

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
 Data File : VN071818.D
 Acq On : 02 Apr 2022 23:23
 Operator : JC\MD
 Sample : N2242-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	62	rBV	346823	1385618	2.99%	0.990%
2	3.134	186	195	212	rVB	609765	1421002	3.07%	1.015%
3	3.516	250	260	274	rBV	249598	625300	1.35%	0.447%
4	5.157	531	539	570	rVB7	279426	1590632	3.43%	1.137%
5	5.616	602	617	637	rBV2	425269	1513482	3.27%	1.081%
6	6.469	754	762	775	rVB2	176262	534918	1.16%	0.382%
7	6.904	825	836	850	rBV	174764	508883	1.10%	0.364%
8	7.145	867	877	887	rBV	624501	1829257	3.95%	1.307%
9	7.845	988	996	1006	rVB	195173	482629	1.04%	0.345%
10	8.022	1016	1026	1030	rBV	438442	1045649	2.26%	0.747%
11	8.086	1030	1037	1046	rVV2	1058854	2664369	5.75%	1.904%
12	8.169	1046	1051	1064	rVB3	196500	521528	1.13%	0.373%
13	8.457	1088	1100	1111	rBV	3874952	9429964	20.36%	6.738%
14	8.598	1113	1124	1125	rBV4	229832	608727	1.31%	0.435%
15	8.963	1177	1186	1199	rBV	1371629	3037618	6.56%	2.170%
16	10.439	1429	1437	1442	rBV	2120811	3870846	8.36%	2.766%
17	10.504	1442	1448	1461	rVB	3709146	6935089	14.98%	4.955%
18	11.739	1650	1658	1668	rBV	2022047	3625441	7.83%	2.590%
19	11.839	1668	1675	1685	rVV	5304773	8973057	19.38%	6.411%
