

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
 Data File : VX029652.D
 Acq On : 21 Jun 2022 09:38
 Operator : JC/MD
 Sample : N3354-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-59

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	42	rBV2	40580	61915	4.68%	0.744%
2	2.343	199	206	211	rBV	27129	53187	4.02%	0.639%
3	2.782	269	278	288	rBV	26845	56761	4.29%	0.682%
4	3.117	324	333	348	rVB2	13772	32941	2.49%	0.396%
5	4.440	538	550	562	rBV7	4788	17903	1.35%	0.215%
6	5.129	653	663	675	rVB5	5181	18597	1.41%	0.224%
7	5.391	694	706	722	rBV	145921	427197	32.29%	5.135%
8	5.556	722	733	748	rVB	271696	774662	58.56%	9.311%
9	5.958	789	799	817	rBV	156029	414102	31.30%	4.977%
10	6.251	834	847	861	rBV	134770	397330	30.04%	4.776%
11	6.763	920	931	952	rBV	412808	988495	74.72%	11.881%
12	7.604	1059	1069	1077	rVB2	8935	21136	1.60%	0.254%
13	7.988	1123	1132	1142	rVB	74881	150530	11.38%	1.809%
14	8.110	1142	1152	1161	rBV	128279	254729	19.26%	3.062%
15	8.653	1229	1241	1256	rBV	829630	1322880	100.00%	15.900%
16	8.958	1285	1291	1300	rVB	59202	97633	7.38%	1.173%
17	9.049	1300	1306	1314	rBV	59739	92212	6.97%	1.108%
18	9.165	1320	1325	1335	rVB	24491	43164	3.26%	0.519%
19	10.055	1465	1471	1485	rBV	817673	1106088	83.61%	13.295%
20	10.280	1503	1508	1518	rVB6	9444	22439	1.70%	0.270%
21	11.079	1634	1639	1646	rBV	611610	810602	61.28%	9.743%
22	12.024	1788	1794	1799	rBV	823122	1004290	75.92%	12.071%
23	12.475	1863	1868	1873	rVB	37666	48631	3.68%	0.585%
24	12.719	1903	1908	1912	rVV3	24705	36003	2.72%	0.433%
25	12.841	1925	1928	1932	rVB	13030	15891	1.20%	0.191%
26	13.036	1955	1960	1966	rVB	15692	21579	1.63%	0.259%
27	13.195	1982	1986	1990	rVV	11930	14996	1.13%	0.180%
