

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
 Data File : VN073710.D
 Acq On : 03 Aug 2022 14:35
 Operator : JC\MD
 Sample : N3971-15
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-23R

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	48	58	63	rBV2	36635	66731	3.98%	0.504%
2	2.399	80	87	96	rBV	216733	340579	20.32%	2.573%
3	2.704	133	139	144	rBV6	12781	29984	1.79%	0.226%
4	3.087	194	204	214	rBV	275163	616119	36.76%	4.654%
5	3.457	257	267	277	rBV4	9636	24750	1.48%	0.187%
6	3.934	336	348	361	rVB4	20823	58103	3.47%	0.439%
7	4.228	391	398	414	rVB2	20265	64070	3.82%	0.484%
8	4.510	434	446	459	rBV	75596	243896	14.55%	1.842%
9	5.004	518	530	536	rBV4	15459	57357	3.42%	0.433%
10	5.104	536	547	568	rVB2	75483	288421	17.21%	2.179%
11	5.534	610	620	633	rBV3	17180	61183	3.65%	0.462%
12	6.516	778	787	798	rBV6	14761	47721	2.85%	0.360%
13	7.069	868	881	889	rBV3	44793	138299	8.25%	1.045%
14	7.139	889	893	903	rVB5	15604	38915	2.32%	0.294%
15	7.239	903	910	914	rBV2	7378	18147	1.08%	0.137%
16	7.339	920	927	939	rVB	33495	82856	4.94%	0.626%
17	7.769	993	1000	1009	rVB8	7251	17585	1.05%	0.133%
18	7.951	1021	1031	1036	rBV	259465	619282	36.95%	4.678%
19	8.016	1036	1042	1056	rVB2	521493	1231839	73.51%	9.305%
20	8.375	1092	1103	1115	rBV2	282128	712068	42.49%	5.379%
21	8.522	1123	1128	1133	rVV3	10102	20557	1.23%	0.155%
22	8.904	1184	1193	1213	rBV	636879	1311362	78.25%	9.905%
23	9.910	1358	1364	1370	rBV3	12934	23671	1.41%	0.179%
24	10.139	1397	1403	1408	rBV	16312	29201	1.74%	0.221%
25	10.263	1418	1424	1430	rBV5	10092	18496	1.10%	0.140%
26	10.380	1436	1444	1452	rBV	928365	1675837	100.00%	12.658%
27	10.445	1452	1455	1460	rVV2	18935	35567	2.12%	0.269%
28	10.492	1460	1463	1469	rVV3	11418	19824	1.18%	0.150%
29	10.580	1469	1478	1485	rVB7	8825	20327	1.21%	0.154%
30	11.233	1581	1589	1601	rBV2	56259	108639	6.48%	0.821%
