

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020317\
 Data File : BF092781.D
 Acq On : 3 Feb 2017 17:59
 Operator : SJ/MA
 Sample : PB96705BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB96705BL

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-BF013017.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	5.116	262	265	274	rVB	1182149	1599757	34.64%	4.518%
2	5.539	299	302	304	rBV	3577724	3642405	78.87%	10.287%
3	6.567	389	392	394	rBV	3343603	3407176	73.78%	9.623%
4	6.693	401	403	406	rBV	3026053	3515929	76.13%	9.930%
5	6.922	421	423	426	rBV	848097	752699	16.30%	2.126%
6	7.082	434	437	439	rBV	3168272	2787968	60.37%	7.874%
7	7.493	470	473	475	rBV	2292324	2527814	54.74%	7.139%
8	8.213	533	536	538	rBV	922718	1031836	22.34%	2.914%
9	9.287	627	630	633	rBV	3512036	4618151	100.00%	13.043%
10	9.973	687	690	692	rBV	1326336	1370127	29.67%	3.870%
11	10.762	756	759	762	rBV	2159505	2315374	50.14%	6.539%
12	11.459	817	820	822	rBV	1333505	1179379	25.54%	3.331%
13	13.048	956	959	962	rBV	3417468	4157033	90.02%	11.741%
14	14.099	1049	1051	1054	rVB	1254742	1185242	25.66%	3.347%
15	14.945	1121	1125	1128	rBV	154998	197600	4.28%	0.558%
16	15.562	1176	1179	1182	rBV	724525	1118852	24.23%	3.160%

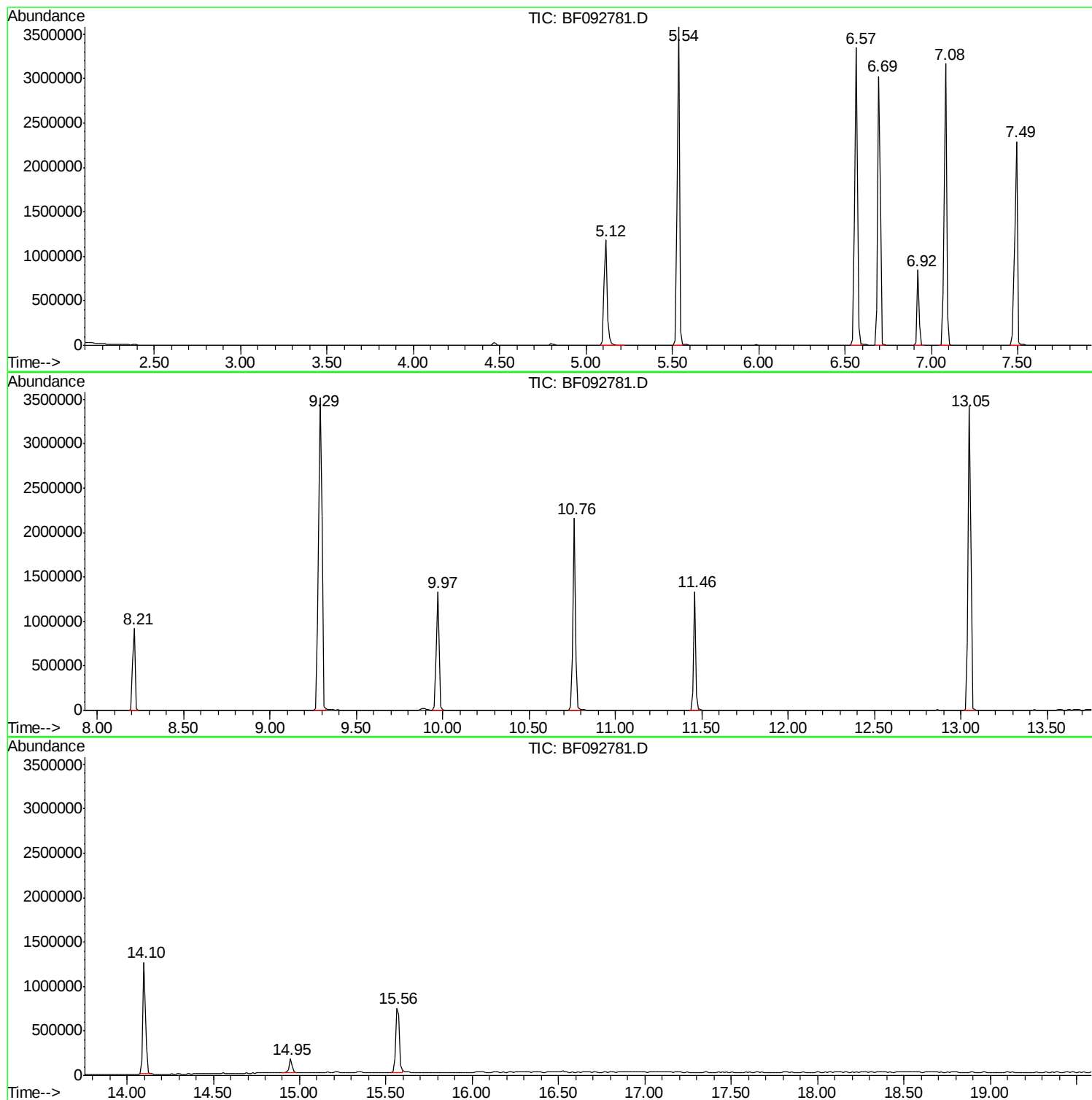
Sum of corrected areas: 35407342

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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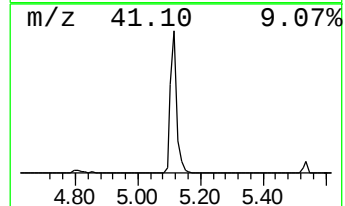
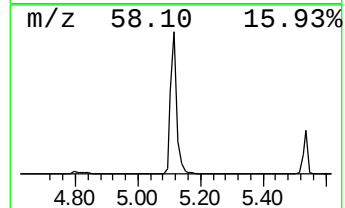
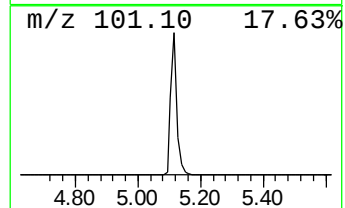
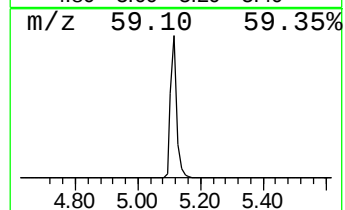
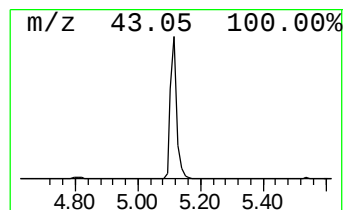
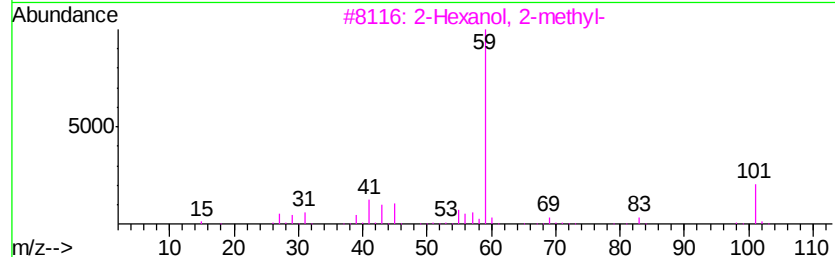
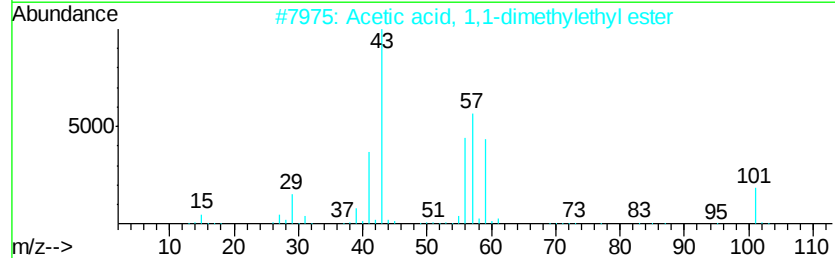