20	11.945	1685	1693	1707	rVV	24653869	46308569	100.00%	33.087%
21	12.274	1737	1749	1760	rBV	3848452	6471189	13.97%	4.624%
22	12.574	1794	1800	1807	rVB	401321	650770	1.41%	0.465%
23	12.727	1818	1826	1836	rBV	1607784	2660597	5.75%	1.901%
24	12.916	1852	1858	1863	rBV	368408	610906	1.32%	0.436%
25	12.980	1863	1869	1873	rBV	3046922	5383331	11.62%	3.846%
26	13.057	1878	1882	1889	rVB	1717742	2712615	5.86%	1.938%
27	13.216	1901	1909	1919	rBV	1342795	2186644	4.72%	1.562%
28	13.363	1922	1934	1949	rVV	5551169	8991584	19.42%	6.424%
29	13.668	1979	1986	1989	rBV	1803263	3207056	6.93%	2.291%
30	13.698	1989	1991	2008	rVB	1766969	2610753	5.64%	1.865%
31	13.874	2015	2021	2037	rVB2	1711014	3609661	7.79%	2.579%
32	14.215	2074	2079	2084	rVB	298366	465820	1.01%	0.333%
33	14.321	2092	2097	2107	rVB2	337756	570564	1.23%	0.408%
34	14.574	2136	2140	2145	rVB	343512	513993	1.11%	0.367%
35	14.927	2191	2200	2206	rBV2	459694	909571	1.96%	0.650%
36	15.504	2285	2298	2309	rBV	762639	1490651	3.22%	1.065%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Title : SW846 8260

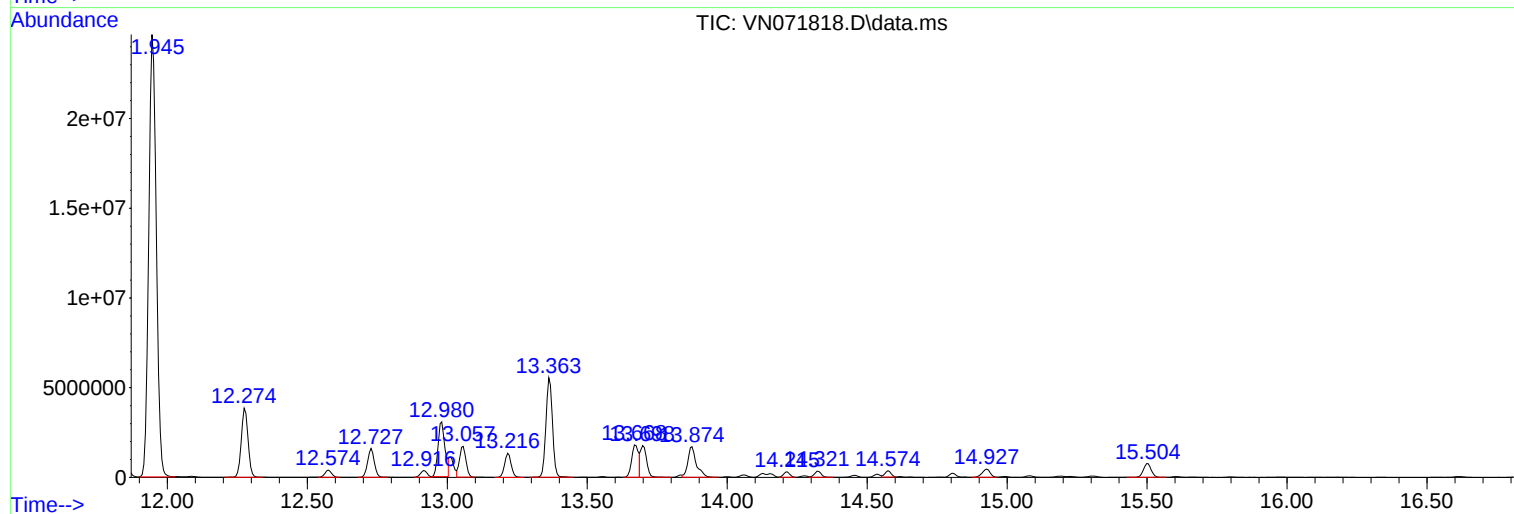
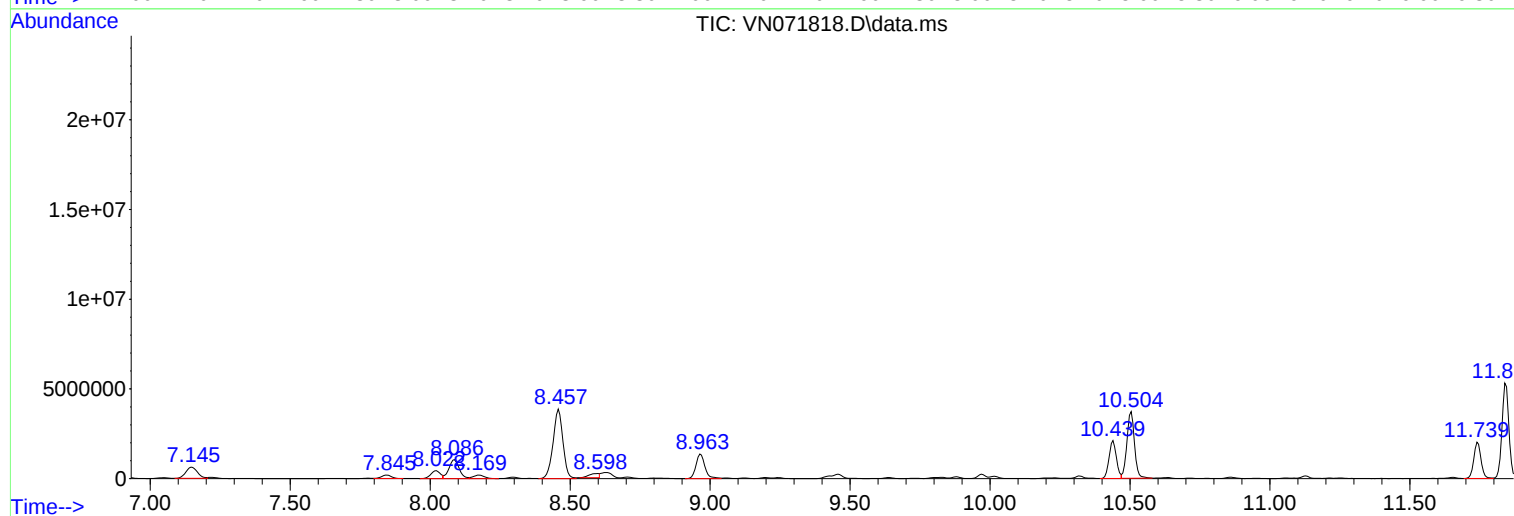
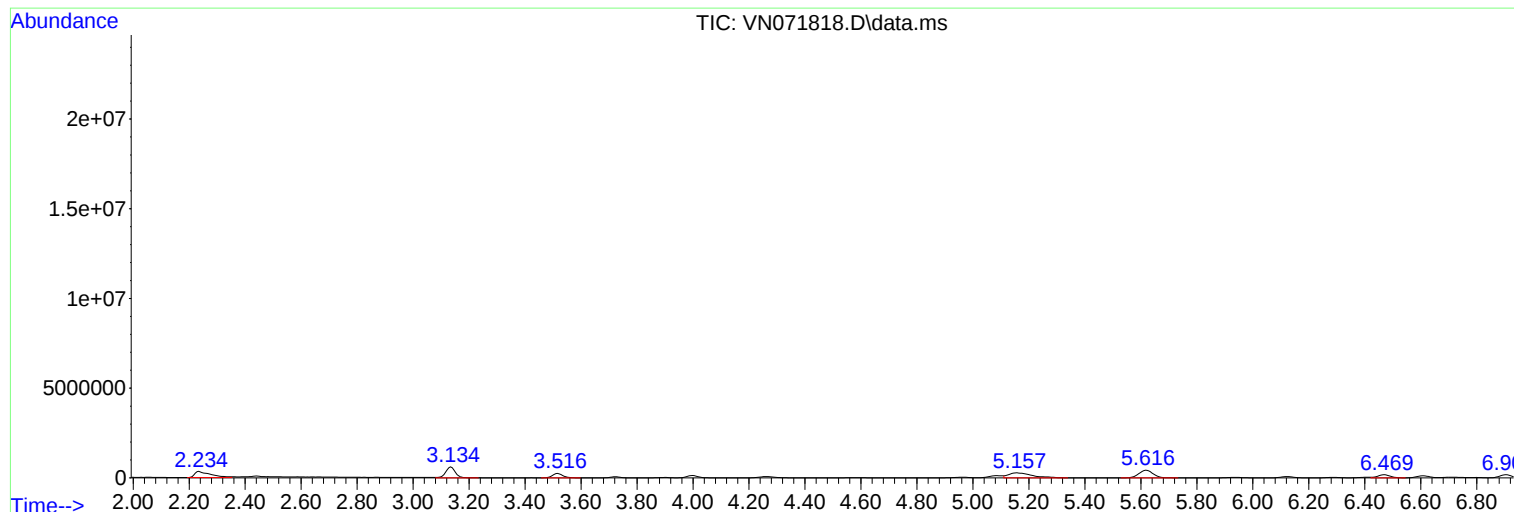
