

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042221\
 Data File : VY004592.D
 Acq On : 22 Apr 2021 17:58
 Operator : SY/MD
 Sample : M2111-04
 Misc : 5.07G/5ML/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-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_Y\methods\82Y041221S.M

Title : SW846 8260

Signal : TIC: VY004592.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	46	63	64	rBV5	6386	27068	2.55%	0.504%
2	4.729	467	477	487	rBV3	4271	13630	1.29%	0.254%
3	7.728	960	969	975	rBV	96710	234827	22.15%	4.372%
4	7.801	975	981	996	rVB	167242	375164	35.38%	6.985%
5	8.155	1025	1039	1049	rBV2	107538	277796	26.20%	5.172%
6	8.697	1119	1128	1138	rBV	277462	538297	50.77%	10.022%
7	9.752	1296	1301	1308	rVB3	7078	12925	1.22%	0.241%
8	10.185	1365	1372	1380	rBV	468770	782933	73.84%	14.577%
9	10.581	1432	1437	1444	rVB	14251	25261	2.38%	0.470%
10	11.319	1554	1558	1564	rBV	16479	28837	2.72%	0.537%
11	11.496	1580	1587	1595	rBV	423175	685299	64.63%	12.759%
12	12.197	1687	1702	1721	rVB9	47648	342227	32.28%	6.372%
13	12.489	1743	1750	1756	rBV2	337972	560842	52.89%	10.442%
14	13.251	1862	1875	1888	rBV9	38574	201627	19.02%	3.754%
15	13.428	1898	1904	1923	rVB	481515	1060305	100.00%	19.741%
16	13.642	1931	1939	1940	rBV4	22602	44629	4.21%	0.831%
17	13.800	1960	1965	1978	rVB3	38507	117420	11.07%	2.186%
18	15.525	2241	2248	2255	rVB3	16518	41874	3.95%	0.780%

