

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
 Data File : VX035663.D
 Acq On : 15 May 2023 14:26
 Operator : JC/MD
 Sample : 02751-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-PRO-03-89-05072023

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\82X051123W.M
 Title : SW846 8260

Signal : TIC: VX035663.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	312318	309299	26.72%	4.116%
2	1.264	26	29	32	rBV	29187	26178	2.26%	0.348%
3	1.356	40	44	54	rBV2	133869	189845	16.40%	2.526%
4	1.453	58	60	64	rVV	10633	11923	1.03%	0.159%
5	1.496	64	67	76	rVB	18765	22034	1.90%	0.293%
6	1.660	87	94	102	rVV2	9579	16619	1.44%	0.221%
7	1.752	105	109	117	rVB	15223	22763	1.97%	0.303%
8	1.910	130	135	139	rBV	22993	31055	2.68%	0.413%
9	1.965	139	144	155	rVB3	20324	44875	3.88%	0.597%
10	2.166	171	177	182	rBV2	7891	15385	1.33%	0.205%
11	2.288	193	197	205	rVB	8634	15604	1.35%	0.208%
12	3.331	360	368	375	rVB3	6517	16243	1.40%	0.216%
13	4.233	509	516	523	rBV3	4379	12346	1.07%	0.164%
14	5.385	693	705	718	rBV2	132675	381377	32.95%	5.075%
15	5.550	718	732	749	rVB	218817	629633	54.39%	8.379%
16	5.952	788	798	809	rBV	156199	416810	36.01%	5.547%
17	6.763	920	931	948	rBV	359725	868439	75.02%	11.557%
18	7.123	982	990	1003	rBV2	60105	135610	11.72%	1.805%
19	7.574	1058	1064	1072	rBV	16118	32962	2.85%	0.439%
20	8.647	1233	1240	1248	rBV	747215	1157557	100.00%	15.405%
21	8.720	1248	1252	1260	rVB2	11245	18905	1.63%	0.252%
22	9.519	1377	1383	1396	rBV	96878	142675	12.33%	1.899%
23	10.055	1465	1471	1482	rBV	731873	1024025	88.46%	13.628%
