

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
 Data File : VN077898.D
 Acq On : 25 May 2023 13:39
 Operator : JC\MD
 Sample : 02884-03 100X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2002

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\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN077898.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.671	115	122	132	rBV	633721	1112744	46.93%	6.843%
2	2.824	141	148	155	rVB2	26363	61752	2.60%	0.380%
3	3.800	305	314	327	rBV	50799	146659	6.19%	0.902%
4	4.294	387	398	414	rBV	748379	2167560	91.43%	13.331%
5	6.730	802	812	826	rBV2	188991	580911	24.50%	3.573%
6	7.235	889	898	909	rBV4	18511	49718	2.10%	0.306%
7	8.177	1048	1058	1062	rBV	327412	775393	32.71%	4.769%
8	8.229	1062	1067	1079	rVB	592020	1312046	55.34%	8.069%
9	8.588	1119	1128	1142	rBV	326577	740782	31.25%	4.556%
10	9.106	1207	1216	1231	rBV	870003	1793339	75.64%	11.029%
11	9.347	1250	1257	1265	rVB2	23813	51352	2.17%	0.316%
12	10.435	1436	1442	1450	rVB2	20885	41696	1.76%	0.256%
13	10.570	1456	1465	1481	rBV	1254055	2370823	100.00%	14.581%
14	10.806	1496	1505	1515	rBV2	104315	187885	7.92%	1.155%
15	10.953	1522	1530	1538	rBV	64282	115917	4.89%	0.713%
16	11.782	1665	1671	1678	rBV2	41675	73295	3.09%	0.451%
17	11.870	1678	1686	1699	rVV	1079111	1934259	81.59%	11.896%
18	11.976	1699	1704	1710	rVB5	15211	27345	1.15%	0.168%
19	12.800	1837	1844	1847	rBV	24281	39851	1.68%	0.245%
20	12.853	1847	1853	1863	rVB	776138	1393892	58.79%	8.572%
21	13.800	2007	2014	2022	rVV	739715	1258080	53.07%	7.737%
22	15.647	2320	2328	2334	rBV3	12219	24805	1.05%	0.153%

