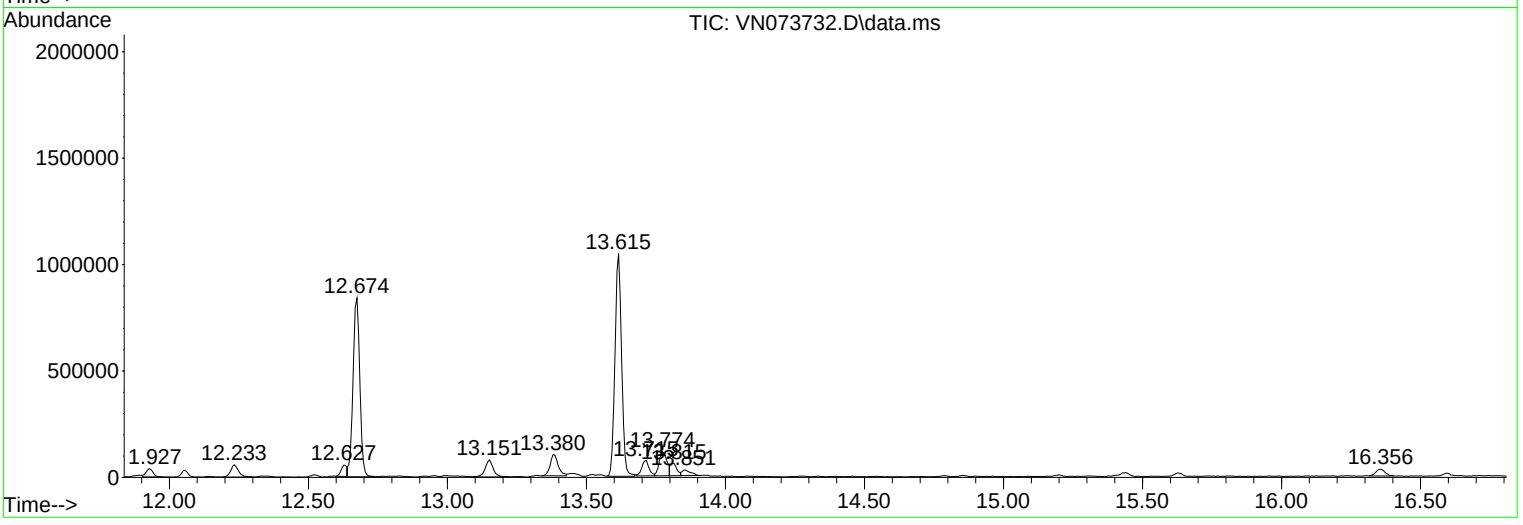
33773-74

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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







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Data File : VN073732.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
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Instrument :
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ClientSampleId :
33773-74

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

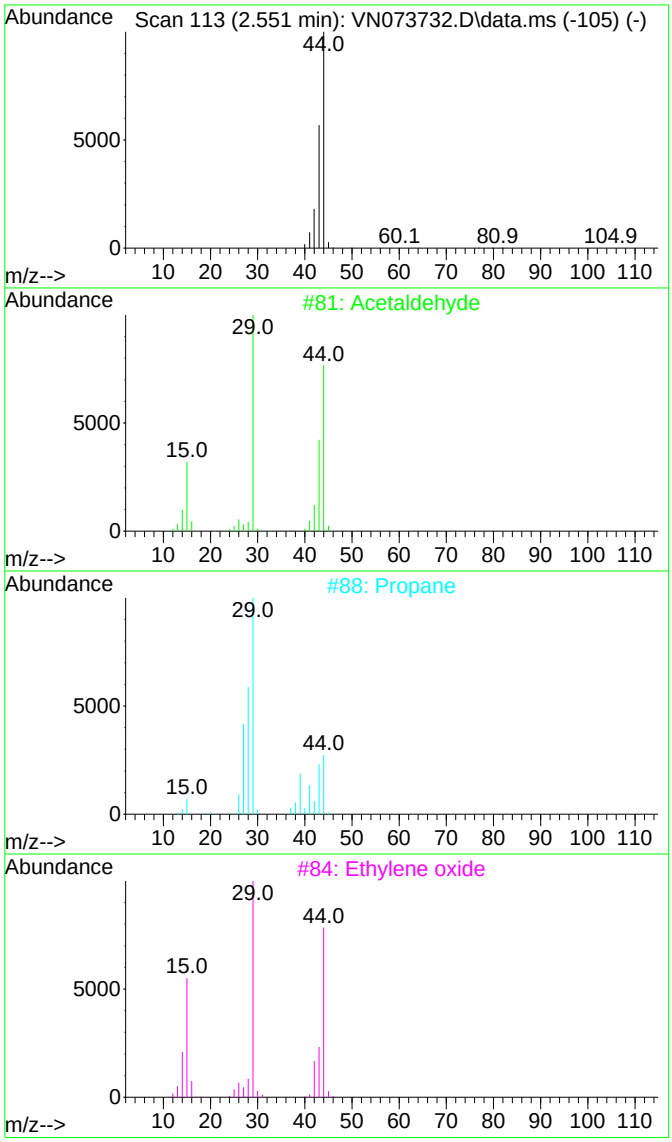
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

