

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040323\
 Data File : VY013177.D
 Acq On : 03 Apr 2023 15:45
 Operator : KP/MD
 Sample : 02165-02
 Misc : 5.52g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-2B

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_Y\methods\82Y033023S.M

Title : SW846 8260

Signal : TIC: VY013177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.954	339	350	362	rBV	3569	9760	2.07%	0.353%
2	4.716	463	475	488	rVB	15750	48375	10.24%	1.748%
3	5.747	633	644	656	rBV3	4072	12684	2.69%	0.458%
4	7.716	953	967	973	rBV2	68589	168982	35.78%	6.107%
5	7.783	973	978	988	rVV	111225	252384	53.44%	9.121%
6	8.136	1027	1036	1046	rBV	67704	150492	31.86%	5.439%
7	8.319	1059	1066	1081	rVB2	16509	41033	8.69%	1.483%
8	8.685	1118	1126	1141	rVB	173192	337308	71.42%	12.190%
9	9.185	1202	1208	1212	rBV4	4183	6877	1.46%	0.249%
10	9.240	1212	1217	1223	rVV3	3888	7744	1.64%	0.280%
11	9.612	1271	1278	1286	rBV	17166	35247	7.46%	1.274%
12	9.746	1293	1300	1308	rBV2	21940	46598	9.87%	1.684%
13	10.112	1350	1360	1364	rBV2	5176	9999	2.12%	0.361%
14	10.179	1364	1371	1379	rVB	275505	472301	100.00%	17.069%
15	11.490	1578	1586	1595	rBV	249267	414220	87.70%	14.970%
16	12.483	1741	1749	1758	rBV	196858	318230	67.38%	11.501%
17	13.282	1872	1880	1886	rBV4	5145	8582	1.82%	0.310%
18	13.422	1895	1903	1909	rBV	257092	393644	83.35%	14.226%
19	13.477	1909	1912	1917	rVV3	4594	9315	1.97%	0.337%
20	13.965	1986	1992	2000	rVB	5075	8489	1.80%	0.307%
21	14.294	2038	2046	2051	rVB2	5009	7493	1.59%	0.271%
22	15.312	2204	2213	2219	rBV2	3838	7296	1.54%	0.264%