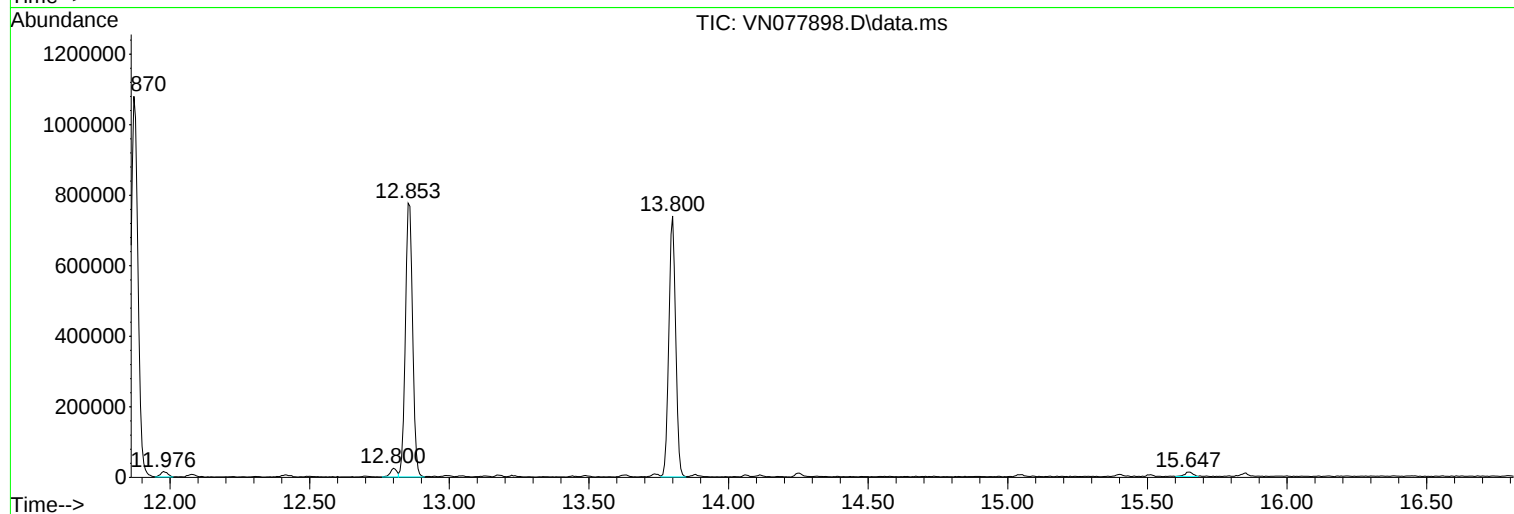
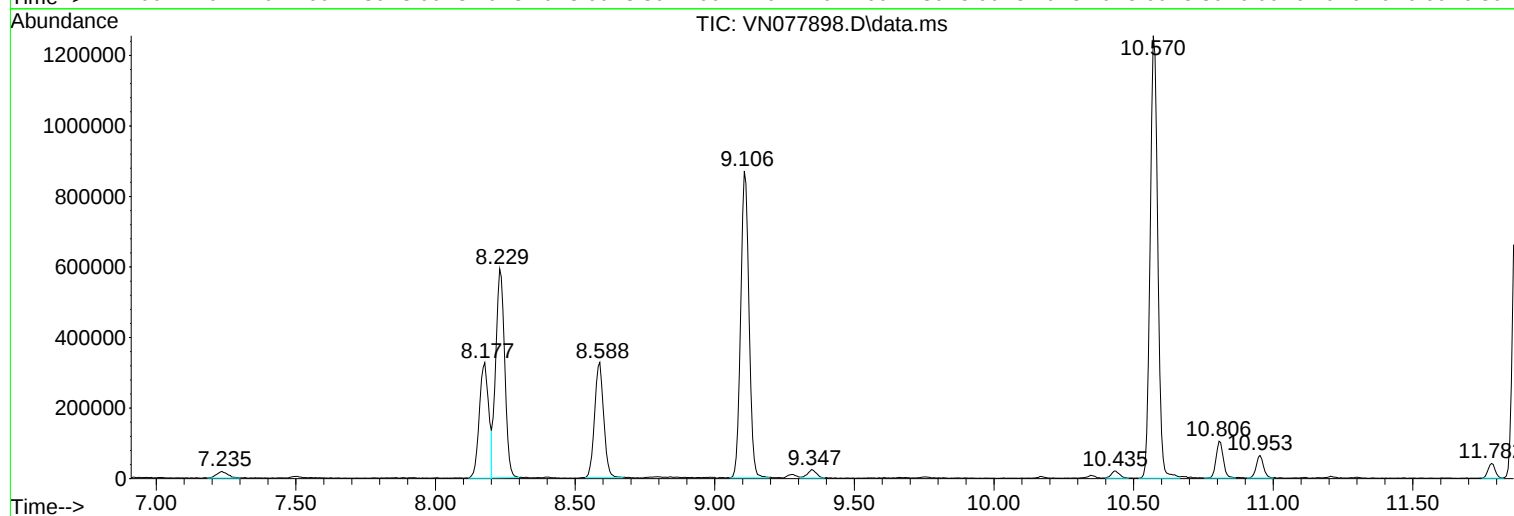
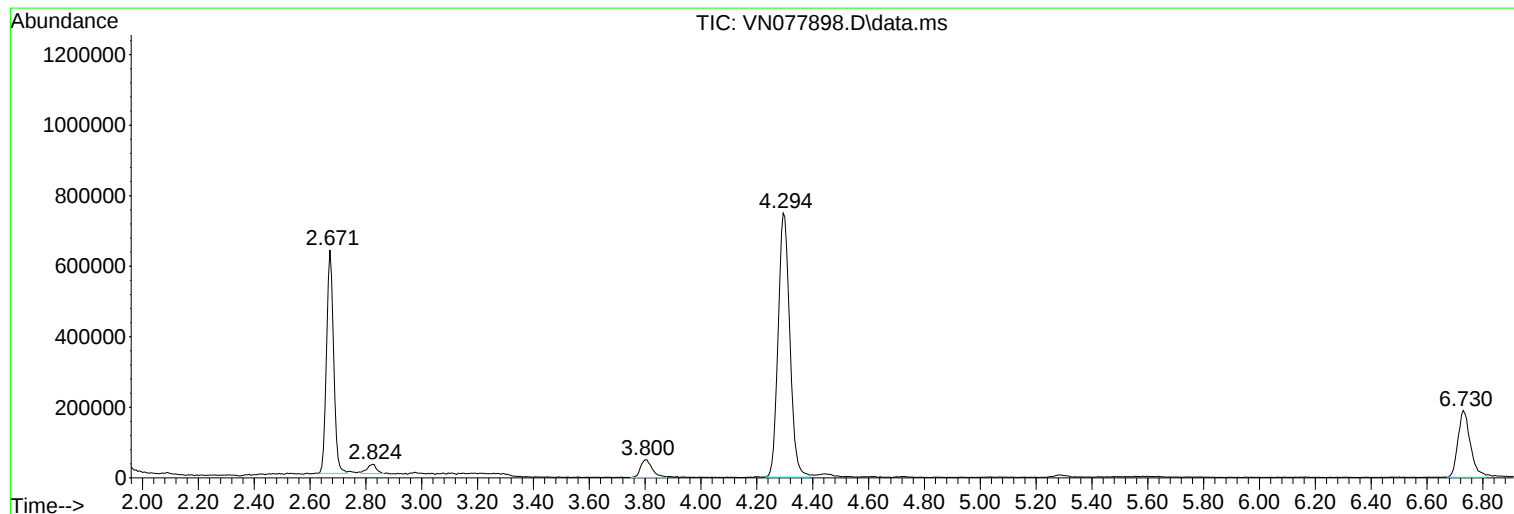
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Quant Title : SW846 8260

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



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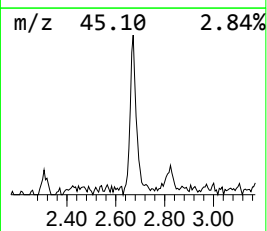
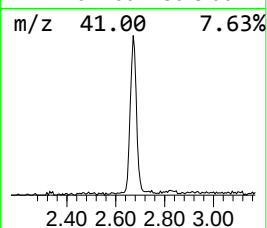
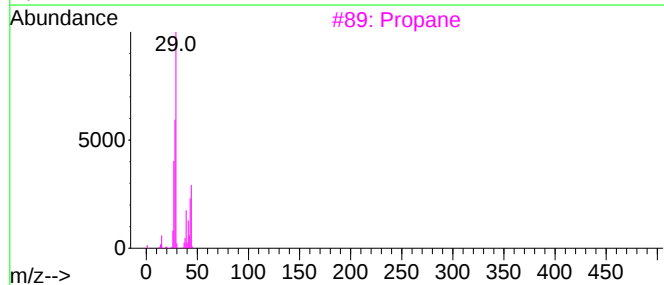
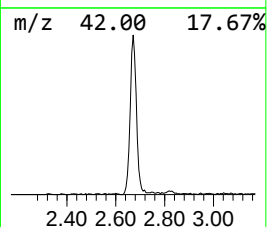
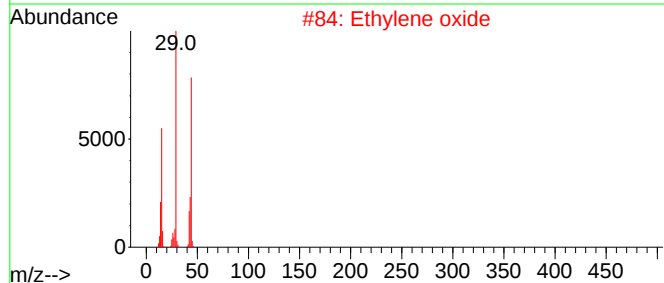
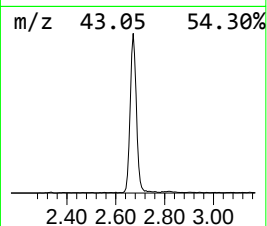
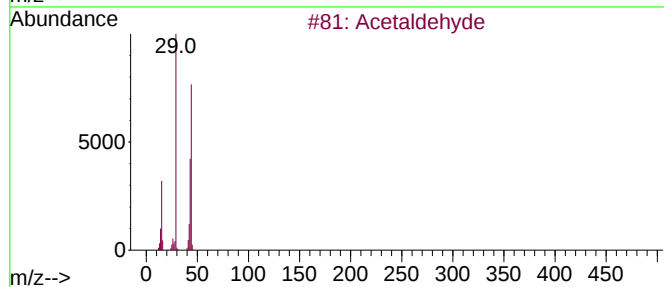
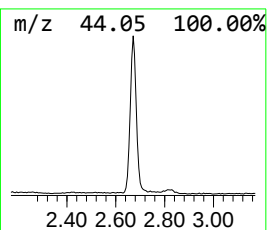
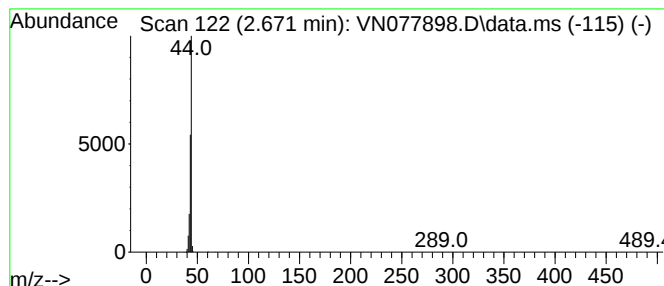
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.671	42.40 ug/l	1112740	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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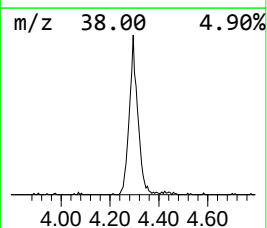
