

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071384.D
 Acq On : 18 Mar 2022 19:56
 Operator : JC\MD
 Sample : N2015-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-06

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\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071384.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	43	rBV	125068	195431	4.59%	0.769%
2	2.263	43	47	63	rVB3	183651	557695	13.09%	2.194%
3	2.434	71	76	84	rVB	164783	256440	6.02%	1.009%
4	3.128	189	194	206	rVB5	25601	62555	1.47%	0.246%
5	5.075	512	525	538	rBV2	44949	169566	3.98%	0.667%
6	5.616	605	617	632	rBV2	68688	242639	5.70%	0.955%
7	7.039	849	859	875	rBV3	55316	194870	4.58%	0.767%
8	7.322	897	907	920	rBV6	21499	65235	1.53%	0.257%
9	8.022	1014	1026	1031	rBV	510422	1256830	29.51%	4.945%
10	8.086	1031	1037	1047	rVB	969986	2175432	51.07%	8.559%
11	8.433	1086	1096	1111	rBV	592776	1368635	32.13%	5.385%
12	8.616	1112	1127	1137	rBV2	375946	1007831	23.66%	3.965%
13	8.963	1176	1186	1207	rBV	1493715	3056640	71.76%	12.026%
14	9.592	1286	1293	1300	rVB2	29641	58740	1.38%	0.231%
15	9.880	1333	1342	1352	rBV	181674	354578	8.32%	1.395%
16	10.010	1355	1364	1374	rBV	377186	768227	18.04%	3.022%
17	10.369	1416	1425	1429	rBV2	39529	75583	1.77%	0.297%
18	10.439	1429	1437	1457	rVB	2329210	4259330	100.00%	16.758%
19	11.739	1650	1658	1672	rBV	2073088	3752031	88.09%	14.762%
20	12.727	1819	1826	1839	rBV	1686707	2841372	66.71%	11.179%
21	13.674	1975	1987	1999	rBV	1571508	2697690	63.34%	10.614%

