

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
 Data File : VN074309.D
 Acq On : 03 Sep 2022 01:03
 Operator : JC\MD
 Sample : N4355-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-34

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\82N090222W.M
 Title : SW846 8260

Signal : TIC: VN074309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.404	74	88	95	rBV2	82974	192660	2.78%	0.942%
2	2.704	131	139	145	rBV4	49688	126299	1.82%	0.618%
3	3.087	196	204	214	rVB	181853	408330	5.89%	1.997%
4	5.116	536	549	563	rVB2	37547	141600	2.04%	0.693%
5	5.275	565	576	590	rBV3	134133	480182	6.92%	2.349%
6	5.534	607	620	633	rBV3	139155	501331	7.23%	2.452%
7	6.410	757	769	781	rBV5	37292	125255	1.81%	0.613%
8	7.063	878	880	889	rVB3	43726	88893	1.28%	0.435%
9	7.951	1020	1031	1036	rBV	243468	590586	8.51%	2.889%
10	8.016	1036	1042	1052	rVB	431412	1003036	14.46%	4.906%
11	8.392	1094	1106	1123	rBV	2843367	6938109	100.00%	33.939%
12	8.904	1184	1193	1208	rBV	609878	1282474	18.48%	6.273%
13	10.139	1396	1403	1416	rBV4	32935	80889	1.17%	0.396%
