

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070552.D
 Acq On : 10 Jan 2022 19:00
 Operator : JC/MD
 Sample : N1015-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30915

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.030	10	15	48	rVB2	113030	236667	2.29%	0.393%
2	2.239	83	93	109	rBV3	99631	256321	2.48%	0.426%
3	2.593	216	225	245	rVB	106111	184676	1.79%	0.307%
4	4.143	781	803	833	rBV	643989	1835328	17.77%	3.047%
5	4.285	834	856	904	rVB	1301615	3837087	37.15%	6.371%
6	4.578	940	965	1005	rBV	930975	3023980	29.28%	5.021%
7	6.581	1686	1712	1766	rBV2	1700078	5595739	54.18%	9.290%
8	7.335	1975	1993	2019	rVB2	135976	358969	3.48%	0.596%
9	7.657	2094	2113	2141	rBV3	40682	113668	1.10%	0.189%
10	7.839	2158	2181	2207	rBV	425143	1016963	9.85%	1.688%
11	8.021	2228	2249	2260	rBV	675954	1619694	15.68%	2.689%
12	8.083	2260	2272	2305	rVB	1309022	2985485	28.91%	4.957%
13	8.437	2383	2404	2432	rBV2	902998	2271446	21.99%	3.771%
14	8.965	2581	2601	2638	rBV	2002098	4117135	39.86%	6.835%
15	9.268	2699	2714	2730	rVB3	66237	129106	1.25%	0.214%
16	10.293	3058	3096	3126	rBV4	105561	570083	5.52%	0.946%
17	10.440	3133	3151	3167	rBV	3014825	5654936	54.75%	9.389%
18	10.682	3226	3241	3262	rBV	640242	1138551	11.02%	1.890%
19	10.827	3281	3295	3323	rBV	545184	994894	9.63%	1.652%
20	11.143	3381	3413	3464	rBV2	2748646	10328048	100.00%	17.147%
21	11.741	3611	3636	3664	rBV	2824740	5861550	56.75%	9.732%
22	12.728	3980	4004	4027	rBV	2217642	3933153	38.08%	6.530%
23	13.672	4341	4356	4378	rBV	2179277	3746957	36.28%	6.221%
24	13.769	4380	4392	4408	rVB2	251173	421236	4.08%	0.699%

