

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100521\
 Data File : VX024574.D
 Acq On : 05 Oct 2021 16:26
 Operator : JC/MD
 Sample : M3989-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 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\82X092321W.M

Title : SW846 8260

Signal : TIC: VX024574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	29	rBV	15878	21673	2.48%	0.370%
2	1.276	29	31	36	rVB4	5781	10487	1.20%	0.179%
3	2.971	301	309	319	rBV2	4358	9902	1.13%	0.169%
4	3.123	326	334	343	rBV2	26957	60723	6.96%	1.036%
5	4.458	544	553	563	rBV4	3443	10343	1.18%	0.177%
6	5.397	695	707	722	rBV	100721	290202	33.25%	4.952%
7	5.562	722	734	752	rVB	157633	440933	50.51%	7.525%
8	5.964	789	800	814	rBV	105083	281173	32.21%	4.798%
9	6.257	834	848	860	rBV	219531	662751	75.93%	11.310%
10	6.769	921	932	948	rBV	259185	613553	70.29%	10.470%
11	7.604	1060	1069	1080	rVB3	16887	37322	4.28%	0.637%
12	7.988	1122	1132	1144	rBV	228464	444266	50.90%	7.582%
13	8.110	1144	1152	1164	rVB	64955	130383	14.94%	2.225%
14	8.653	1227	1241	1250	rBV	553261	872878	100.00%	14.896%
15	10.055	1466	1471	1484	rVB	540246	716204	82.05%	12.222%
16	11.085	1634	1640	1651	rBV	451896	579334	66.37%	9.887%
17	12.024	1789	1794	1802	rBV	560476	677701	77.64%	11.565%

