

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
 Data File : BM040338.D
 Acq On : 21 Jun 2023 17:16
 Operator : MA/JU
 Sample : 03251-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-01

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_M\Methods\8270-BM061323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.434	189	195	210	rVB	1901864	2614476	25.20%	4.914%
2	5.046	293	299	314	rBV	4229253	5592170	53.90%	10.511%
3	5.510	372	378	391	rBV	1542444	2282676	22.00%	4.291%
4	6.134	478	484	494	rBV	644361	910431	8.78%	1.711%
5	7.122	645	652	667	rBV	848826	1363748	13.14%	2.563%
6	7.957	786	794	804	rBV	964405	1540657	14.85%	2.896%
7	9.128	984	993	1010	rBV	3216691	5324380	51.32%	10.008%
8	10.769	1265	1272	1283	rBV	1195161	2038281	19.65%	3.831%
9	13.228	1683	1690	1704	rBV	7265747	10375132	100.00%	19.501%
10	14.598	1914	1923	1939	rBV	1569346	2234994	21.54%	4.201%
11	15.951	2147	2153	2159	rBV	104651	155279	1.50%	0.292%
12	16.086	2169	2176	2193	rBV	2773542	4011821	38.67%	7.541%
13	17.339	2383	2389	2404	rBV	1476540	2132873	20.56%	4.009%
14	19.956	2829	2834	2845	rBV	7413170	8843061	85.23%	16.621%