14	10.380	1436	1444	1452	rBV	927373	1691283	24.38%	8.273%
15	10.580	1468	1478	1485	rBV3	58117	109085	1.57%	0.534%
16	10.657	1485	1491	1498	rVB2	57005	98743	1.42%	0.483%
17	11.069	1556	1561	1570	rVB2	74903	136771	1.97%	0.669%
18	11.680	1657	1665	1676	rBV	925902	1644215	23.70%	8.043%
19	11.786	1676	1683	1693	rVB	210674	375674	5.41%	1.838%
20	12.521	1801	1808	1816	rBV2	69437	121598	1.75%	0.595%
21	12.668	1826	1833	1843	rBV	765969	1273416	18.35%	6.229%
22	12.857	1857	1865	1873	rVB	51435	87503	1.26%	0.428%
23	13.610	1986	1993	2006	rBV	979305	1629755	23.49%	7.972%
24	13.815	2017	2028	2034	rBV	322691	593475	8.55%	2.903%
25	14.268	2099	2105	2112	rVB	135432	228676	3.30%	1.119%
26	14.474	2132	2140	2143	rBV	54859	86952	1.25%	0.425%
27	14.515	2143	2147	2153	rVB	56207	88658	1.28%	0.434%
28	14.868	2199	2207	2213	rBV3	95563	165101	2.38%	0.808%
29	15.239	2262	2270	2277	rVB4	32862	82525	1.19%	0.404%
30	16.733	2516	2524	2531	rBV3	29938	69936	1.01%	0.342%

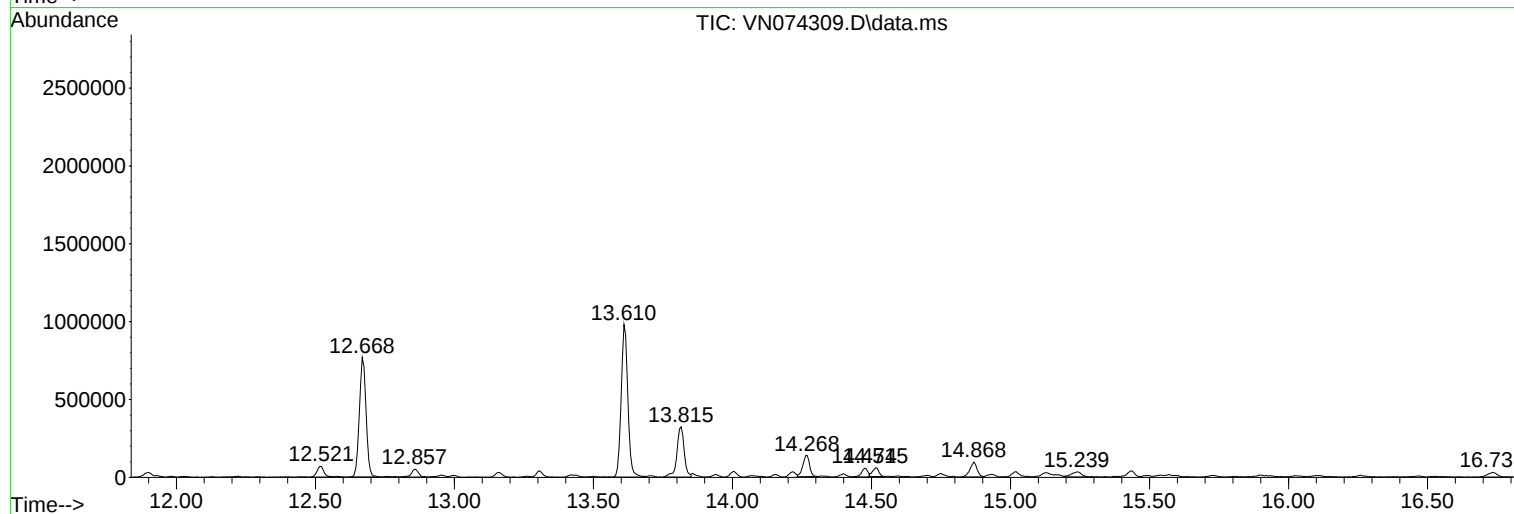
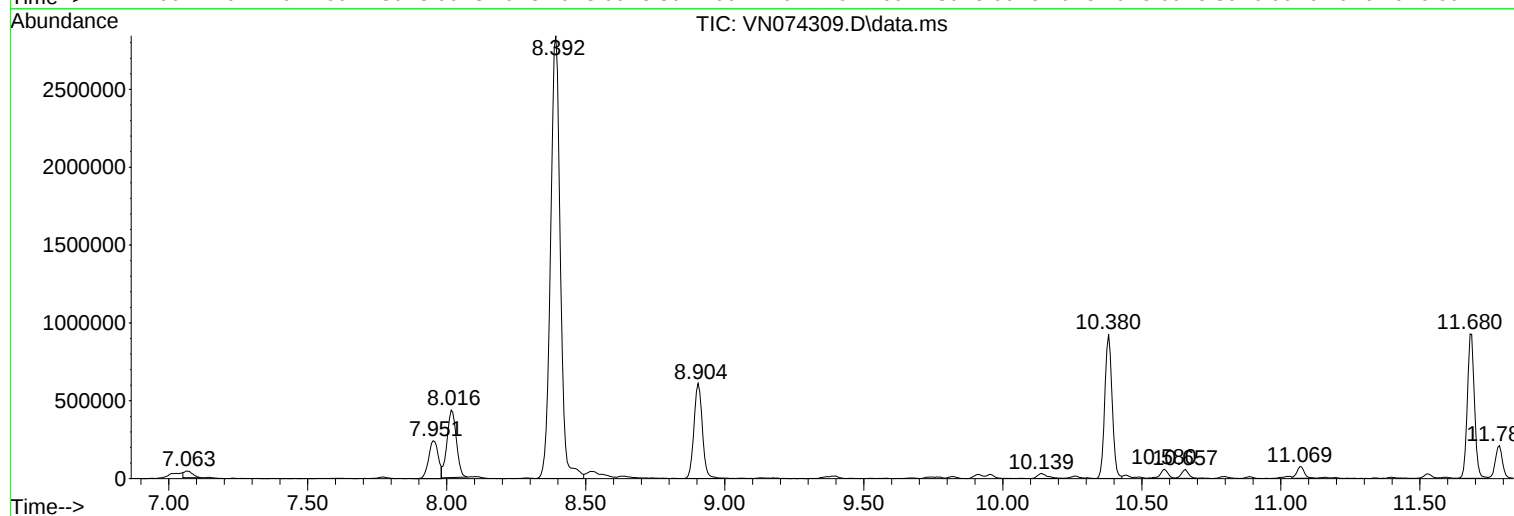
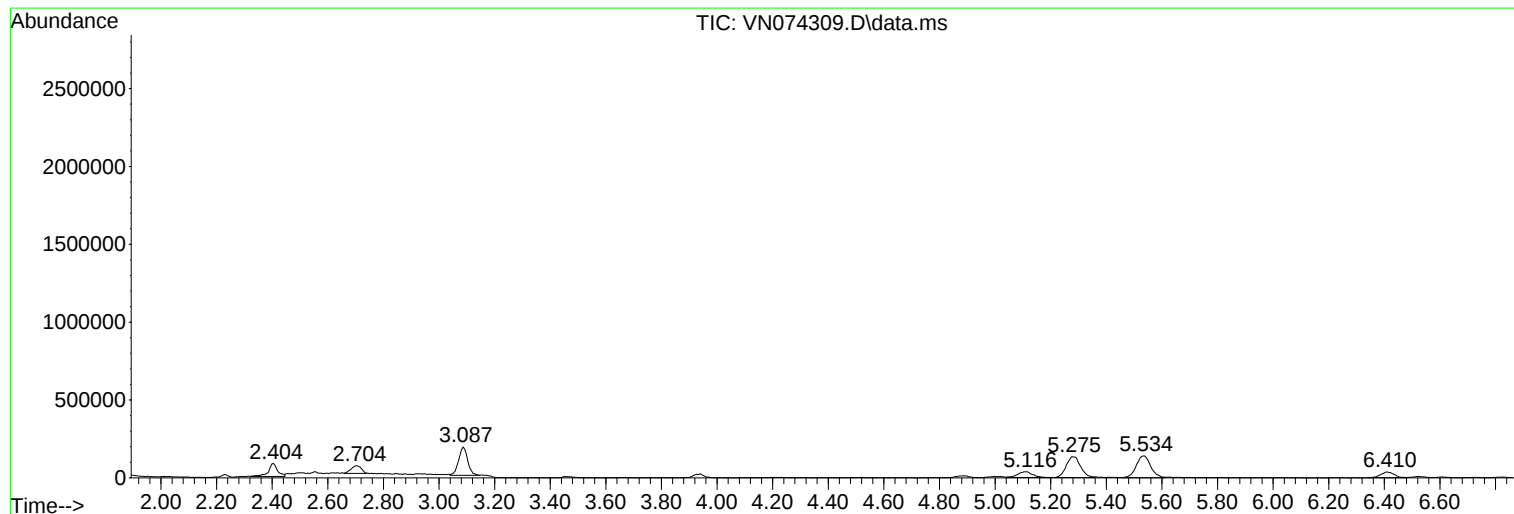