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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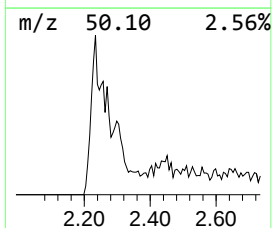
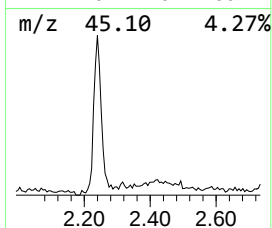
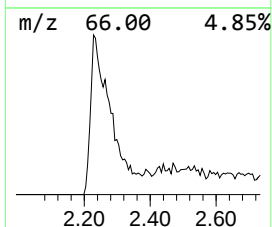
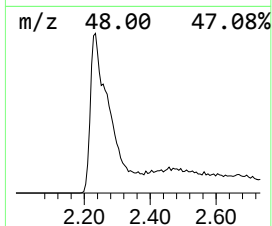
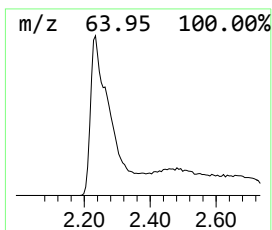
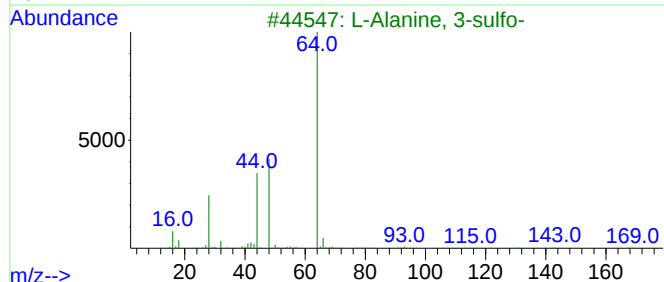
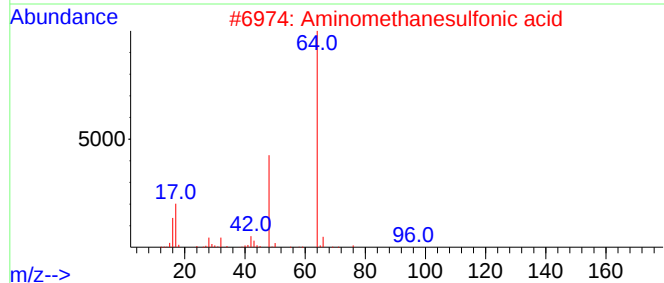
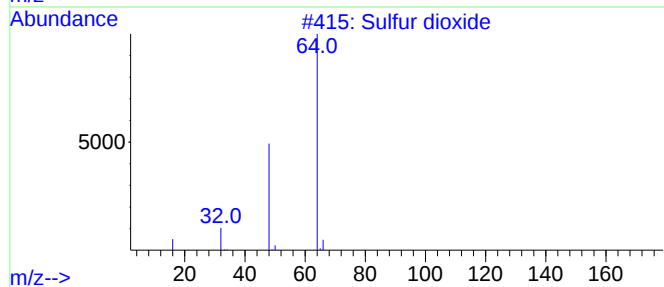
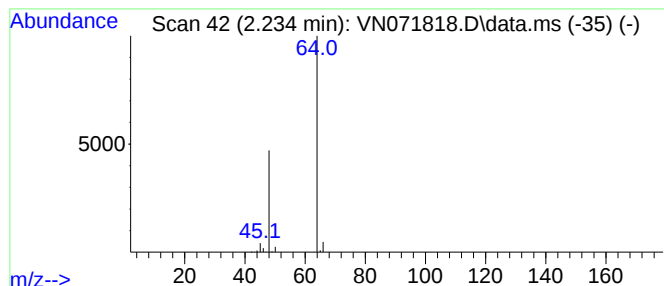
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	26.00 ug/l	1385620	Pentafluorobenzene	8.086

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	74
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



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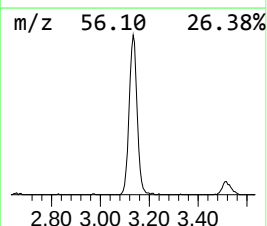
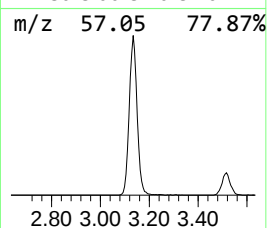
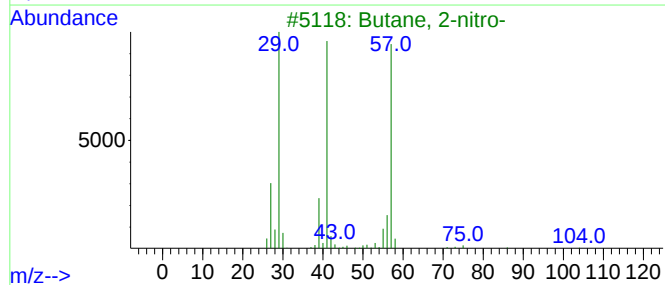
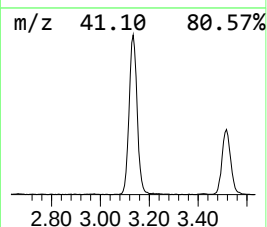
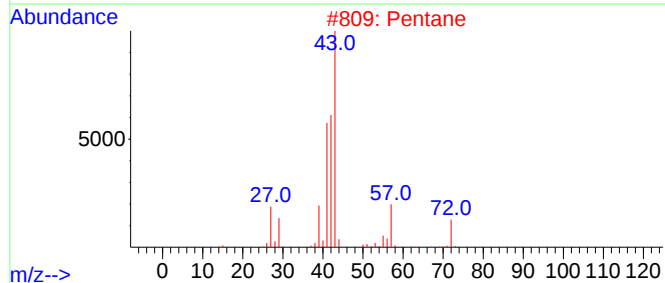
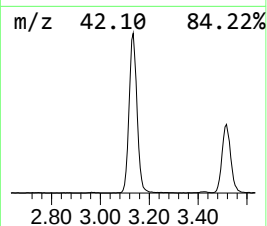
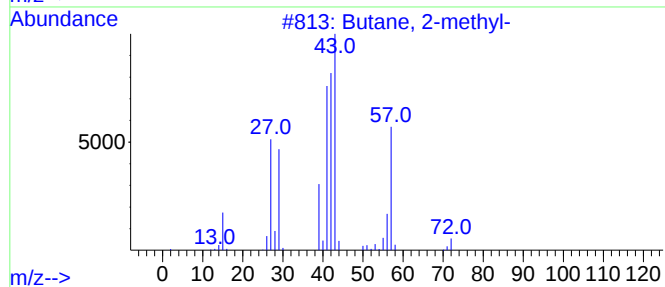
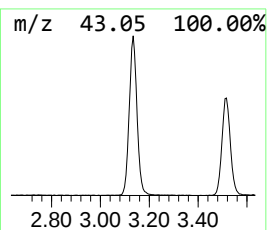
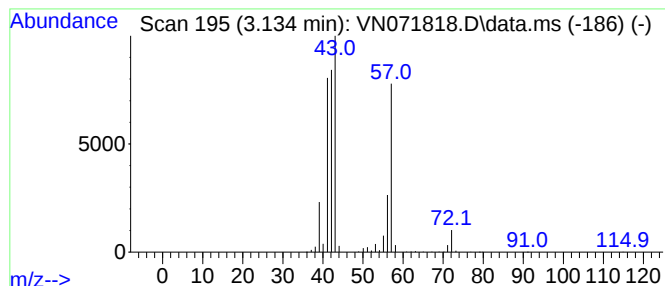
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Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	26.67 ug/l	1421000	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	43