24	10.854	1594	1602	1610	rBV	43393	56196	4.85%	0.748%
25	11.079	1634	1639	1652	rVB	646058	802785	69.35%	10.683%
26	11.927	1771	1778	1788	rBV2	34235	45350	3.92%	0.604%
27	12.018	1788	1793	1801	rBV	737670	936889	80.94%	12.468%
28	12.853	1926	1930	1943	rVB	35647	48025	4.15%	0.639%
29	15.542	2363	2371	2381	rBV2	25564	46006	3.97%	0.612%
30	16.469	2517	2523	2533	rBV3	19890	36952	3.19%	0.492%

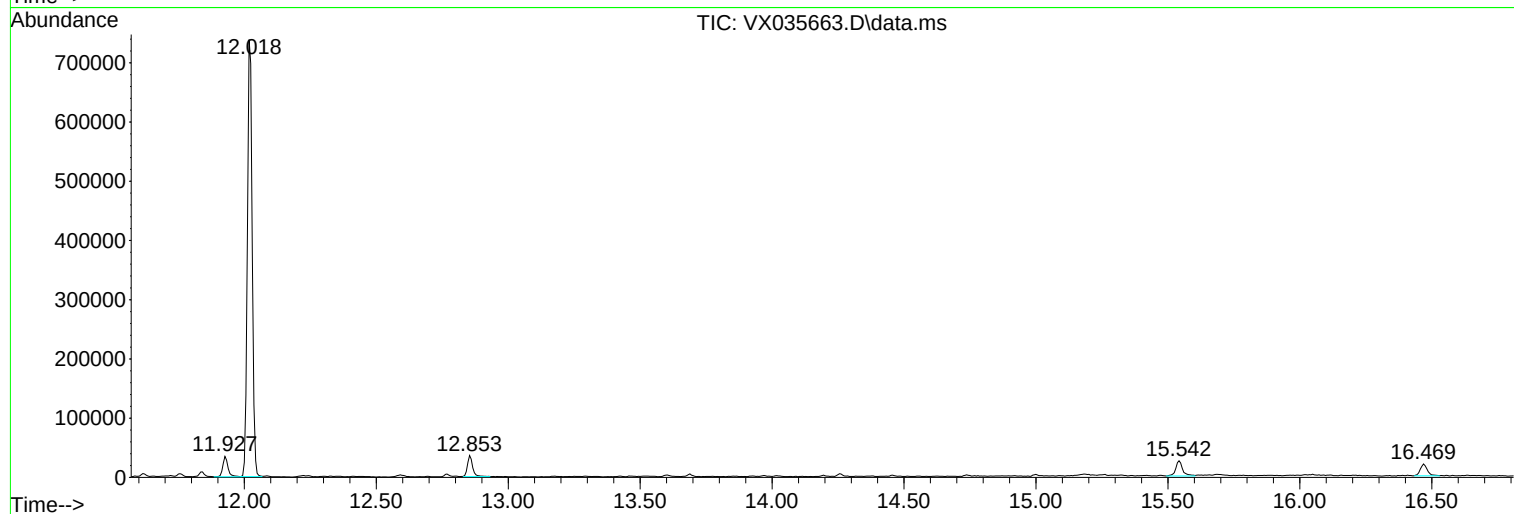
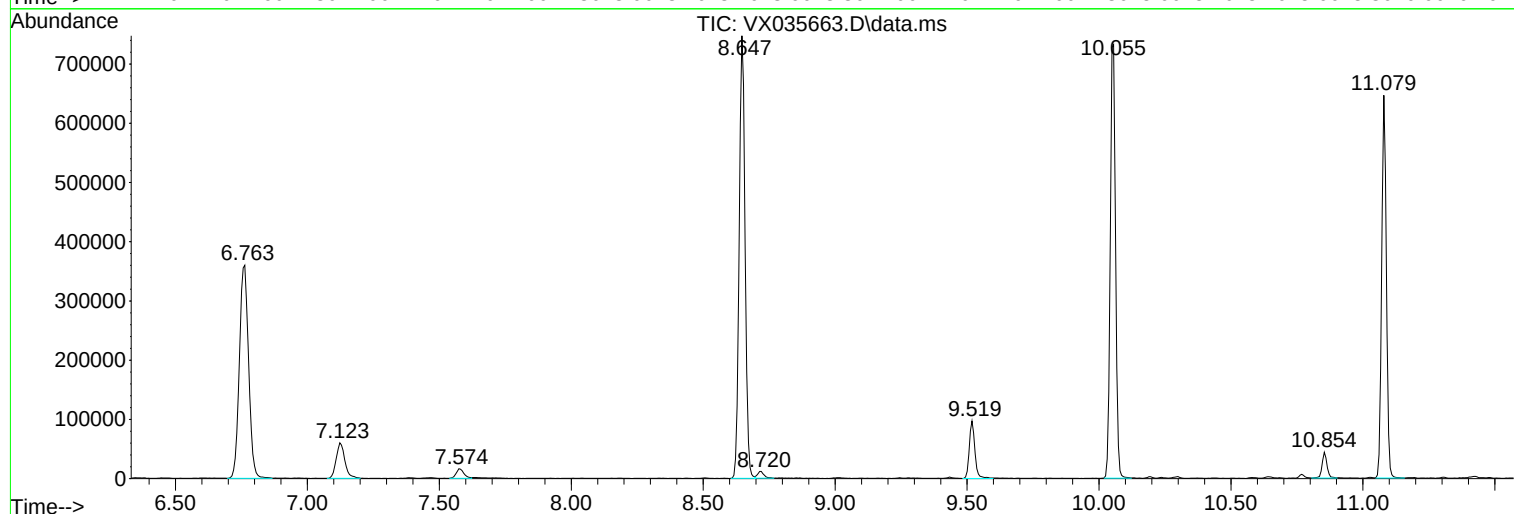
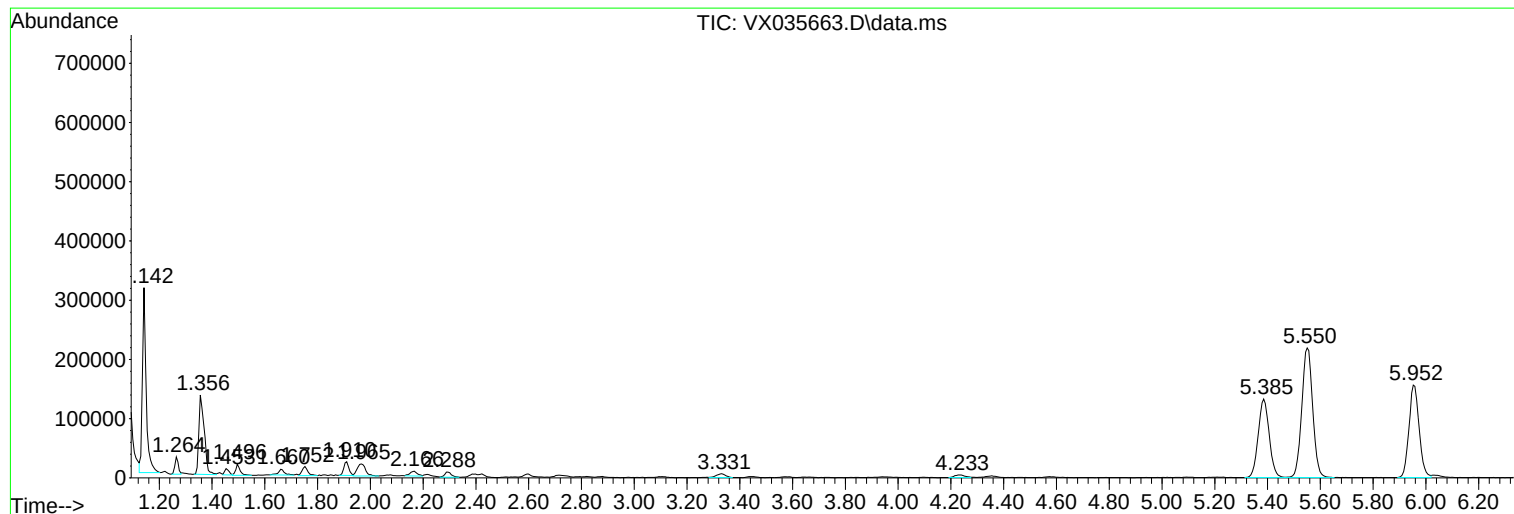
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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



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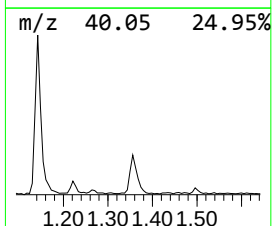
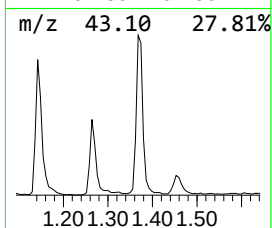
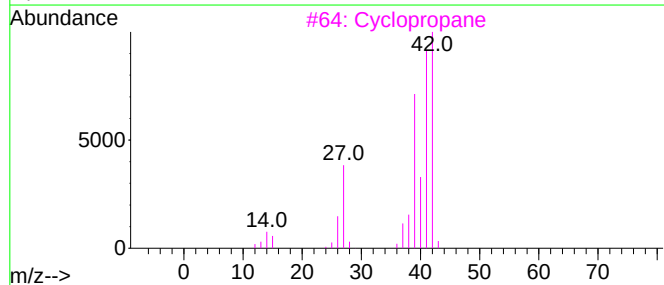