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



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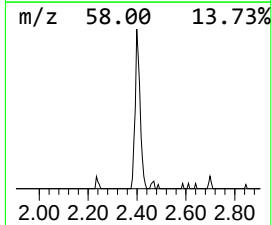
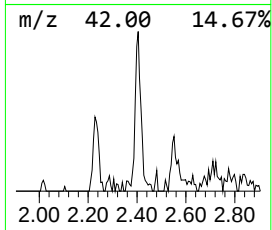
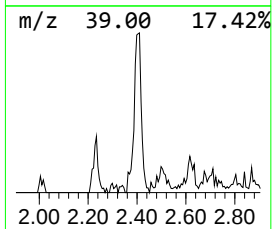
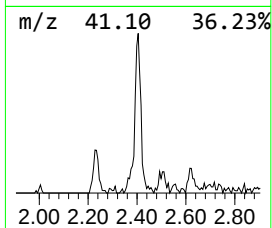
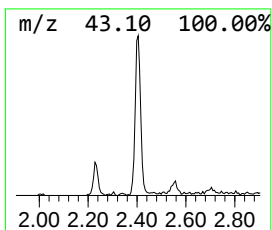
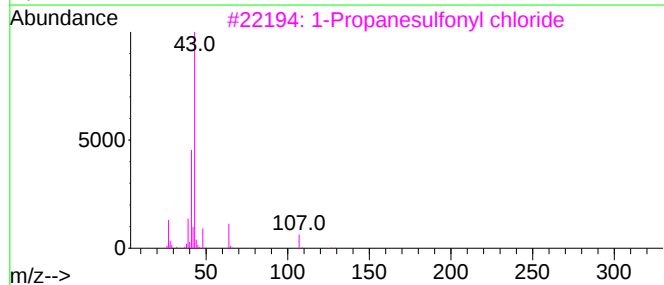
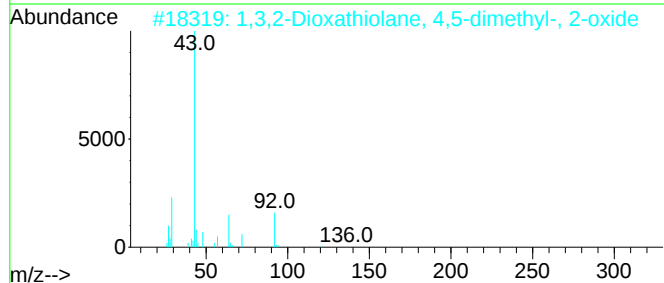
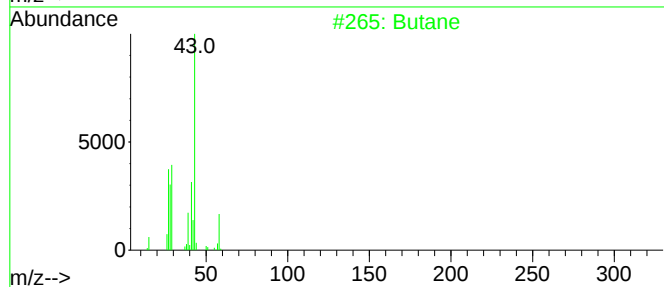
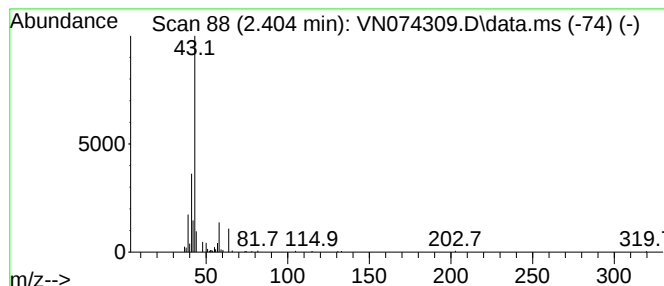
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.404 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.404	9.60 ug/l	192660	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	47
2	1,3,2-Dioxathiolane, 4,5-dimethy...			136	C4H8O3S	004440-90-8	33
3	1-Propanesulfonyl chloride			142	C3H7ClO2S	010147-36-1	9
4	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
5	Formic acid, chloro-, (3,4,4-tri...			194	C7H11ClO4	107323-92-2	9



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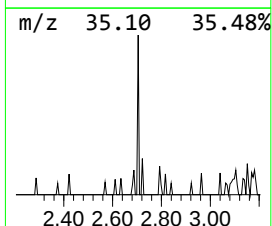
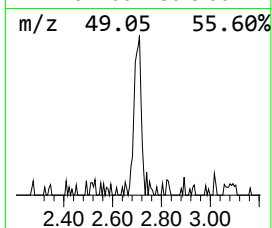
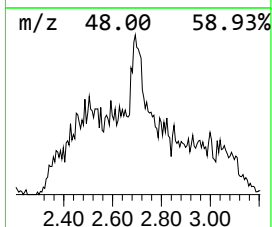
