

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
 Data File : VX046496.D
 Acq On : 04 Jun 2025 13:28
 Operator : JC/MD
 Sample : Q2175-05 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 52525-B

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_X\Method\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046496.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	31	rBV	22891	35358	7.60%	1.280%
2	1.453	56	60	68	rVB	25137	31741	6.83%	1.149%
3	1.569	70	79	80	rBV6	8576	18917	4.07%	0.685%
4	5.385	691	705	721	rBV2	52669	157162	33.80%	5.689%
5	5.550	721	732	747	rVV	78135	222364	47.83%	8.050%
6	5.952	788	798	813	rBV	60241	164051	35.28%	5.939%
7	6.757	921	930	949	rBV	138476	334775	72.00%	12.119%
8	8.647	1234	1240	1250	rBV	295433	464934	100.00%	16.831%
9	10.055	1465	1471	1480	rBV	298640	425754	91.57%	15.413%
10	10.299	1506	1511	1516	rBV3	3284	5554	1.19%	0.201%
11	11.079	1634	1639	1651	rBV	259004	331857	71.38%	12.013%
12	12.018	1788	1793	1802	rBV	310130	394235	84.79%	14.272%
13	12.585	1875	1886	1901	rBV2	14734	32611	7.01%	1.181%
14	12.817	1919	1924	1938	rVB2	2436	10365	2.23%	0.375%
15	13.103	1960	1971	1972	rBV2	2920	7083	1.52%	0.256%
16	13.780	2076	2082	2089	rBV	6530	9447	2.03%	0.342%
17	14.188	2145	2149	2164	rBV2	19926	40335	8.68%	1.460%
18	14.634	2216	2222	2227	rBV	15219	21569	4.64%	0.781%
19	14.780	2241	2246	2250	rBV	9562	12757	2.74%	0.462%
20	15.475	2356	2360	2370	rVB3	6204	11465	2.47%	0.415%
21	15.615	2376	2383	2386	rBV2	7285	12156	2.61%	0.440%
22	15.652	2386	2389	2393	rVB3	4578	6407	1.38%	0.232%
23	15.841	2412	2420	2425	rVB5	2959	5943	1.28%	0.215%
24	16.475	2519	2524	2532	rBV	3299	5546	1.19%	0.201%

