

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
 Data File : VU049549.D
 Acq On : 30 Jun 2022 06:39
 Operator : SY/MD
 Sample : N3476-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 52422

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_U\Method\82U062722W.M

Title : SW846 8260

Signal : TIC: VU049549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.636	390	403	416	rBV	7488	15171	1.10%	0.188%
2	5.289	1212	1228	1241	rBV	208149	440811	31.89%	5.470%
3	5.372	1241	1254	1276	rVB	356615	730887	52.88%	9.069%
4	5.700	1340	1356	1377	rBV2	225260	465851	33.70%	5.780%
5	6.247	1512	1526	1552	rBV	529157	1008823	72.99%	12.518%
6	7.896	2025	2039	2057	rBV	798560	1382168	100.00%	17.150%
7	9.417	2498	2512	2536	rBV	728798	1221534	88.38%	15.157%
8	10.632	2878	2890	2911	rBV	600121	967129	69.97%	12.000%
9	11.742	3228	3235	3244	rVV2	27199	40694	2.94%	0.505%
10	11.812	3245	3257	3282	rVB	771950	1237398	89.53%	15.354%
11	16.192	4613	4619	4633	rVB2	90775	135243	9.78%	1.678%
12	16.539	4722	4727	4737	rVB3	121805	176254	12.75%	2.187%
13	17.420	4996	5001	5011	rVB2	162296	237199	17.16%	2.943%

