

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
 Data File : VN079520.D
 Acq On : 11 Oct 2023 16:24
 Operator : JC\MD
 Sample : 04823-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOTES-2

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\82N100523W.M
 Title : SW846 8260

Signal : TIC: VN079520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.659	109	120	132	rBV	6430806	11168156	29.02%	6.589%
2	4.236	386	388	389	rBV	43001697	28393717	73.78%	16.753%
3	4.430	416	421	462	rVB2	2722542	9844737	25.58%	5.809%
4	4.718	464	470	484	rVB	160927	524916	1.36%	0.310%
5	5.583	598	617	634	rBV	243923	860254	2.24%	0.508%
6	6.783	791	821	839	rBV	10126866	38483273	100.00%	22.706%
7	7.230	886	897	907	rBV2	153038	425522	1.11%	0.251%
8	8.171	1048	1057	1061	rBV	449261	1005091	2.61%	0.593%
9	8.230	1061	1067	1081	rVB	679245	1539071	4.00%	0.908%
10	8.606	1115	1131	1138	rBV3	979089	2998222	7.79%	1.769%
11	8.982	1183	1195	1200	rBV2	253678	569287	1.48%	0.336%
12	9.106	1209	1216	1232	rVB	1109771	2276338	5.92%	1.343%
13	9.641	1295	1307	1320	rBV8	134815	608078	1.58%	0.359%
14	10.571	1457	1465	1470	rBV	1628505	3006307	7.81%	1.774%
15	10.635	1470	1476	1483	rVV	2185098	4044636	10.51%	2.386%
16	10.724	1483	1491	1498	rVV	7456985	12947979	33.65%	7.640%
17	10.806	1498	1505	1521	rVV	7116711	12297130	31.95%	7.256%
18	10.947	1521	1529	1545	rVB	3985722	6851362	17.80%	4.042%
19	11.353	1592	1598	1617	rVB	212365	494542	1.29%	0.292%
20	11.829	1672	1679	1683	rBV2	4085989	7708212	20.03%	4.548%
21	11.871	1683	1686	1690	rVV	1572891	2593219	6.74%	1.530%
22	11.912	1690	1693	1698	rVV	762394	1234937	3.21%	0.729%
23	11.971	1698	1703	1712	rVV	440716	829731	2.16%	0.490%
24	12.071	1713	1720	1730	rVB	1290357	2400234	6.24%	1.416%
25	12.218	1737	1745	1756	rVB2	270915	563891	1.47%	0.333%
26	12.406	1771	1777	1793	rVB2	718226	1454396	3.78%	0.858%
27	12.800	1836	1844	1848	rBV	995322	1631743	4.24%	0.963%
28	12.853	1848	1853	1865	rVB	1218530	2118946	5.51%	1.250%
29	13.482	1952	1960	1966	rBV2	355208	728847	1.89%	0.430%
30	13.635	1980	1986	1991	rBV	356182	544652	1.42%	0.321%
31	13.794	2006	2013	2023	rBV2	1369726	2478607	6.44%	1.462%
32	14.182	2073	2079	2085	rVB2	253983	466000	1.21%	0.275%
33	15.641	2314	2327	2340	rBV	3270084	6394797	16.62%	3.773%

