

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073689.D
 Acq On : 02 Aug 2022 16:01
 Operator : JC\MD
 Sample : N3971-15
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 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: VN073689.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	54	58	63	rVB	35921	50242	2.99%	0.378%
2	2.399	76	87	94	rBV	232916	372249	22.12%	2.800%
3	2.704	132	139	149	rVB4	21905	72758	4.32%	0.547%
4	3.081	194	203	217	rVB	284881	641749	38.14%	4.827%
5	3.451	259	266	277	rVB6	10371	27792	1.65%	0.209%
6	3.922	337	346	359	rBV2	23149	60883	3.62%	0.458%
7	4.228	390	398	408	rBV2	17727	48780	2.90%	0.367%
8	4.510	435	446	459	rBV2	75964	234503	13.94%	1.764%
9	4.998	516	529	535	rBV6	15571	57851	3.44%	0.435%
10	5.110	537	548	568	rVB3	76521	289326	17.19%	2.176%
11	5.534	608	620	634	rBV4	17660	63374	3.77%	0.477%
12	6.516	776	787	799	rBV7	14739	50645	3.01%	0.381%
13	7.069	869	881	889	rBV3	43716	137640	8.18%	1.035%
14	7.139	889	893	902	rVB4	17550	41401	2.46%	0.311%
15	7.339	920	927	940	rVB2	36367	89361	5.31%	0.672%
16	7.951	1022	1031	1036	rBV	260165	623096	37.03%	4.686%
17	8.022	1036	1043	1054	rVV2	525771	1259220	74.84%	9.471%
18	8.375	1092	1103	1114	rBV2	276290	726435	43.17%	5.464%
19	8.522	1123	1128	1133	rVV2	10022	21736	1.29%	0.163%
20	8.904	1184	1193	1210	rBV	634355	1304999	77.56%	9.815%
21	9.910	1357	1364	1371	rBV3	13164	25952	1.54%	0.195%
22	10.139	1397	1403	1409	rBV2	14663	30907	1.84%	0.232%
23	10.263	1418	1424	1430	rBV4	11861	20614	1.23%	0.155%
24	10.380	1436	1444	1452	rBV	917753	1682650	100.00%	12.655%
25	10.439	1453	1454	1459	rVV3	18475	28172	1.67%	0.212%
26	10.492	1459	1463	1470	rVV5	10889	22218	1.32%	0.167%
27	10.580	1470	1478	1484	rVV6	8540	20855	1.24%	0.157%
28	11.233	1581	1589	1600	rBV	59218	111284	6.61%	0.837%
29	11.686	1657	1666	1677	rBV	903838	1591415	94.58%	11.969%
30	11.786	1677	1683	1690	rVV	81776	147793	8.78%	1.112%