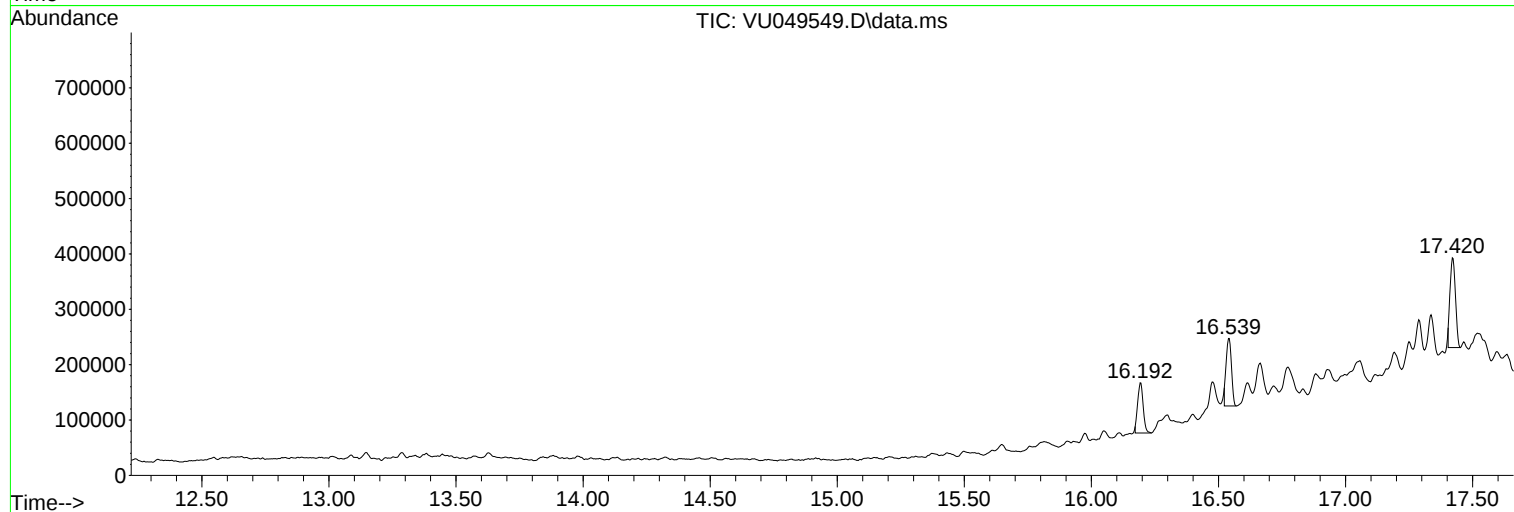
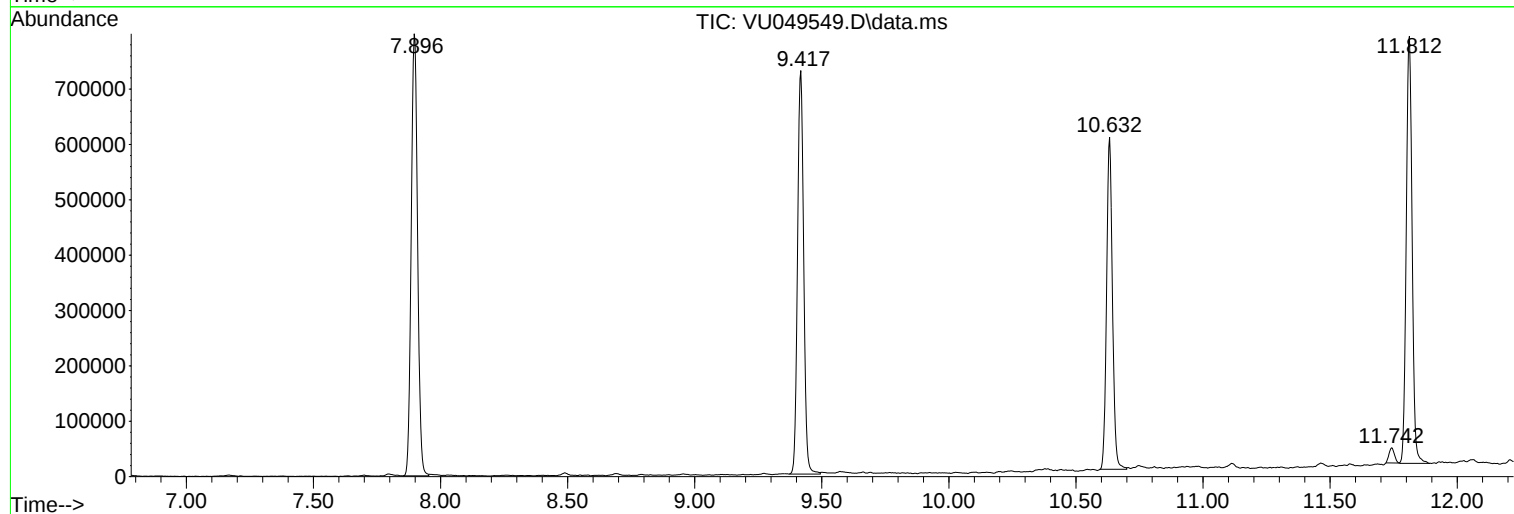
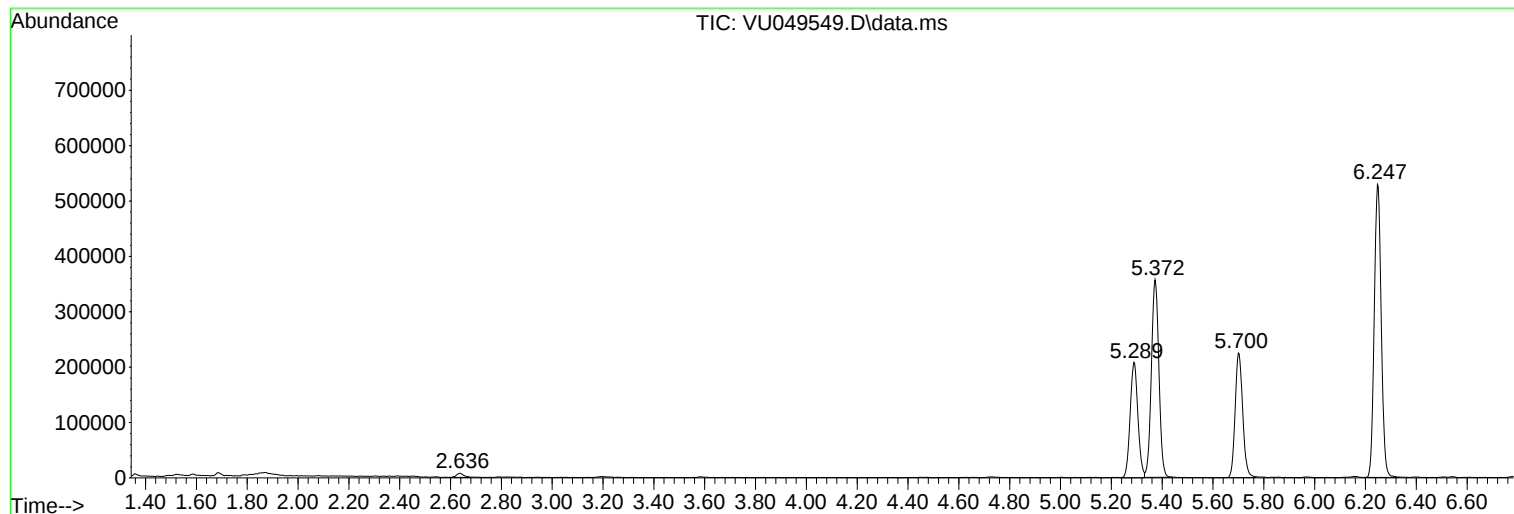
Sum of corrected areas: 8059162