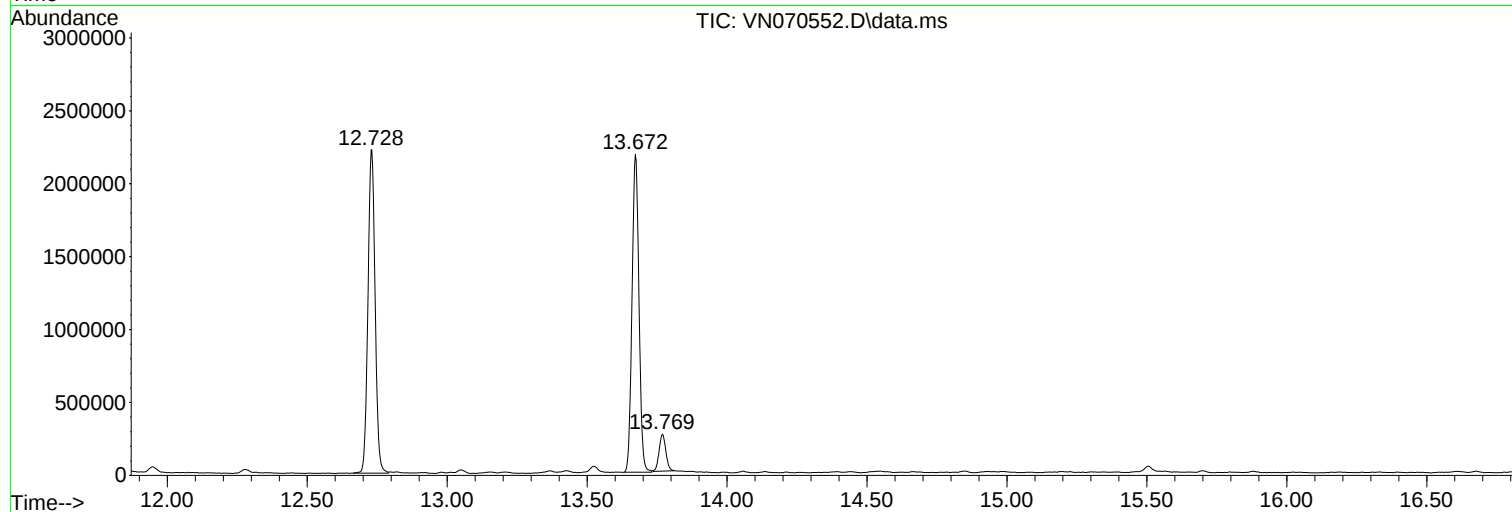
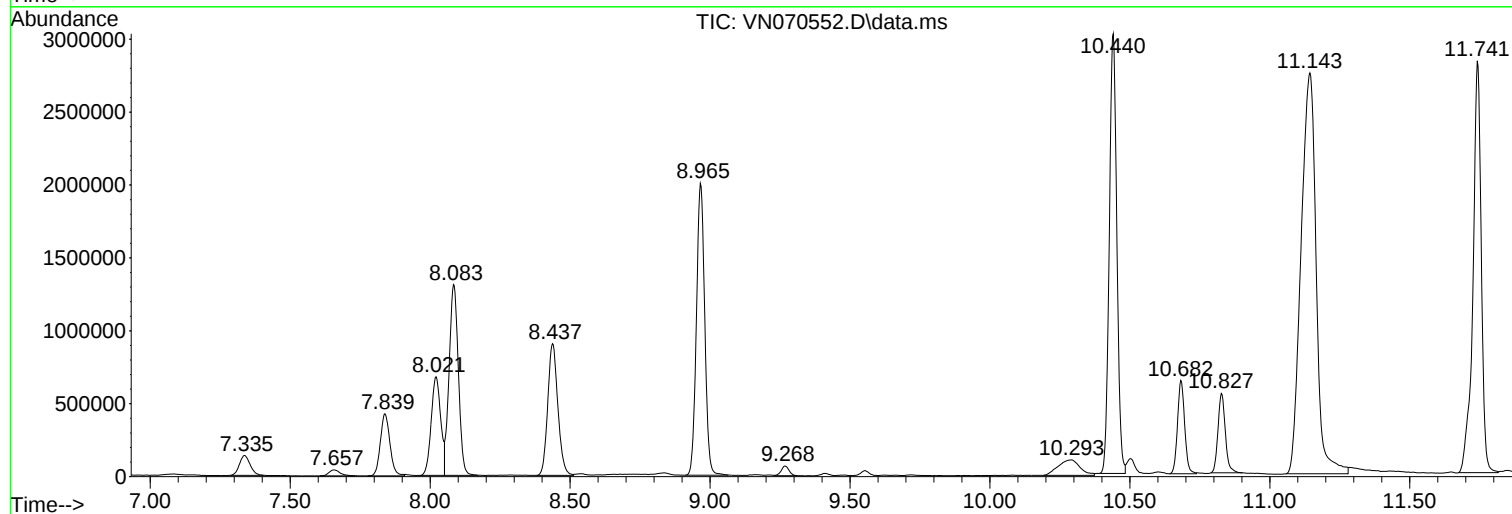
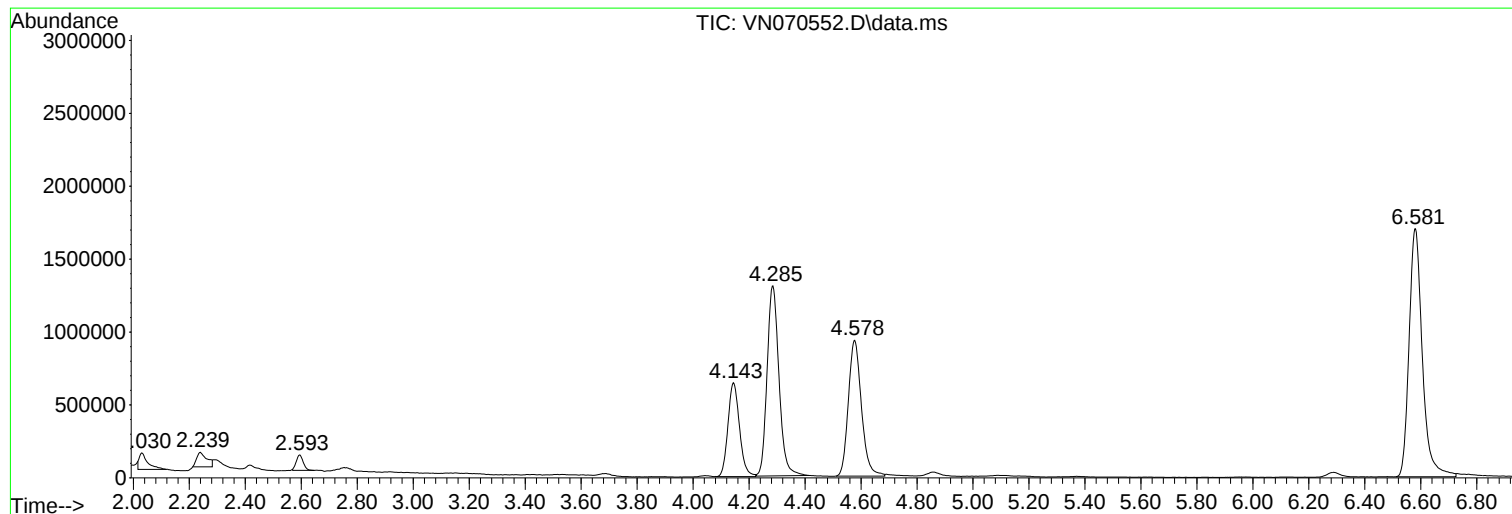
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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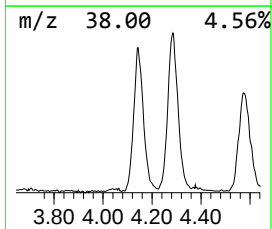
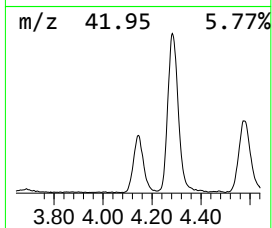
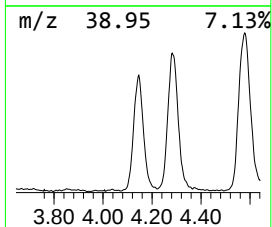
