

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY091919\
 Data File : VY000089.D
 Acq On : 19 Sep 2019 19:48
 Operator : SY/MD
 Sample : K4862-08
 Misc : 5.04g/5.00ml/MSVOA Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CSA-4-4-1

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_Y\METHODS\82Y091719S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.697	13	18	35	rVV	615162	932705	100.00%	25.037%
2	4.715	501	513	521	rBV7	6106	19805	2.12%	0.532%
3	7.720	996	1006	1012	rBV2	75564	181333	19.44%	4.868%
4	7.793	1012	1018	1029	rVB2	127627	286846	30.75%	7.700%
5	8.147	1067	1076	1086	rVB2	77481	178461	19.13%	4.791%
6	8.689	1155	1165	1174	rBV	224236	432417	46.36%	11.608%
7	9.982	1371	1377	1384	rBV2	32198	60994	6.54%	1.637%
8	10.177	1398	1409	1417	rBV	325917	556918	59.71%	14.950%
9	11.488	1617	1624	1633	rVB	269456	429131	46.01%	11.519%
10	12.475	1777	1786	1793	rBV	161020	261677	28.06%	7.024%
11	12.805	1835	1840	1847	rVB3	6403	11002	1.18%	0.295%
12	13.420	1935	1941	1948	rBV	179092	281458	30.18%	7.555%
13	13.756	1988	1996	2006	rBV4	13972	32301	3.46%	0.867%
14	14.304	2081	2086	2091	rBV5	8049	12405	1.33%	0.333%
15	14.505	2111	2119	2126	rBV2	30003	47857	5.13%	1.285%

