

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
 Data File : BF139000.D
 Acq On : 14 Aug 2024 18:14
 Operator : RC/JU
 Sample : P3548-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 289

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_F\Methods\8270-BF073024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139000.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	503	523	rVB	21267	34546	3.64%	0.730%
2	5.469	569	574	601	rBV	343525	532439	56.03%	11.251%
3	6.481	741	746	765	rBV	380576	553885	58.29%	11.704%
4	6.681	772	780	792	rBV	8216	17868	1.88%	0.378%
5	6.834	802	806	814	rVB	203575	244671	25.75%	5.170%
6	7.398	897	902	921	rBV	254718	327903	34.51%	6.929%
7	8.116	1019	1024	1041	rBV	240827	298894	31.46%	6.316%
8	8.434	1074	1078	1093	rBV	33411	54696	5.76%	1.156%
9	9.186	1201	1206	1217	rBV	313181	389849	41.03%	8.238%
10	9.863	1317	1321	1331	rBV	216581	271228	28.54%	5.731%
11	9.963	1331	1338	1354	rBV	598861	950223	100.00%	20.079%
12	10.657	1451	1456	1471	rVB	153711	197680	20.80%	4.177%
13	11.351	1569	1574	1583	rBV	168167	210800	22.18%	4.454%
14	12.933	1838	1843	1848	rBV	217472	263358	27.72%	5.565%
15	13.851	1993	1999	2008	rBV7	3558	11426	1.20%	0.241%
16	13.998	2019	2024	2036	rVB	154560	210447	22.15%	4.447%
17	15.074	2198	2207	2215	rBV8	4118	9888	1.04%	0.209%
18	15.462	2267	2273	2283	rVB	97158	152699	16.07%	3.227%

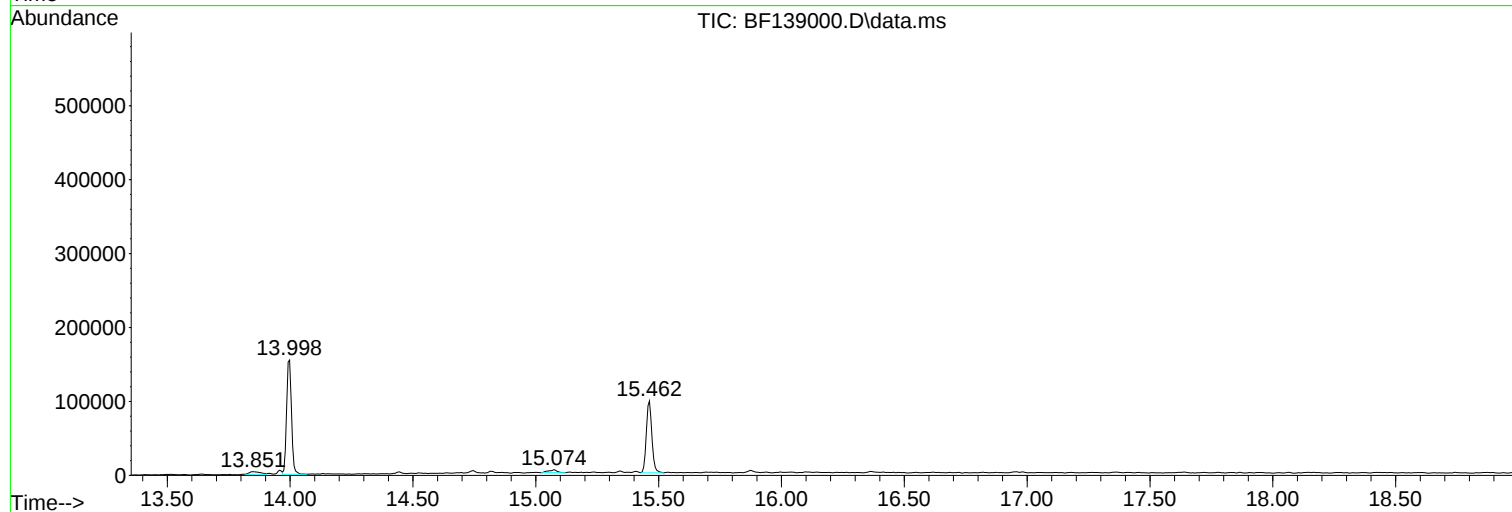
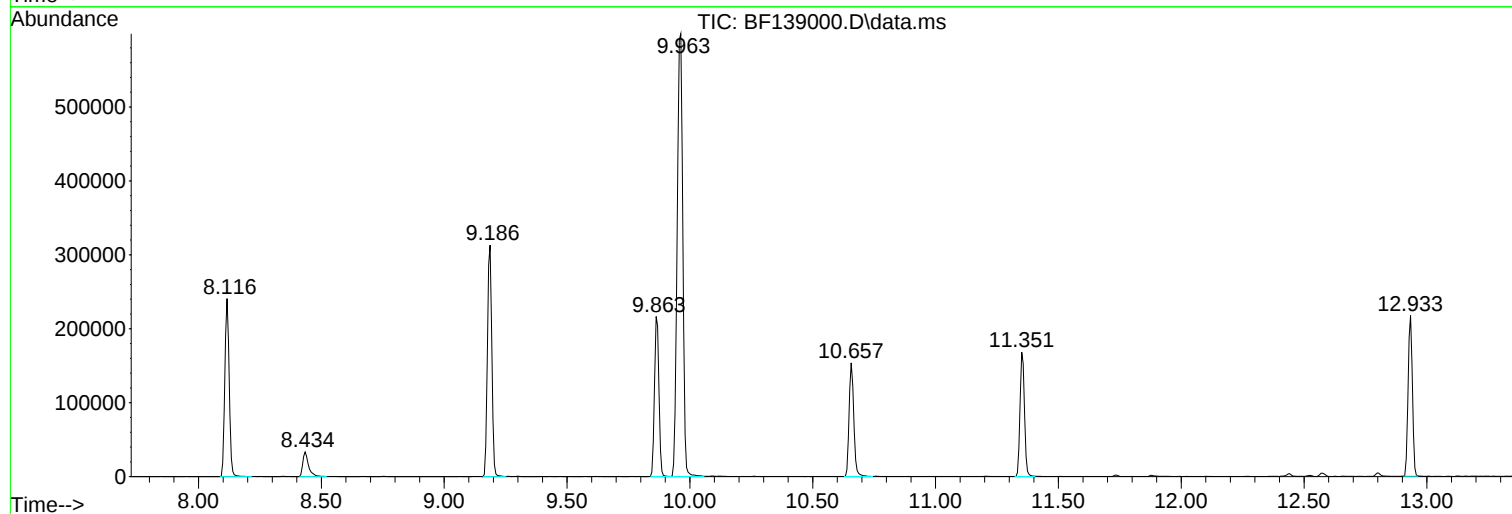
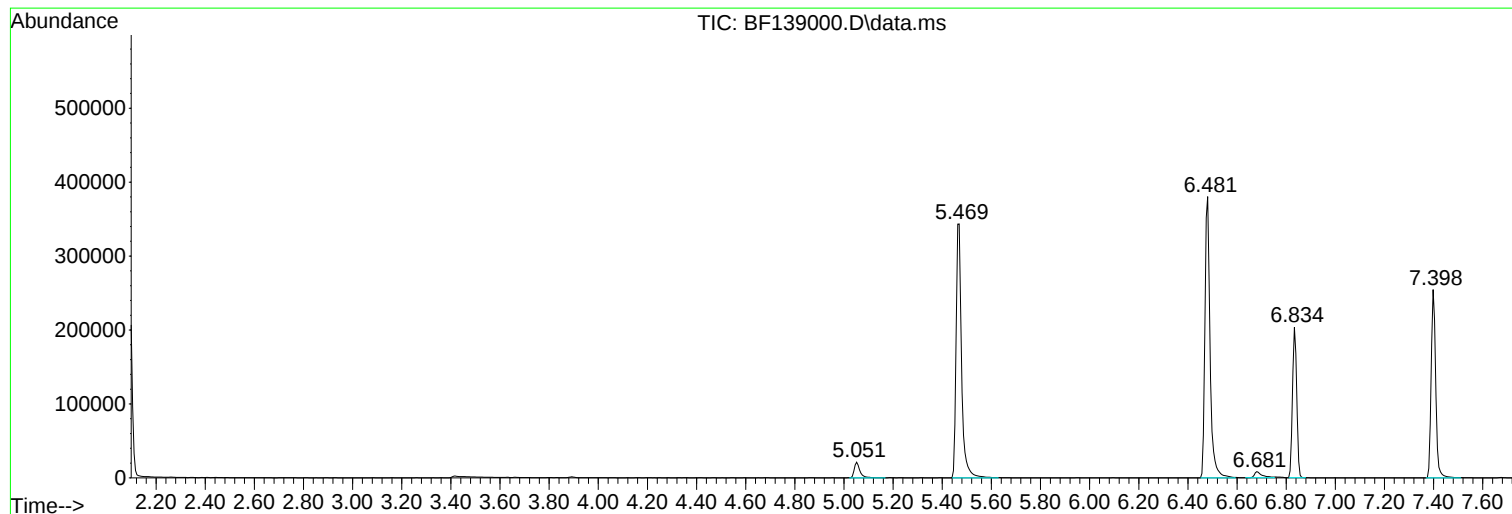
Sum of corrected areas: 4732500

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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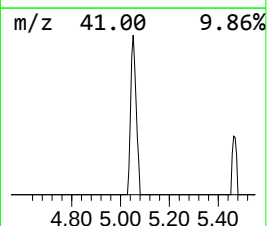