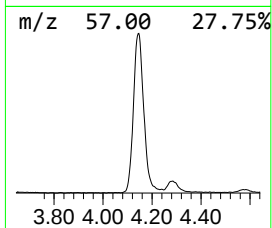
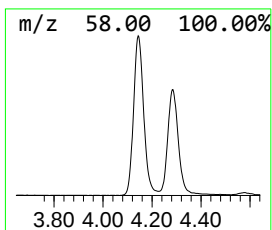
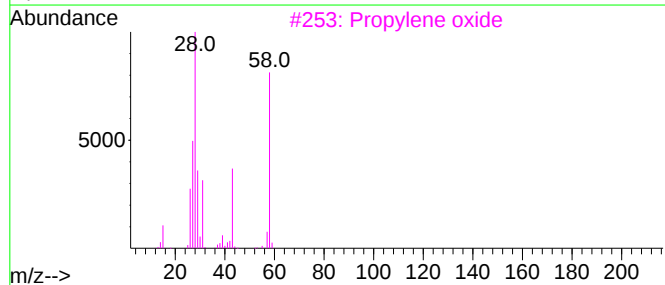
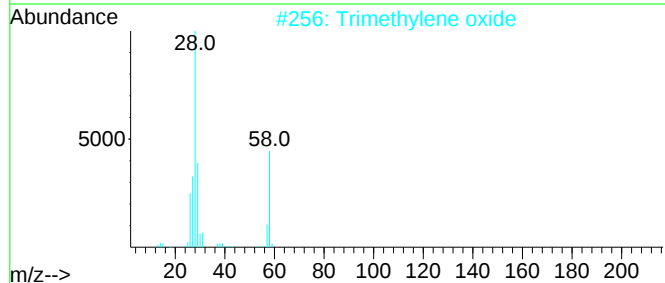
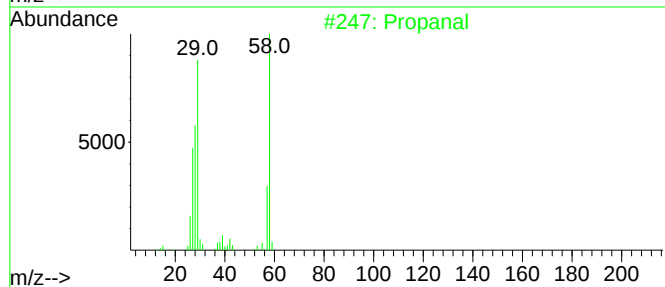
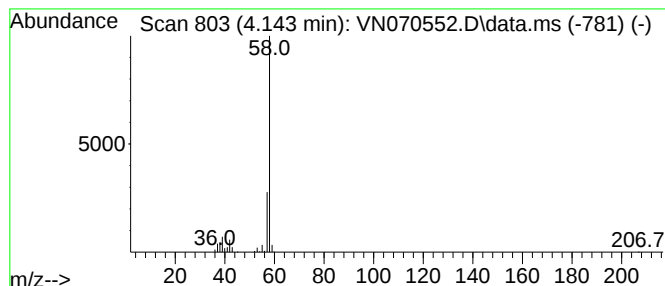
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.143	30.74 ug/l	1835330	Pentafluorobenzene	8.086

