

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
 Data File : VN082384.D
 Acq On : 29 May 2024 20:43
 Operator : JC\MD
 Sample : P2609-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 509

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.812	140	146	155	rVB2	5729	12263	1.08%	0.187%
2	4.436	413	422	432	rBV	9998	30434	2.68%	0.463%
3	7.224	886	896	910	rBV3	27833	78658	6.94%	1.197%
4	8.171	1047	1057	1061	rBV	149062	353852	31.21%	5.386%
5	8.224	1061	1066	1081	rVB	249289	562905	49.65%	8.567%
6	8.583	1111	1127	1135	rBV	172299	402105	35.46%	6.120%
7	8.659	1135	1140	1141	rBV3	14720	23309	2.06%	0.355%
8	9.106	1207	1216	1227	rBV	384161	799293	70.49%	12.165%
9	9.271	1238	1244	1253	rVB5	5336	12614	1.11%	0.192%
10	10.571	1456	1465	1475	rBV	628027	1133851	100.00%	17.257%
11	11.865	1672	1685	1696	rBV	561915	1010455	89.12%	15.379%
12	12.853	1844	1853	1864	rVB	445513	776349	68.47%	11.816%
13	13.259	1915	1922	1932	rBV	161891	261452	23.06%	3.979%
14	13.506	1956	1964	1973	rBV	60003	100785	8.89%	1.534%
15	13.794	2004	2013	2026	rBV	544739	943560	83.22%	14.361%
16	15.394	2279	2285	2291	rBV3	16870	28767	2.54%	0.438%
17	15.812	2354	2356	2366	rVB5	7177	13683	1.21%	0.208%
18	16.164	2412	2416	2423	rVB5	7819	14553	1.28%	0.221%
19	16.506	2469	2474	2482	rVB5	5940	11516	1.02%	0.175%

