

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
 Data File : BG048476.D
 Acq On : 23 Mar 2021 19:11
 Operator : CG/JU
 Sample : M1746-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-3

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.177	309	313	319	rBV	19522	29767	1.06%	0.233%
2	5.652	387	394	406	rBV	546080	875094	31.20%	6.848%
3	7.251	657	666	678	rBV	601566	1033958	36.87%	8.091%
4	8.103	805	811	818	rBV	145298	247709	8.83%	1.938%
5	9.266	999	1009	1016	rBV	375157	654662	23.34%	5.123%
6	10.923	1284	1291	1300	rBV	194478	358000	12.76%	2.801%
7	13.367	1700	1707	1714	rVB	982234	1466072	52.27%	11.472%
8	14.742	1935	1941	1948	rVB	355797	553250	19.73%	4.329%
9	16.228	2186	2194	2201	rBV	1029781	1568333	55.92%	12.272%
10	17.492	2403	2409	2415	rBV	519215	786016	28.03%	6.151%
11	18.373	2553	2559	2572	rBV2	160882	244984	8.73%	1.917%
12	19.542	2754	2758	2765	rVB	46092	67516	2.41%	0.528%
13	19.642	2771	2775	2783	rVB3	36274	56334	2.01%	0.441%
14	19.906	2816	2820	2824	rVB	48804	60985	2.17%	0.477%
15	20.100	2847	2853	2858	rVB	2161708	2804630	100.00%	21.947%
16	20.776	2962	2968	2972	rVB8	17133	29771	1.06%	0.233%
17	21.416	3072	3077	3089	rBV4	132403	335926	11.98%	2.629%
18	21.781	3133	3139	3145	rBV2	468759	814732	29.05%	6.375%
19	25.112	3697	3706	3717	rBV2	277040	791638	28.23%	6.195%

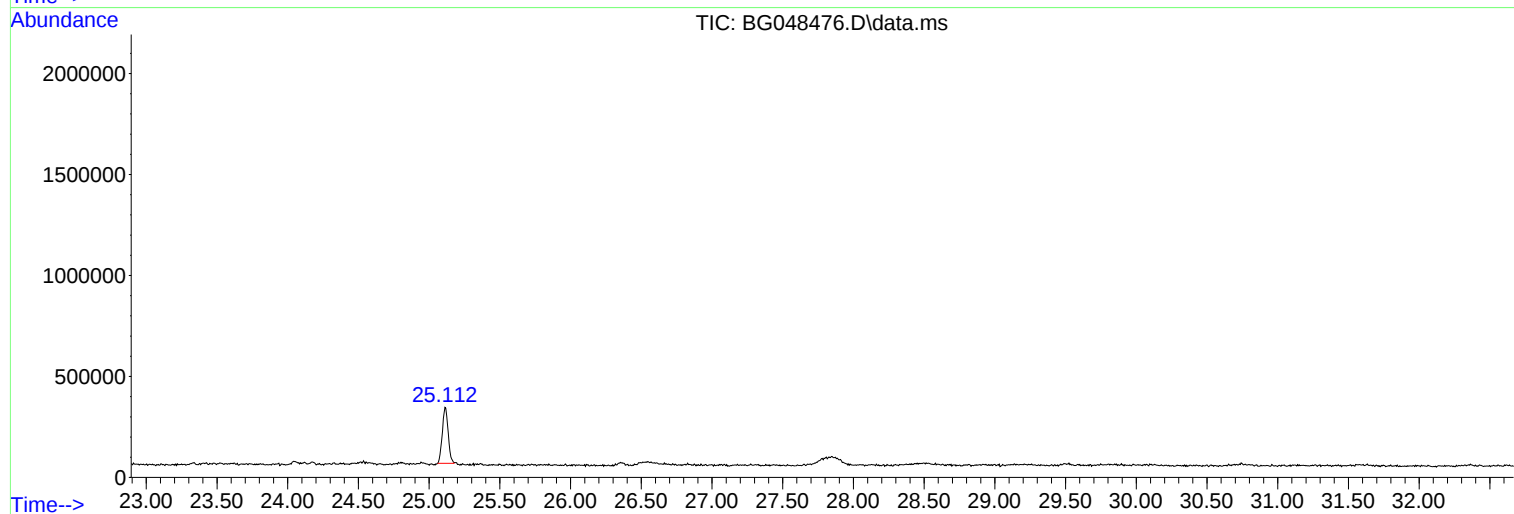
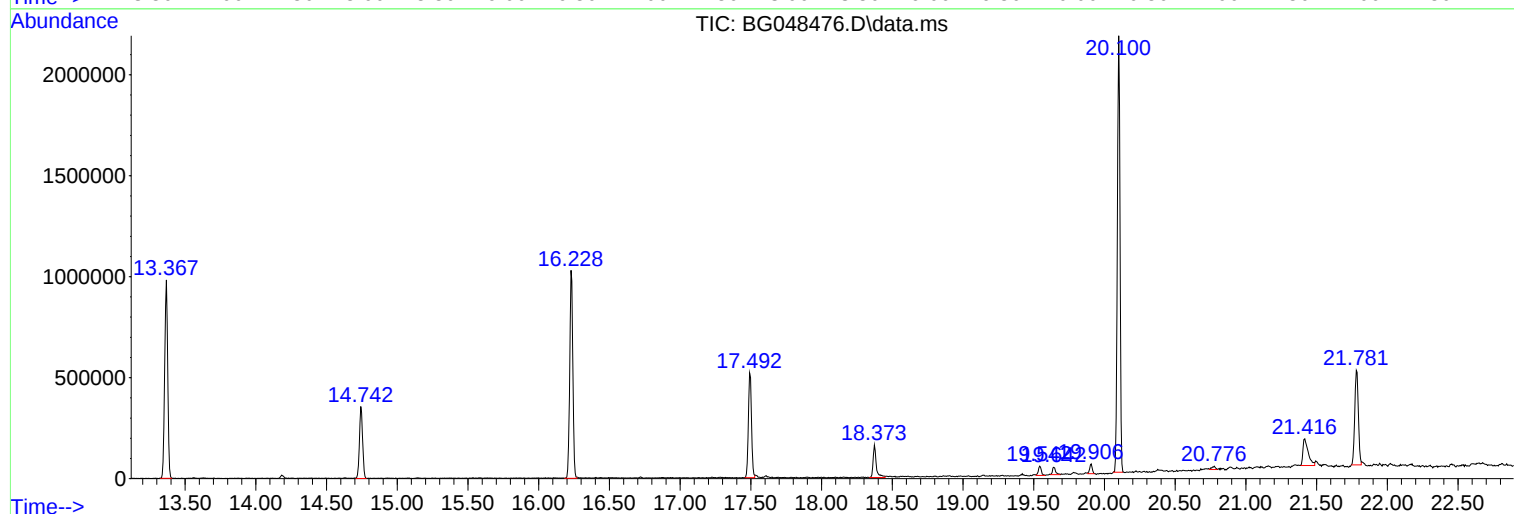
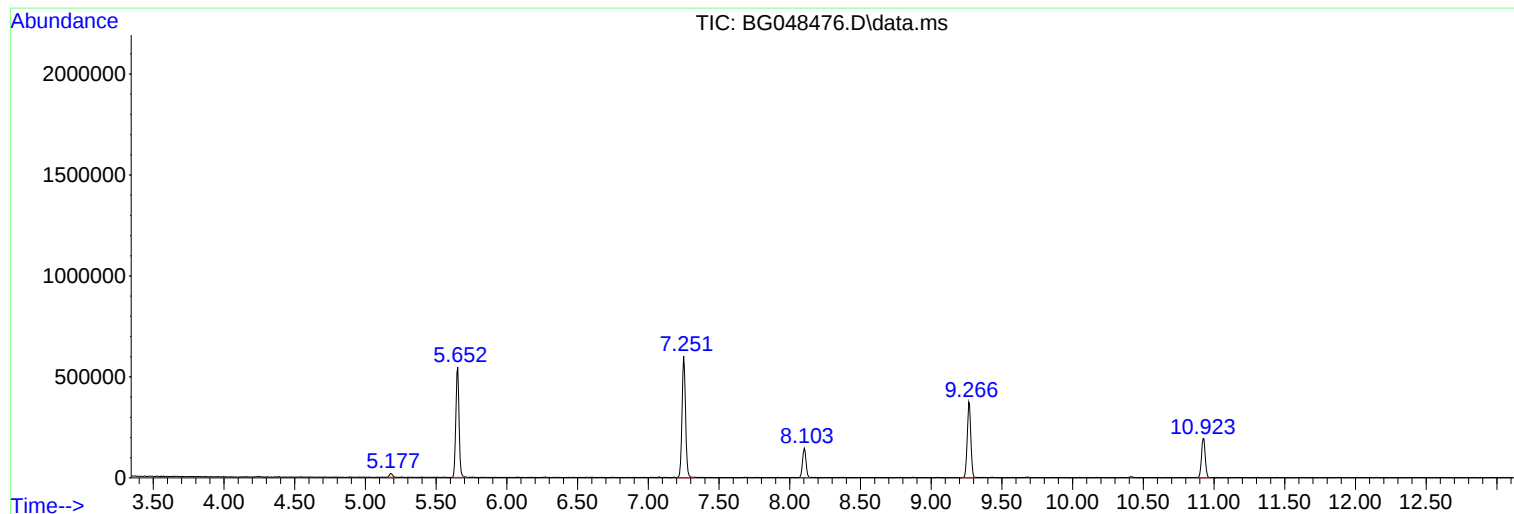
Sum of corrected areas: 12779377

