

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040121\
 Data File : VX021719.D
 Acq On : 01 Apr 2021 19:24
 Operator : JC/MD
 Sample : M1895-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2R

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\82X032421W.M

Title : SW846 8260

Signal : TIC: VX021719.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	79	86	89	rVB6	2406	4993	1.29%	0.176%
2	3.011	319	327	337	rVB2	3377	7942	2.06%	0.279%
3	3.164	344	353	366	rBV	22444	53885	13.95%	1.894%
4	5.464	731	744	757	rBV	49245	136130	35.25%	4.786%
5	5.629	760	772	790	rVV	68387	190231	49.26%	6.688%
6	6.029	829	840	853	rBV	51033	135776	35.16%	4.773%
7	6.317	874	889	901	rBV	118464	356512	92.32%	12.534%
8	6.829	966	976	989	rBV	115334	276492	71.60%	9.721%
9	7.653	1108	1116	1127	rVB	9855	22054	5.71%	0.775%
10	8.035	1171	1181	1191	rBV	128226	247087	63.99%	8.687%
11	8.159	1193	1202	1211	rVB	36158	71492	18.51%	2.513%
12	8.694	1282	1293	1308	rBV	246810	386151	100.00%	13.576%
13	10.094	1525	1531	1538	rBV	261203	354237	91.74%	12.454%
14	11.118	1699	1705	1716	rBV	212429	274036	70.97%	9.634%
15	11.930	1840	1843	1847	rVB	3862	4835	1.25%	0.170%
16	12.059	1860	1865	1874	rVB	258037	322559	83.53%	11.340%