31	11.898	1693	1702	1713	rVB3	19864	41570	2.47%	0.313%
32	12.521	1800	1808	1814	rBV	56434	98374	5.85%	0.740%
33	12.674	1826	1834	1846	rBV	738645	1238656	73.61%	9.316%
34	12.863	1861	1866	1876	rVB	39397	64731	3.85%	0.487%
35	13.615	1986	1994	2004	rBV	884902	1464148	87.01%	11.012%
36	13.710	2006	2010	2016	rVV2	49352	82050	4.88%	0.617%

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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	13.780	2018	2022	2023	rVV	16182	20134	1.20%	0.151%
38	13.815	2023	2028	2036	rVB2	169160	275846	16.39%	2.075%
39	14.162	2081	2087	2093	rVB3	9539	17075	1.01%	0.128%
40	14.268	2099	2105	2113	rVB	23493	41090	2.44%	0.309%
41	14.480	2132	2141	2146	rBV4	11508	22055	1.31%	0.166%
42	15.433	2295	2303	2312	rVB	35004	74410	4.42%	0.560%

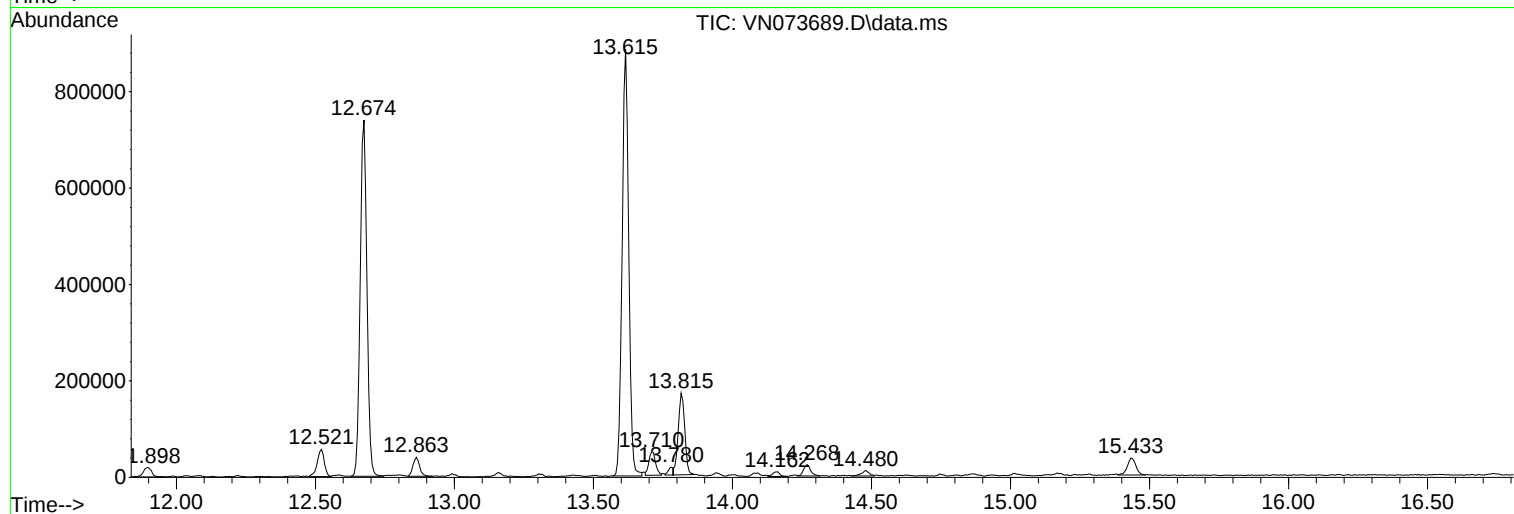
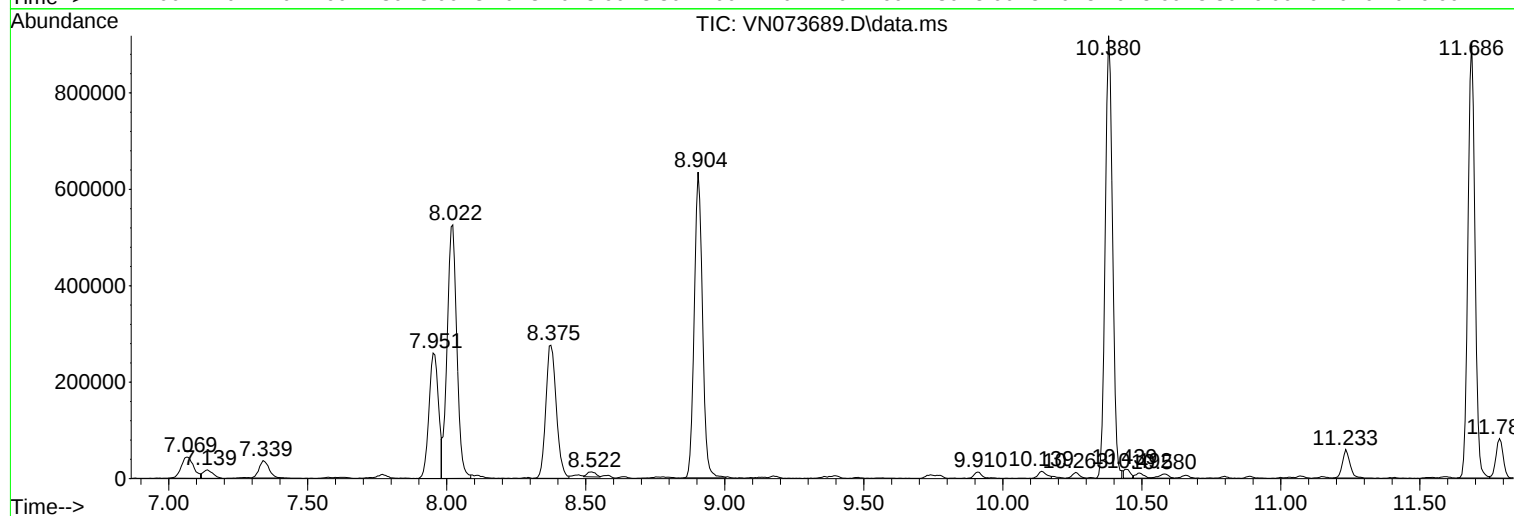
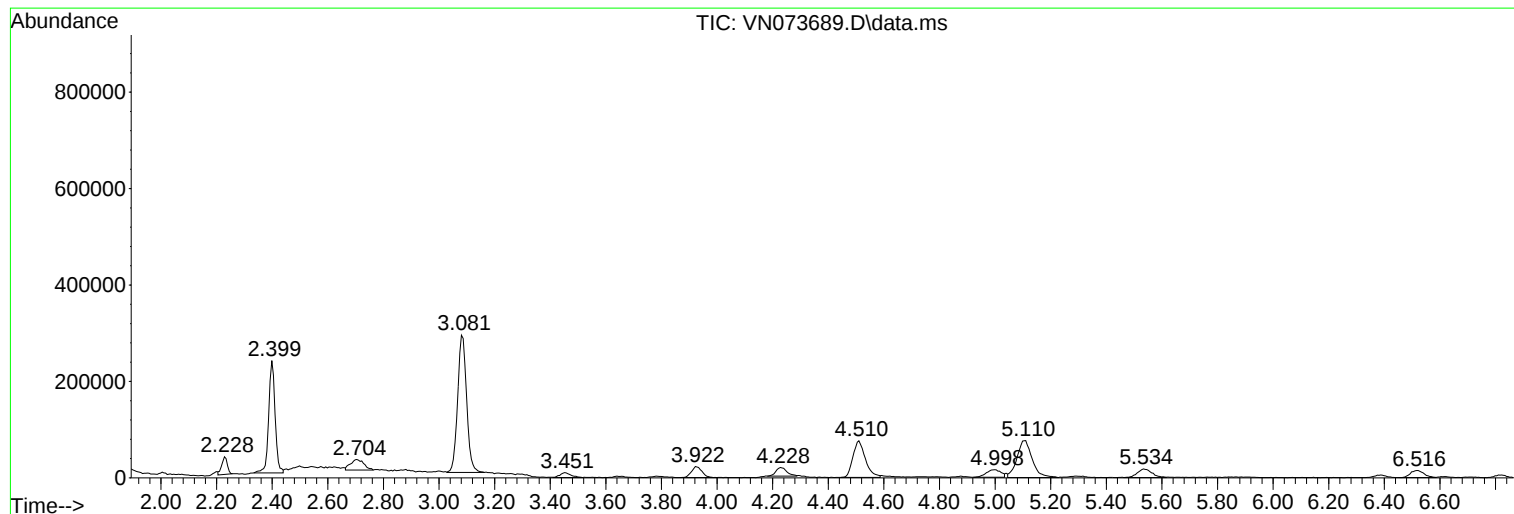