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			Propylene oxide	58	C3H6O	000075-56-9	7
4			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5
5			Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	4



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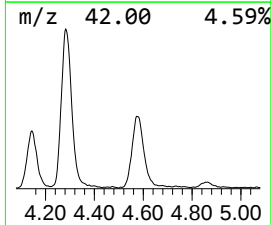
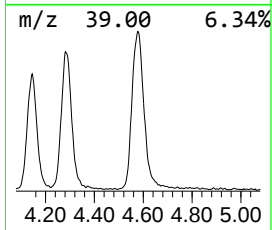
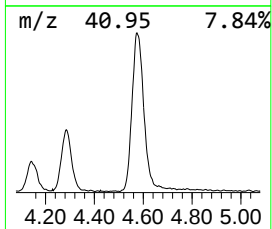
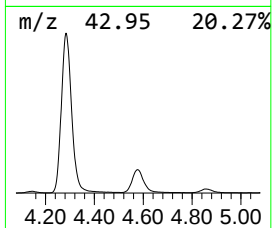
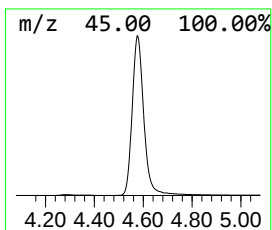
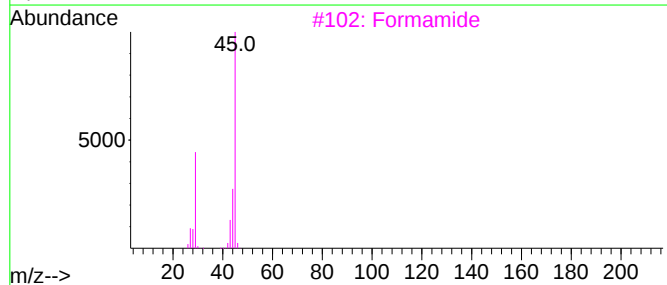
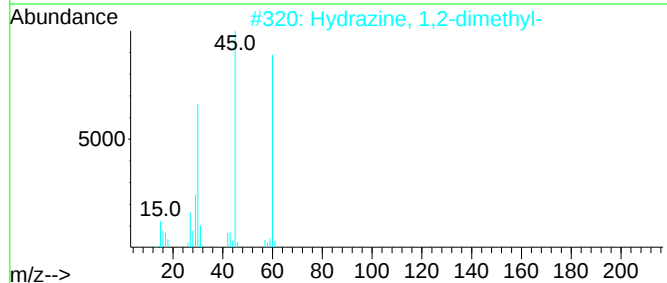
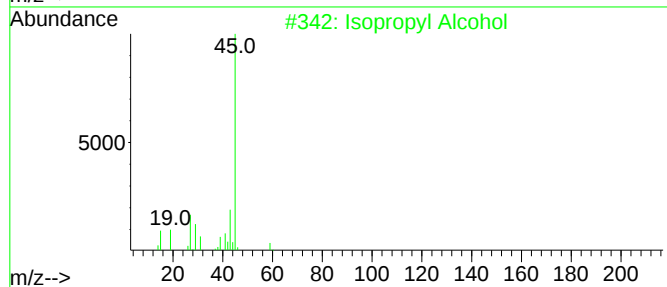
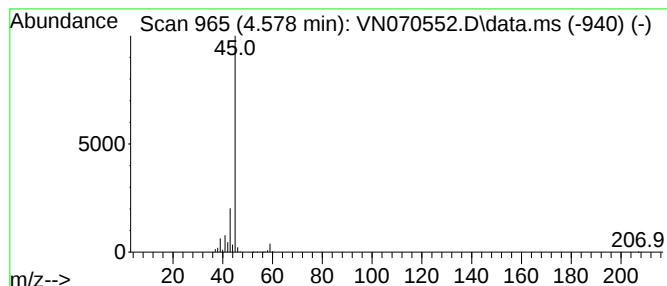
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.578	50.64 ug/l	3023980	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Formamide	45	CH3NO	000075-12-7	5
4			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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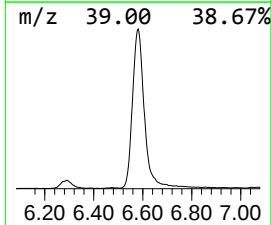
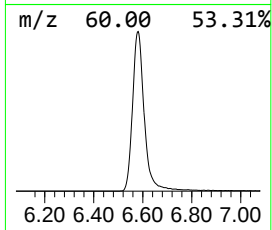
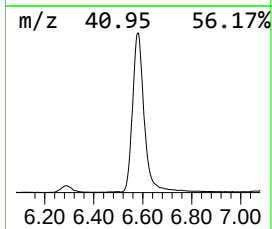
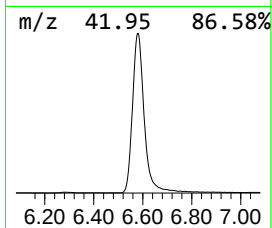
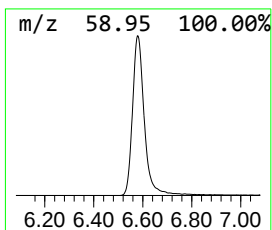
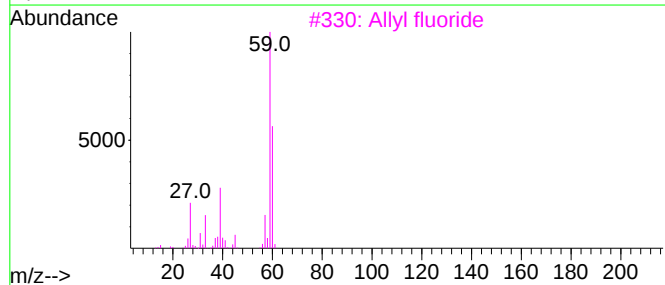
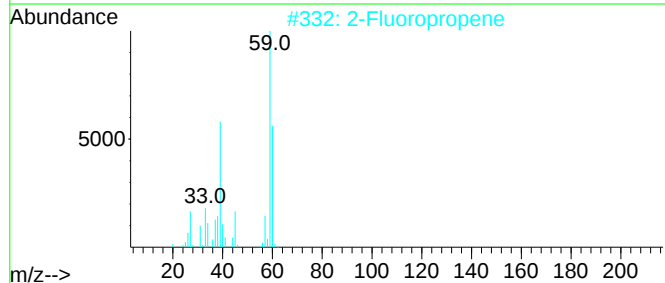
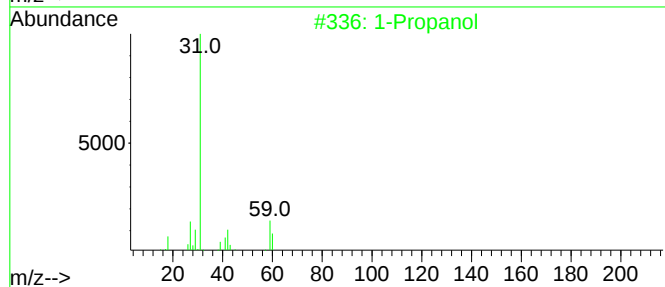
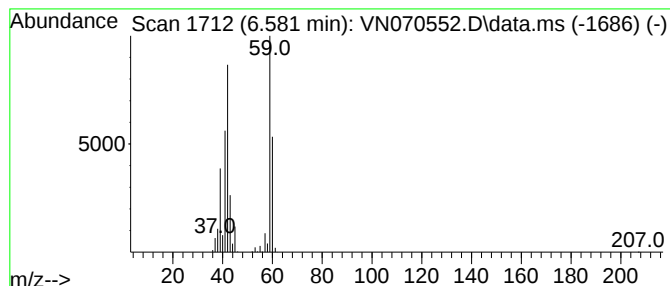
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	93.72 ug/l	5595740	Pentafluorobenzene	8.086

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	38
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	10
5			Cyclopropane	42	C3H6	000075-19-4	9



