LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036951.D
Acq On : 11 Aug 2023 19:15
Operator : JC/MD
Sample : IBLK
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
IBLK

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_X\Method\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.581	69	81	82	rBV4	4259	12191	1.54%	0.240%
2	4.587	563	574	583	rBV2	4627	15660	1.98%	0.308%
3	5.385	694	705	720	rBV	90050	263269	33.29%	5.180%
4	5.550	720	732	746	rVV	142150	410382	51.89%	8.075%
5	5.958	788	799	821	rBV	96809	255112	32.26%	5.020%
6	6.763	921	931	949	rBV	240173	574209	72.60%	11.299%
7	8.647	1228	1240	1255	rBV	497298	790884	100.00%	15.562%
8	10.055	1465	1471	1485	rBV	547897	727950	92.04%	14.324%
9	11.079	1634	1639	1651	rBV	445558	583159	73.74%	11.475%
10	11.750	1745	1749	1757	rVB	7741	10891	1.38%	0.214%
11	12.024	1788	1794	1802	rBV	572450	743091	93.96%	14.622%
12	14.615	2216	2219	2221	rBV3	6955	9518	1.20%	0.187%
13	14.755	2238	2242	2244	rBV4	11173	14009	1.77%	0.276%
14	14.792	2244	2248	2252	rVB4	8760	13339	1.69%	0.262%
15	14.841	2253	2256	2260	rBV5	9997	15931	2.01%	0.313%
16	14.963	2268	2276	2283	rBV8	16237	45458	5.75%	0.894%
17	15.213	2313	2317	2320	rVB	23919	26594	3.36%	0.523%
18	15.371	2341	2343	2346	rBV3	10948	11328	1.43%	0.223%
19	15.414	2346	2350	2355	rBV	52600	79535	10.06%	1.565%
20	15.481	2357	2361	2368	rBV5	28366	63662	8.05%	1.253%
21	15.615	2379	2383	2385	rBV	25669	36188	4.58%	0.712%
22	15.743	2400	2404	2409	rVB2	78369	121840	15.41%	2.397%
23	15.816	2412	2416	2419	rBV5	21893	44053	5.57%	0.867%
24	16.091	2457	2461	2464	rBV6	18480	32787	4.15%	0.645%
25	16.609	2542	2546	2551	rVB8	30525	51483	6.51%	1.013%
26	16.706	2557	2562	2568	rVB3	66434	129485	16.37%	2.548%