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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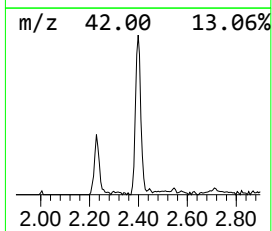
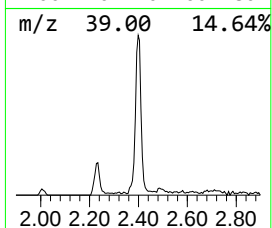
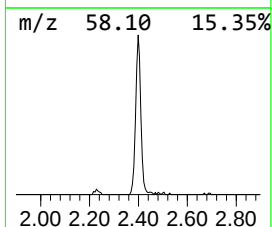
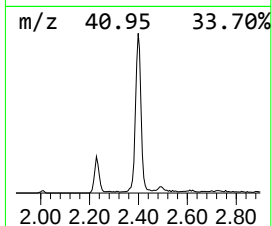
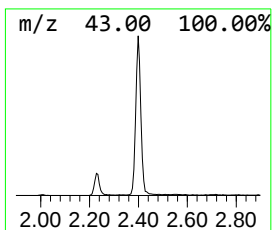
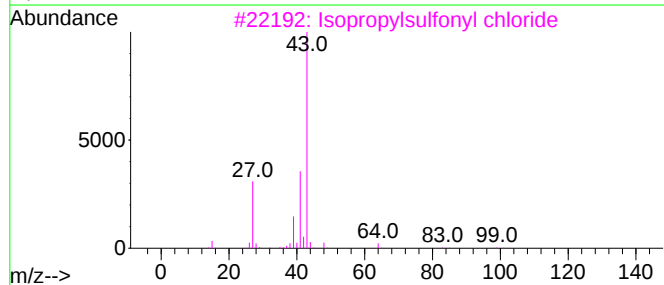
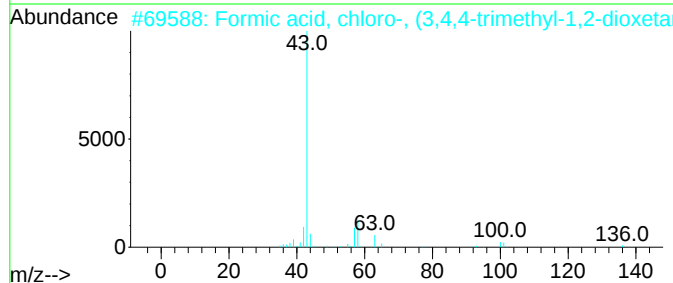
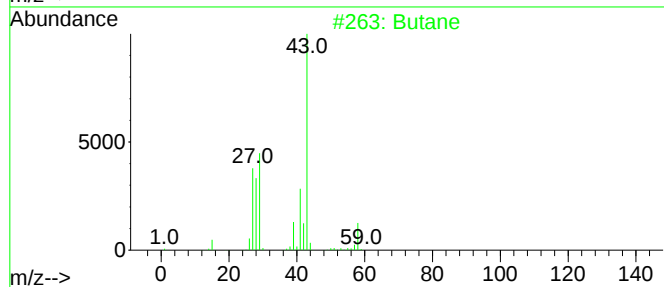
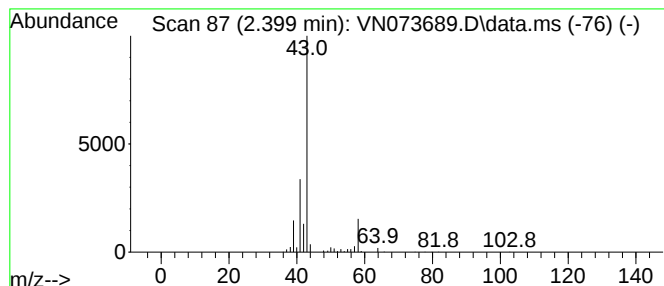
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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	14.78 ug/l	372249	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	38
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	25
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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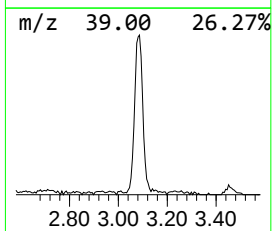
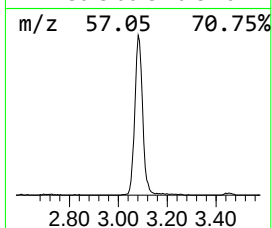
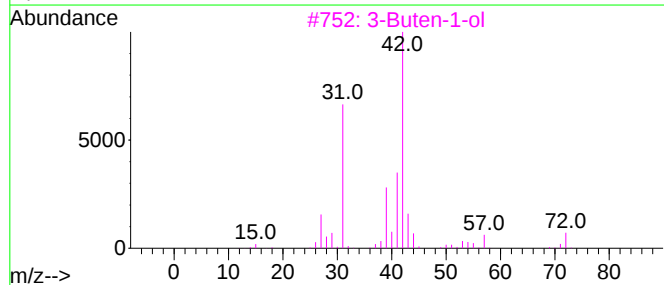
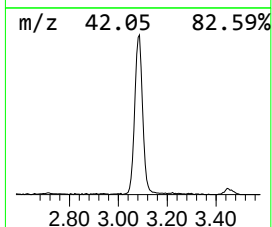