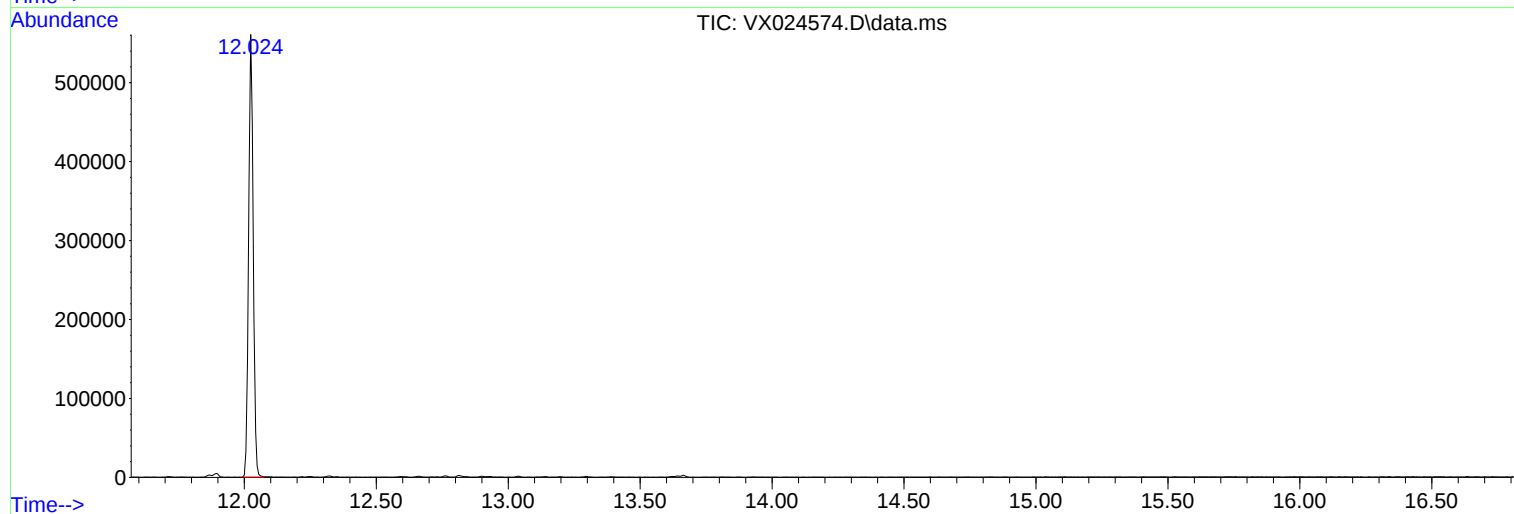
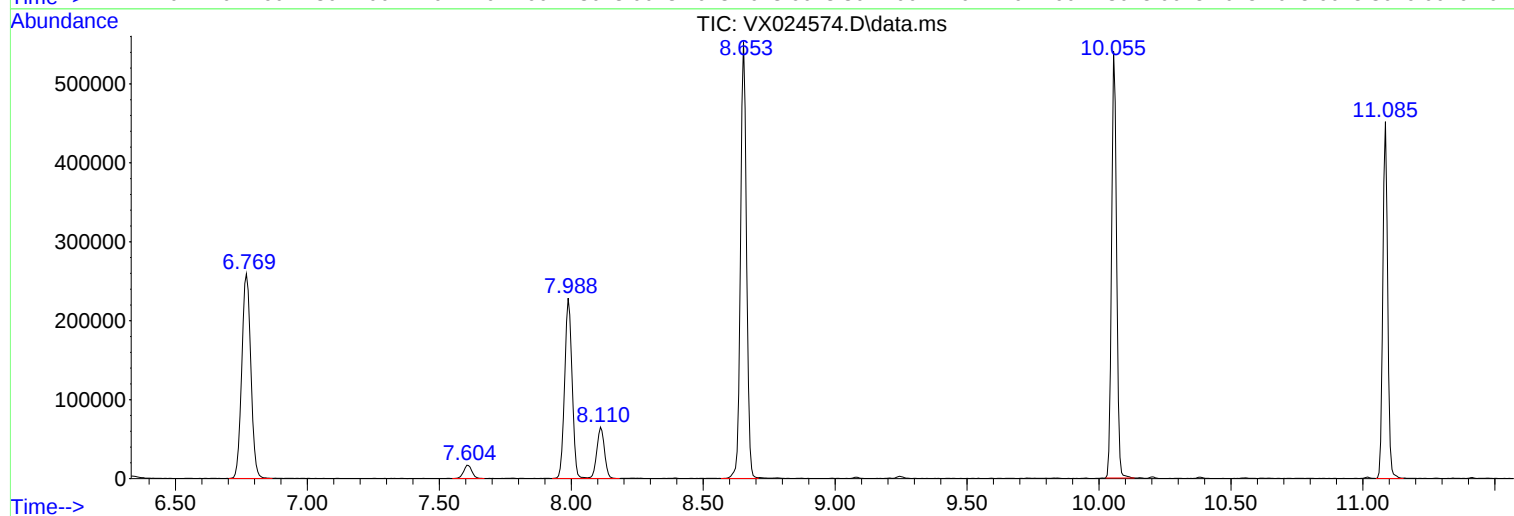
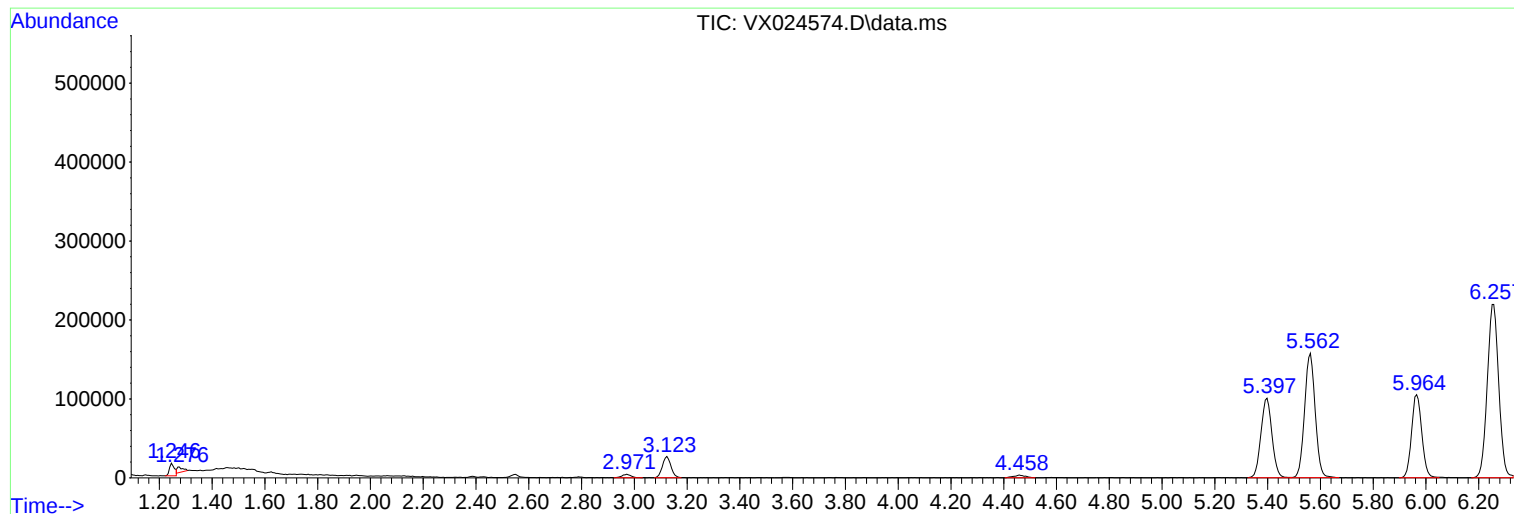
Sum of corrected areas: 5859828