Sum of corrected areas: 5082008

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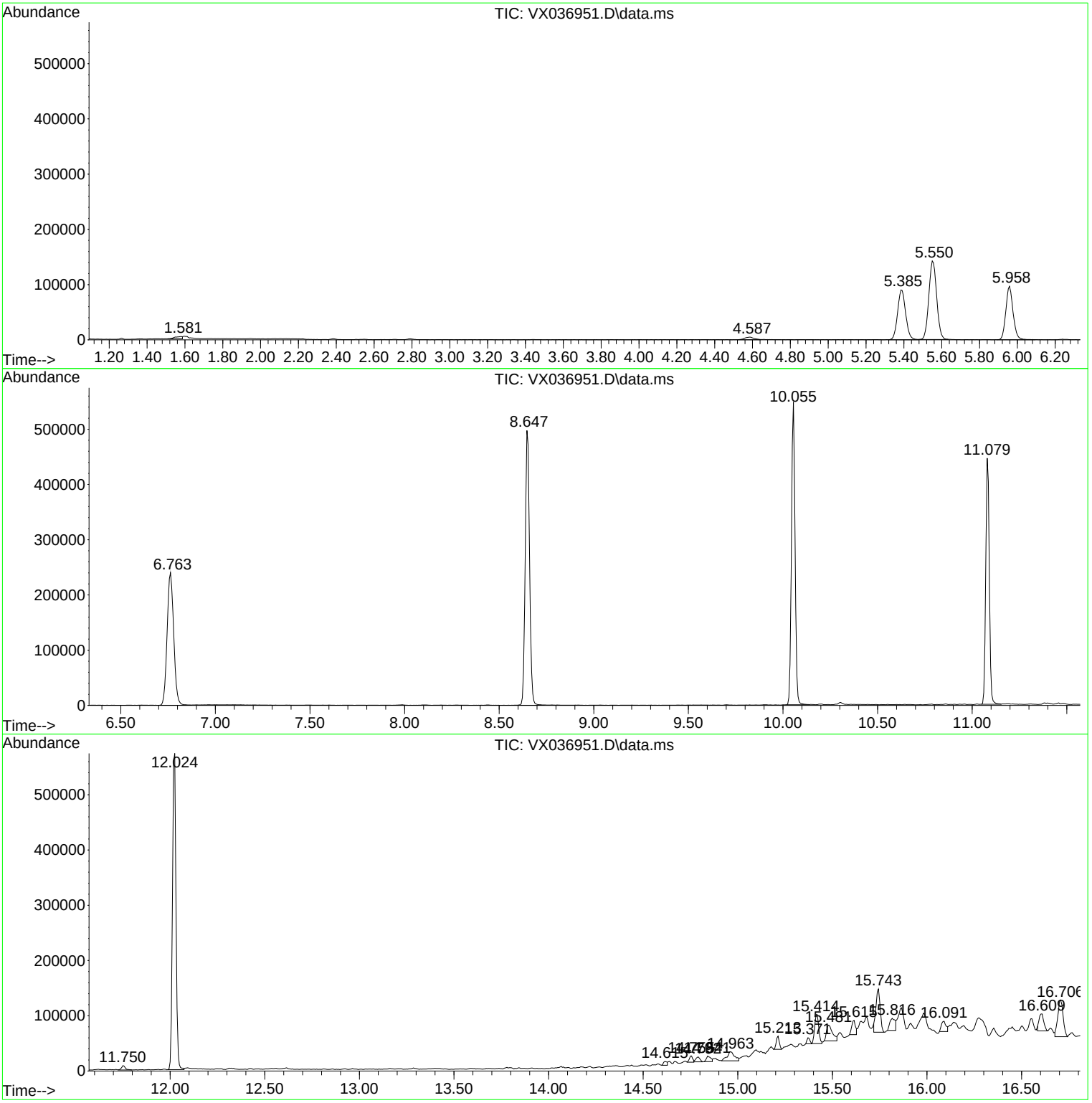
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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TIC Library : C:\Database\NIST20.L
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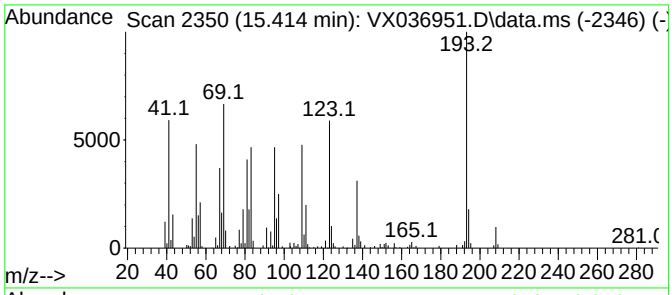
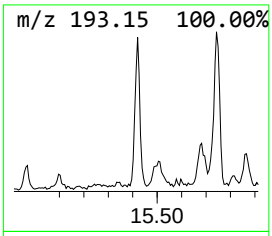
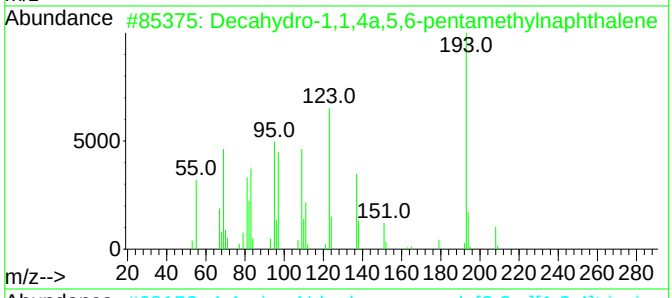
****
Peak Number 1 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

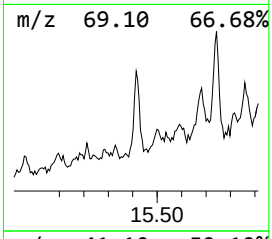
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	5.35 ug/l	79535	1,4-Dichlorobenzene-d4	12.024

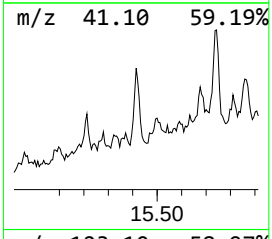
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	27
3	Arsenous acid, tripropyl ester	252	C9H21AsO3	015606-91-4	27
4	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5	1H-Pyrazole, 3,5-bis(1,1-dimethy...	208	C13H24N2	125281-21-2	22