31	11.686	1656	1666	1677	rBV	918274	1618058	96.55%	12.222%
32	11.786	1677	1683	1691	rVV2	81854	145424	8.68%	1.098%
33	11.892	1694	1701	1712	rVB2	25578	54753	3.27%	0.414%
34	12.516	1797	1807	1814	rBV2	53019	95025	5.67%	0.718%
35	12.674	1826	1834	1843	rBV	764893	1274185	76.03%	9.624%
36	12.863	1860	1866	1873	rVB	42797	65730	3.92%	0.496%

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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\82N072822W.M
Title : SW846 8260

37	13.616	1986	1994	2005	rBV	904768	1551381	92.57%	11.718%
38	13.710	2005	2010	2017	rVB2	44445	78147	4.66%	0.590%
39	13.815	2023	2028	2034	rVB	157970	253968	15.15%	1.918%
40	14.268	2099	2105	2111	rBV3	21196	35670	2.13%	0.269%
41	14.474	2133	2140	2151	rVB6	9573	20442	1.22%	0.154%
42	15.433	2297	2303	2310	rVB2	13052	24933	1.49%	0.188%

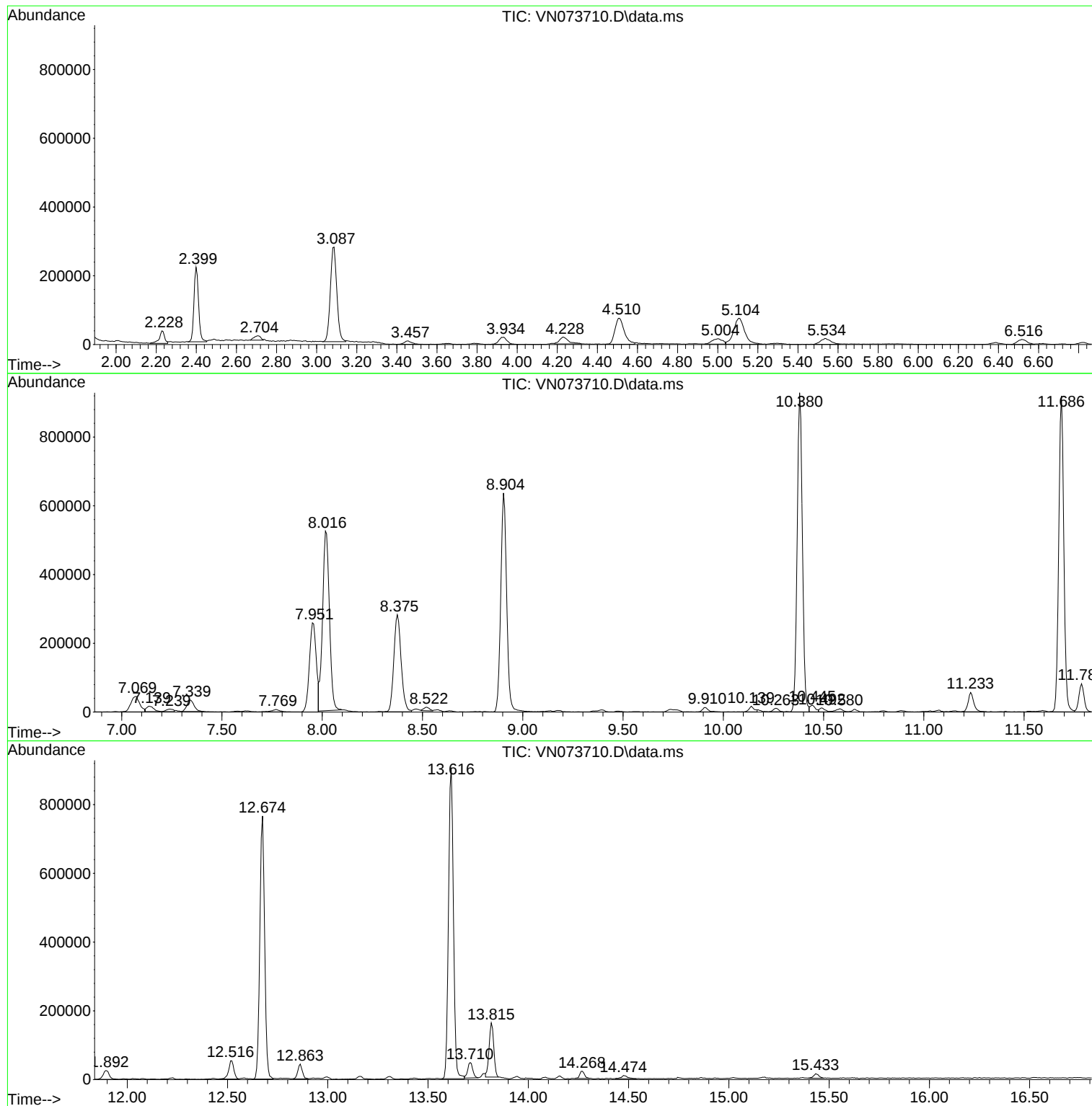