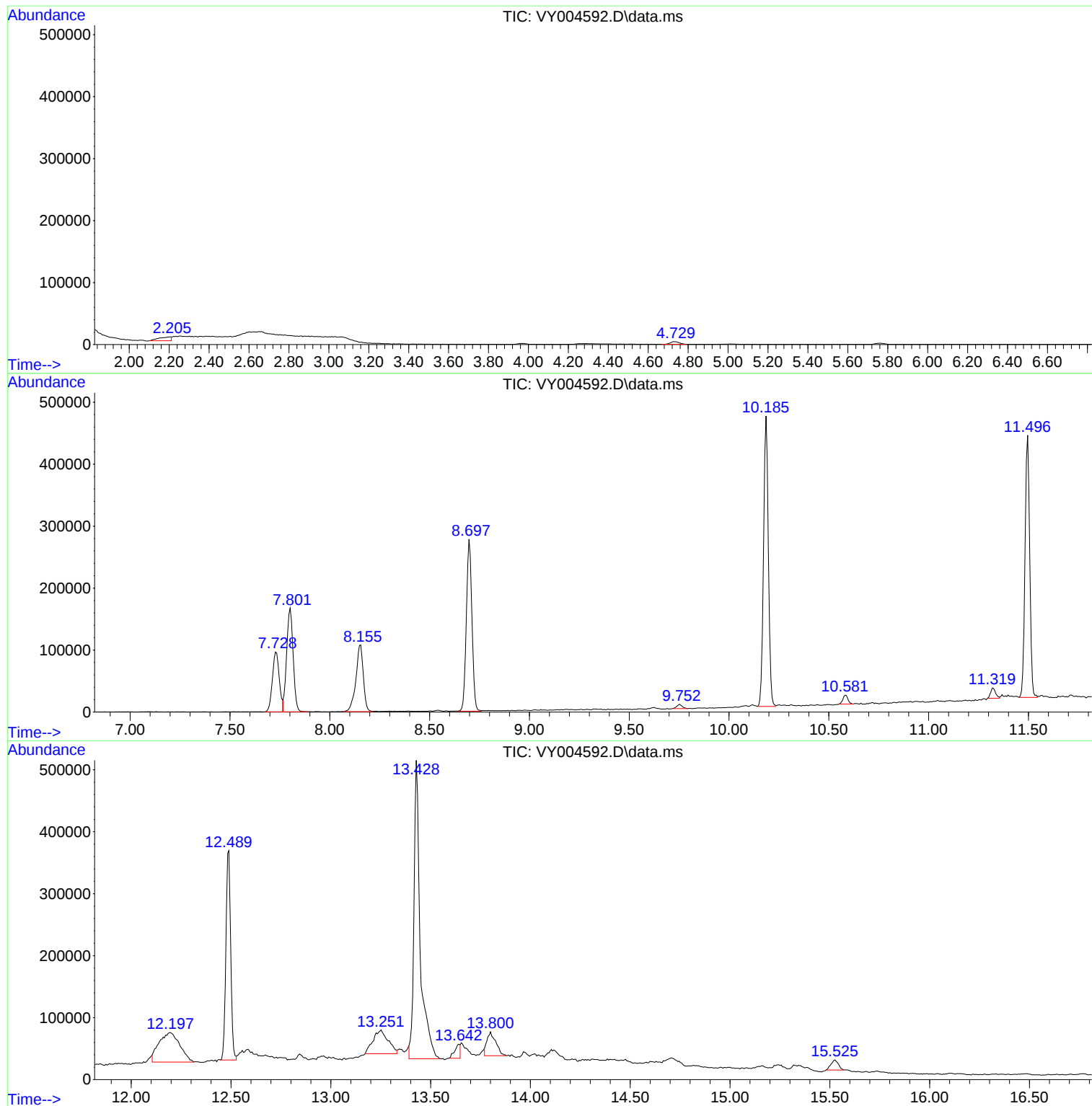
Sum of corrected areas: 5370961

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_Y
ClientSampled :
S-4

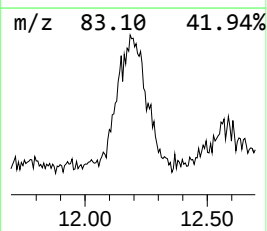
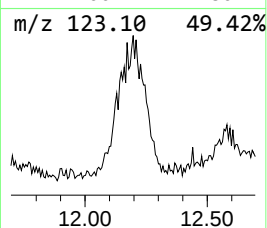
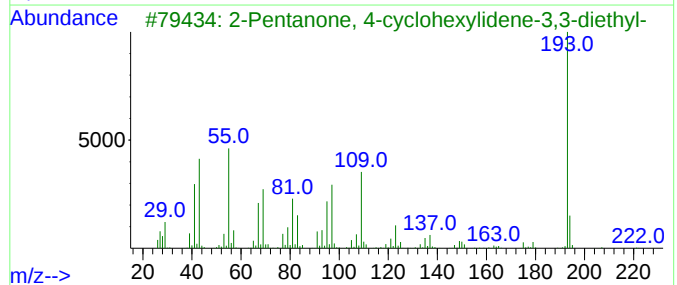
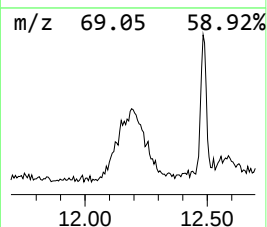
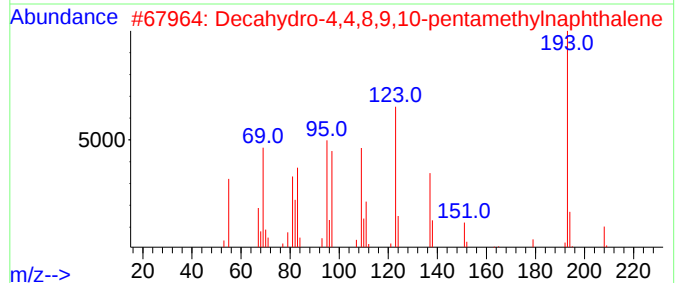
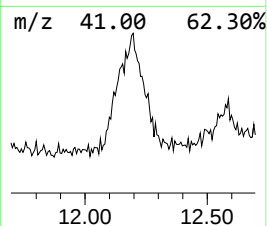
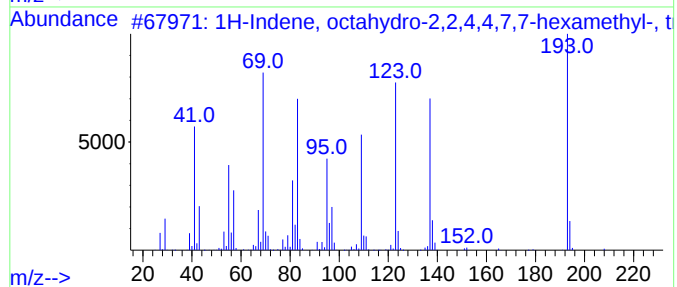
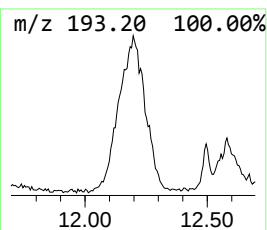
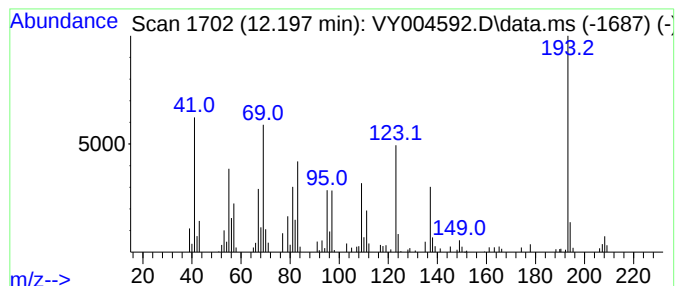
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

