

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
 Data File : VN074966.D
 Acq On : 21 Oct 2022 17:00
 Operator : JC\MD
 Sample : N5222-12
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-5

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\82N102022W.M
 Title : SW846 8260

Signal : TIC: VN074966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	35	41	50	rBV	171944	430789	6.71%	1.282%
2	2.848	125	135	146	rVB6	142477	528819	8.24%	1.573%
3	3.242	197	202	215	rVB8	74065	262337	4.09%	0.781%
4	5.818	624	640	653	rBV3	136443	465586	7.25%	1.385%
5	8.171	1030	1040	1045	rBV	798414	1937008	30.17%	5.763%
6	8.230	1045	1050	1060	rVV2	943007	2146841	33.44%	6.387%
7	8.335	1060	1068	1077	rVB5	56718	150496	2.34%	0.448%
8	8.453	1077	1088	1094	rBV7	32008	73269	1.14%	0.218%
9	8.582	1101	1110	1121	rBV	904244	2078525	32.38%	6.184%
10	8.735	1126	1136	1137	rVV5	49631	112545	1.75%	0.335%
11	8.777	1137	1143	1154	rVV6	227271	622307	9.69%	1.852%
12	9.106	1188	1199	1213	rBV	1302738	2750349	42.84%	8.183%
13	9.565	1266	1277	1280	rBV6	43728	92747	1.44%	0.276%
14	10.018	1348	1354	1361	rVB2	82808	171388	2.67%	0.510%
15	10.147	1364	1376	1382	rBV3	121491	266568	4.15%	0.793%
16	10.318	1400	1405	1413	rBV7	46707	122406	1.91%	0.364%
17	10.571	1440	1448	1466	rBV	3397204	6419777	100.00%	19.101%
18	10.735	1466	1476	1477	rBV5	38782	66530	1.04%	0.198%
19	10.918	1501	1507	1512	rBV5	36730	79330	1.24%	0.236%
20	10.988	1512	1519	1527	rVV5	72157	217179	3.38%	0.646%
21	11.106	1535	1539	1545	rVB4	59047	106341	1.66%	0.316%
22	11.247	1558	1563	1570	rBV3	70425	138531	2.16%	0.412%
23	11.694	1631	1639	1646	rBV7	26546	67734	1.06%	0.202%
24	11.865	1660	1668	1677	rBV	1974023	3549834	55.30%	10.562%
25	11.965	1681	1685	1691	rVV6	46415	89486	1.39%	0.266%
26	12.853	1827	1836	1847	rBV	2343539	4048960	63.07%	12.047%
27	13.335	1911	1918	1926	rBV3	36632	70066	1.09%	0.208%
28	13.612	1958	1965	1973	rVB5	29322	75211	1.17%	0.224%
29	13.794	1989	1996	2006	rVB	2306410	3943455	61.43%	11.733%
30	13.953	2017	2023	2027	rBV	333367	518844	8.08%	1.544%
