

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
 Data File : VN074583.D
 Acq On : 19 Sep 2022 14:01
 Operator : JC\MD
 Sample : N4526-03 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 INF-0907

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\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074583.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	47	52	61	rBV	140410	303129	14.12%	1.395%
2	2.399	83	87	91	rBV	46378	64336	3.00%	0.296%
3	2.687	131	136	141	rBV3	47170	120784	5.63%	0.556%
4	3.069	194	201	214	rVB2	315940	768298	35.78%	3.535%
5	3.446	255	265	278	rBV3	63932	175004	8.15%	0.805%
6	3.652	294	300	305	rBV3	12422	23858	1.11%	0.110%
7	4.881	497	509	515	rBV6	16601	51335	2.39%	0.236%
8	4.987	517	527	528	rBV	30147	54418	2.53%	0.250%
9	5.075	534	542	544	rBV7	28845	63738	2.97%	0.293%
10	5.528	607	619	631	rBV5	33417	122538	5.71%	0.564%
11	6.028	693	704	713	rBV4	13702	42570	1.98%	0.196%
12	6.381	750	764	776	rVB2	27225	82252	3.83%	0.378%
13	6.516	778	787	795	rBV7	14753	44393	2.07%	0.204%
14	6.610	795	803	810	rBV4	9682	29156	1.36%	0.134%
15	6.810	827	837	848	rBV7	19433	59180	2.76%	0.272%
16	7.063	871	880	894	rVB3	110179	350574	16.33%	1.613%
17	7.245	902	911	920	rBV2	25943	81931	3.82%	0.377%
18	7.775	993	1001	1009	rVB2	26459	65527	3.05%	0.301%