3			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10
4			1-Butene	56	C4H8	000106-98-9	10
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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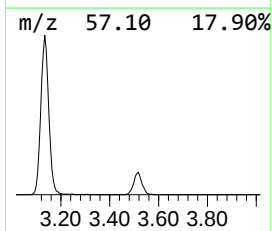
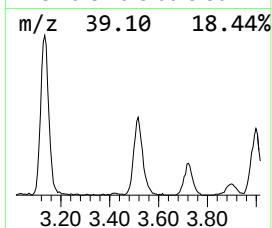
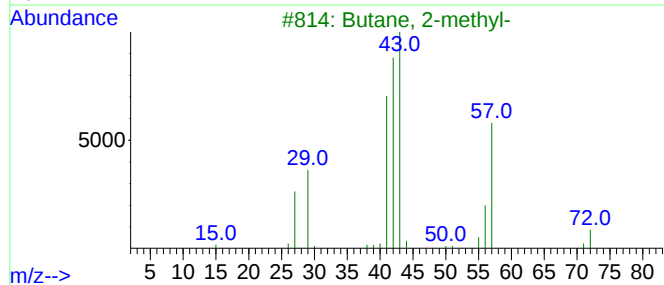
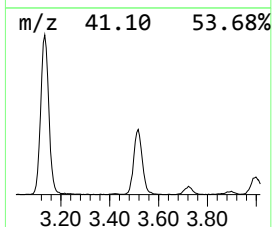
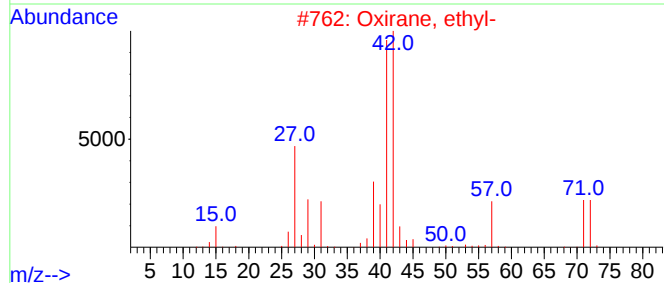
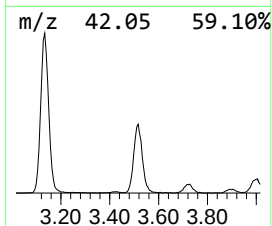
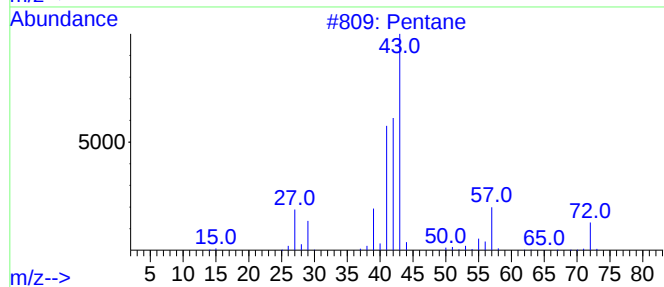
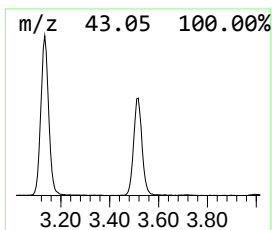
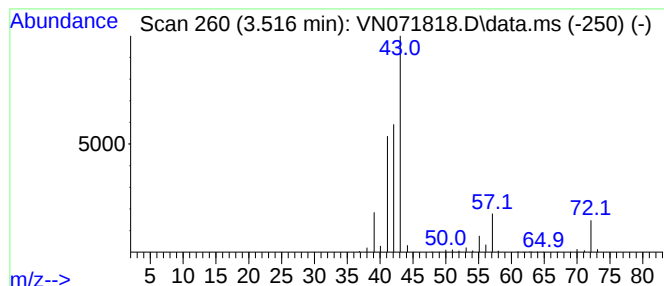
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	11.73 ug/l	625300	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	87
2	Oxirane, ethyl-			72	C4H8O	000106-88-7	50
3	Butane, 2-methyl-			72	C5H12	000078-78-4	38
4	Diaziridine,3,3-dimethyl-			72	C3H8N2	004901-76-2	32
5	Butanal, 2-ethyl-			100	C6H12O	000097-96-1	10



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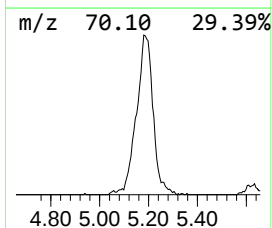
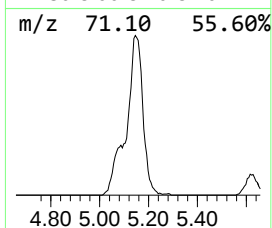
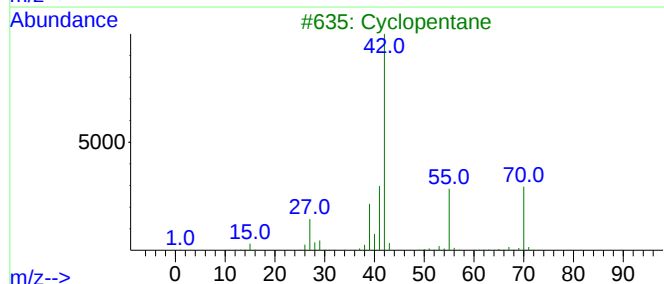
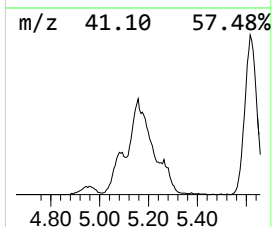
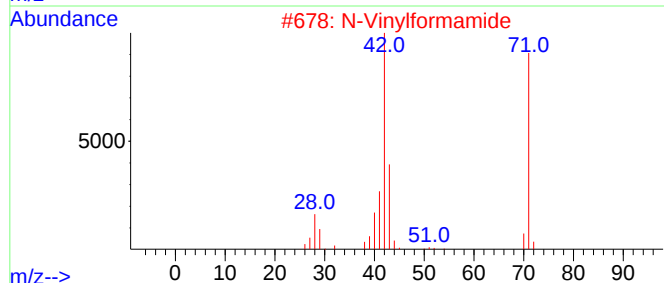
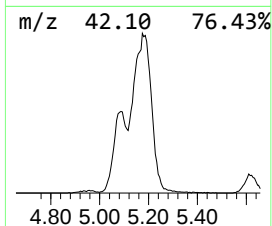