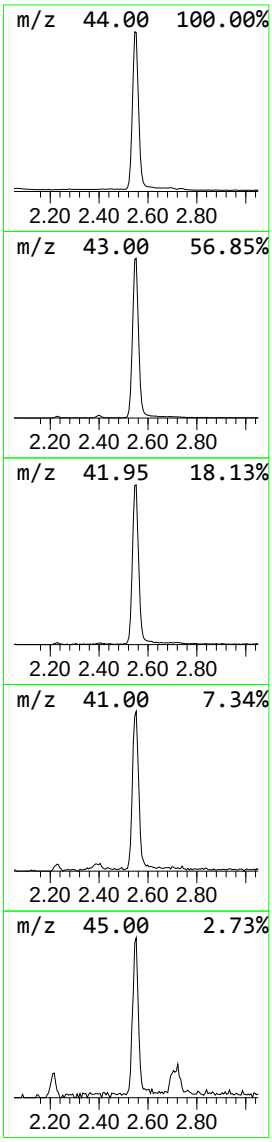
****

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.551	53.71 ug/l	1247580	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	Alanine	89	C3H7NO2	000056-41-7	4





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Data File : VN073732.D
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Operator : JC\MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

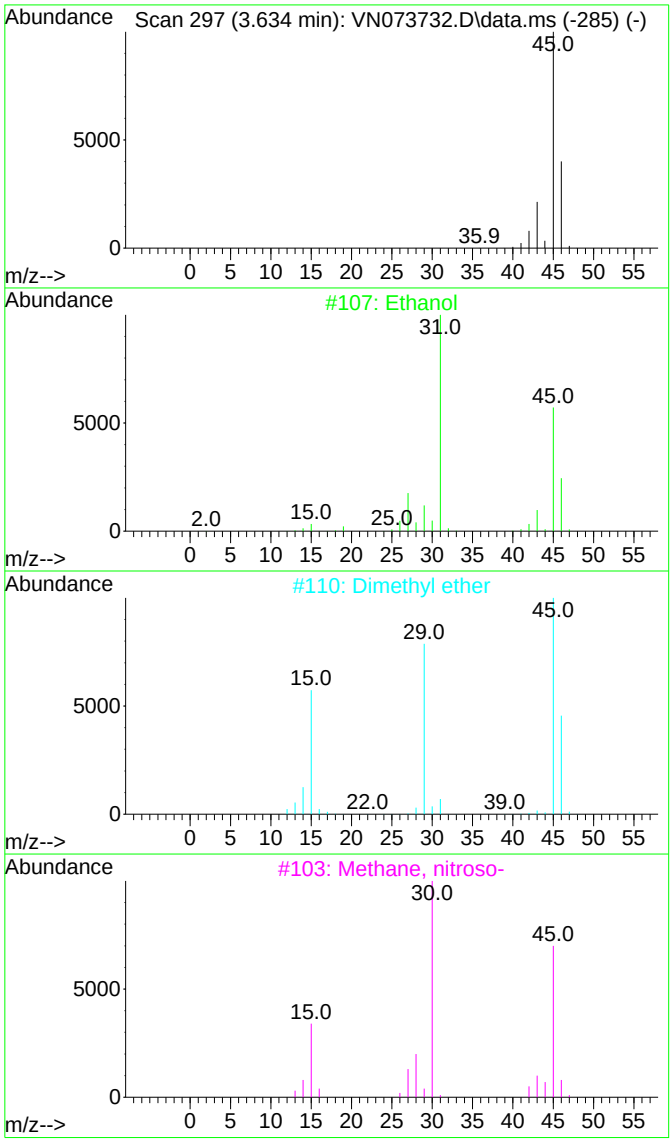
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

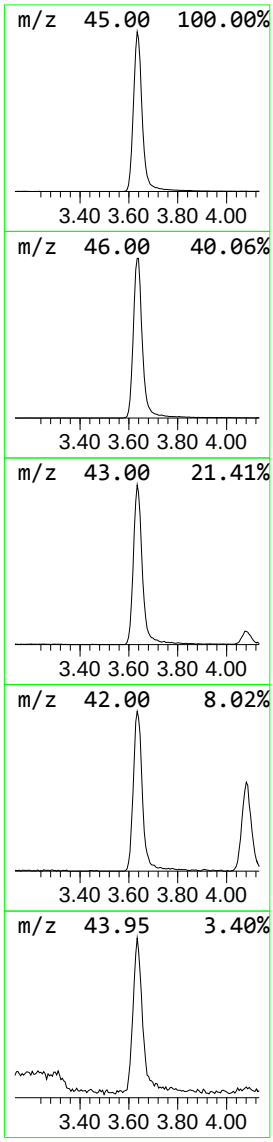
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	105.21 ug/l	2444000	Pentafluorobenzene	8.016

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073732.D
Acq On : 04 Aug 2022 13:27
Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