19	7.951	1020	1031	1036	rBV2	241336	578229	26.93%	2.660%
20	8.016	1036	1042	1052	rVV2	420094	999225	46.53%	4.597%
21	8.104	1052	1057	1067	rVB6	31664	81480	3.79%	0.375%
22	8.228	1069	1078	1083	rBV4	11357	25548	1.19%	0.118%
23	8.387	1094	1105	1116	rBV3	805179	2147261	100.00%	9.879%
24	8.516	1120	1127	1132	rVV10	23007	56287	2.62%	0.259%
25	8.634	1144	1147	1155	rVB8	11212	24673	1.15%	0.114%
26	8.904	1184	1193	1205	rBV	634152	1323403	61.63%	6.089%
27	9.175	1235	1239	1247	rVB7	11192	23236	1.08%	0.107%
28	9.363	1264	1271	1272	rBV4	19315	31595	1.47%	0.145%
29	9.392	1272	1276	1284	rVB5	33866	69906	3.26%	0.322%
30	9.910	1358	1364	1367	rBV3	16332	27225	1.27%	0.125%
31	9.951	1367	1371	1378	rVB5	17936	36654	1.71%	0.169%
32	10.257	1418	1423	1430	rBV5	19220	41802	1.95%	0.192%
33	10.381	1436	1444	1450	rBV	965156	1757947	81.87%	8.088%
34	10.445	1450	1455	1462	rVB2	186151	341356	15.90%	1.570%
35	10.580	1473	1478	1484	rVB5	12143	23975	1.12%	0.110%
36	10.810	1511	1517	1525	rVB8	9753	24484	1.14%	0.113%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
 Data File : VN074583.D
 Acq On : 19 Sep 2022 14:01
 Operator : JC\MD
 Sample : N4526-03 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 INF-0907

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\82N091522W.M