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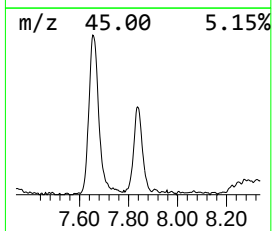
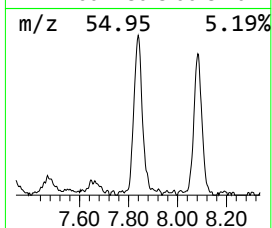
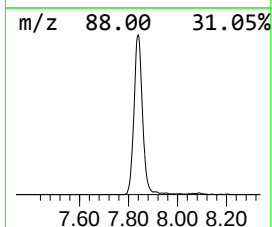
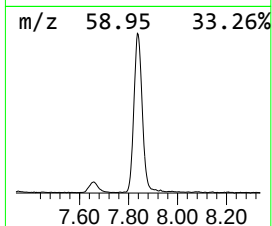
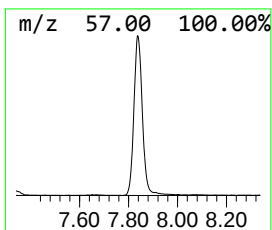
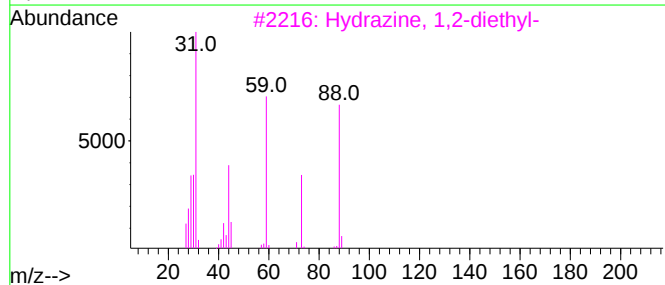
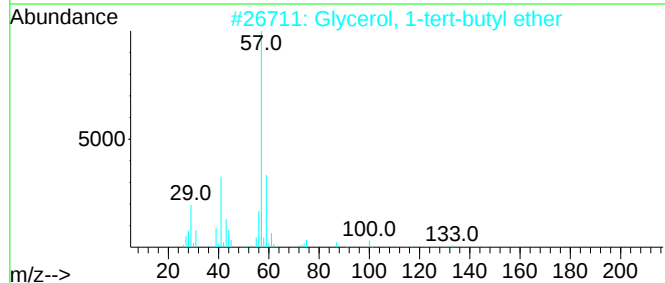
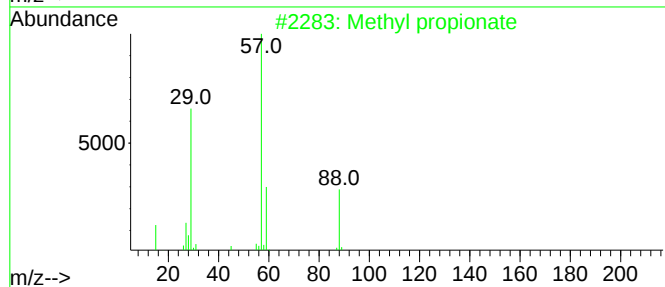
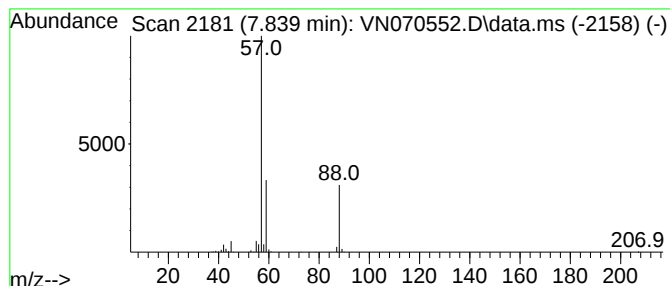
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Peak Number 4 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.839	17.03 ug/l	1016960	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl propionate	88	C4H8O2	000554-12-1	90
2			Glycerol, 1-tert-butyl ether	148	C7H16O3	1010381-75-8	28
3			Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9
4			Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	9
5			tert-Butyl isopropyl carbonate	160	C8H16O3	030221-21-7	9



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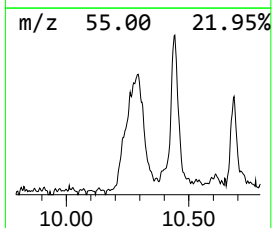
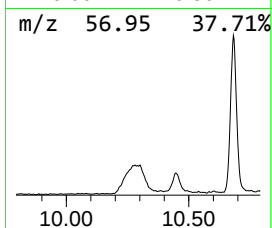
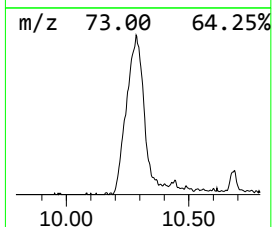
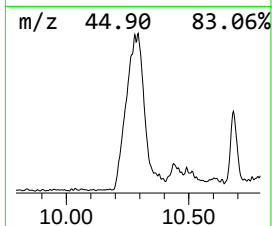
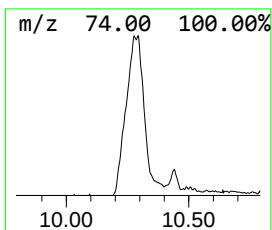
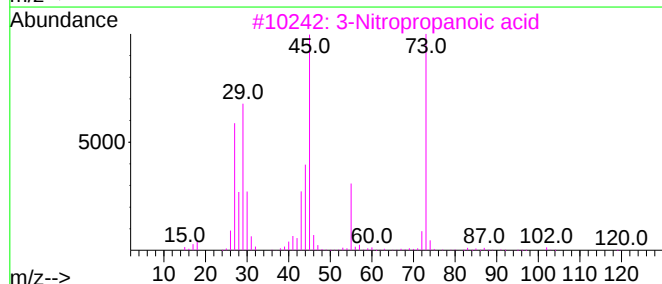
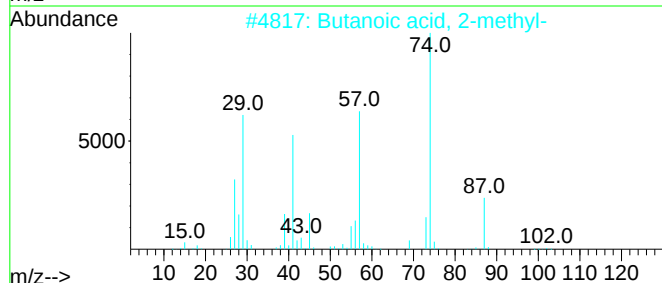
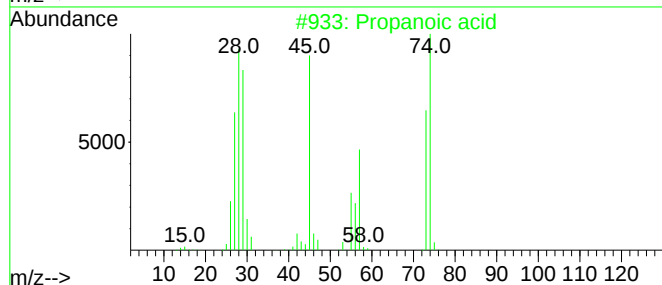
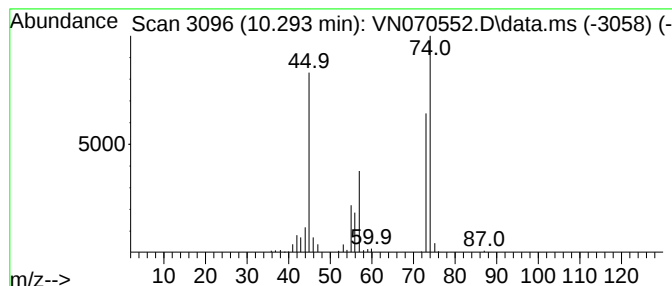
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.293	6.92 ug/l	570083	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid	74	C3H6O2	000079-09-4	90
2			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	25
3			3-Nitropropanoic acid	119	C3H5NO4	000504-88-1	17
4			N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	9
5			Methane, nitroso-	45	CH3NO	000865-40-7	9