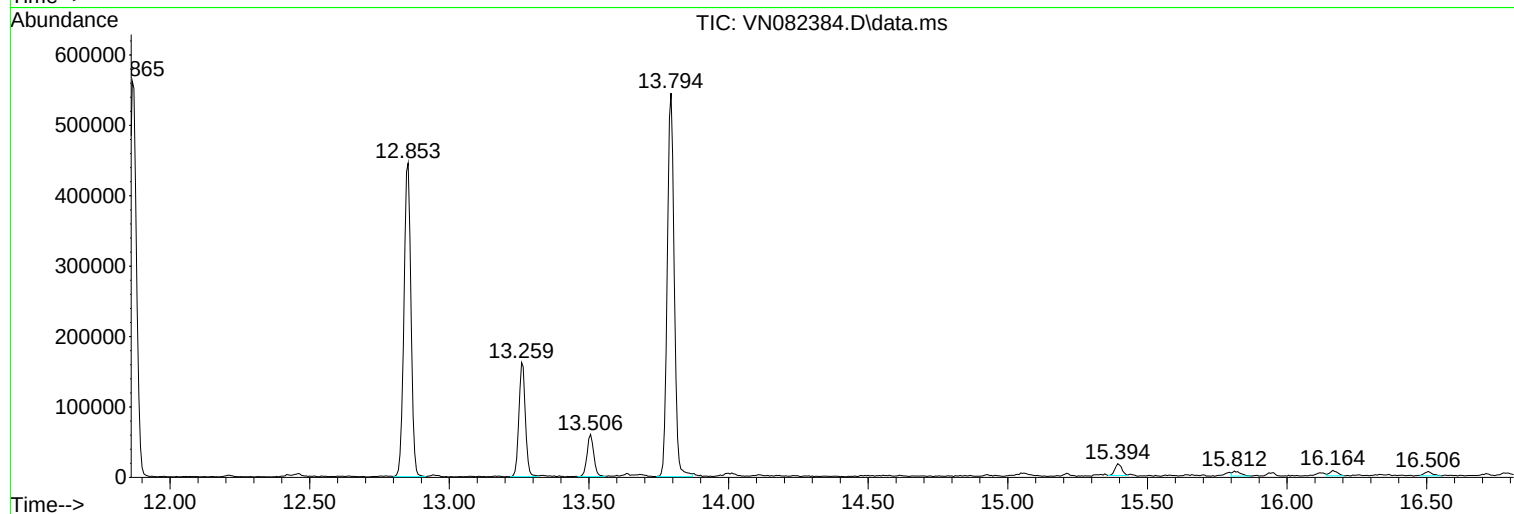
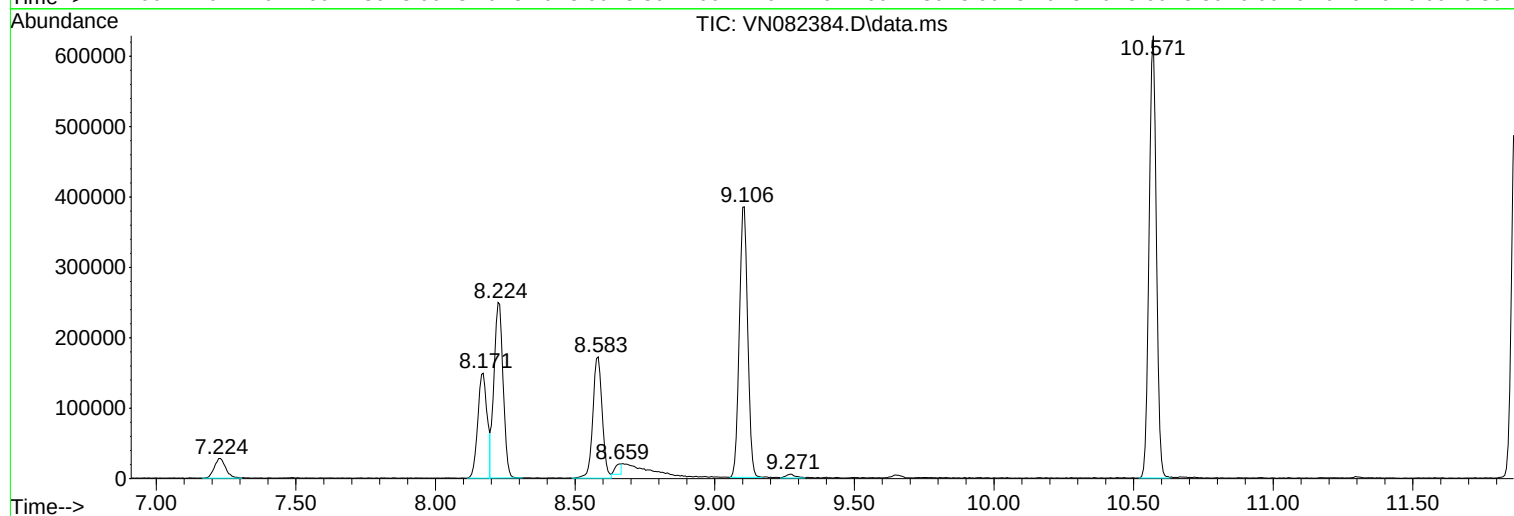
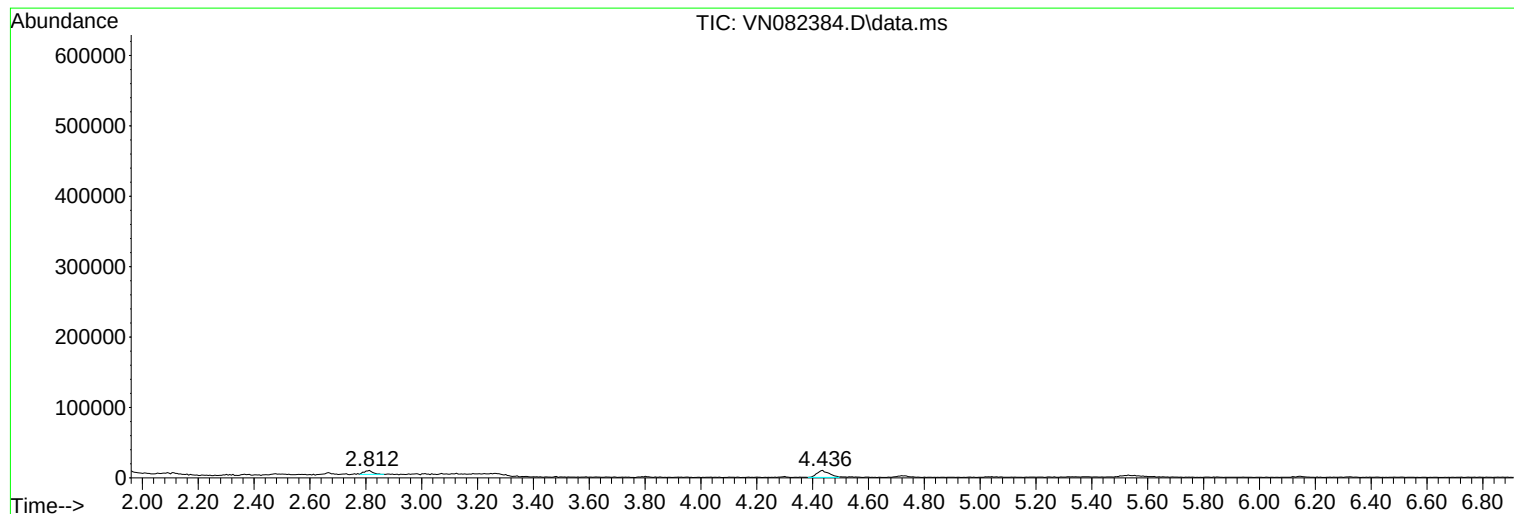
Sum of corrected areas: 6570404