 Title : SW846 8260

37	11.686	1658	1666	1676	rBV	999863	1741737	81.11%	8.013%
38	11.786	1676	1683	1694	rVV	501529	859148	40.01%	3.953%
39	11.898	1694	1702	1713	rVV	1048989	2066606	96.24%	9.508%
40	12.222	1747	1757	1763	rBV	75257	125981	5.87%	0.580%
41	12.522	1803	1808	1815	rVB3	71810	118692	5.53%	0.546%
42	12.674	1826	1834	1844	rBV	824303	1358786	63.28%	6.251%
43	12.863	1859	1866	1871	rBV2	128571	208593	9.71%	0.960%
44	12.927	1871	1877	1879	rVV2	57297	102431	4.77%	0.471%
45	12.957	1879	1882	1886	rVV	126004	200870	9.35%	0.924%
46	13.004	1886	1890	1896	rVB2	137239	220577	10.27%	1.015%
47	13.163	1908	1917	1924	rBV2	131462	216166	10.07%	0.995%
48	13.310	1935	1942	1950	rBV	514588	811166	37.78%	3.732%
49	13.616	1987	1994	2005	rBV2	1003138	2083012	97.01%	9.583%
50	13.816	2017	2028	2044	rVB	327985	654624	30.49%	3.012%
51	14.010	2055	2061	2067	rVB3	24088	40771	1.90%	0.188%
52	14.074	2067	2072	2075	rBV3	23499	37371	1.74%	0.172%
53	14.157	2080	2086	2093	rBV	58878	89350	4.16%	0.411%
54	14.221	2093	2097	2100	rBV4	17979	27326	1.27%	0.126%
55	14.268	2100	2105	2111	rVB3	69350	115557	5.38%	0.532%
56	14.398	2118	2127	2133	rBV3	17414	29839	1.39%	0.137%
57	14.486	2135	2142	2144	rBV2	37255	61914	2.88%	0.285%
58	14.521	2144	2148	2153	rVB3	32286	47221	2.20%	0.217%