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092321W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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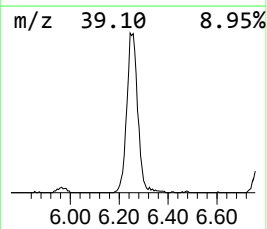
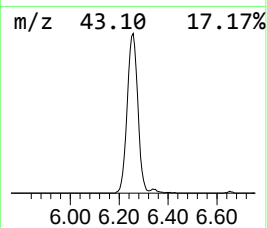
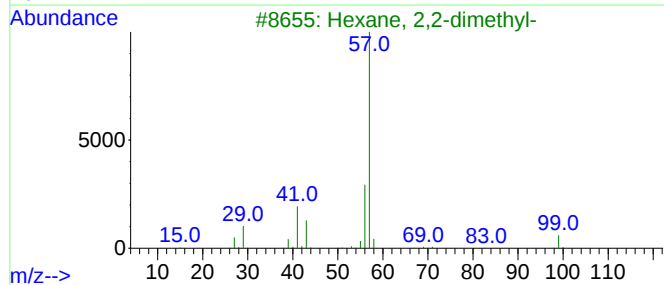
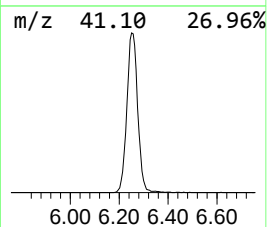
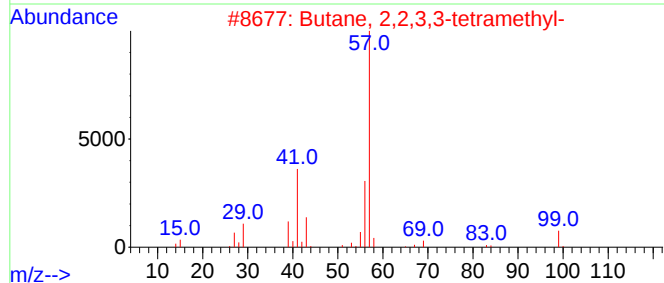
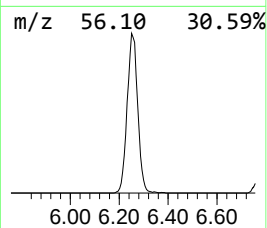
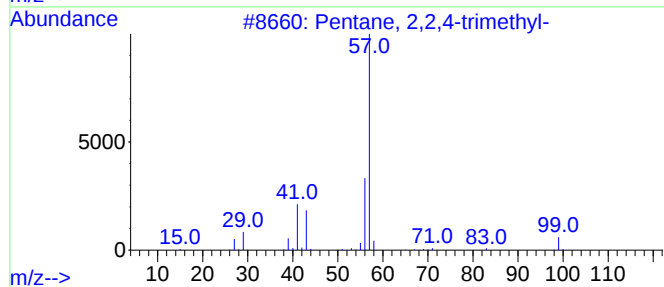
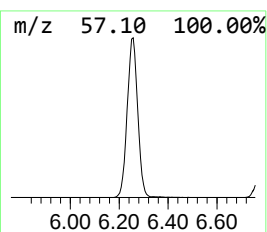
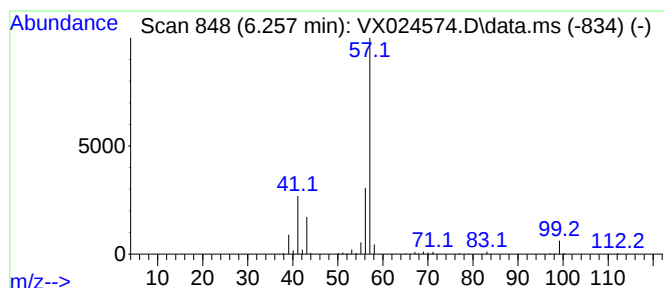
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092321W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.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.
6.257	54.01 ug/l	662751	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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MSVOA_X
ClientSampleId :
MW-2R