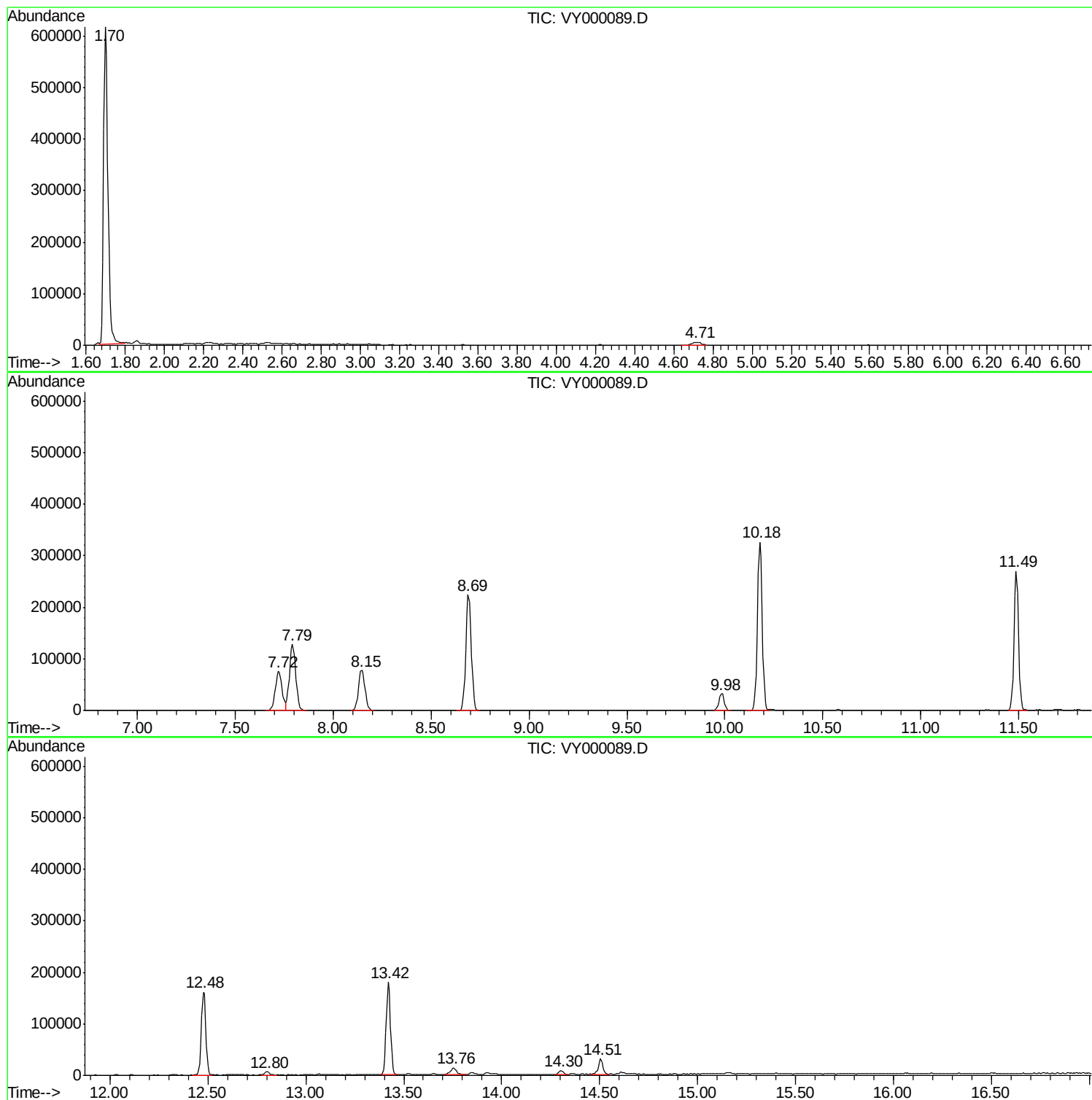
Sum of corrected areas: 3725310

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Quant Title : SW846 8260

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



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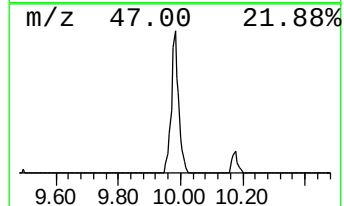
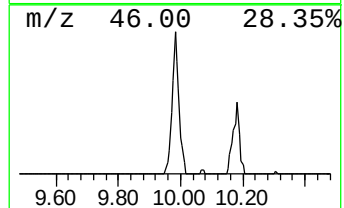