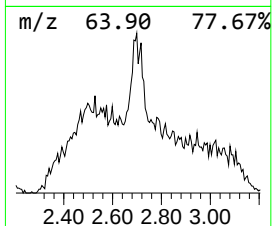
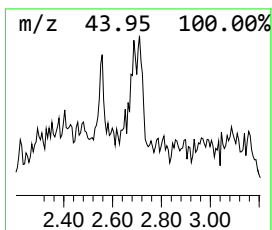
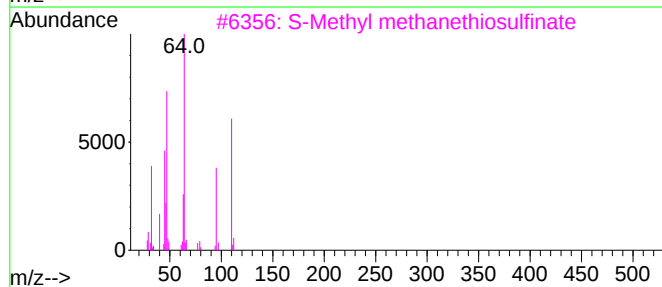
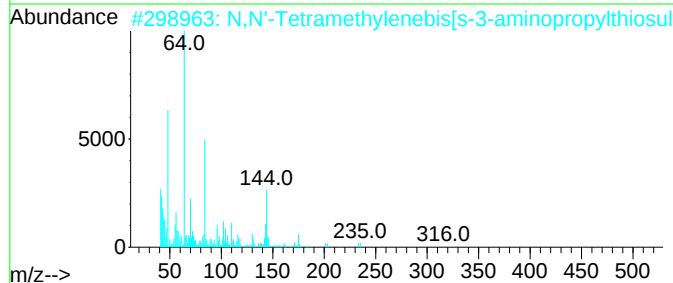
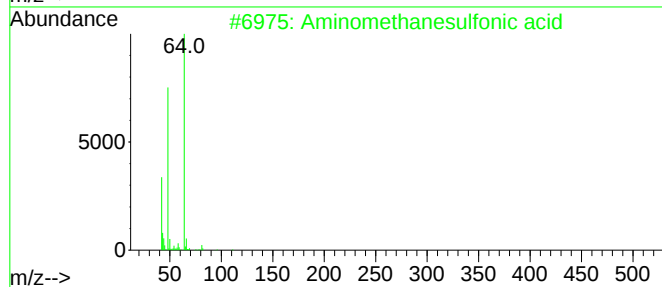
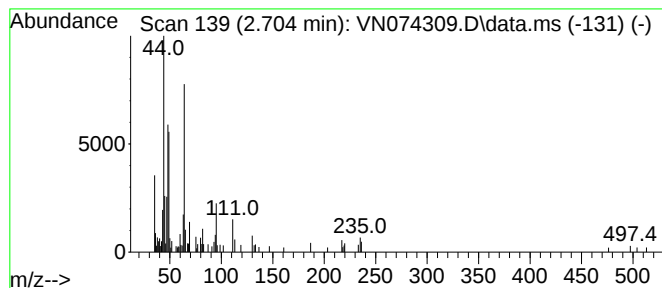
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.704 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.704	6.30 ug/l	126299	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	37
2			N,N'-Tetramethylenebis[s-3-amino...	396	C10H24N2O6S4	035871-61-5	25
3			S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	25
4			1-[1-Bromo-2-(2,2,3,3-tetrafluor...	328	C12H10BrF5	1000223-18-3	17
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	9



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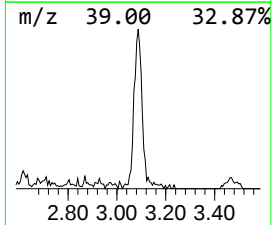
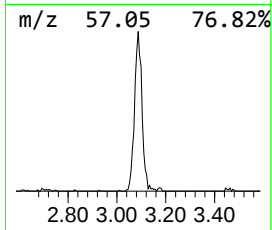
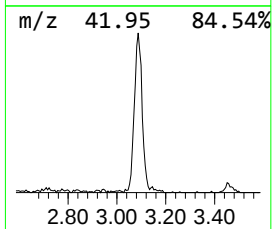
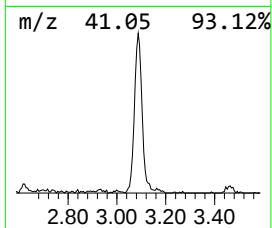
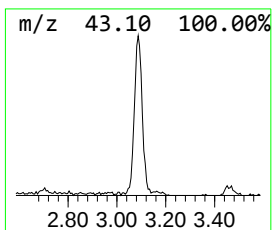
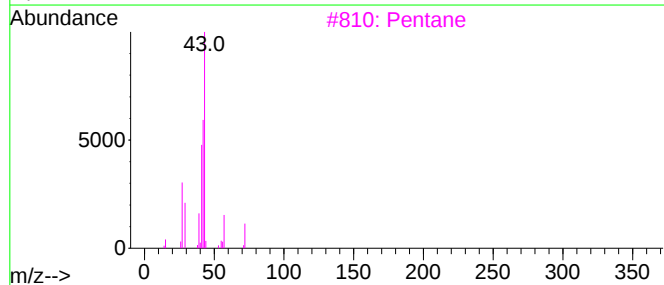
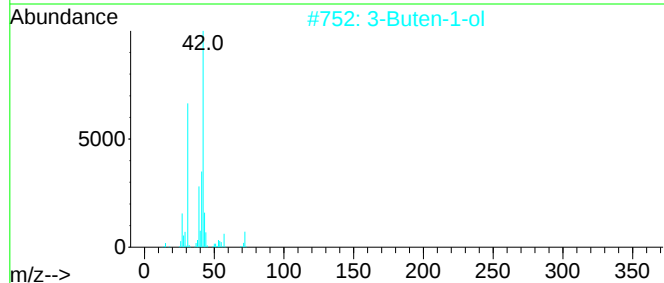
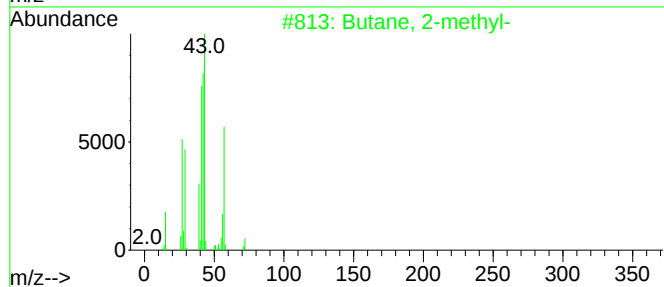
