

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
 Data File : VN080367.D
 Acq On : 05 Dec 2023 15:34
 Operator : JC\MD
 Sample : 05616-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1151

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\82N111623W.M
 Title : SW846 8260

Signal : TIC: VN080367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	15	22	30	rVB	95043	134575	12.58%	1.499%
2	2.295	52	58	60	rBV3	8593	16288	1.52%	0.181%
3	2.483	85	90	93	rBV6	5693	11320	1.06%	0.126%
4	2.659	115	120	131	rVB2	27761	55262	5.16%	0.615%
5	4.430	413	421	427	rBV3	16235	40904	3.82%	0.456%
6	7.224	887	896	908	rBV	113111	314238	29.37%	3.500%
7	8.165	1046	1056	1061	rBV	169615	401840	37.55%	4.476%
8	8.224	1061	1066	1080	rVB2	230107	530526	49.58%	5.909%
9	8.582	1119	1127	1140	rVB2	161027	405585	37.90%	4.517%
10	8.812	1162	1166	1172	rVB5	4984	10883	1.02%	0.121%
11	9.100	1207	1215	1225	rVB	352281	717331	67.04%	7.989%
12	9.265	1238	1243	1249	rBV3	14000	27756	2.59%	0.309%
13	9.659	1304	1310	1320	rBV2	24840	54538	5.10%	0.607%
14	10.571	1456	1465	1471	rBV	562692	1047589	97.90%	11.668%
15	10.629	1471	1475	1481	rVB2	47201	88434	8.26%	0.985%
16	11.865	1678	1685	1695	rVB	552659	989137	92.44%	11.017%
17	11.965	1698	1702	1706	rBV2	11254	15573	1.46%	0.173%
18	12.070	1714	1720	1728	rBV2	39012	71381	6.67%	0.795%
19	12.212	1736	1744	1748	rVB6	5760	11145	1.04%	0.124%
20	12.341	1762	1766	1770	rBV4	11407	16783	1.57%	0.187%
21	12.394	1770	1775	1781	rBV3	21989	45954	4.29%	0.512%
22	12.853	1844	1853	1862	rBV	479331	835669	78.10%	9.307%
23	13.123	1888	1899	1911	rVB	135112	288170	26.93%	3.210%
24	13.341	1930	1936	1942	rBV	89490	140349	13.12%	1.563%
25	13.482	1955	1960	1964	rBV4	9983	18362	1.72%	0.205%
26	13.523	1965	1967	1974	rVB5	8243	14303	1.34%	0.159%
27	13.688	1988	1995	2002	rBV	488173	802613	75.01%	8.939%
28	13.794	2006	2013	2020	rVV	621787	1070022	100.00%	11.917%
29	13.876	2020	2027	2033	rVV2	188806	319571	29.87%	3.559%
30	13.953	2036	2040	2045	rVV4	17692	32634	3.05%	0.363%
31	14.006	2045	2049	2056	rVB6	10650	22328	2.09%	0.249%
32	14.253	2085	2091	2098	rBV8	10080	21685	2.03%	0.242%
33	14.482	2125	2130	2136	rBV5	11680	23992	2.24%	0.267%
34	14.576	2138	2146	2147	rBV6	7474	13821	1.29%	0.154%
35	14.623	2148	2154	2159	rVB7	18683	41498	3.88%	0.462%
36	14.794	2177	2183	2188	rBV10	17940	33051	3.09%	0.368%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

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\82N111623W.M
Title : SW846 8260

37	15.082	2222	2232	2234	rBV9	15166	27972	2.61%	0.312%
38	15.235	2253	2258	2261	rBV5	7699	13940	1.30%	0.155%
39	15.347	2271	2277	2281	rBV4	38933	64590	6.04%	0.719%
40	15.400	2281	2286	2295	rVB3	46294	83488	7.80%	0.930%
41	15.506	2301	2304	2313	rVB5	7461	14380	1.34%	0.160%
42	15.611	2313	2322	2335	rBV8	21365	89131	8.33%	0.993%