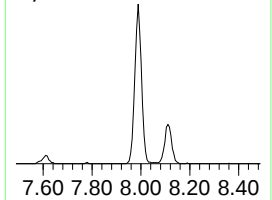
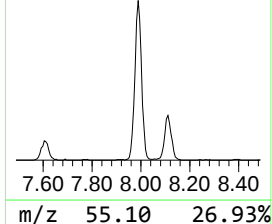
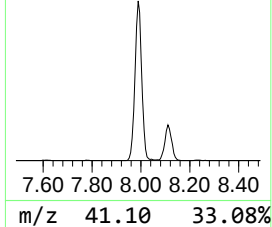
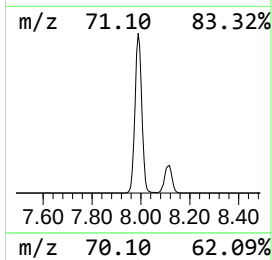
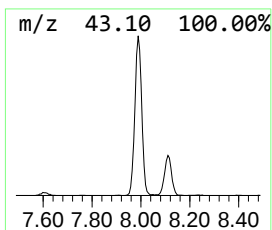
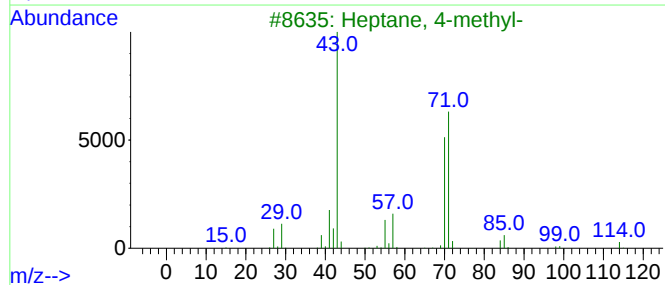
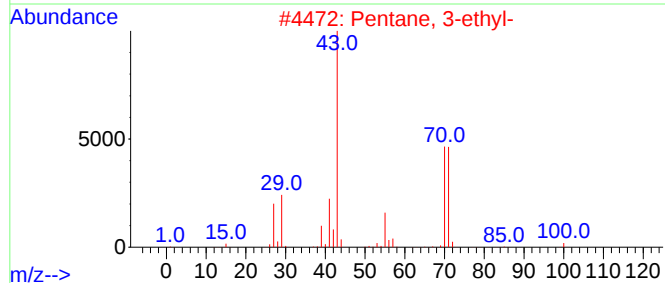
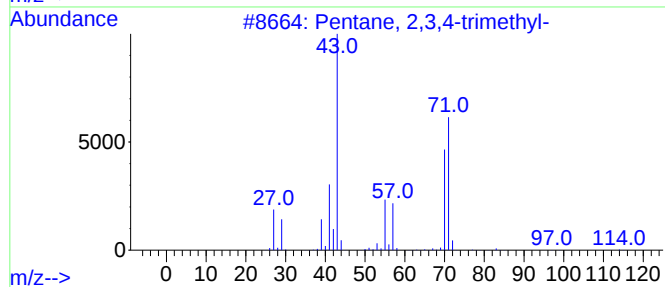
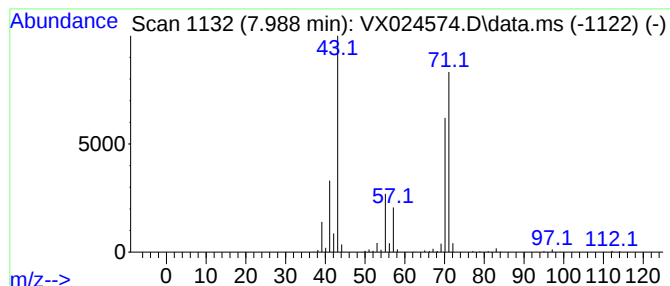
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092321W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
7.988	36.20 ug/l	444266	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5			3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	74