15	21.521	3095	3100	3111	rBV	1329582	1807915	17.43%	3.398%
16	23.939	3506	3511	3523	rVB	989512	1974989	19.04%	3.712%

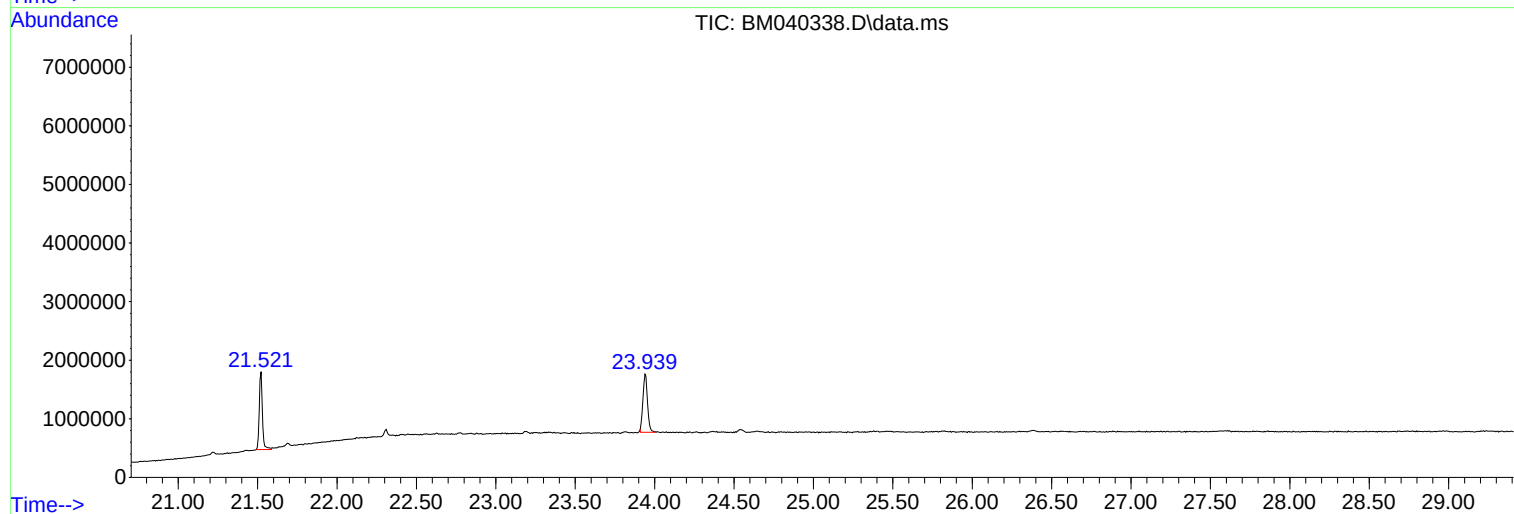
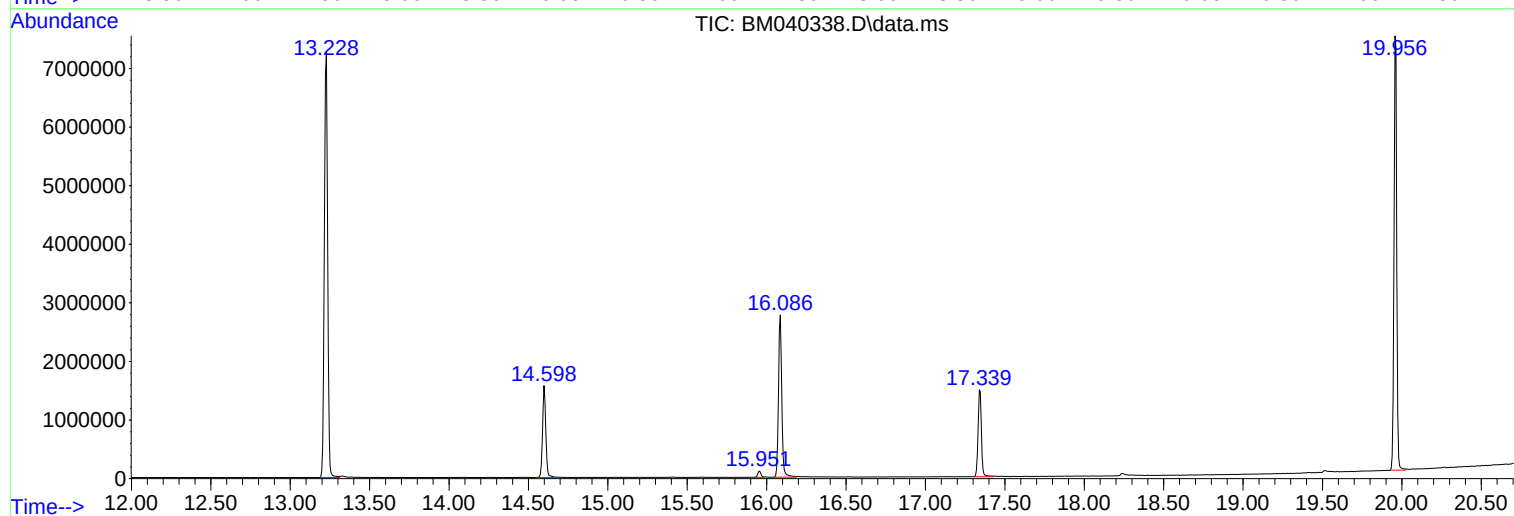
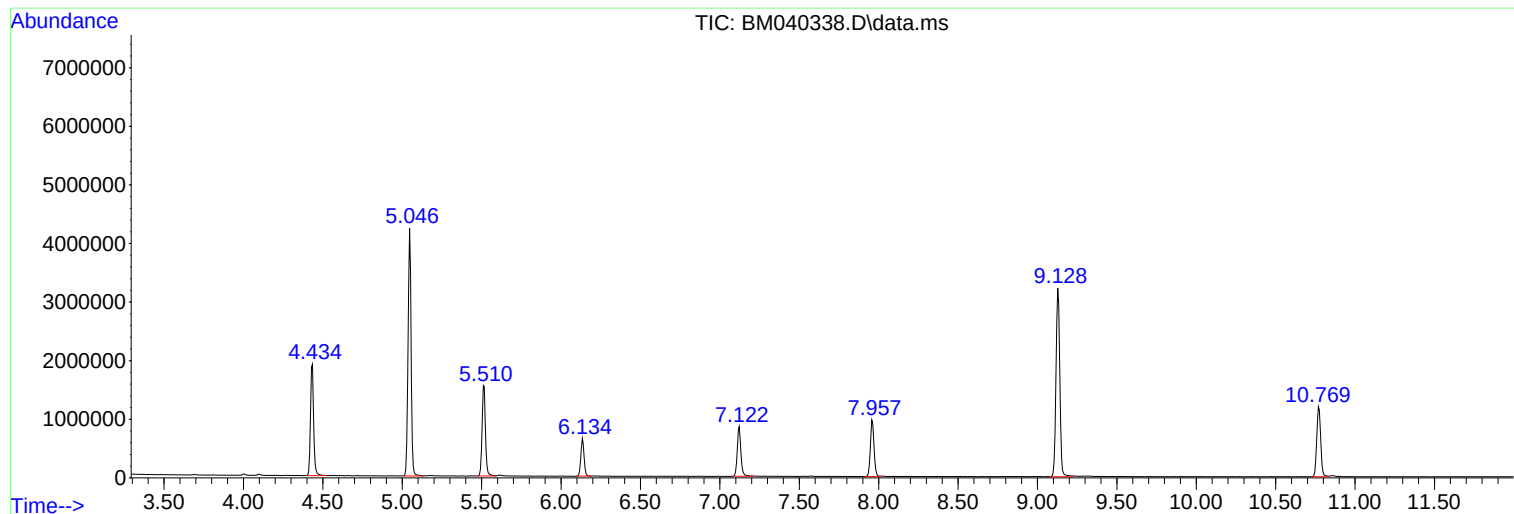
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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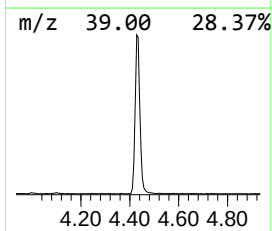
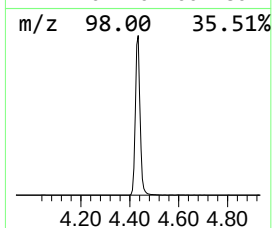
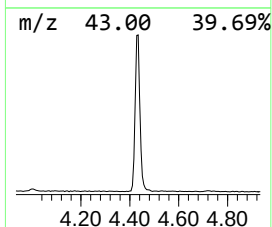
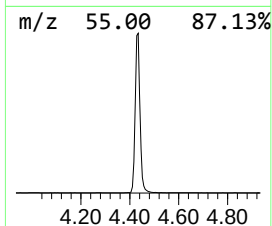
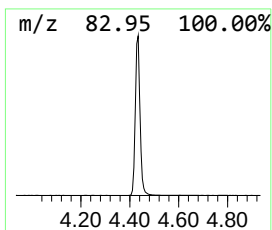
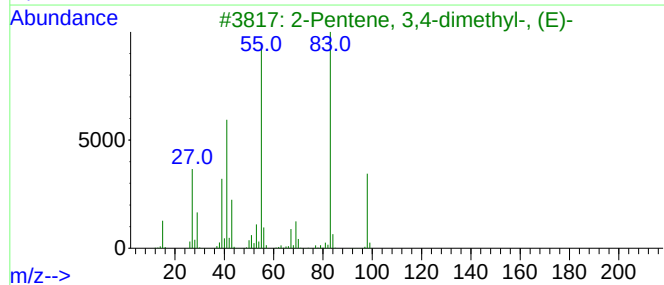