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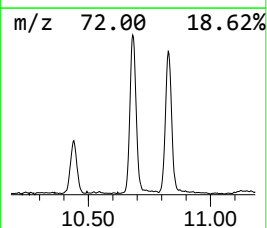
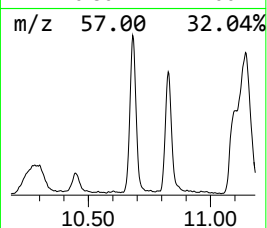
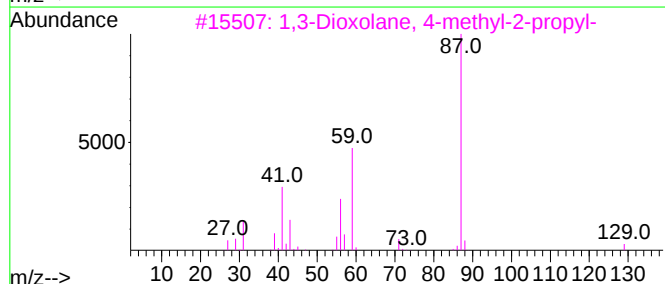
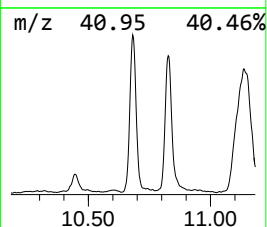
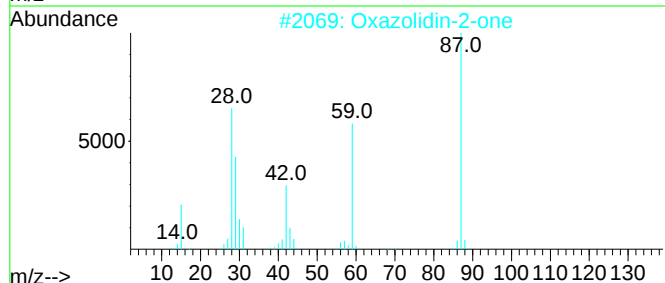
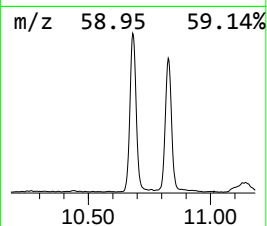
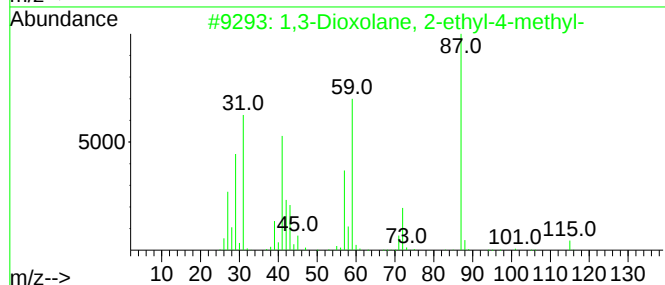
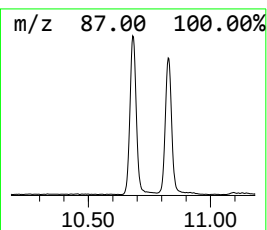
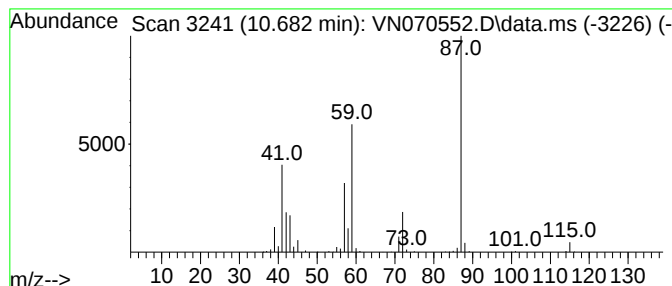
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.682	9.71 ug/l	1138550	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	95
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070552.D
Acq On : 10 Jan 2022 19:00
Operator : JC/MD
Sample : N1015-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