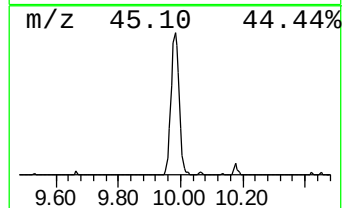
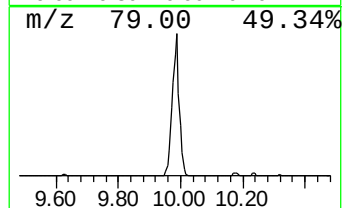
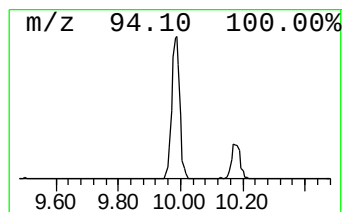
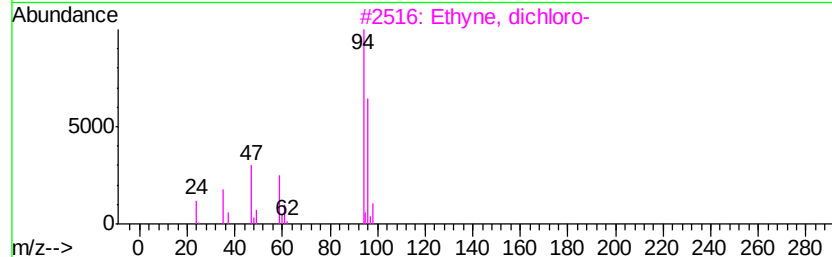
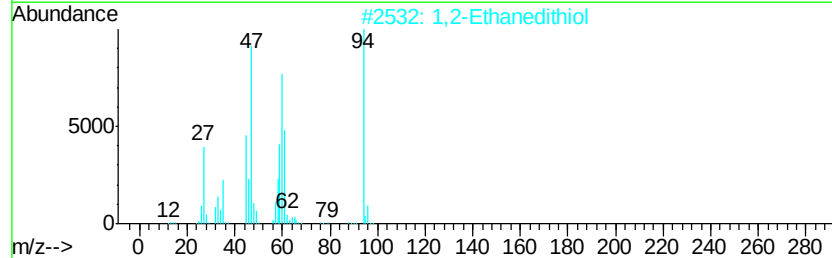
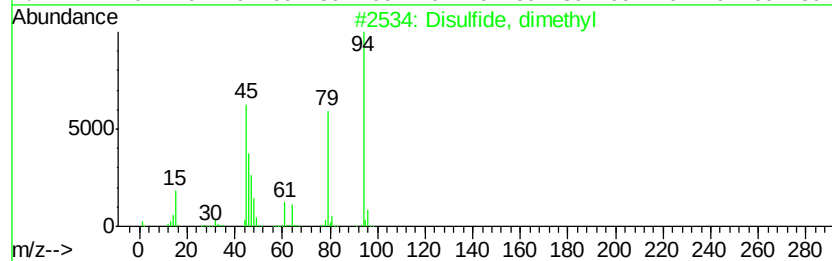
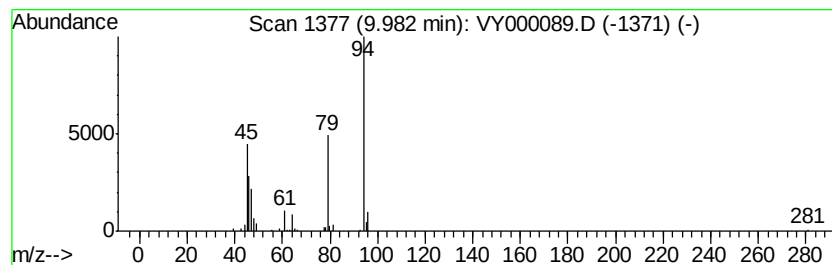
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y091719S.M
Quant Title : SW846 8260