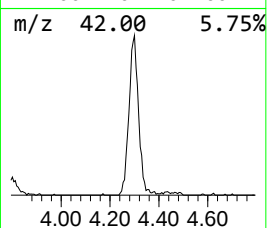
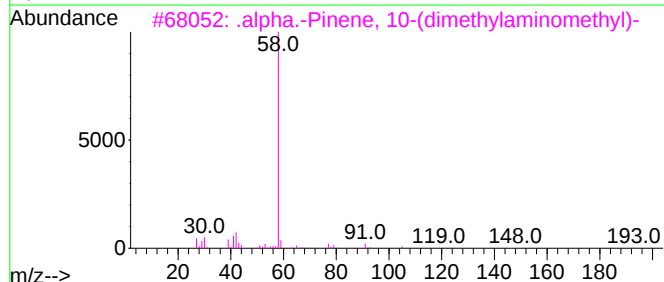
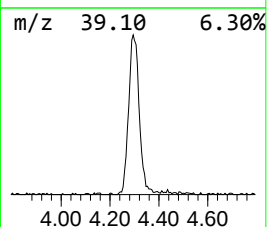
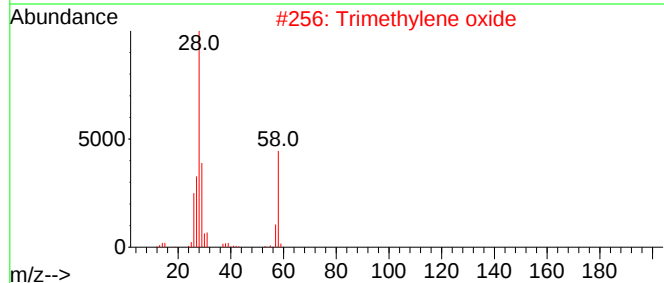
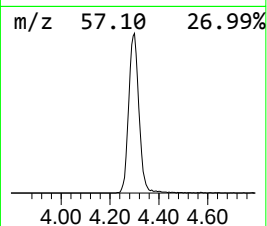
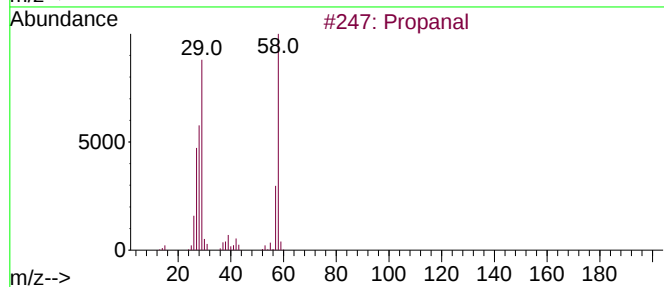
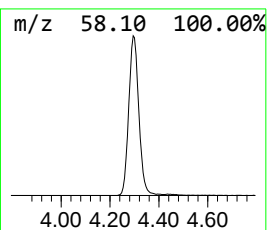
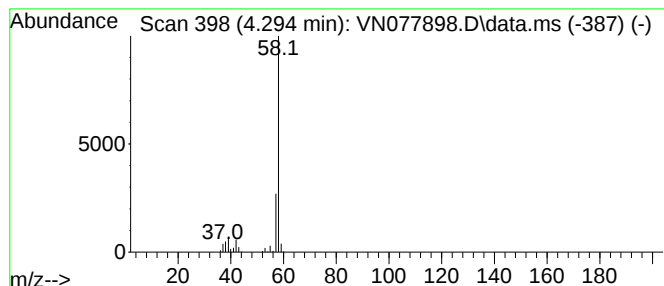
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Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	82.60 ug/l	2167560	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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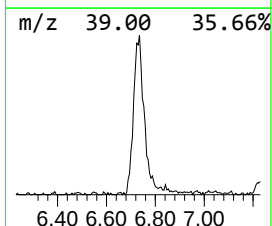
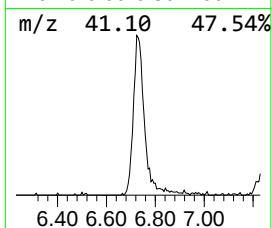
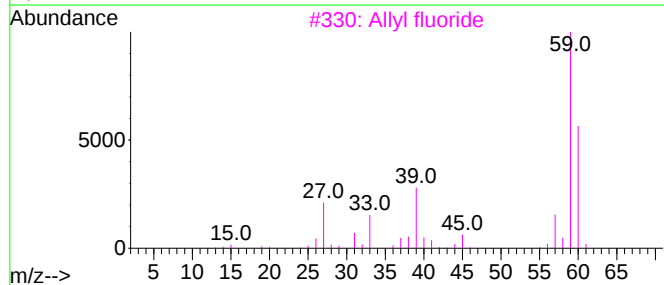
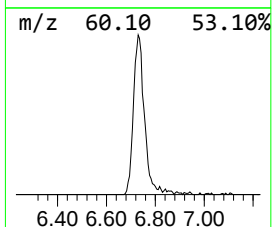