28	13.237	1990	1993	1999	rVB3	9317	13994	1.06%	0.168%

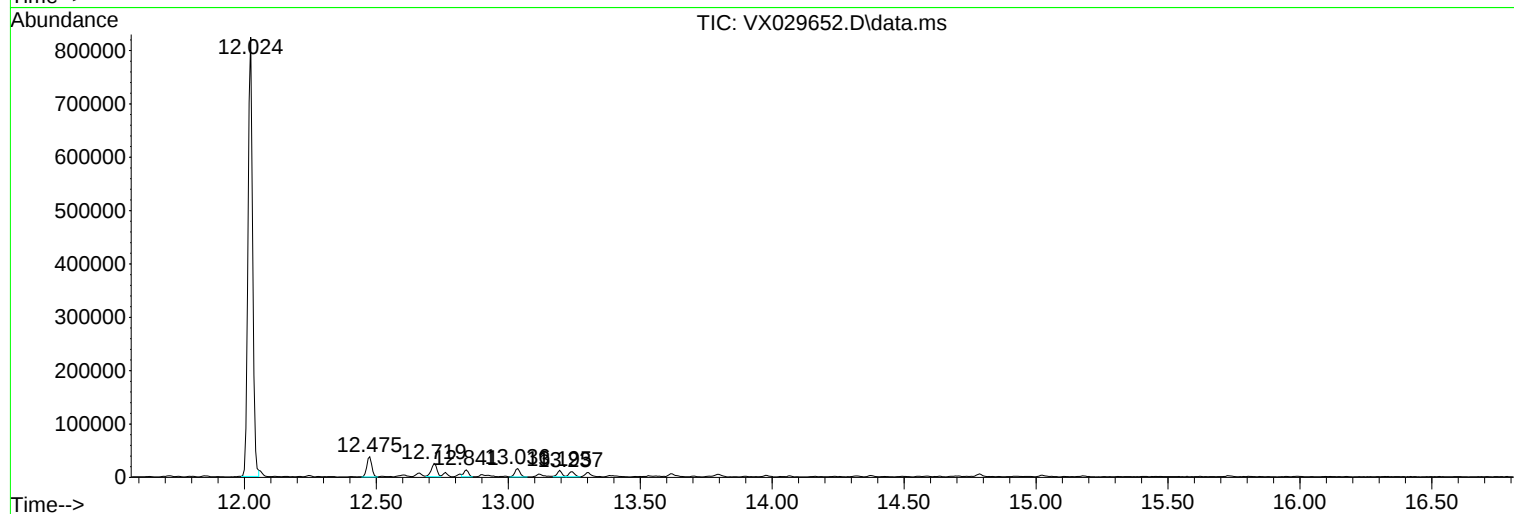
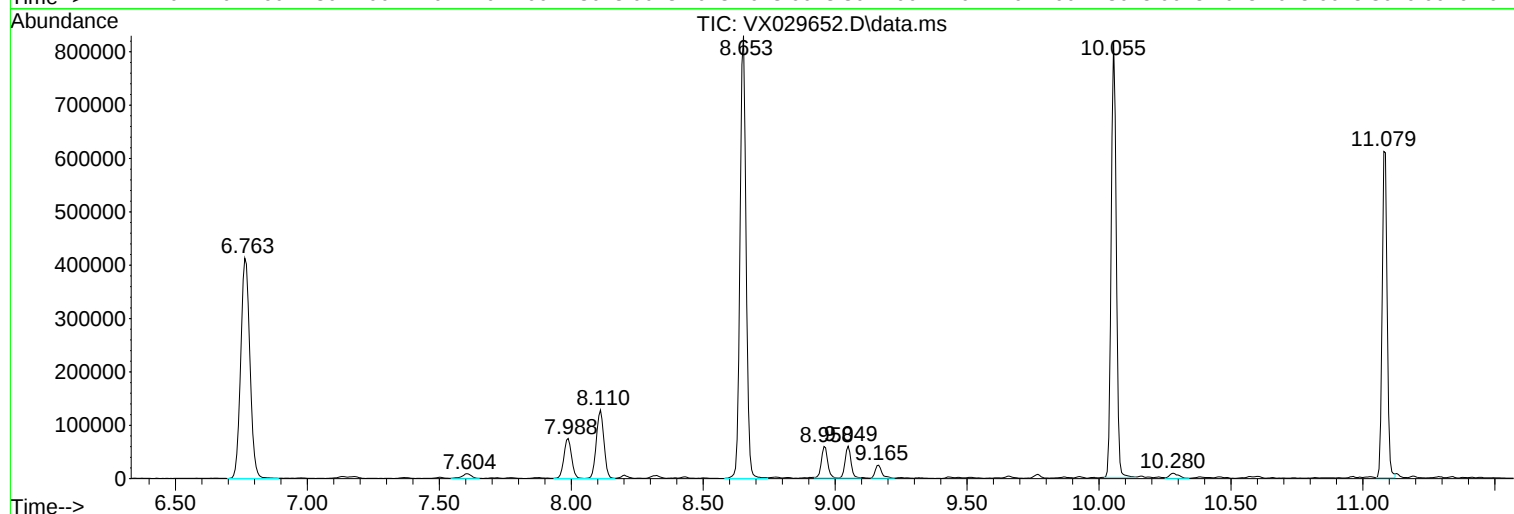
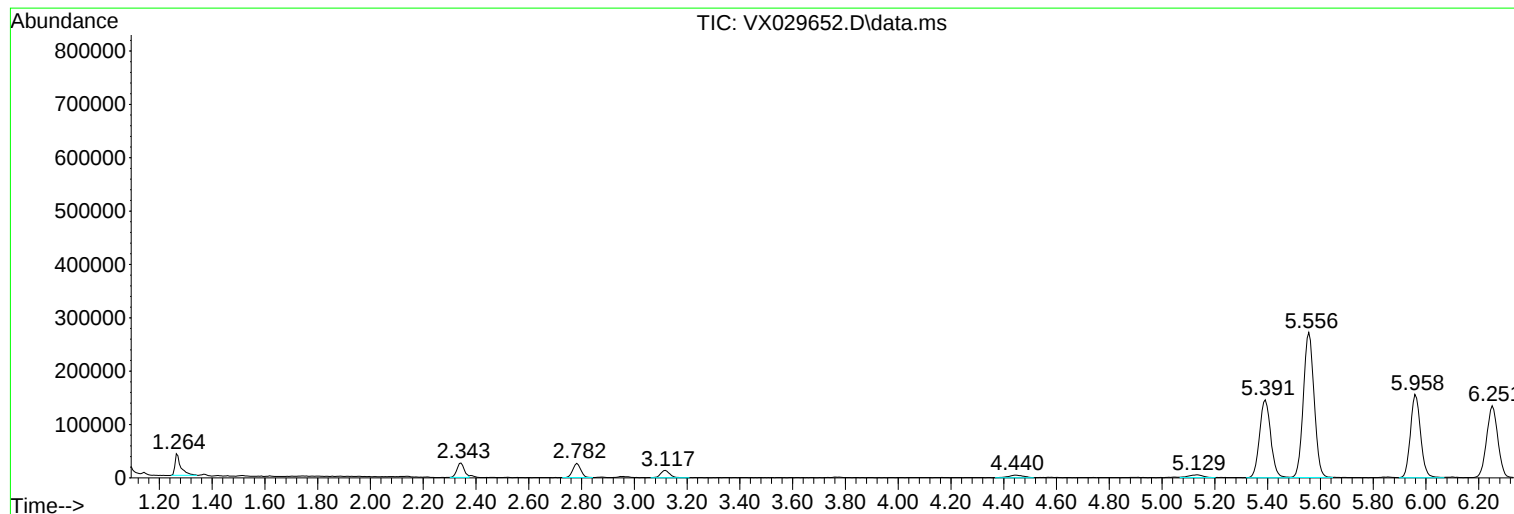
Sum of corrected areas: 8319887

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Instrument :
MSVOA_X
ClientSampleId :
MW-59

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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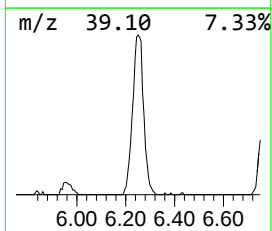
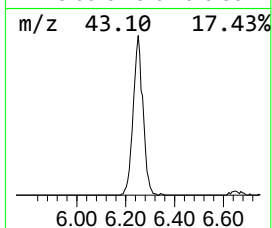
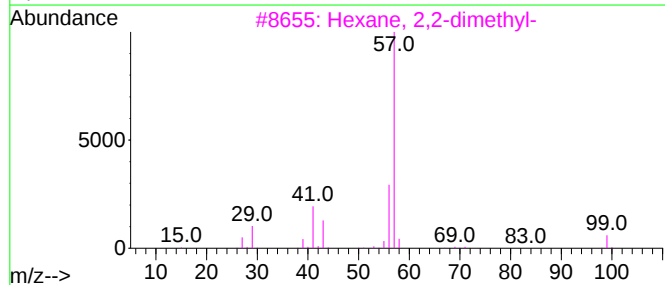
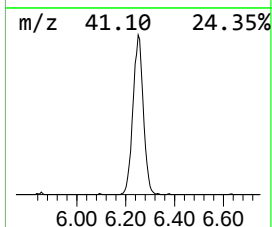
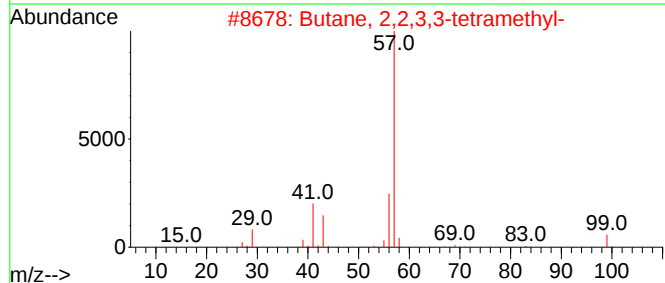
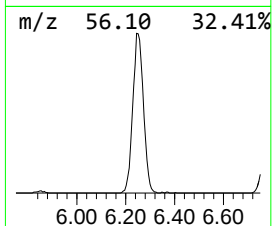
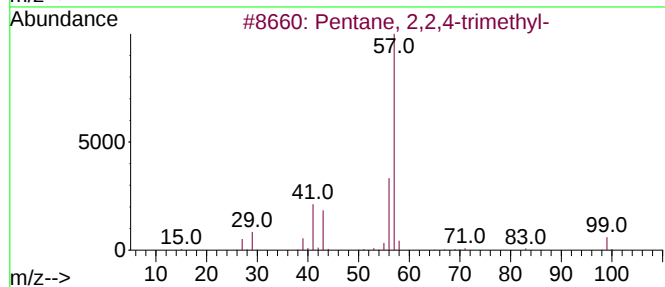
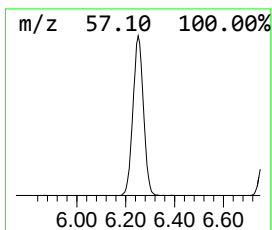
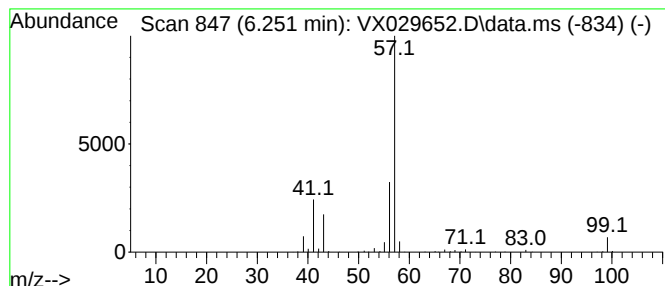