59	14.751	2182	2187	2193	rBV2	40772	63882	2.98%	0.294%
60	14.868	2199	2207	2214	rBV5	79088	162435	7.56%	0.747%
61	15.439	2297	2304	2311	rBV	93942	174532	8.13%	0.803%

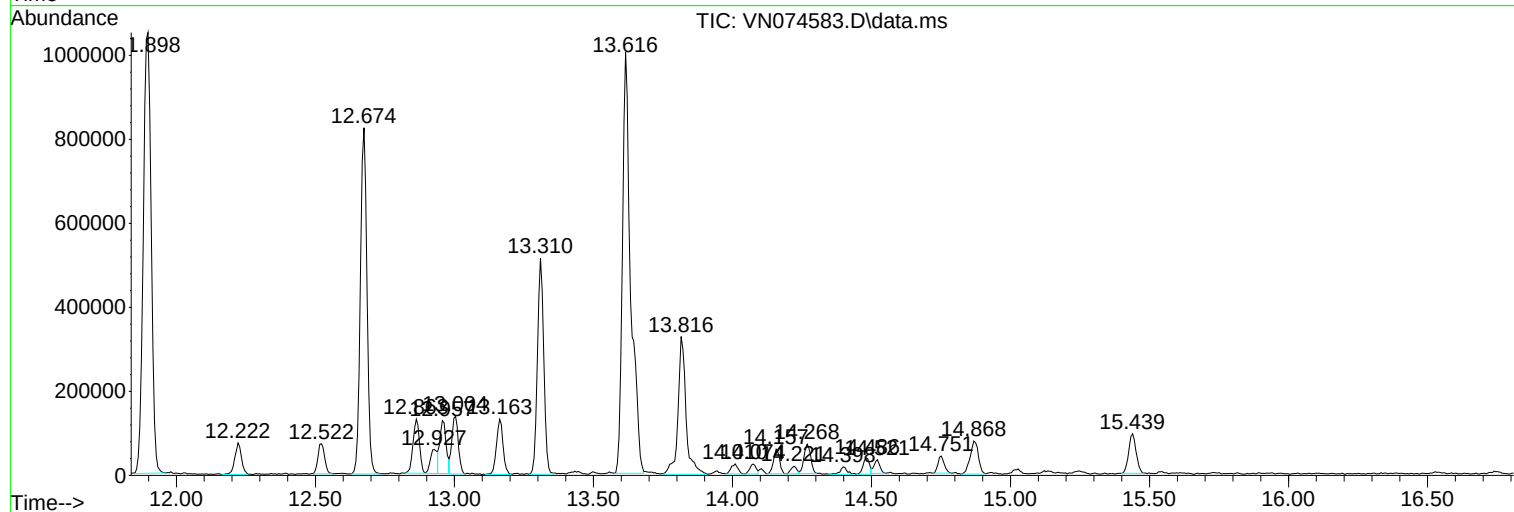
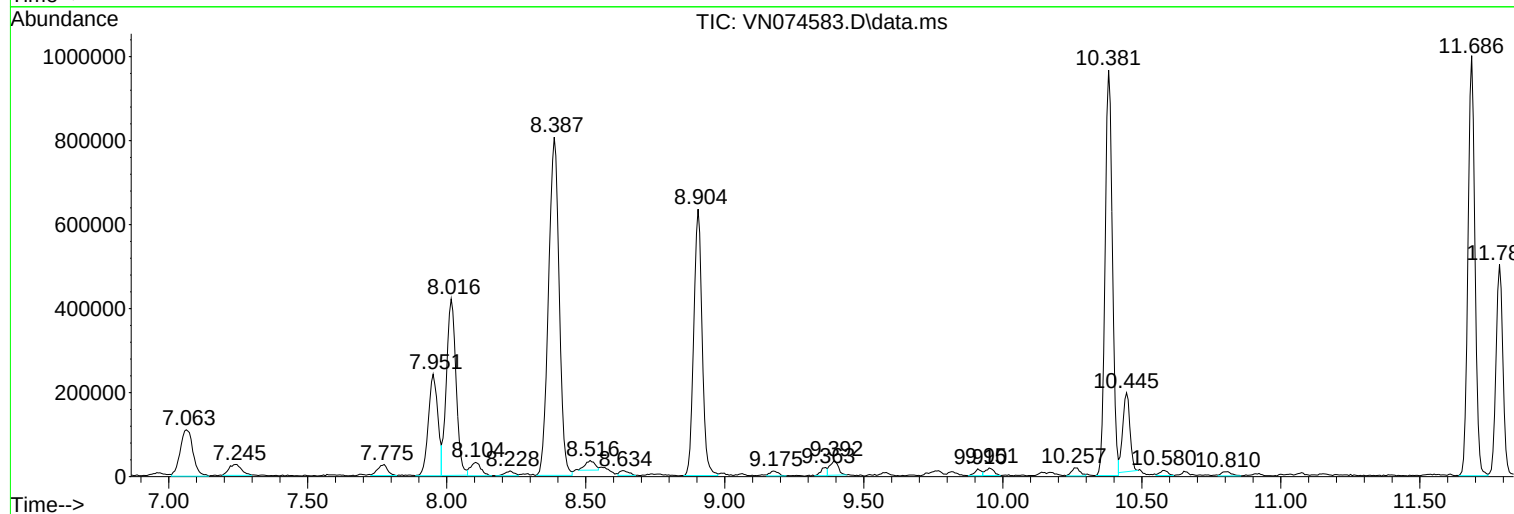
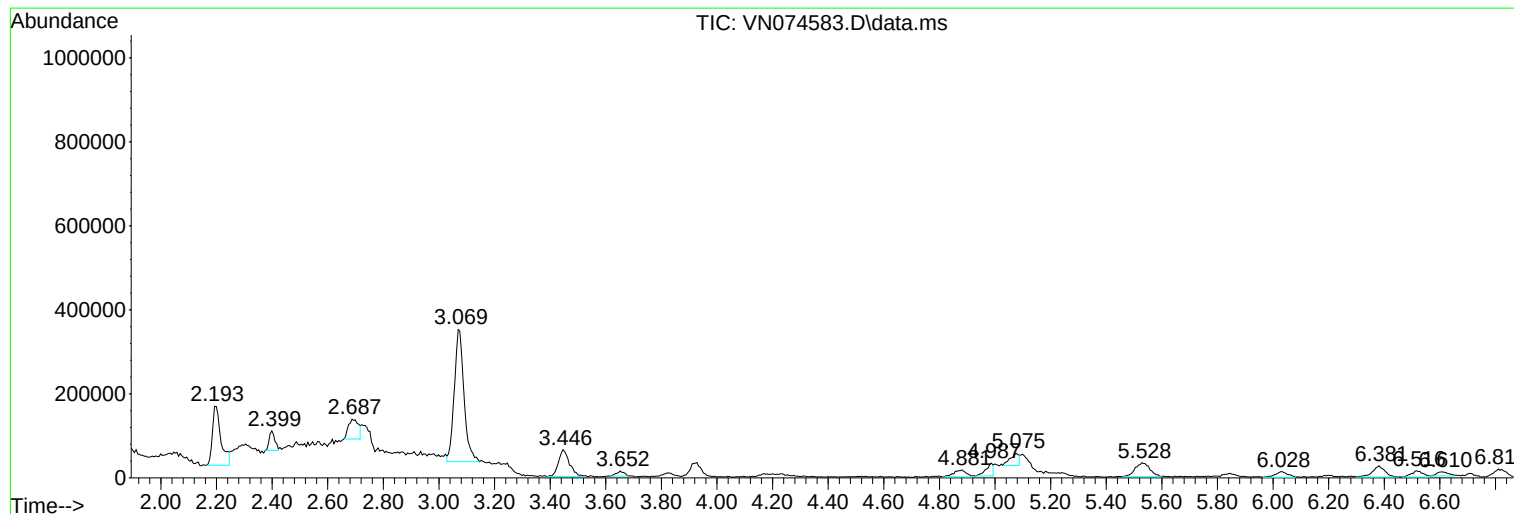
Sum of corrected areas: 21735894

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

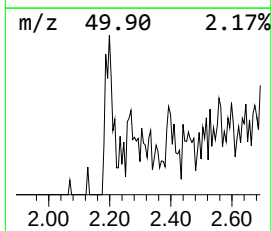
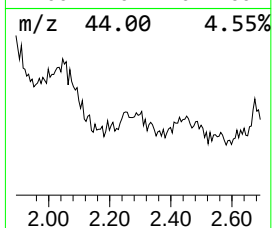
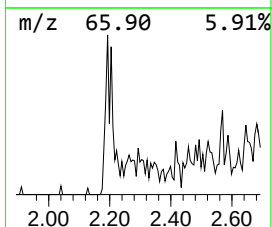
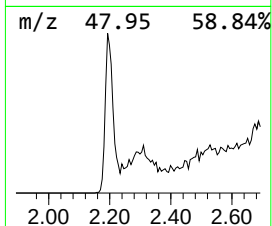
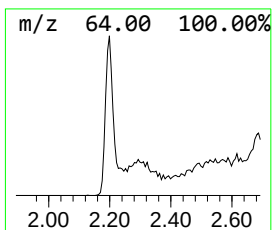
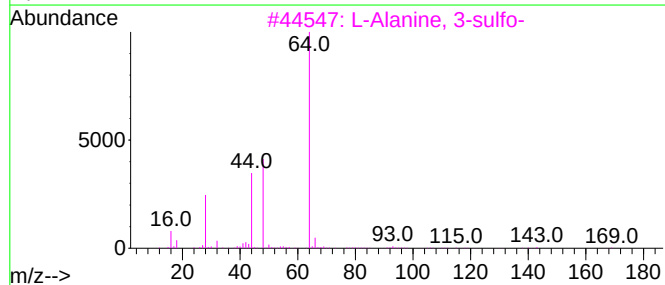
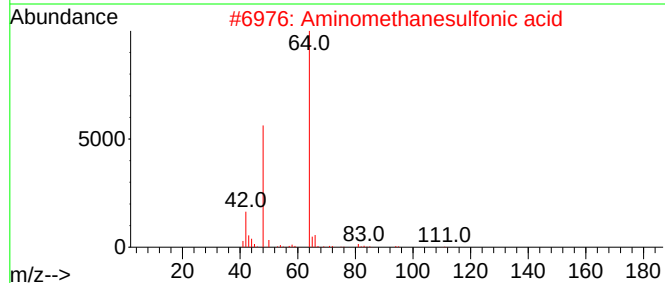
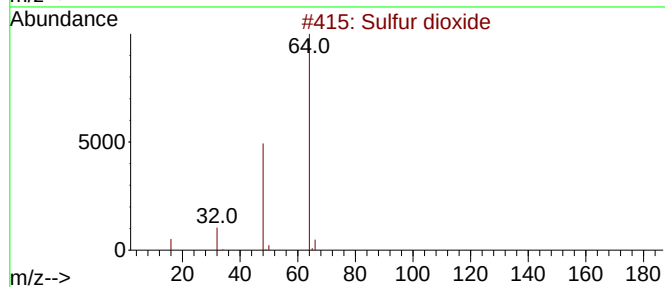
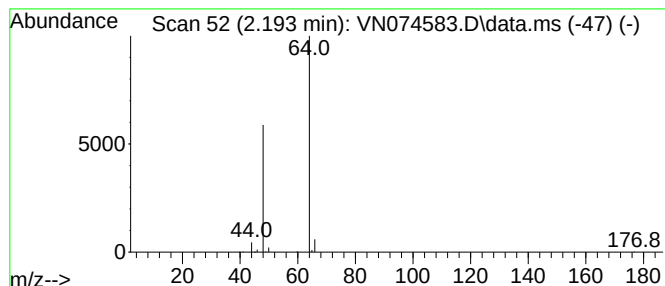
Instrument :
MSVOA_N
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.193	15.17 ug/l	303129	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

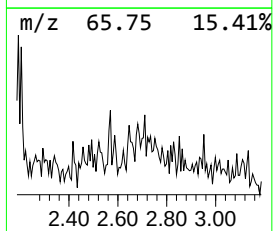
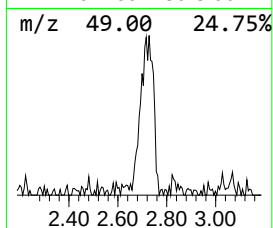
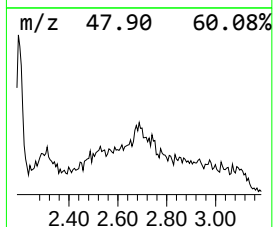
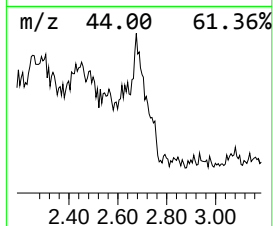
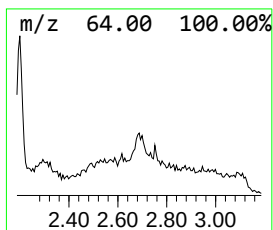
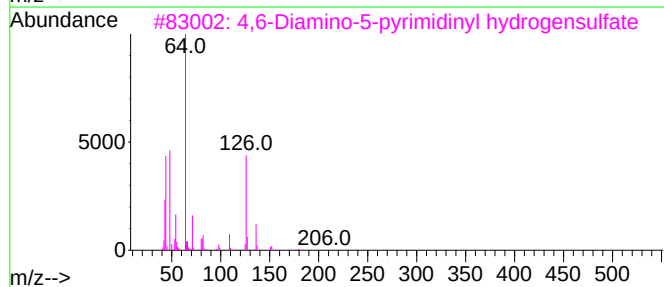
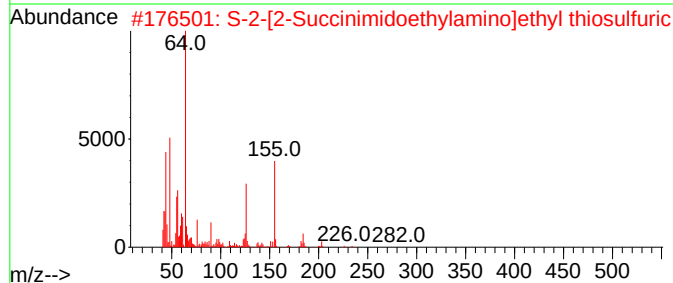
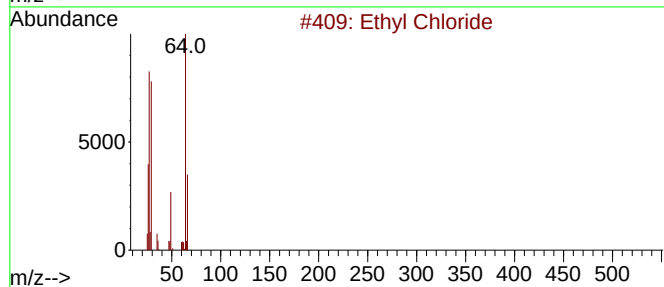