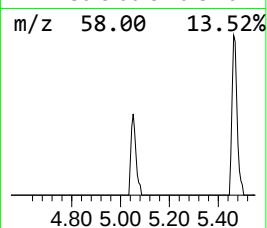
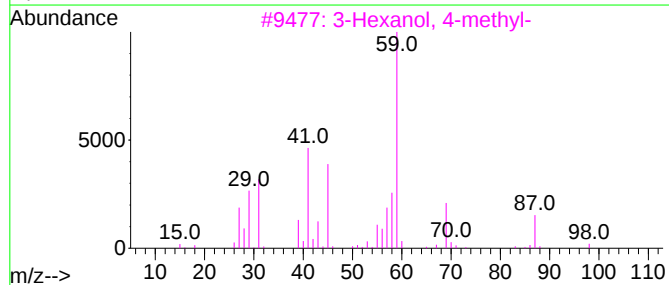
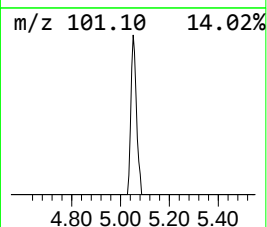
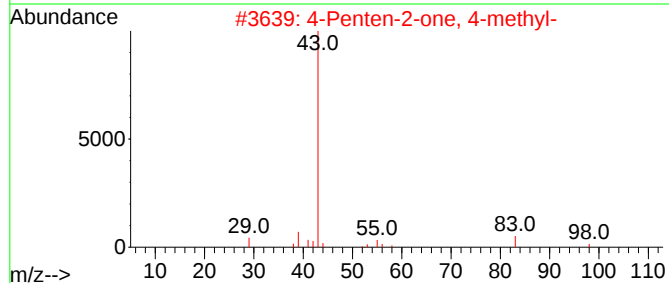
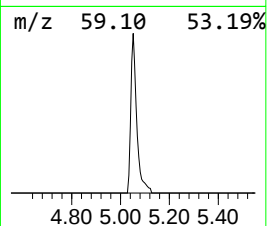
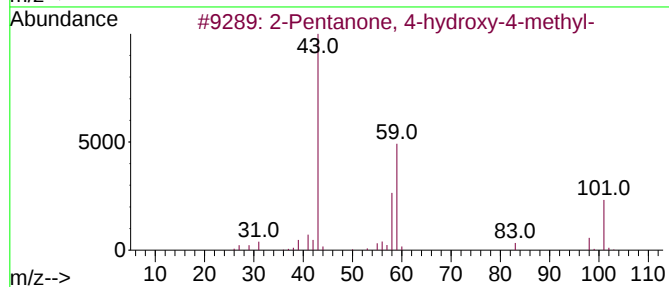
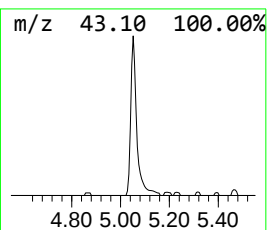
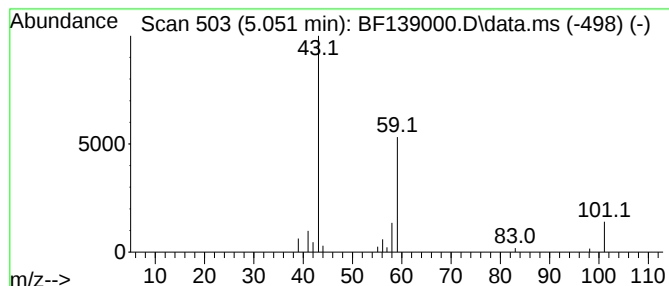
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.82 ng	34546	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	
5	Diacetamide	101	C4H7NO2	000625-77-4	7	



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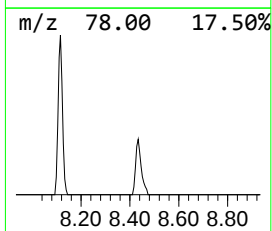
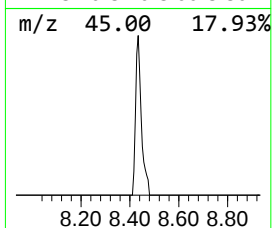
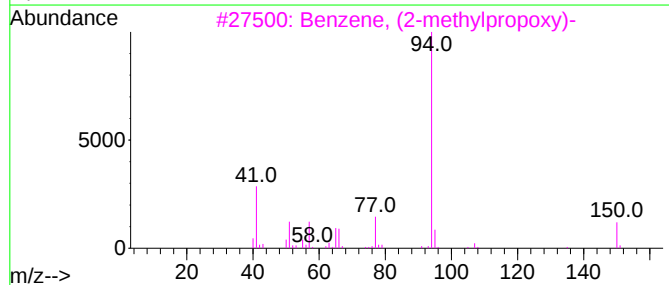
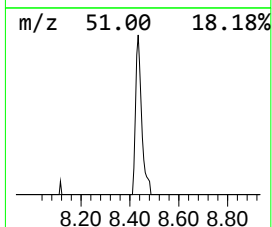