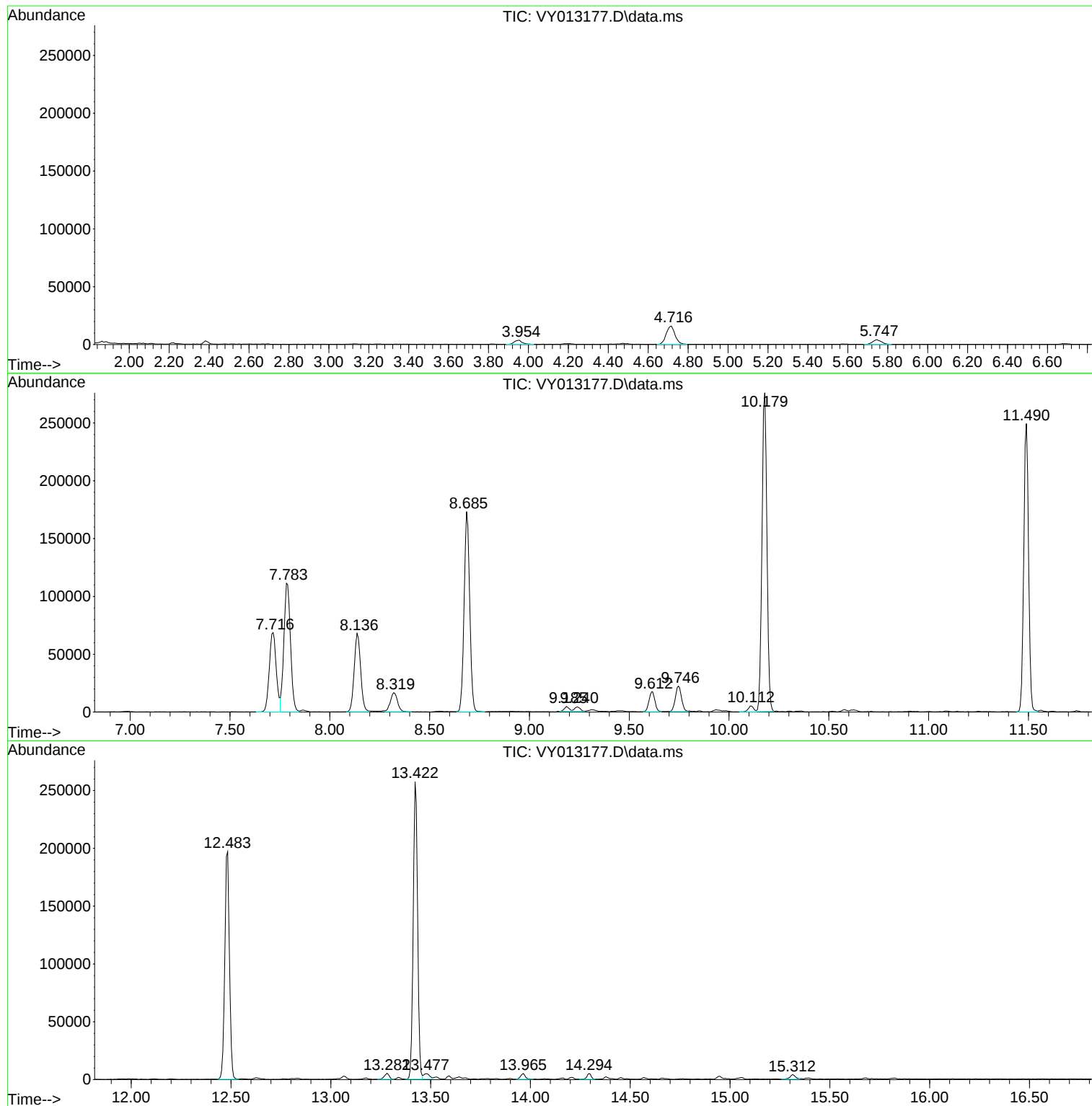
Sum of corrected areas: 2767053

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y033023S.M
Quant Title : SW846 8260

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



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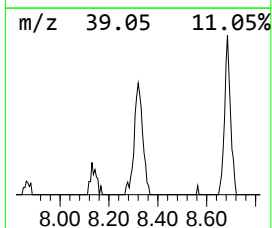
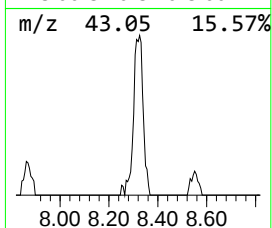
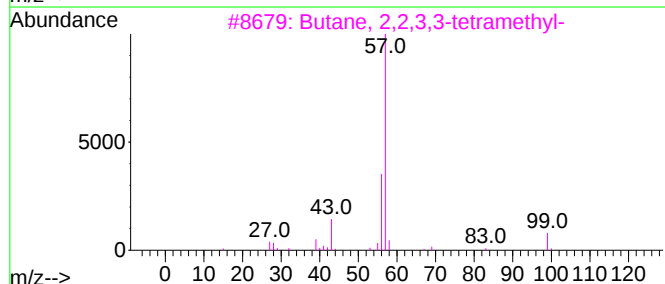
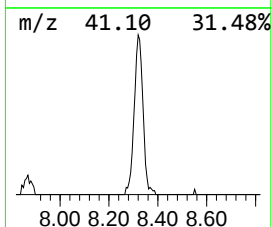
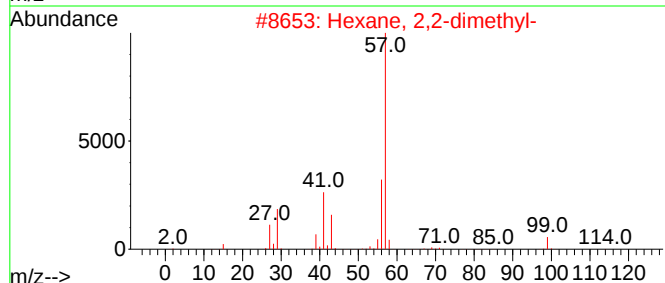
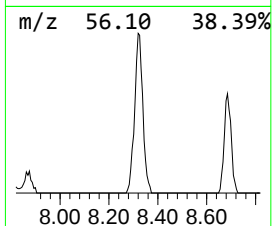
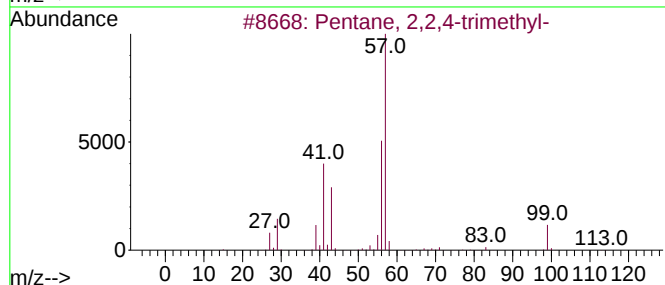
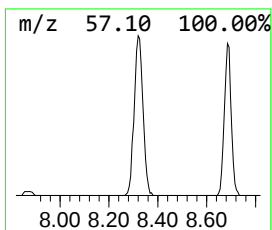
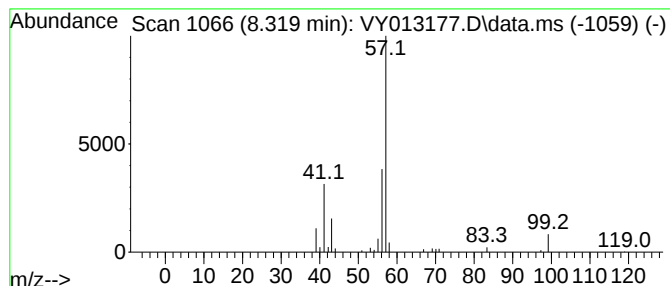
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y033023S.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.319	6.08 ug/l	41033	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	64