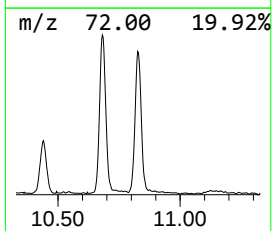
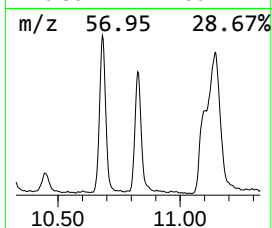
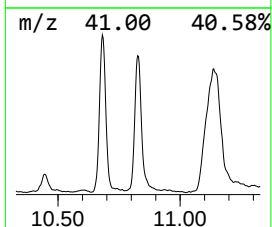
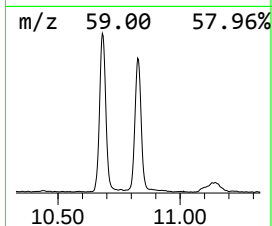
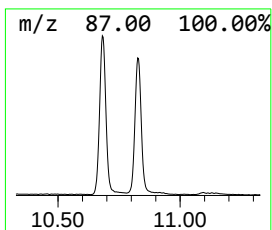
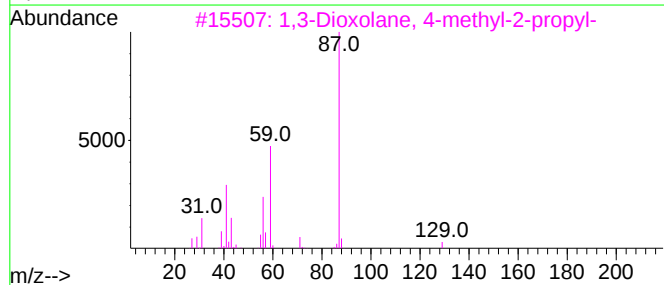
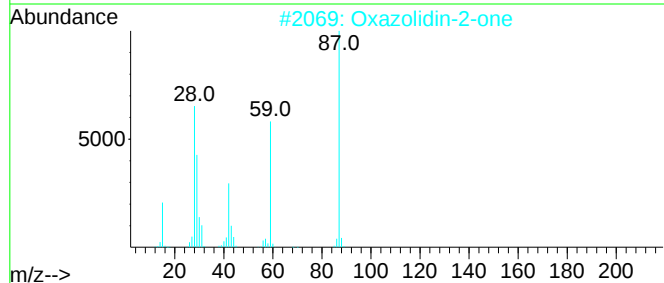
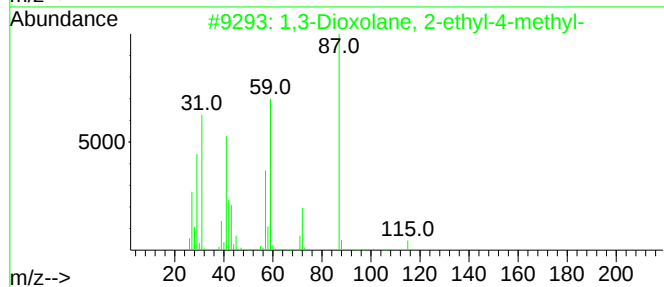
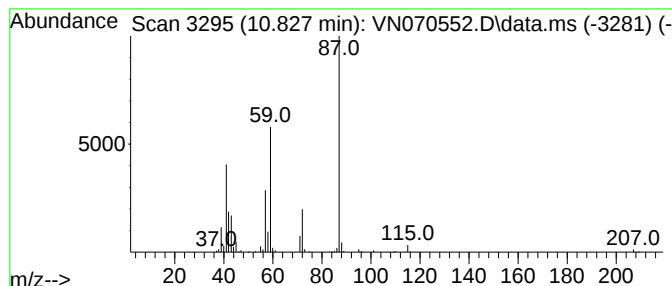
Instrument :
MSVOA_N
ClientSampleId :
30915

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 7 Oxazolidin-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.827	8.49 ug/l	994894	Chlorobenzene-d5	11.744	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	95
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	58
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070552.D
Acq On : 10 Jan 2022 19:00
Operator : JC/MD
Sample : N1015-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30915

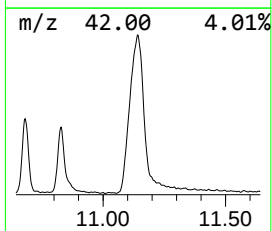
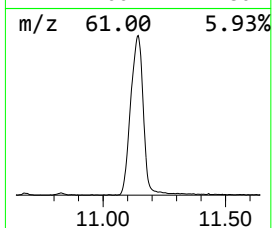
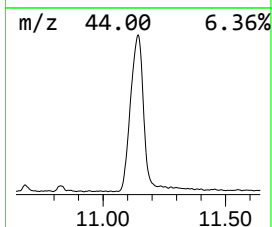
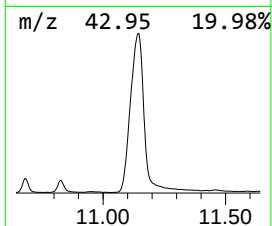
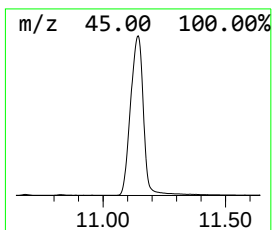
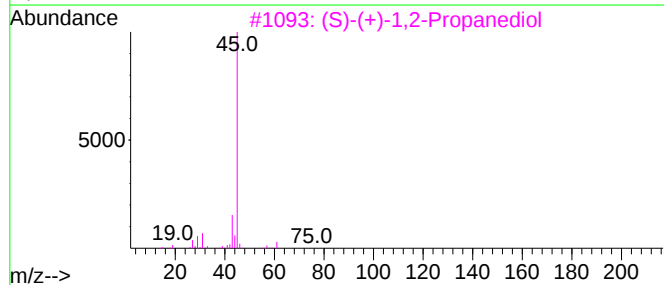
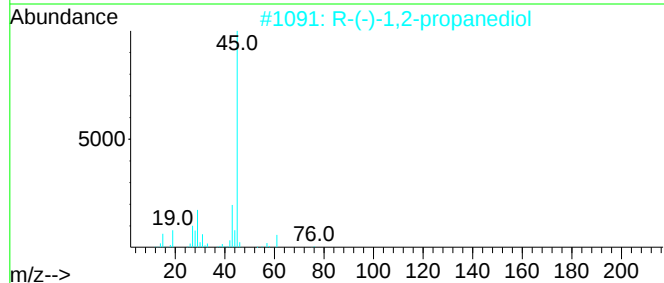
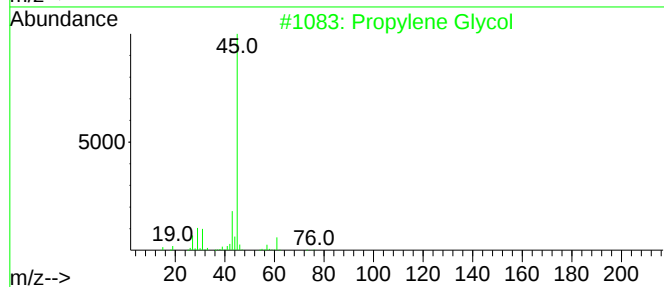
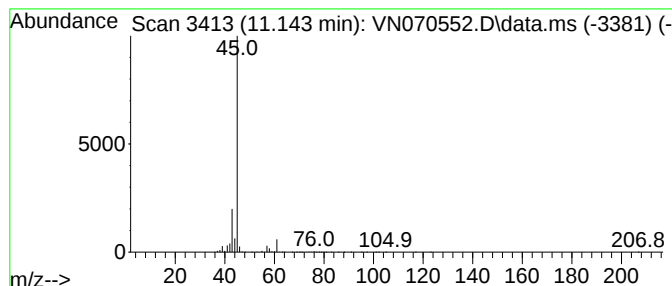
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Quant Title : SW846 8260

