

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
 Data File : VN073709.D
 Acq On : 03 Aug 2022 14:11
 Operator : JC\MD
 Sample : N3971-10 20X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-14

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: VN073709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	77	87	93	rBV	33817	56829	1.10%	0.228%
2	3.081	195	203	217	rVB	210992	478257	9.22%	1.921%
3	3.457	257	267	279	rVB3	43073	114462	2.21%	0.460%
4	3.934	338	348	357	rVB2	23099	61593	1.19%	0.247%
5	7.069	870	881	890	rBV3	62343	180226	3.48%	0.724%
6	7.239	900	910	922	rBV2	54744	158492	3.06%	0.637%
7	7.951	1020	1031	1037	rBV	263610	650342	12.54%	2.612%
8	8.016	1037	1042	1068	rVB	478500	1099127	21.19%	4.415%
9	8.381	1091	1104	1115	rBV4	365353	1034158	19.94%	4.154%
10	8.904	1181	1193	1207	rBV	662085	1343343	25.90%	5.396%
11	10.380	1436	1444	1450	rBV	937018	1669602	32.19%	6.707%
12	10.445	1450	1455	1461	rVB	173920	307802	5.94%	1.236%
13	11.686	1657	1666	1676	rBV	959931	1640302	31.63%	6.589%
14	11.786	1676	1683	1693	rVV	702711	1163628	22.44%	4.674%
15	11.892	1693	1701	1720	rVB	2804101	5186113	100.00%	20.833%
16	12.222	1748	1757	1768	rBV	1346724	2179630	42.03%	8.756%
17	12.521	1800	1808	1814	rVB	52596	84268	1.62%	0.339%
18	12.674	1826	1834	1845	rBV	839216	1366460	26.35%	5.489%
19	12.863	1860	1866	1871	rBV	101388	161281	3.11%	0.648%
20	12.921	1871	1876	1880	rVV	449937	776166	14.97%	3.118%
21	12.957	1880	1882	1886	rVV	195059	267536	5.16%	1.075%
22	13.004	1886	1890	1897	rVB	230728	360562	6.95%	1.448%
23	13.163	1910	1917	1925	rBV	290653	467752	9.02%	1.879%
24	13.310	1934	1942	1955	rBV	846681	1326756	25.58%	5.330%