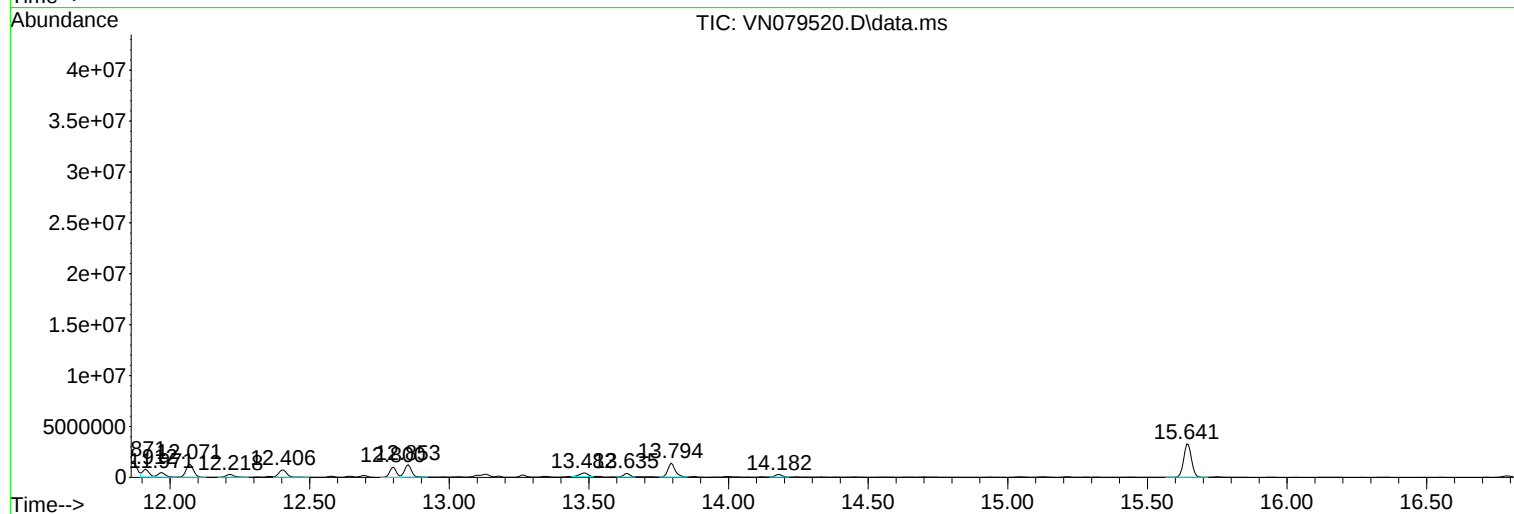
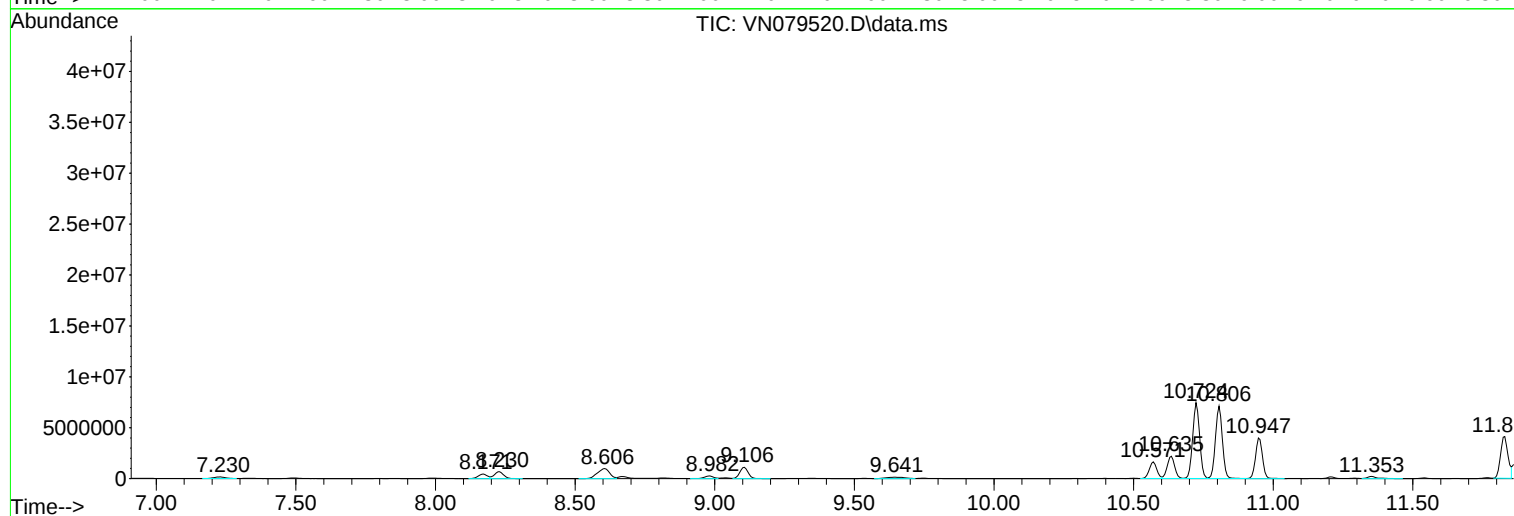
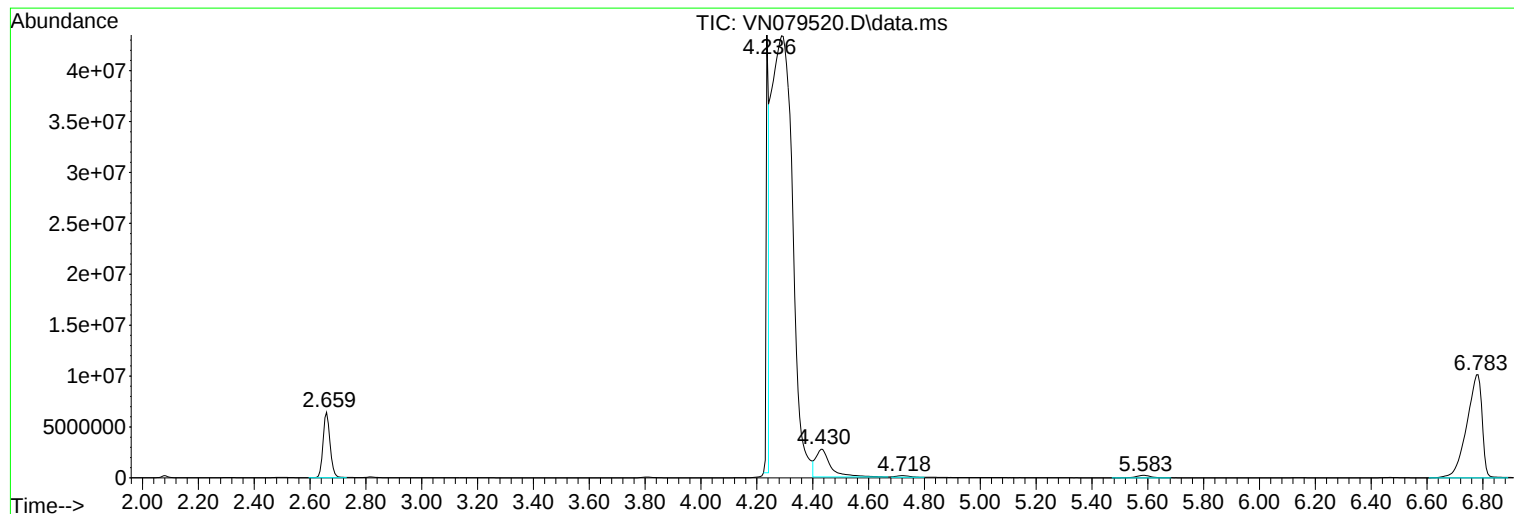
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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