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

Peak Number 8 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.143	88.10 ug/l	10328000	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070552.D
Acq On : 10 Jan 2022 19:00
Operator : JC/MD
Sample : N1015-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30915

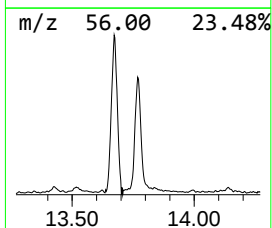
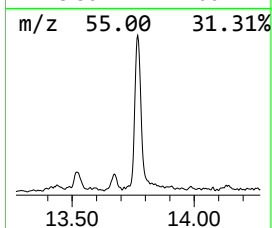
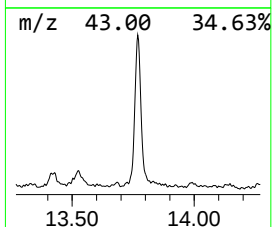
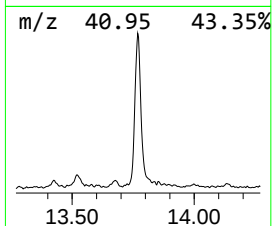
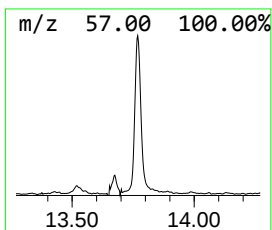
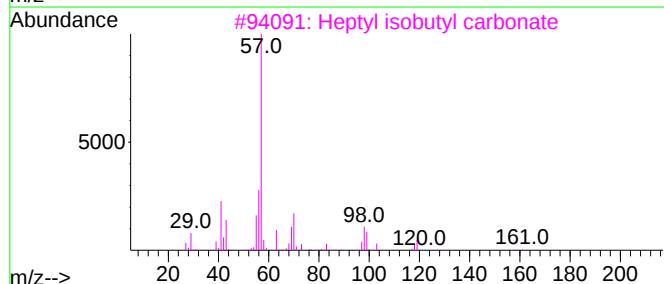
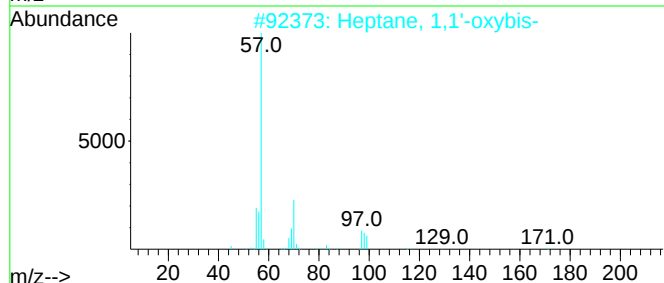
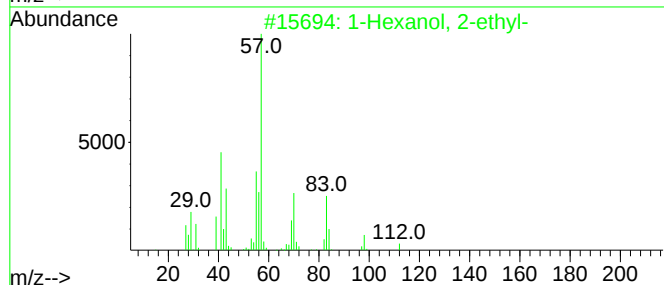
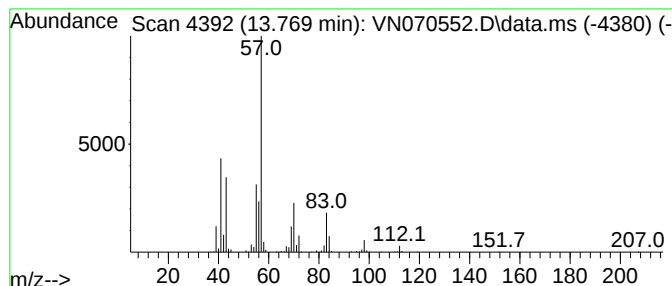
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	5.62 ug/l	421236	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
4			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	56
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070552.D
Acq On : 10 Jan 2022 19:00
Operator : JC/MD
Sample : N1015-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30915

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.143	30.7	ug/l	1835330	1	8.086	2985490	50.0
Isopropyl Alcohol	4.578	50.6	ug/l	3023980	1	8.086	2985490	50.0
1-Propanol	6.581	93.7	ug/l	5595740	1	8.086	2985490	50.0
Methyl propionate	7.839	17.0	ug/l	1016960	1	8.086	2985490	50.0
Propanoic acid	10.293	6.9	ug/l	570083	2	8.965	4117140	50.0
1,3-Dioxolane, ...	10.682	9.7	ug/l	1138550	3	11.744	5861550	50.0
Oxazolidin-2-one	10.827	8.5	ug/l	994894	3	11.744	5861550	50.0
Propylene Glycol	11.143	88.1	ug/l	10328000	3	11.744	5861550	50.0
1-Hexanol, 2-et...	13.769	5.6	ug/l	421236	4	13.672	3746960	50.0