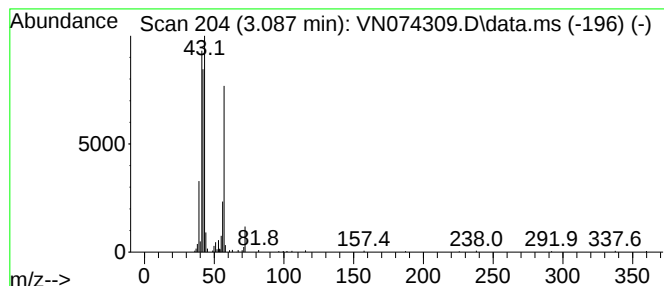
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Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	20.35 ug/l	408330	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	91
2	3-Buten-1-ol			72	C4H8O	000627-27-0	46
3	Pentane			72	C5H12	000109-66-0	42
4	1-Propanol, 2-methyl-			74	C4H10O	000078-83-1	36
5	1-Propanol, 2-chloro-2-methyl-			108	C4H9ClO	000558-38-3	36



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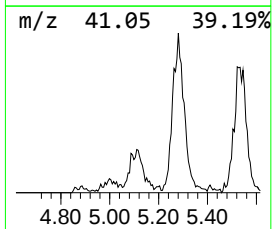
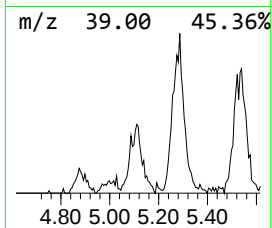
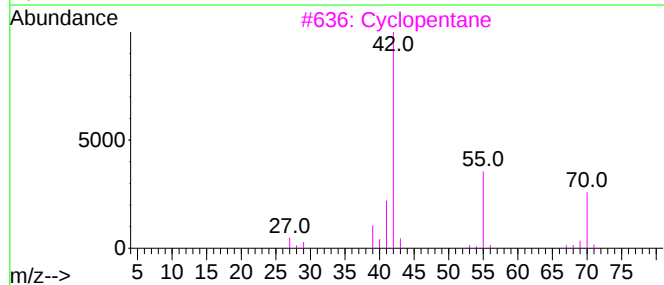
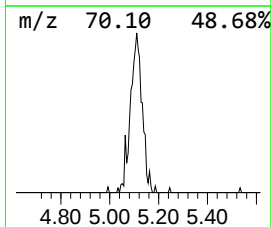
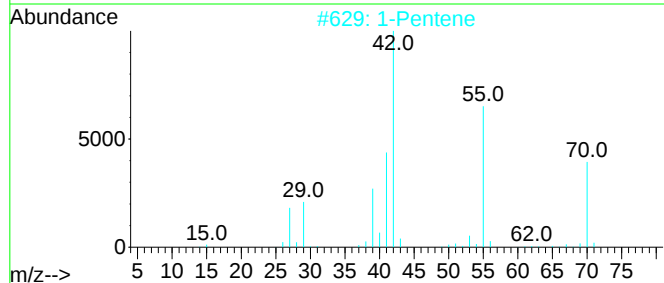
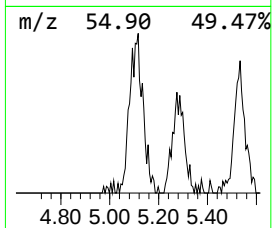
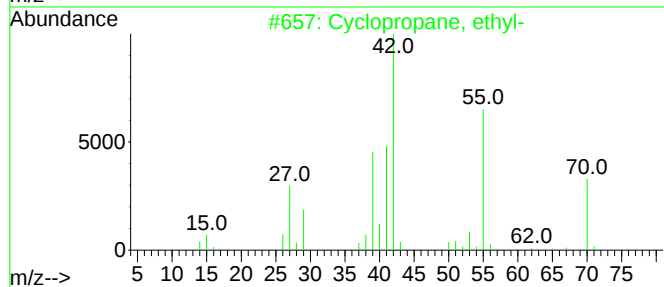
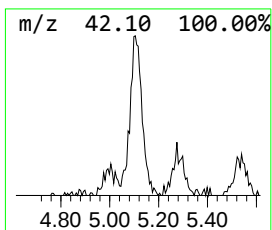
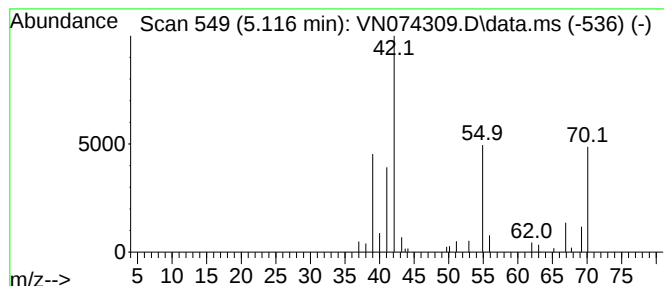
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Peak Number 4 Cyclopropane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	7.06 ug/l	141600	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
2			1-Pentene	70	C5H10	000109-67-1	50
