

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050418\
 Data File : VU023616.D
 Acq On : 03 May 2018 22:11
 Operator : MD/SY
 Sample : J2630-09
 Misc : 25mL/MSVOA U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : W:\HPCHEM1\MSVOA U\METHOD\SOMUTR050418WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

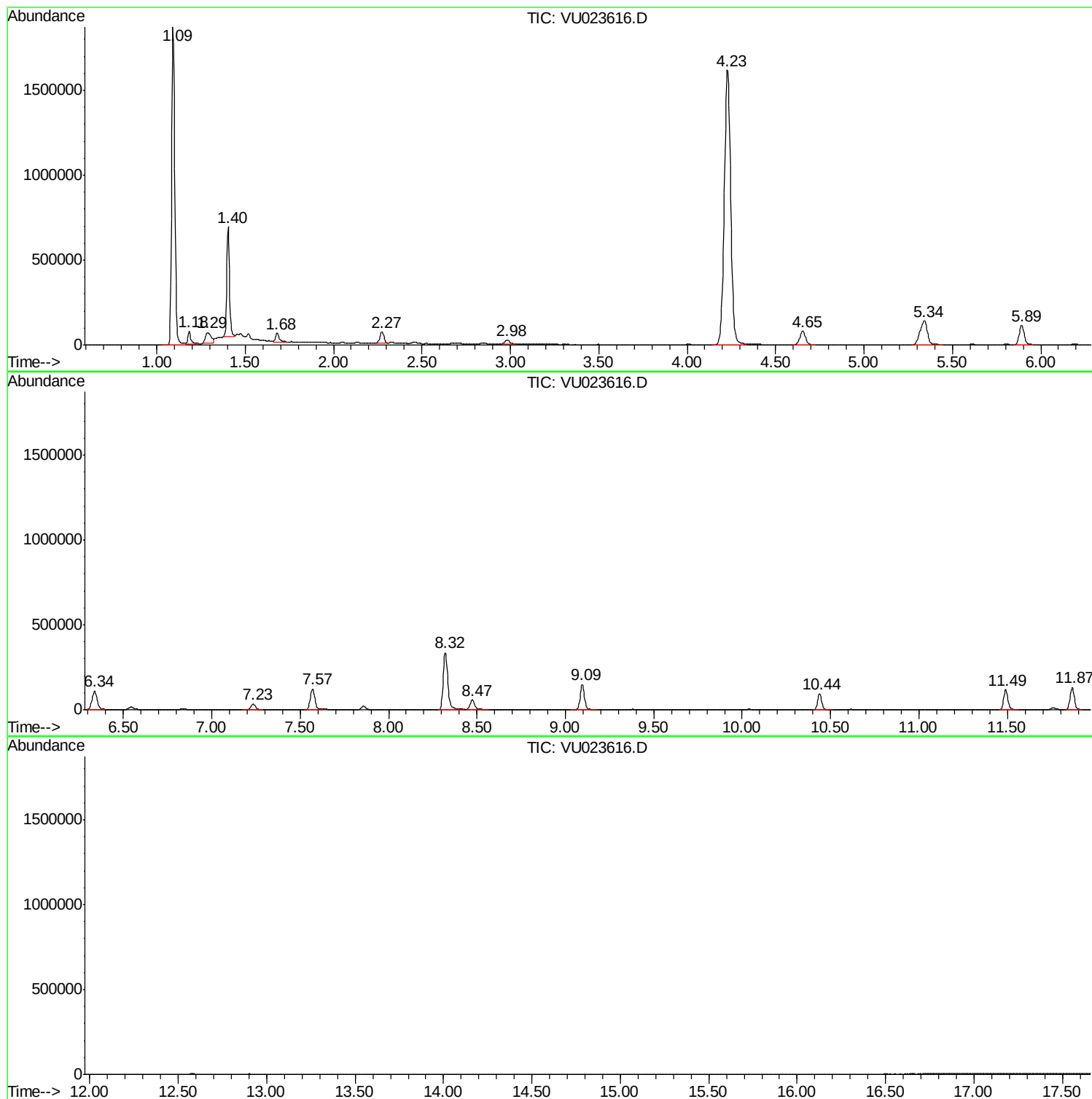
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.092	137	156	178	rBV	1873546	2300702	56.86%	22.288%
2	1.182	178	184	202	rVB	73646	84031	2.08%	0.814%
3	1.288	207	217	227	rBV	64887	148536	3.67%	1.439%
4	1.404	245	253	265	rBV	646085	698856	17.27%	6.770%
5	1.680	333	339	357	rVB	51587	75283	1.86%	0.729%
6	2.275	514	524	534	rVB	63865	97553	2.41%	0.945%
7	2.982	735	744	759	rVB	23130	42834	1.06%	0.415%
8	4.227	1105	1131	1165	rBV	1620129	4046551	100.00%	39.200%