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

Peak Number 2 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	7.05 ug/l	60994	1,4-Difluorobenzene	8.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2		1,2-Ethanedithiol	94	C2H6S2	000540-63-6	47
3		Ethvne, dichloro-	94	C2Cl2	007572-29-4	38
4		Diethyl chloromalonate	194	C7H11ClO4	014064-10-9	9
5		Succinic acid, di(cyclohex-2-eny...	306	C18H26O4	1000330-19-3	9



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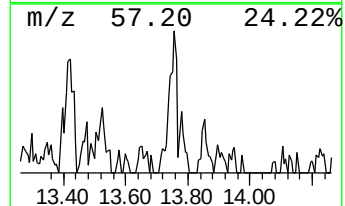
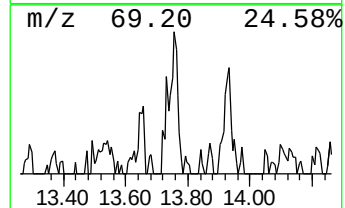
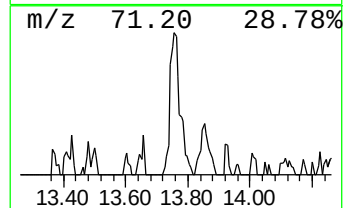
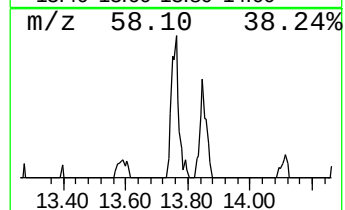
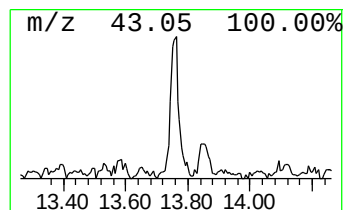
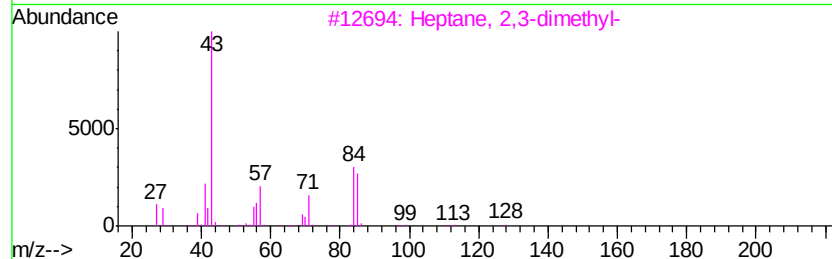
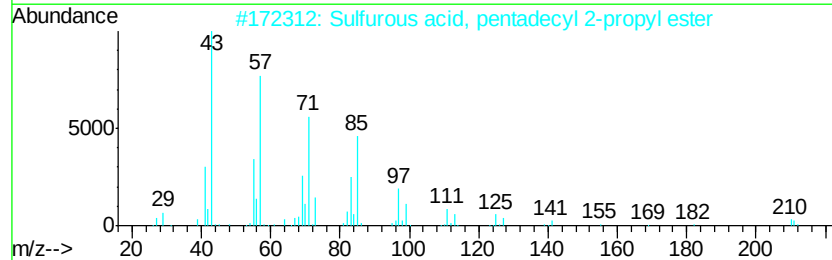
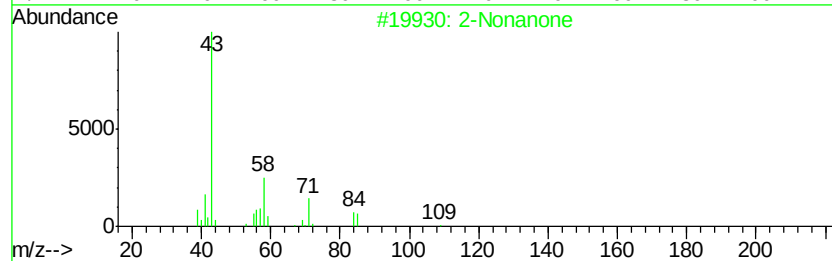
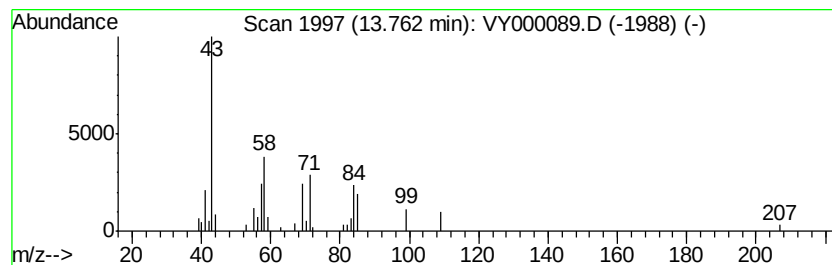
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Peak Number 3 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.76	5.74 ug/l	32301	1,4-Dichlorobenzene-d4		13.42		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanone	142	C9H18O	000821-55-6	53
2			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	38
3			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	38
4			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	38
5			Octane, 4-methyl-	128	C9H20	002216-34-4	35