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

Peak Number 1 1H-Indene, octahydro-2,2,4,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.197	24.97 ug/l	342227	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	59
2			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	43
3			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
4			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	27
5			Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	22



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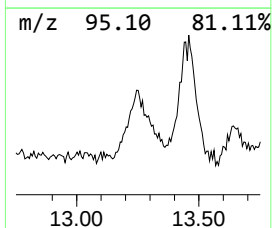
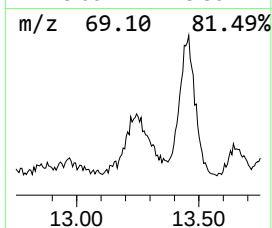
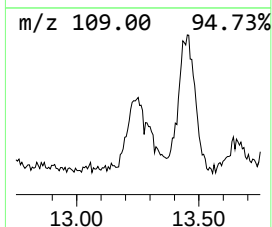
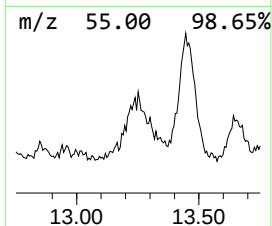
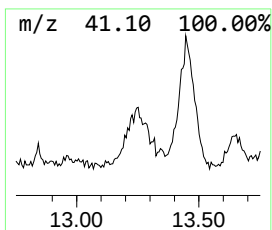
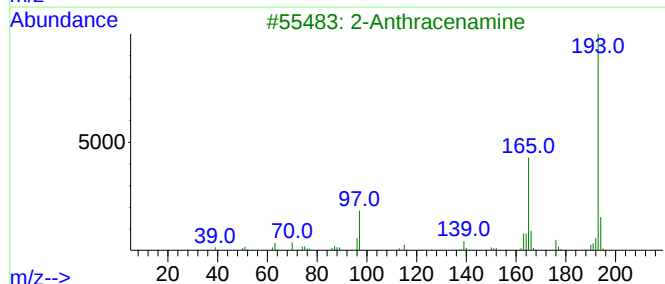
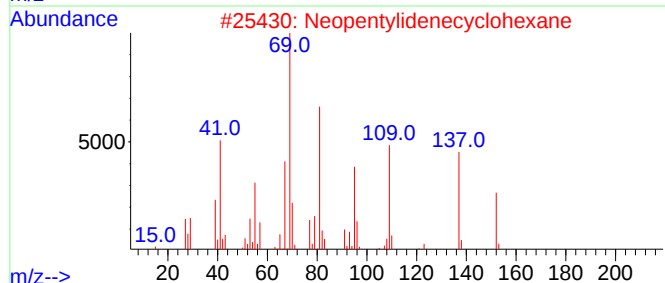
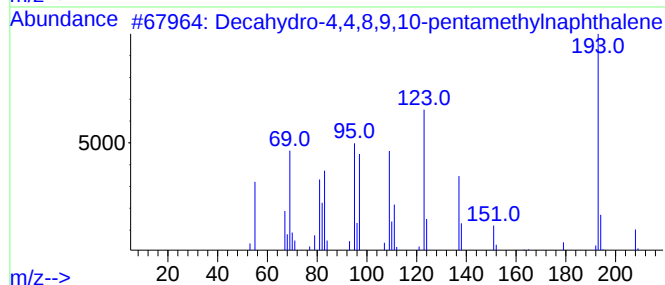
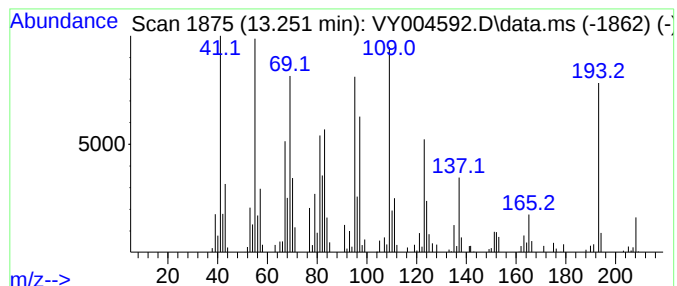
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Peak Number 2 Decahydro-4,4,8,9,10-pentam... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	9.51 ug/l	201627	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
2			Neopentylidenecyclohexane	152	C11H20	039546-80-0	30
3			2-Anthracenamine	193	C14H11N	000613-13-8	25
4			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	25
5			1,2-Cyclohexanediol, cyclic sulf...	162	C6H10O3S	019456-19-0	25