3			Cyclopentane	70	C5H10	000287-92-3	9
4			Ethoxyacetylene	70	C4H6O	000927-80-0	9
5			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	9



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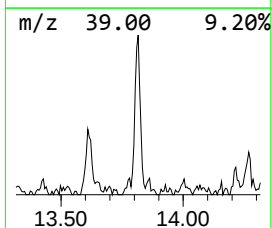
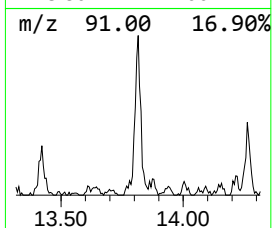
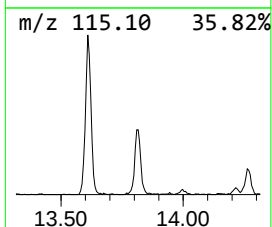
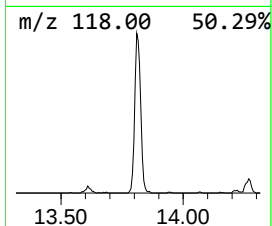
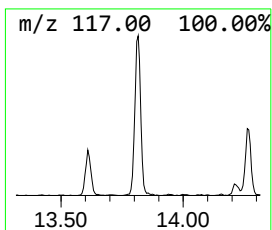
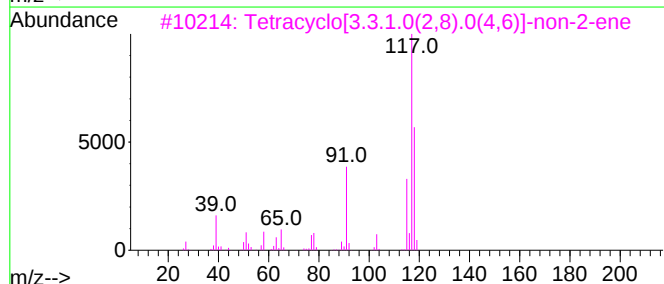
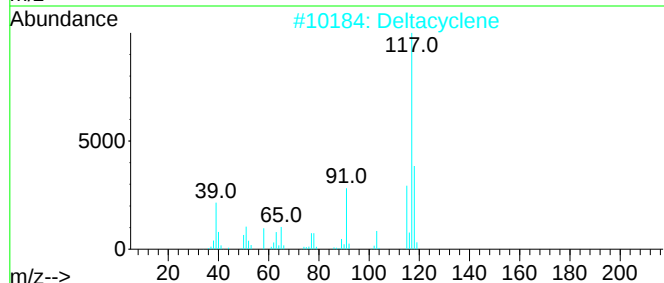
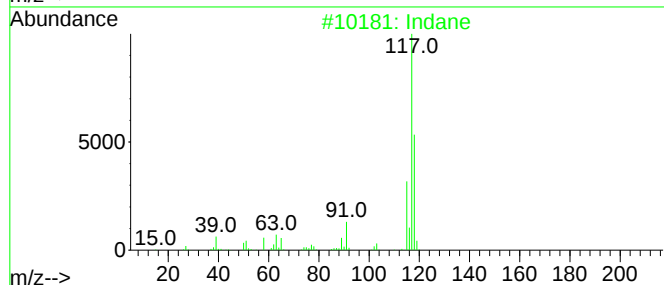
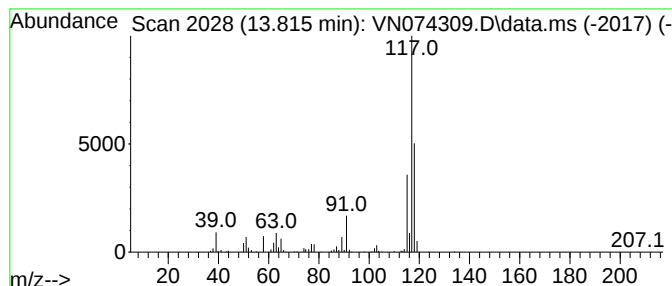
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	18.21 ug/l	593475	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Deltacyclene	118	C9H10	007785-10-6	81
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64



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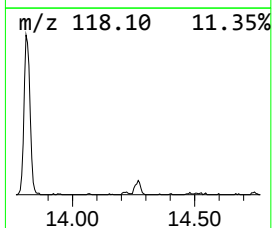
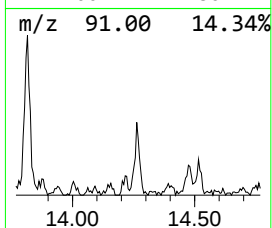
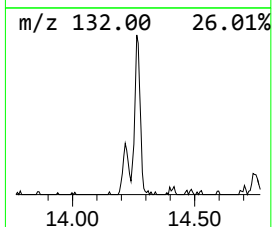
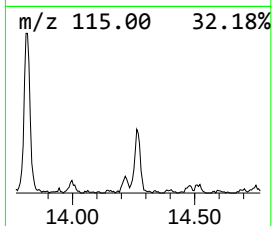
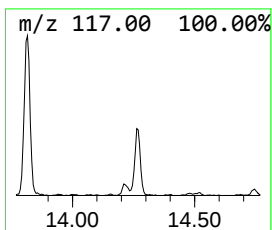