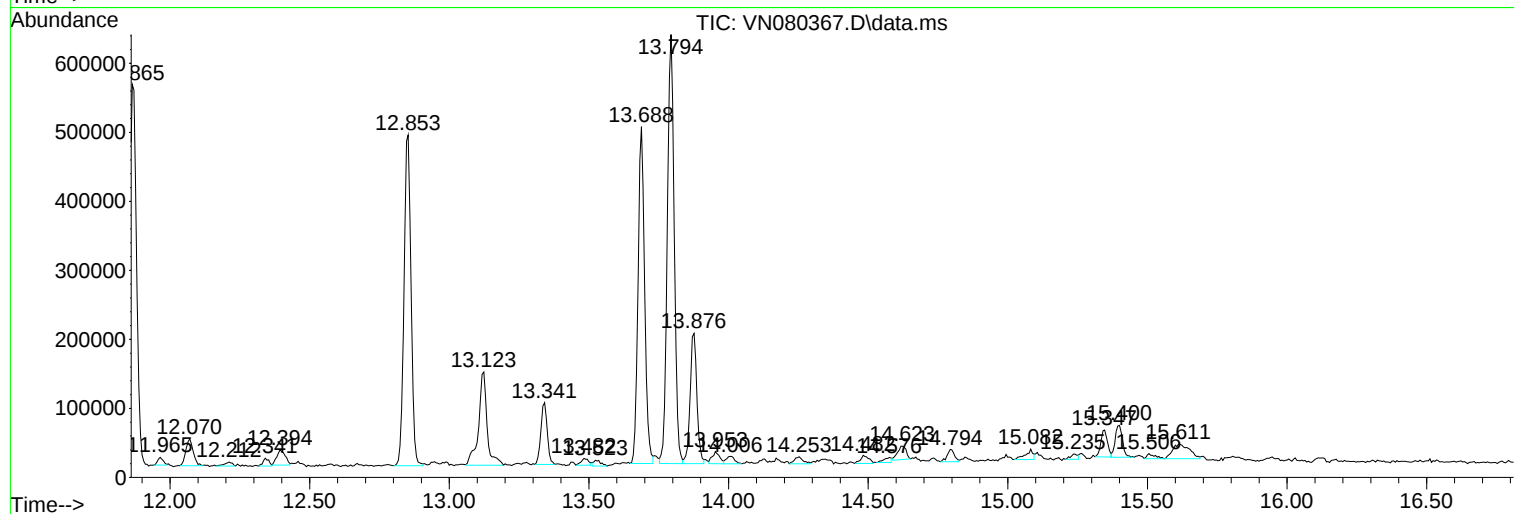
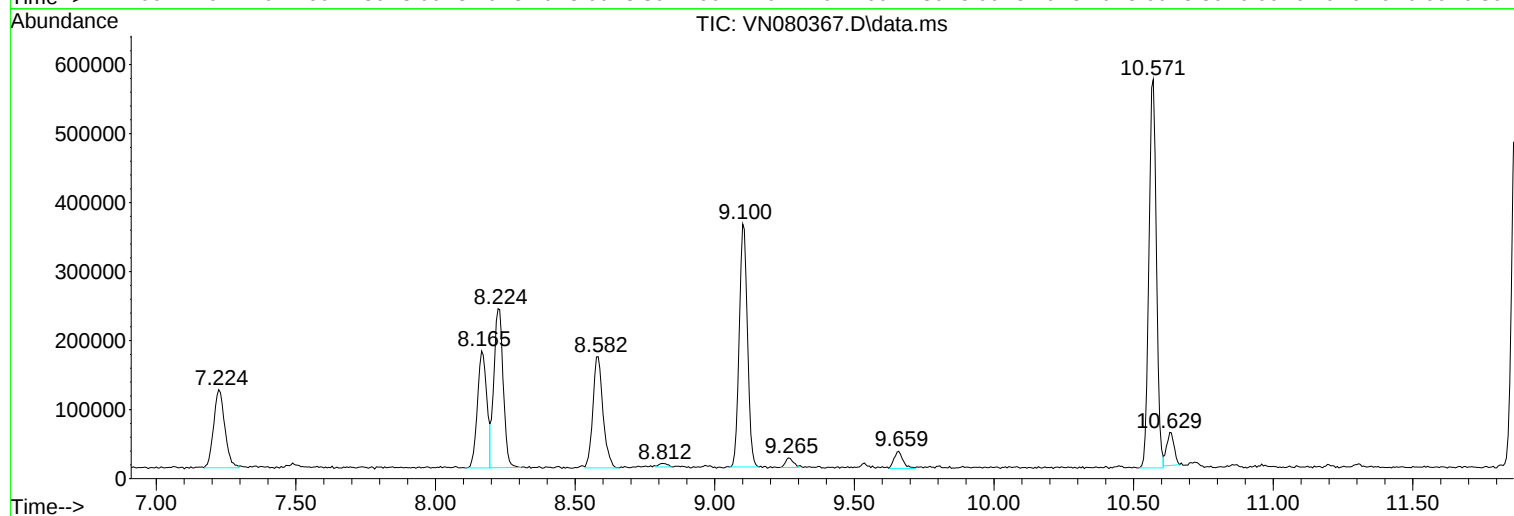
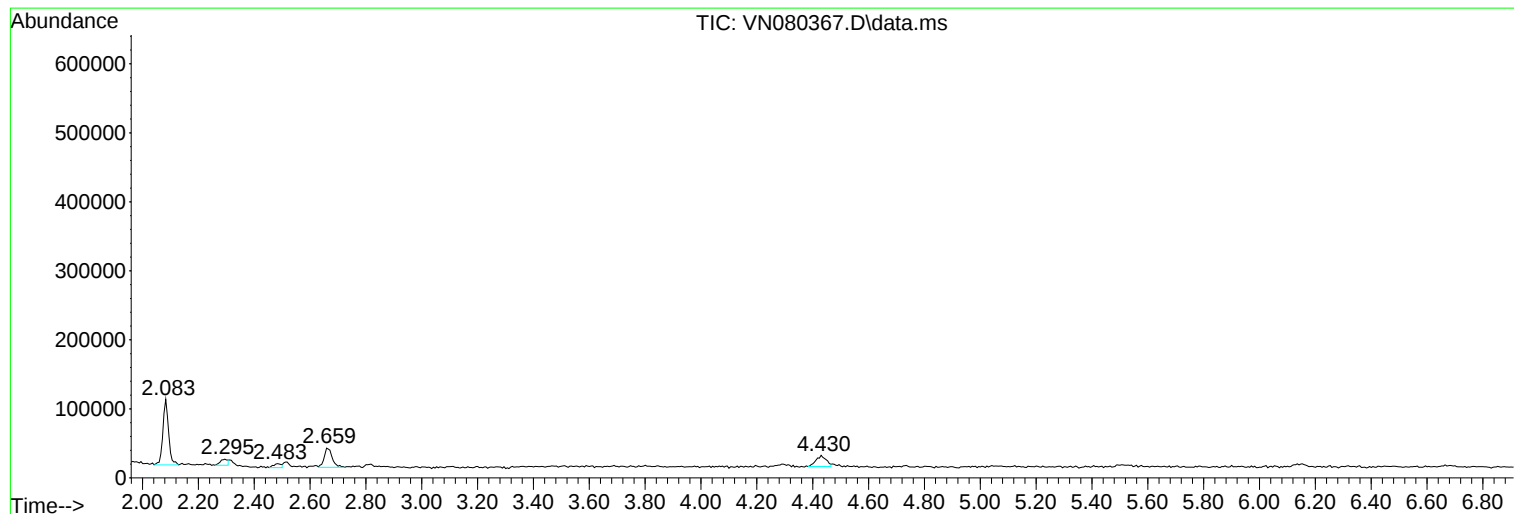
Sum of corrected areas: 8978611