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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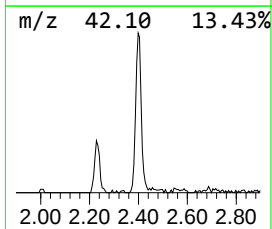
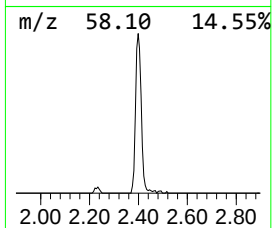
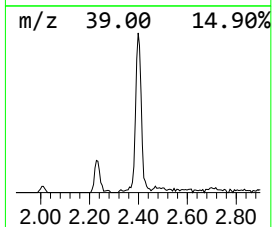
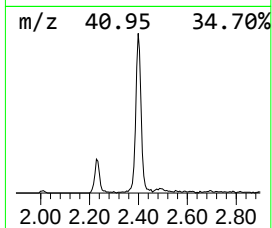
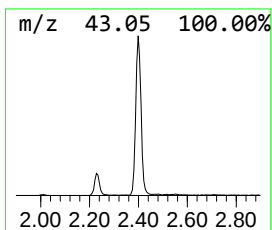
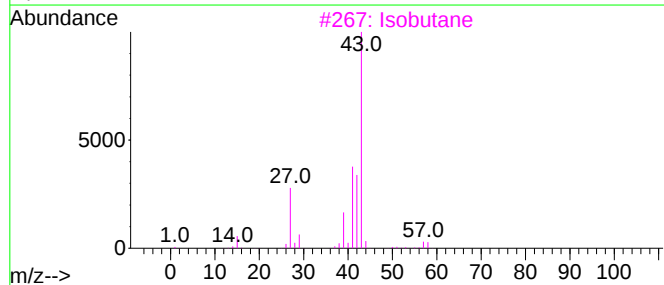
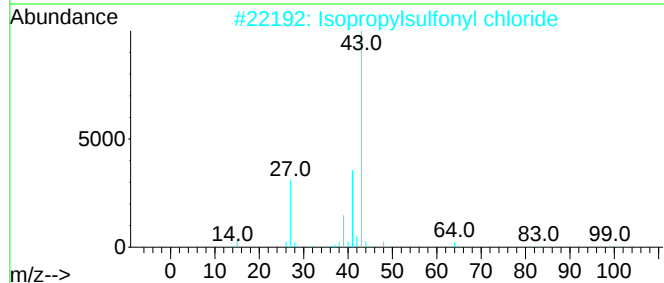
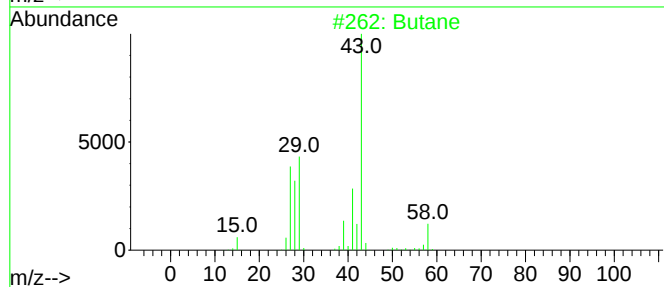
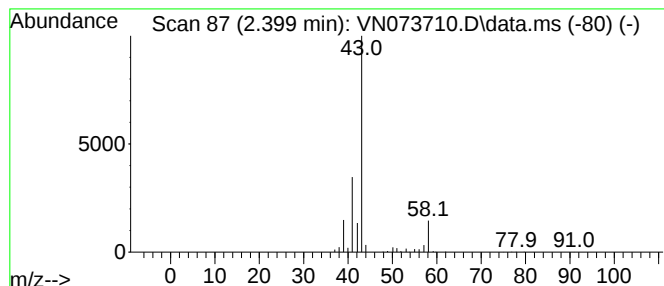
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	13.82 ug/l	340579	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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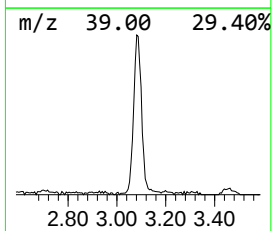
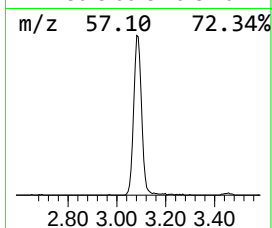
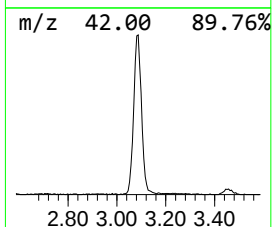
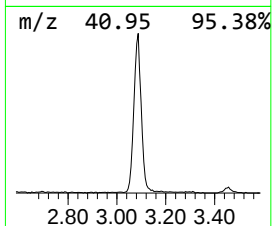
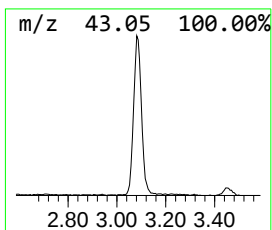
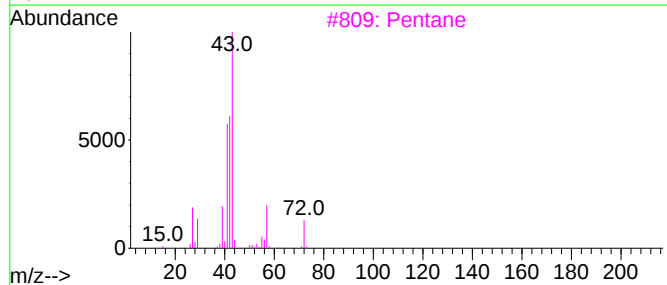
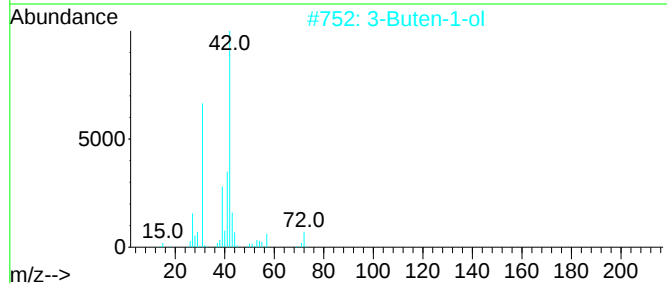
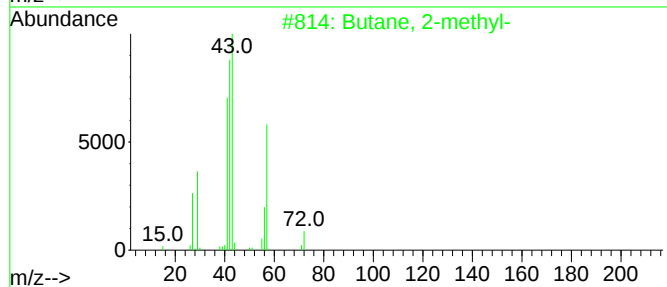