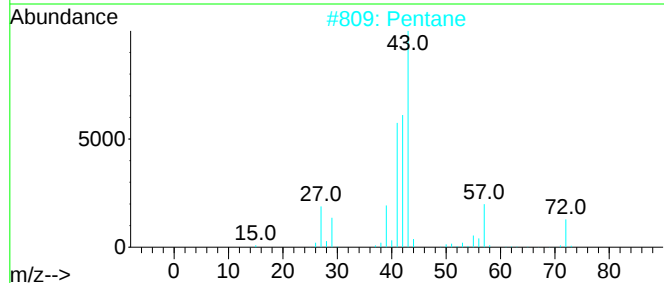
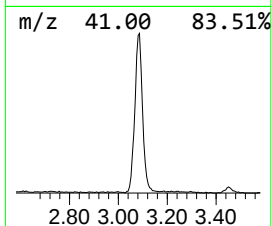
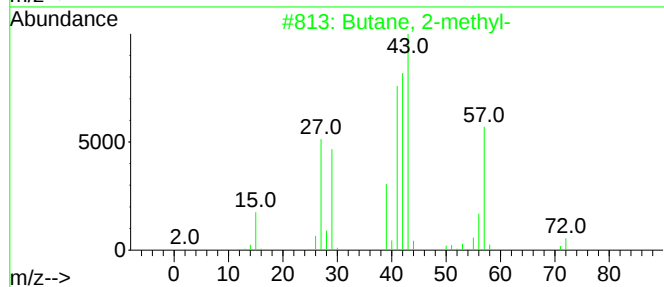
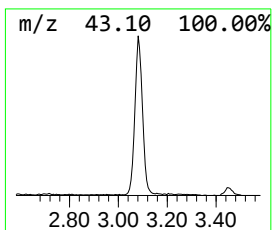
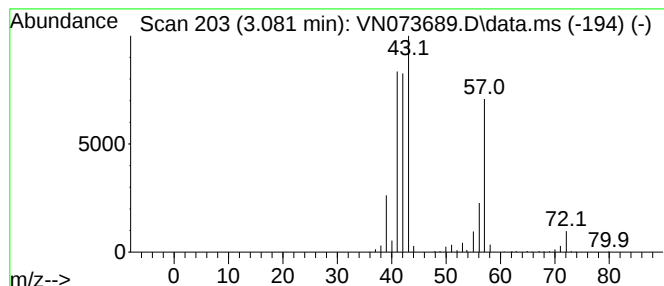
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	25.48 ug/l	641749	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	38
3			3-Buten-1-ol	72	C4H8O	000627-27-0	38
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5			Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	10



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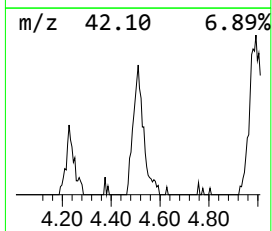
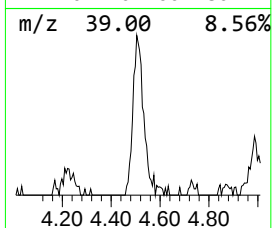
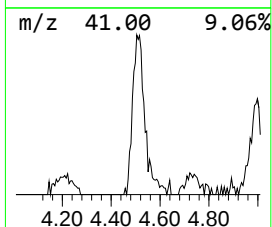
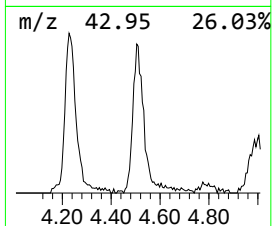
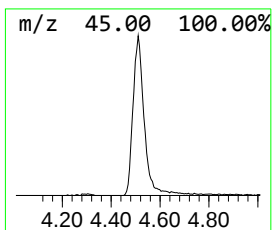
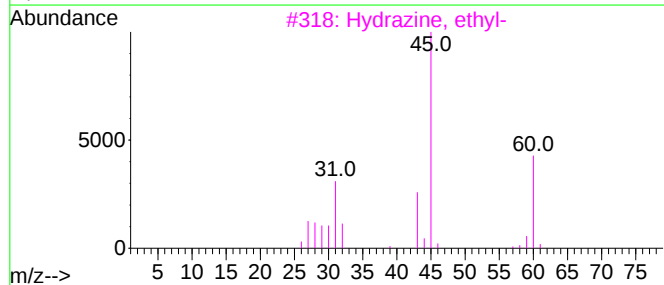
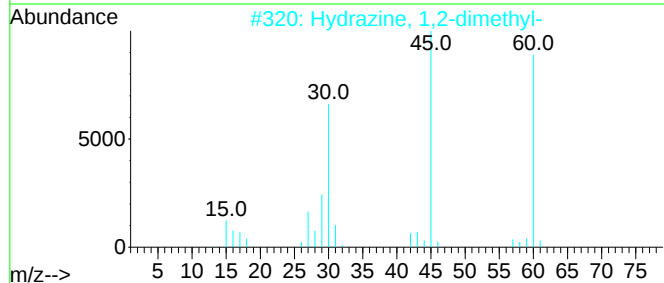
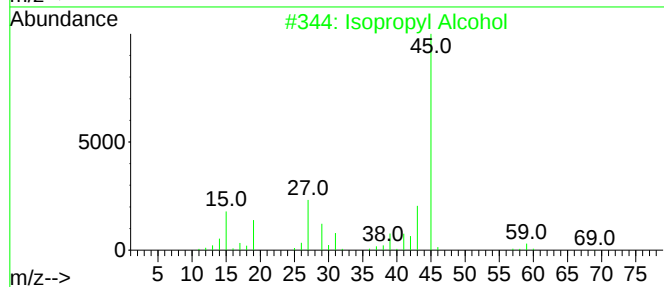
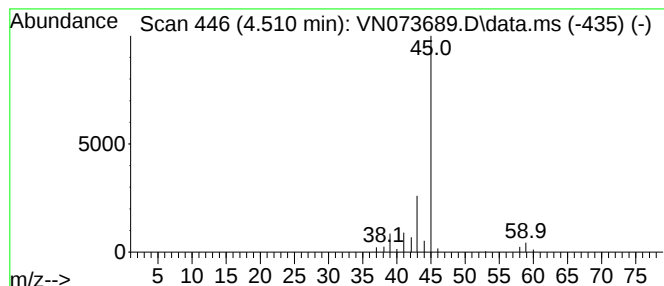