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Quant Title : SW846 8260

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



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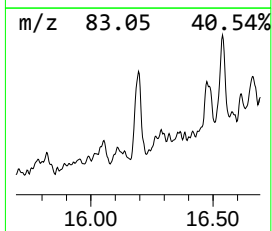
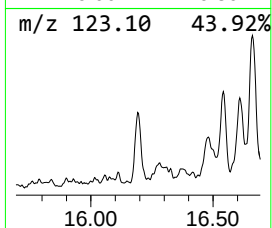
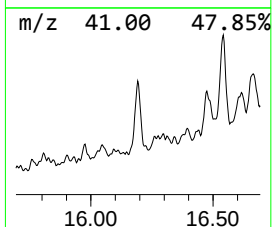
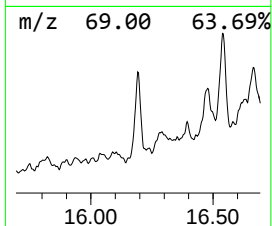
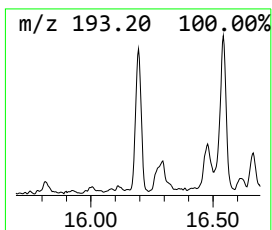
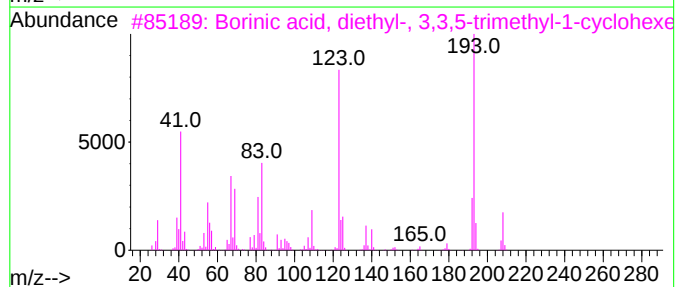
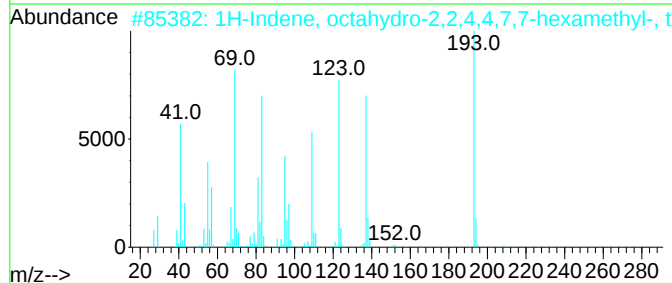
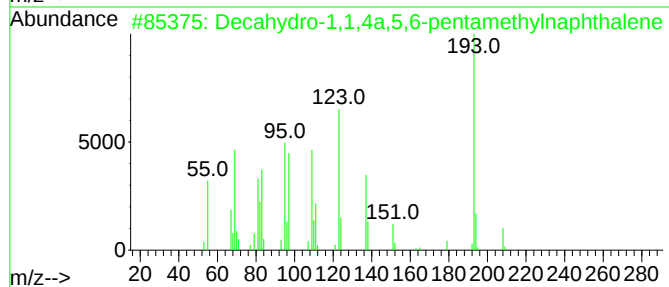
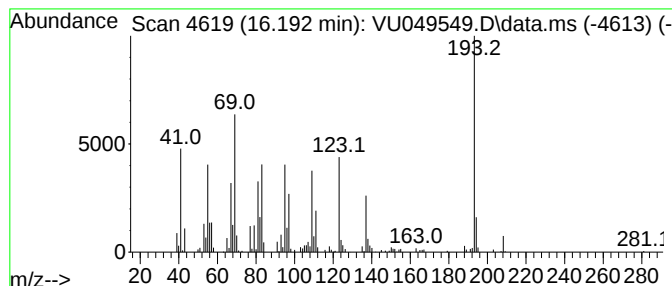
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.M
Quant Title : SW846 8260