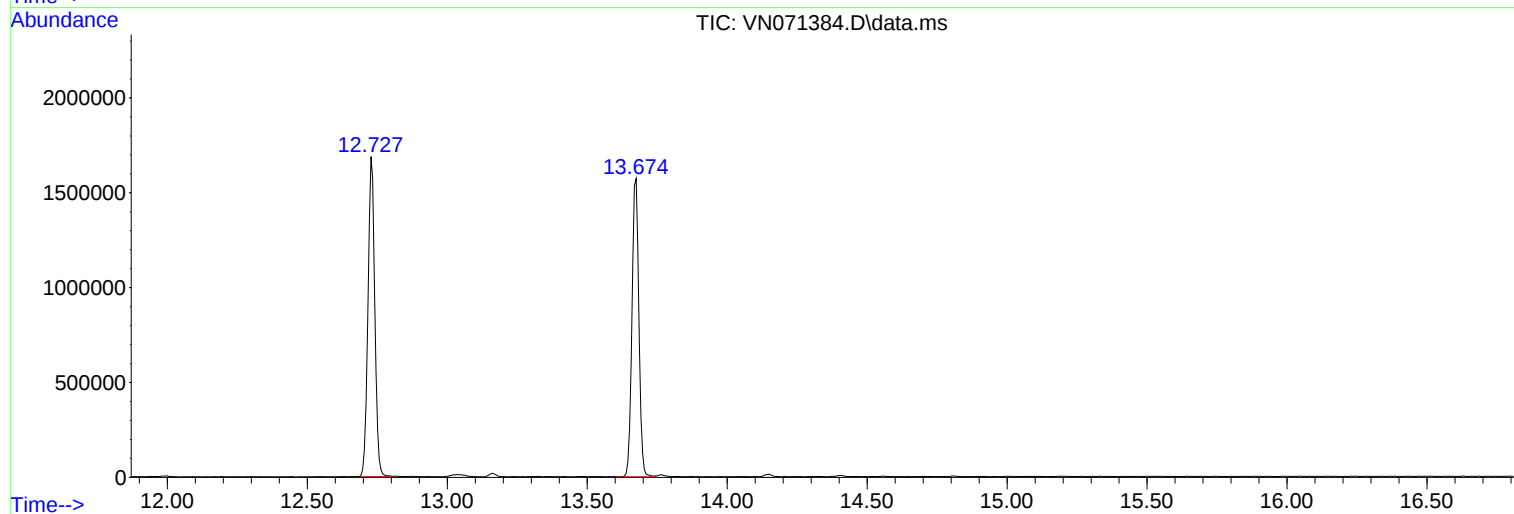
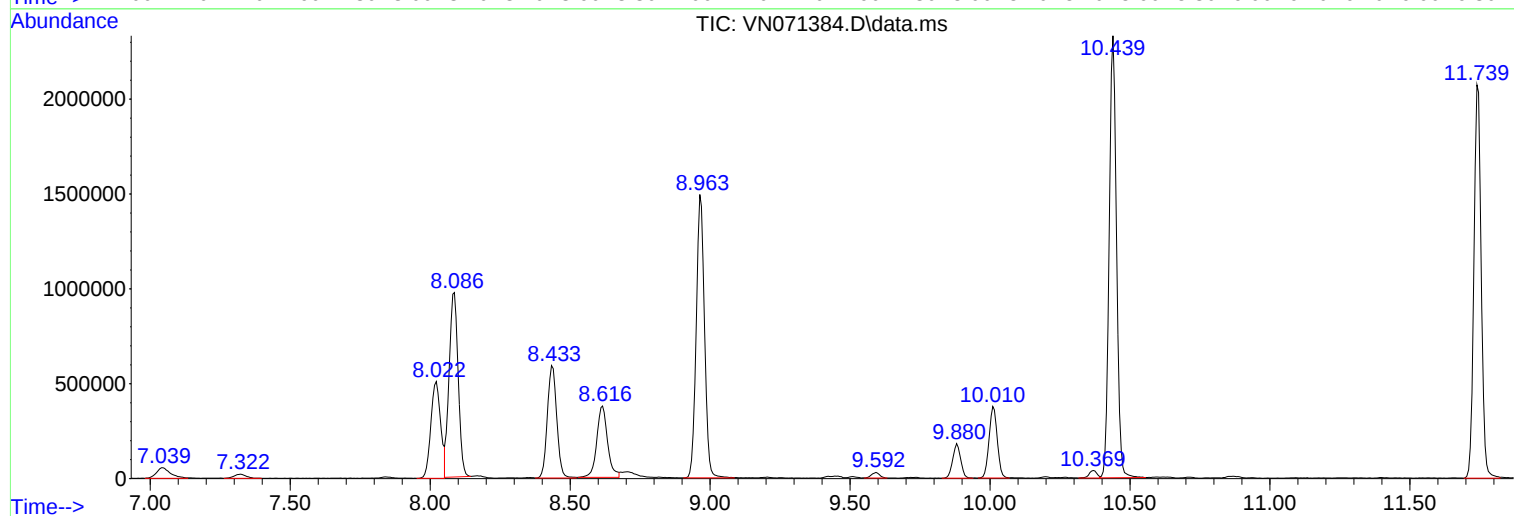
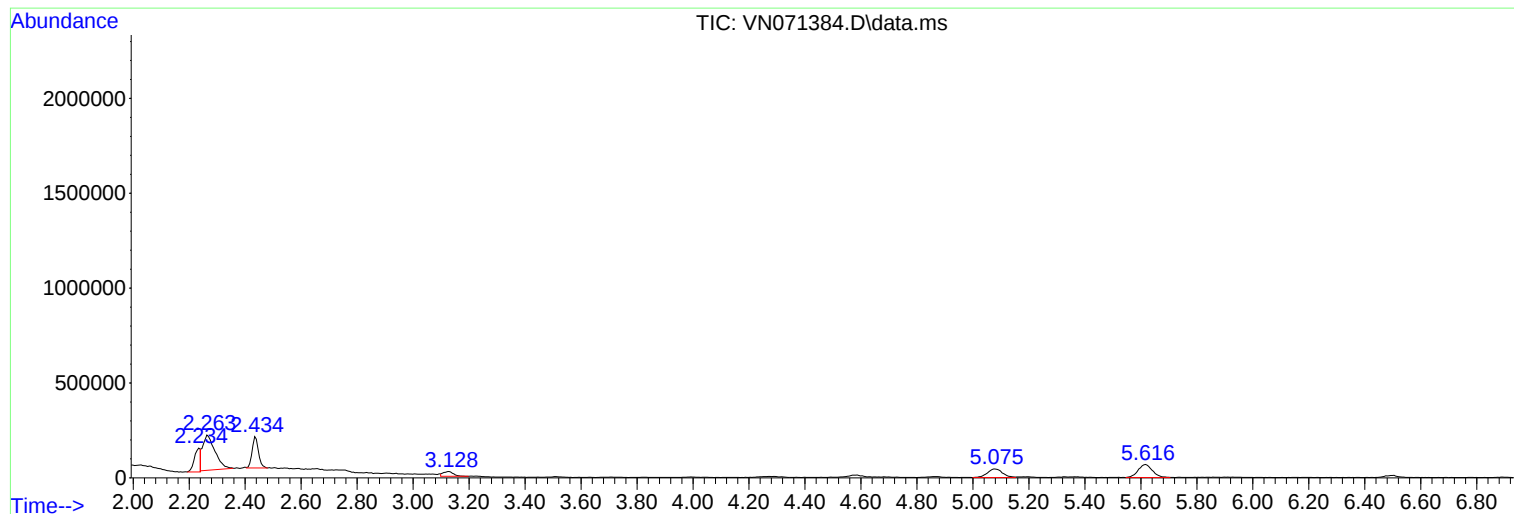
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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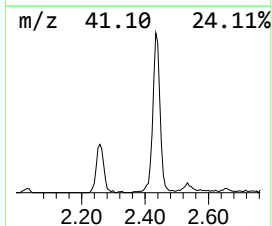
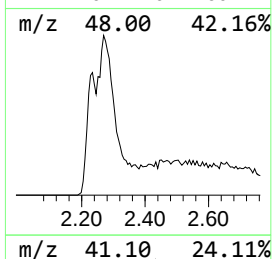
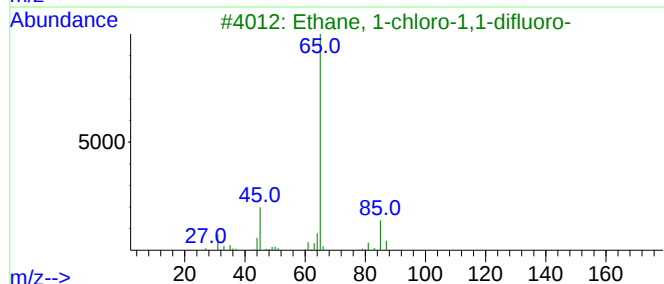
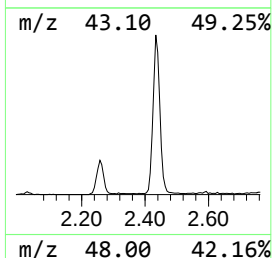
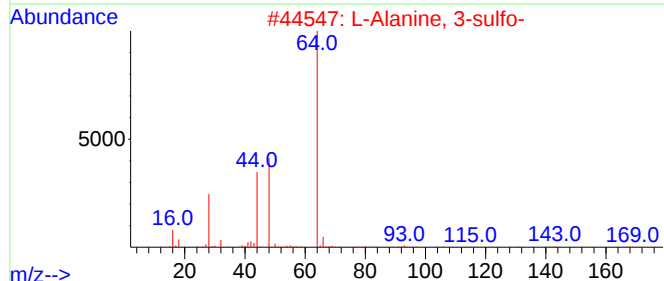
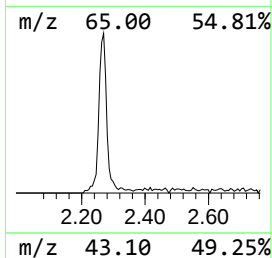
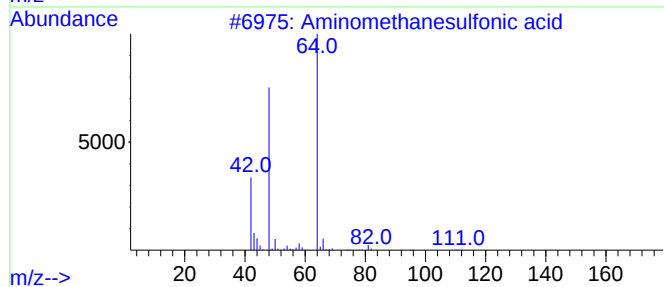
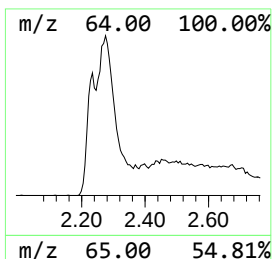
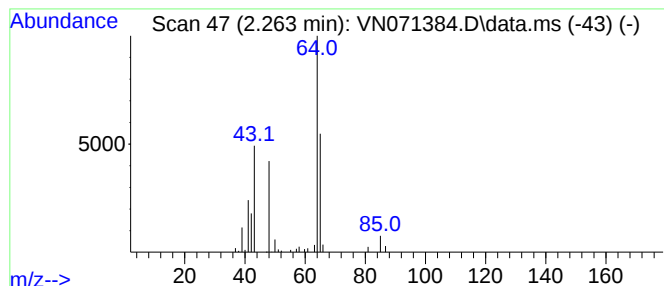
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.263 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	12.82 ug/l	557695	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	10