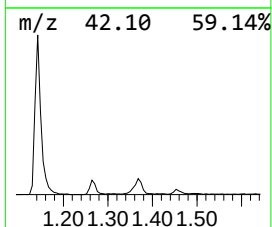
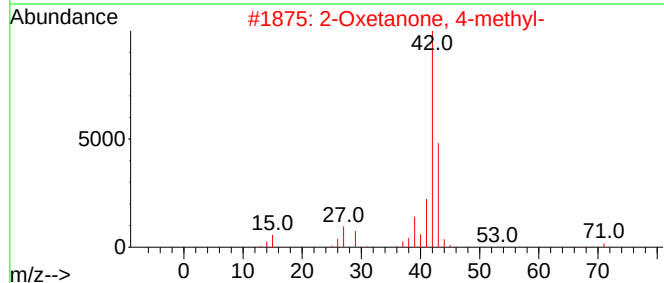
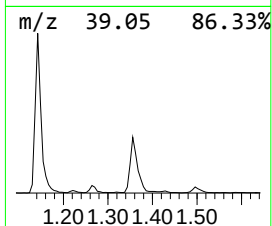
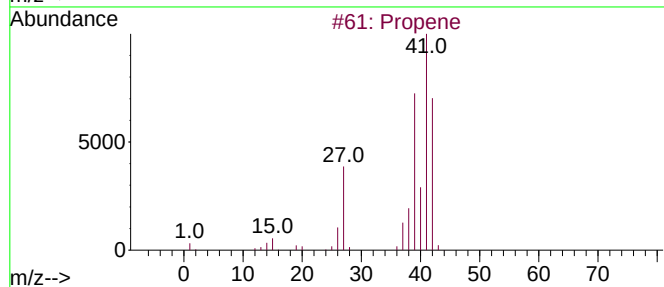
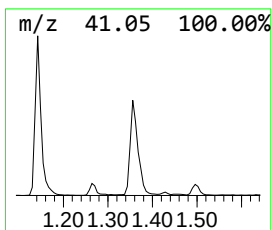
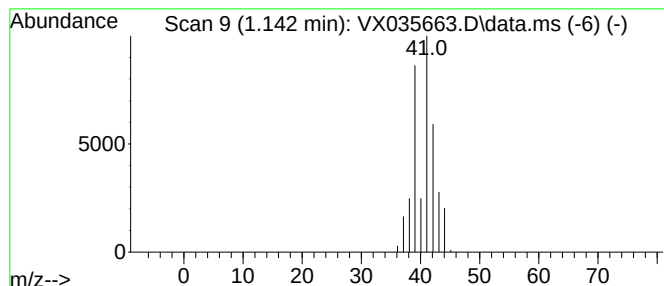
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	24.56 ug/l	309299	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	83
2			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
3			Cyclopropane	42	C3H6	000075-19-4	7
4			Cyclopropene	40	C3H4	002781-85-3	5
5			4-Amino-1-butanol	89	C4H11NO	013325-10-5	1



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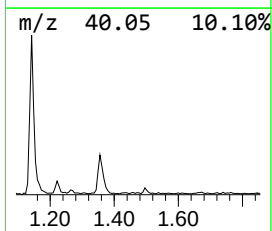
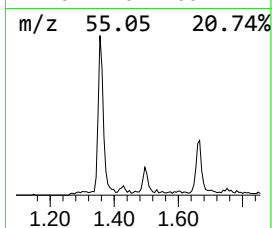
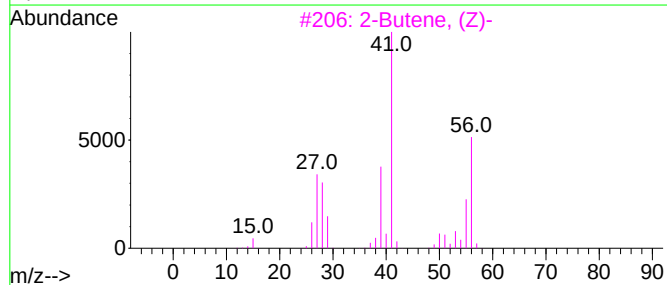
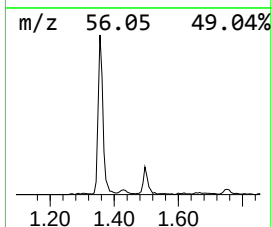
