

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071122\
 Data File : VN073420.D
 Acq On : 11 Jul 2022 15:30
 Operator : JC\MD
 Sample : N3651-12
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SW-4

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	49	54	57	rBV2	9701	18958	1.42%	0.205%
2	4.510	438	446	457	rBV3	11674	36736	2.76%	0.397%
3	4.987	516	527	543	rBV2	14513	58166	4.37%	0.628%
4	5.293	568	579	588	rBV3	6104	21720	1.63%	0.235%
5	5.534	611	620	621	rBV2	7810	16881	1.27%	0.182%
6	7.951	1021	1031	1036	rBV2	200219	481187	36.14%	5.199%
7	8.016	1036	1042	1055	rVB	365673	841370	63.19%	9.091%
8	8.369	1093	1102	1115	rBV	216844	492641	37.00%	5.323%
9	8.545	1123	1132	1142	rBV	132046	316680	23.78%	3.422%
10	8.904	1184	1193	1206	rBV	527187	1102207	82.78%	11.910%
11	9.534	1292	1300	1306	rVB2	15197	32984	2.48%	0.356%
12	9.816	1340	1348	1359	rVB2	129578	261481	19.64%	2.825%
13	9.951	1359	1371	1383	rBV2	186071	401177	30.13%	4.335%
14	10.310	1427	1432	1436	rBV3	14445	23557	1.77%	0.255%
15	10.381	1436	1444	1459	rVB	705842	1322372	99.32%	14.289%
16	10.581	1465	1478	1484	rBV2	37679	74188	5.57%	0.802%
17	10.657	1484	1491	1497	rVB2	33544	62465	4.69%	0.675%
18	11.686	1656	1666	1681	rVB	746581	1331470	100.00%	14.387%
19	12.669	1826	1833	1844	rBV	596051	1030335	77.38%	11.133%
20	13.610	1985	1993	2006	rBV	778754	1310767	98.45%	14.163%
21	14.345	2112	2118	2123	rVB4	9646	17419	1.31%	0.188%