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

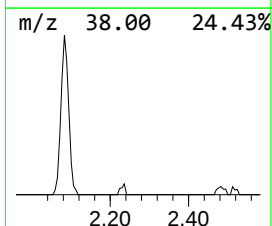
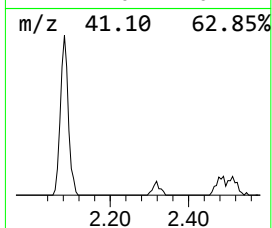
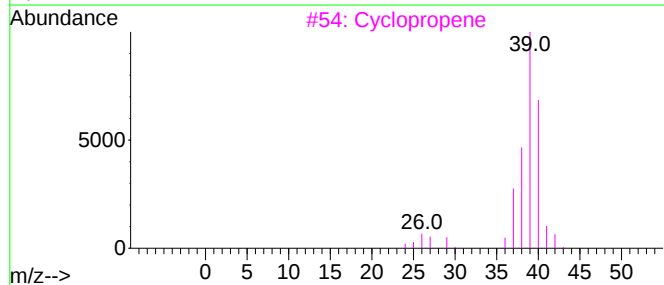
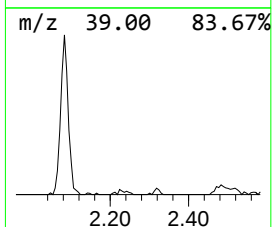
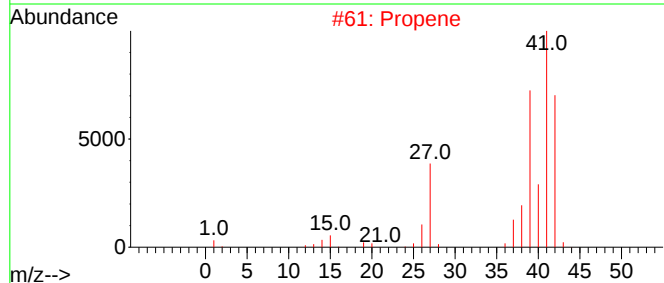
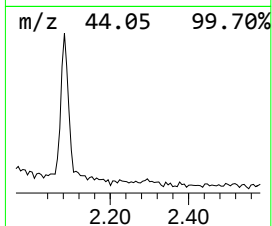
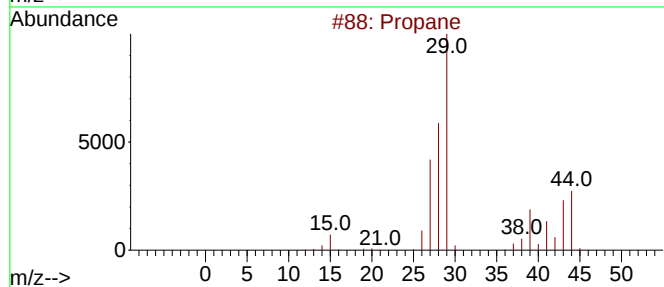
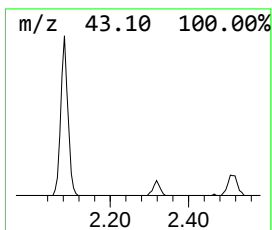
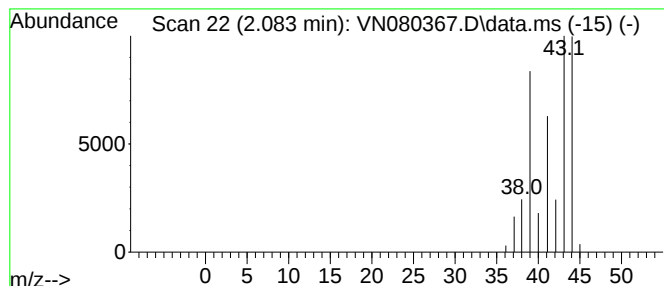
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	12.68 ug/l	134575	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Propene			42	C3H6	000115-07-1	9
3	Cyclopropene			40	C3H4	002781-85-3	4
4	Alanine			89	C3H7NO2	000056-41-7	2
5	Butanenitrile			69	C4H7N	000109-74-0	2