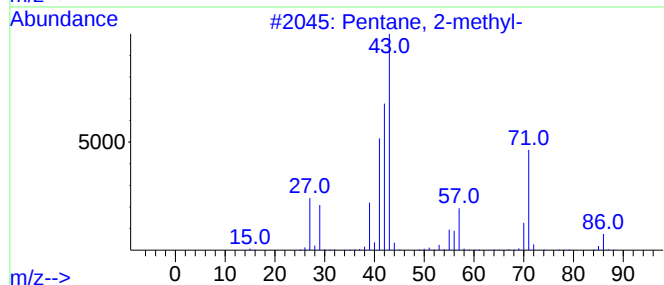
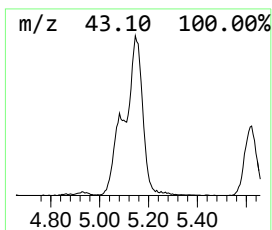
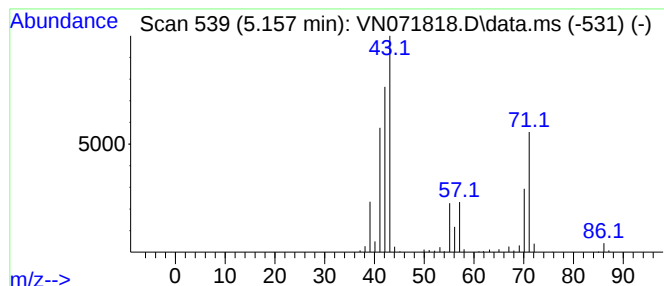
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	29.85 ug/l	1590630	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	86
2			N-Vinylformamide	71	C3H5NO	013162-05-5	50
3			Cyclopentane	70	C5H10	000287-92-3	43
4			Butane, 2-methyl-	72	C5H12	000078-78-4	40
5			Pentane	72	C5H12	000109-66-0	38



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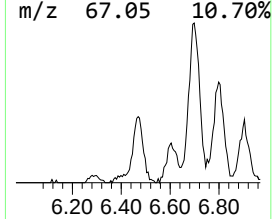
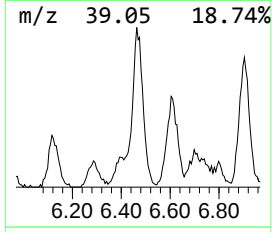
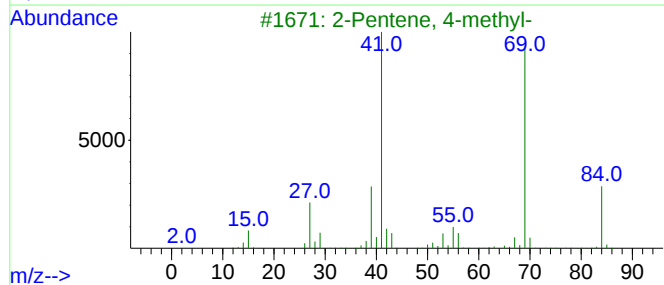
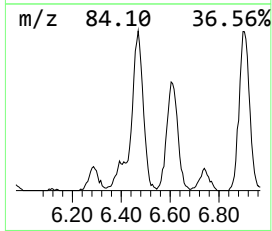
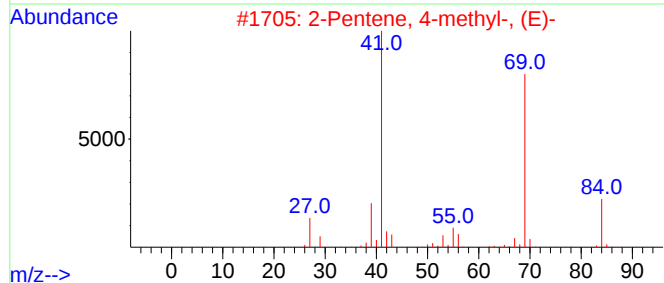
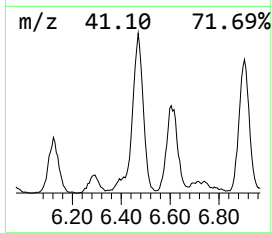
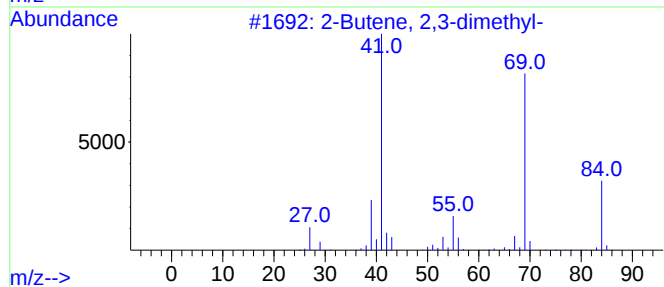
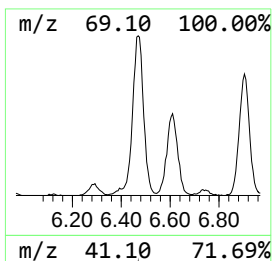
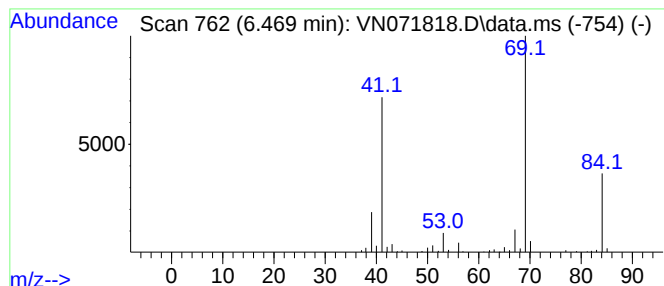
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 5 2-Butene, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.469	10.04 ug/l	534918	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	90
2			2-Pentene, 4-methyl-, (E)-	84	C6H12	000674-76-0	86
3			2-Pentene, 4-methyl-	84	C6H12	004461-48-7	86
4			2-Pentene, 2-methyl-	84	C6H12	000625-27-4	78