31	13.994	2027	2030	2034	rVV	183588	292585	4.56%	0.871%
32	14.035	2034	2037	2045	rVB	94105	142920	2.23%	0.425%
33	14.270	2068	2077	2083	rBV2	64615	124950	1.95%	0.372%
34	14.447	2100	2107	2114	rVB	460072	768270	11.97%	2.286%
35	14.659	2136	2143	2150	rVB2	121602	210741	3.28%	0.627%
36	14.929	2185	2189	2197	rVB5	49750	93628	1.46%	0.279%

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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

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37	15.317	2248	2255	2262	rBV4	78847	165906	2.58%	0.494%
38	15.429	2268	2274	2282	rVB5	56062	133019	2.07%	0.396%
39	15.641	2305	2310	2316	rVB2	39104	74846	1.17%	0.223%

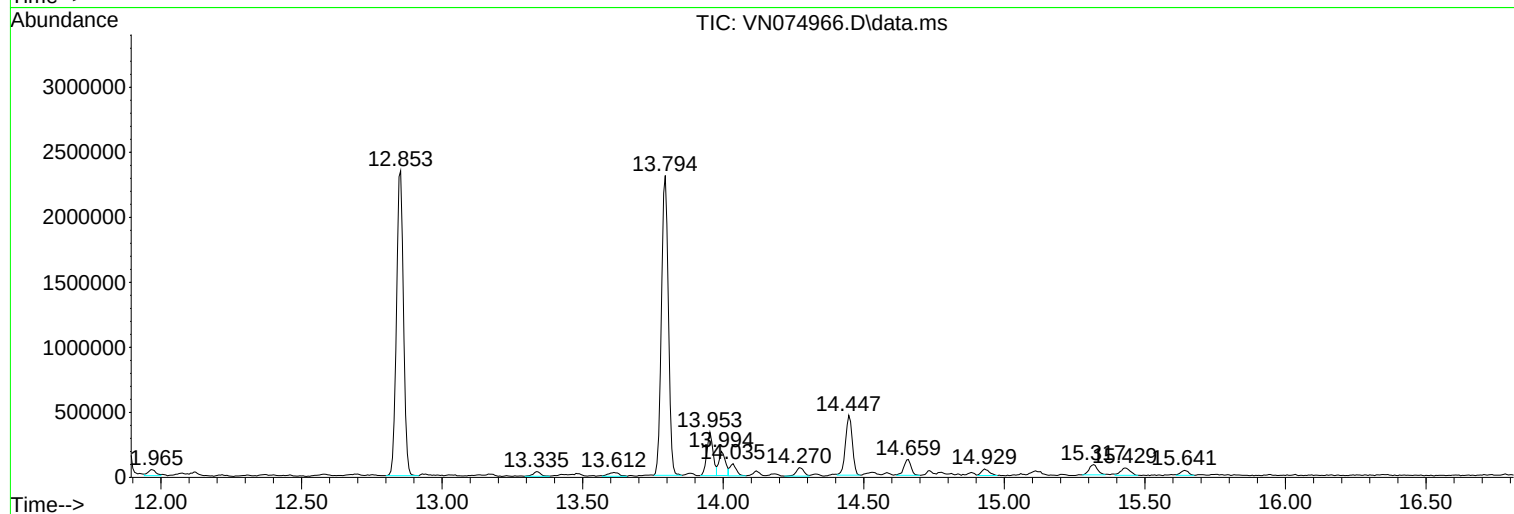
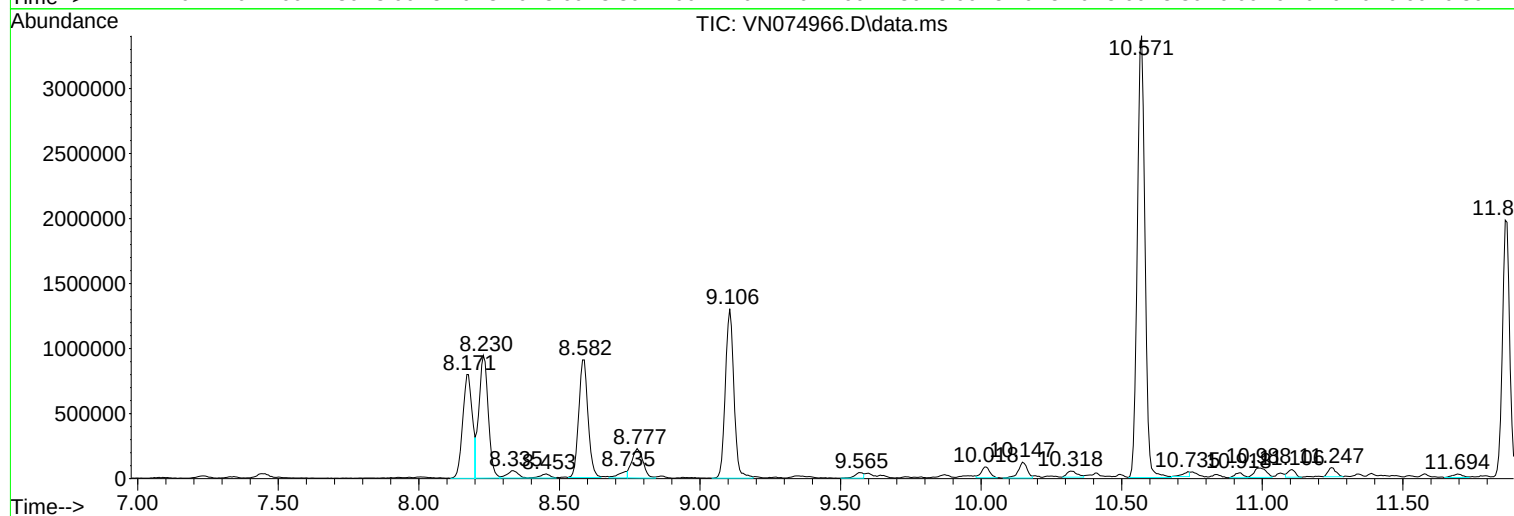
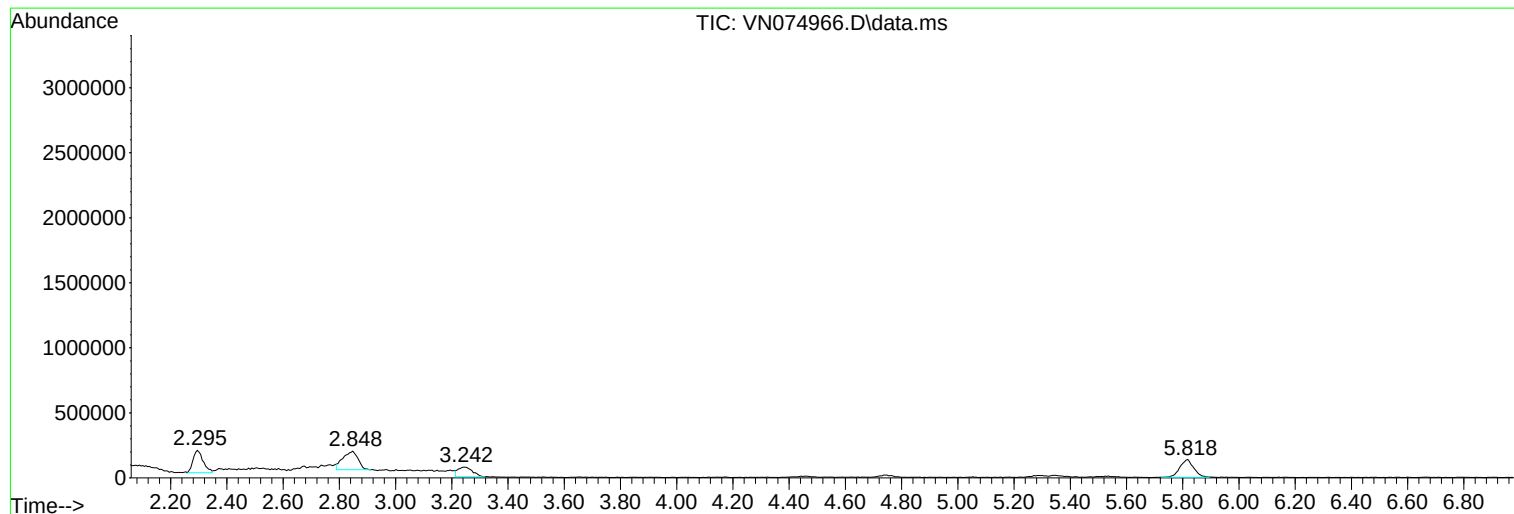
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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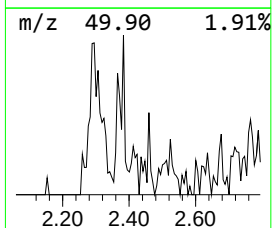
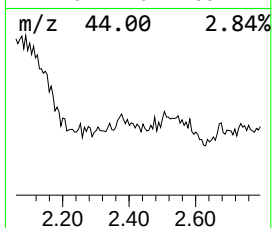
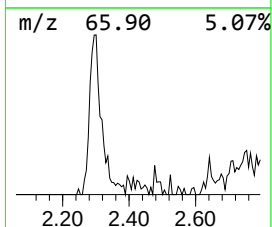