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Instrument :
MSVOA_X
ClientSampleId :
MW-2R

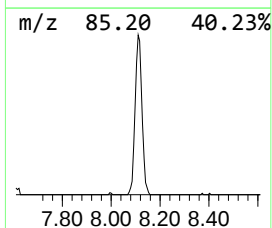
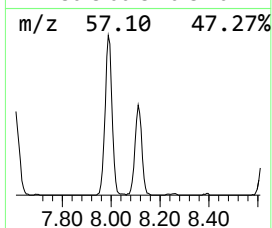
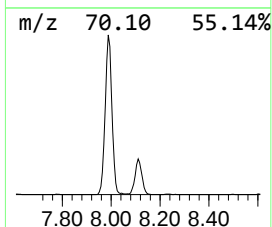
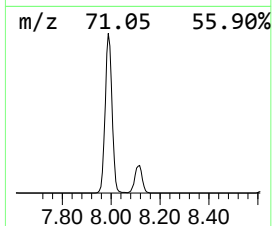
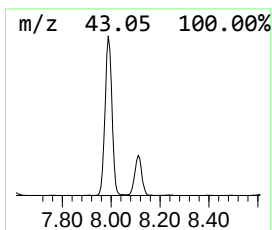
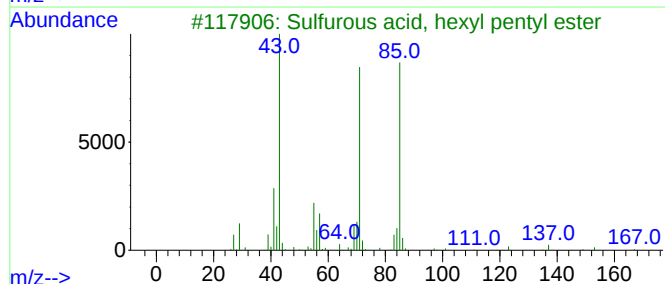
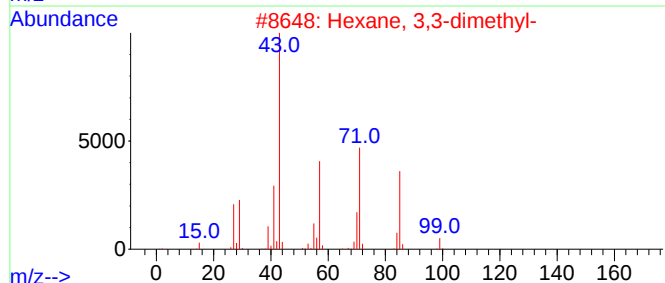
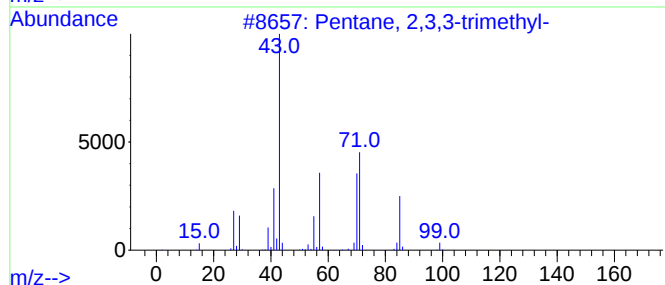
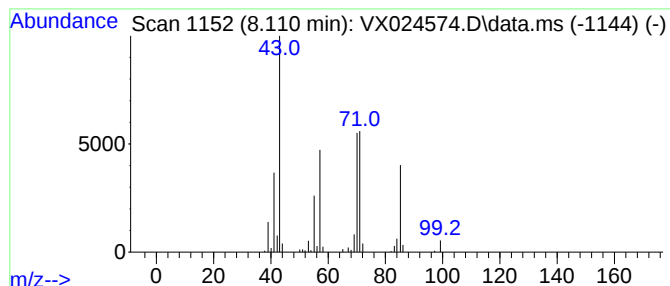
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092321W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
8.110	10.63 ug/l	130383	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5			Octane, 4-methyl-	128	C9H20	002216-34-4	50



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092321W.M
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-...	6.257	54.0	ug/l	662751	2	6.769	613553	50.0
Pentane, 2,3,4-...	7.988	36.2	ug/l	444266	2	6.769	613553	50.0
Pentane, 2,3,3-...	8.110	10.6	ug/l	130383	2	6.769	613553	50.0