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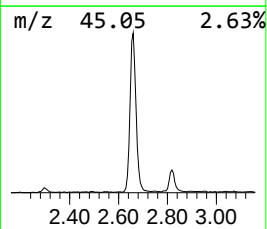
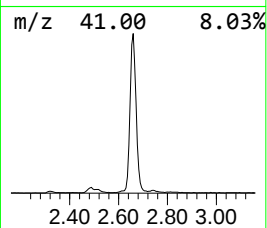
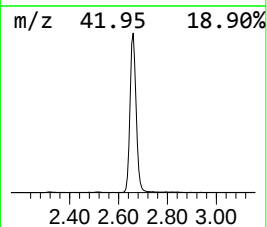
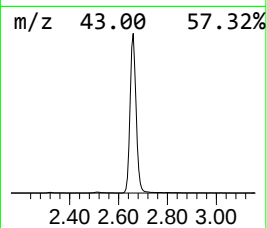
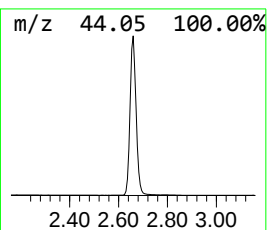
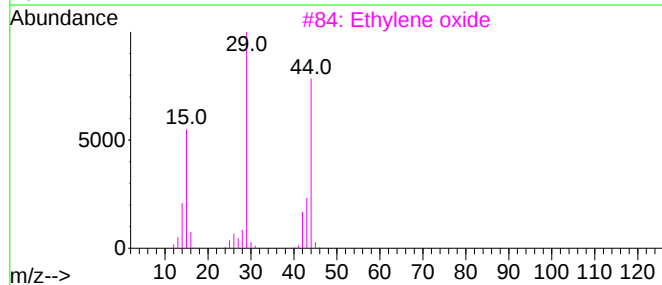
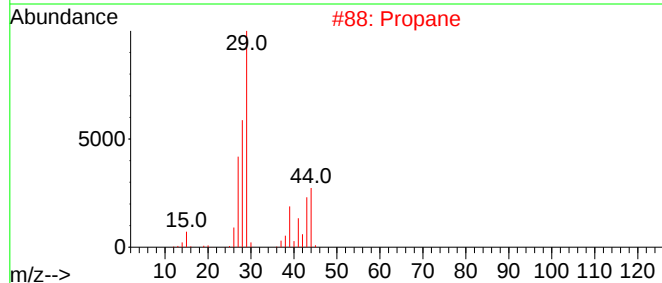
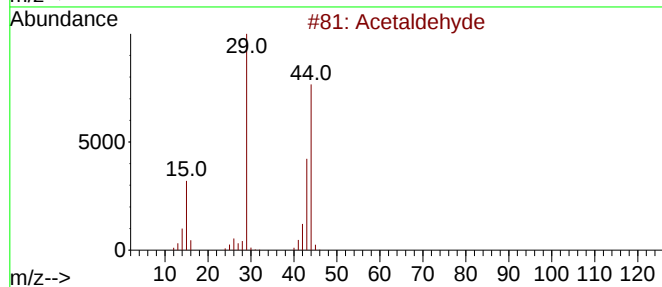
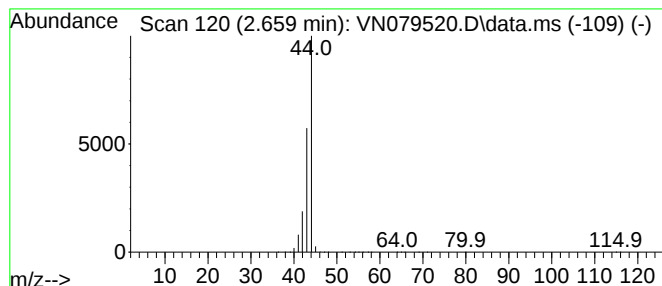
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.659	362.82 ug/l	11168200	Pentafluorobenzene	8.230

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			Hydrogen isocyanate	43	CHNO	000075-13-8	3
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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Instrument :
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ClientSampleId :
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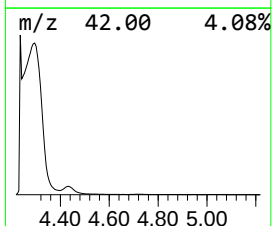
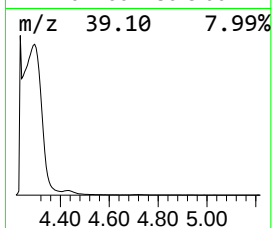
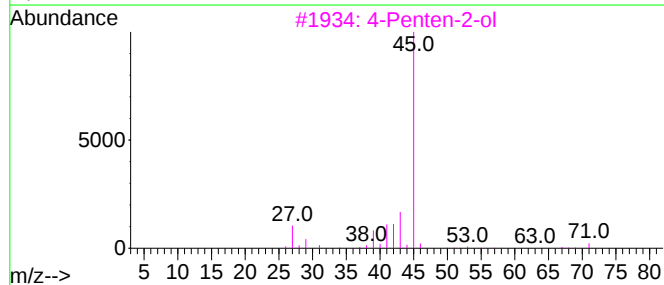
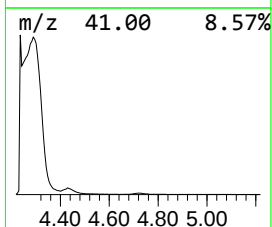
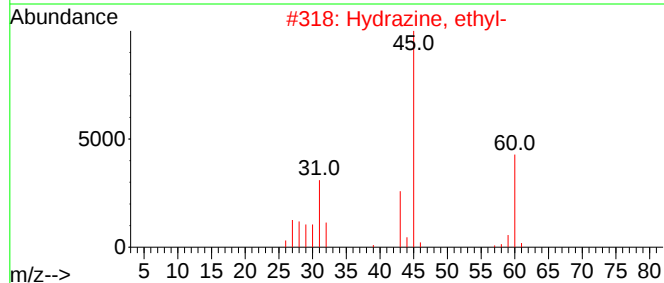
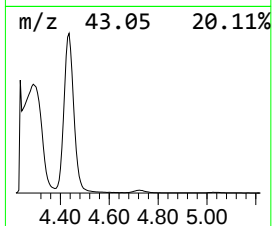
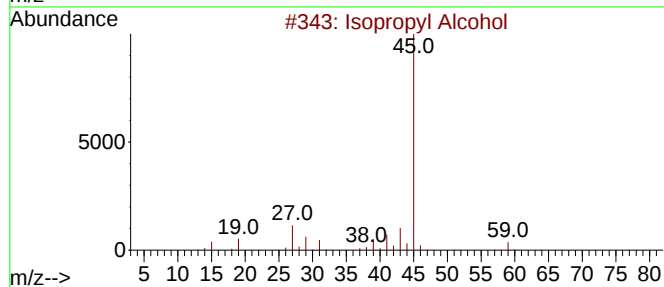
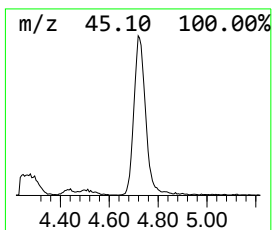
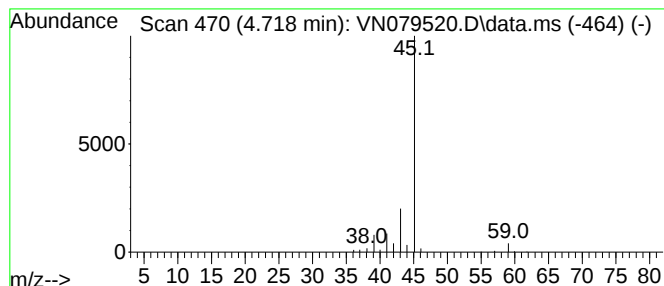
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.718	17.05 ug/l	524916	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3			4-Penten-2-ol	86	C5H10O	000625-31-0	4
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4
5			Formamide	45	CH3NO	000075-12-7	4