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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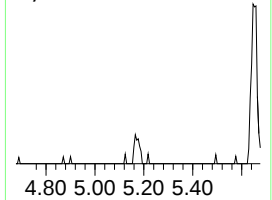
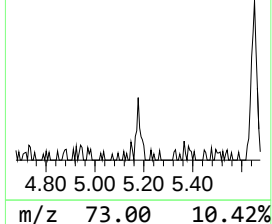
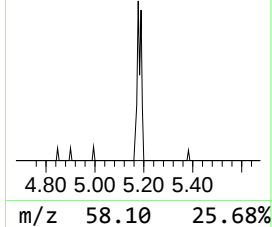
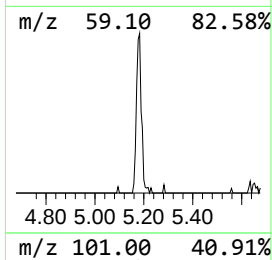
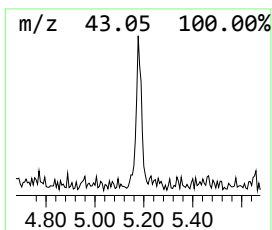
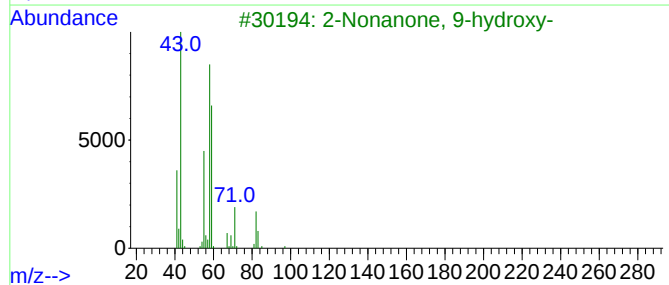
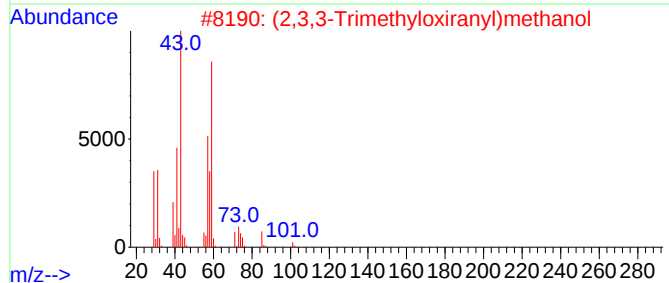
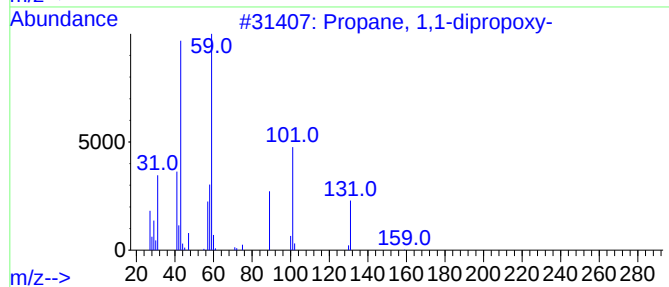
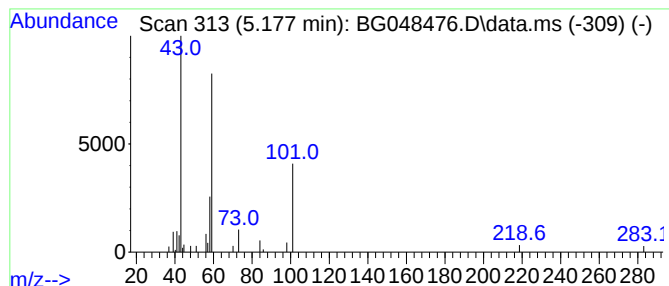
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.177 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	2.40 ng	29767	1,4-Dichlorobenzene-d4	8.103

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	40
2			(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	36
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	23