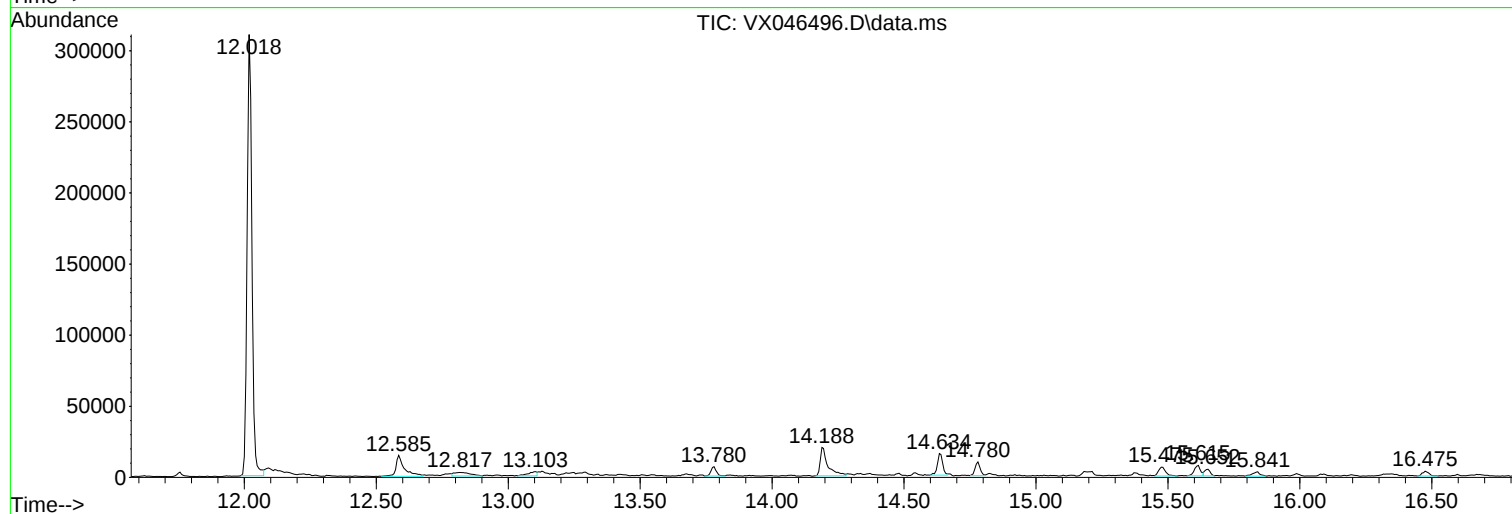
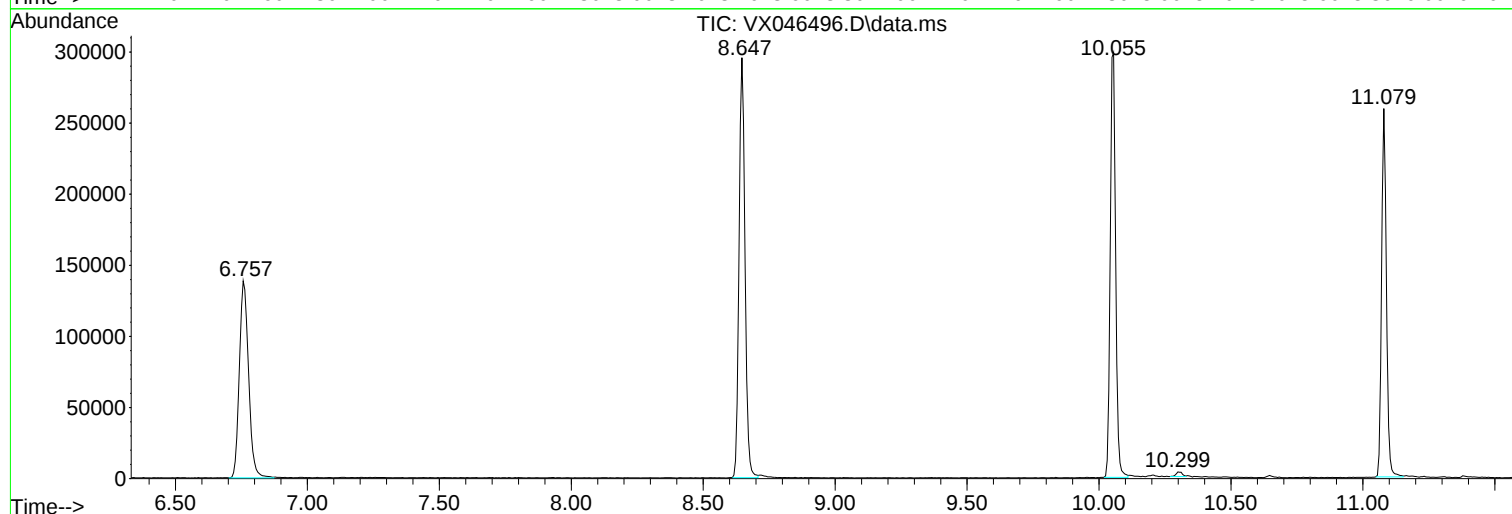
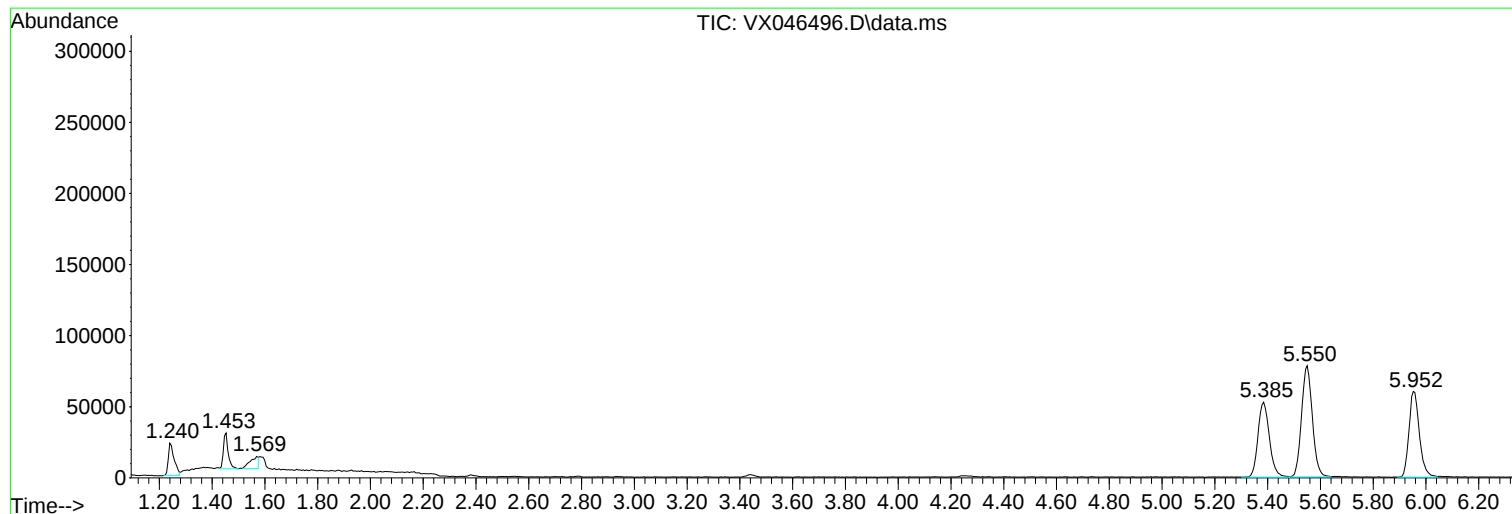
Sum of corrected areas: 2762386

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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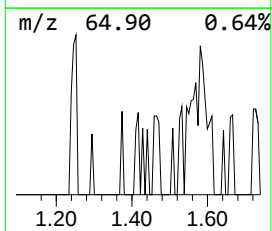
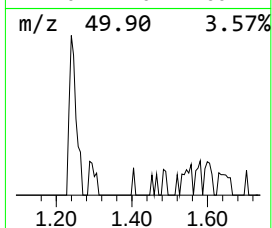
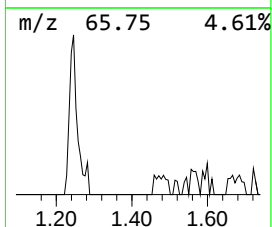
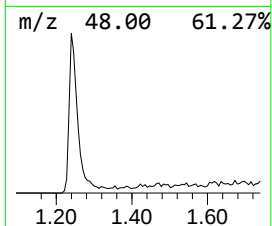
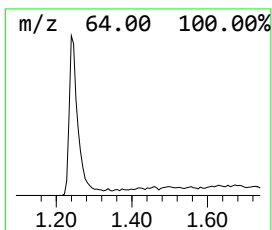
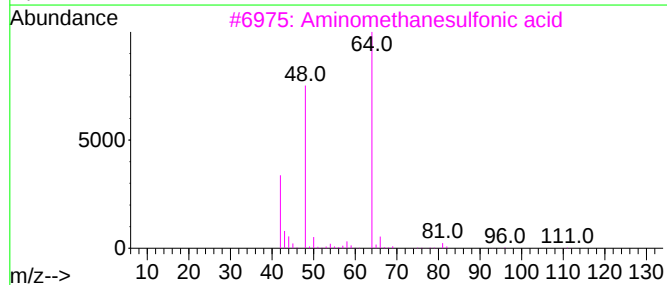
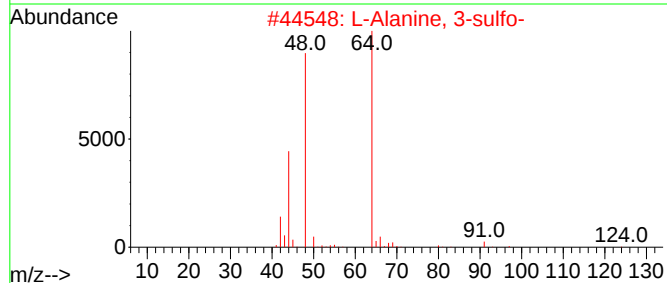
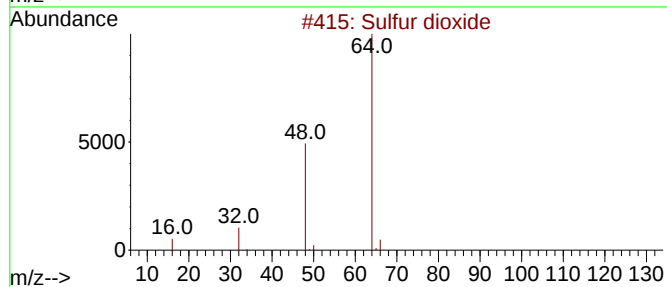
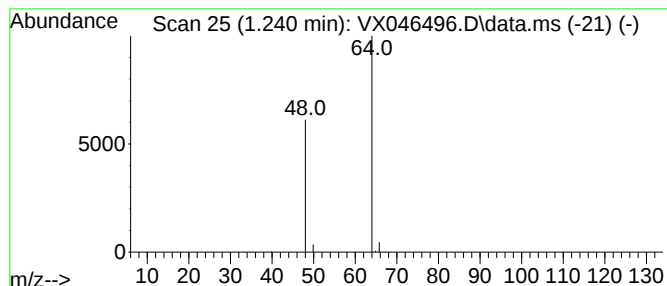
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	7.95 ug/l	35358	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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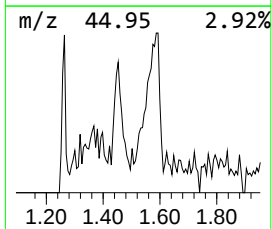