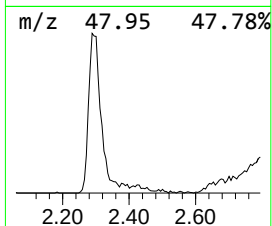
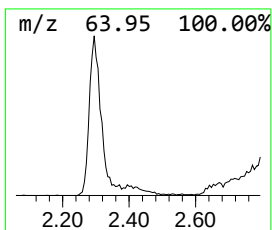
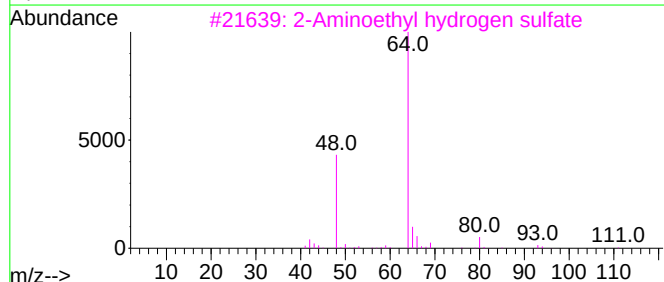
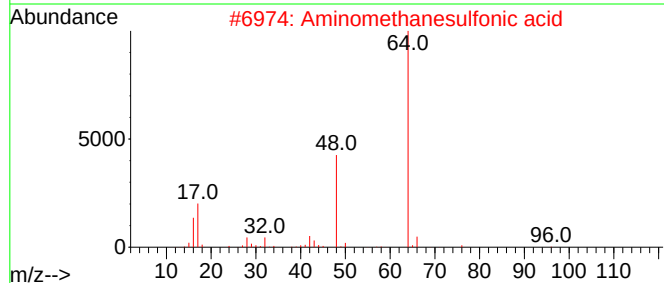
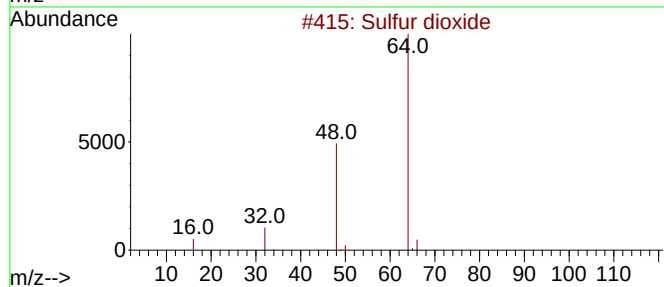
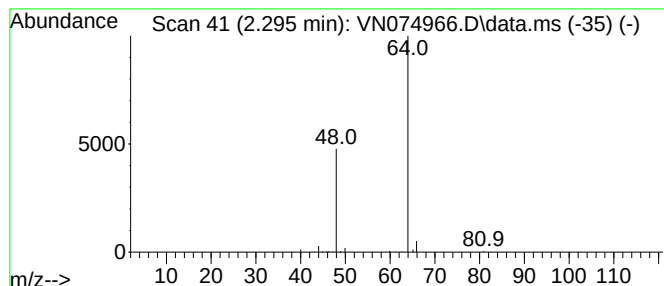
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	10.03 ug/l	430789	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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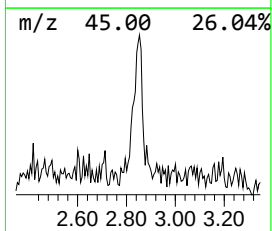
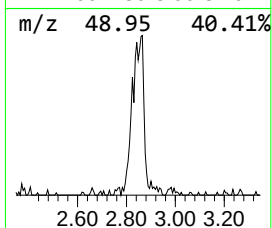
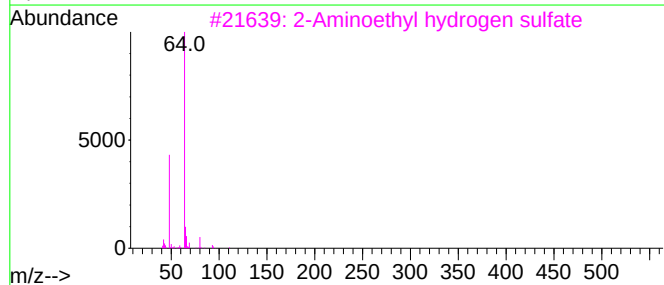
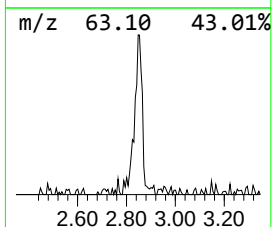
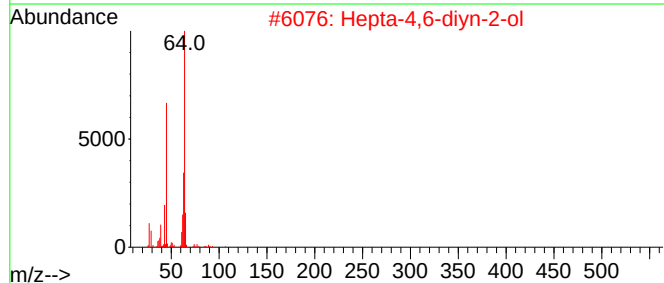
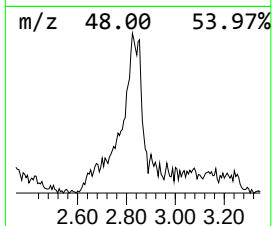
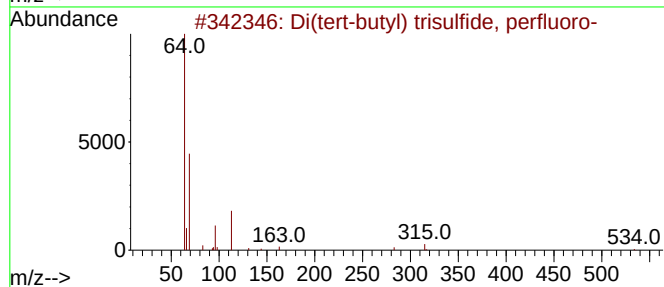
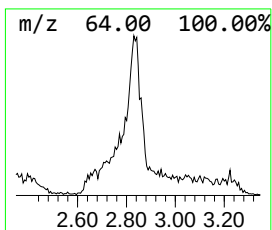
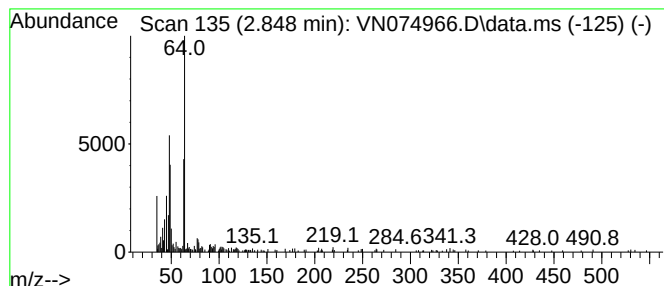
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Di(tert-butyl) trisulfide, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.848	12.32 ug/l	528819	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	83		