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Quant Title : SW846 8260

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



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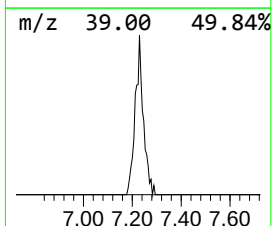
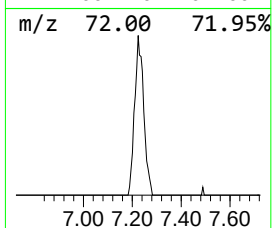
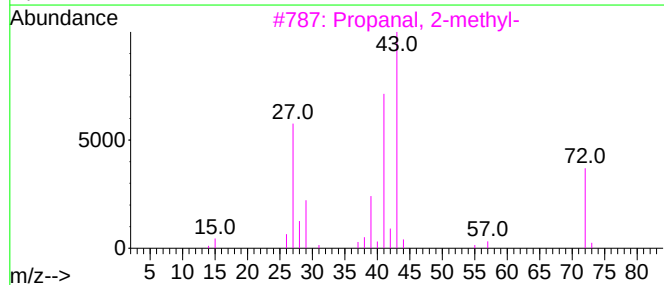
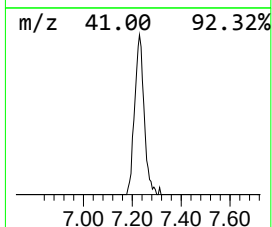
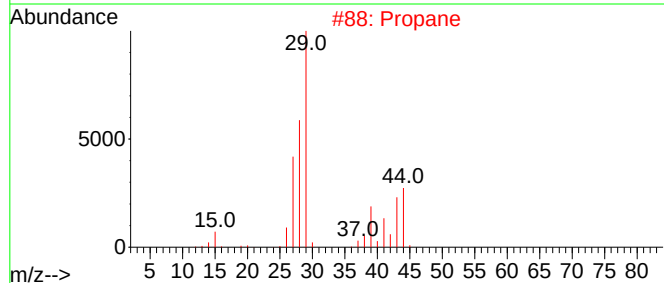
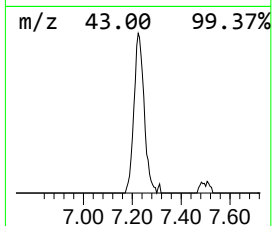
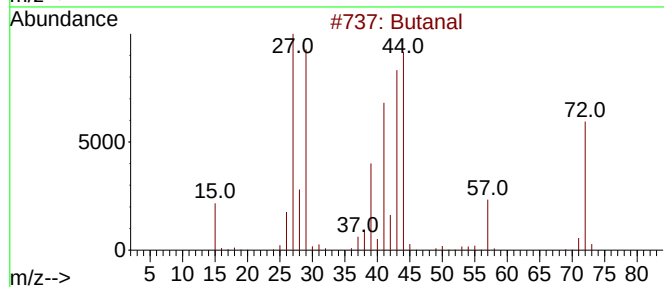
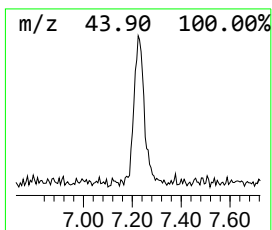
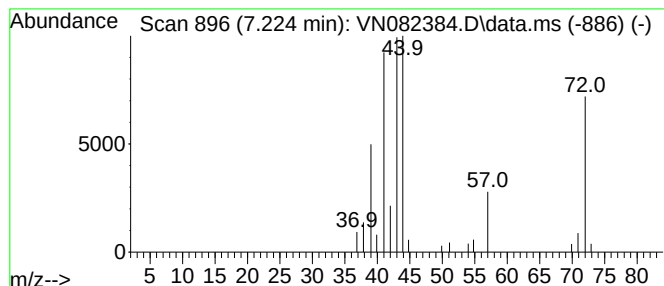
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	6.99 ug/l	78658	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	59
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	32
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	17



