

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
 Data File : VN069170.D
 Acq On : 25 Oct 2021 23:11
 Operator : JC/MD
 Sample : M4334-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 STORAGE-BLANK-REF-6

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\82N101221W.M
 Title : SW846 8260

Signal : TIC: VN069170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	82	93	110	rBV5	16929	39419	1.33%	0.201%
2	4.151	780	806	848	rBV	384589	1128757	37.95%	5.743%
3	4.578	940	965	998	rBV2	27499	92943	3.12%	0.473%
4	6.294	1583	1605	1622	rBV4	11175	35212	1.18%	0.179%
5	6.578	1691	1711	1748	rBV2	37397	129905	4.37%	0.661%
6	7.316	1962	1986	2015	rBV2	47378	139265	4.68%	0.709%
7	8.027	2228	2251	2261	rBV	340858	797525	26.81%	4.058%
8	8.088	2262	2274	2305	rVB	661654	1534578	51.59%	7.808%
9	8.440	2383	2405	2434	rBV	370015	856873	28.81%	4.360%
10	8.971	2583	2603	2635	rBV	968818	2005410	67.42%	10.204%
11	9.558	2804	2822	2838	rBV3	14408	31329	1.05%	0.159%
12	10.446	3131	3153	3184	rBV	1479883	2835343	95.32%	14.427%
13	11.746	3611	3638	3667	rVV	1451055	2974545	100.00%	15.135%
14	11.859	3670	3680	3708	rVB7	19523	49462	1.66%	0.252%