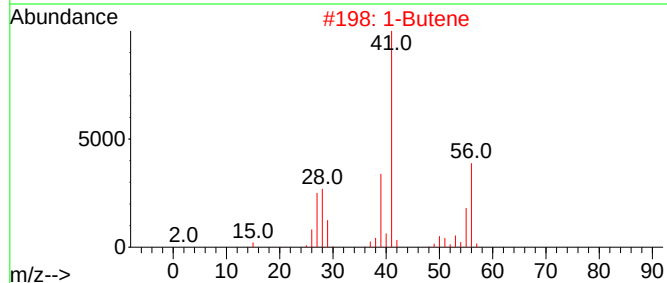
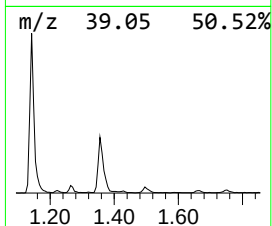
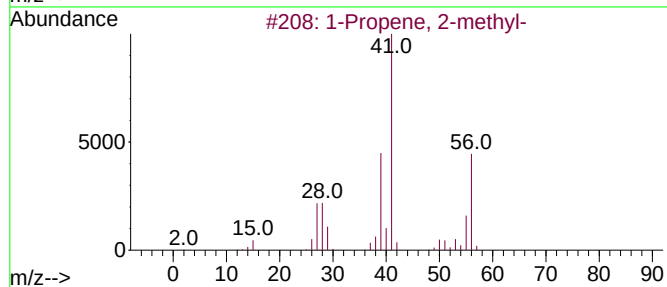
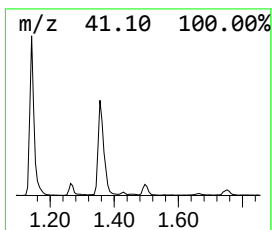
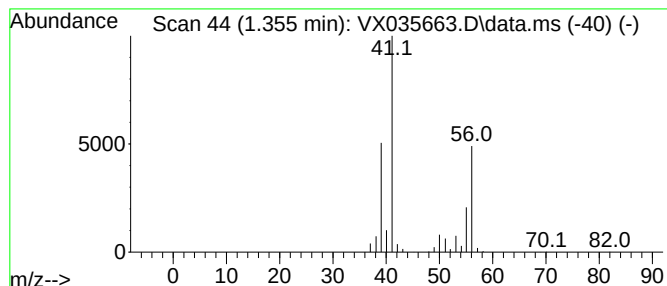
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Peak Number 2 1-Propene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.355	15.08 ug/l	189845	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90	
2	1-Butene	56	C4H8	000106-98-9	87	
3	2-Butene, (Z)-	56	C4H8	000590-18-1	80	
4	2-Butene	56	C4H8	000107-01-7	72	
5	Cyclobutane	56	C4H8	000287-23-0	49	



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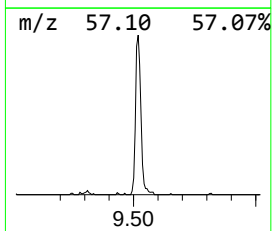
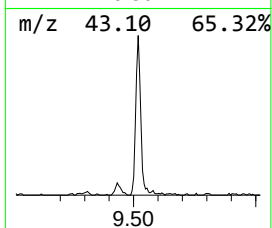
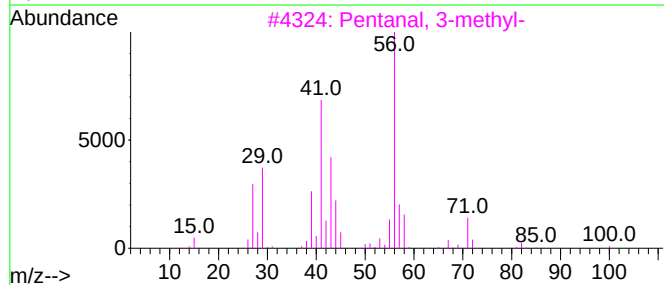
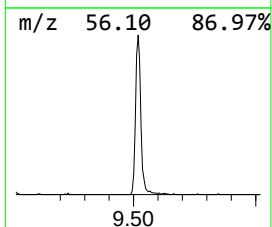