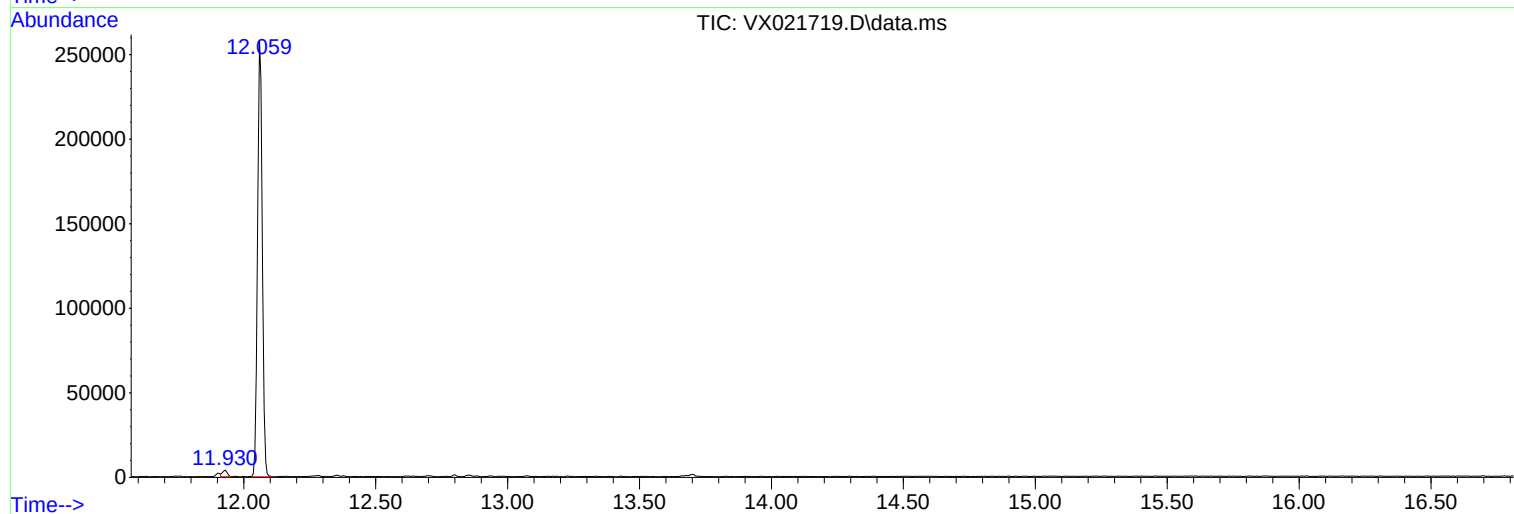
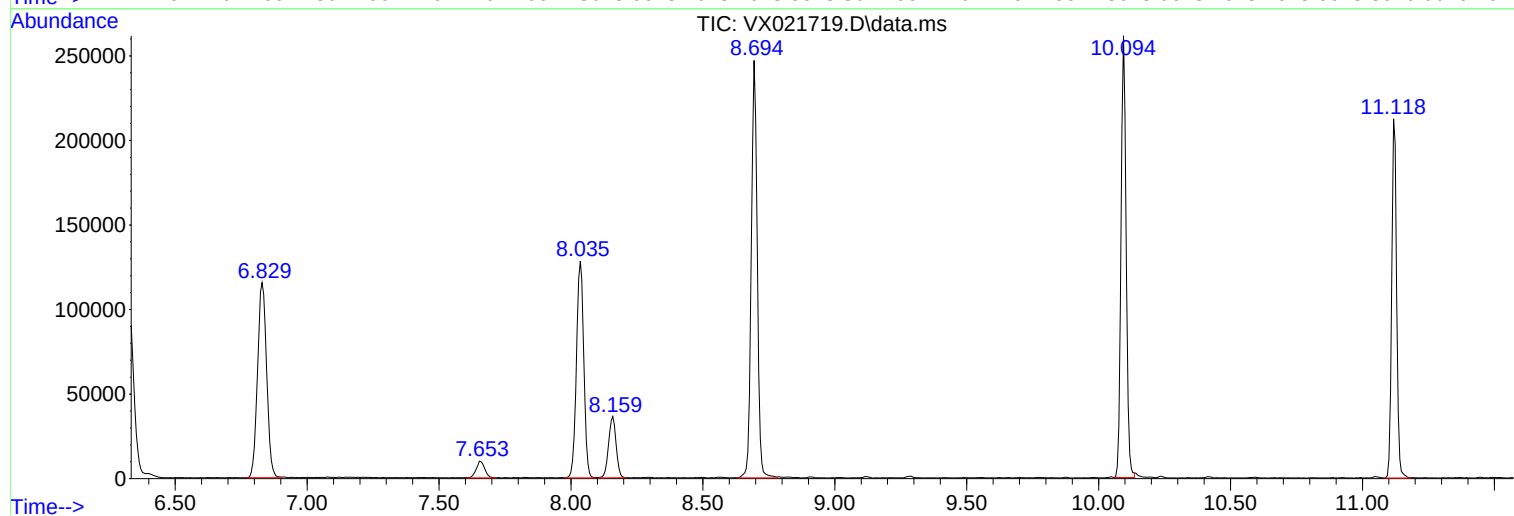
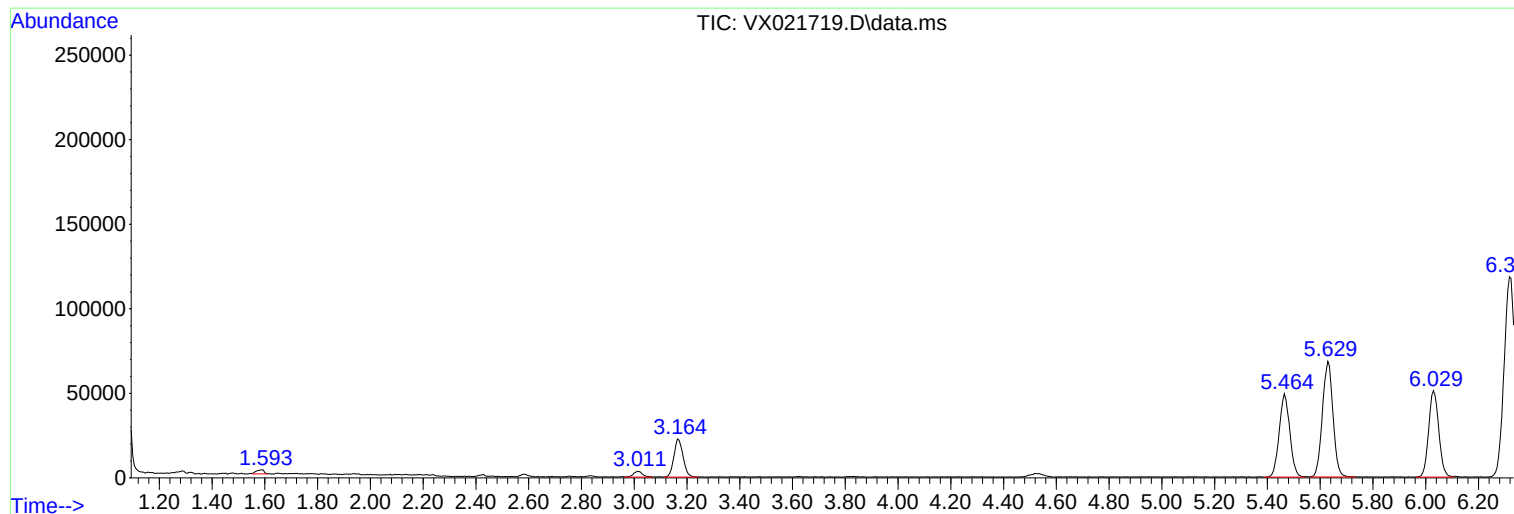
Sum of corrected areas: 2844412