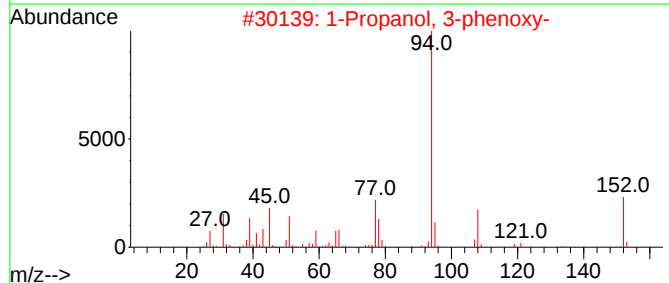
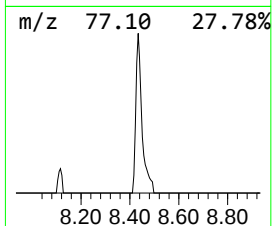
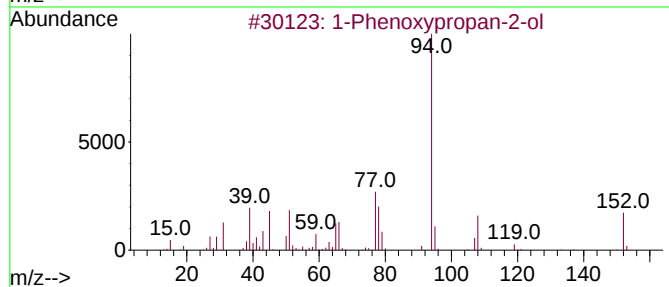
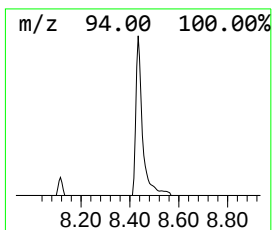
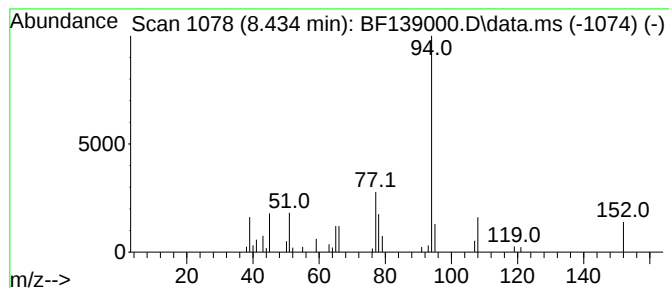
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	3.66 ng	54696	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol			152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-			152	C9H12O2	006180-61-6	91
3	Benzene, (2-methylpropoxy)-			150	C10H14O	001126-75-6	53
4	Ethanol, 2-phenoxy-			138	C8H10O2	000122-99-6	50
5	DL-Gabaculine			139	C7H9NO2	059556-18-2	45



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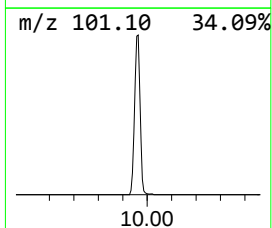
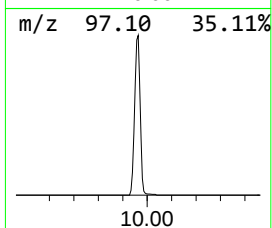
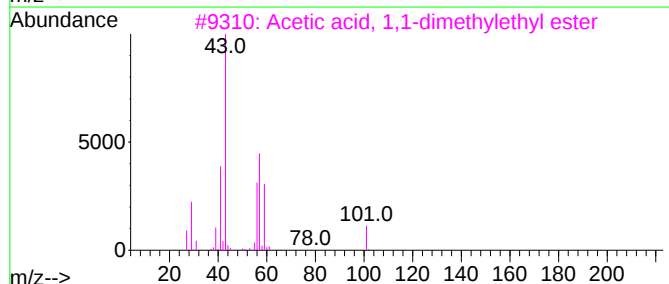
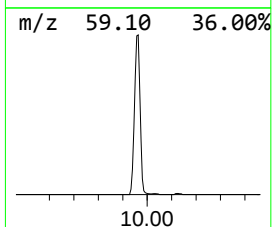