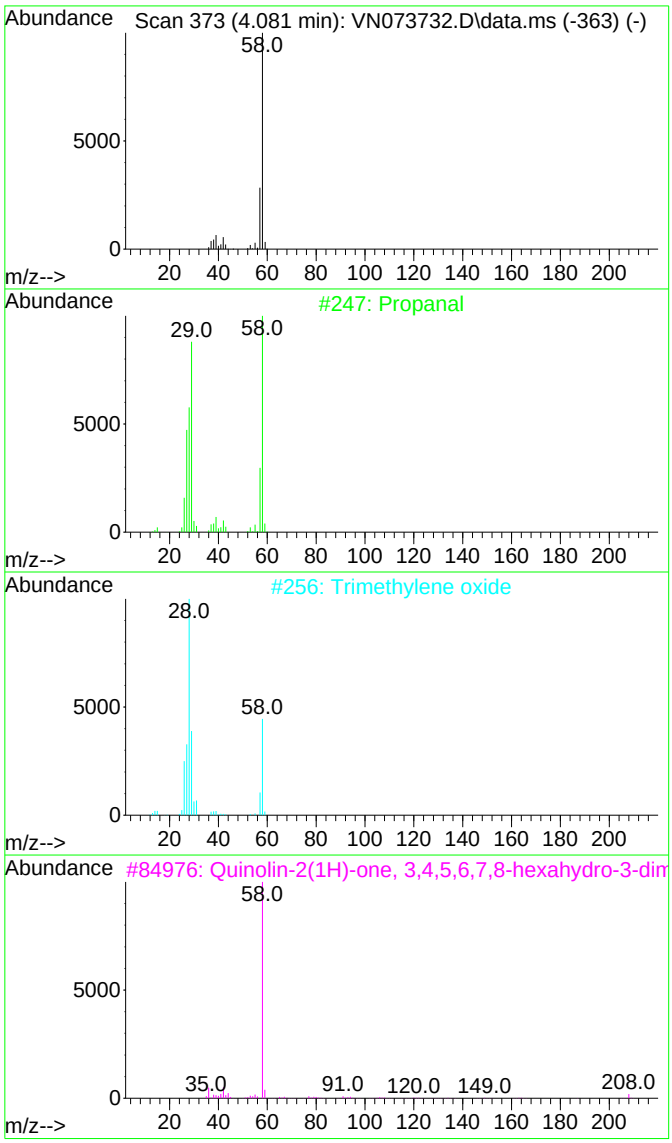
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

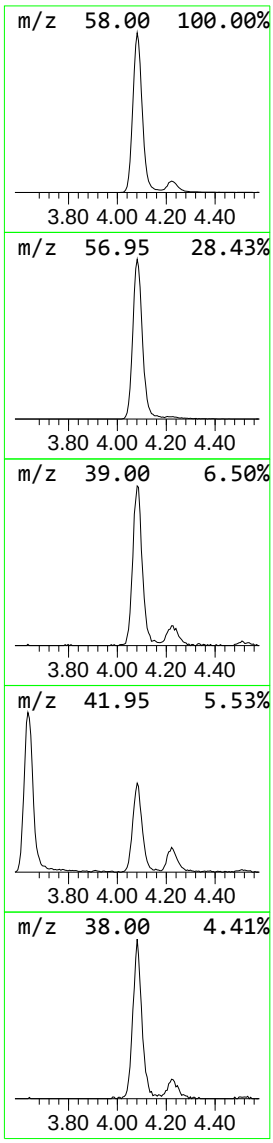
****

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.081	83.57 ug/l	1941300	Pentafluorobenzene	8.016

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	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073732.D
Acq On : 04 Aug 2022 13:27
Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

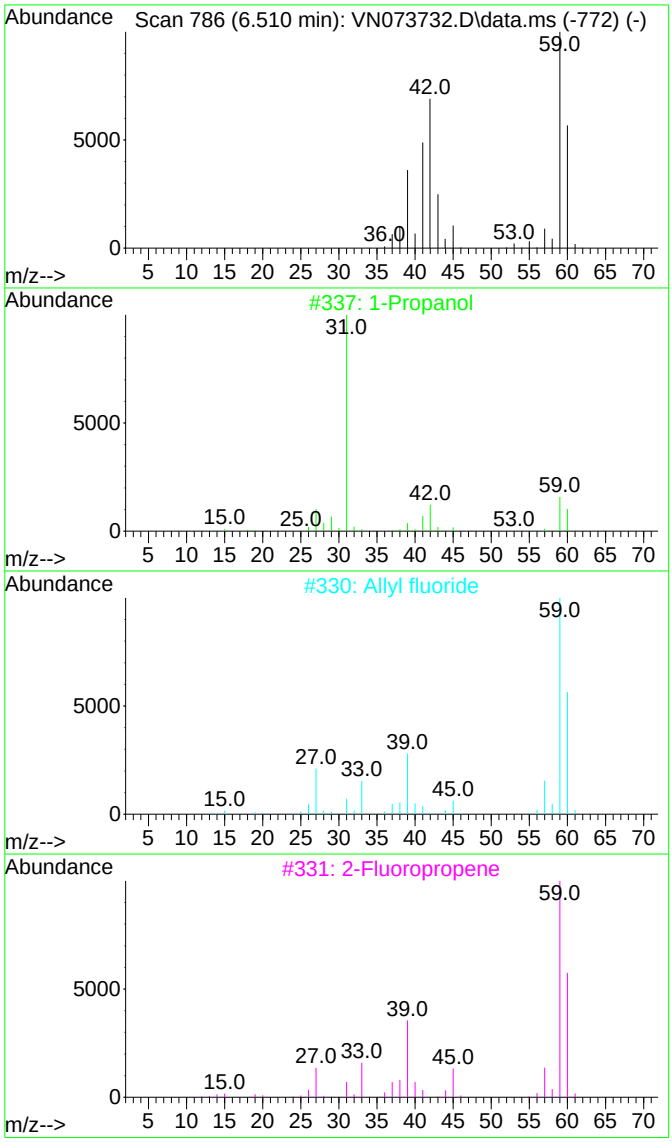
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