2	Hepta-4,6-diyn-2-ol	108	C7H8O	1000154-66-3	38		
3	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	32		
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	27		
5	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	23		



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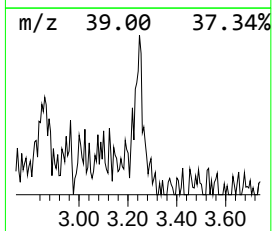
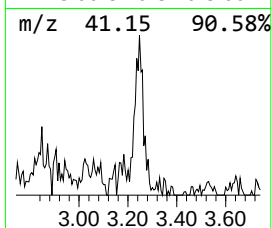
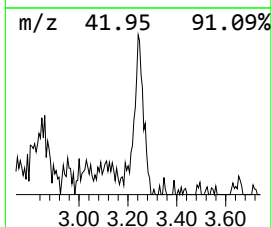
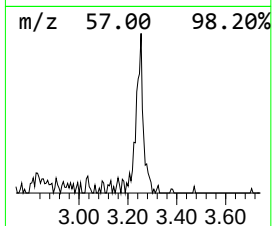
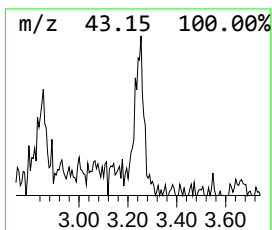
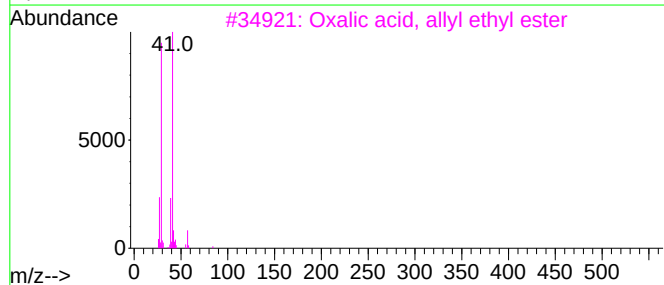
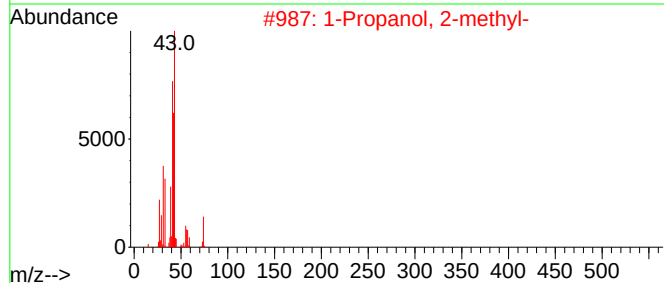
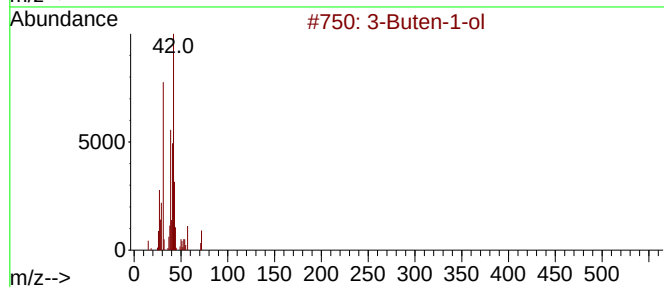
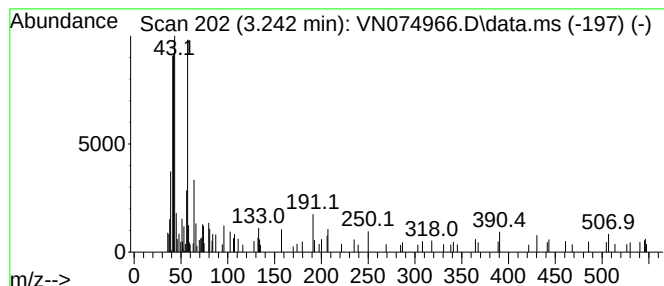
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown3.242 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.242	6.11 ug/l	262337	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-1-ol			72	C4H8O	000627-27-0	47
2	1-Propanol, 2-methyl-			74	C4H10O	000078-83-1	9
3	Oxalic acid, allyl ethyl ester			158	C7H10O4	1000309-22-8	9