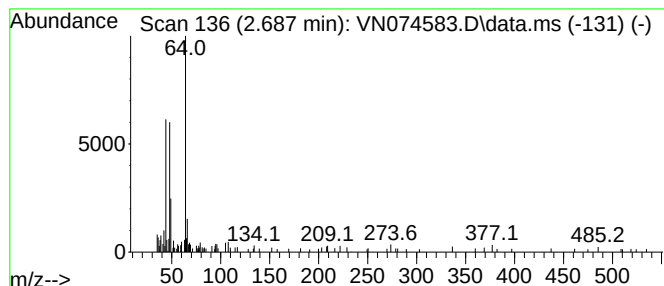
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethyl Chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	6.04 ug/l	120784	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	72
2			S-2-[2-Succinimidoethylamino]eth...	282	C8H14N2O5S2	031701-74-3	39
3			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	39
4			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	39
5			2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

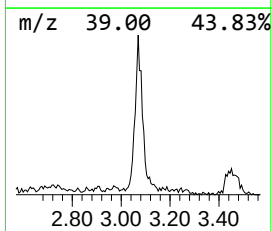
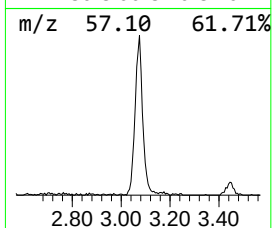
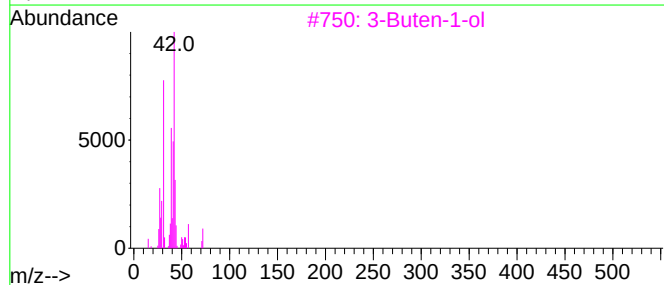
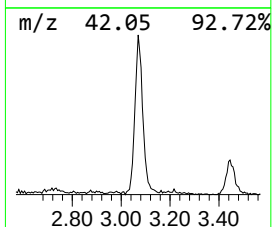
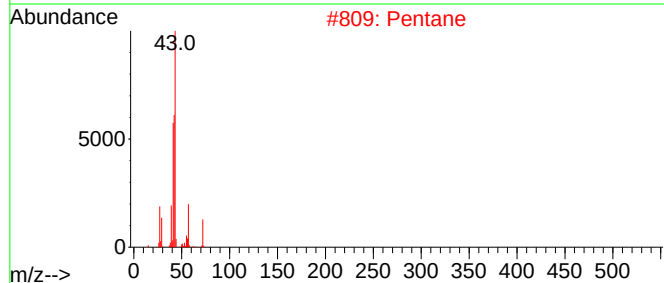
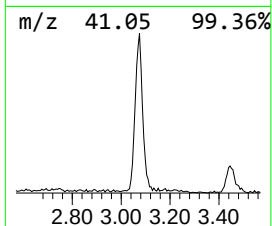
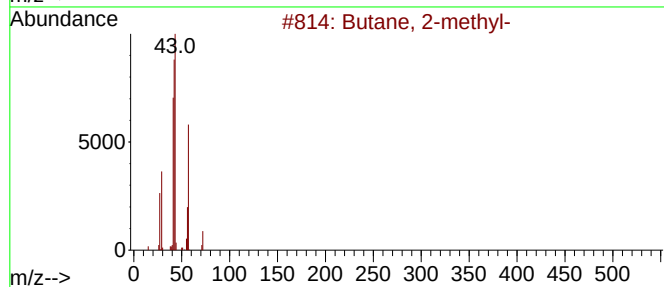
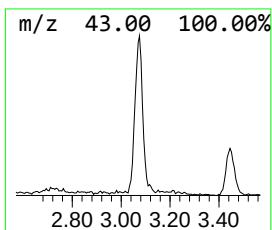
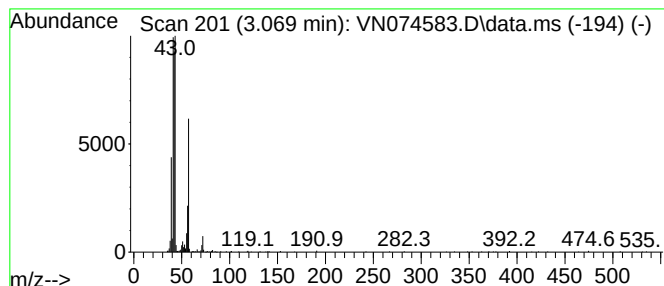
Instrument :
MSVOA_N
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown3.069 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.069	38.44 ug/l	768298	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	49
2	Pentane	72	C5H12	000109-66-0	39
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	Ethenamine, N-methyl-N-nitroso-	86	C3H6N2O	004549-40-0	28
5	Acetamide, N-[3-(4-bromophenyl)-...	326	C13H15BrN2O3	1000295-71-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