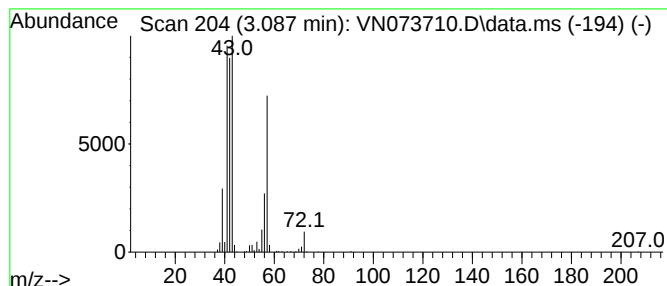
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	25.01 ug/l	616119	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	50
3			Pentane	72	C5H12	000109-66-0	33
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	16



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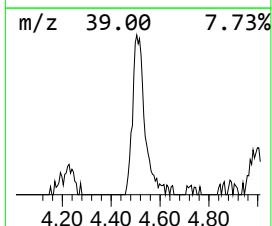
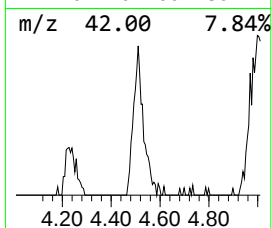
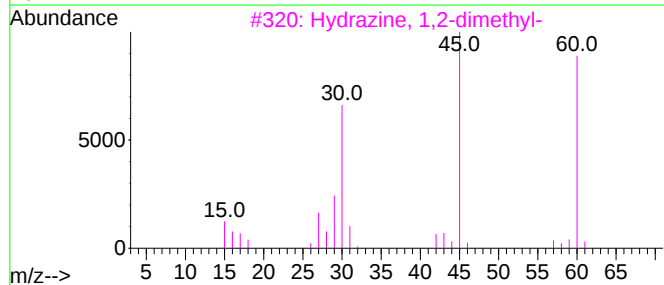
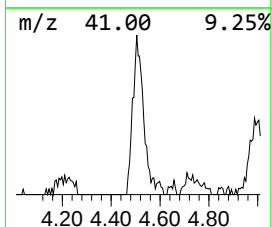
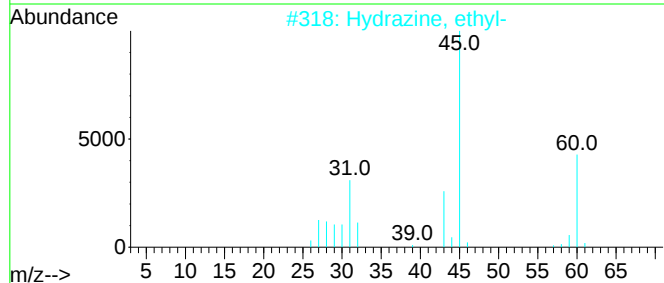
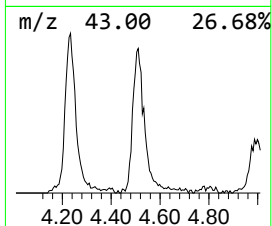
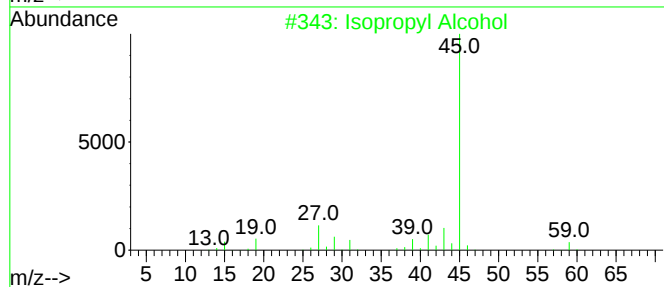
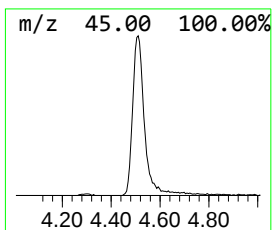
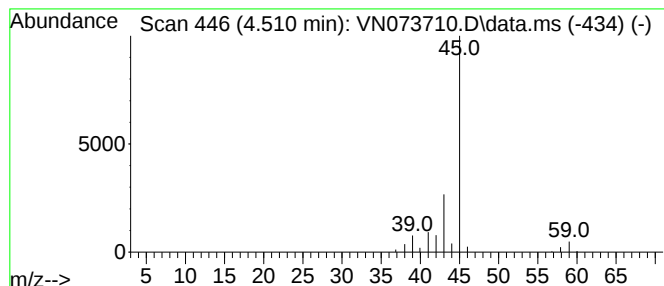
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	9.90 ug/l	243896	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			4-Penten-2-ol	86	C5H10O	000625-31-0	9
5			Formamide	45	CH3NO	000075-12-7	4