15	12.358	3850	3866	3881	rBV4	15973	35059	1.18%	0.178%
16	12.733	3988	4006	4027	rBV2	1481852	2649042	89.06%	13.479%
17	12.908	4053	4071	4079	rBV5	21402	53997	1.82%	0.275%
18	13.527	4287	4302	4323	rBV2	112829	211046	7.10%	1.074%
19	13.678	4341	4358	4375	rBV	1249912	2116613	71.16%	10.770%
20	14.141	4518	4531	4547	rVB2	38656	67234	2.26%	0.342%
21	14.351	4593	4609	4621	rBV5	15206	33217	1.12%	0.169%
22	14.426	4624	4637	4659	rVV4	58738	128319	4.31%	0.653%
23	14.689	4706	4735	4759	rBV8	182406	720837	24.23%	3.668%
24	14.785	4761	4771	4788	rVB2	90557	169305	5.69%	0.861%
25	14.997	4838	4850	4878	rVB2	88703	176420	5.93%	0.898%
26	15.348	4962	4981	5010	rBV2	200413	434737	14.62%	2.212%
27	15.517	5035	5044	5069	rVB3	84641	175648	5.91%	0.894%
28	15.885	5171	5181	5199	rVB6	15719	31536	1.06%	0.160%

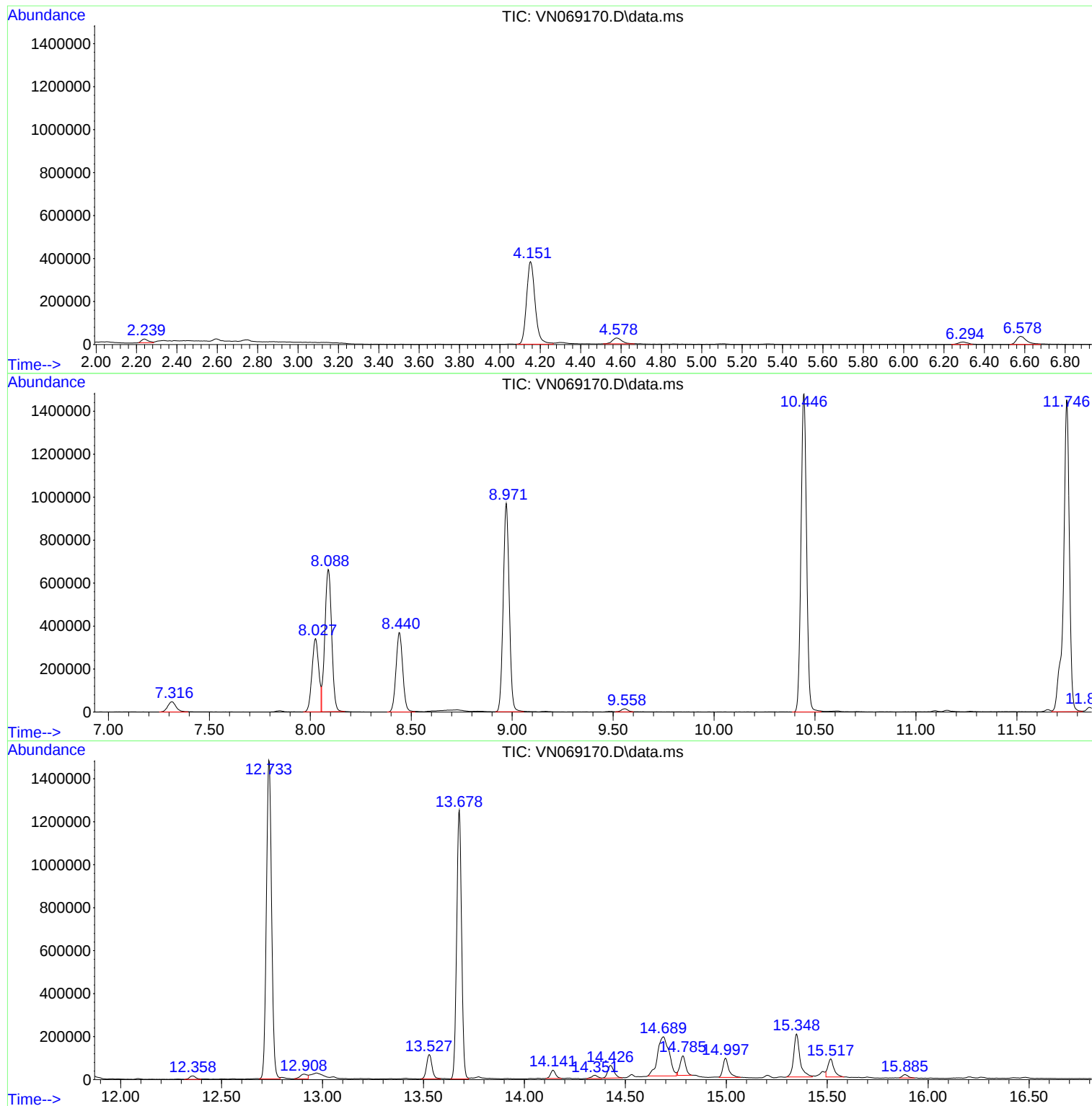
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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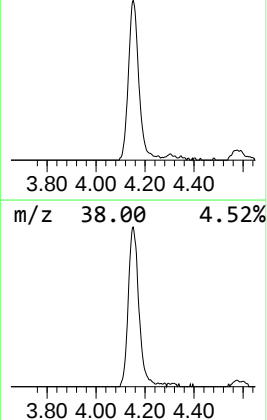
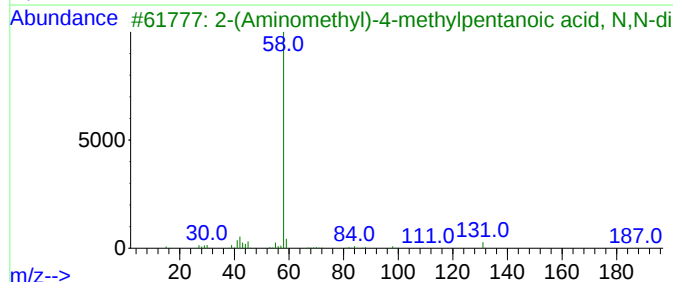
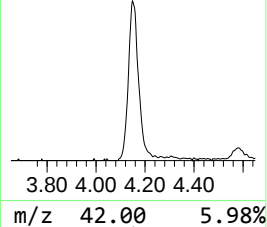
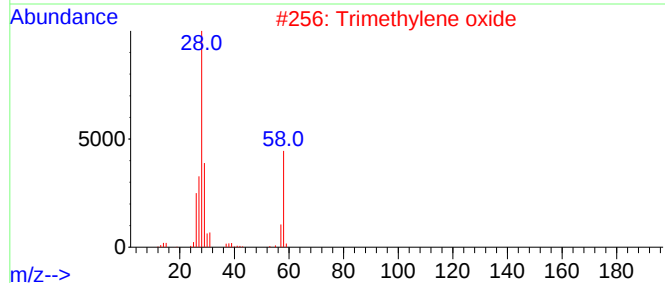