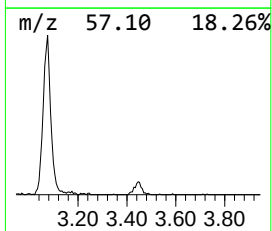
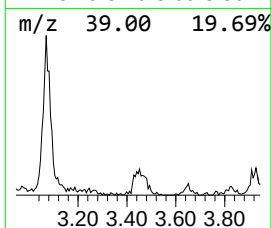
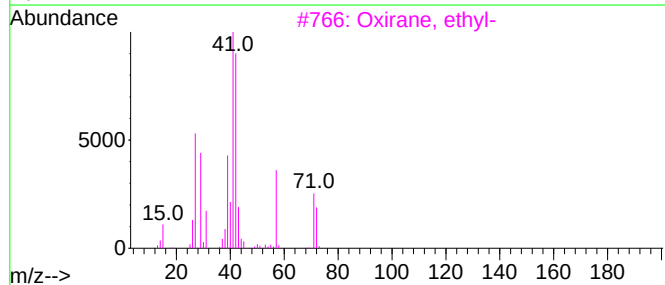
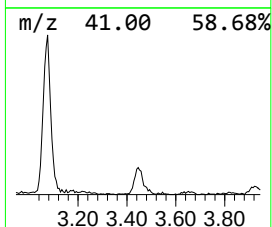
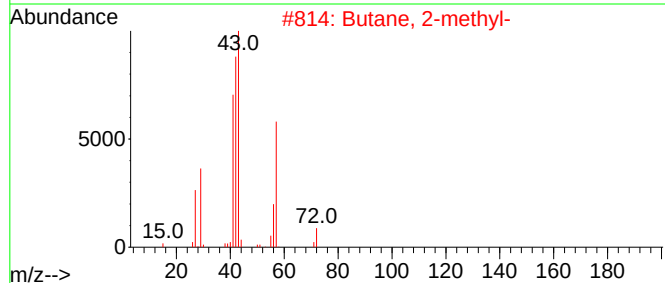
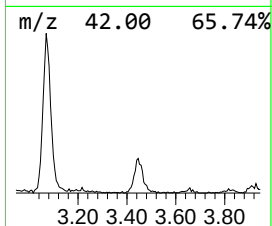
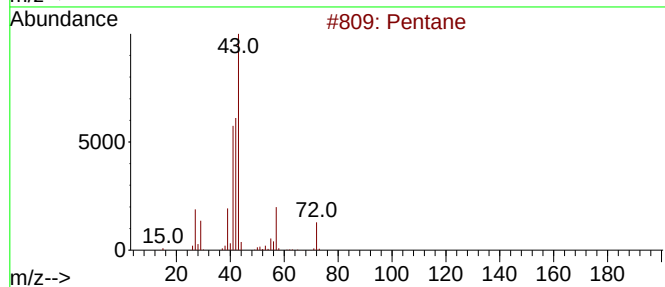
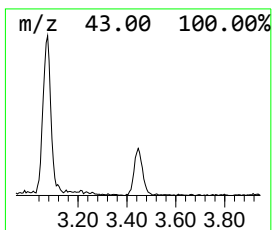
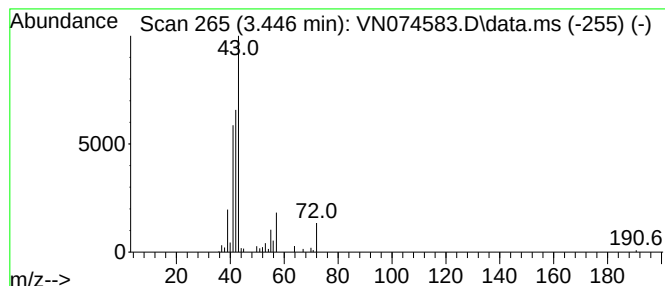
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.446	8.76 ug/l	175004	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Butane, 2-methyl-	72	C5H12	000078-78-4	38
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	17
4	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	17
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

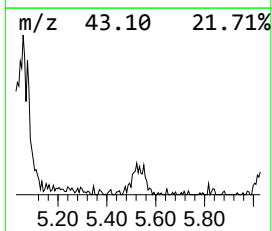
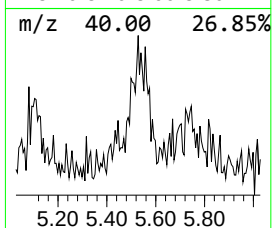
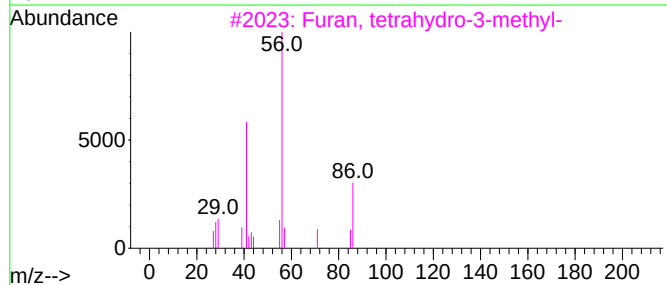
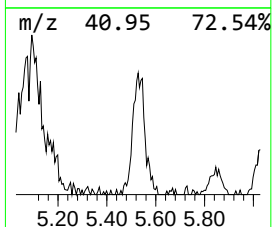
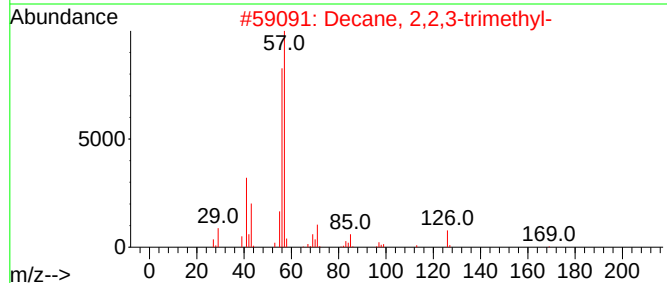
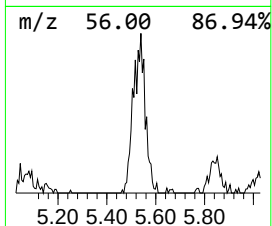
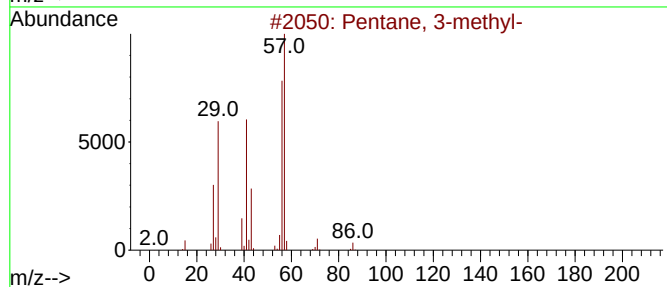
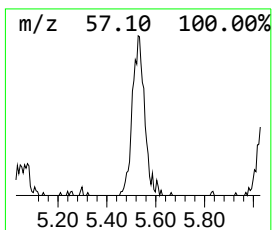
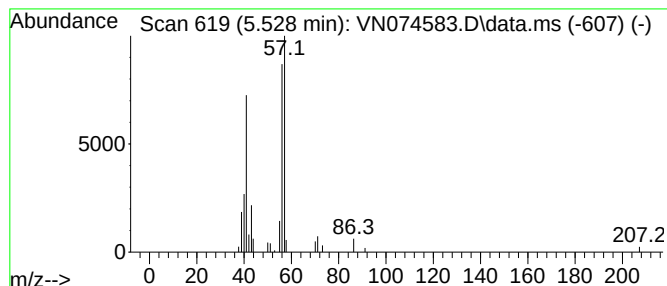
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.528	6.13 ug/l	122538	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	56