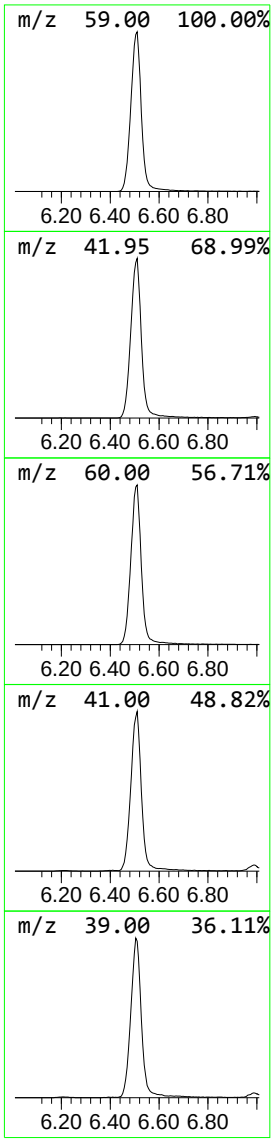
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	225.75 ug/l	5243910	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	53
3	2-Fluoropropene	60	C3H5F	001184-60-7	50
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	12
5	Cyclopropane	42	C3H6	000075-19-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
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Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

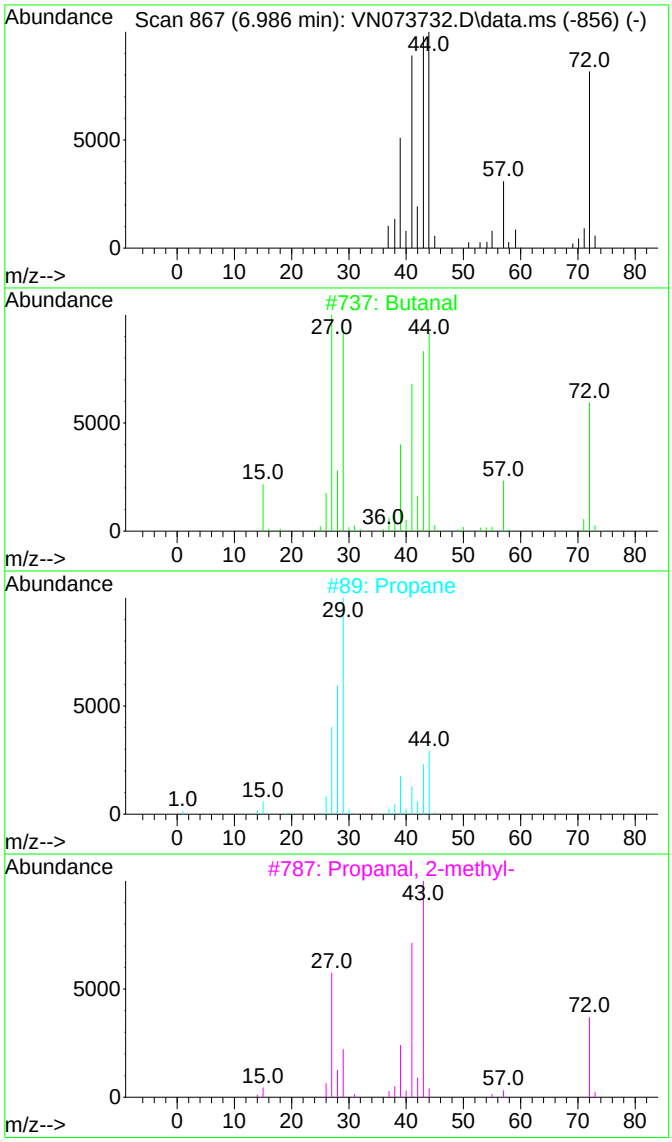
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

