

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050817\
 Data File : BF094994.D
 Acq On : 8 May 2017 22:45
 Operator : SJ/MA
 Sample : I2976-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-TANK001-02

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.013	519	523	545	rBV	245123	480569	17.85%	2.243%
2	5.654	627	632	662	rBV	1281038	2089627	77.62%	9.752%
3	5.919	673	677	684	rVB	16624	29486	1.10%	0.138%
4	7.254	900	904	920	rBV	1181825	2048688	76.10%	9.561%
5	7.372	920	924	943	rVB	1624832	2432062	90.34%	11.350%
6	7.713	978	982	992	rVB	482403	551484	20.48%	2.574%
7	7.948	1017	1022	1033	rBV	1487568	1749364	64.98%	8.164%
8	8.613	1126	1135	1157	rBV	1029902	1403917	52.15%	6.552%
9	9.225	1235	1239	1244	rBV	41230	47259	1.76%	0.221%
10	9.730	1321	1325	1341	rBV	561930	799101	29.68%	3.729%
11	11.507	1622	1627	1639	rBV	2223412	2692234	100.00%	12.565%
12	12.195	1740	1744	1757	rBV	235180	321845	11.95%	1.502%
13	12.560	1801	1806	1819	rBV2	627967	864463	32.11%	4.034%