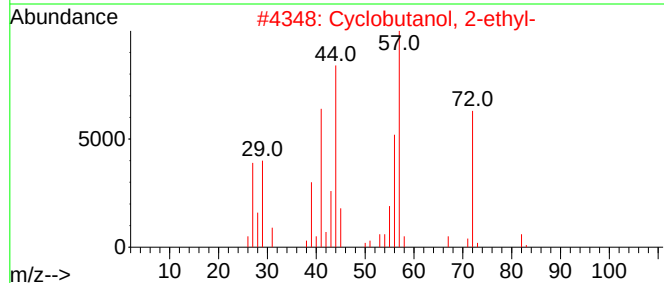
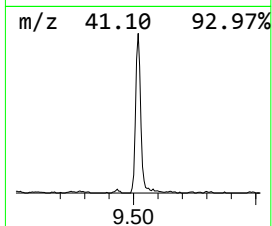
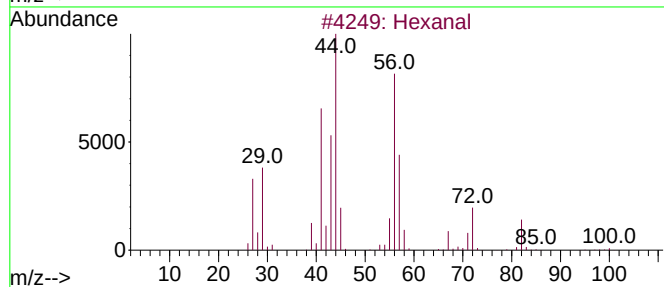
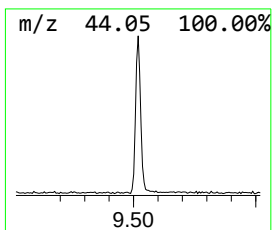
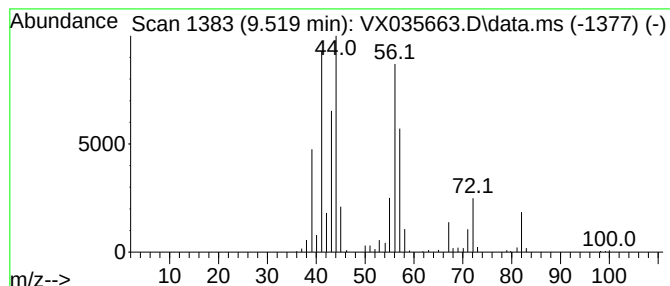
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	6.97 ug/l	142675	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	87
2			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
3			Pentanal, 3-methyl-	100	C6H12O	015877-57-3	35
4			Butanal	72	C4H8O	000123-72-8	22
5			Glutaraldehyde	100	C5H8O2	000111-30-8	16



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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
Propene	1.142	24.6	ug/l	309299	1	5.550	629633	50.0
1-Propene, 2-me...	1.355	15.1	ug/l	189845	1	5.550	629633	50.0
Hexanal	9.519	7.0	ug/l	142675	3	10.055	1024030	50.0