5			2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

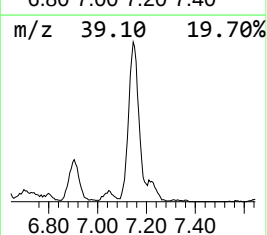
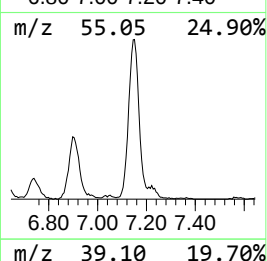
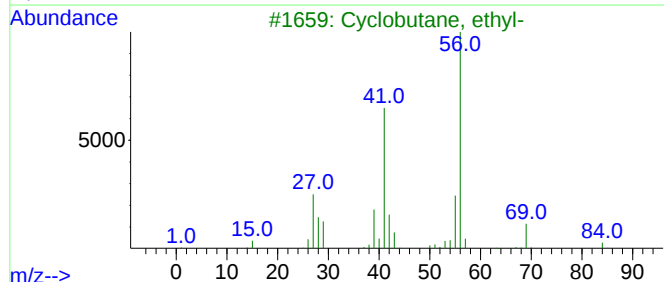
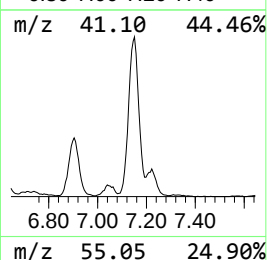
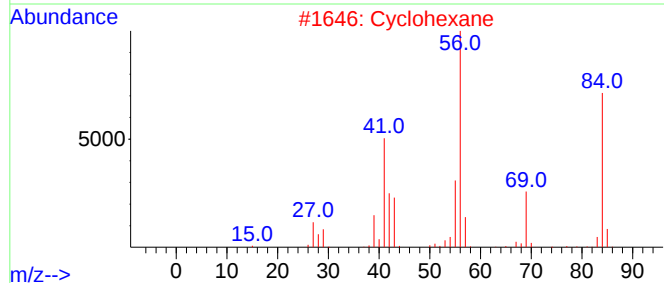
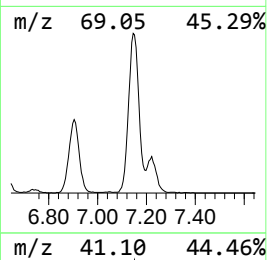
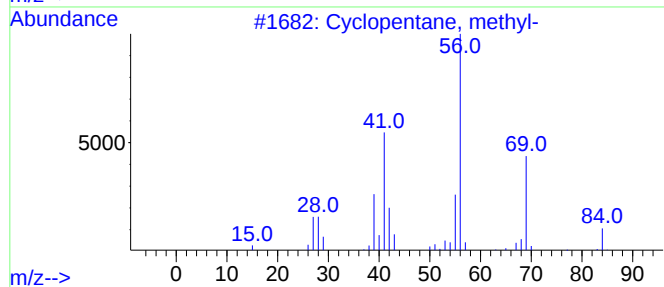
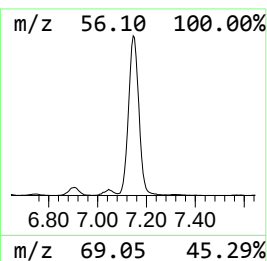
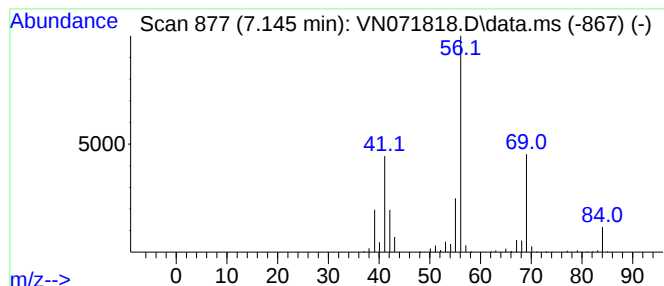
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	34.33 ug/l	1829260	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	83
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

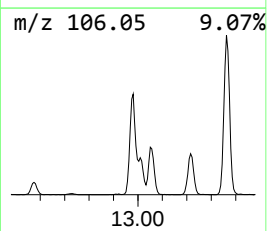
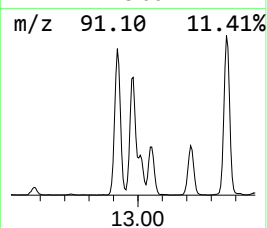
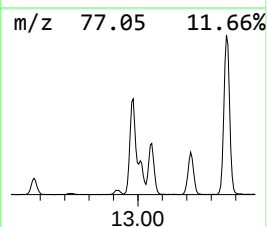
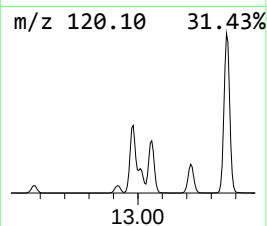
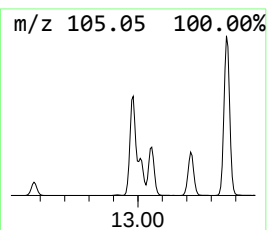
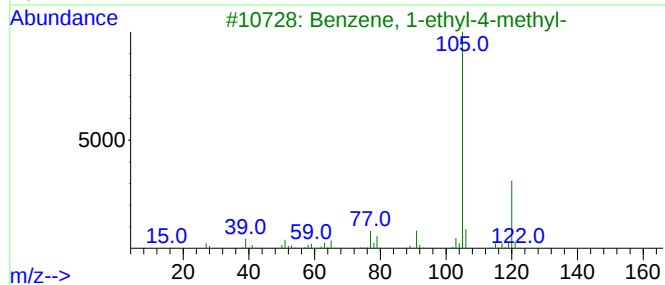
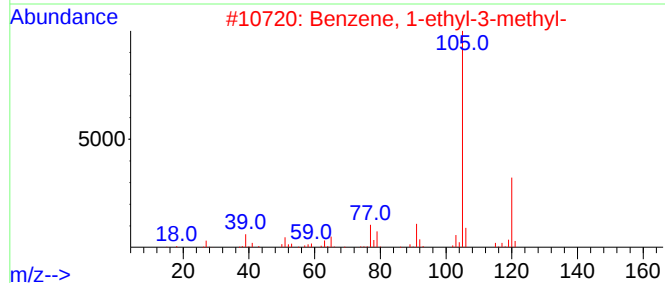
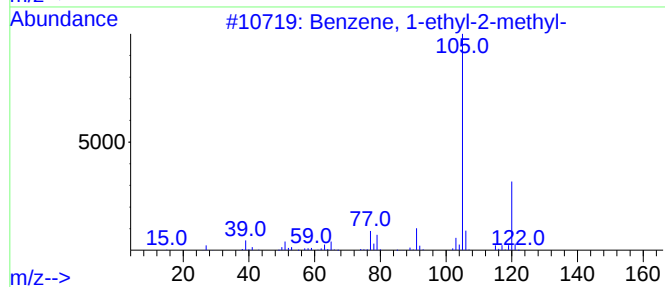
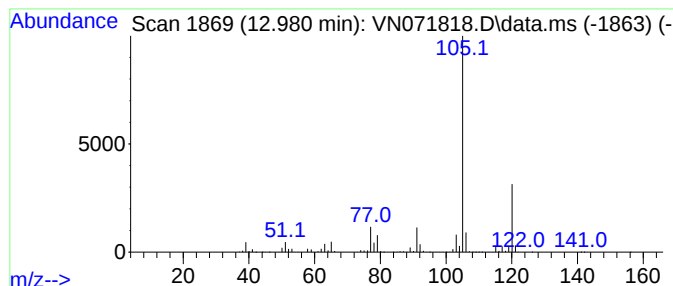
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	83.93 ug/l	5383330	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
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\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