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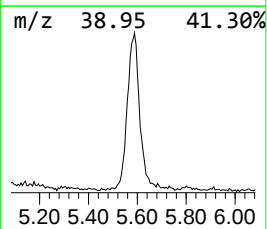
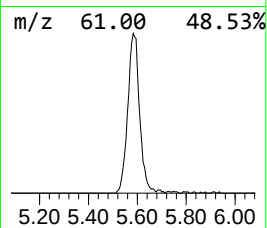
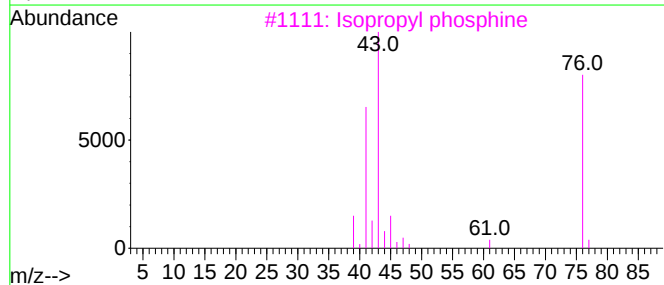
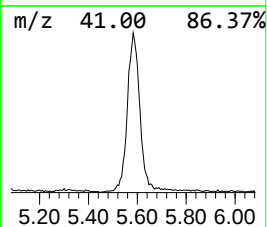
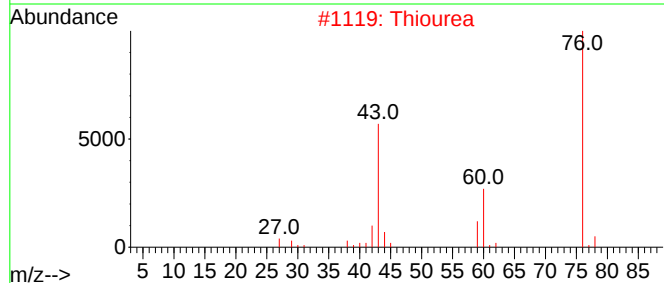
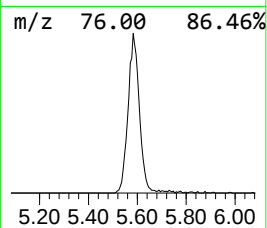
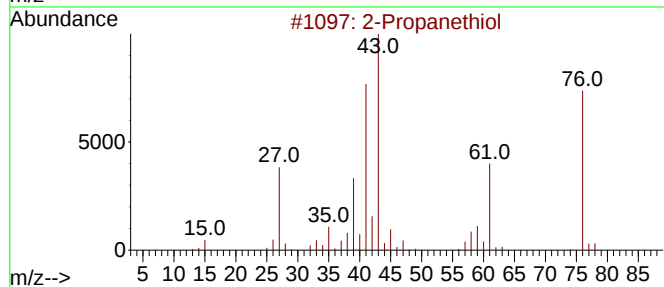
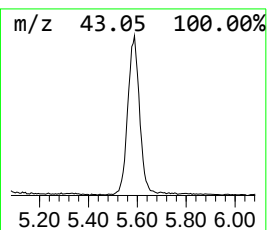
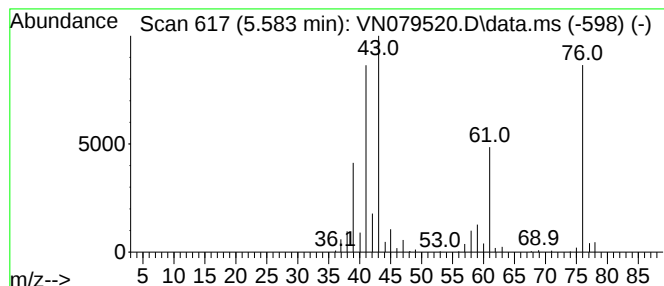
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Propanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.583	27.95 ug/l	860254	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol	76	C3H8S	000075-33-2	93
2			Thiourea	76	CH4N2S	000062-56-6	59
3			Isopropyl phosphine	76	C3H9P	004538-29-8	45
4			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9
5			4,4'-Diisothiocyanatostilbene-2,...	454	C16H10N2O6S4	053005-05-3	9