4	N-[9-(Hydroxyimino)-2-methyl-5,1...			251	C7H5N7O4	1000436-04-1	9
5	17a-Ethyl-3.beta.-methoxy-17a-az...			345	C22H35NO2	149942-11-0	8



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ClientSampleId :
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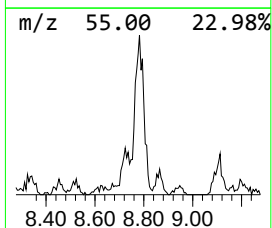
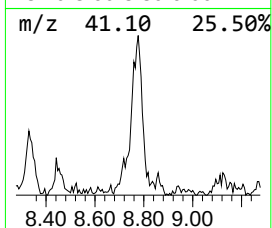
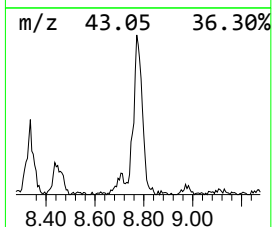
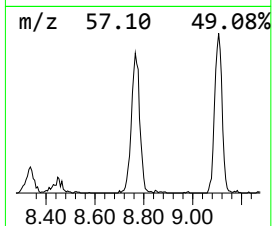
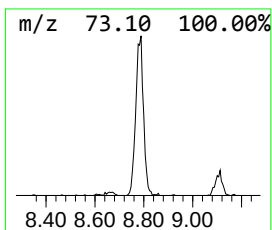
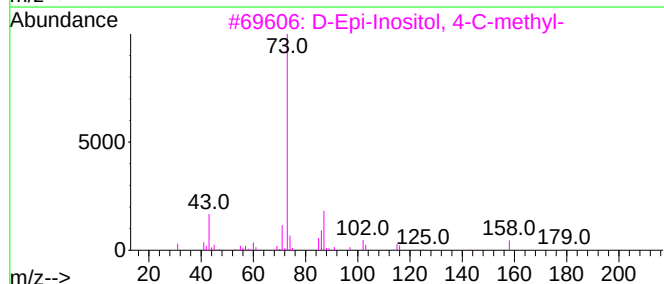
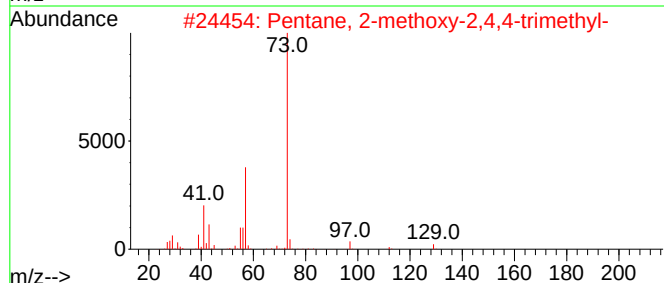
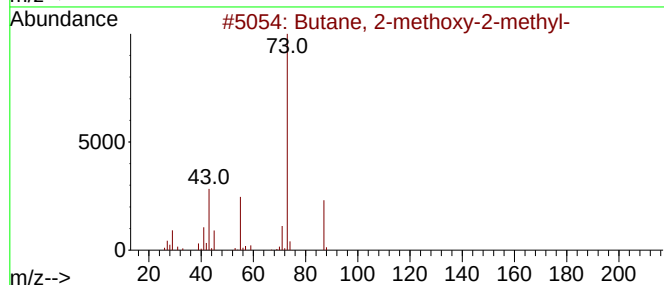
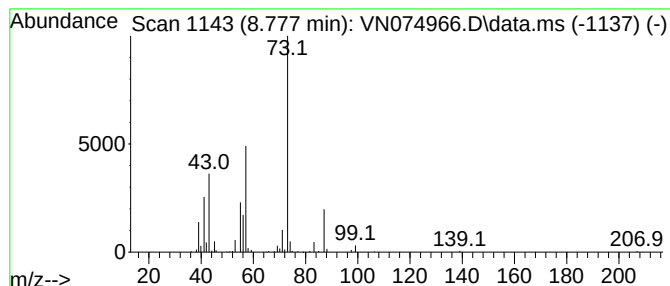
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Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.777	11.31 ug/l	622307	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2			Pentane, 2-methoxy-2,4,4-trimethyl-	144	C9H20O	062108-41-2	37
3			D-Epi-Inositol, 4-C-methyl-	194	C7H14O6	040788-89-4	33
4			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	28