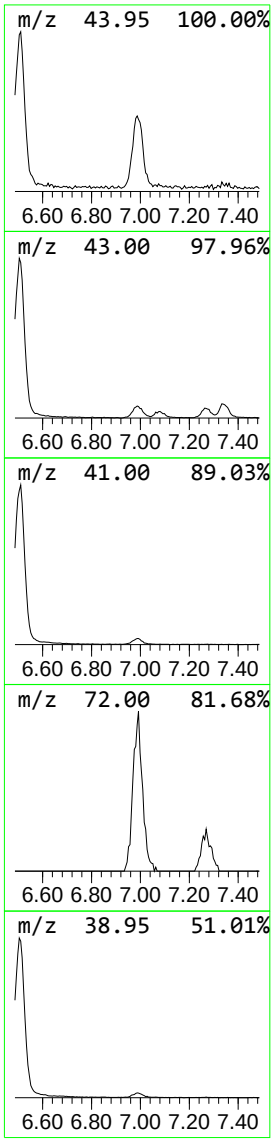
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.986	5.97 ug/l	138646	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	32





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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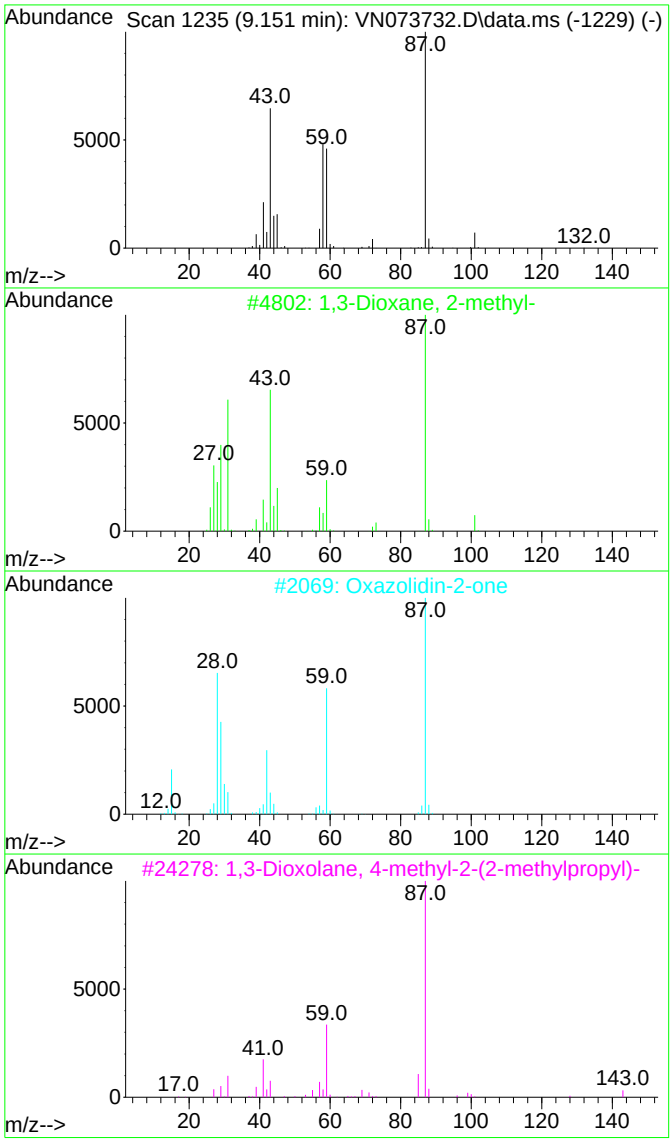
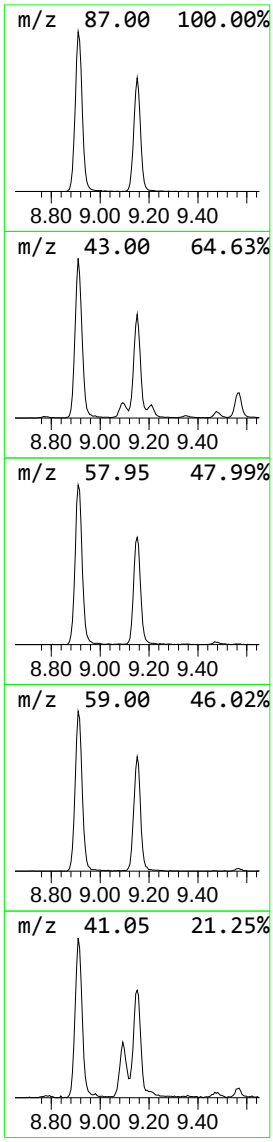
****
Peak Number 6 1,3-Dioxane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	15.44 ug/l	841103	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	33