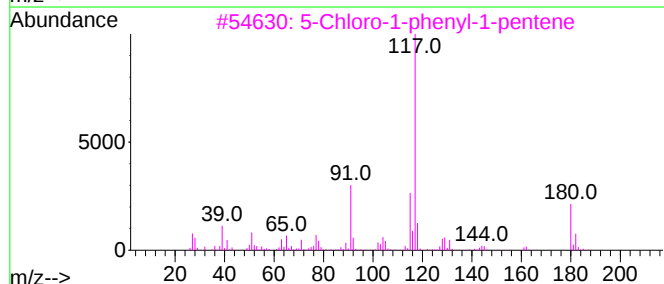
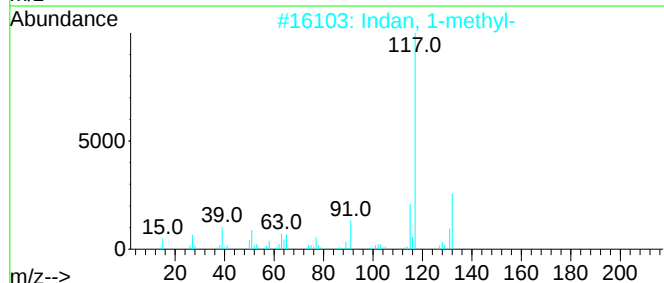
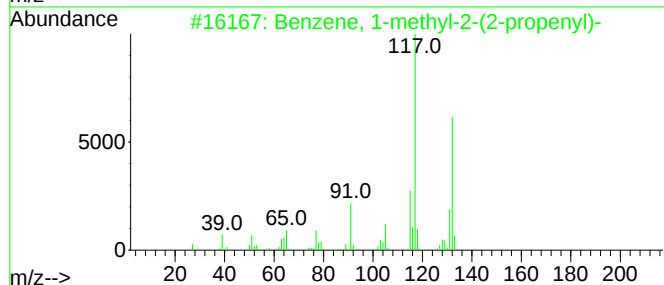
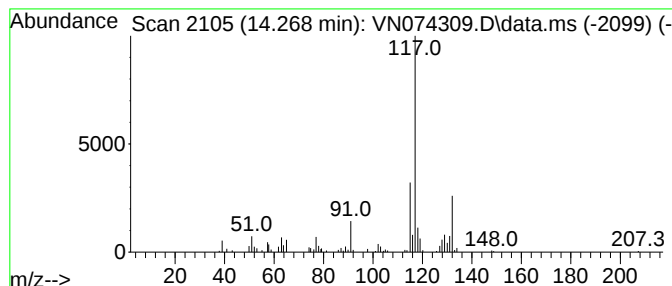
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-2-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	7.02 ug/l	228676	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	78
2			Indan, 1-methyl-	132	C10H12	000767-58-8	76
3			5-Chloro-1-phenyl-1-pentene	180	C11H13Cl	016424-50-3	64
4			Hex-1-enylbenzene	160	C12H16	000828-15-9	64
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074309.D
Acq On : 03 Sep 2022 01:03
Operator : JC\MD
Sample : N4355-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 32 Sample Multiplier: 1

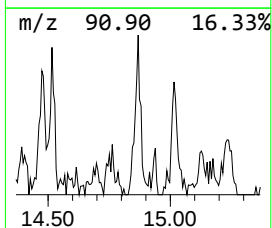
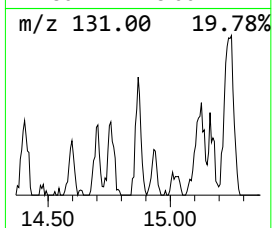
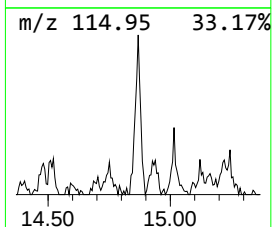
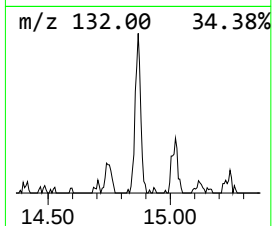
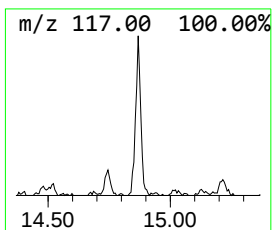
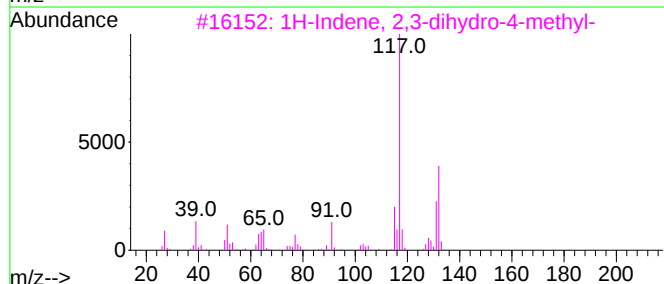
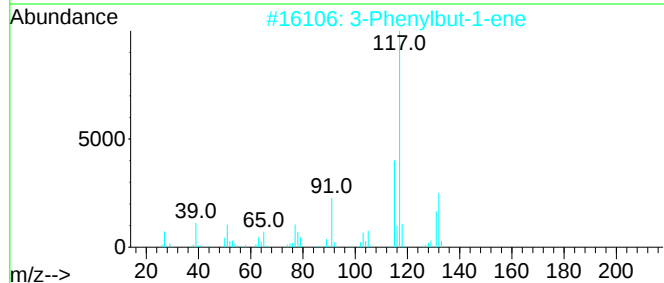
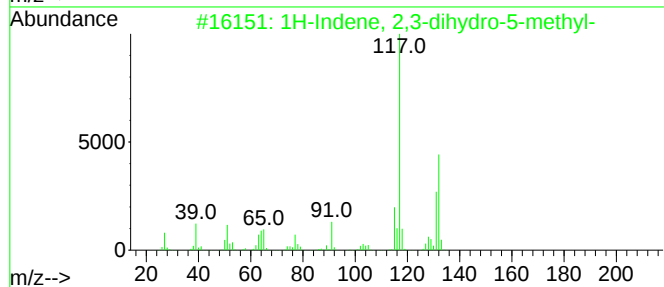
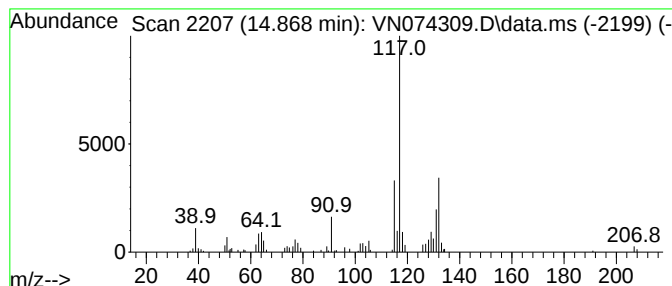
Instrument :
MSVOA_N
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.868	5.07 ug/l	165101	1,4-Dichlorobenzene-d4		13.610	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-		132	C10H12	000874-35-1	91
2	3-Phenylbut-1-ene		132	C10H12	000934-10-1	90
3	1H-Indene, 2,3-dihydro-4-methyl-		132	C10H12	000824-22-6	87
4	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	83
5	Benzene, (1-methyl-1-propenyl)-,...		132	C10H12	000768-00-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074309.D
Acq On : 03 Sep 2022 01:03
Operator : JC\MD
Sample : N4355-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.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
unknown2.404	2.404	9.6	ug/l	192660	1	8.016	1003040	50.0
unknown2.704	2.704	6.3	ug/l	126299	1	8.016	1003040	50.0
Butane, 2-methyl-	3.087	20.4	ug/l	408330	1	8.016	1003040	50.0
Cyclopropane, e...	5.116	7.1	ug/l	141600	1	8.016	1003040	50.0
Indane	13.816	18.2	ug/l	593475	4	13.610	1629760	50.0
Benzene, 1-meth...	14.268	7.0	ug/l	228676	4	13.610	1629760	50.0
1H-Indene, 2,3-...	14.868	5.1	ug/l	165101	4	13.610	1629760	50.0