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-2

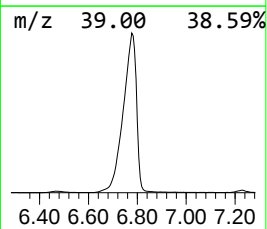
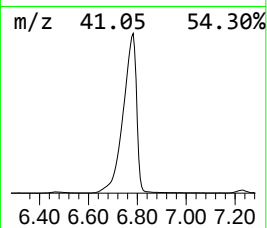
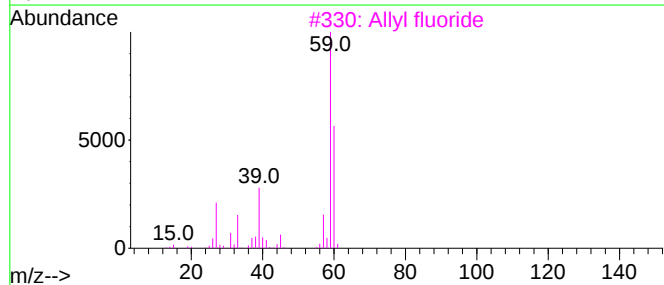
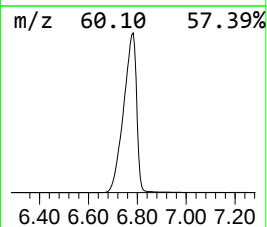
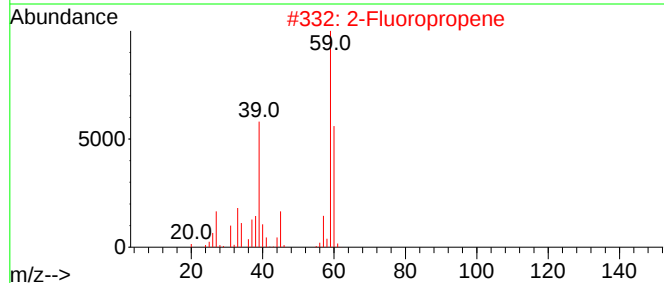
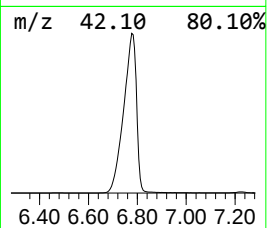
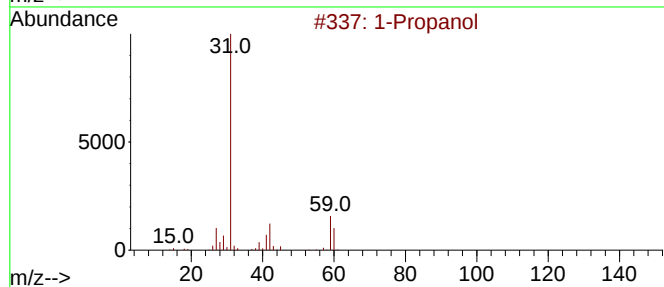
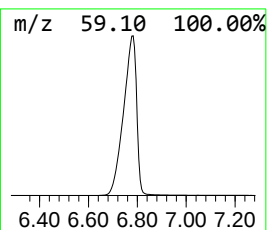
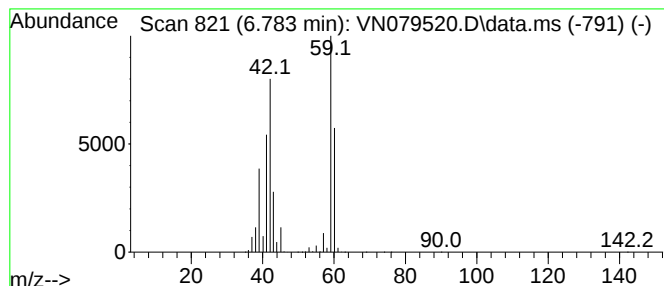
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.783	1250.21 ug/l	38483300	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	64
2			2-Fluoropropene	60	C3H5F	001184-60-7	50
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			Cyclopropane	42	C3H6	000075-19-4	32
5			Formamidoxime	60	CH4N2O	000624-82-8	9



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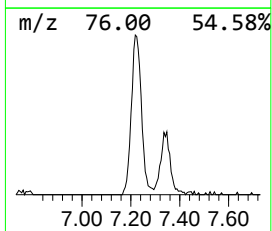
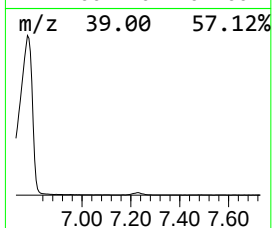
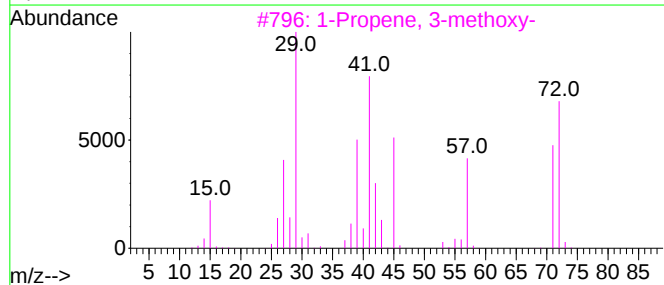
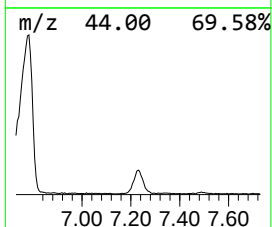
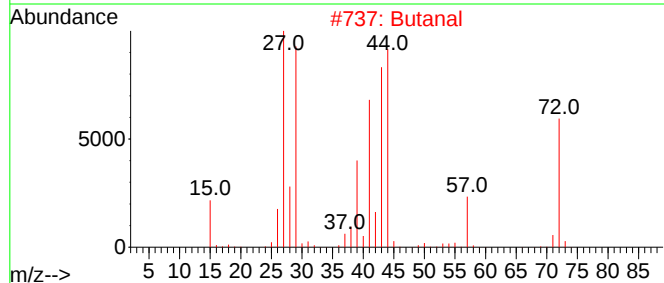
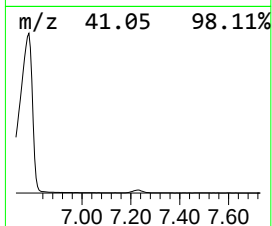
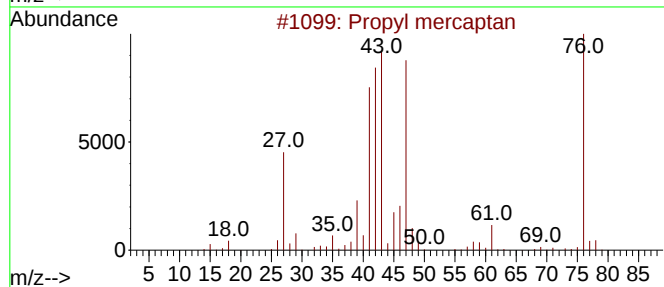
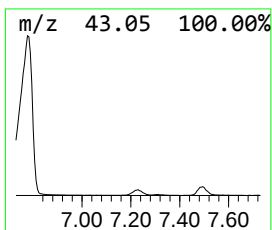
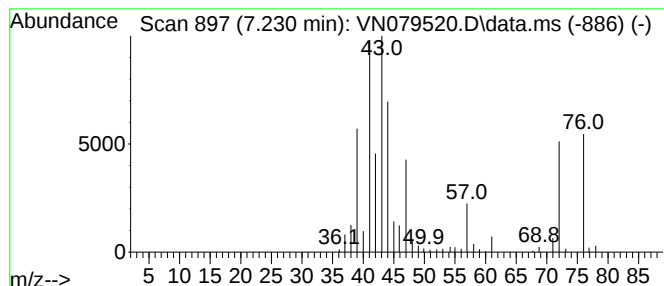
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 6 Propyl mercaptan Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	13.82 ug/l	425522	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propyl mercaptan	76	C3H8S	000107-03-9	55
2			Butanal	72	C4H8O	000123-72-8	25
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
4			Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	23
5			Propene	42	C3H6	000115-07-1	14