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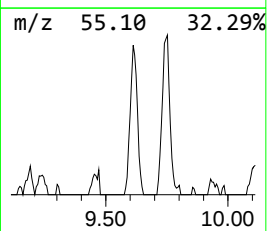
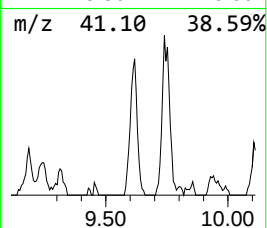
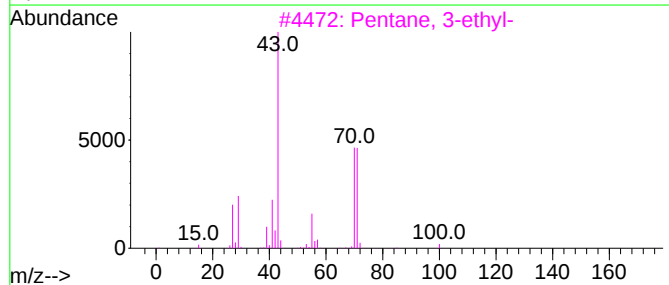
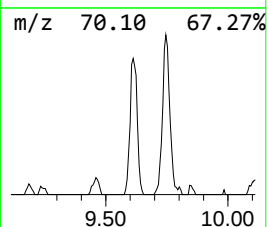
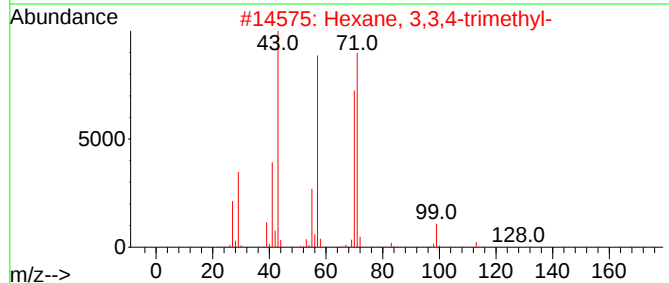
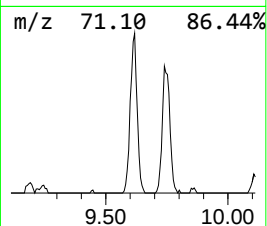
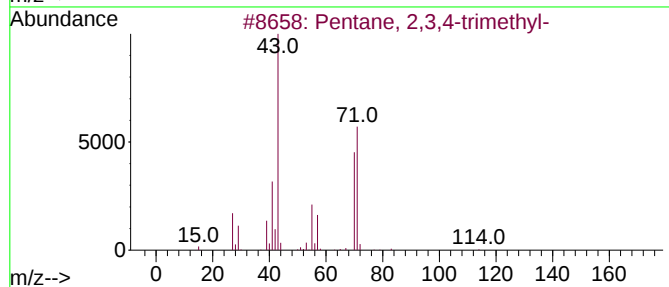
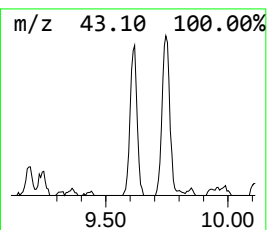
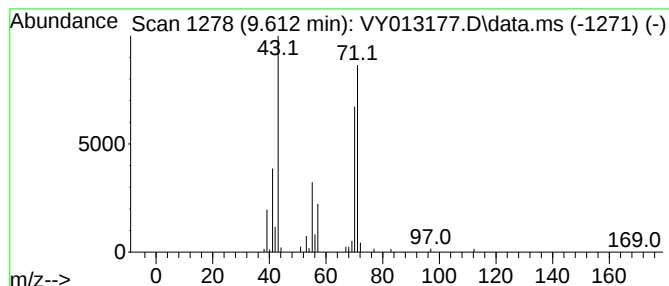
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Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.612	5.22 ug/l	35247	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	74