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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



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Instrument :
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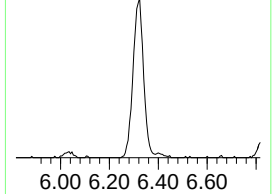
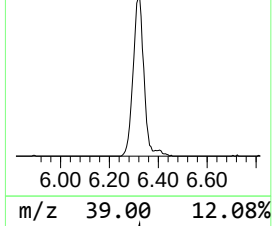
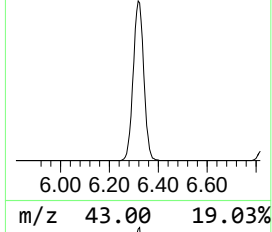
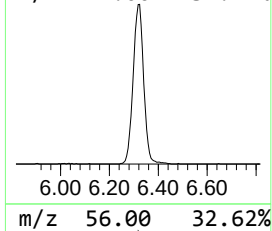
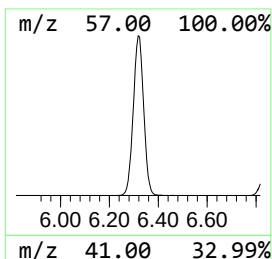
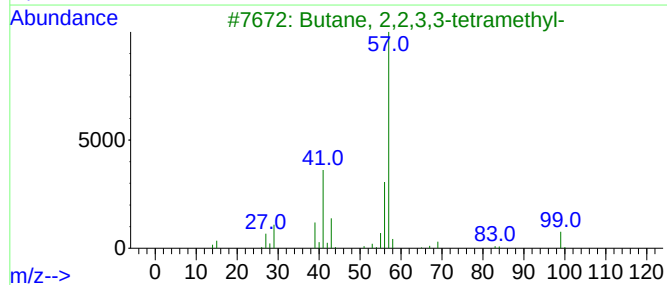
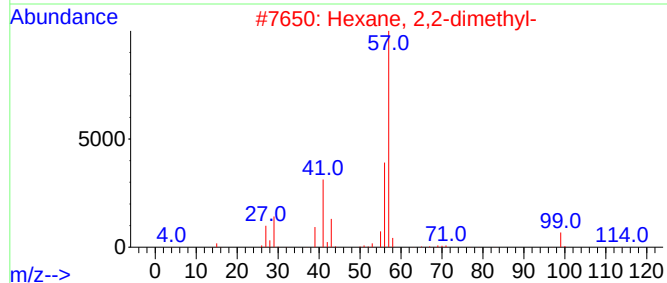
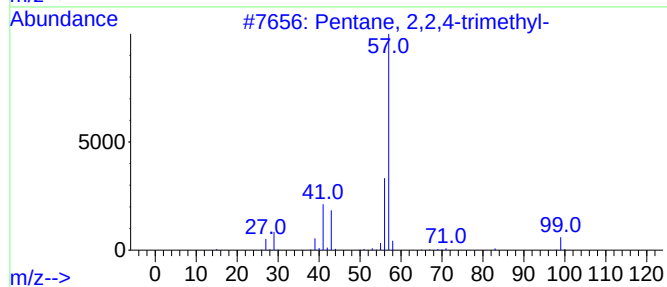
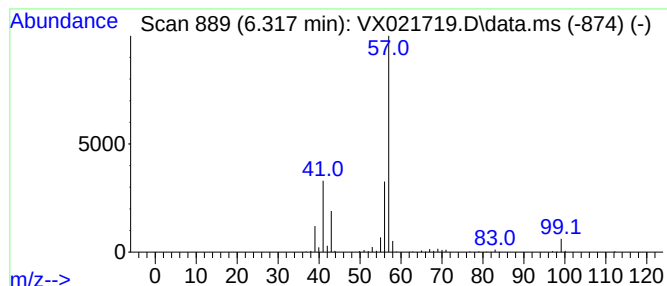
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.317	64.47 ug/l	356512	1,4-Difluorobenzene	6.829