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

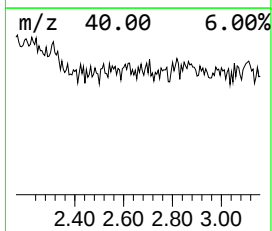
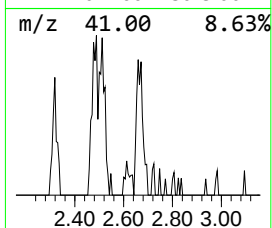
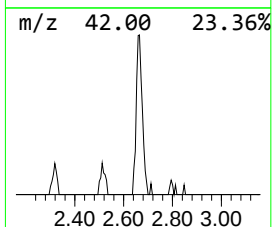
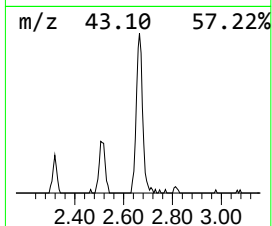
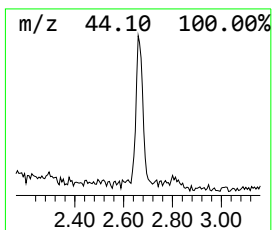
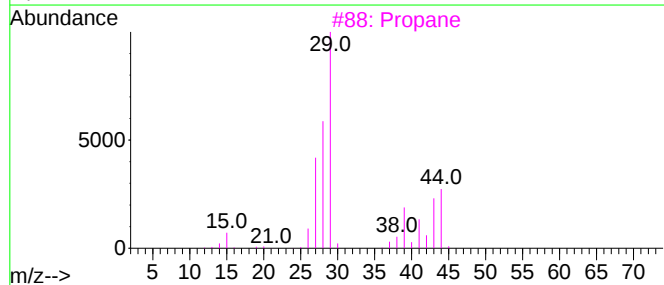
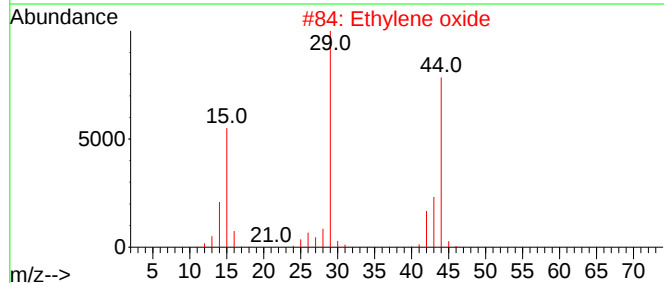
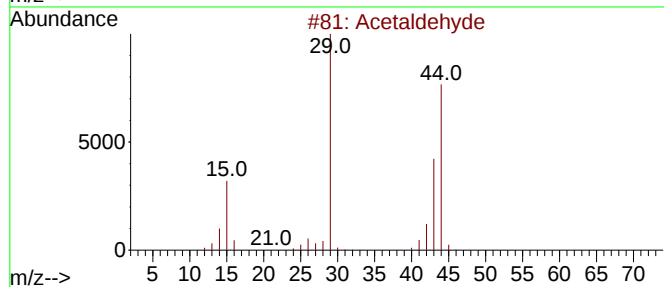
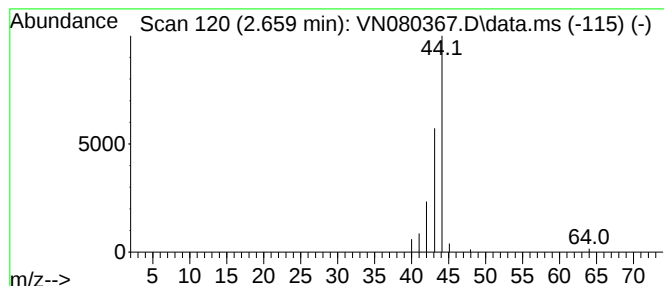
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.659	5.21 ug/l	55262	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Silane, methyl-	46	CH6Si	000992-94-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