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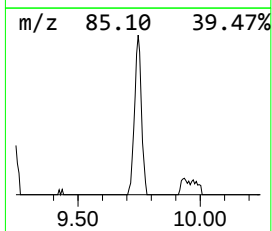
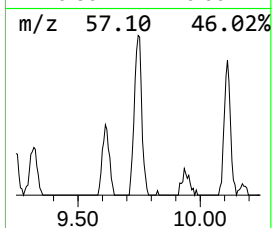
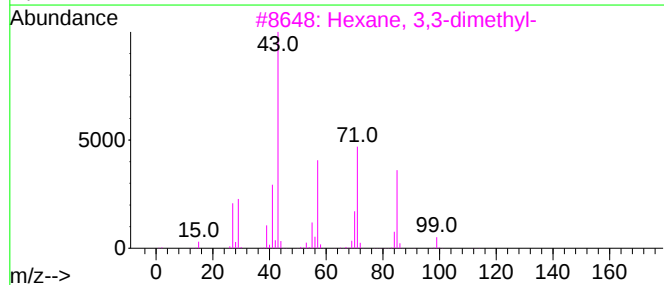
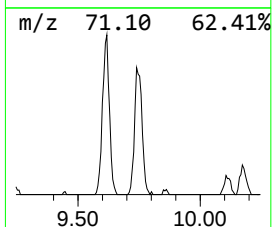
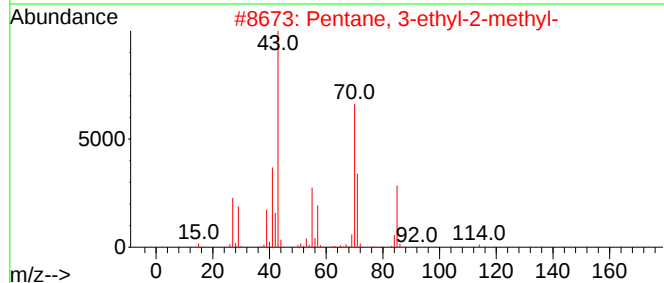
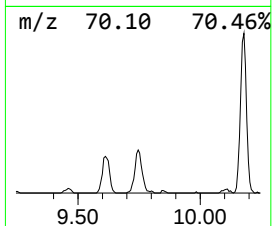
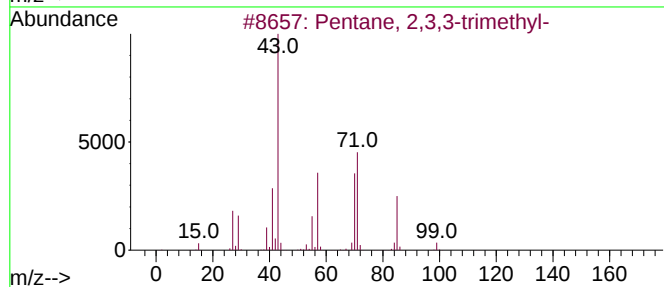
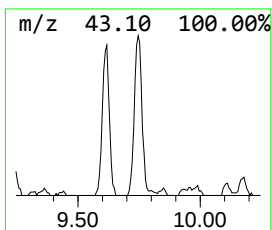
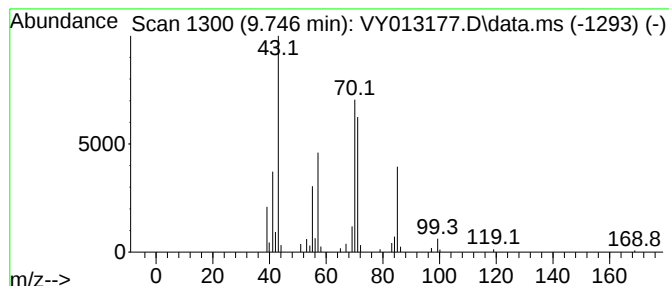
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.746	6.91 ug/l	46598	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	59
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	53
5			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	53



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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
Pentane, 2,2,4-...	8.319	6.1	ug/l	41033	2	8.685	337308	50.0
Pentane, 2,3,4-...	9.612	5.2	ug/l	35247	2	8.685	337308	50.0
Pentane, 2,3,3-...	9.746	6.9	ug/l	46598	2	8.685	337308	50.0