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23R

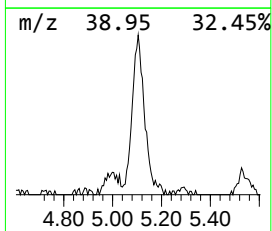
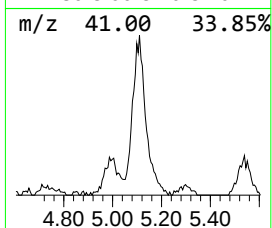
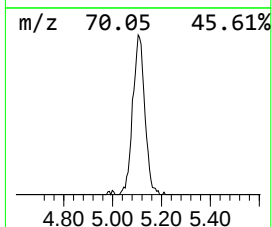
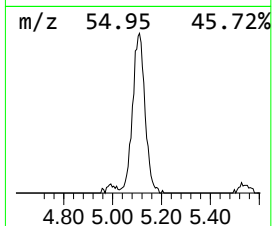
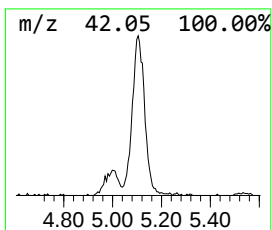
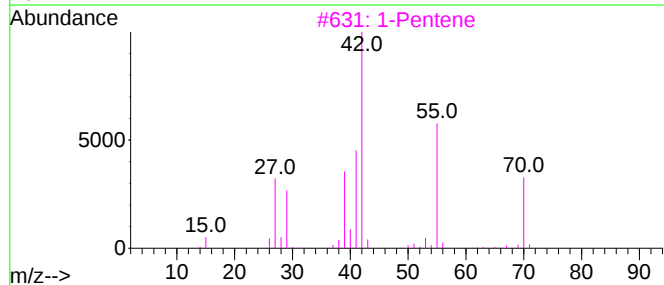
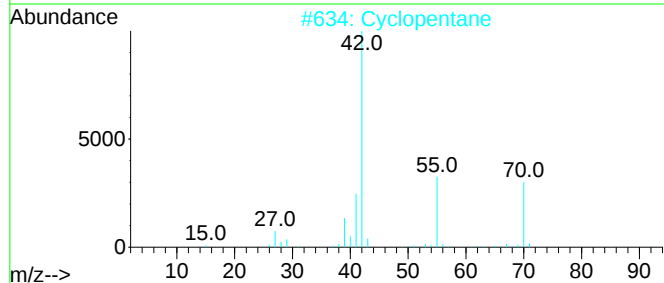
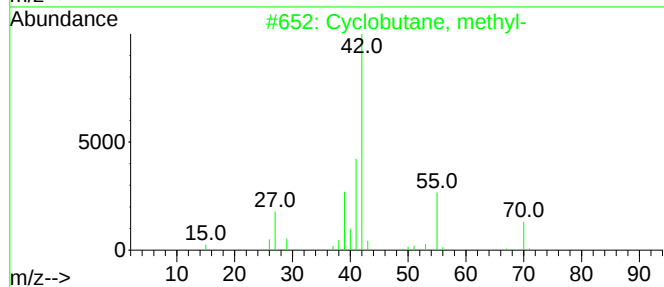
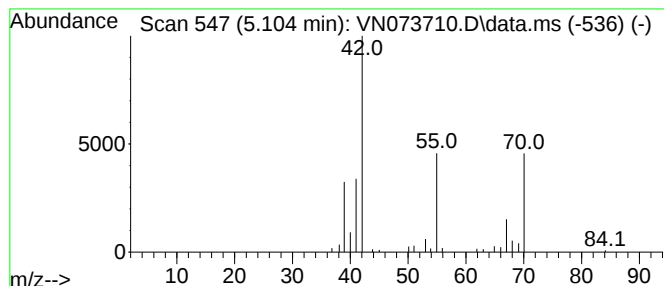
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclobutane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	11.71 ug/l	288421	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			Cyclopentane	70	C5H10	000287-92-3	72
3			1-Pentene	70	C5H10	000109-67-1	59
4			3-Buten-1-ol	72	C4H8O	000627-27-0	9
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	9



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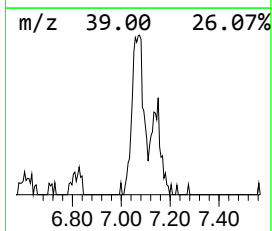
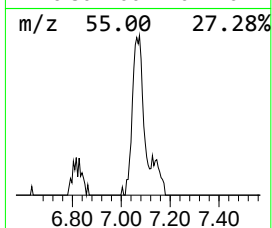