2		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3		Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	9
4		Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5		Sulfur dioxide	64	O2S	007446-09-5	3



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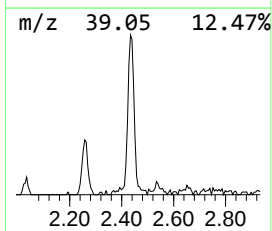
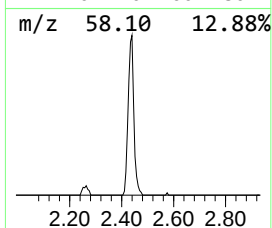
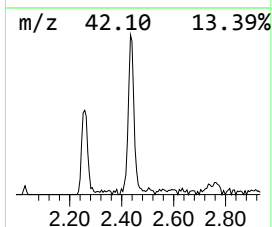
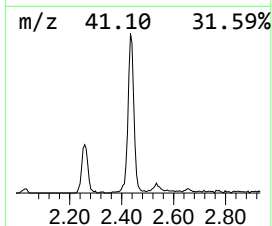
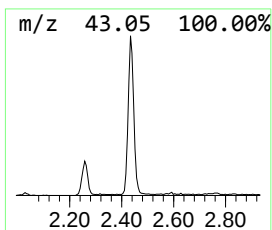
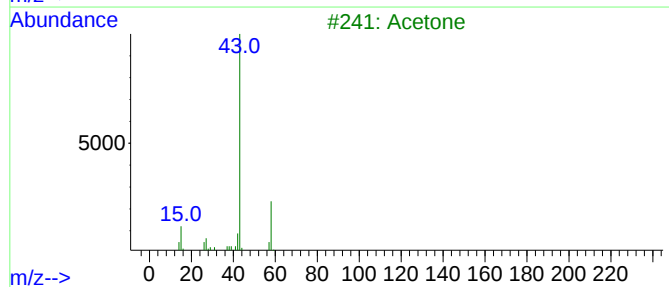
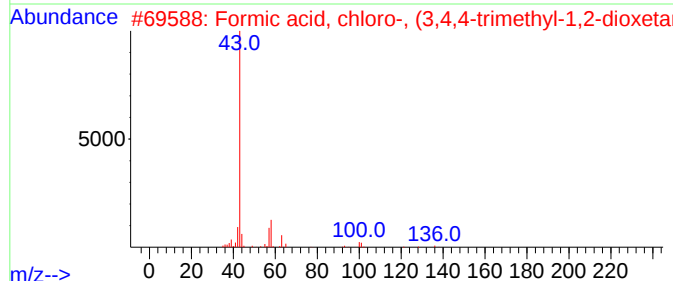
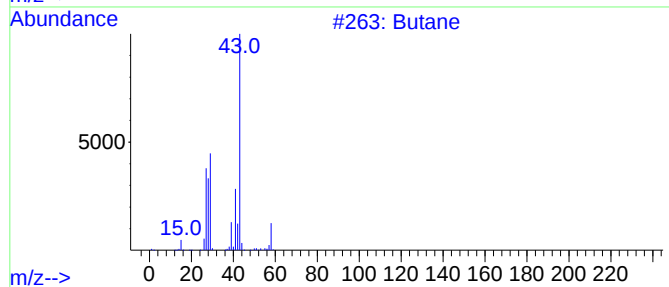
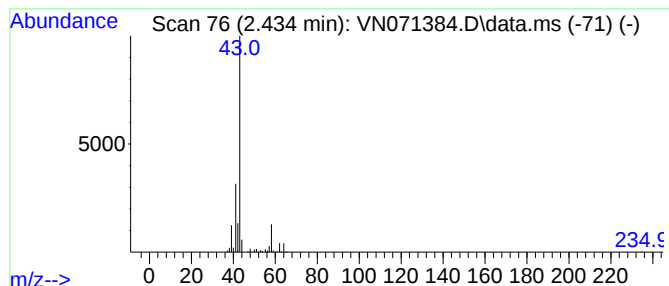
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	5.89 ug/l	256440	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	58