25	13.616	1986	1994	2007	rBV2	1055760	2247059	43.33%	9.026%
26	13.816	2023	2028	2043	rVB2	149738	292240	5.64%	1.174%
27	14.868	2199	2207	2212	rBV3	29061	54548	1.05%	0.219%
28	15.439	2295	2304	2311	rBV	83671	165555	3.19%	0.665%

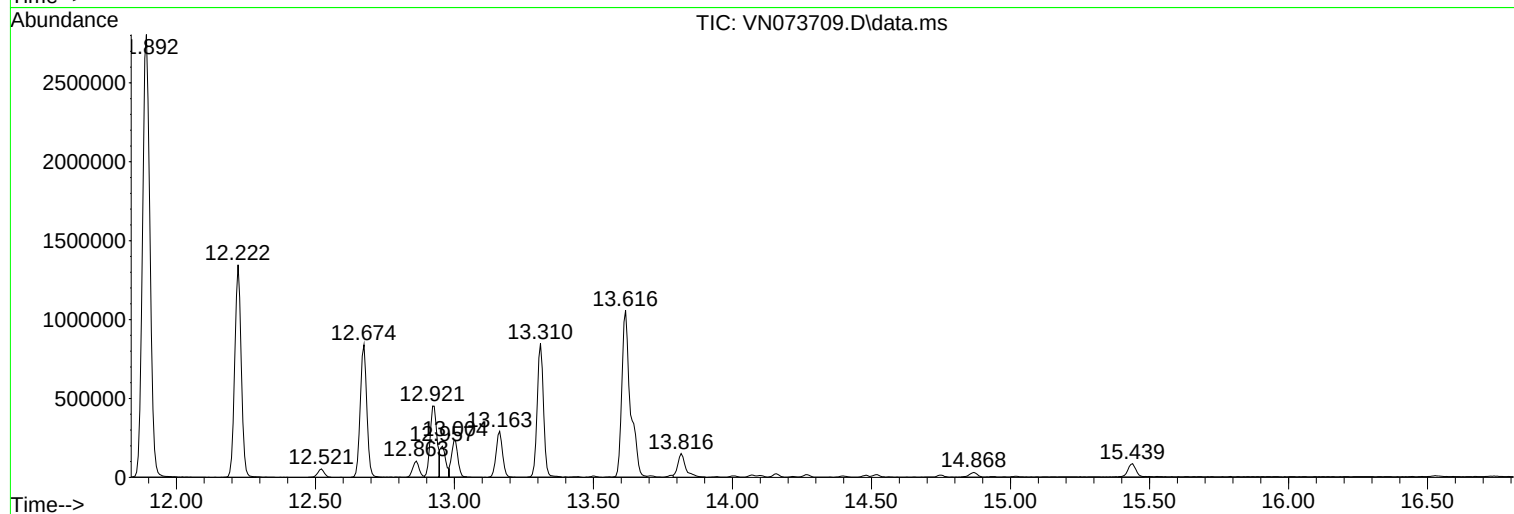
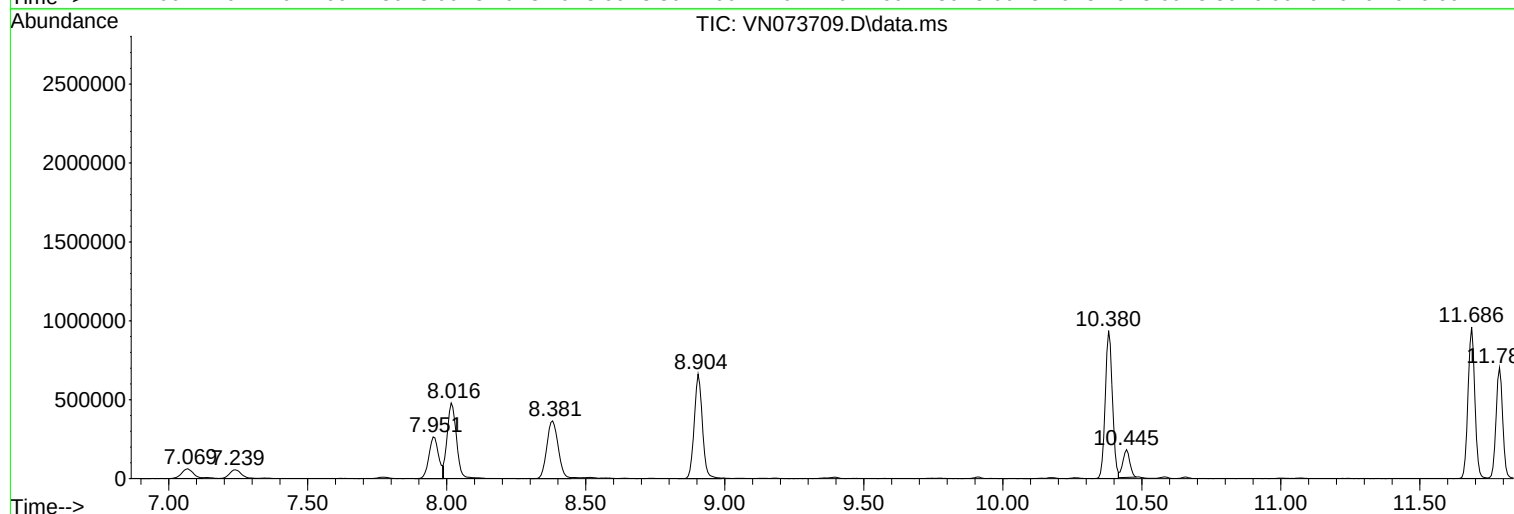
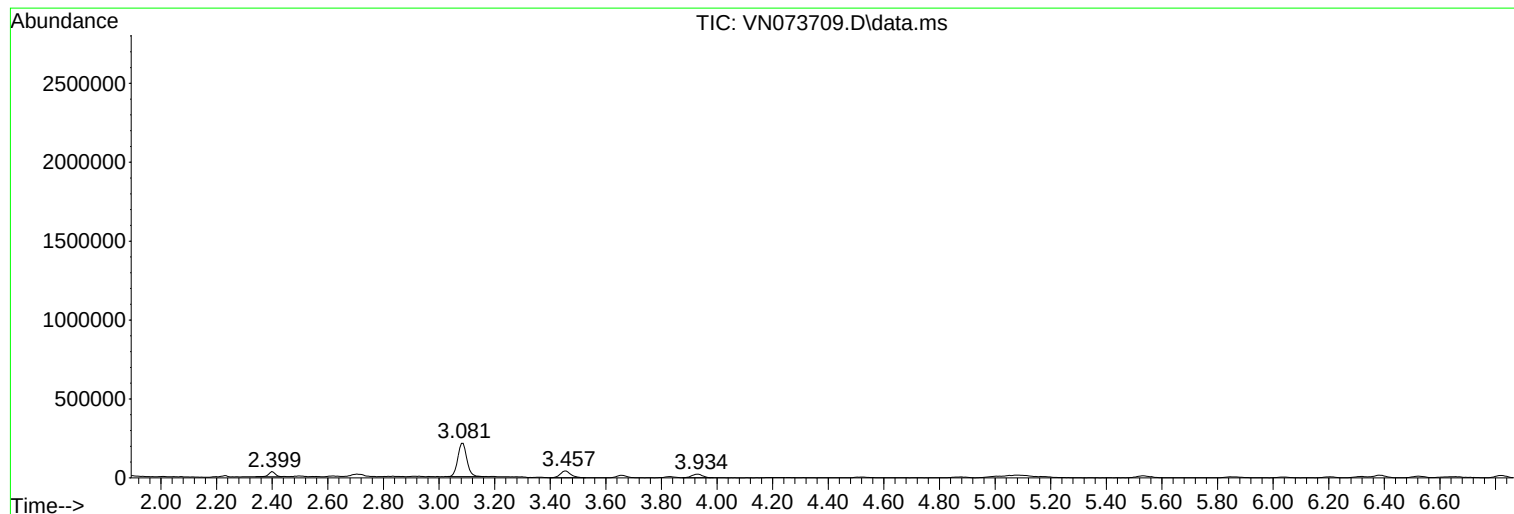
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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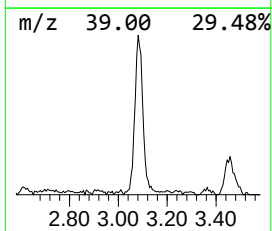
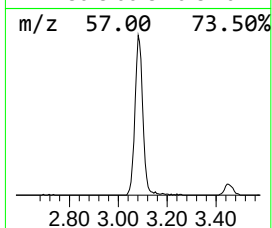
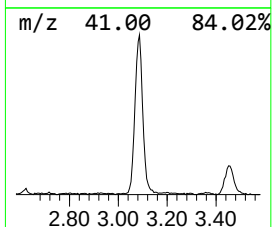
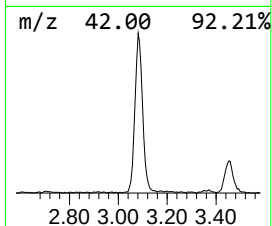
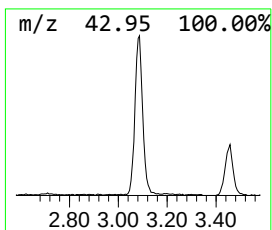
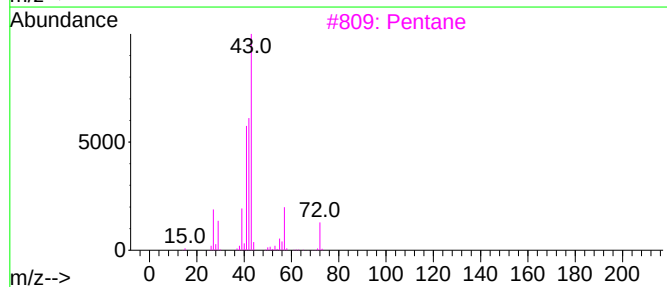
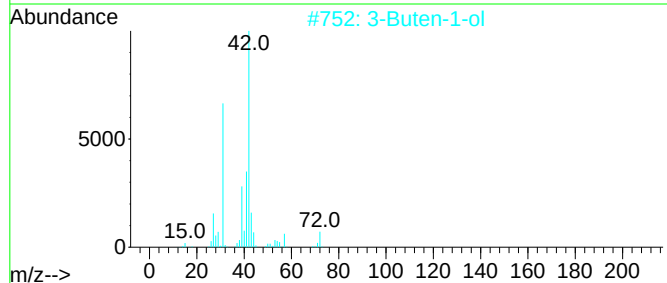
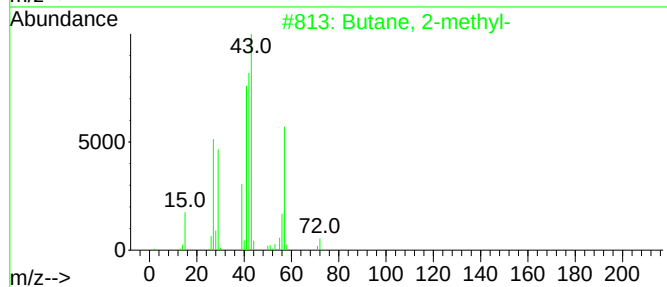