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	9.31 ug/l	234503	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
5			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



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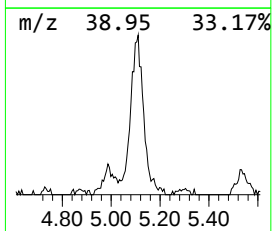
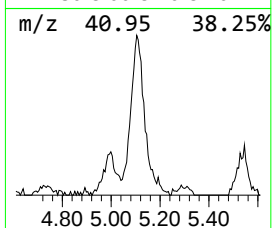
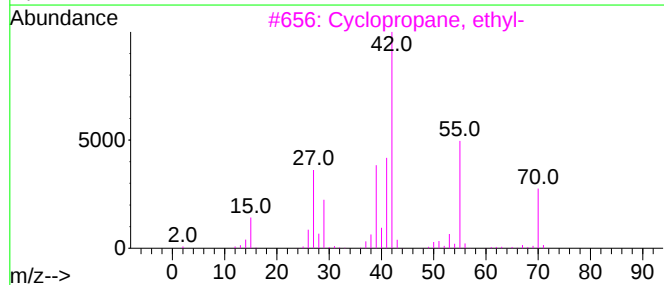
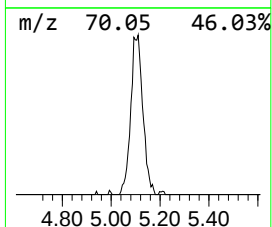
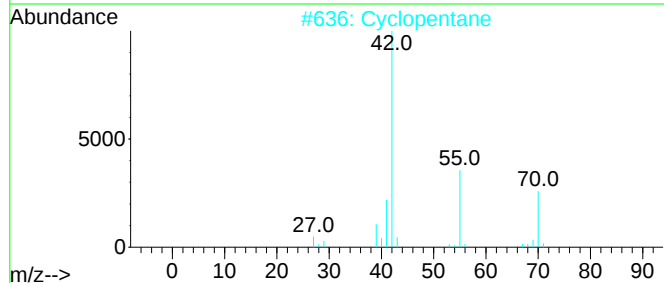
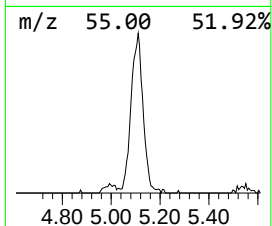
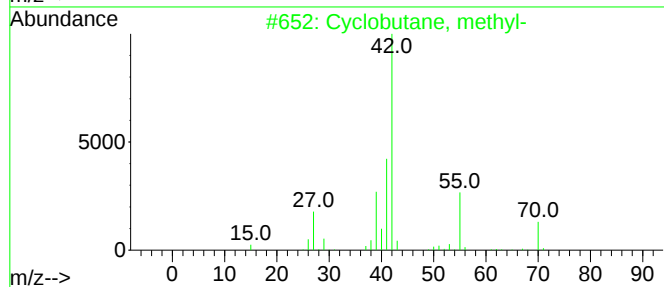
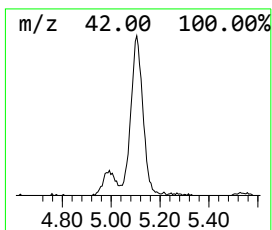
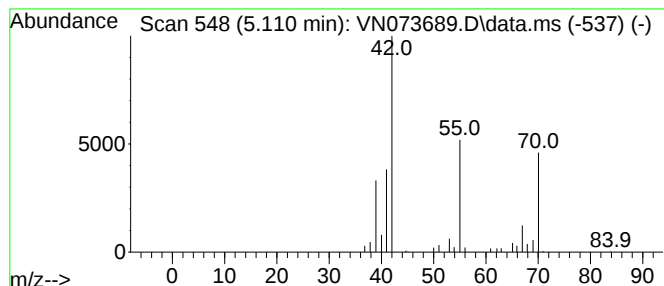
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclobutane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	11.49 ug/l	289326	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2		Cyclopentane	70	C5H10	000287-92-3	72
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
4		1-Pentene	70	C5H10	000109-67-1	59
5		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	43