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	36
3			Acetone	58	C3H6O	000067-64-1	4
4			1-Propanol, 2-chloro-	94	C3H7ClO	000078-89-7	4
5			Cyclobutylamine	71	C4H9N	002516-34-9	4



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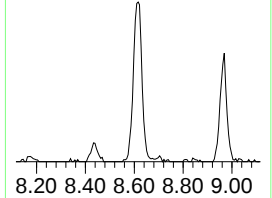
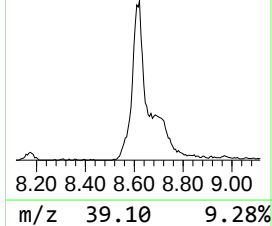
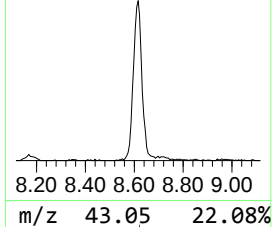
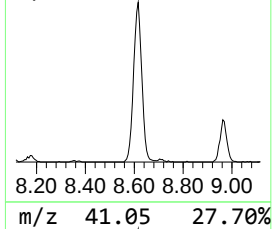
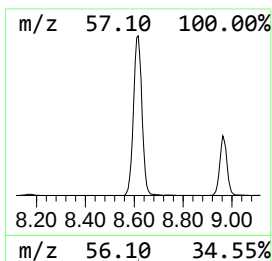
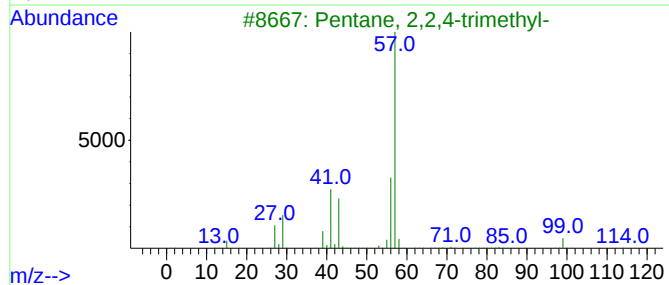
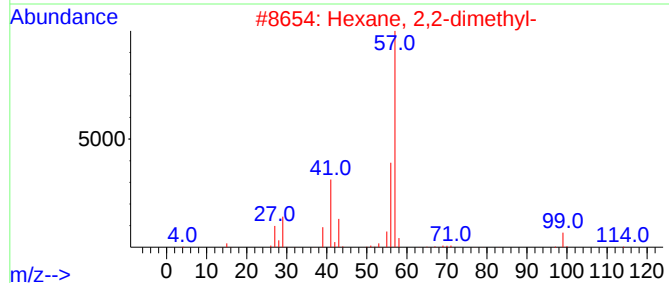
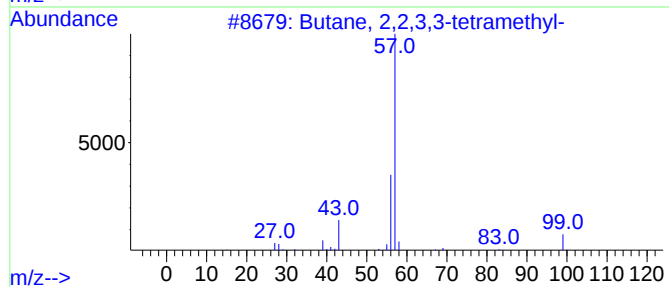
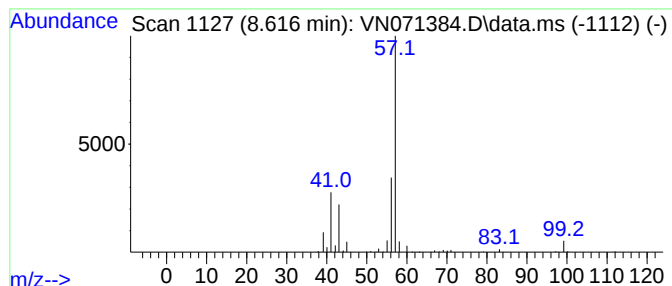
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Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	16.49 ug/l	1007830	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53