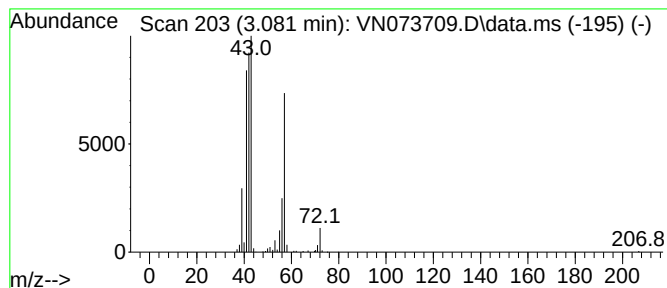
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	21.76 ug/l	478257	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Pentane	72	C5H12	000109-66-0	32
4			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	27
5			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12



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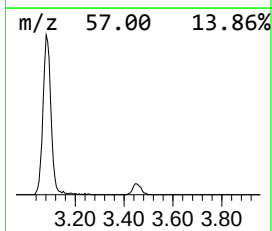
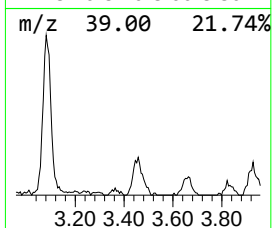
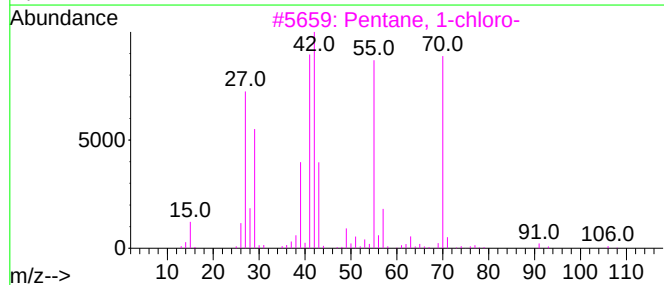
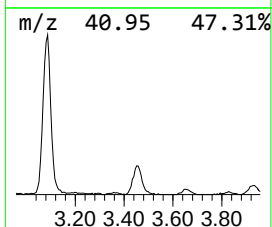
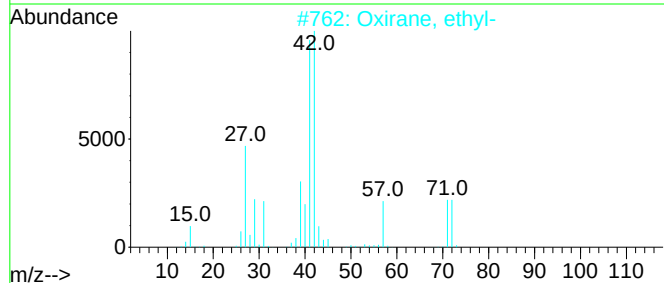
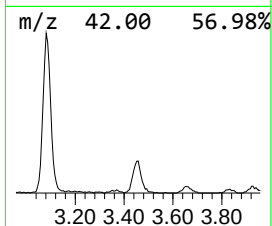
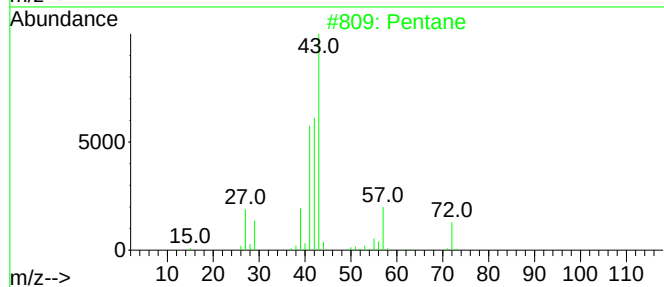
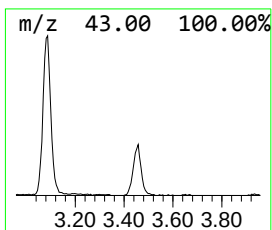
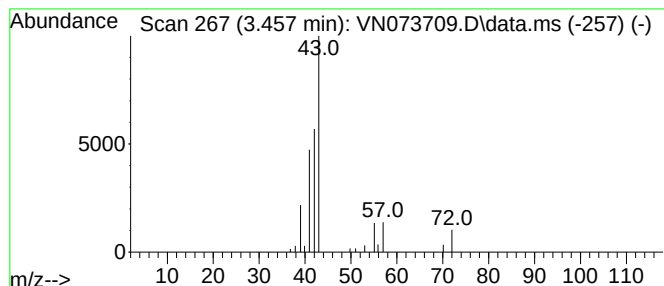
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	5.21 ug/l	114462	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	90