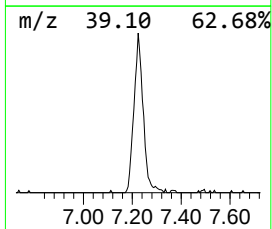
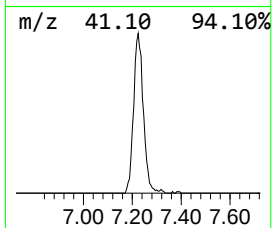
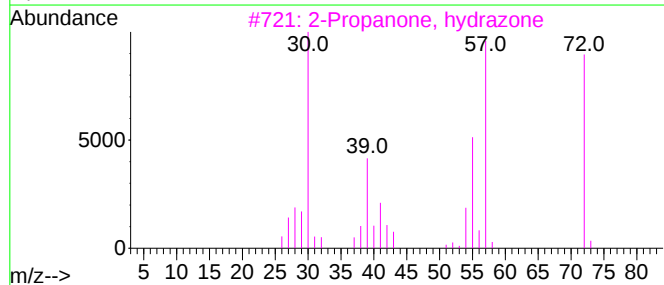
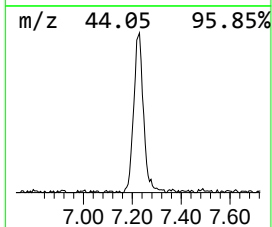
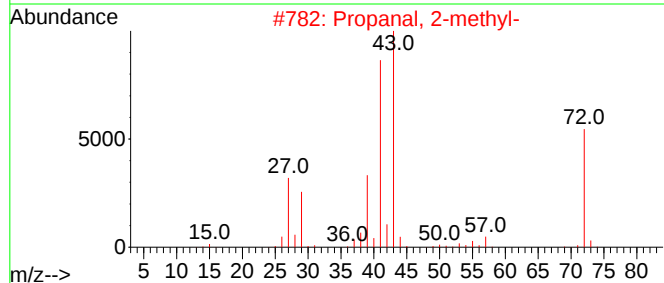
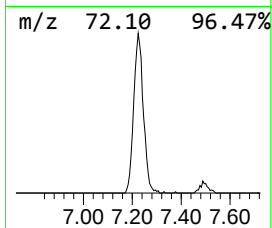
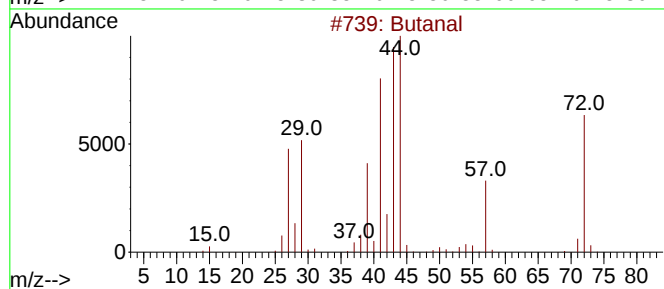
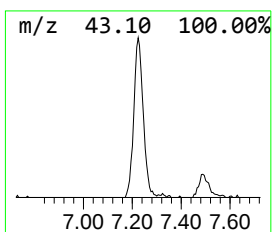
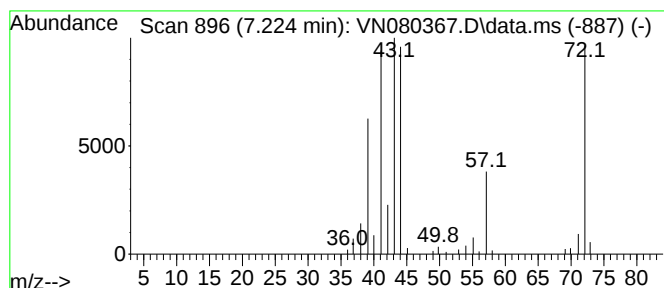
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	29.62 ug/l	314238	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	72
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
4			Propane	44	C3H8	000074-98-6	35
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