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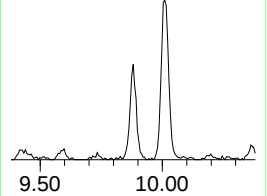
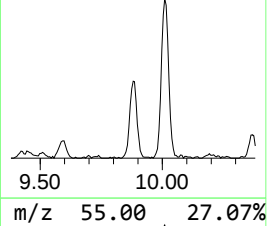
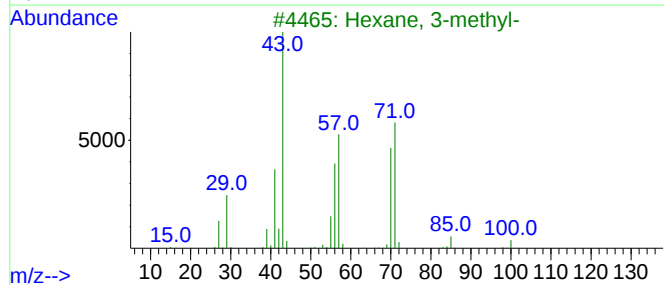
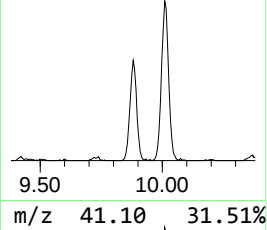
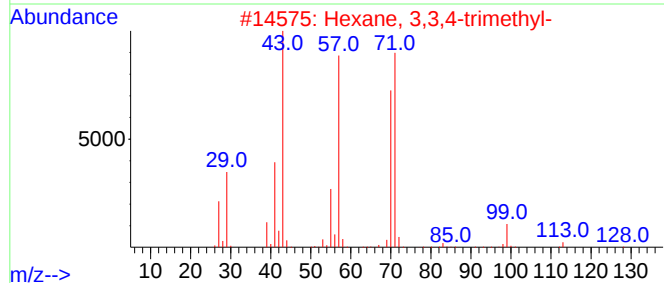
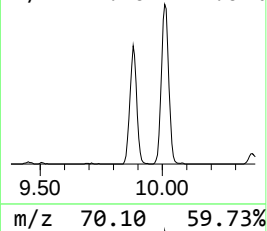
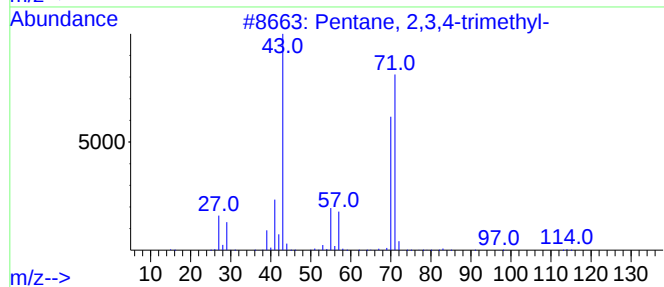
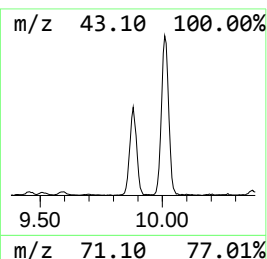
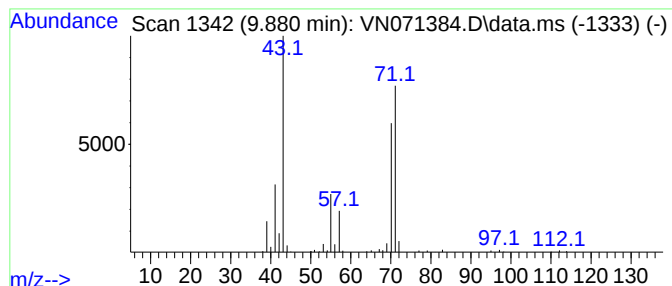
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	5.80 ug/l	354578	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	83
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78



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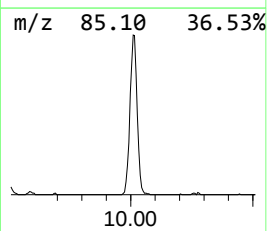