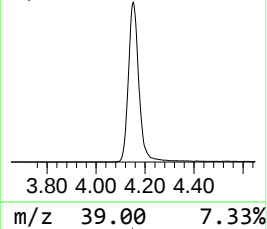
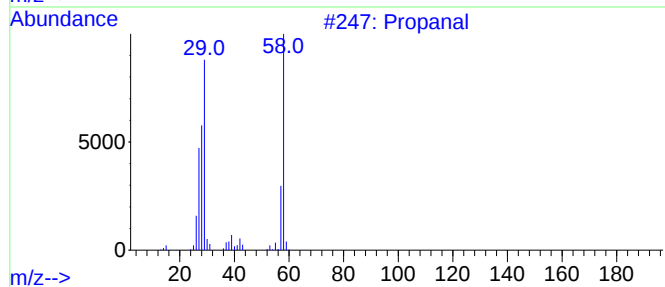
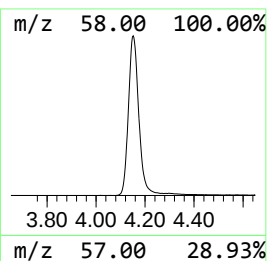
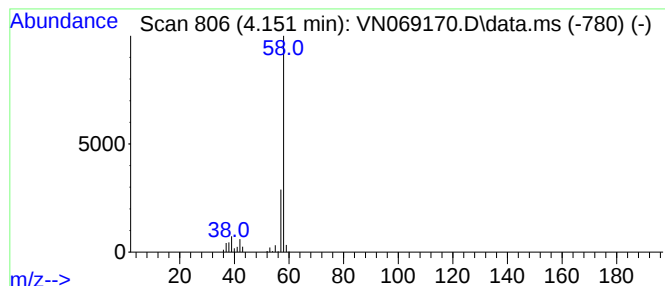
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.151	36.78 ug/l	1128760	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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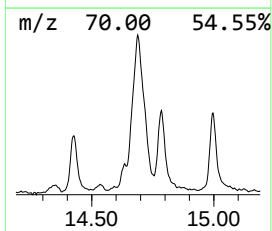
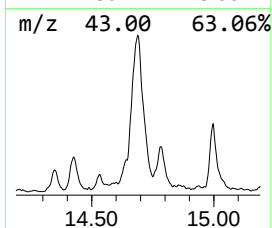
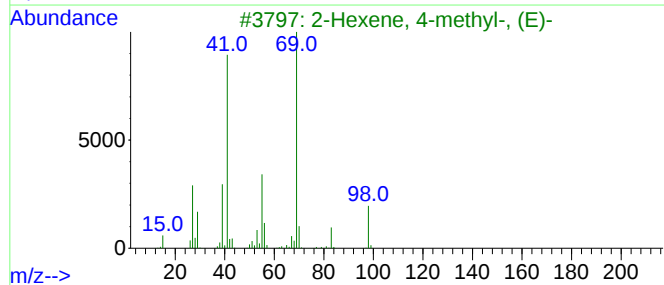
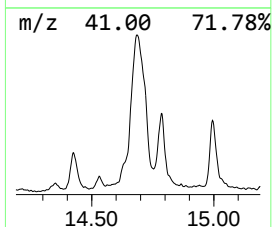
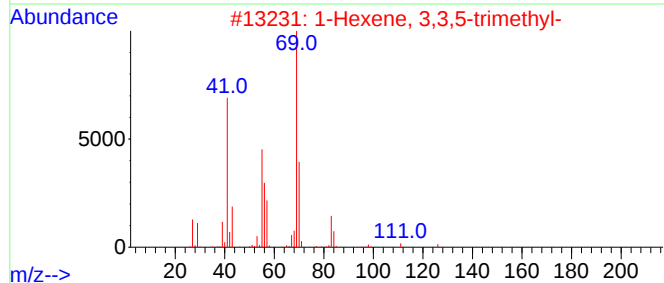
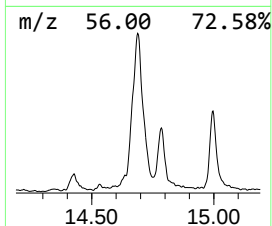
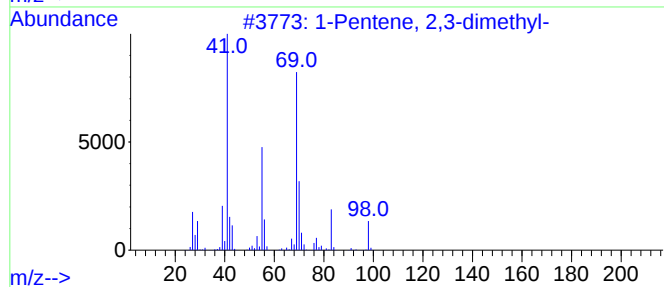
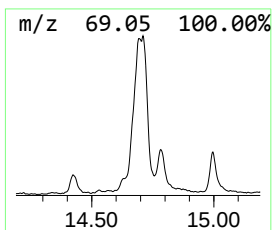
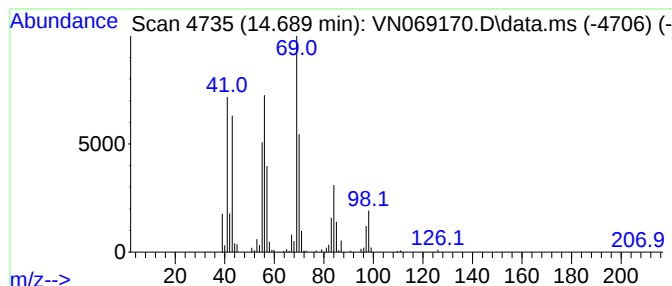
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Peak Number 2 unknown14.689 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.689	17.03 ug/l	720837	1,4-Dichlorobenzene-d4	13.678

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	46
2		1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	43
3		2-Hexene, 4-methyl-, (E)-	98	C7H14	003683-22-5	43
4		3-Methyl-3-hexene	98	C7H14	003404-65-7	43