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	20.10 ug/l	397330	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
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		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	47



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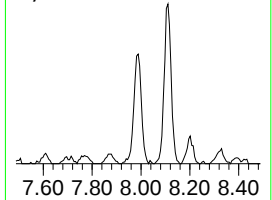
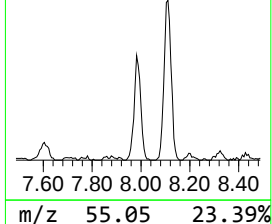
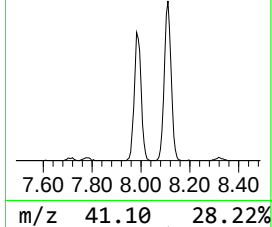
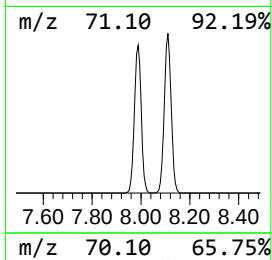
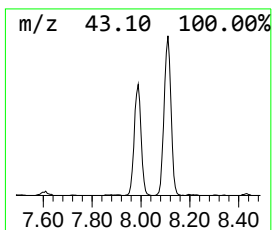
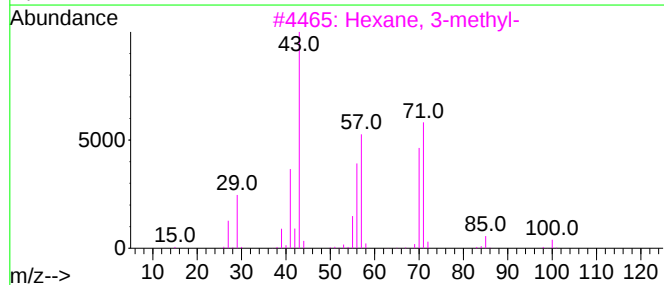
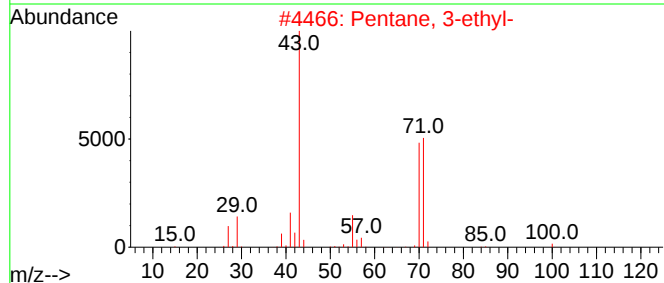
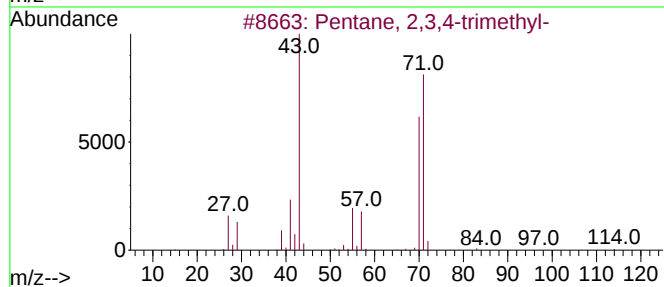
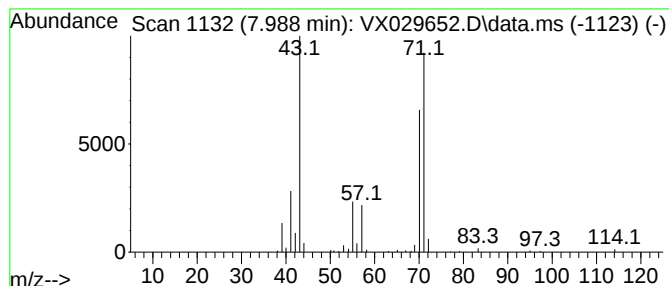
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Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	7.61 ug/l	150530	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72