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Quant Title : SW846 8260

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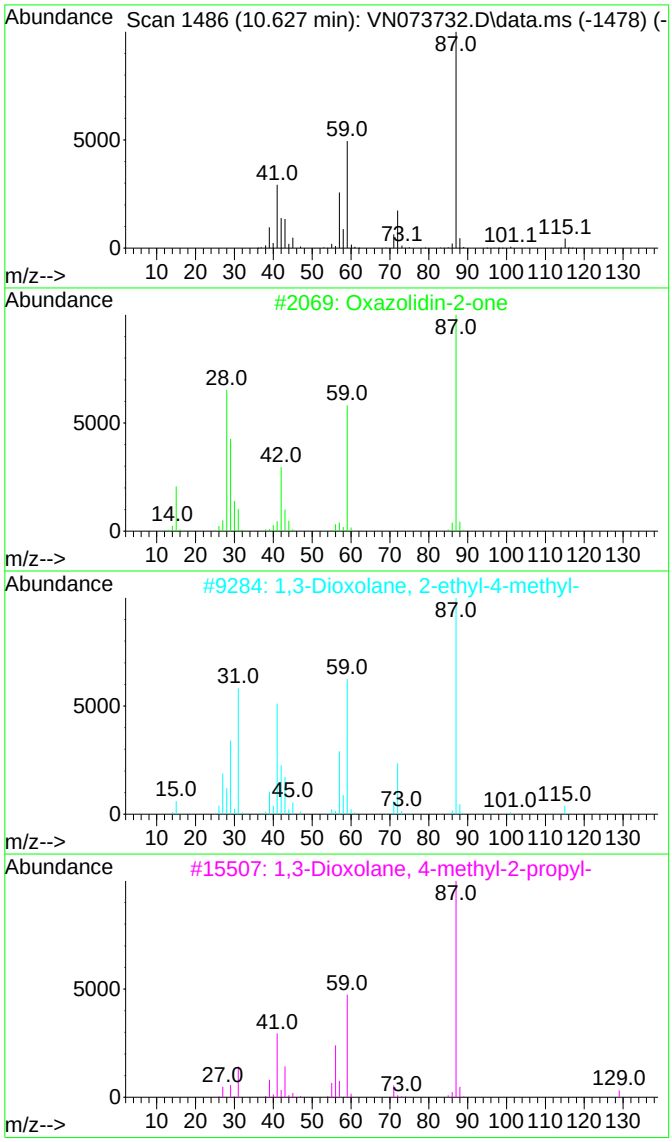
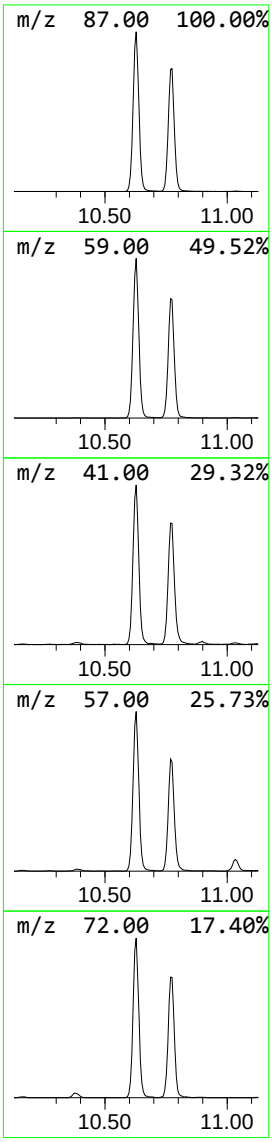
****

Peak Number 7 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.627	85.16 ug/l	3488280	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
2	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	76
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	50





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ClientSampleId :
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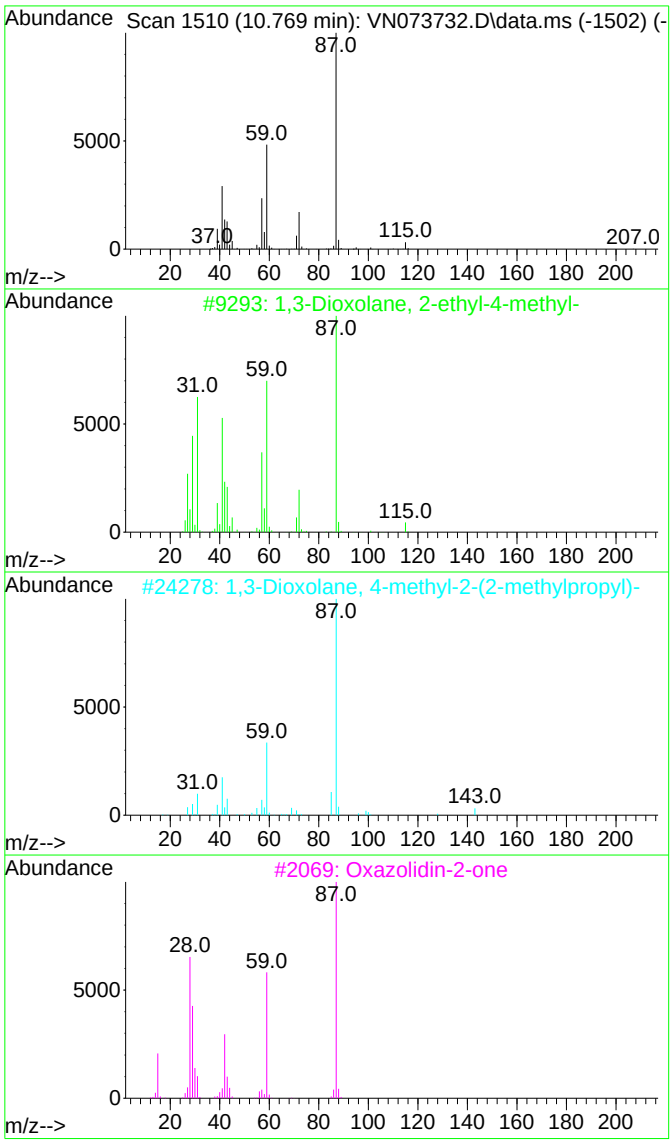
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