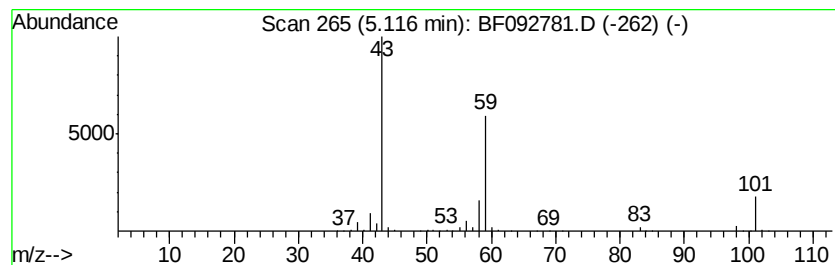
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	42.51 ng	1599760	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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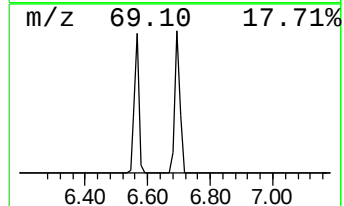
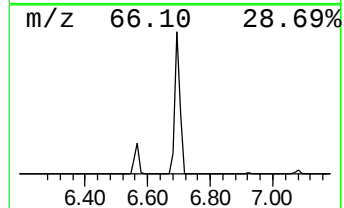
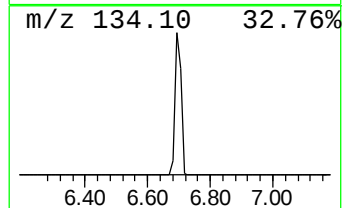
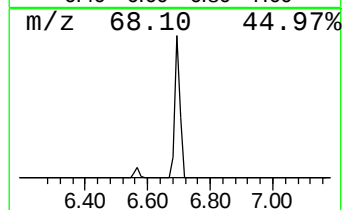
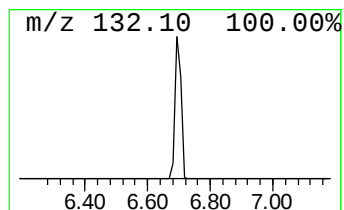
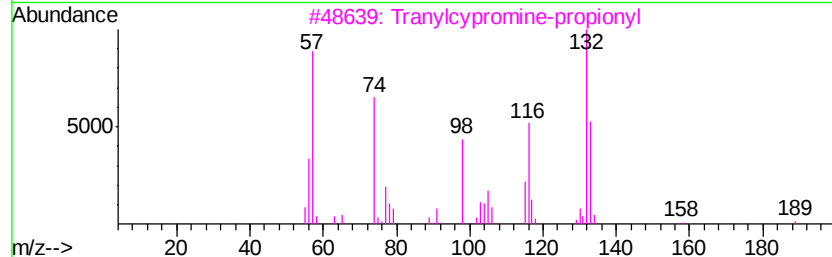
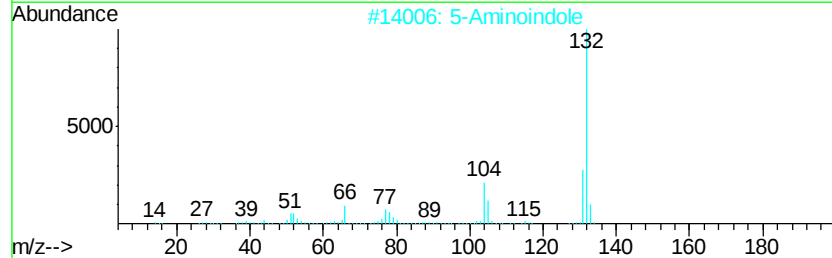
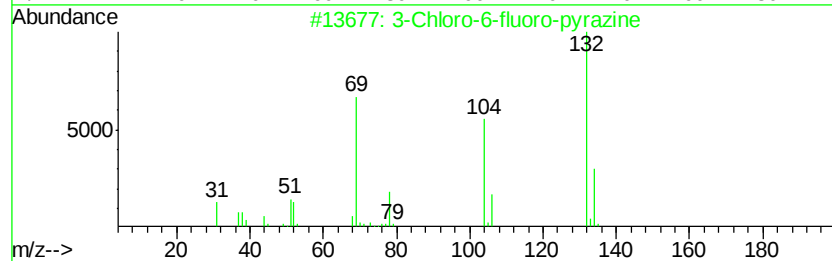
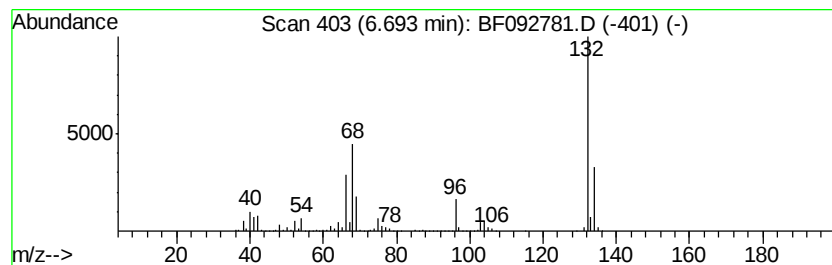
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	93.42 ng	3515930	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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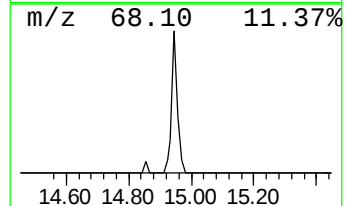