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			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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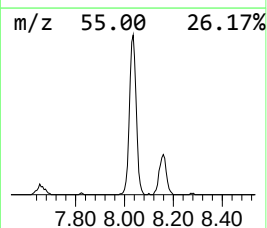
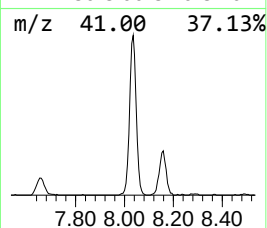
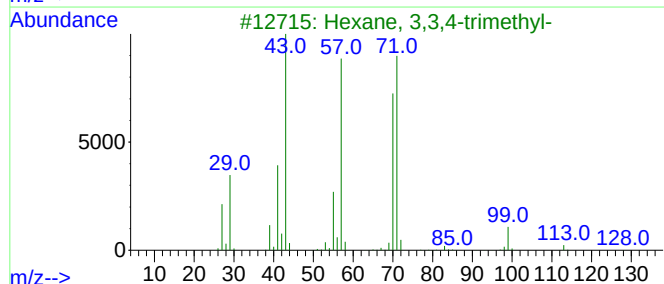
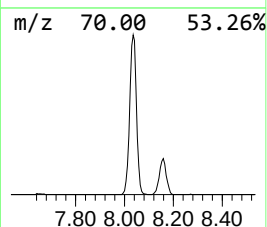
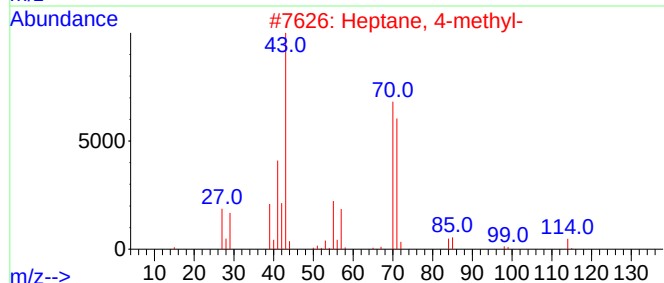
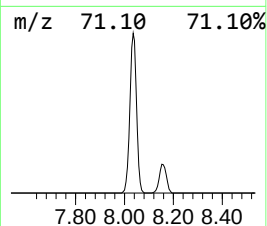
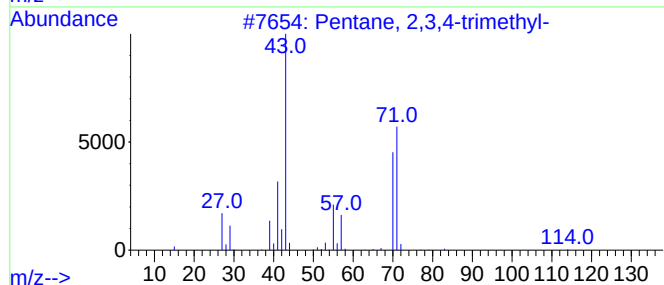
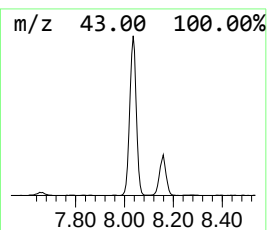
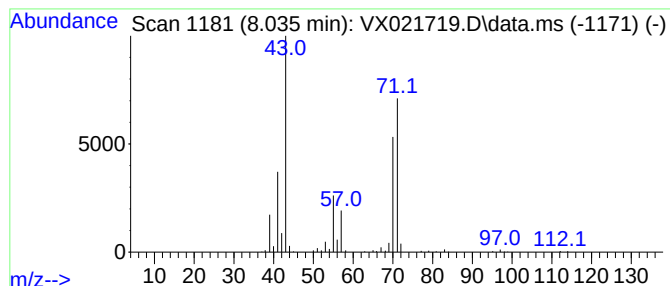
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.035	44.68 ug/l	247087	1,4-Difluorobenzene	6.829