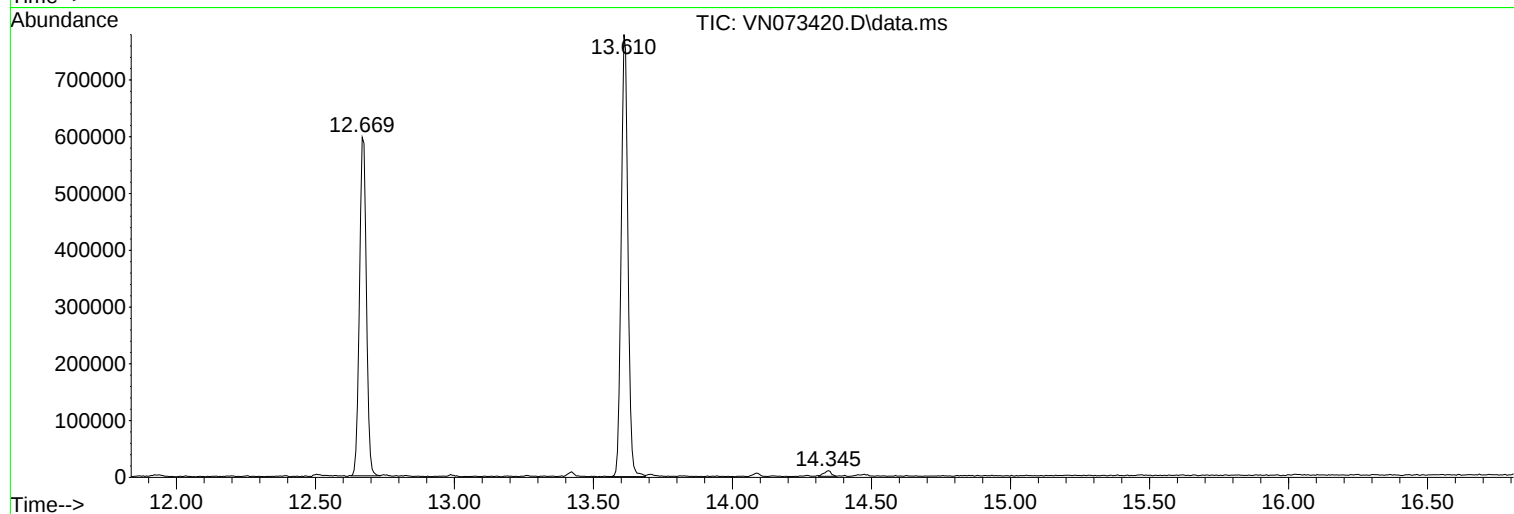
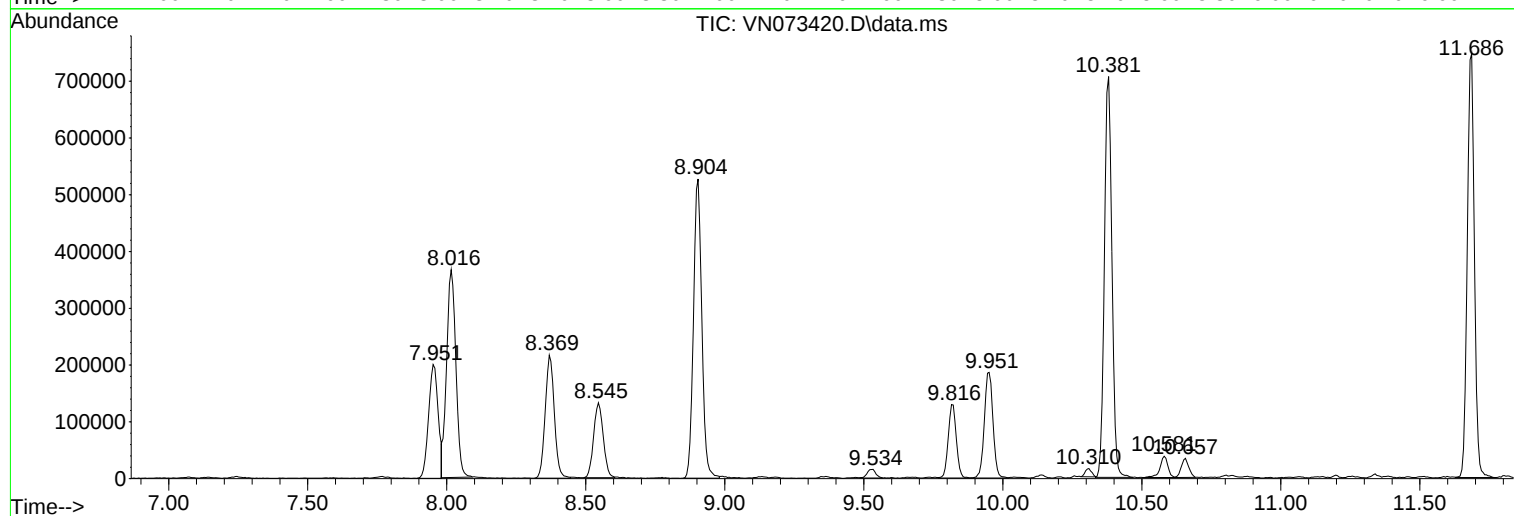
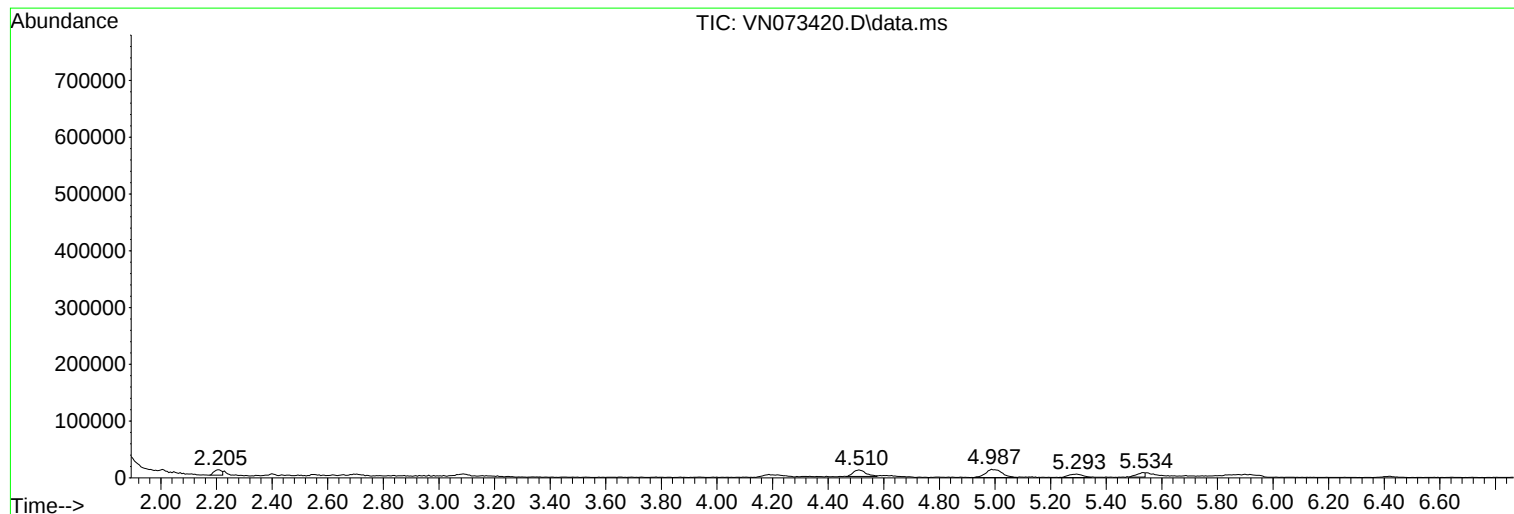
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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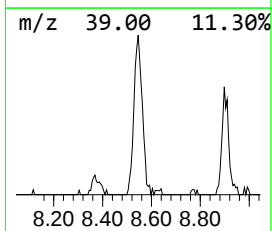
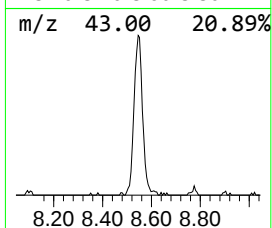
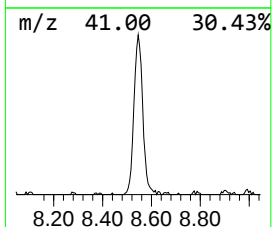
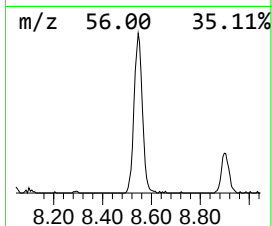
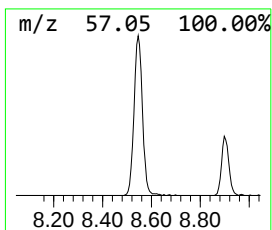
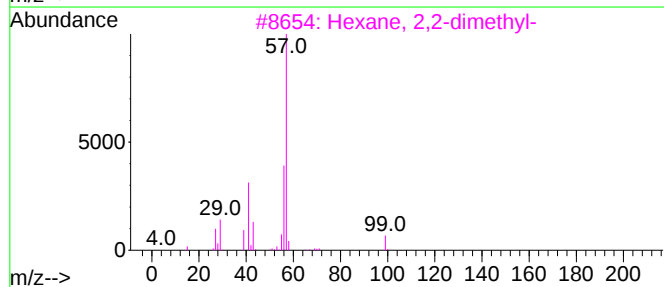
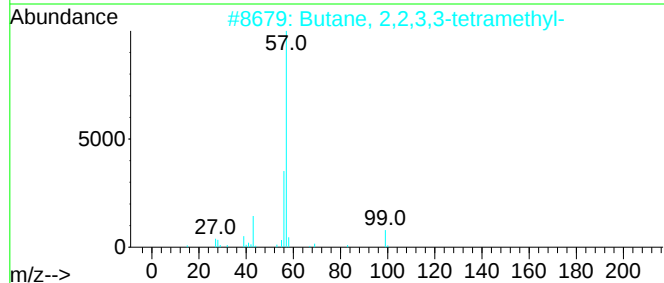
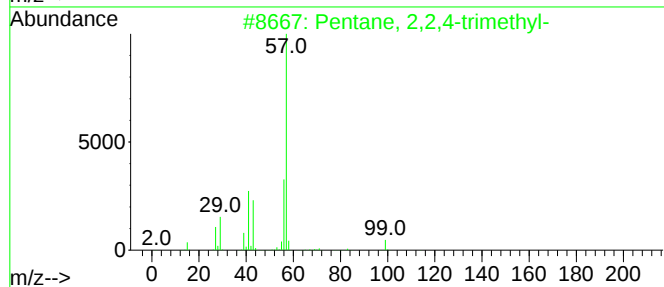
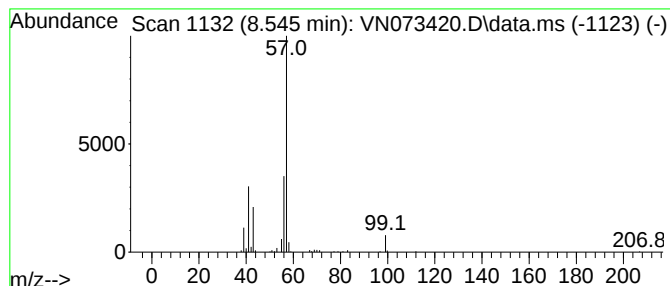
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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.