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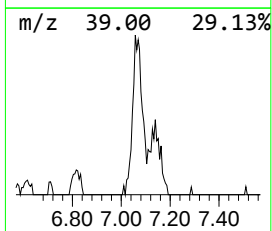
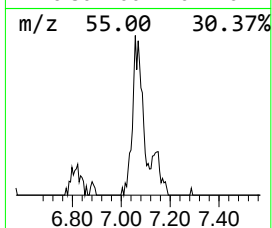
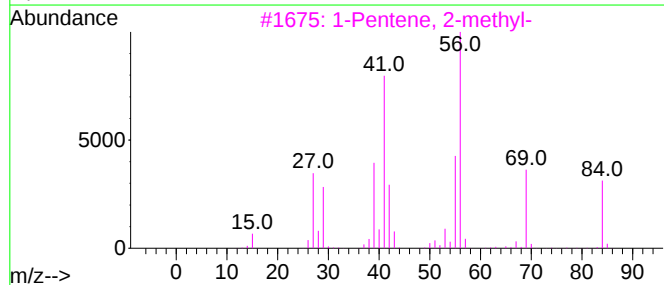
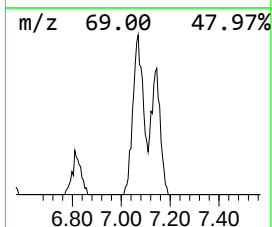
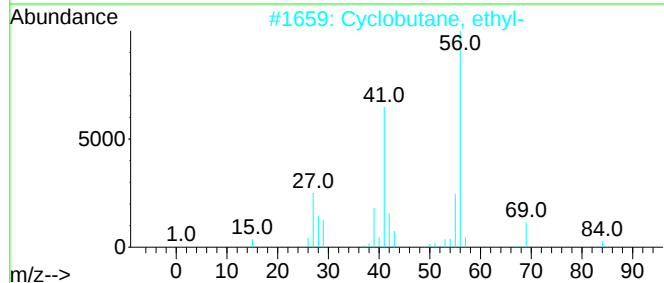
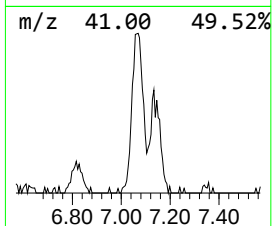
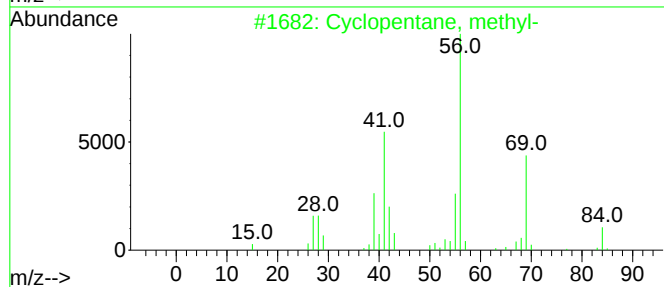
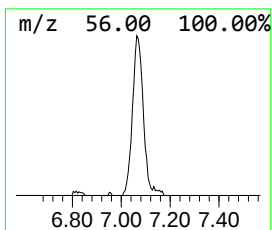
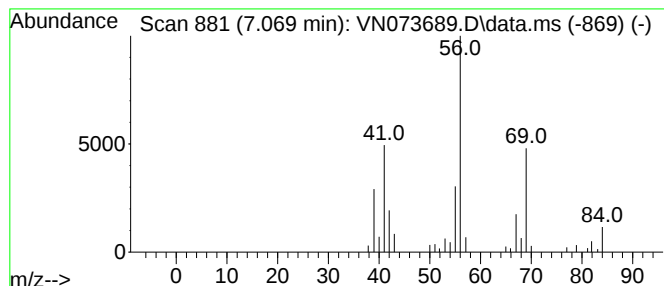
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	5.47 ug/l	137640	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	45
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073689.D
Acq On : 02 Aug 2022 16:01
Operator : JC\MD
Sample : N3971-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23R

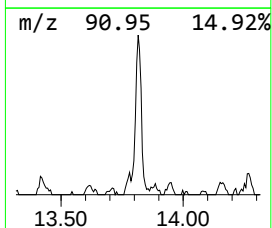
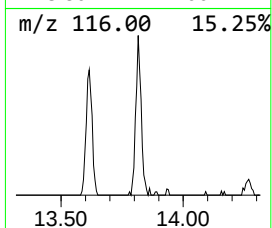
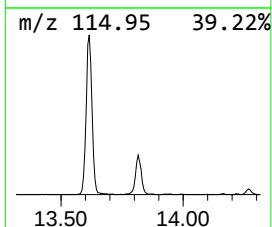
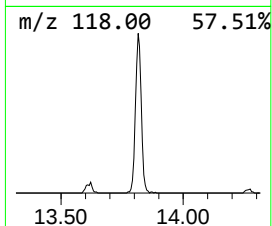
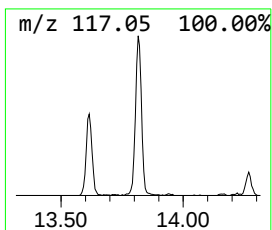