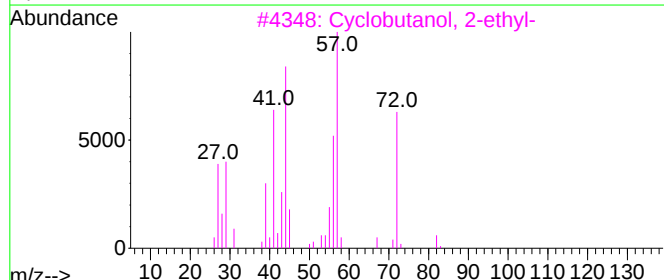
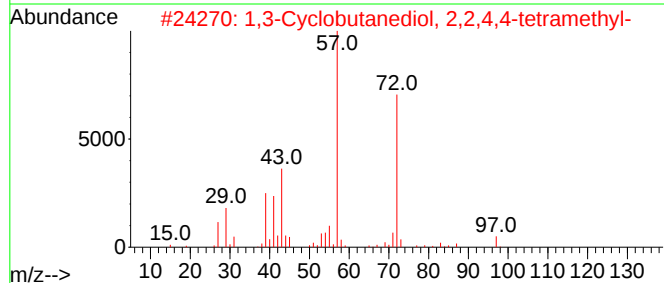
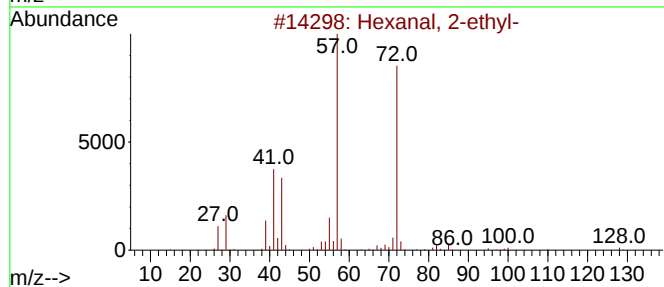
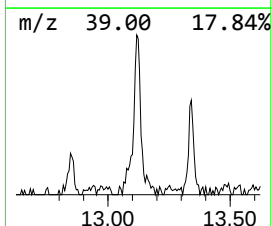
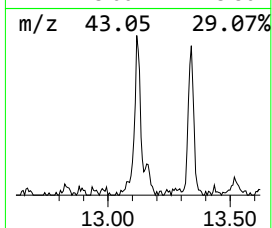
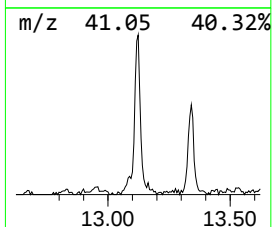
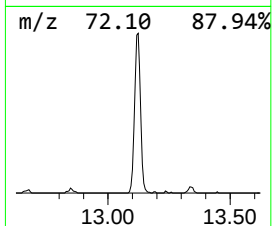
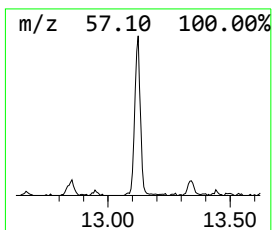
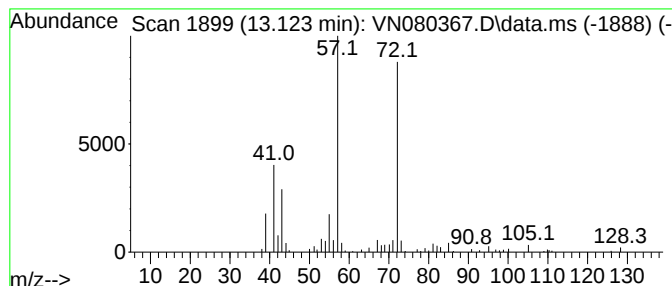
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 4 Hexanal, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.123	13.47 ug/l	288170	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	90
2			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	64
3			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	64
4			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	64
5			Methylephedrine	179	C11H17NO	000552-79-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

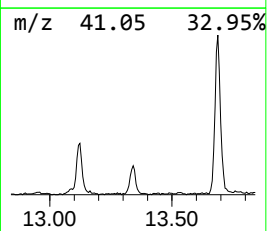
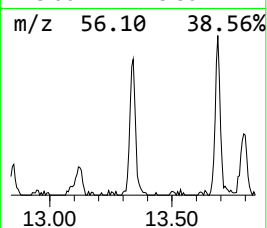
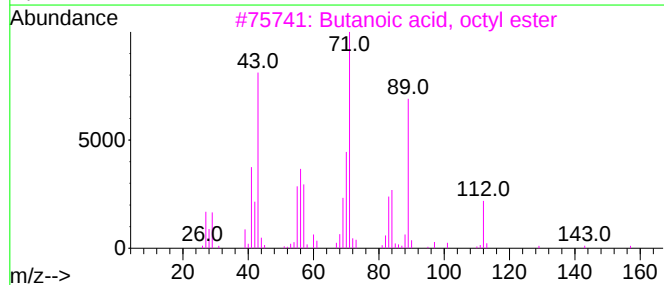
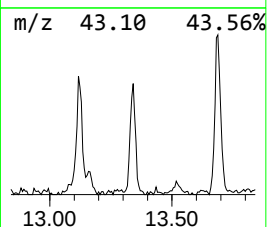
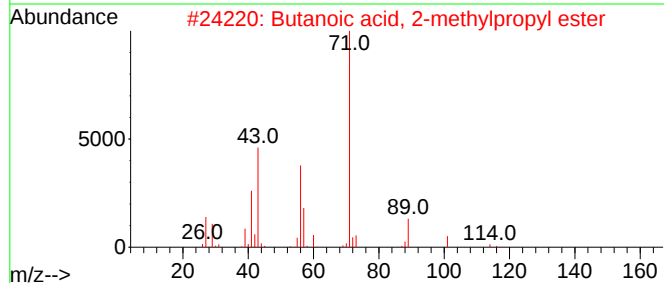
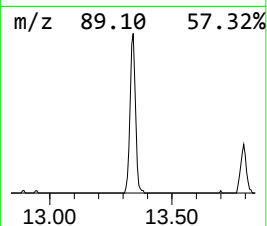
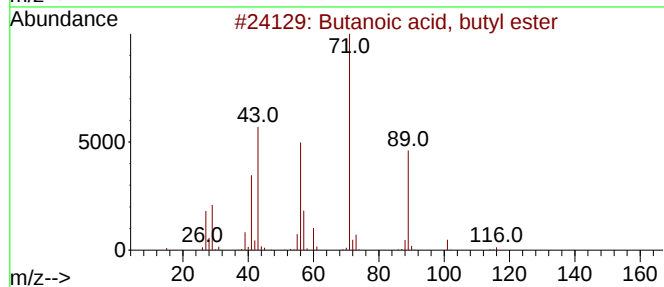
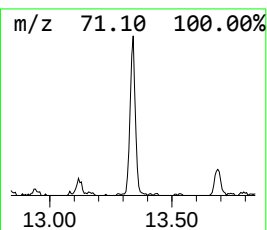
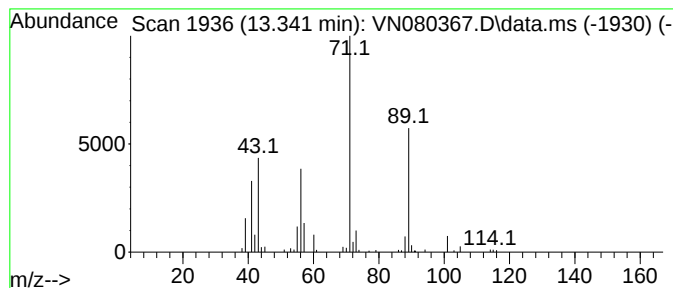
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	6.56 ug/l	140349	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	74
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	56
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	56
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