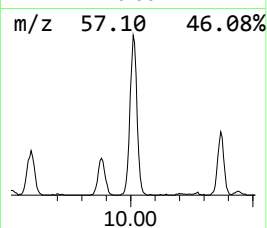
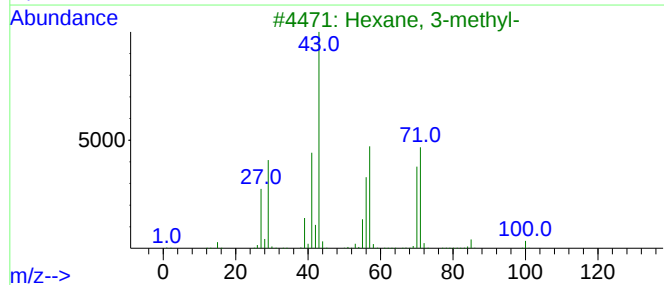
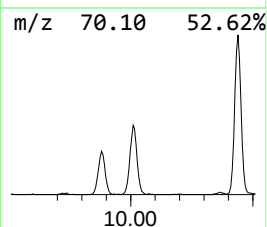
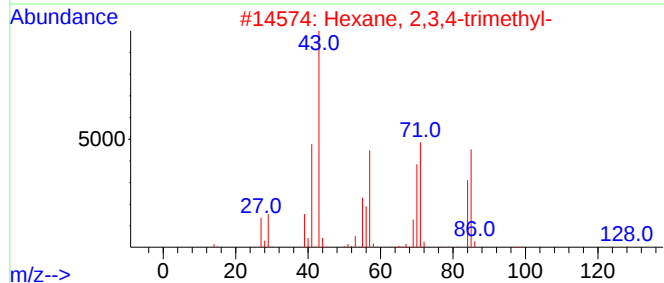
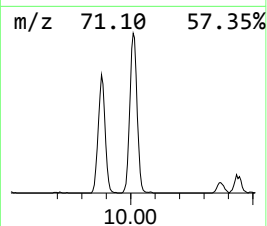
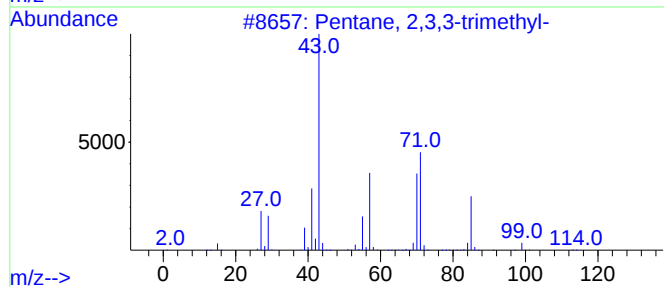
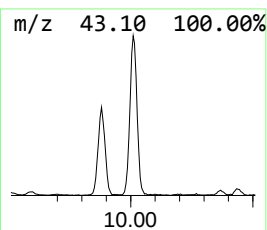
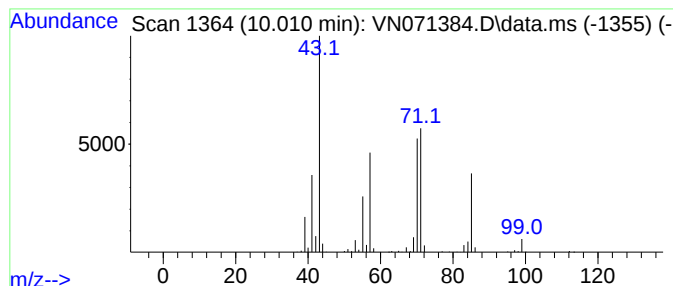
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	12.57 ug/l	768227	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.263	2.263	12.8	ug/l	557695	1	8.086	2175430	50.0
Butane	2.434	5.9	ug/l	256440	1	8.086	2175430	50.0
Butane, 2,2,3,3...	8.616	16.5	ug/l	1007830	2	8.963	3056640	50.0
Pentane, 2,3,4-...	9.880	5.8	ug/l	354578	2	8.963	3056640	50.0
Pentane, 2,3,3-...	10.010	12.6	ug/l	768227	2	8.963	3056640	50.0