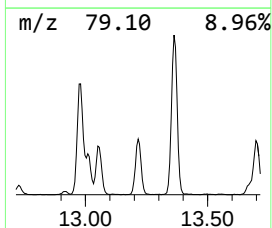
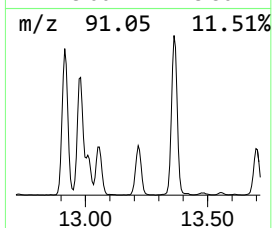
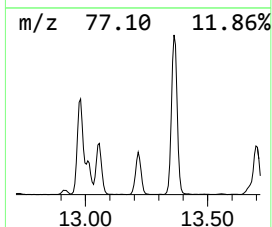
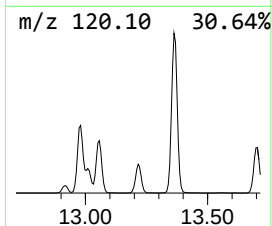
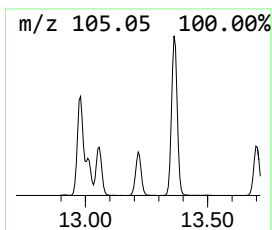
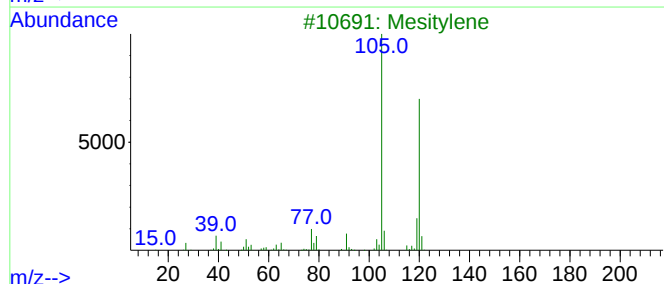
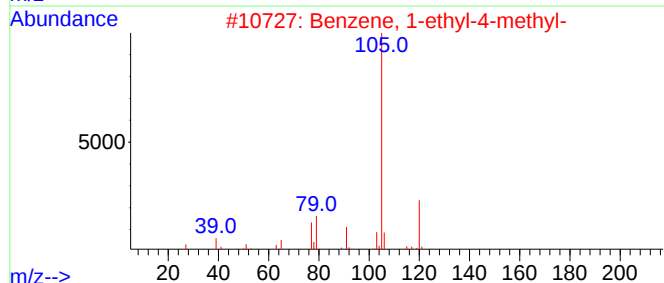
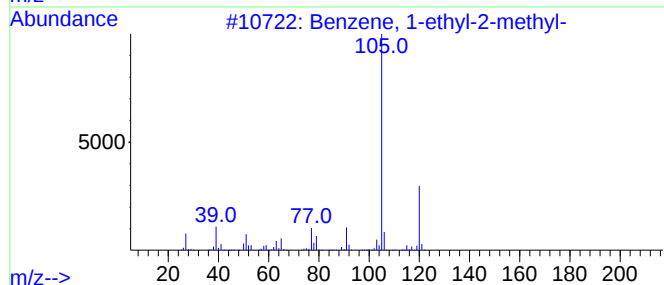
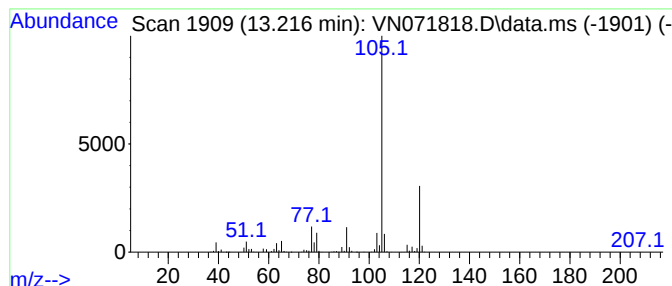
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	34.09 ug/l	2186640	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

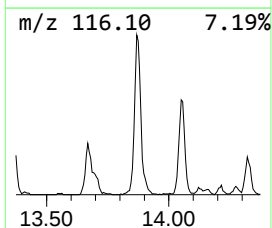
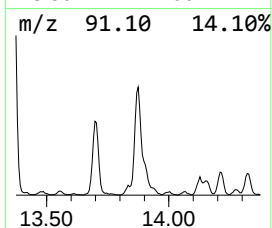
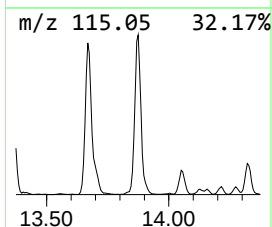
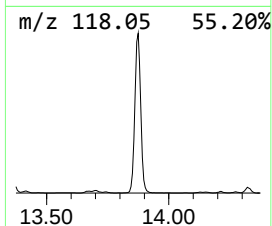
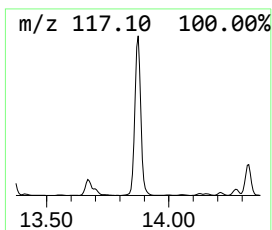
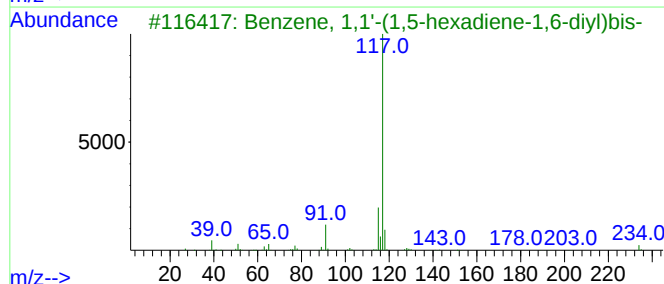
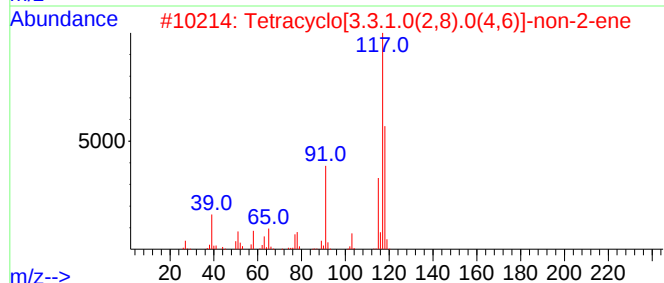
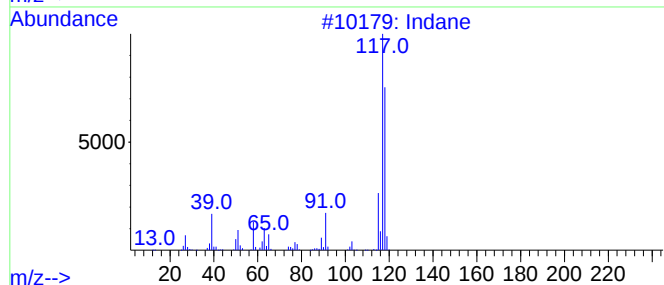
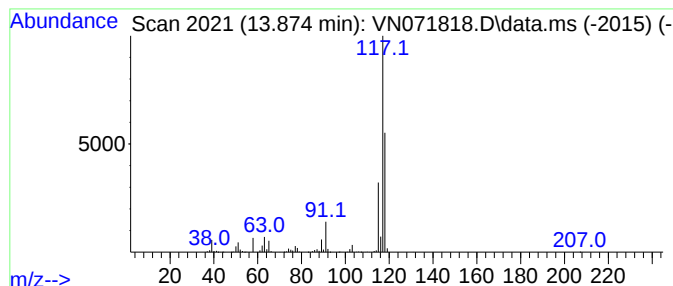
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	56.28 ug/l	3609660	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
3			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
4			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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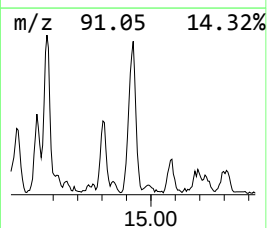