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

Peak Number 1 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.192	5.46 ug/l	135243	1,4-Dichlorobenzene-d4	11.812	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	81
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
4	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
5	Iminostilbene	193	C14H11N	000256-96-2	25



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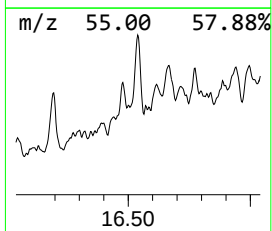
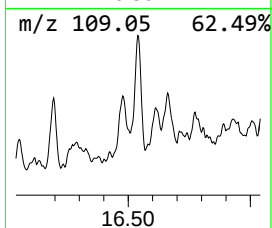
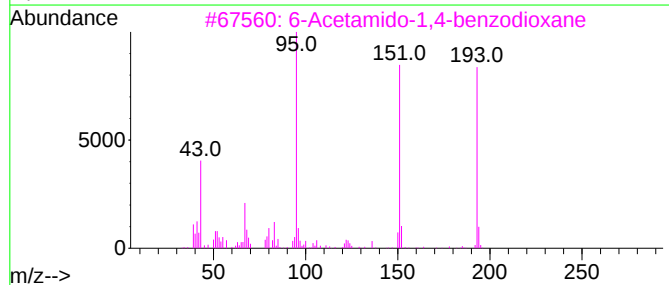
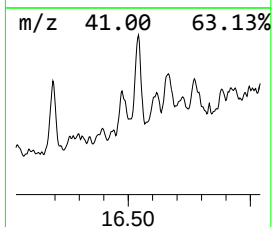
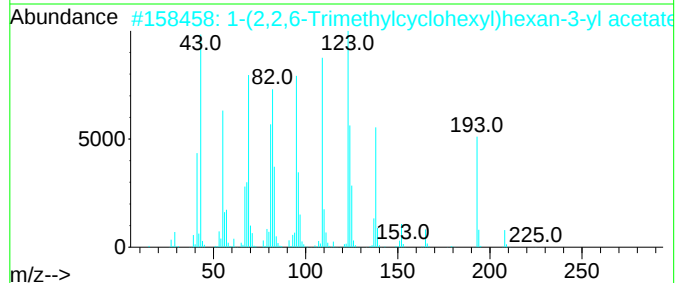
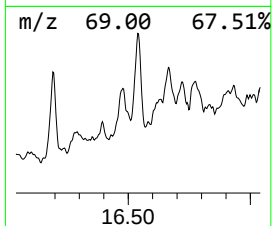
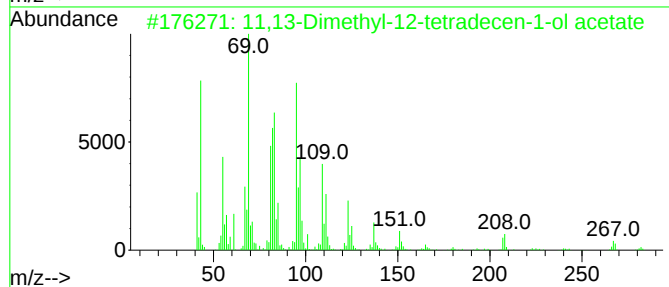
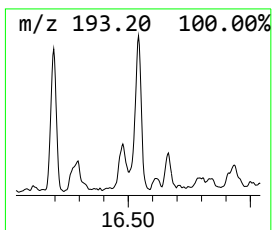
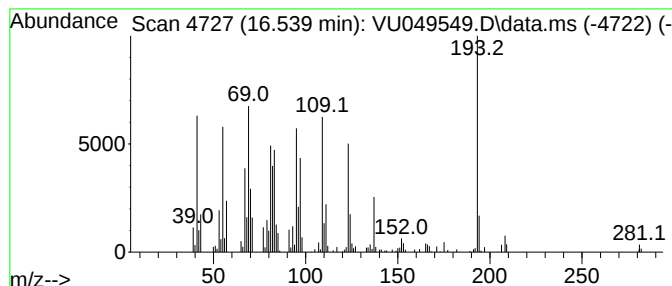
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Peak Number 2 11,13-Dimethyl-12-tetradec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.539	7.12 ug/l	176254	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	50		
2	1-(2,2,6-Trimethylcyclohexyl)hex...	268	C17H32O2	1000498-96-1	38		
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	27		
4	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	25		
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	25		