14	13.407	1946	1950	1956	rBV	37992	43807	1.63%	0.204%
15	13.854	2021	2026	2041	rBV	958190	1394987	51.82%	6.510%
16	14.177	2077	2081	2084	rBV	33915	40815	1.52%	0.190%
17	14.965	2210	2215	2226	rVB2	509918	681161	25.30%	3.179%
18	15.930	2373	2379	2388	rBV2	119764	157958	5.87%	0.737%
19	16.754	2515	2519	2528	rVB2	36284	46138	1.71%	0.215%
20	17.018	2560	2564	2567	rBV2	24651	29805	1.11%	0.139%
21	17.054	2567	2570	2578	rVB	40317	49991	1.86%	0.233%
22	17.289	2605	2610	2618	rBV	1741778	1916261	71.18%	8.943%
23	18.577	2825	2829	2834	rBV6	15515	33678	1.25%	0.157%
24	18.630	2834	2838	2847	rVV	508051	631174	23.44%	2.946%
25	19.324	2954	2956	2960	rVB4	26422	30522	1.13%	0.142%
26	19.653	3009	3012	3016	rBV	51841	51182	1.90%	0.239%
27	19.765	3028	3031	3035	rVB2	22572	27489	1.02%	0.128%
28	19.906	3052	3055	3058	rBV2	25028	33511	1.24%	0.156%
29	20.047	3075	3079	3083	rBV2	37333	52212	1.94%	0.244%
30	20.294	3118	3121	3131	rVV	410098	554194	20.58%	2.586%
31	20.765	3198	3201	3205	rBV	28776	38834	1.44%	0.181%