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	9
4			1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	9



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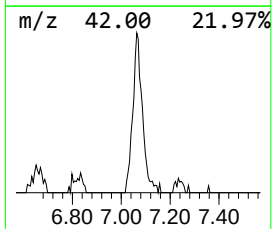
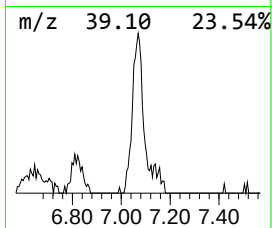
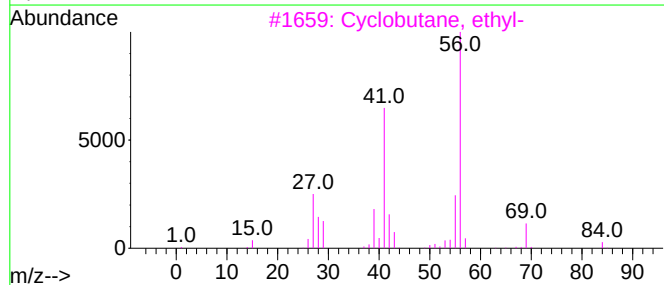
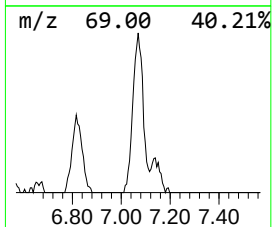
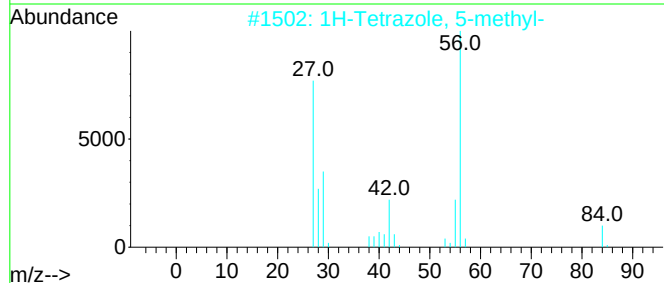
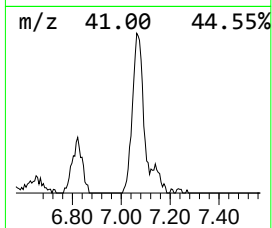
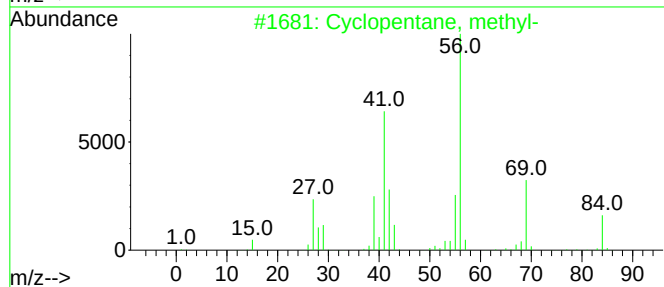
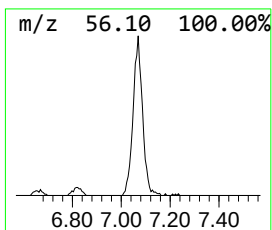
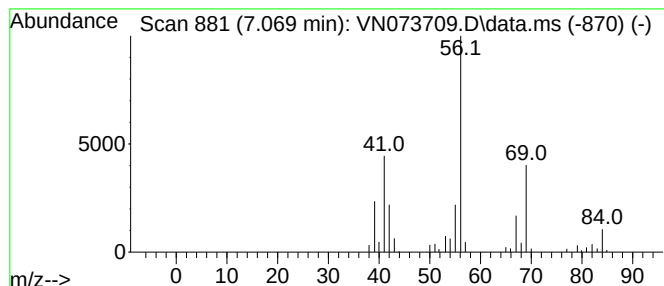
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	8.20 ug/l	180226	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4		Cyclohexane	84	C6H12	000110-82-7	53
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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Instrument :