9	4.654	1247	1264	1284	rVB	79341	182946	4.52%	1.772%
10	5.342	1456	1478	1510	rBV2	140487	414675	10.25%	4.017%
11	5.892	1635	1649	1669	rBV	113842	226063	5.59%	2.190%
12	6.336	1773	1787	1805	rBV	108565	214902	5.31%	2.082%
13	7.233	2048	2066	2082	rBV	32709	57956	1.43%	0.561%
14	7.571	2157	2171	2188	rBV	122887	219810	5.43%	2.129%
15	8.320	2392	2404	2436	rBV	335272	604325	14.93%	5.854%
16	8.474	2441	2452	2480	rVB	56612	102243	2.53%	0.990%
17	9.095	2625	2645	2669	rBV	148120	247847	6.12%	2.401%
18	10.439	3051	3063	3085	rVB	94964	149536	3.70%	1.449%
19	11.490	3379	3390	3412	rBV	118993	193535	4.78%	1.875%
20	11.866	3496	3507	3524	rBV	131684	214604	5.30%	2.079%

Sum of corrected areas: 10322788

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Quant Method : W:\HPCHEM1\MSVOA U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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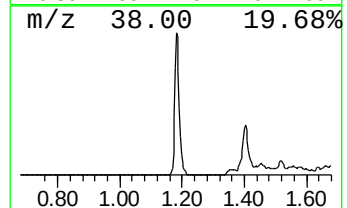
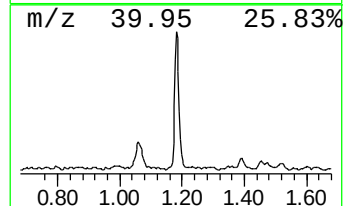
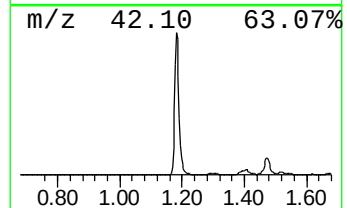
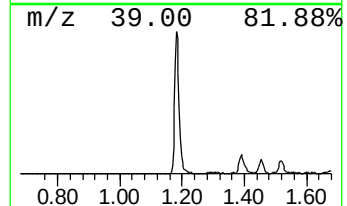
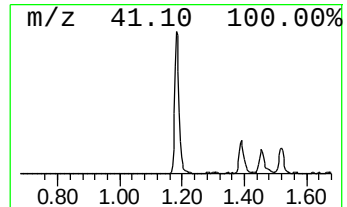
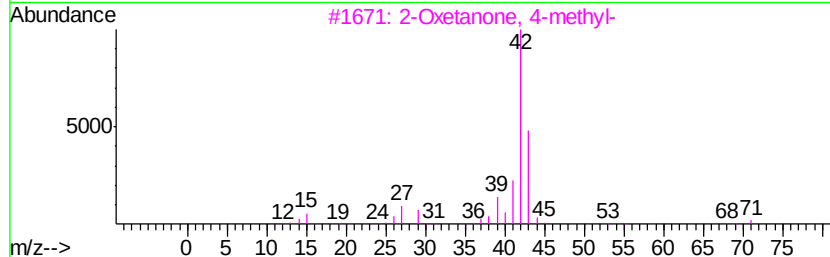
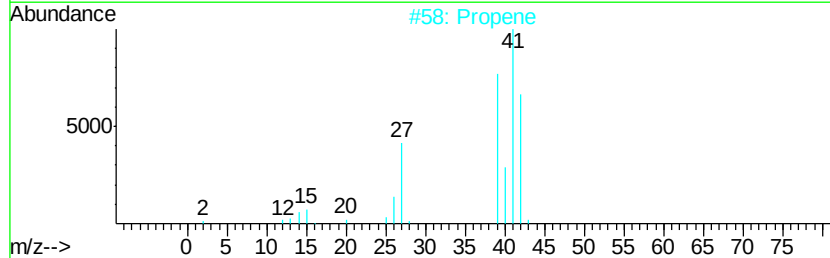
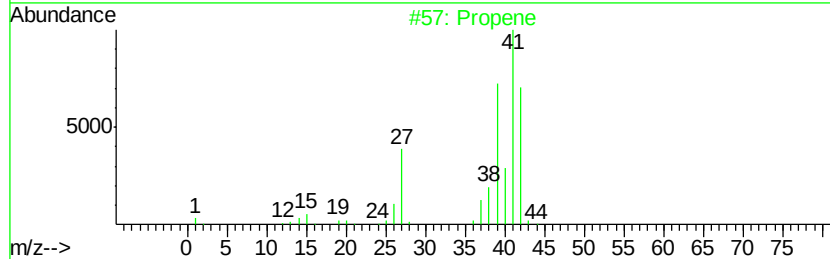
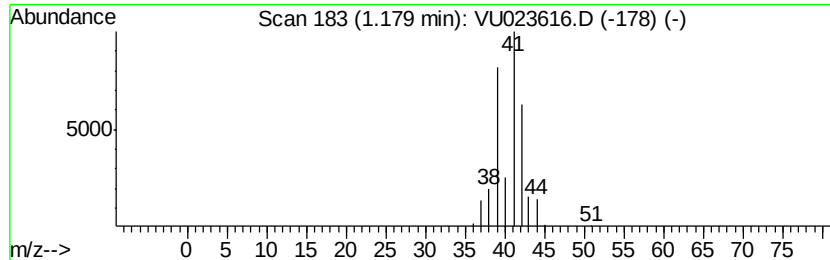
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Peak Number 2 (DEL) Alkane: Cyclic1.18 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	1.86 ug/L	84031	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Propene	42	C3H6	000115-07-1	42
3		2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
4		Cyclopropene	40	C3H4	002781-85-3	9