32	21.194	3269	3274	3278	rBV5	21998	41788	1.55%	0.195%
33	21.683	3354	3357	3364	rVB8	17954	28957	1.08%	0.135%
34	22.253	3449	3454	3462	rVB8	13523	32476	1.21%	0.152%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

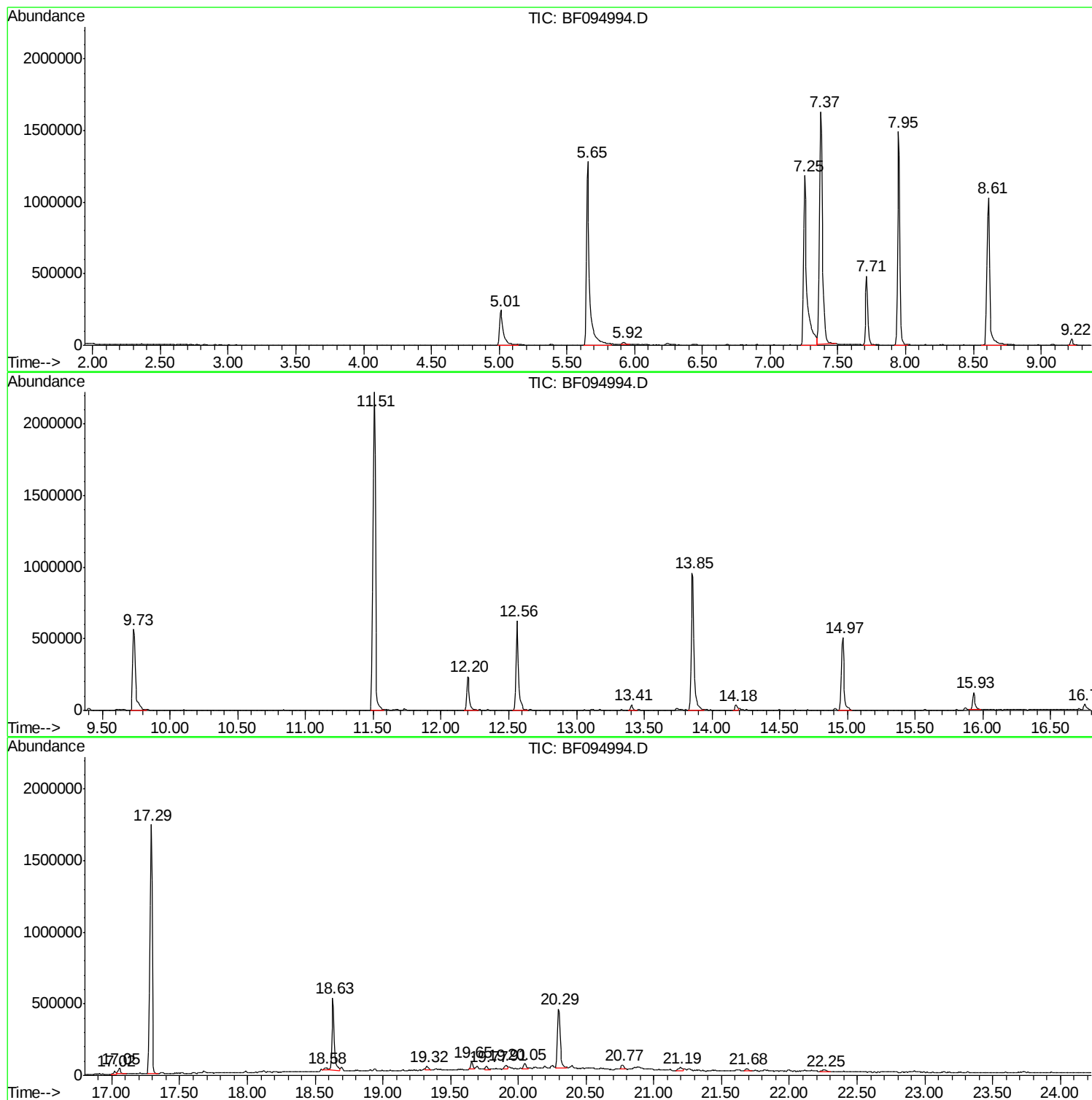
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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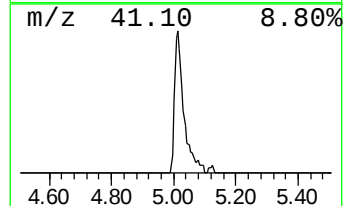
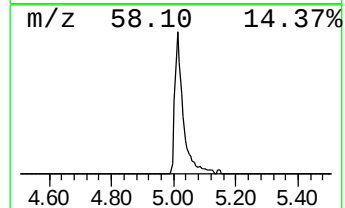
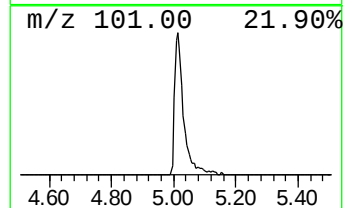
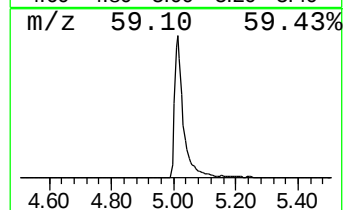
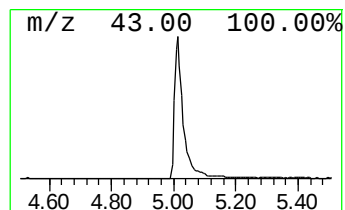
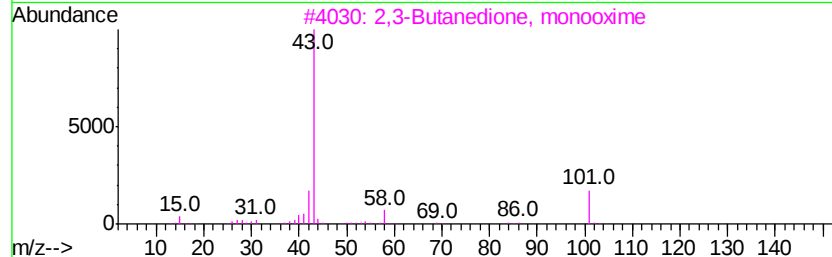
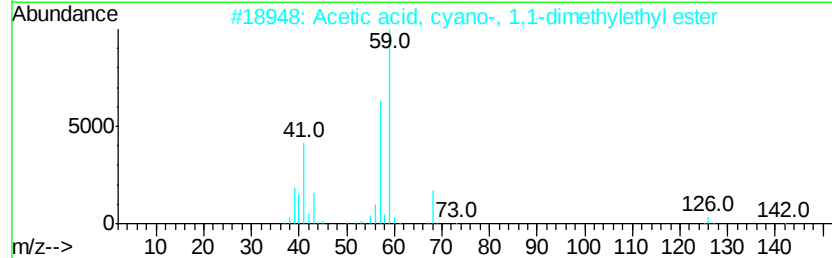
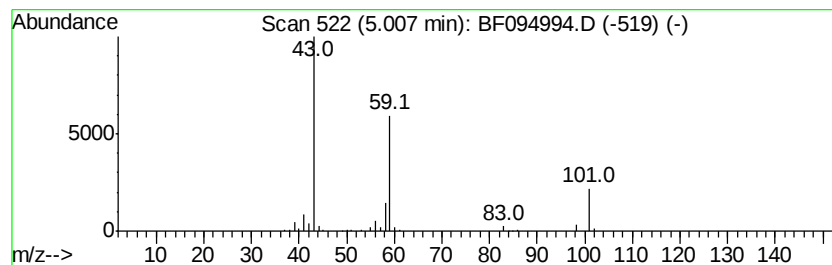
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	17.43 ng	480569	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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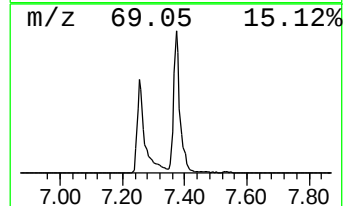
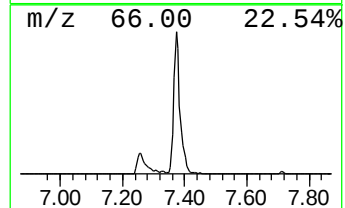