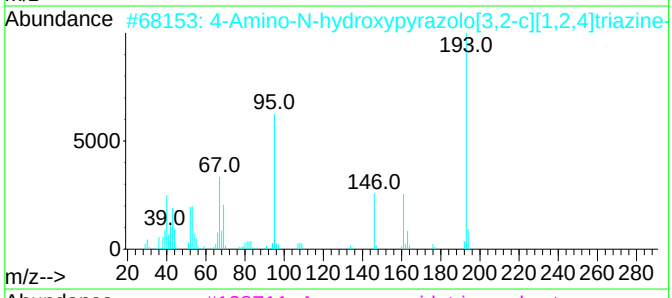


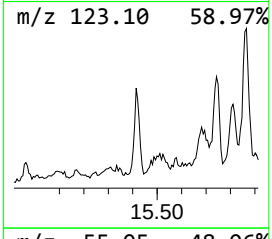


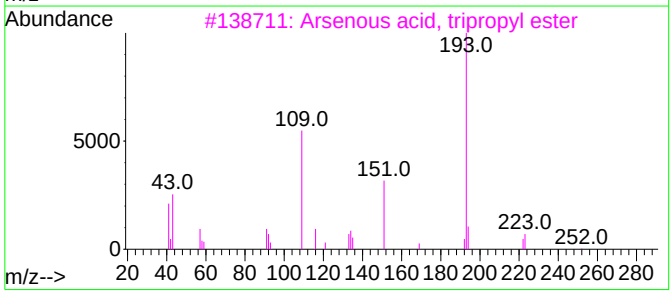


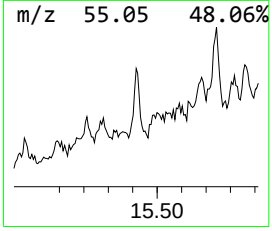












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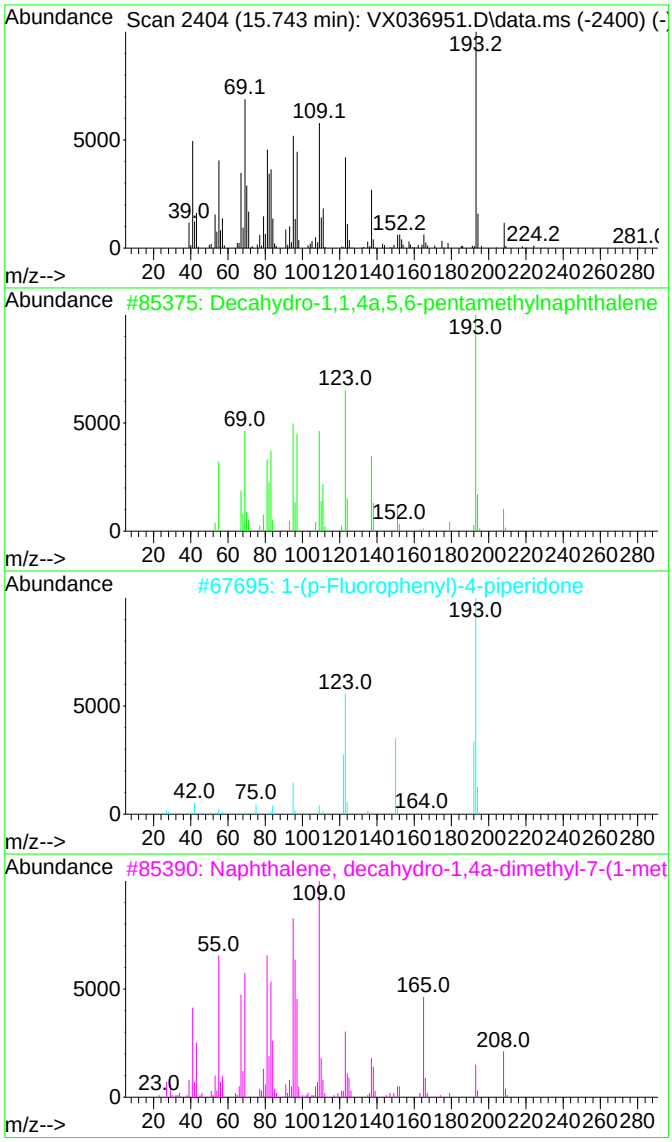
Quant Title : SW846 8260

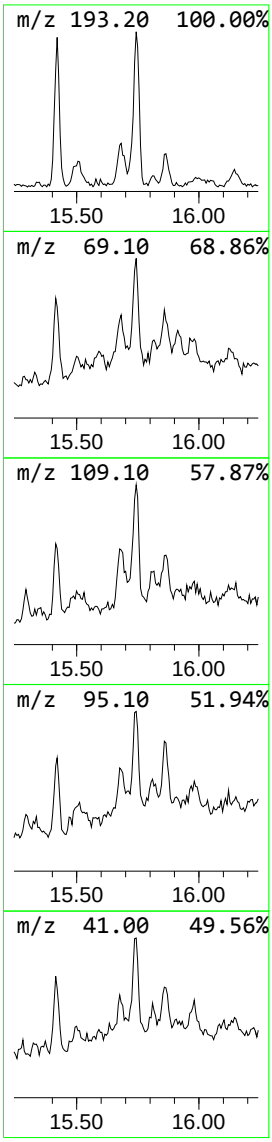
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown15.743 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	8.20 ug/l	121840	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	38
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
5	Iminostilbene	193	C14H11N	000256-96-2	30