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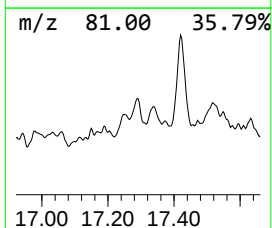
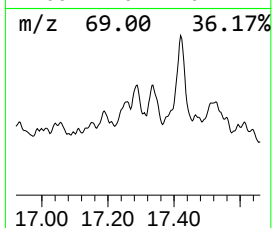
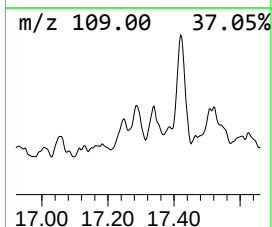
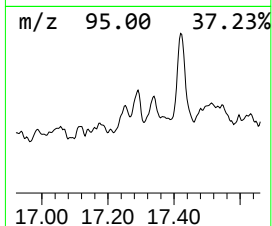
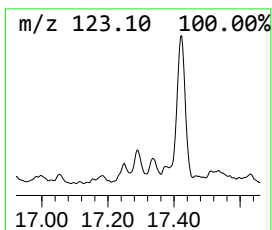
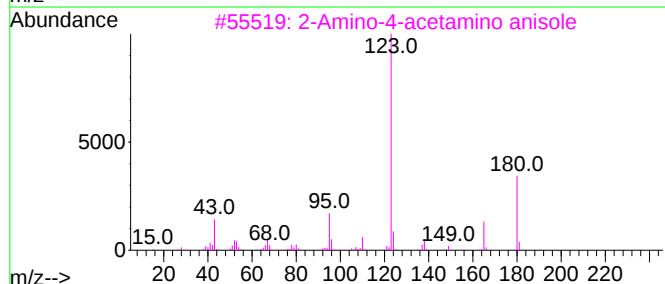
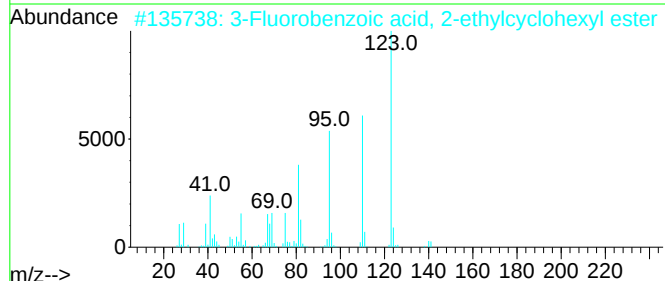
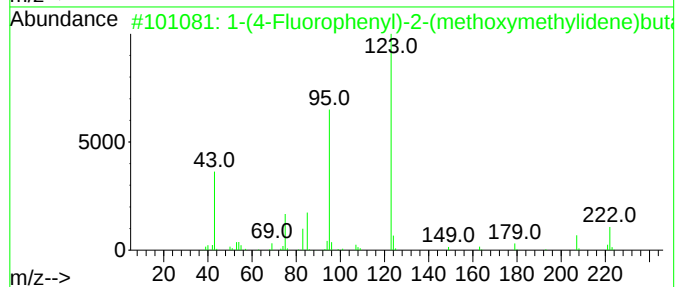
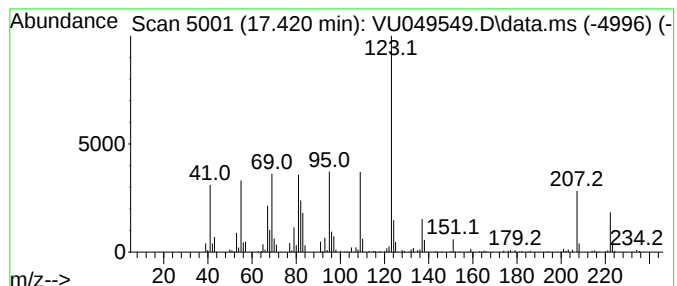
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Peak Number 3 1-(4-Fluorophenyl)-2-(metho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.420	9.58 ug/l	237199	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11F03	1000388-14-4	50		
2	3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19F02	1000279-04-9	50		
3	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	47		
4	Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	47		
5	Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	47		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decahydro-1,1,4...	16.192	5.5	ug/l	135243	4	11.812	1237400	50.0
11,13-Dimethyl-...	16.539	7.1	ug/l	176254	4	11.812	1237400	50.0
1-(4-Fluorophen...	17.420	9.6	ug/l	237199	4	11.812	1237400	50.0