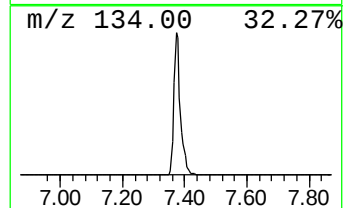
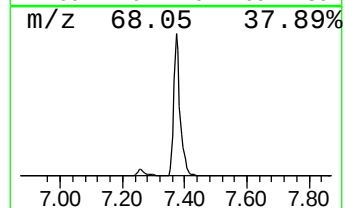
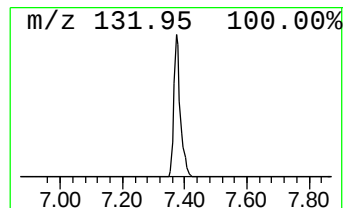
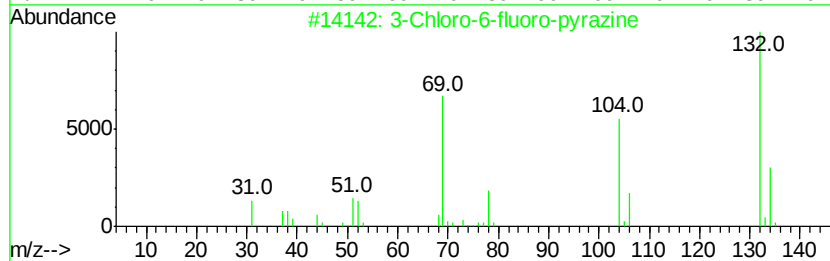
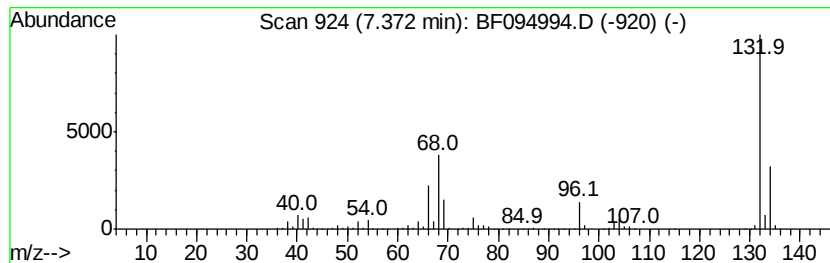
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.37	88.20 ng	2432060	1,4-Dichlorobenzene-d4	7.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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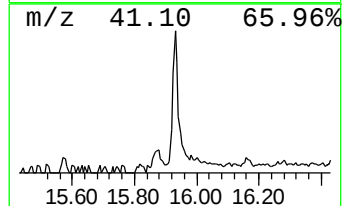
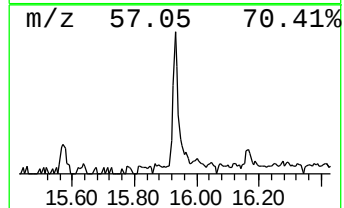
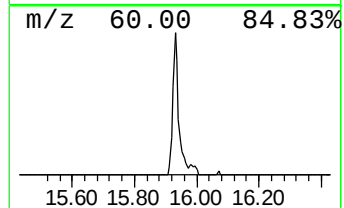
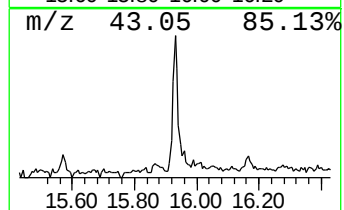
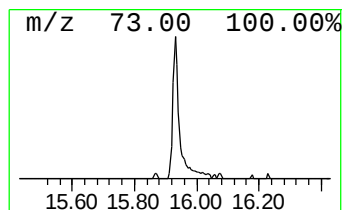
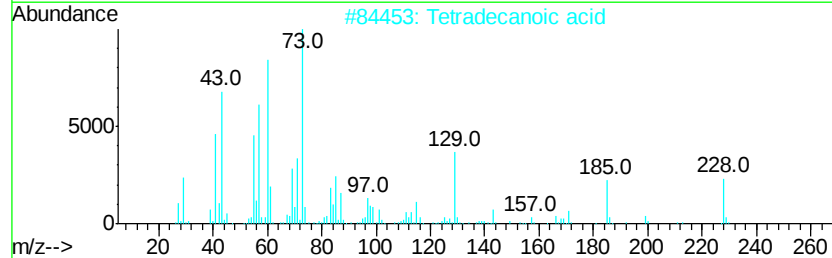
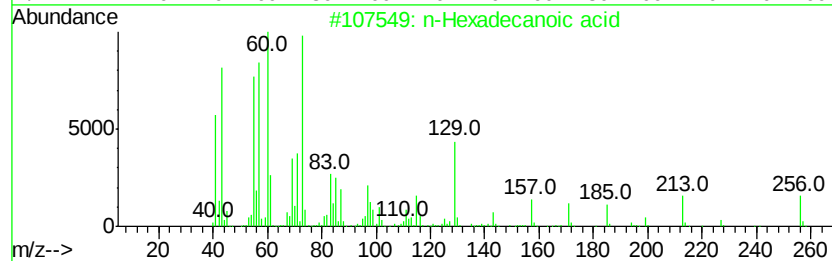
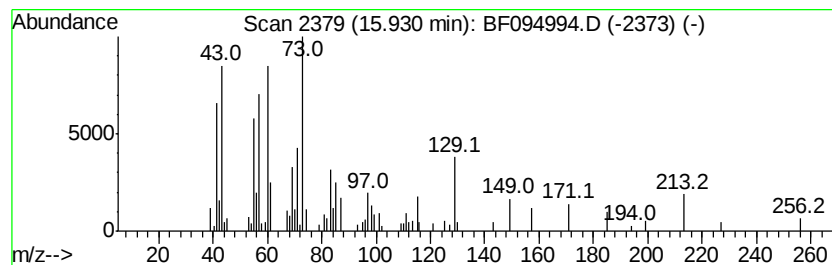
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.64 ng	157958	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	17.4	ng	480569	1	7.71	551484	20.0
unknown7.37	7.37	88.2	ng	2432060	1	7.71	551484	20.0
n-Hexadecanoic acid	15.93	4.6	ng	157958	4	14.97	681161	20.0