8.545	14.37 ug/l	316680	1,4-Difluorobenzene	8.904

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			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59



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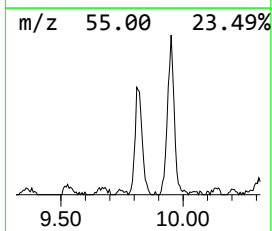
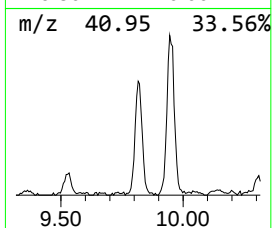
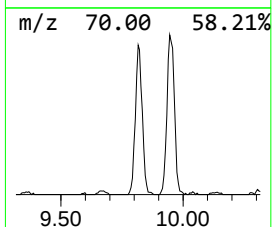
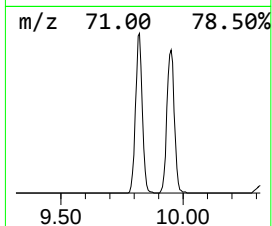
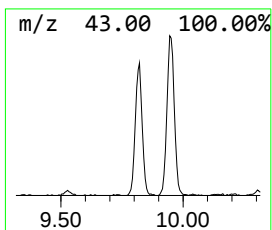
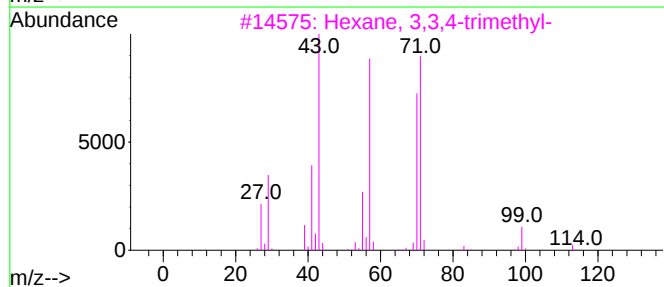
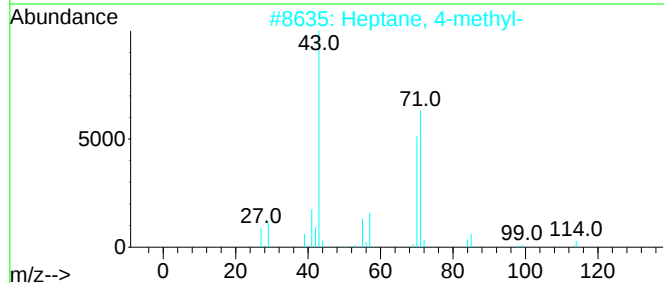
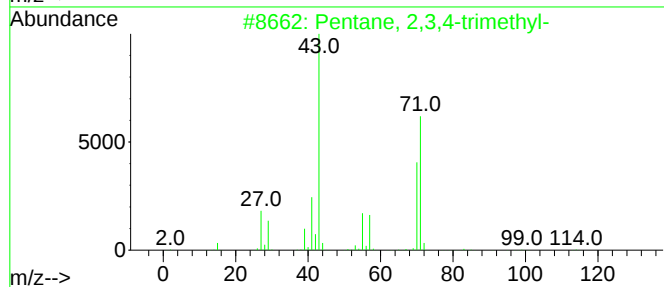
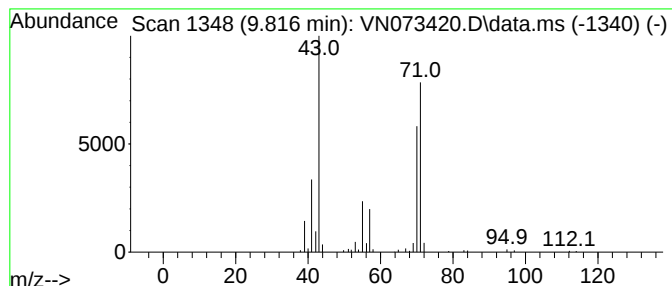
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Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	11.86 ug/l	261481	1,4-Difluorobenzene	8.904

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	83