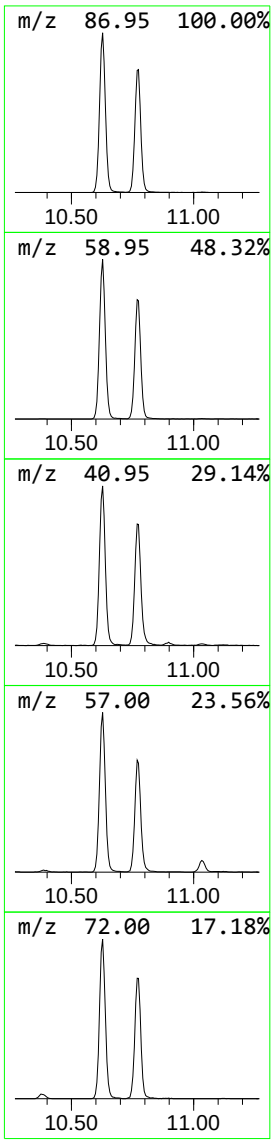
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	68.11 ug/l	2790010	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	56
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073732.D
Acq On : 04 Aug 2022 13:27
Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

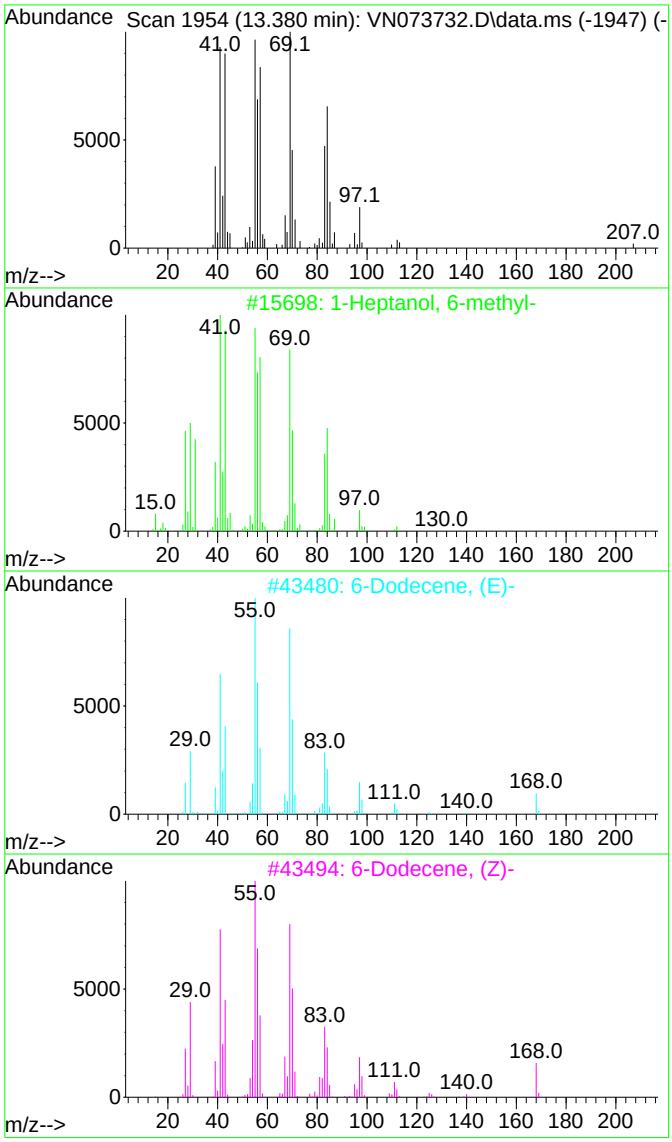
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

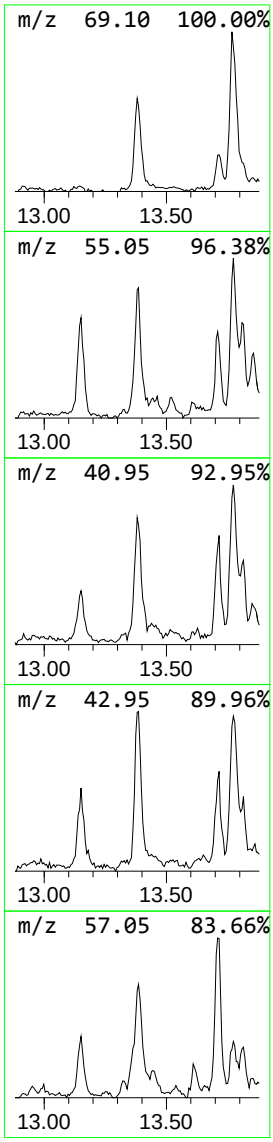
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Heptanol, 6-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.380	5.81 ug/l	201818	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	78
2	6-Dodecene, (E)-	168	C12H24	007206-17-9	59
3	6-Dodecene, (Z)-	168	C12H24	007206-29-3	59
4	4-Decene, 3-methyl-, (E)-	154	C11H22	062338-47-0	47
5	Hexanal, 3,3-dimethyl-	128	C8H16O	055320-57-5	43