5			Morpholine	87	C4H9NO	000110-91-8	25



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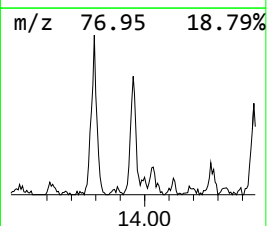
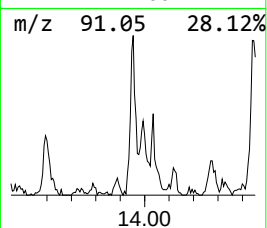
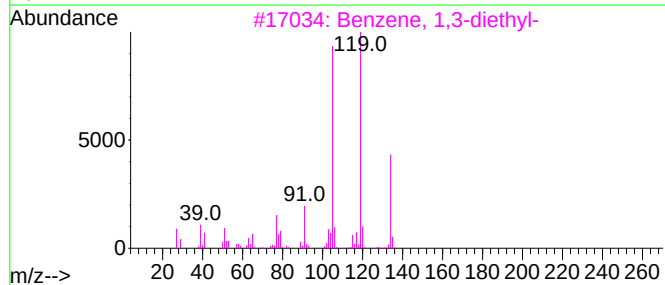
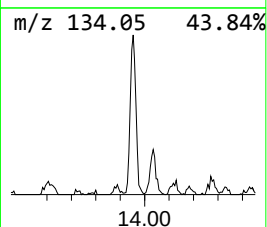
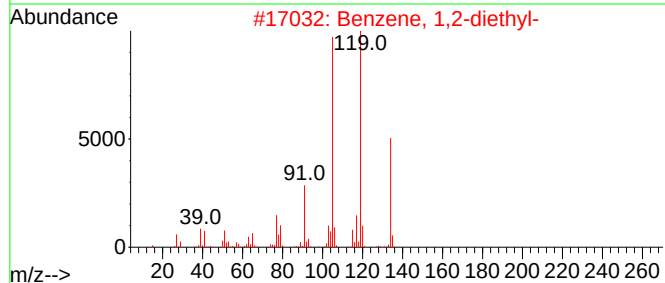
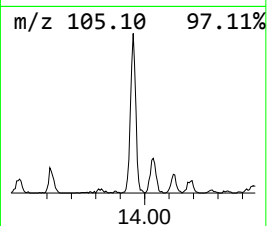
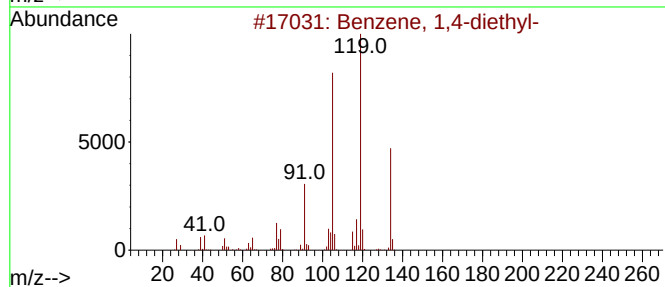
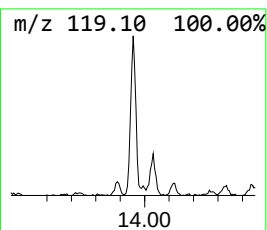
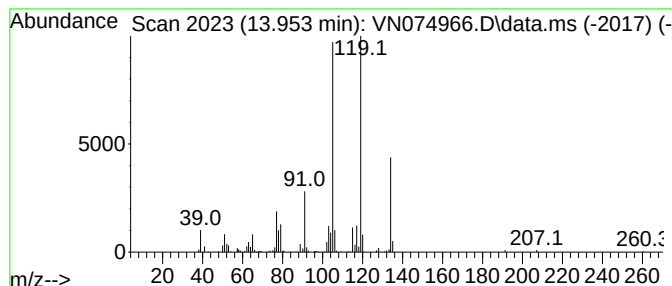
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,4-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.953	6.58 ug/l	518844	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074966.D
Acq On : 21 Oct 2022 17:00
Operator : JC\MD
Sample : N5222-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

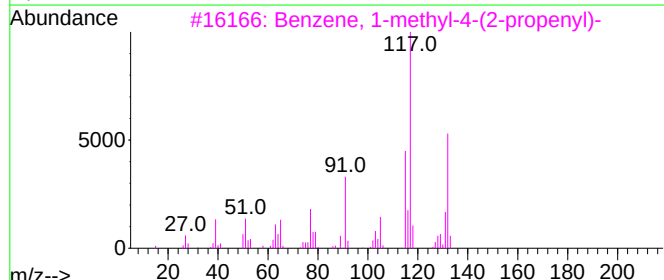
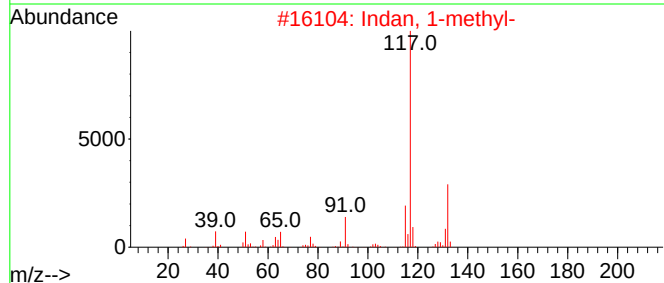
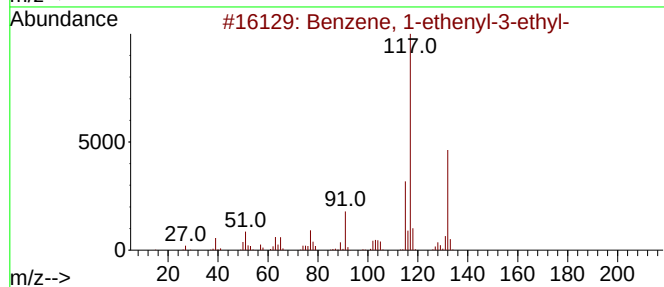
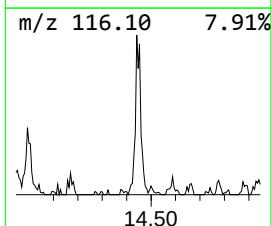
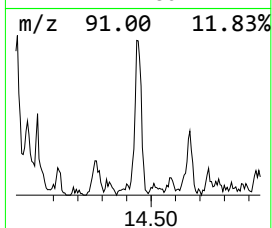
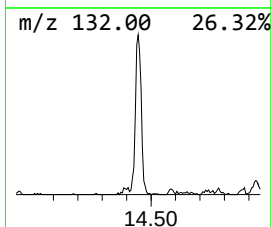