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TOTES-2

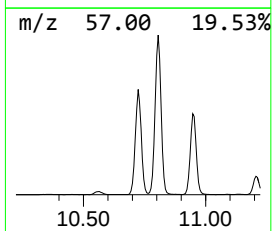
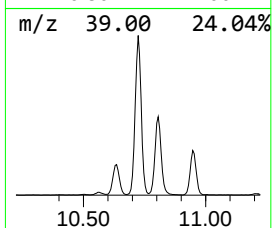
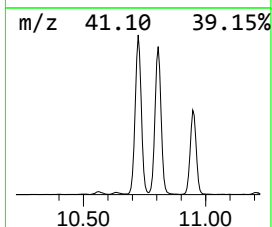
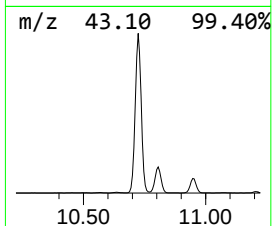
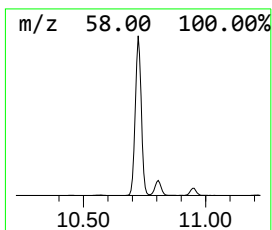
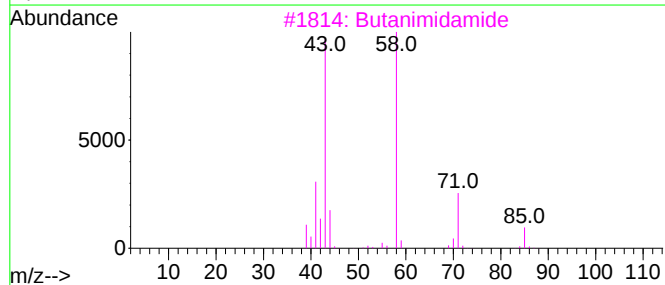
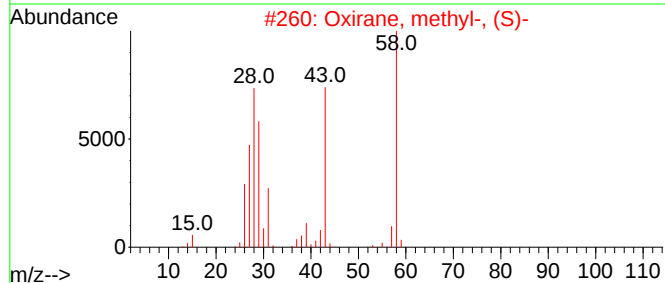
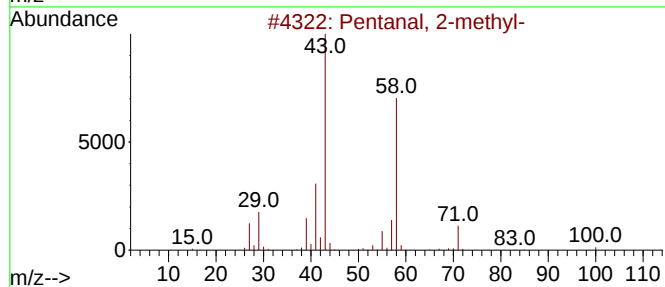
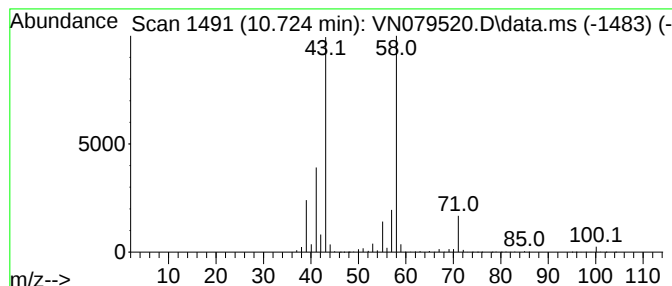
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Quant Title : SW846 8260

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

Peak Number 7 Pentanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.724	249.65 ug/l	12948000	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	91
2			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	72
3			Butanimidamide	86	C4H10N2	000107-90-4	64
4			2-Propenoic acid, 2-(dimethylami...	143	C7H13NO2	002439-35-2	45
5			2-Hexanone	100	C6H12O	000591-78-6	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
Data File : VN079520.D
Acq On : 11 Oct 2023 16:24
Operator : JC\MD
Sample : 04823-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