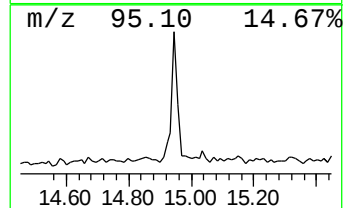
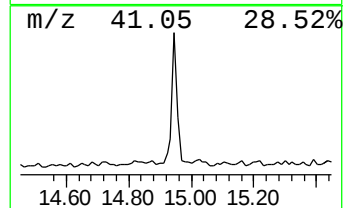
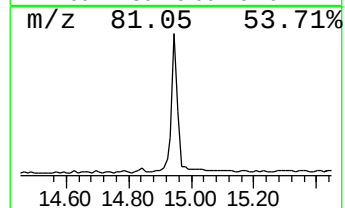
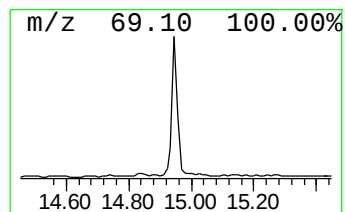
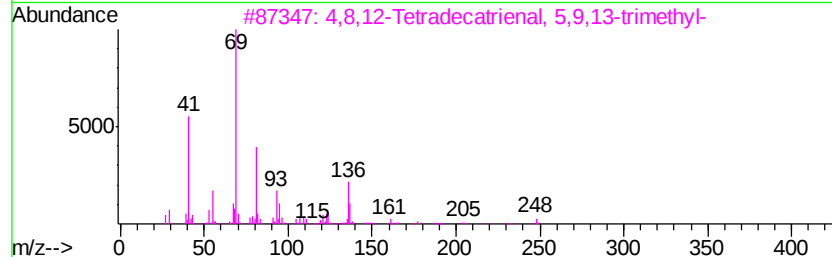
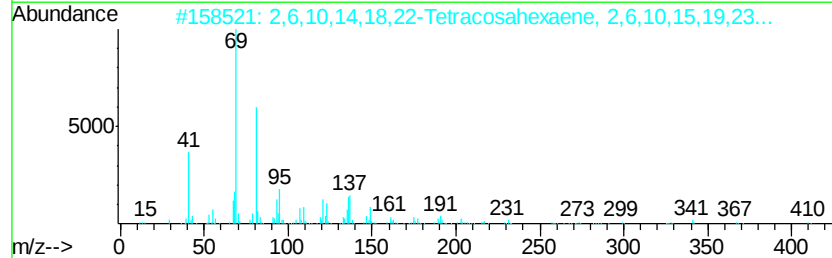
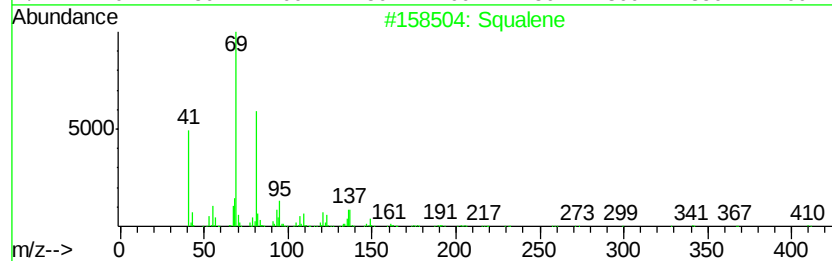
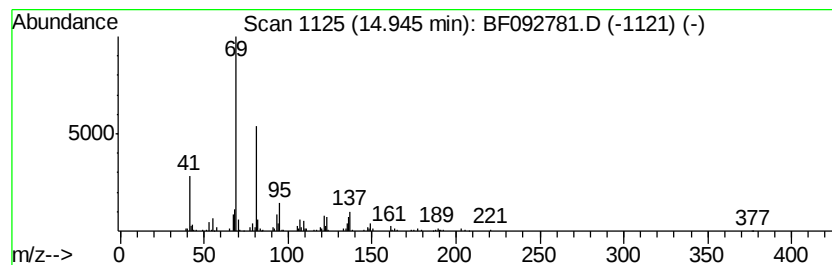
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Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.53 ng	197600	Perylene-d12	15.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	72
4	2,6,10,14-Hexadecatetraenoic aci...	332 C22H36O2	024035-35-6	72
5	Trideca-1,7,11-triene-1,1-dicarb...	270 C18H26N2	1000161-46-0	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	42.5	ng	1599760	1	6.92	752699	20.0
unknown6.69	6.69	93.4	ng	3515930	1	6.92	752699	20.0
Squalene	14.95	3.5	ng	197600	6	15.57	1118850	20.0