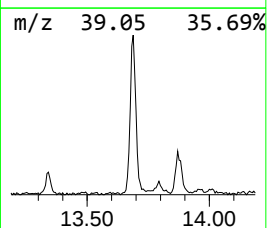
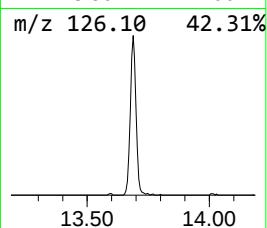
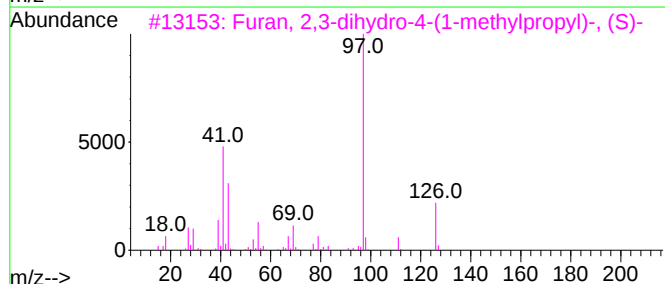
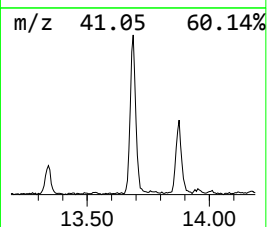
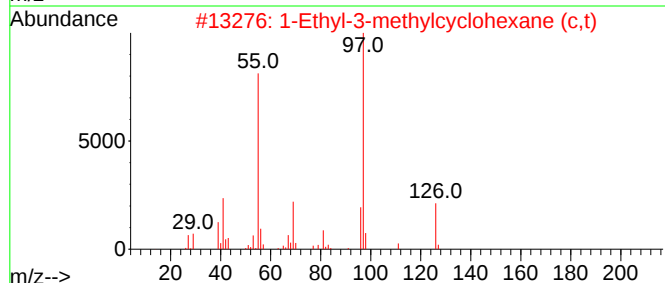
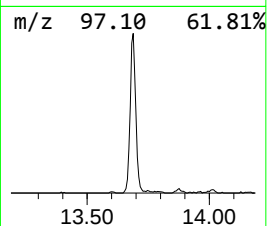
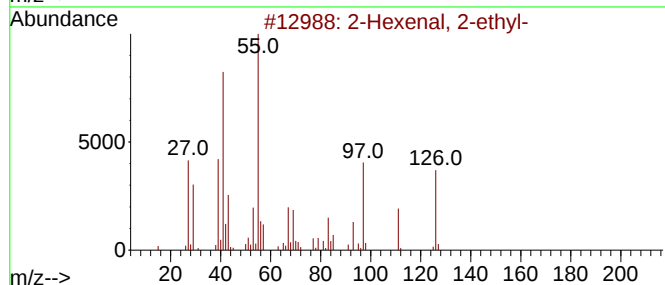
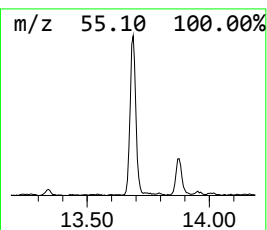
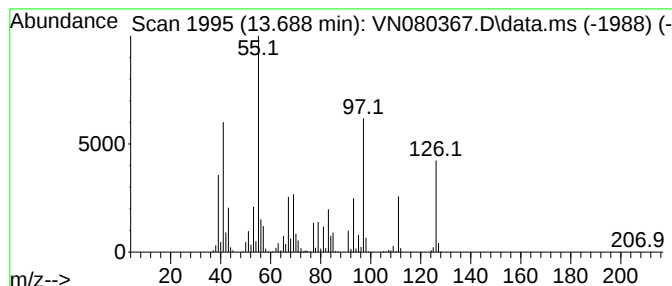
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Hexenal, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	37.50 ug/l	802613	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	95
2			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	47
3			Furan, 2,3-dihydro-4-(1-methylpr...	126	C8H14O	034379-54-9	43
4			3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	43
5			5-Hydroxymethylfurfural	126	C6H6O3	000067-47-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