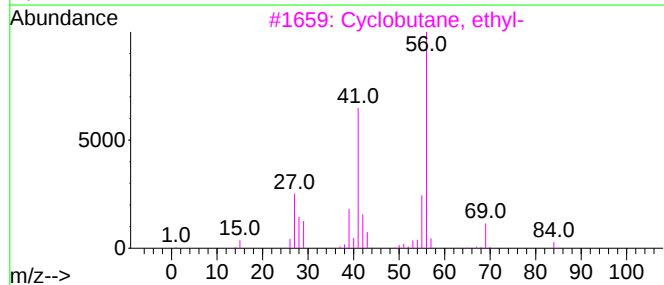
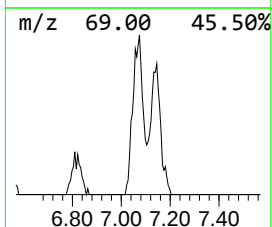
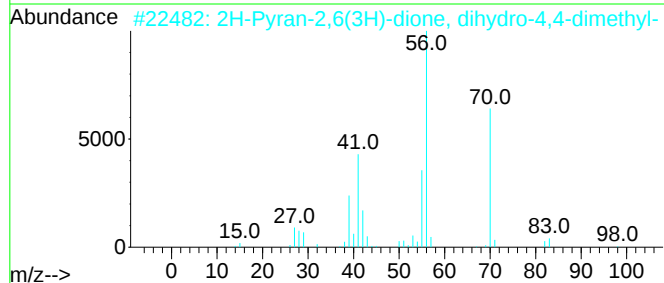
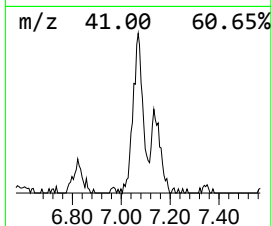
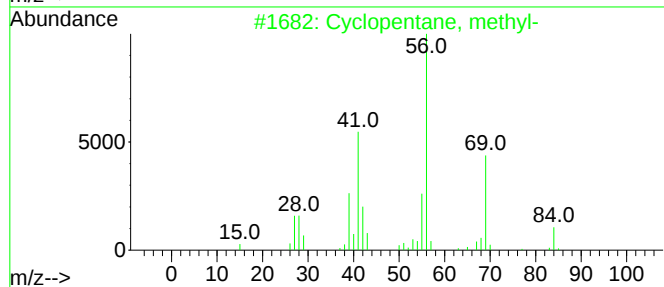
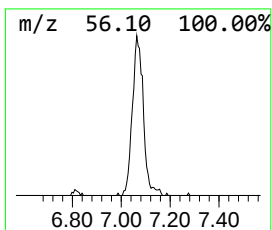
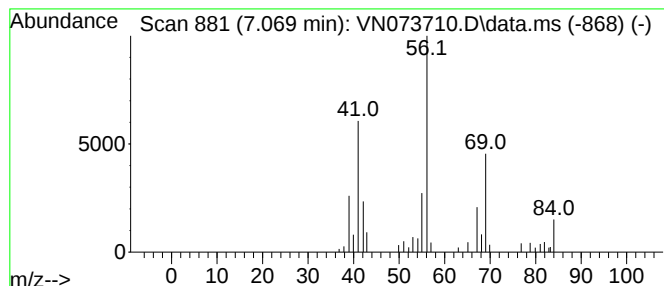
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	5.61 ug/l	138299	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	76
2			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
4			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	38
5			Cyclobutane	56	C4H8	000287-23-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073710.D
Acq On : 03 Aug 2022 14:35
Operator : JC\MD
Sample : N3971-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23R

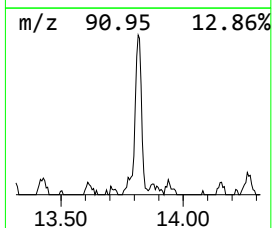
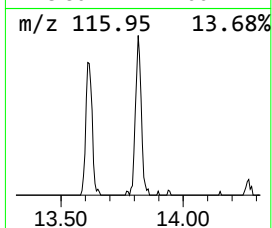
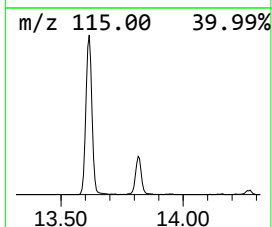
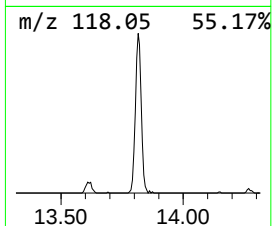