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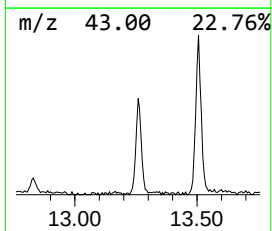
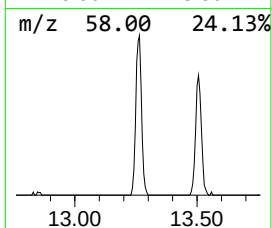
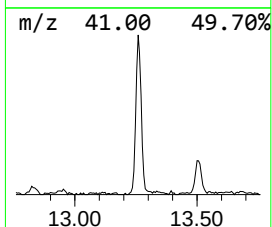
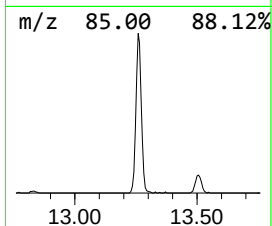
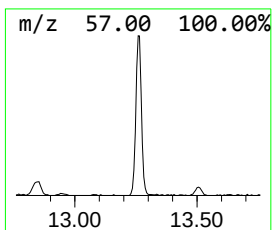
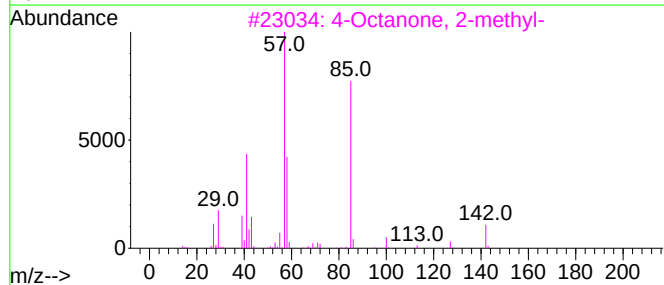
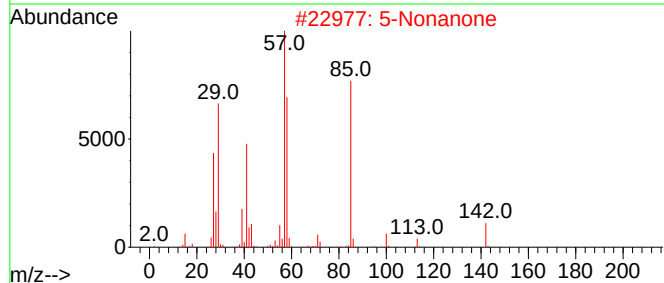
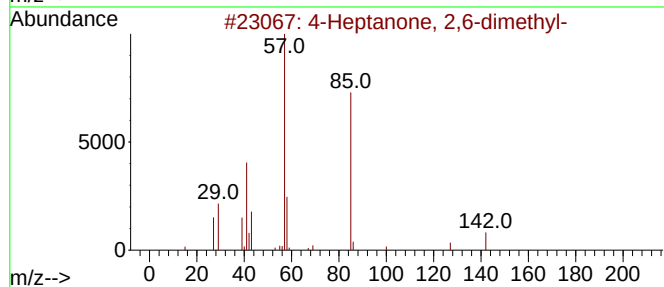
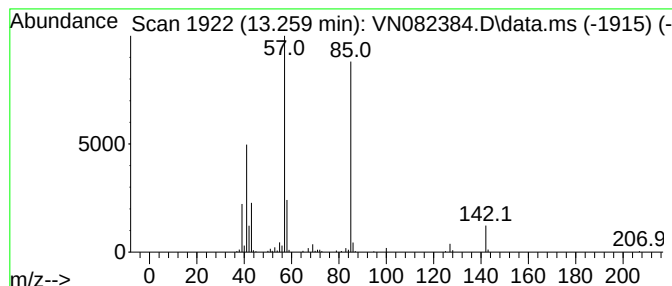
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Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	13.85 ug/l	261452	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			5-Nonanone	142	C9H18O	000502-56-7	72
3			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
4			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5			Pentanoic acid, 4-methyl-2-oxo-,...	144	C7H12O3	003682-43-7	59