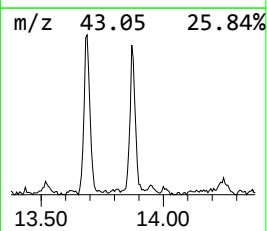
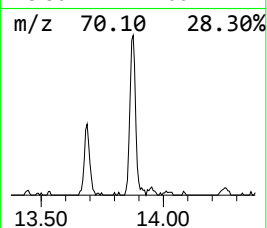
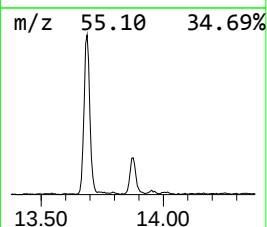
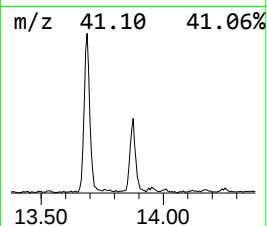
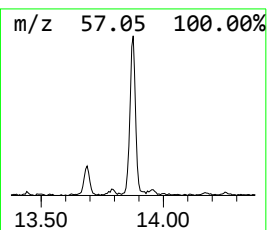
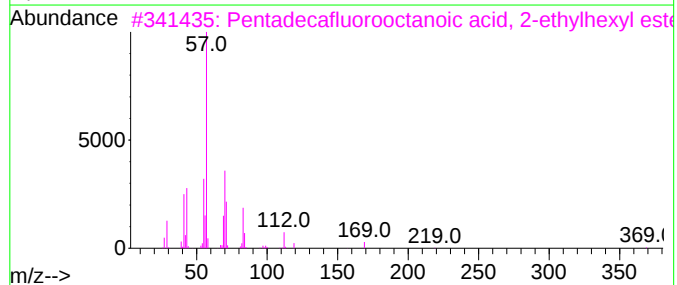
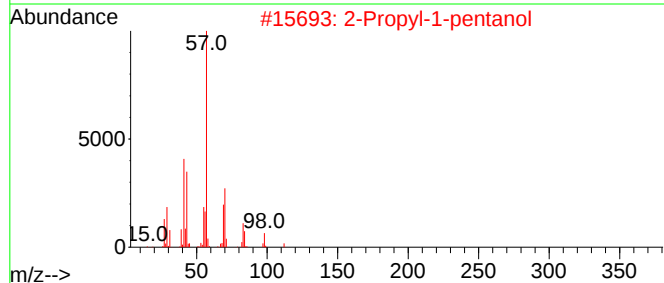
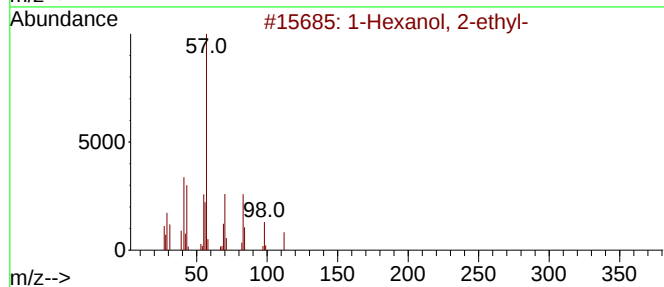
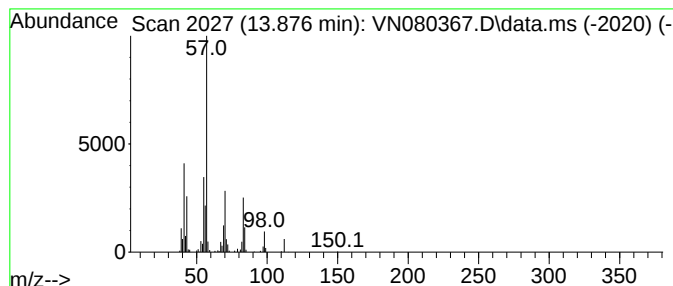
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	14.93 ug/l	319571	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080367.D
Acq On : 05 Dec 2023 15:34
Operator : JC\MD
Sample : 05616-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.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
Propane	2.083	12.7	ug/l	134575	1	8.229	530526	50.0
Acetaldehyde	2.659	5.2	ug/l	55262	1	8.229	530526	50.0
Butanal	7.224	29.6	ug/l	314238	1	8.229	530526	50.0
Hexanal, 2-ethyl-	13.123	13.5	ug/l	288170	4	13.794	1070020	50.0
Butanoic acid, ...	13.341	6.6	ug/l	140349	4	13.794	1070020	50.0
2-Hexenal, 2-et...	13.688	37.5	ug/l	802613	4	13.794	1070020	50.0
1-Hexanol, 2-et...	13.876	14.9	ug/l	319571	4	13.794	1070020	50.0