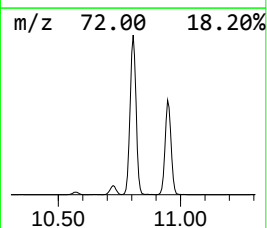
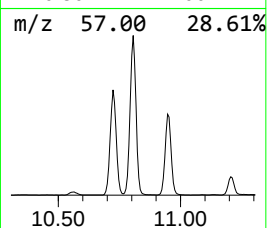
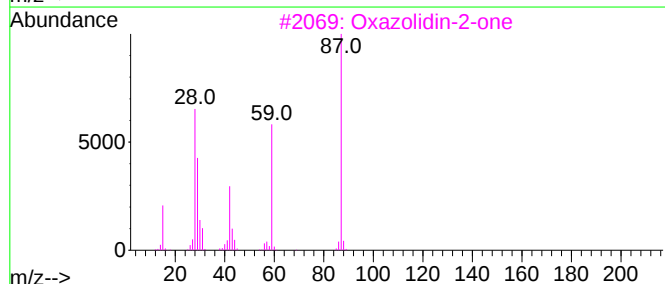
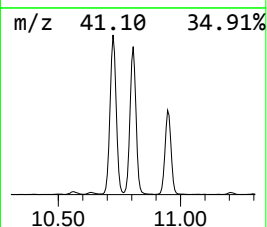
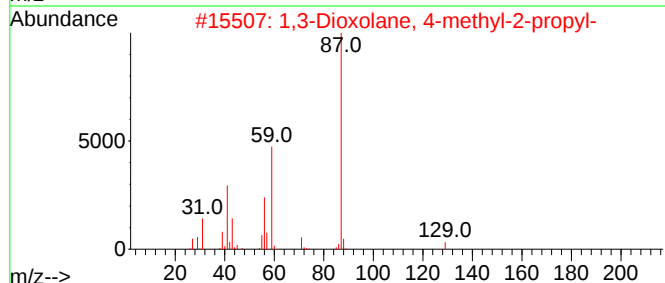
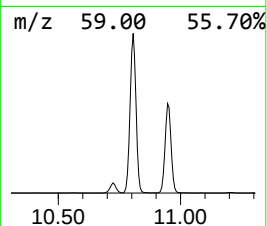
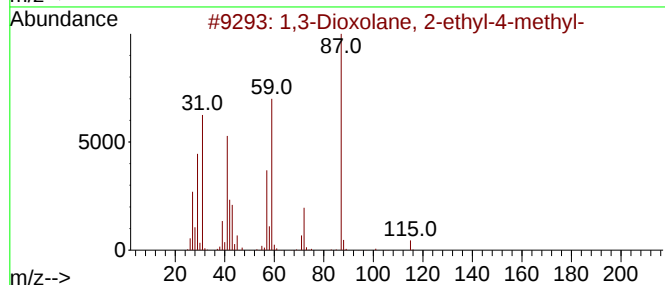
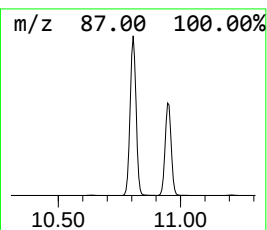
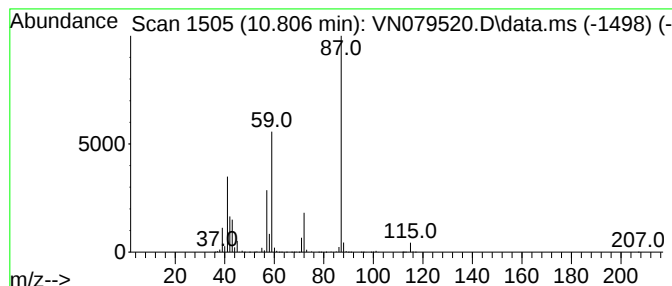
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ClientSampleId :
TOTES-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.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.	
10.806	237.10 ug/l	12297100	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	91
2	1,3-Dioxolane, 4-methyl-2-propyl-		130	C7H14O2	004352-99-2	72
3	Oxazolidin-2-one		87	C3H5NO2	000497-25-6	72
4	Acetamide, N-ethyl-		87	C4H9NO	000625-50-3	50
5	Ethanol, 2-[2-(2-methoxyethoxy)e...		206	C9H18O5	003610-27-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
Data File : VN079520.D
Acq On : 11 Oct 2023 16:24
Operator : JC\MD
Sample : 04823-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-2

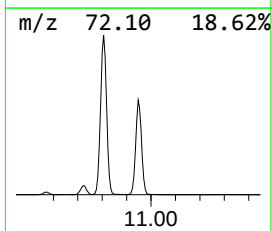
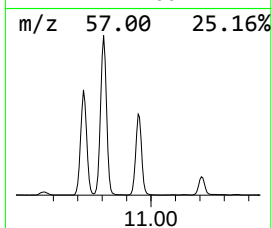
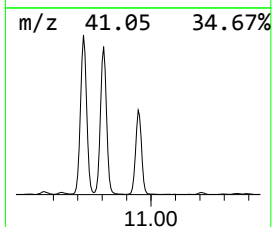
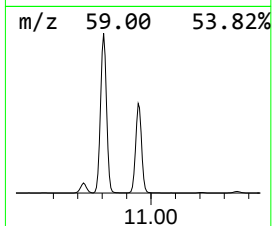
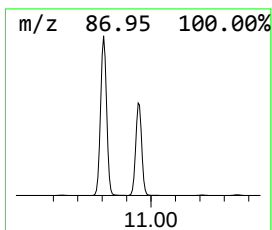
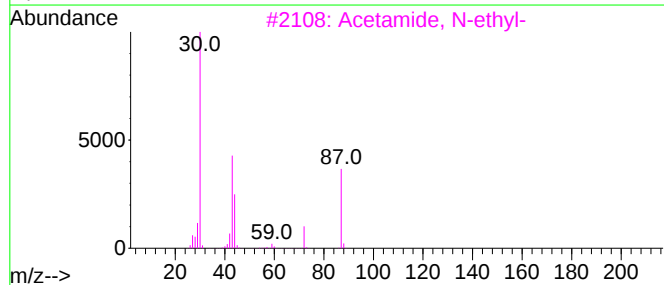
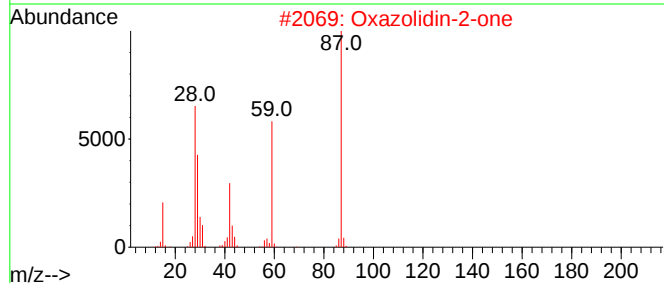
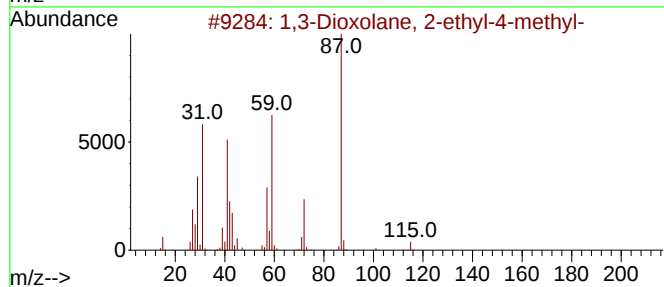
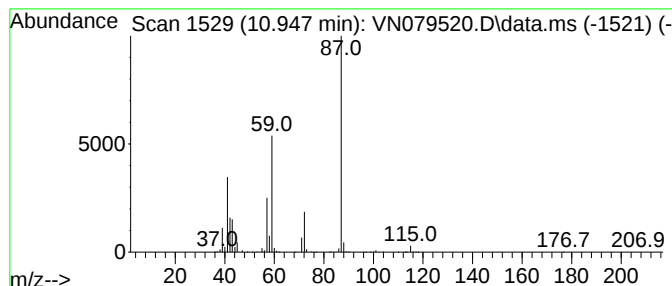
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Quant Title : SW846 8260