3			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	53
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	50
5			Propanoic acid, 2-bromo-, butyl ...	208	C7H13BrO2	041145-84-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

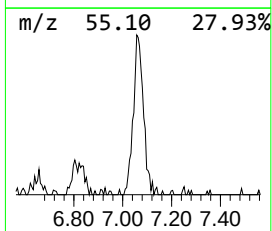
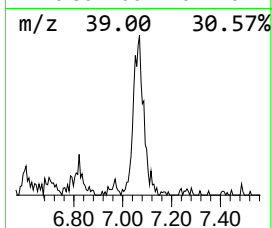
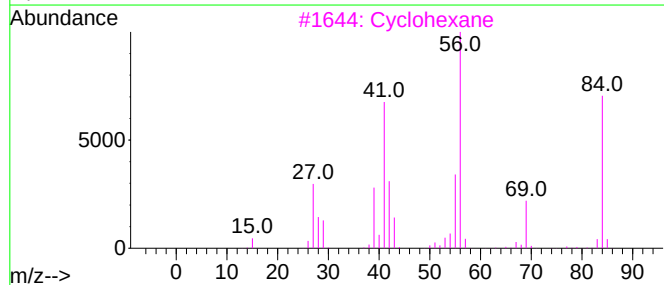
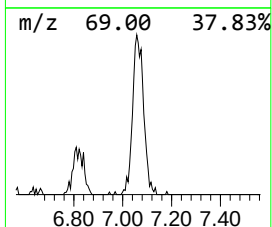
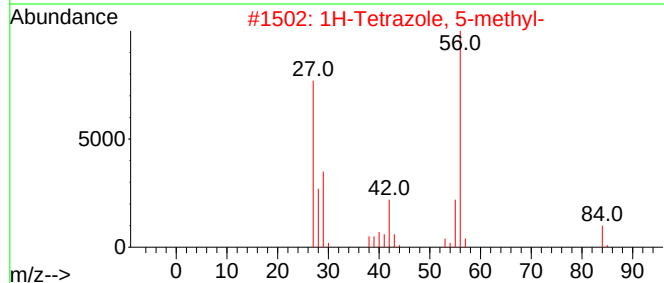
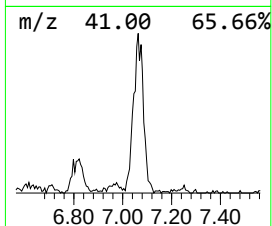
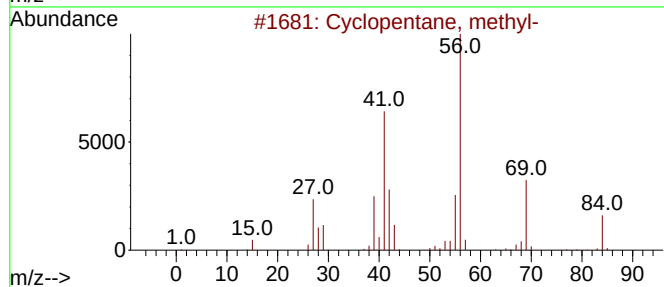
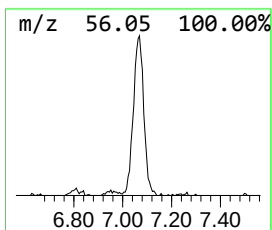
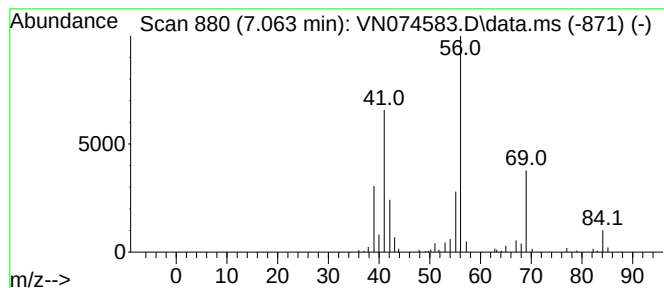
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	17.54 ug/l	350574	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3		Cyclohexane	84	C6H12	000110-82-7	78
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
5		Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

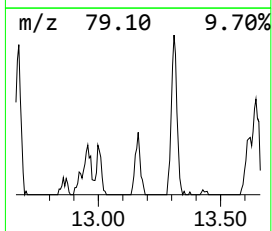
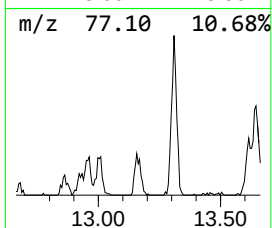
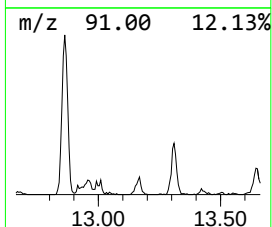
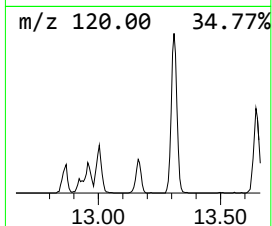
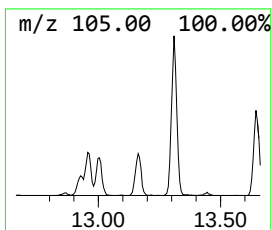
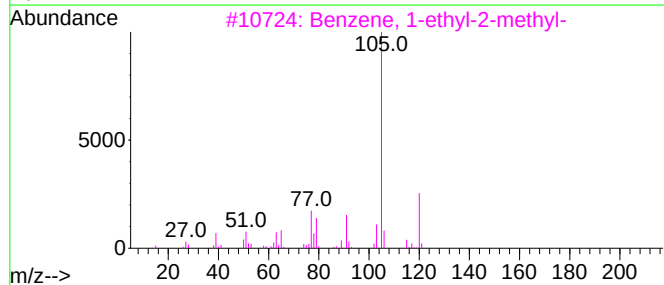
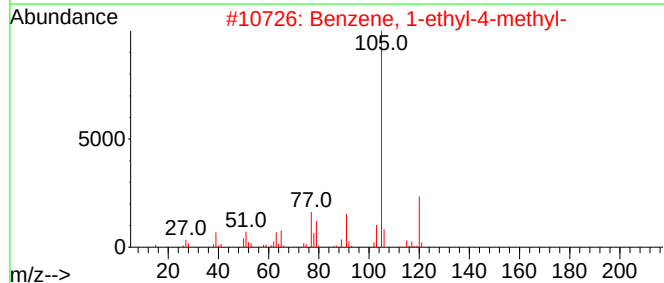
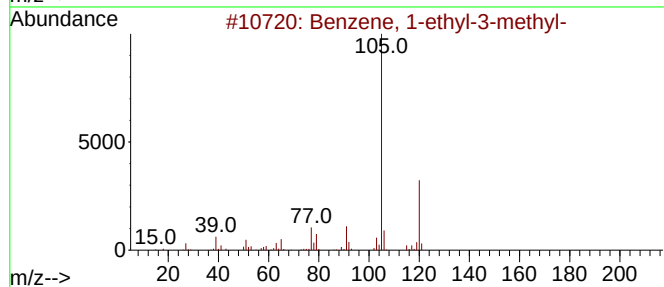
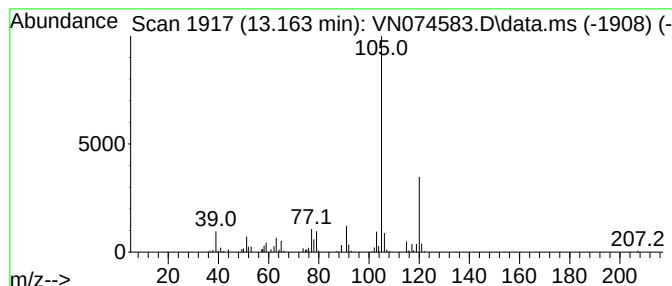