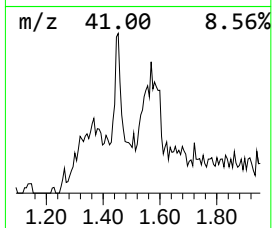
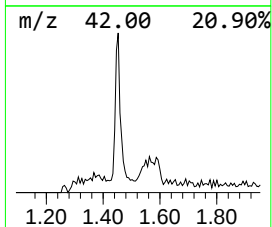
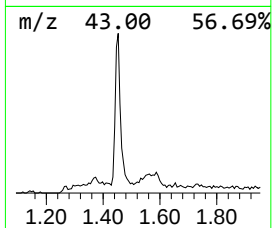
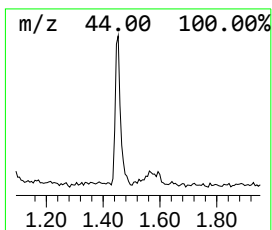
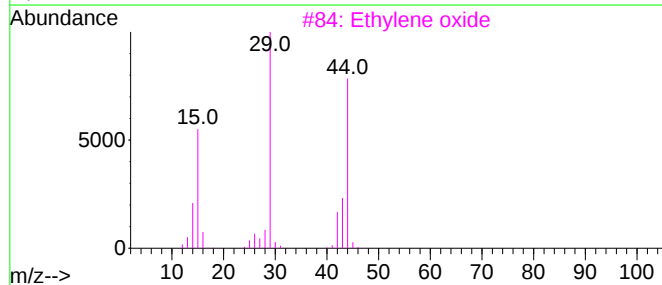
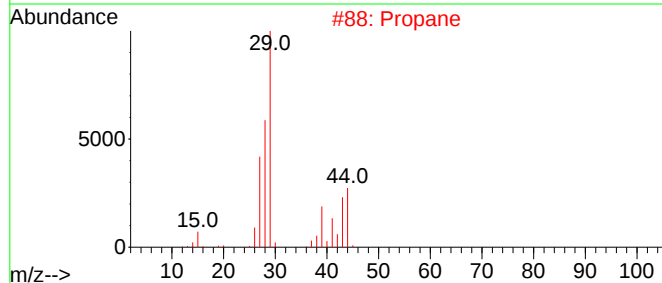
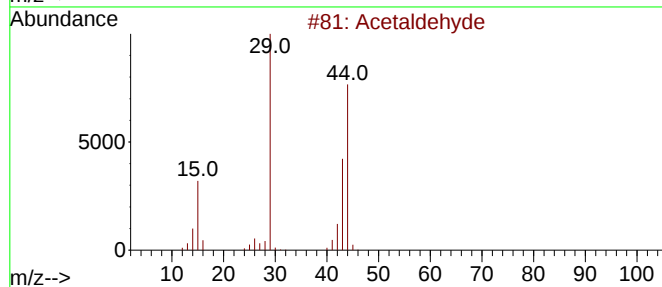
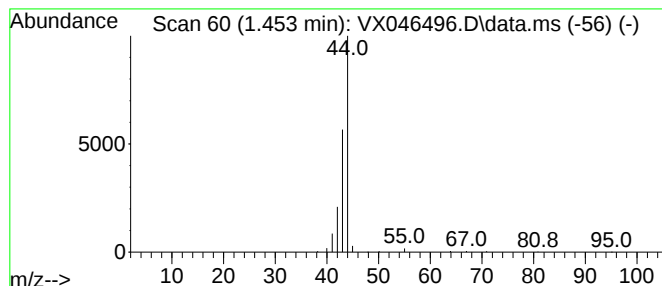
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Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	7.14 ug/l	31741	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			1-Propanol, 2-amino-, (+/-)-	75	C3H9NO	006168-72-5	4
5			D-Alanine	89	C3H7NO2	000338-69-2	4



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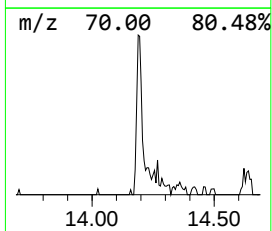
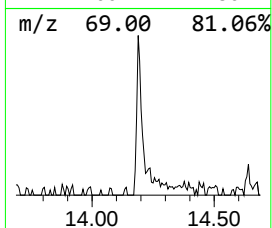
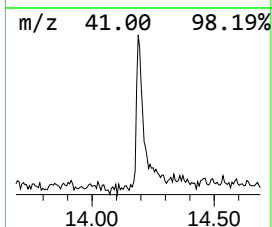
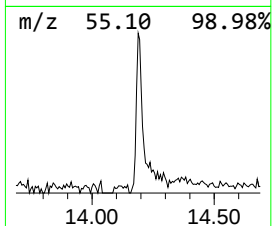