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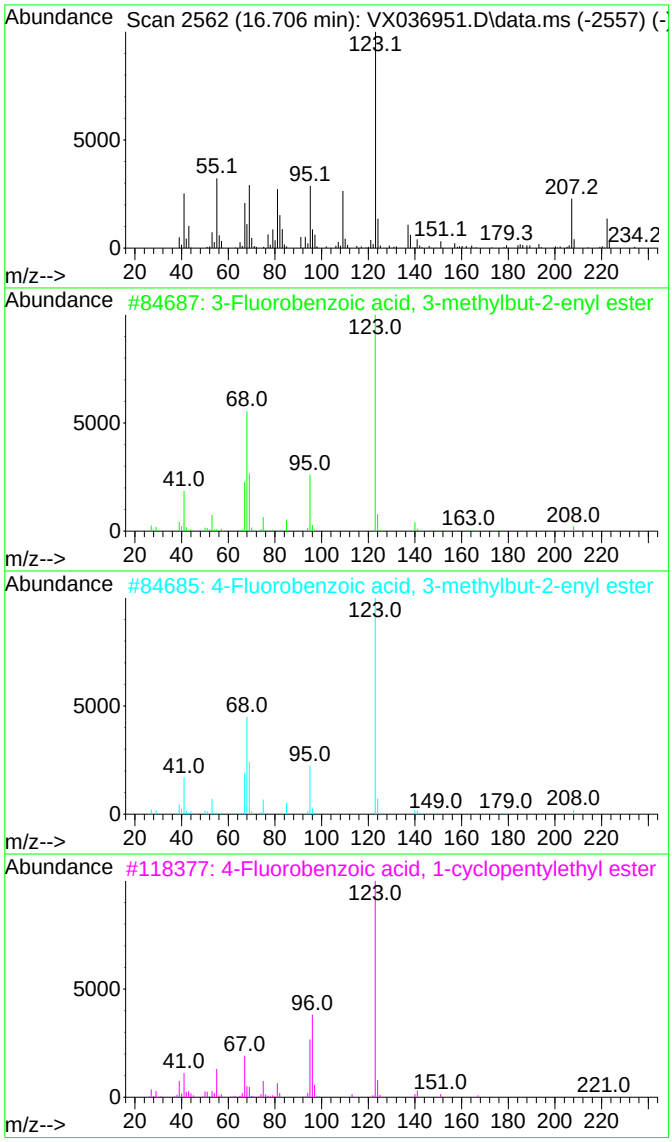
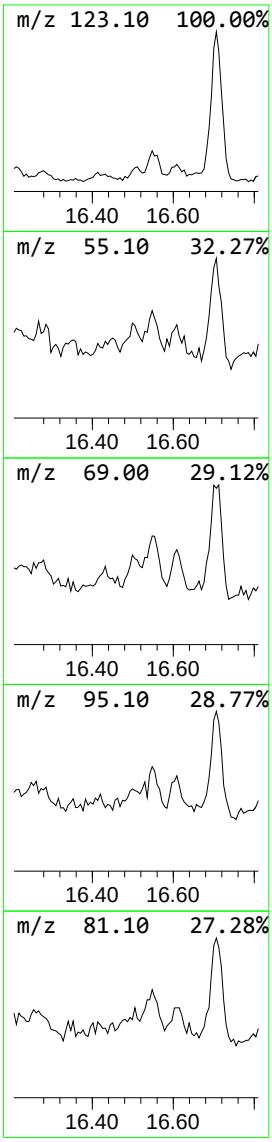
****
Peak Number 3 3-Fluorobenzoic acid, 3-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	8.71 ug/l	129485	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	52
2	4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	52
3	4-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000279-05-8	50
4	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	49
5	4-Fluorobenzoic acid, hex-4-yn-3...	220	C13H13FO2	1000299-15-3	46





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Decahydro-1,1,4...	15.414	5.3	ug/l	79535	4	12.024	743091	50.0
unknown15.743	15.743	8.2	ug/l	121840	4	12.024	743091	50.0
3-Fluorobenzoic...	16.706	8.7	ug/l	129485	4	12.024	743091	50.0