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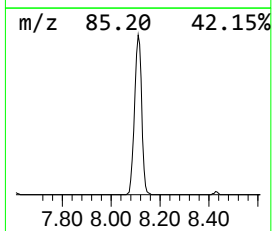
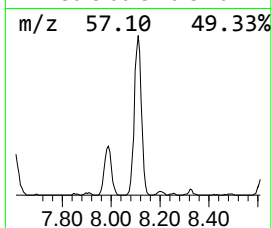
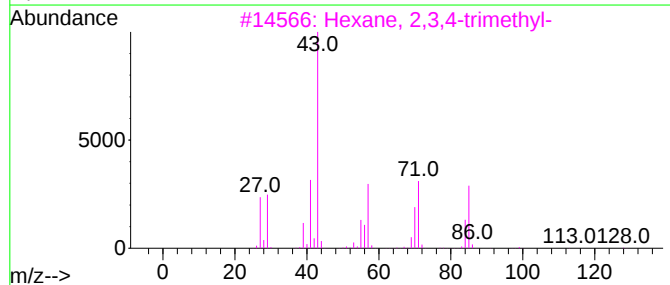
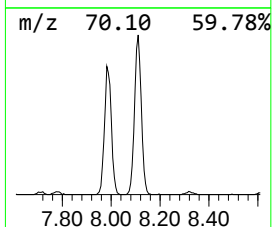
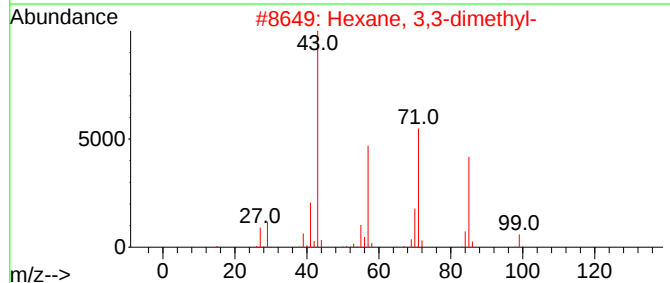
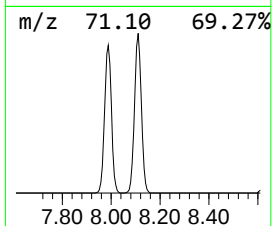
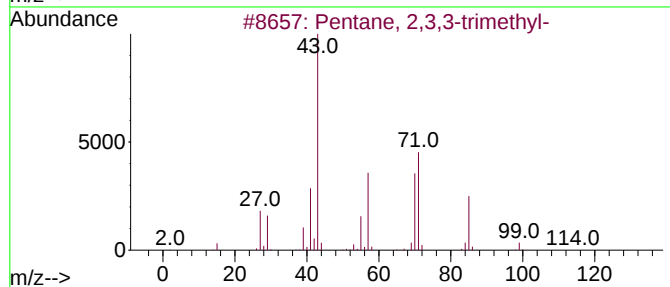
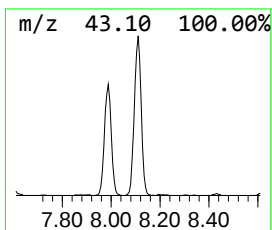
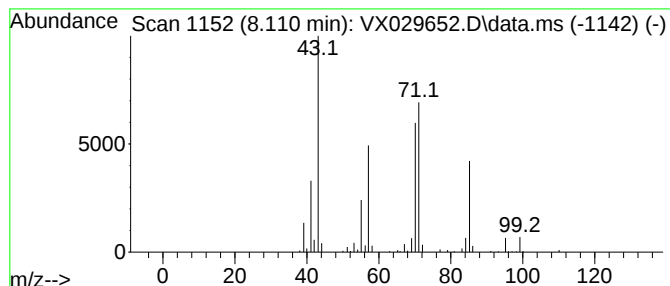
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	12.88 ug/l	254729	1,4-Difluorobenzene	6.763

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	72
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	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-...	6.251	20.1	ug/l	397330	2	6.763	988495	50.0
Pentane, 2,3,4-...	7.988	7.6	ug/l	150530	2	6.763	988495	50.0
Pentane, 2,3,3-...	8.110	12.9	ug/l	254729	2	6.763	988495	50.0