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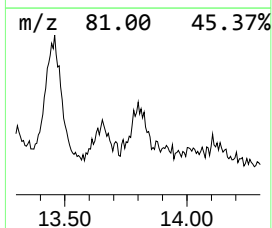
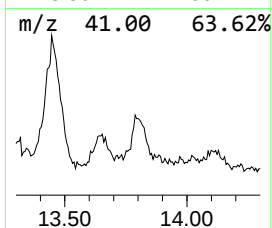
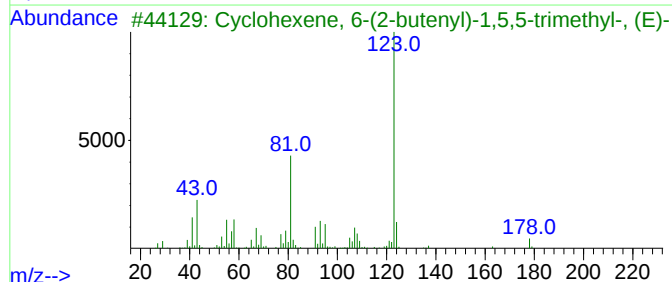
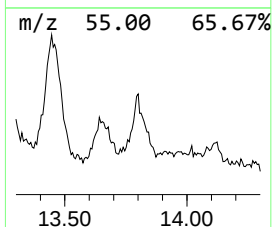
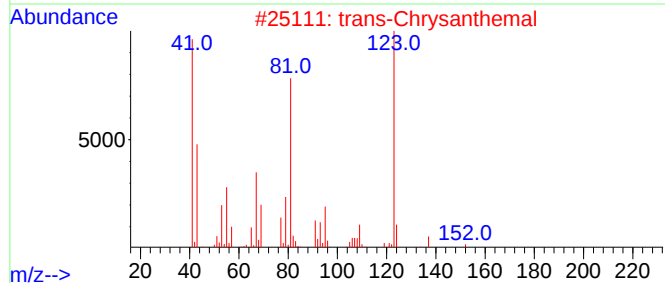
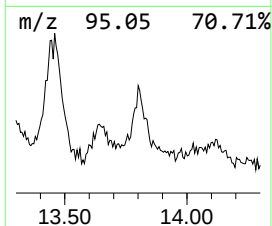
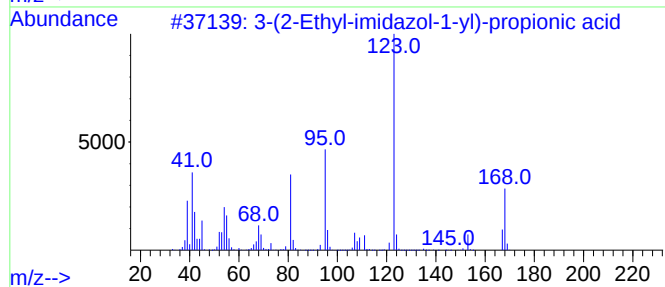
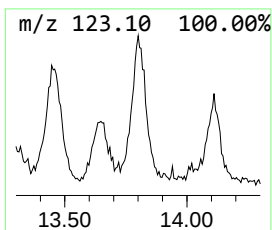
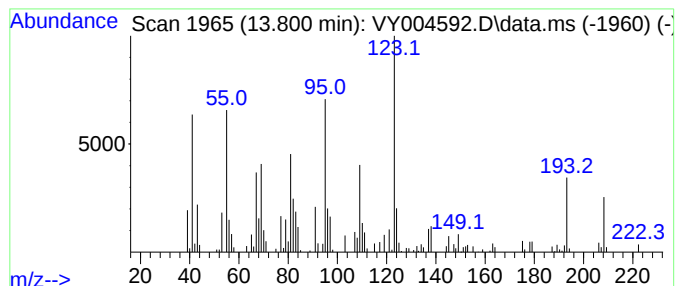
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Peak Number 3 unknown13.800 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.800	5.54 ug/l	117420	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1000277-78-0	38		
2	trans-Chrysanthemal	152	C10H16O	020104-05-6	27		
3	Cyclohexene, 6-(2-butenyl)-1,5,5...	178	C13H22	053941-16-5	27		
4	Furan, 2-(1,1-dimethylethyl)-4-m...	138	C9H14O	006141-68-0	27		
5	Octopamine	153	C8H11NO2	000104-14-3	27		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-Indene, octa...	12.197	25.0	ug/l	342227	3	11.496	685299	50.0
Decahydro-4,4,8...	13.251	9.5	ug/l	201627	4	13.428	1060310	50.0
unknown13.800	13.800	5.5	ug/l	117420	4	13.428	1060310	50.0