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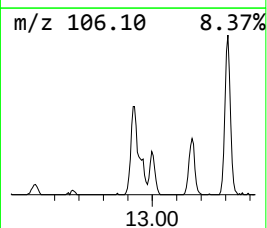
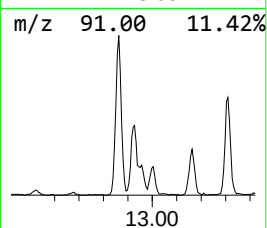
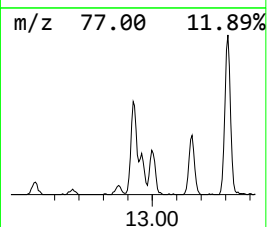
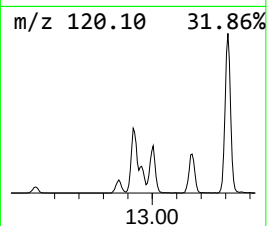
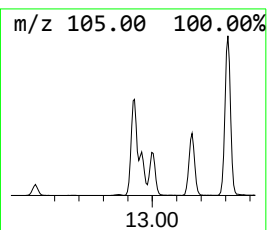
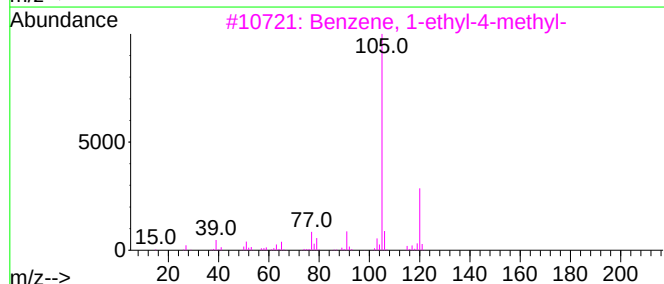
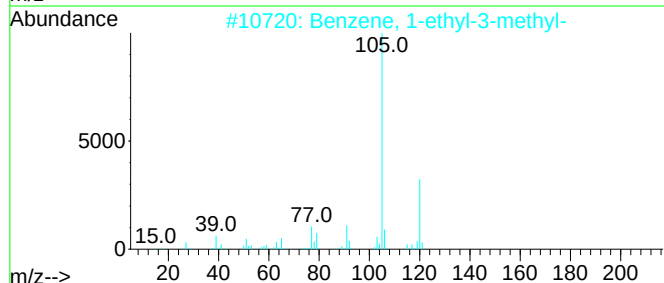
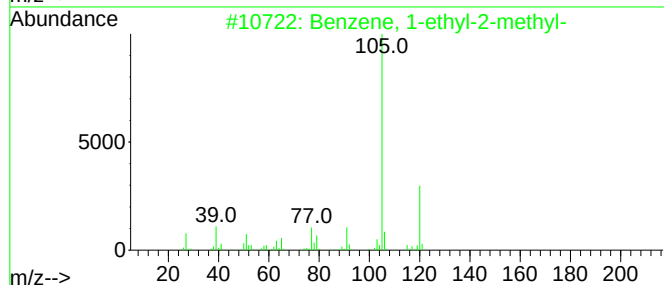
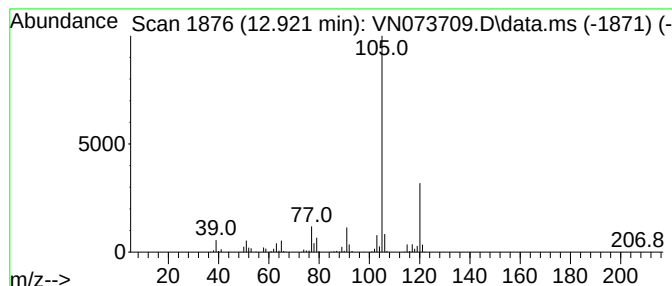
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	17.27 ug/l	776166	1,4-Dichlorobenzene-d4	13.616

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



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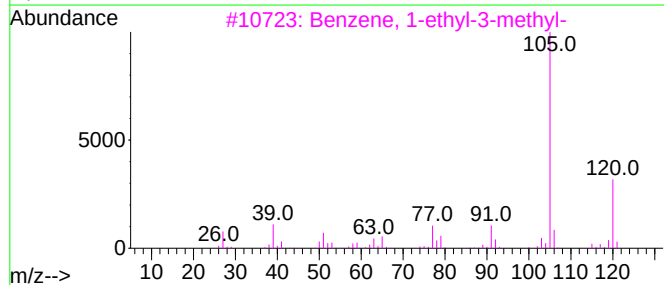
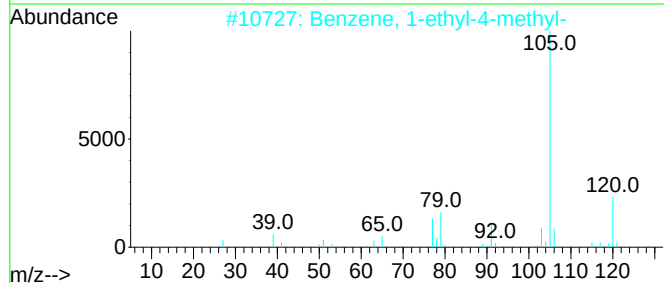
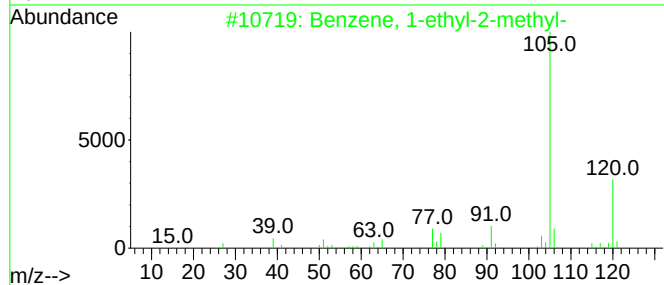