5		1-Heptene	98	C7H14	000592-76-7	41



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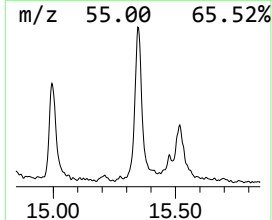
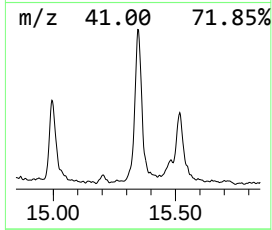
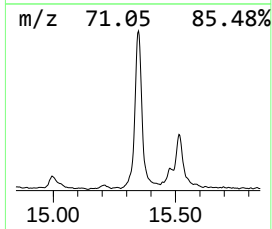
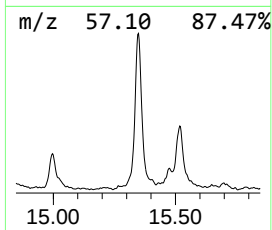
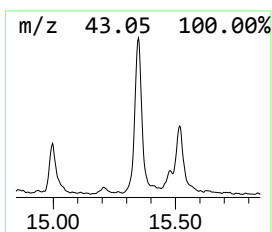
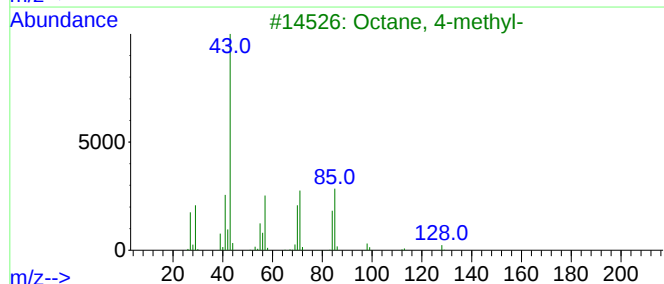
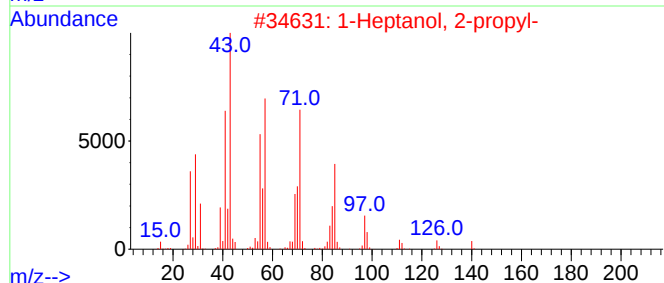
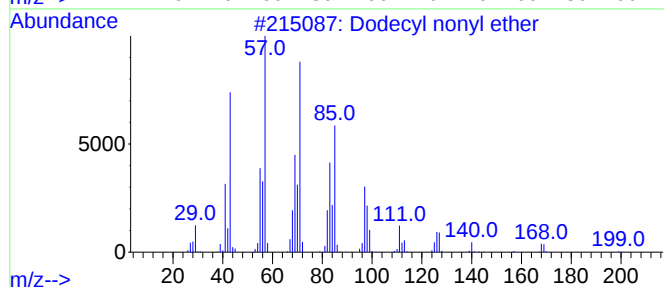
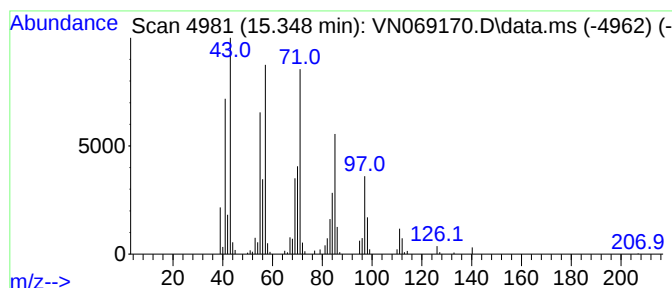
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Peak Number 3 Dodecyl nonyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.348	10.27 ug/l	434737	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyl nonyl ether	312	C21H44O	1000406-37-5	78
2			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
3			Octane, 4-methyl-	128	C9H20	002216-34-4	47
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	43
5			1-Tetradecene	196	C14H28	001120-36-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.151	36.8	ug/l	1128760	1	8.088	1534580	50.0
unknown14.689	14.689	17.0	ug/l	720837	4	13.678	2116610	50.0
Dodecyl nonyl e...	15.348	10.3	ug/l	434737	4	13.678	2116610	50.0