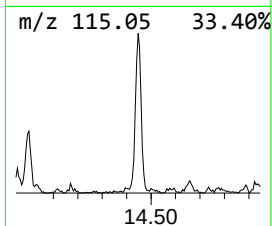
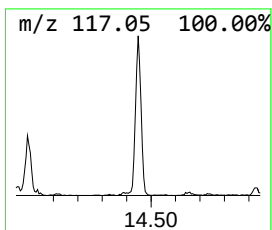
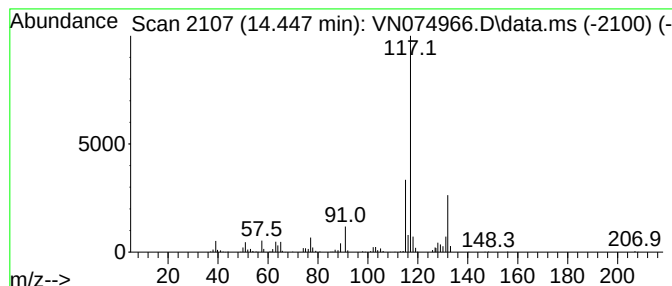
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	9.74 ug/l	768270	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
2			Indan, 1-methyl-	132	C10H12	000767-58-8	83
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
4			1H-Indene, 1-ethyl-2,3-dihydro-	146	C11H14	004830-99-3	53
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074966.D
Acq On : 21 Oct 2022 17:00
Operator : JC\MD
Sample : N5222-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.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
Sulfur dioxide	2.295	10.0	ug/l	430789	1	8.230	2146840	50.0
Di(tert-butyl) ...	2.848	12.3	ug/l	528819	1	8.230	2146840	50.0
unknown3.242	3.242	6.1	ug/l	262337	1	8.230	2146840	50.0
Butane, 2-metho...	8.777	11.3	ug/l	622307	2	9.106	2750350	50.0
Benzene, 1,4-di...	13.953	6.6	ug/l	518844	4	13.794	3943460	50.0
Benzene, 1-ethe...	14.447	9.7	ug/l	768270	4	13.794	3943460	50.0