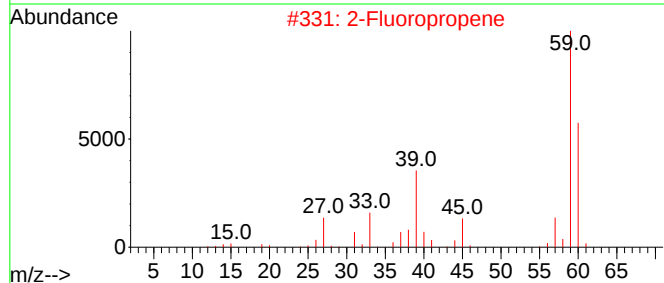
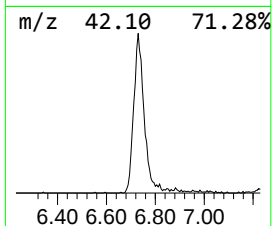
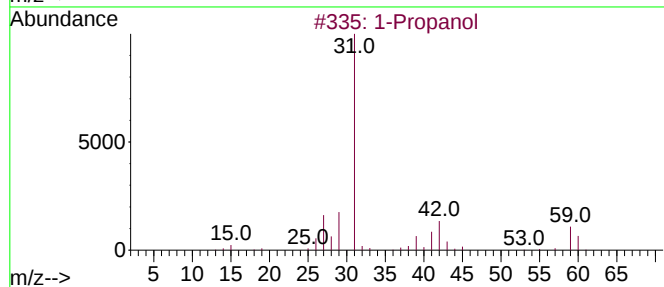
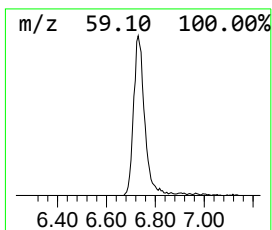
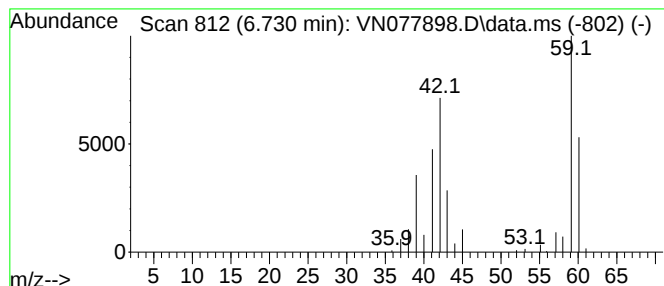
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.730	22.14 ug/l	580911	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	2-Fluoropropene			60	C3H5F	001184-60-7	64
3	Allyl fluoride			60	C3H5F	000818-92-8	53
4	Formamidoxime			60	CH4N2O	000624-82-8	16
5	Cyclopropane			42	C3H6	000075-19-4	9



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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
Acetaldehyde	2.671	42.4	ug/l	1112740	1	8.235	1312050	50.0
Propanal	4.294	82.6	ug/l	2167560	1	8.235	1312050	50.0
1-Propanol	6.730	22.1	ug/l	580911	1	8.235	1312050	50.0