5		Cyclopropane	42	C3H6	000075-19-4	9



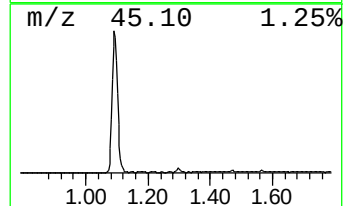
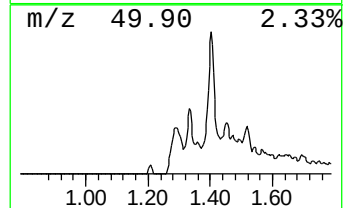
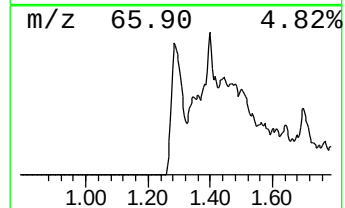
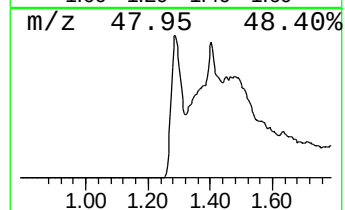
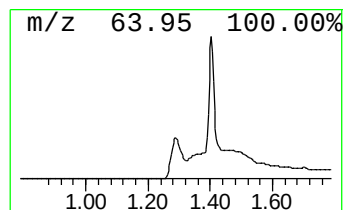
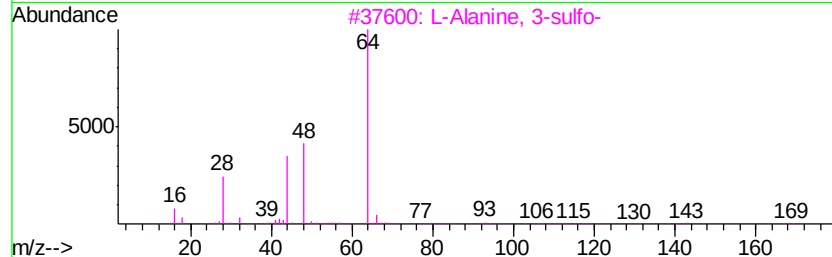
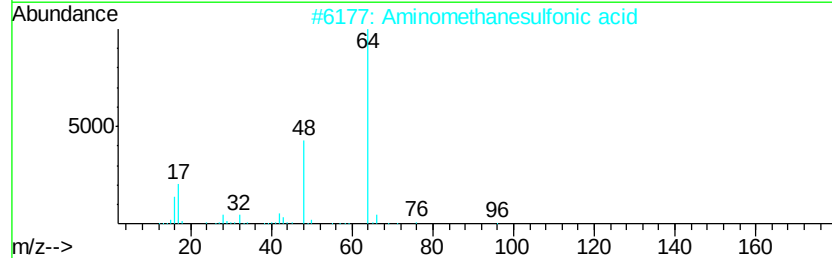
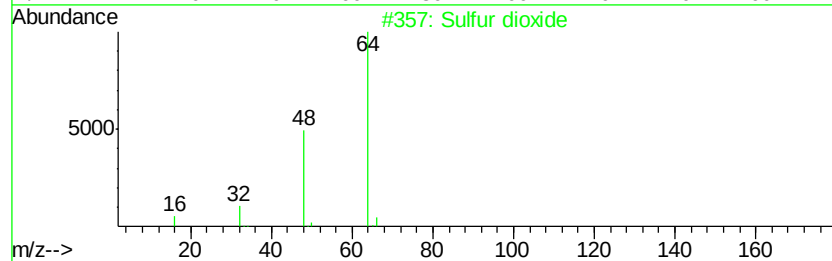
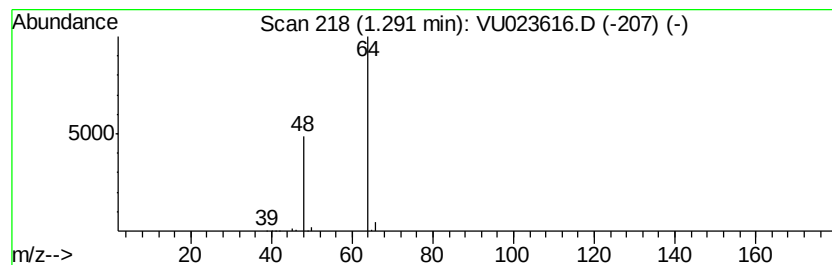
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Peak Number 3 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.29	3.29 ug/L	148536	1,4-Difluorobenzene	5.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	9
5	Ethene, 1,1-difluoro-		64	C2H2F2	000075-38-7	4



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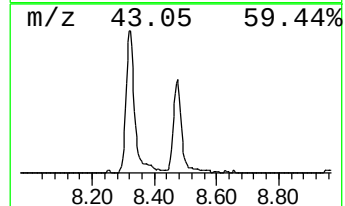