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

Peak Number 9 Oxazolidin-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	132.10 ug/l	6851360	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	94
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50
5			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
Data File : VN079520.D
Acq On : 11 Oct 2023 16:24
Operator : JC\MD
Sample : 04823-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-2

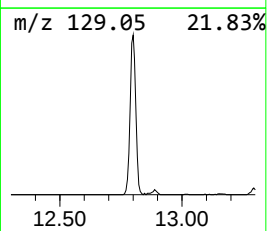
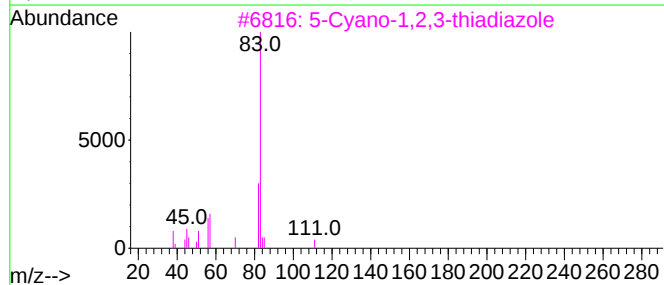
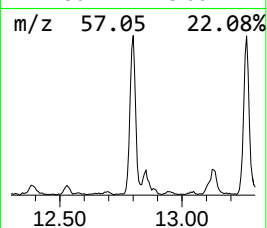
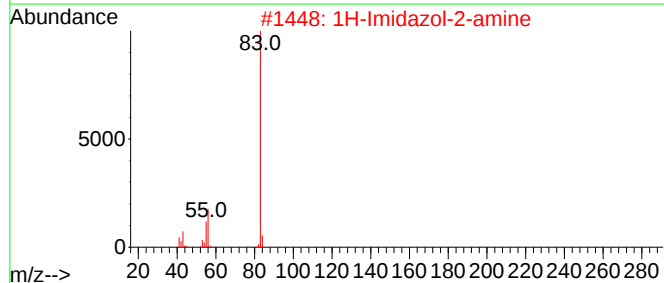
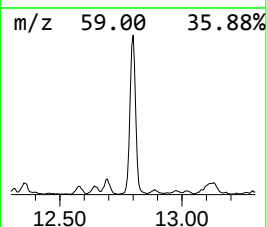
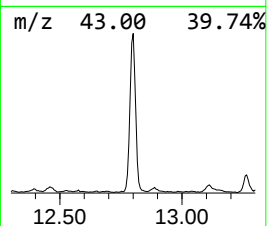
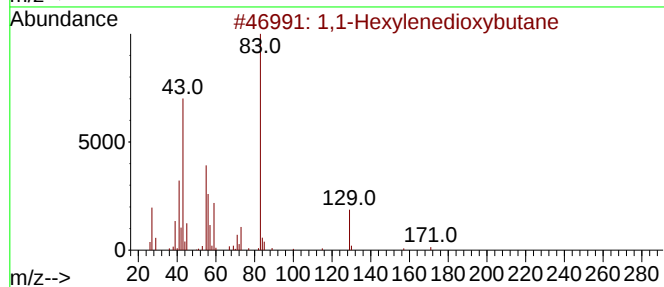
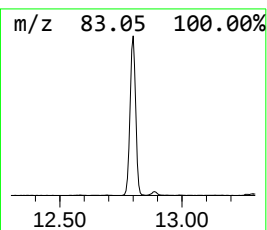
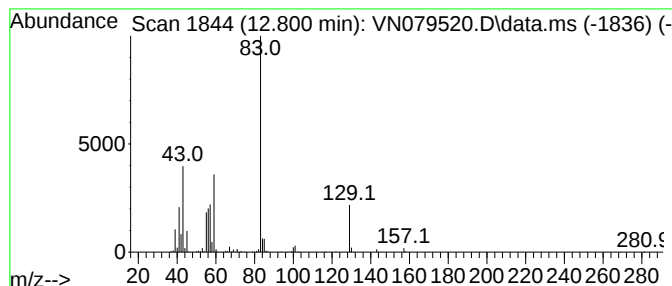
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Quant Title : SW846 8260

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

Peak Number 10 1,1-Hexylenedioxybutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.800	31.46 ug/l	1631740	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	56
2			1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	50
3			5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	42
4			Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	36
5			N-(Piperidin-3-yl)acetamide	142	C7H14N2O	005810-55-9	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
Data File : VN079520.D
Acq On : 11 Oct 2023 16:24
Operator : JC\MD
Sample : 04823-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.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
Acetaldehyde	2.659	362.8	ug/l	11168200	1	8.230	1539070	50.0
Isopropyl Alcohol	4.718	17.1	ug/l	524916	1	8.230	1539070	50.0
2-Propanethiol	5.583	27.9	ug/l	860254	1	8.230	1539070	50.0
1-Propanol	6.783	1250.2	ug/l	38483300	1	8.230	1539070	50.0
Propyl mercaptan	7.230	13.8	ug/l	425522	1	8.230	1539070	50.0
Pentanal, 2-met...	10.724	249.7	ug/l	12948000	3	11.871	2593220	50.0
1,3-Dioxolane, ...	10.806	237.1	ug/l	12297100	3	11.871	2593220	50.0
Oxazolidin-2-one	10.947	132.1	ug/l	6851360	3	11.871	2593220	50.0
1,1-Hexylenedio...	12.800	31.5	ug/l	1631740	3	11.871	2593220	50.0