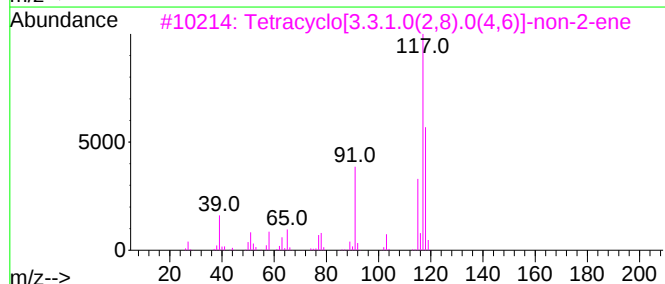
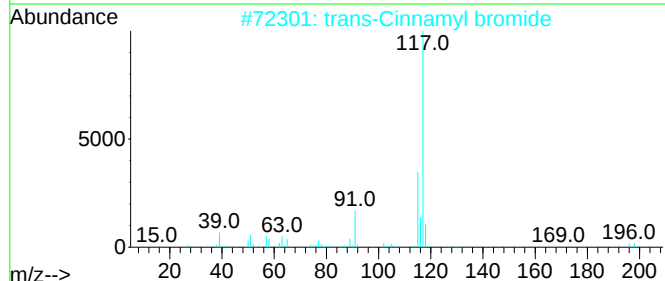
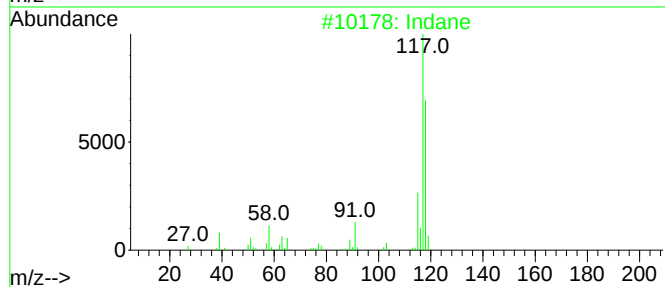
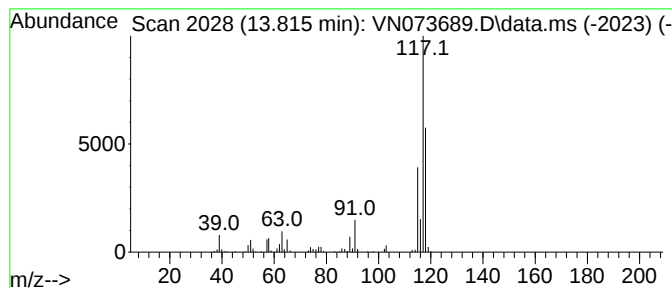
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	9.42 ug/l	275846	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	86
2			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	64
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	53
5			Indole	117	C8H7N	000120-72-9	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073689.D
Acq On : 02 Aug 2022 16:01
Operator : JC\MD
Sample : N3971-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	2.399	14.8	ug/l	372249	1	8.016	1259220	50.0
Butane, 2-methyl-	3.081	25.5	ug/l	641749	1	8.016	1259220	50.0
Isopropyl Alcohol	4.510	9.3	ug/l	234503	1	8.016	1259220	50.0
Cyclobutane, me...	5.110	11.5	ug/l	289326	1	8.016	1259220	50.0
Cyclopentane, m...	7.069	5.5	ug/l	137640	1	8.016	1259220	50.0
Indane	13.815	9.4	ug/l	275846	4	13.615	1464150	50.0