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	5.19 ug/l	216166	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

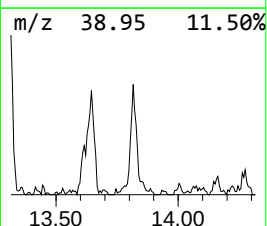
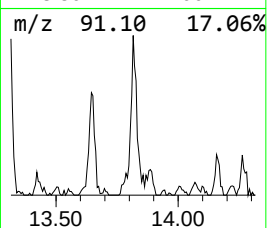
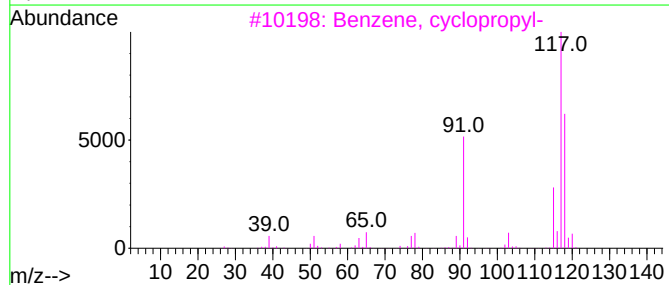
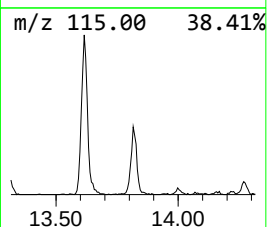
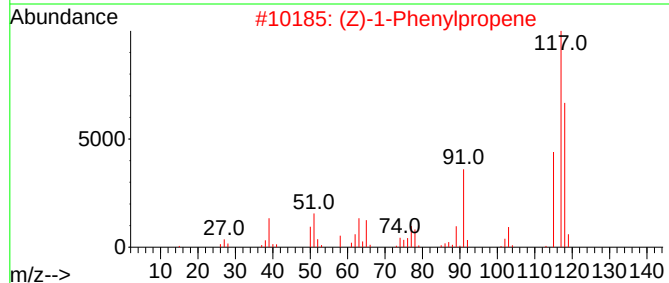
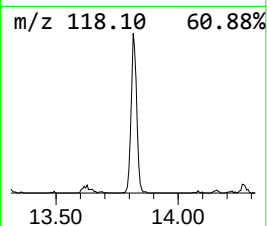
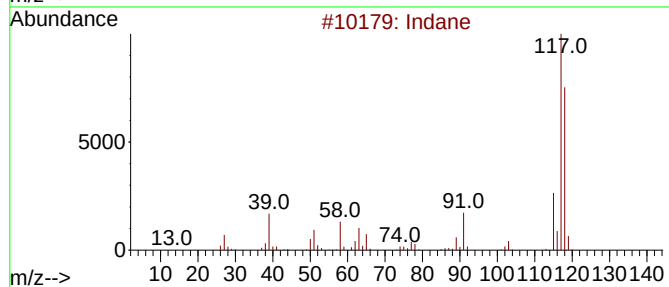
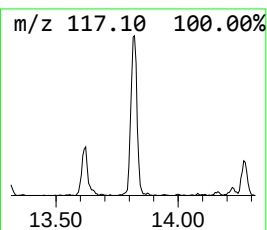
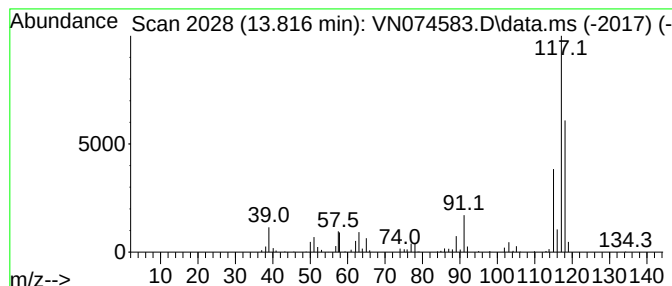
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	15.71 ug/l	654624	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	89
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074583.D
Acq On : 19 Sep 2022 14:01
Operator : JC\MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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	2.193	15.2	ug/l	303129	1	8.016	999225	50.0
Ethyl Chloride	2.687	6.0	ug/l	120784	1	8.016	999225	50.0
unknown3.069	3.069	38.4	ug/l	768298	1	8.016	999225	50.0
Pentane	3.446	8.8	ug/l	175004	1	8.016	999225	50.0
Pentane, 3-methyl-	5.528	6.1	ug/l	122538	1	8.016	999225	50.0
Cyclopentane, m...	7.063	17.5	ug/l	350574	1	8.016	999225	50.0
Benzene, 1-ethy...	13.163	5.2	ug/l	216166	4	13.616	2083010	50.0
Indane	13.816	15.7	ug/l	654624	4	13.616	2083010	50.0