4			Guanidine	59	CH5N3	000113-00-8	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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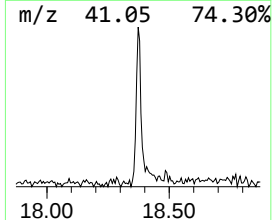
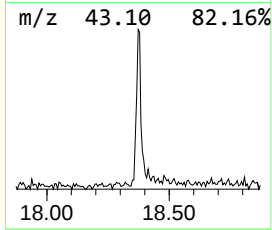
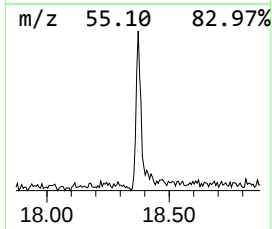
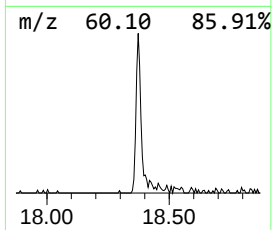
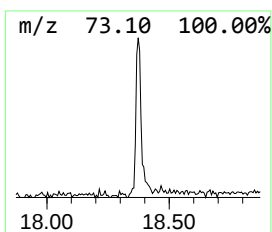
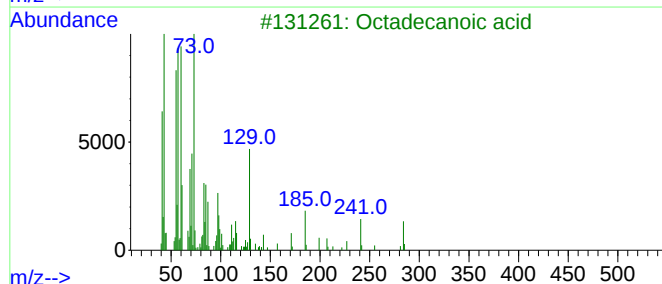
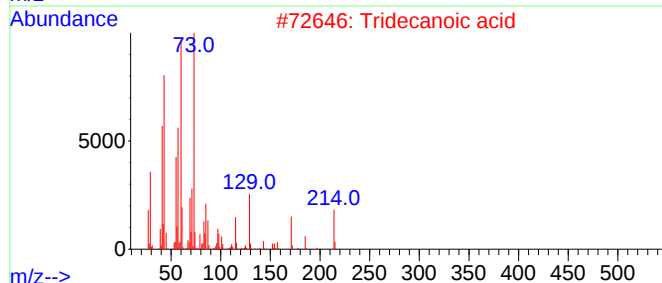
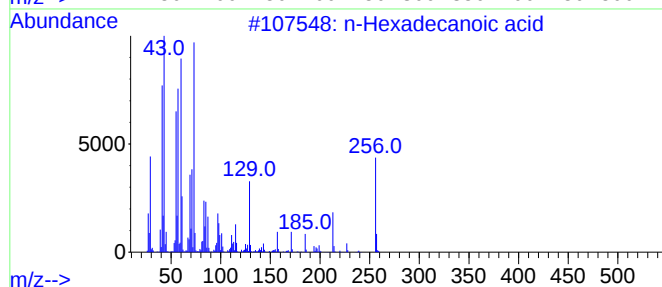
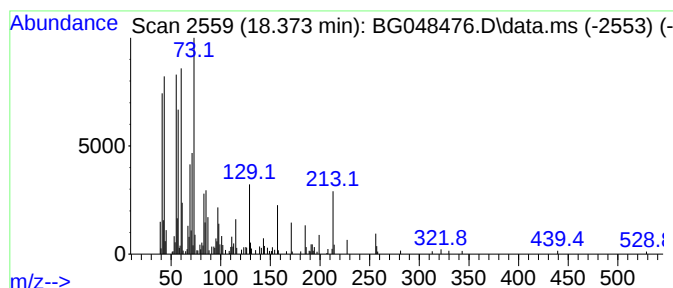
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.373	6.23 ng	244984	Phenanthrene-d10	17.491	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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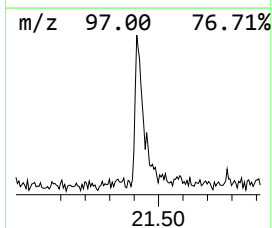
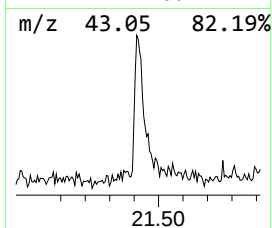