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
4			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	59
5			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	56



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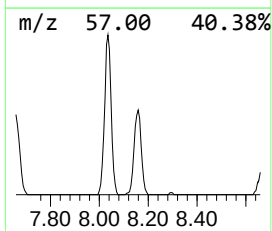
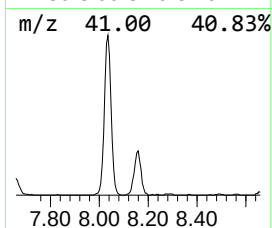
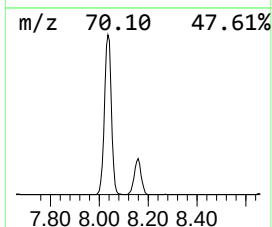
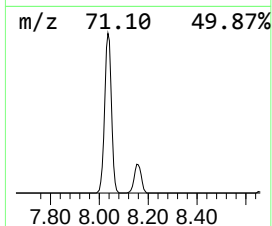
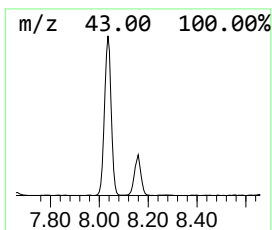
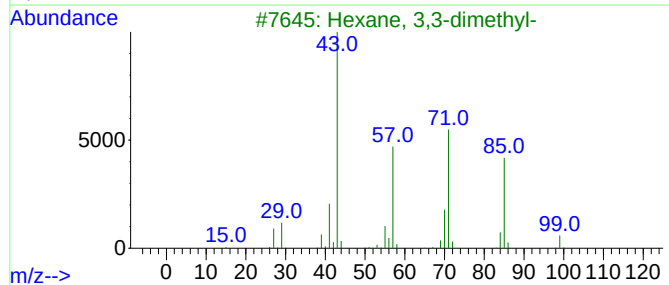
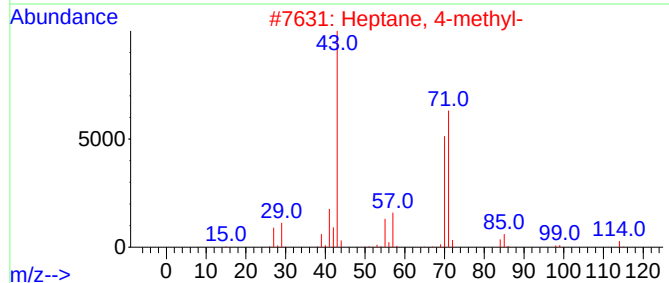
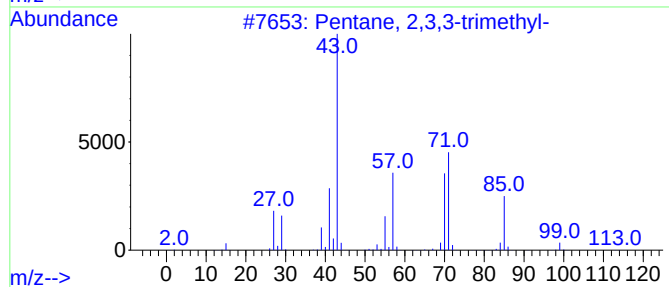
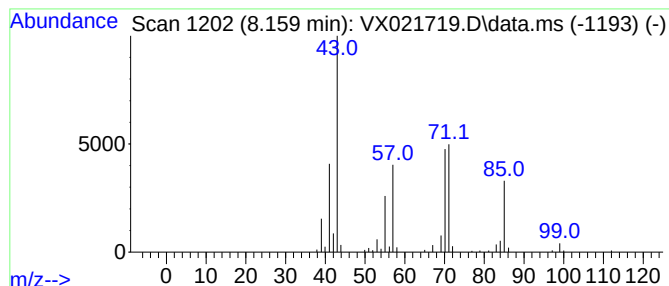
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	12.93 ug/l	71492	1,4-Difluorobenzene	6.829

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Pyrrolidine	71	C4H9N	000123-75-1	50



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,4-...	6.317	64.5	ug/l	356512	2	6.829	276492	50.0
Pentane, 2,3,4-...	8.035	44.7	ug/l	247087	2	6.829	276492	50.0
Pentane, 2,3,3-...	8.159	12.9	ug/l	71492	2	6.829	276492	50.0