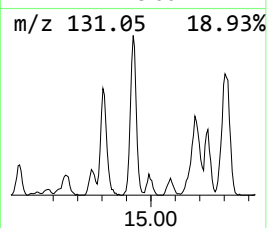
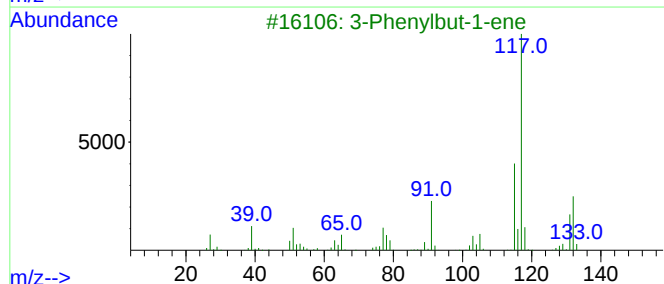
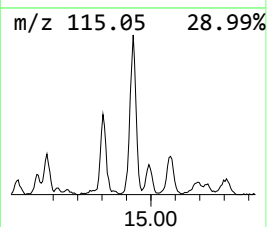
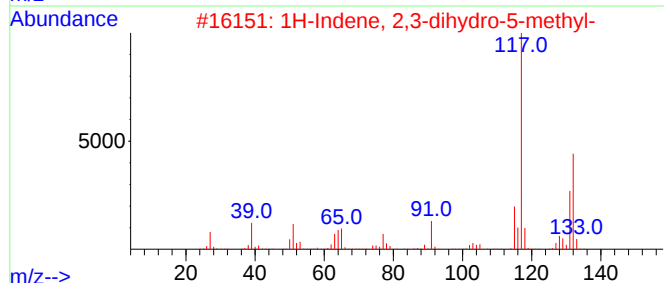
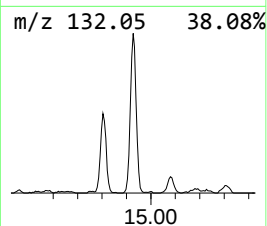
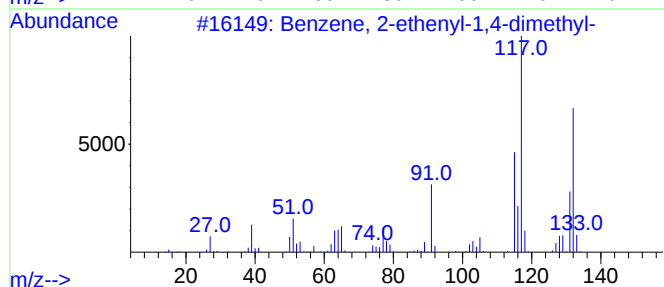
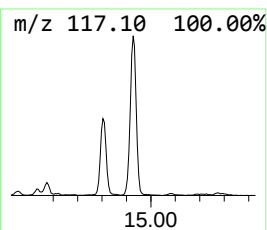
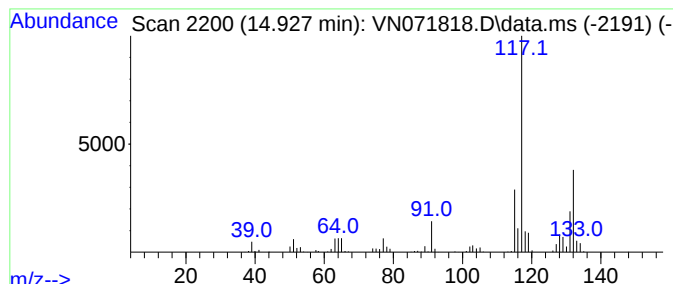
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	14.18 ug/l	909571	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071818.D
Acq On : 02 Apr 2022 23:23
Operator : JC\MD
Sample : N2242-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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
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Butane, 2-methyl-	3.134	26.7	ug/l	1421000	1	8.086	2664370	50.0
Pentane	3.516	11.7	ug/l	625300	1	8.086	2664370	50.0
Pentane, 2-methyl-	5.157	29.9	ug/l	1590630	1	8.086	2664370	50.0
2-Butene, 2,3-d...	6.469	10.0	ug/l	534918	1	8.086	2664370	50.0
Cyclopentane, m...	7.145	34.3	ug/l	1829260	1	8.086	2664370	50.0
Benzene, 1-ethy...	12.980	83.9	ug/l	5383330	4	13.668	3207060	50.0
Benzene, 1-ethy...	13.216	34.1	ug/l	2186640	4	13.668	3207060	50.0
Indane	13.874	56.3	ug/l	3609660	4	13.668	3207060	50.0
Benzene, 2-ethe...	14.927	14.2	ug/l	909571	4	13.668	3207060	50.0