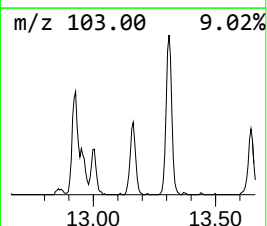
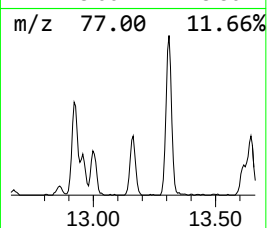
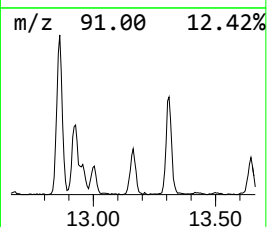
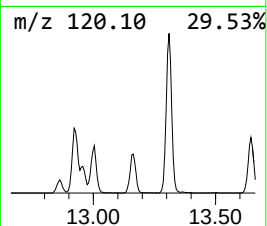
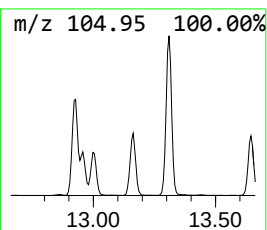
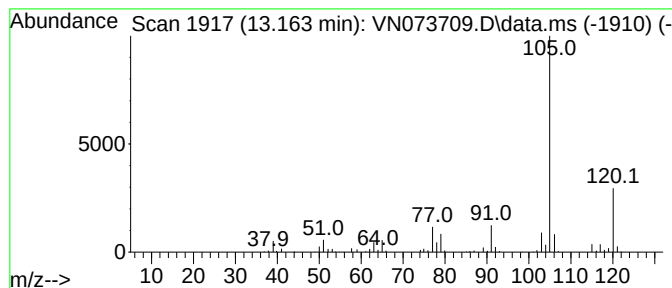
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	10.41 ug/l	467752	1,4-Dichlorobenzene-d4	13.616

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-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	90



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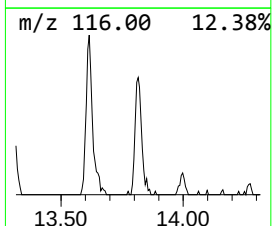
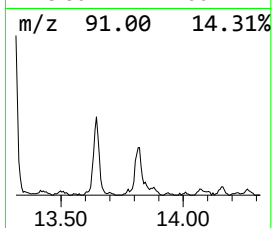
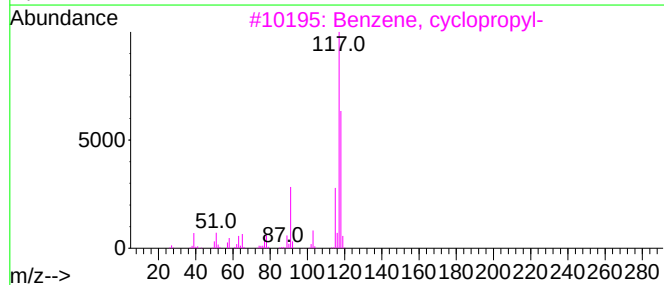
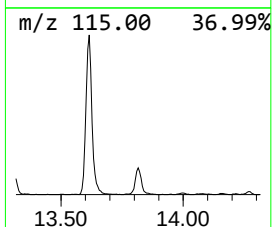
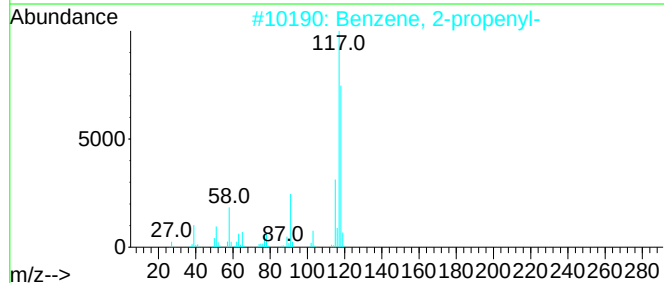
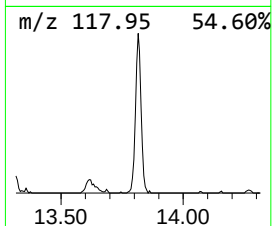
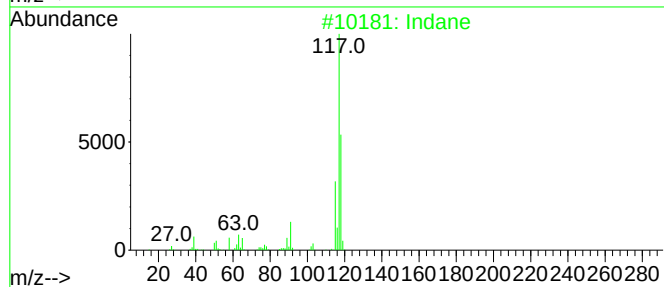