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Instrument :
MSVOA_N
ClientSampleId :
33773-74

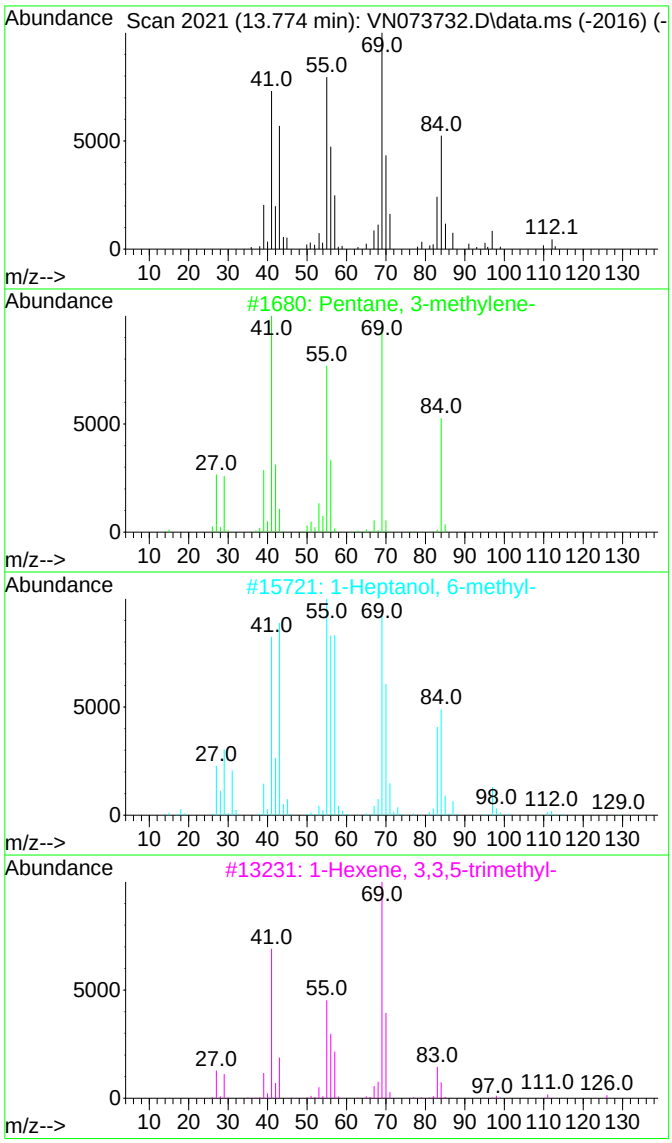
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

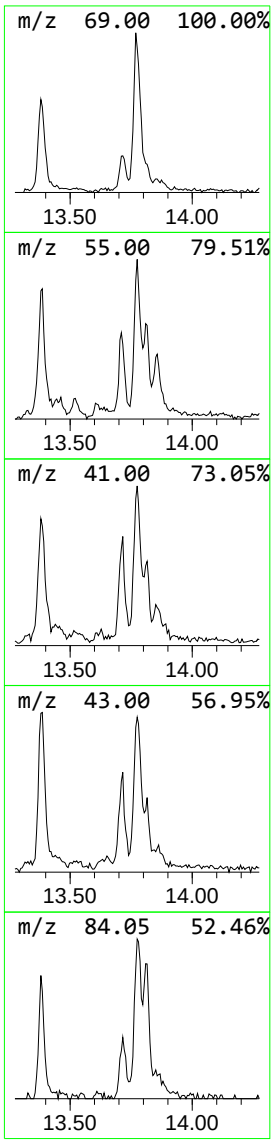
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentane, 3-methylene- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	6.43 ug/l	223362	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methylene-	84	C6H12	000760-21-4	50
2	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	50
3	1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	50
4	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	50
5	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073732.D
Acq On : 04 Aug 2022 13:27
Operator : JC\MD
Sample : N4018-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
33773-74

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Acetaldehyde	2.551	53.7	ug/l	1247580	1	8.016	1161450	50.0
Ethanol	3.634	105.2	ug/l	2444000	1	8.016	1161450	50.0
Propanal	4.081	83.6	ug/l	1941300	1	8.016	1161450	50.0
1-Propanol	6.510	225.8	ug/l	5243910	1	8.016	1161450	50.0
Butanal	6.986	6.0	ug/l	138646	1	8.016	1161450	50.0
1,3-Dioxane, 2-...	9.151	15.4	ug/l	841103	2	8.904	2724050	50.0
Oxazolidin-2-one	10.627	85.2	ug/l	3488280	3	11.686	2048090	50.0
1,3-Dioxolane, ...	10.769	68.1	ug/l	2790010	3	11.686	2048090	50.0
1-Heptanol, 6-m...	13.380	5.8	ug/l	201818	4	13.615	1735760	50.0
Pentane, 3-meth...	13.774	6.4	ug/l	223362	4	13.615	1735760	50.0