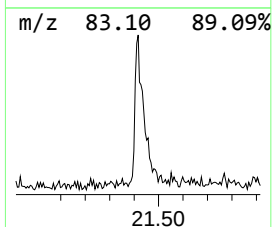
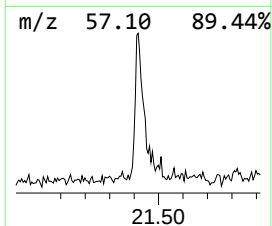
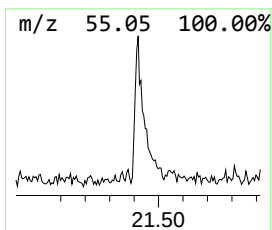
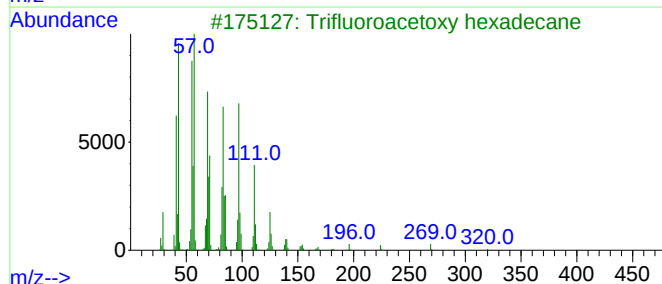
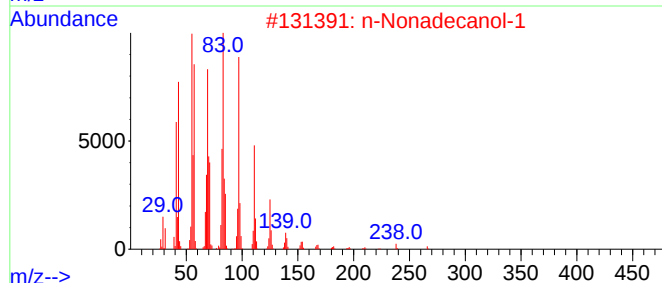
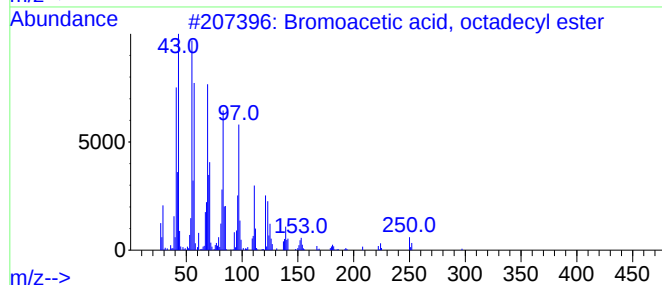
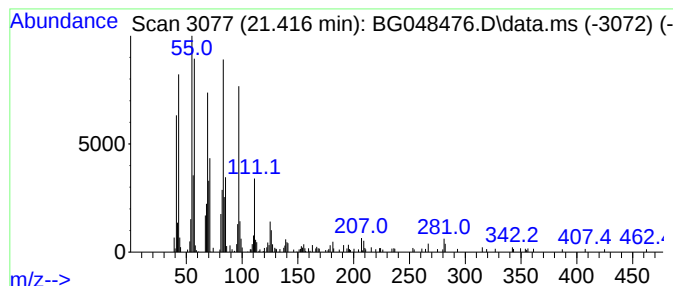
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Peak Number 3 Bromoacetic acid, octadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	8.25 ng	335926	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	76
5			1-Tricosene	322	C23H46	018835-32-0	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.177	5.177	2.4	ng	29767	1	8.103	247709	20.0
n-Hexadecanoic ...	18.373	6.2	ng	244984	4	17.491	786016	20.0
Bromoacetic aci...	21.416	8.3	ng	335926	5	21.781	814732	20.0