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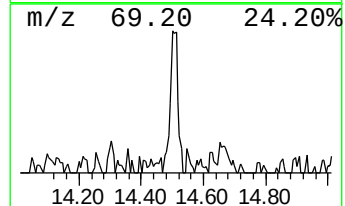
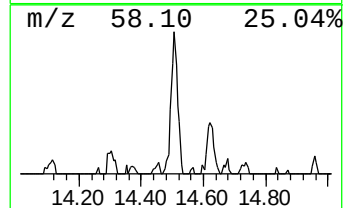
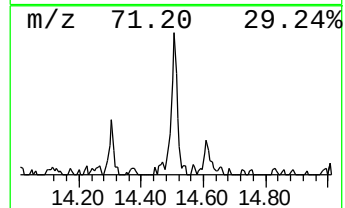
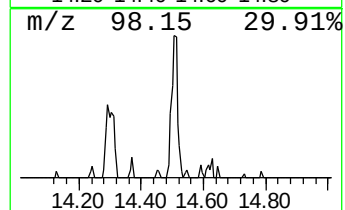
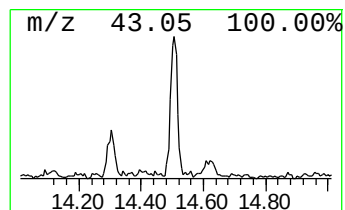
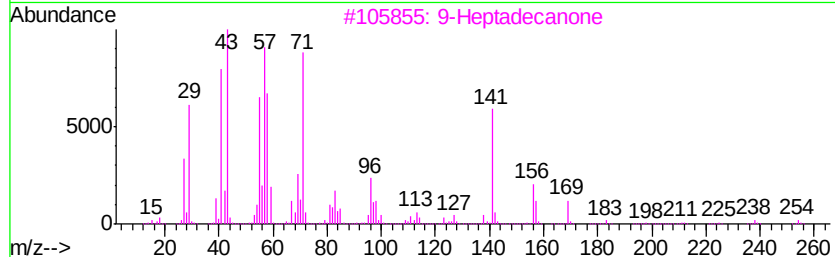
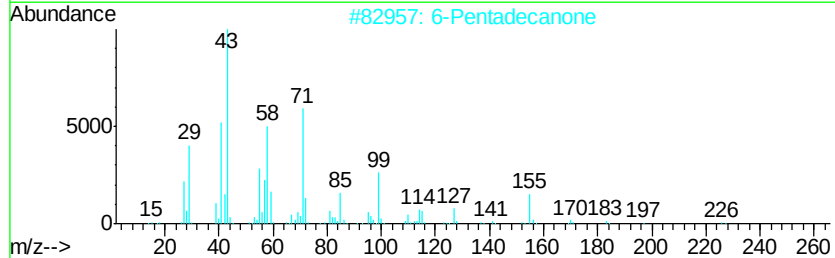
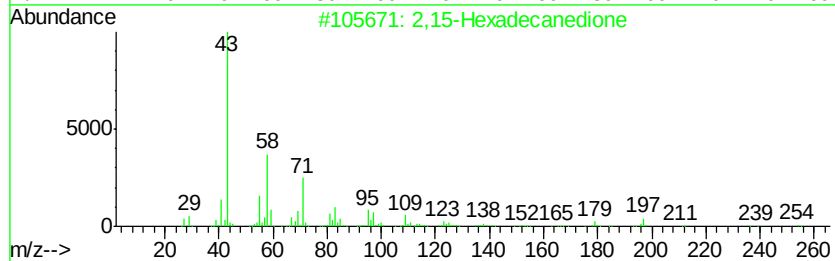
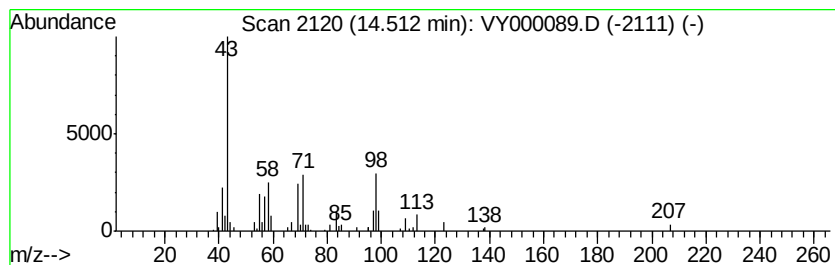
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Peak Number 4 unknown14.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.51	8.50 ug/l	47857	1,4-Dichlorobenzene-d4	13.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,15-Hexadecanedione	254	C16H30O2	018650-13-0	35
2	6-Pentadecanone	226	C15H30O	001001-45-2	32
3	9-Heptadecanone	254	C17H34O	000540-08-9	25
4	2,11-Dodecanedione	198	C12H22O2	007029-09-6	25
5	5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dimethyl	9.98	7.0	ug/l	60994	2	8.69	432417	50.0
2-Nonanone	13.76	5.7	ug/l	32301	4	13.42	281458	50.0
unknown14.51	14.51	8.5	ug/l	47857	4	13.42	281458	50.0