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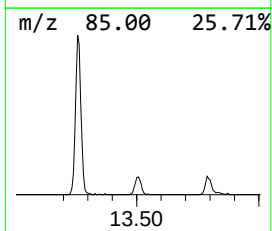
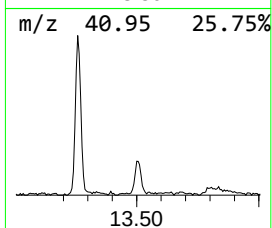
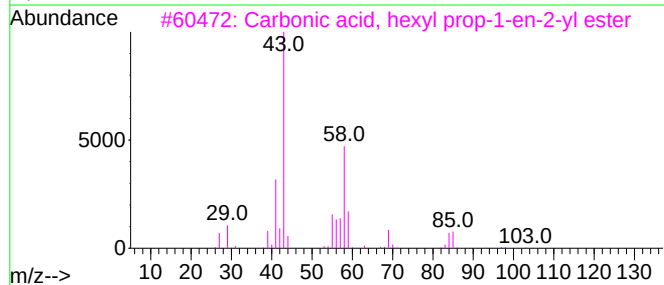
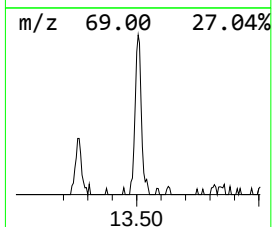
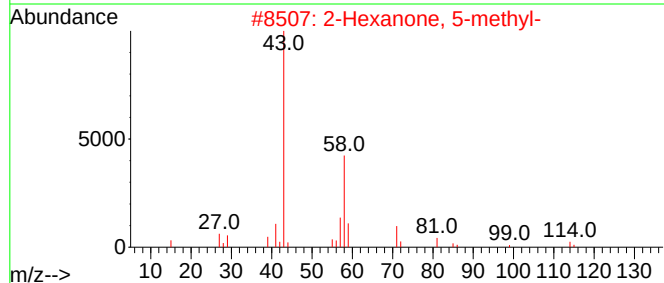
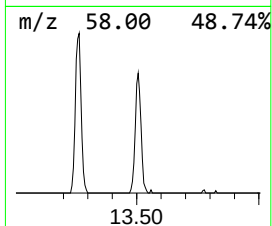
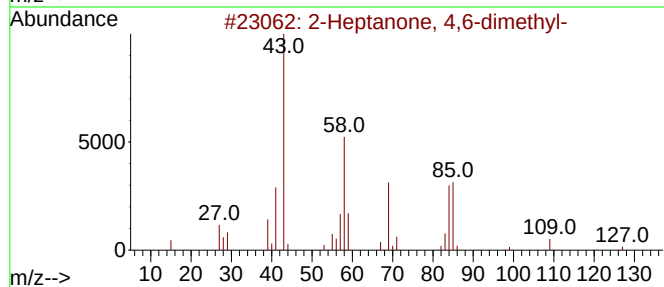
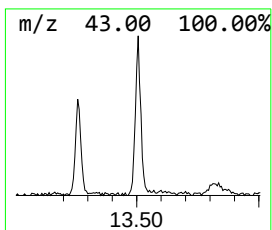
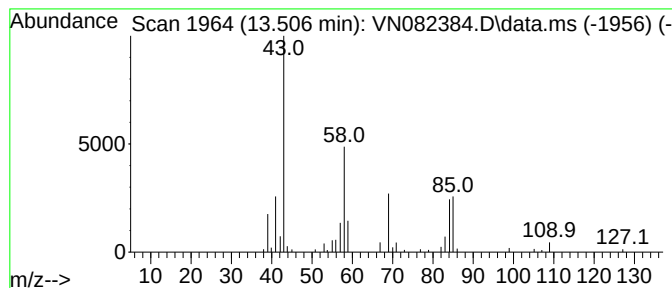
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Peak Number 3 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	5.34 ug/l	100785	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
3			Carbonic acid, hexyl prop-1-en-2-yl ester	186	C10H18O3	1000382-54-2	50
4			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	47
5			3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	43



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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
Butanal	7.224	7.0	ug/l	78658	1	8.230	562905	50.0
4-Heptanone, 2,...	13.259	13.9	ug/l	261452	4	13.794	943560	50.0
2-Heptanone, 4,...	13.506	5.3	ug/l	100785	4	13.794	943560	50.0