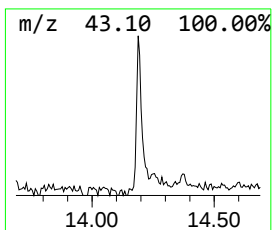
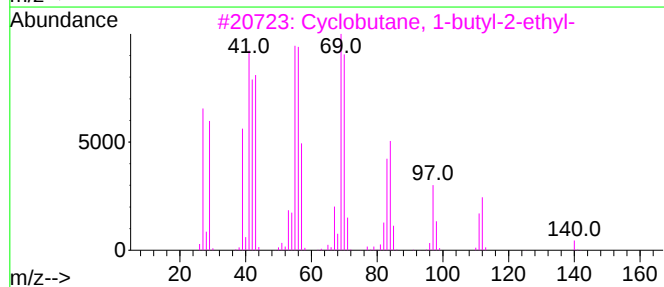
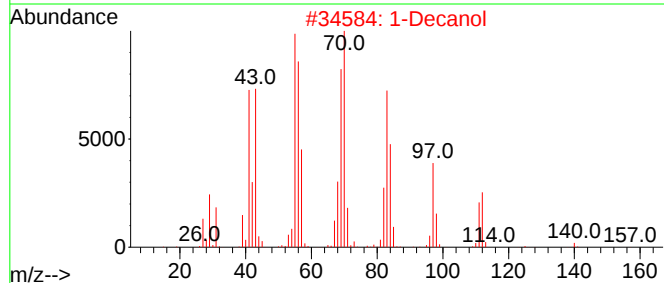
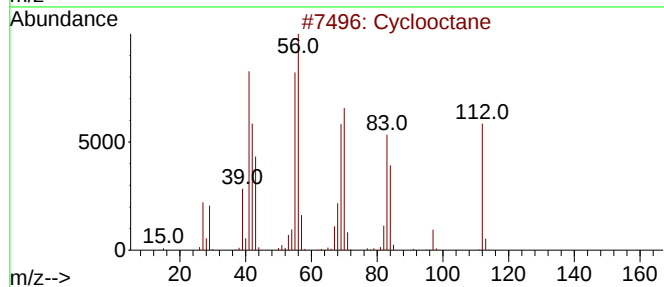
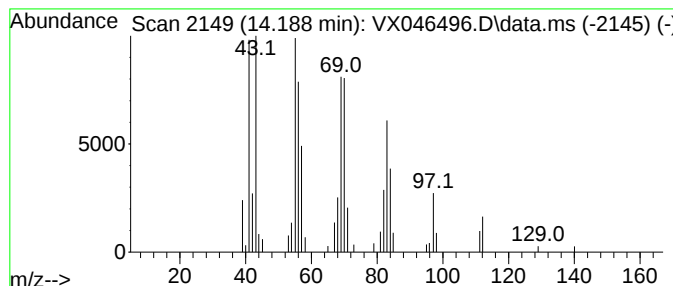
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Peak Number 3 Cyclooctane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	5.12 ug/l	40335	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	87
2			1-Decanol	158	C10H22O	000112-30-1	87
3			Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1010150-67-3	70
4			1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	62
5			Octane, 3-chloro-	148	C8H17Cl	001117-79-9	58



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	8.0	ug/l	35358	1	5.550	222364	50.0
Acetaldehyde	1.453	7.1	ug/l	31741	1	5.550	222364	50.0
Cyclooctane	14.188	5.1	ug/l	40335	4	12.018	394235	50.0