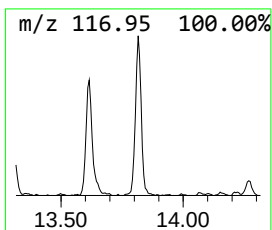
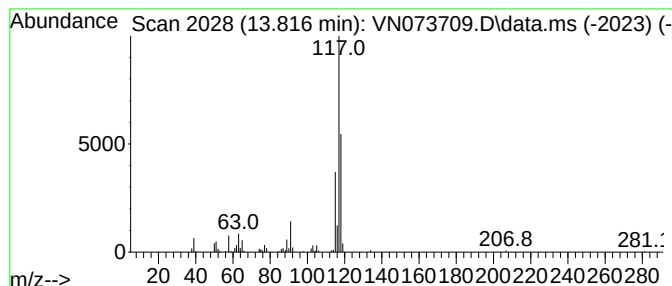
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	6.50 ug/l	292240	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4			Deltacyclene	118	C9H10	007785-10-6	72
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073709.D
Acq On : 03 Aug 2022 14:11
Operator : JC\MD
Sample : N3971-10 20X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

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-methyl-	3.081	21.8	ug/l	478257	1	8.016	1099130	50.0
Pentane	3.457	5.2	ug/l	114462	1	8.016	1099130	50.0
Cyclopentane, m...	7.069	8.2	ug/l	180226	1	8.016	1099130	50.0
Benzene, 1-ethy...	12.922	17.3	ug/l	776166	4	13.616	2247060	50.0
Benzene, 1-ethy...	13.163	10.4	ug/l	467752	4	13.616	2247060	50.0
Indane	13.816	6.5	ug/l	292240	4	13.616	2247060	50.0