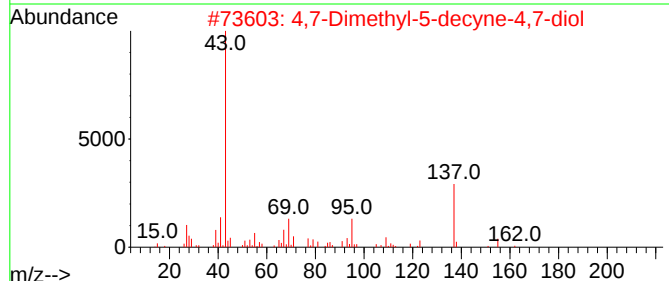
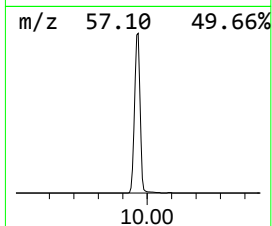
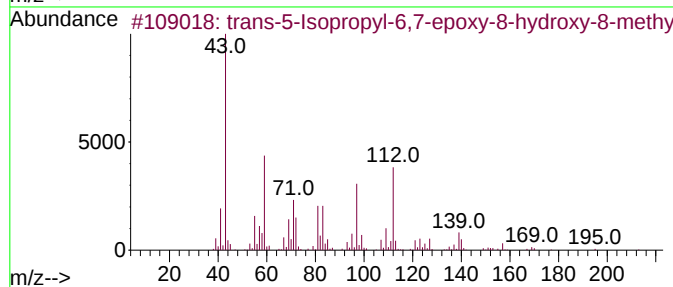
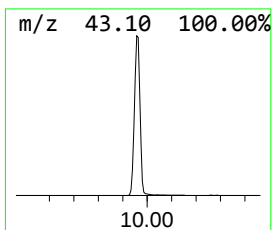
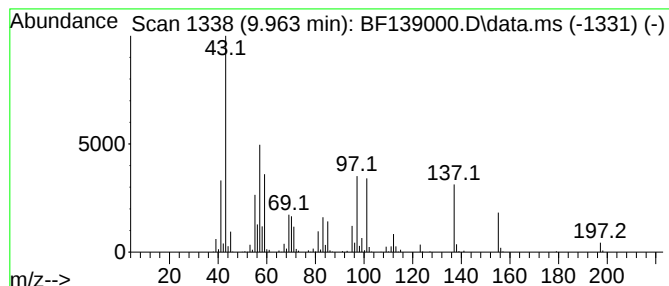
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Peak Number 3 unknown9.963 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	70.07 ng	950223	Acenaphthene-d10	9.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	25
2		4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	12
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4		3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10
5		2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	2.8	ng	34546	1	6.834	244671	20.0
1-Phenoxypropan...	8.434	3.7	ng	54696	2	8.116	298894	20.0
unknown9.963	9.963	70.1	ng	950223	3	9.863	271228	20.0