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	78



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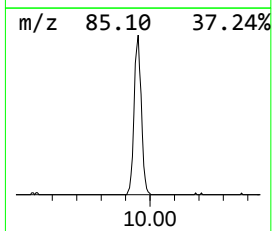
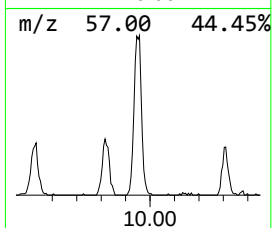
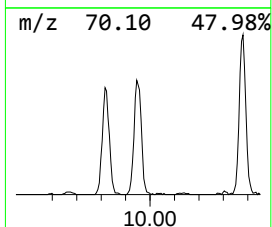
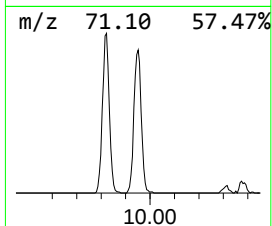
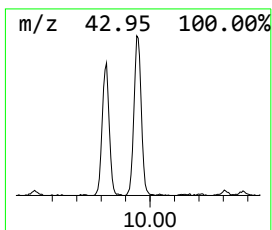
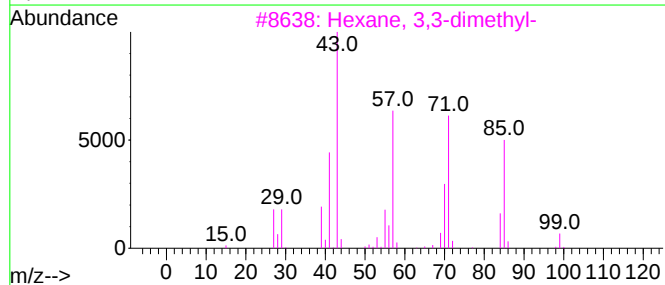
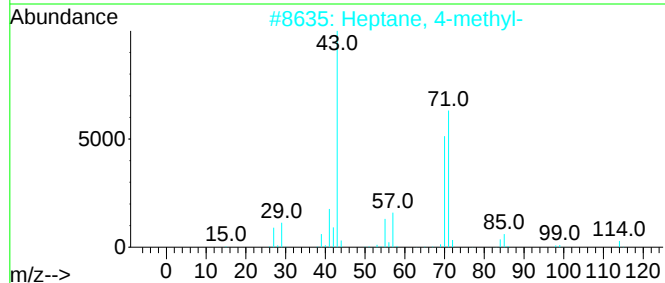
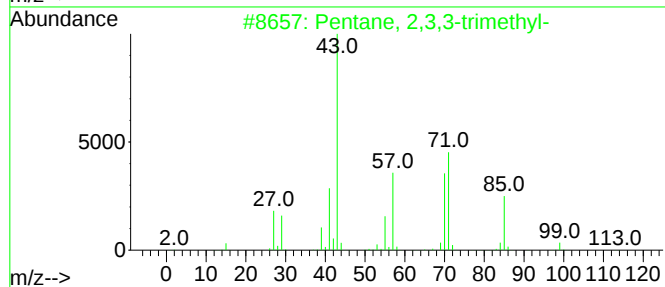
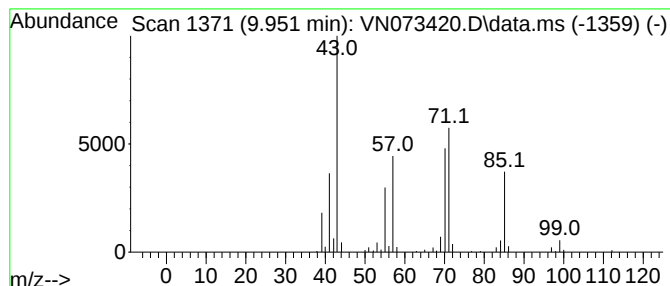
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	18.20 ug/l	401177	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,4-...	8.545	14.4	ug/l	316680	2	8.904	1102210	50.0
Pentane, 2,3,4-...	9.816	11.9	ug/l	261481	2	8.904	1102210	50.0
Pentane, 2,3,3-...	9.951	18.2	ug/l	401177	2	8.904	1102210	50.0