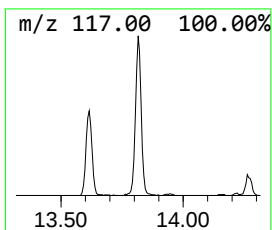
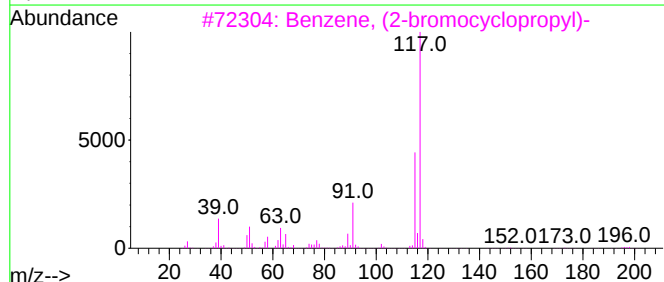
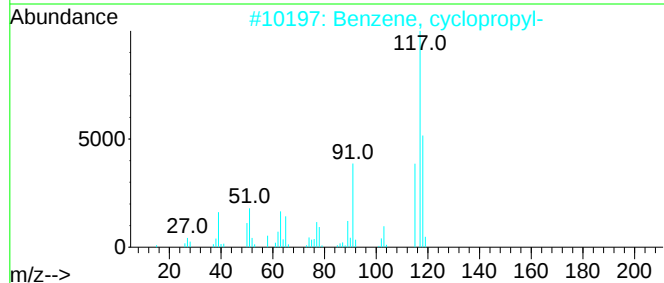
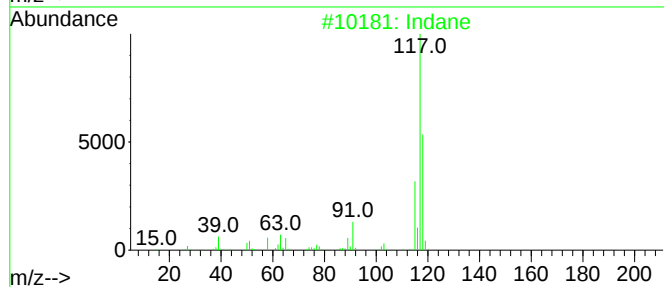
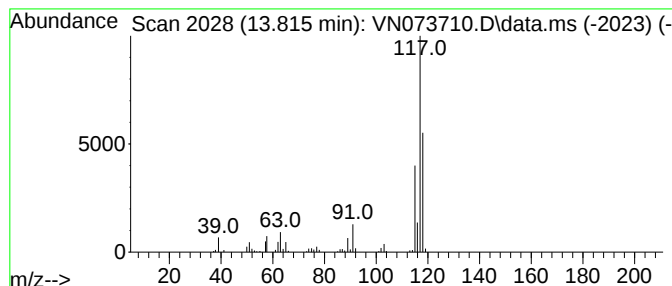
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	8.19 ug/l	253968	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	89
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	62
3			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073710.D
Acq On : 03 Aug 2022 14:35
Operator : JC\MD
Sample : N3971-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Butane	2.399	13.8	ug/l	340579	1	8.016	1231840	50.0
Butane, 2-methyl-	3.087	25.0	ug/l	616119	1	8.016	1231840	50.0
Isopropyl Alcohol	4.510	9.9	ug/l	243896	1	8.016	1231840	50.0
Cyclobutane, me...	5.104	11.7	ug/l	288421	1	8.016	1231840	50.0
Cyclopentane, m...	7.069	5.6	ug/l	138299	1	8.016	1231840	50.0
Indane	13.816	8.2	ug/l	253968	4	13.616	1551380	50.0