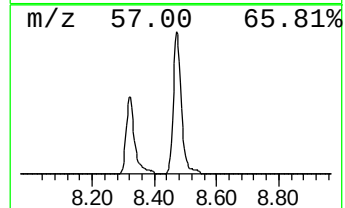
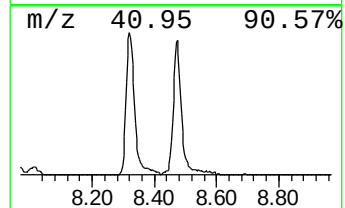
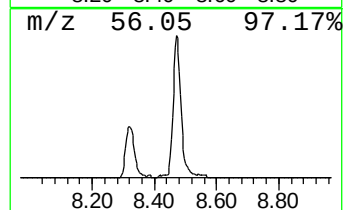
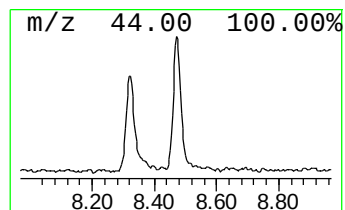
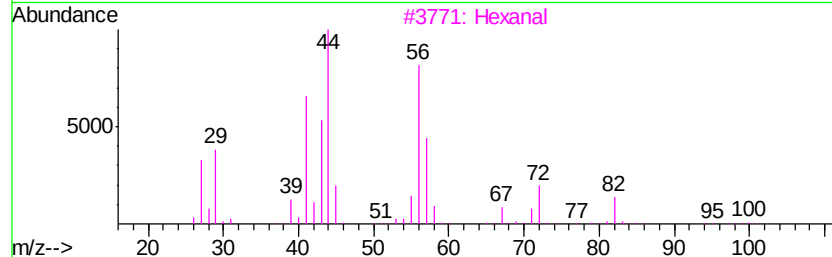
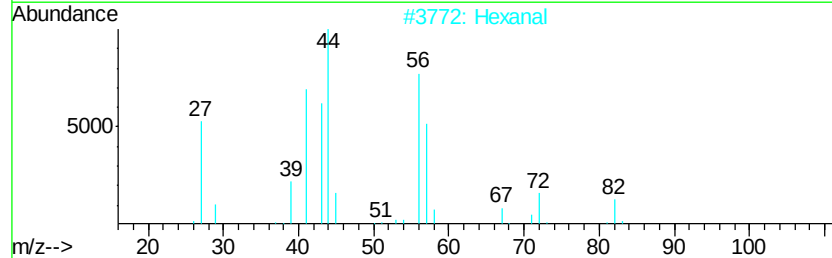
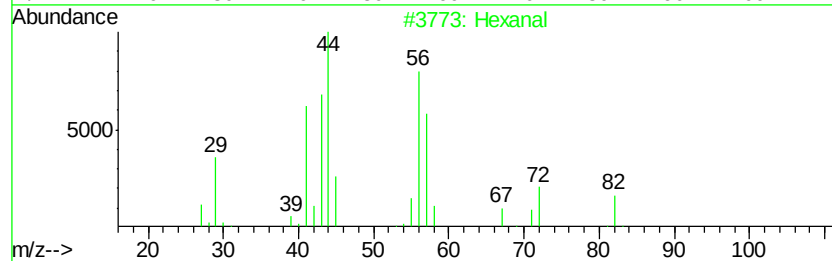
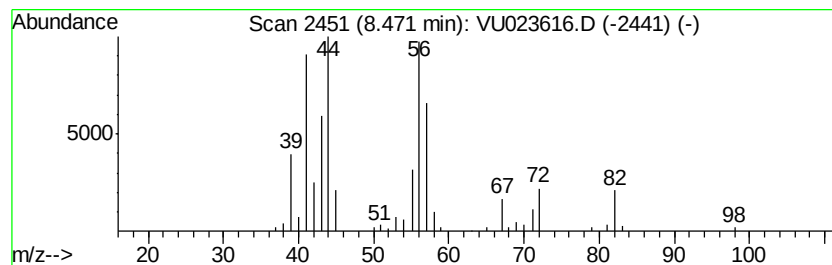
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Peak Number 5 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	2.06 ug/L	102243	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	72
2		Hexanal	100	C6H12O	000066-25-1	64
3		Hexanal	100	C6H12O	000066-25-1	64
4		Hexanal	100	C6H12O	000066-25-1	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.18	1.9	ug/L	84031	1	5.89	226063	5.0
Sulfur dioxide	1.29	3.3	ug/L	148536	1	5.89	226063	5.0
Hexanal	8.47	2.1	ug/L	102243	2	9.09	247847	5.0