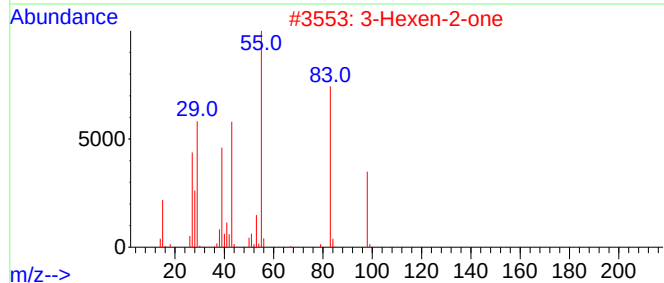
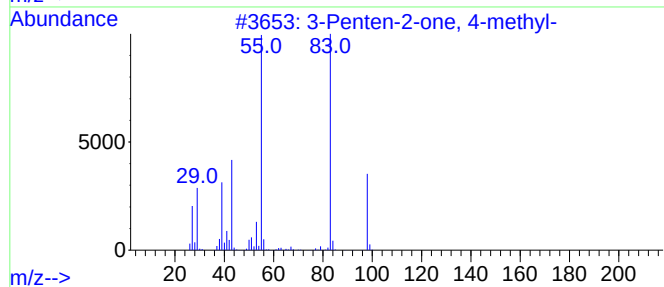
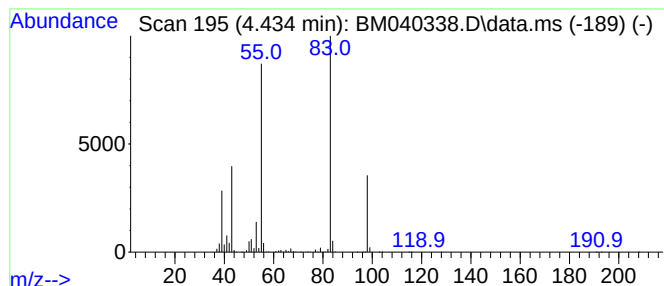
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	33.94 ng	2614480	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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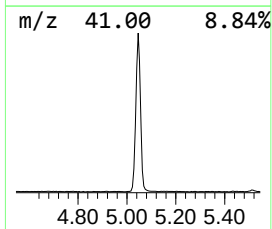
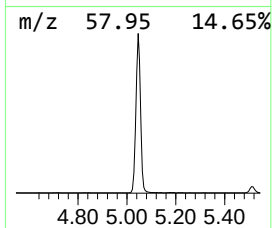
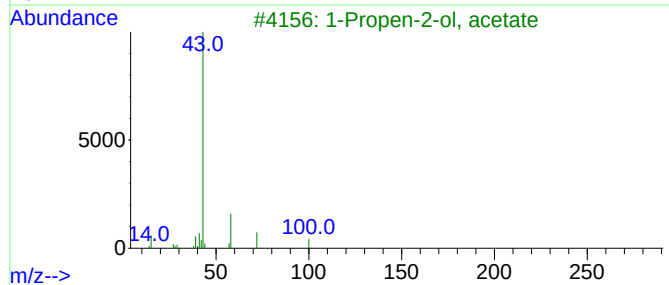
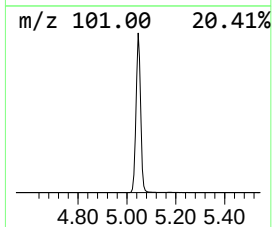
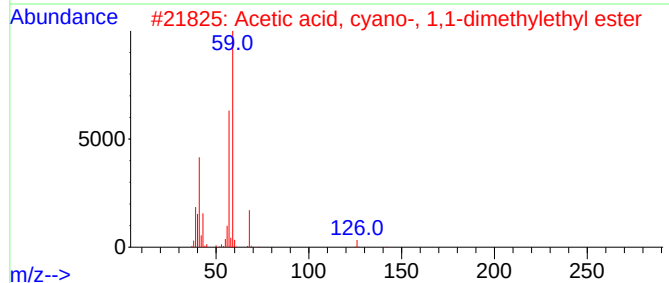
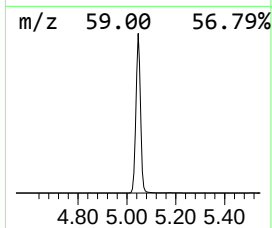
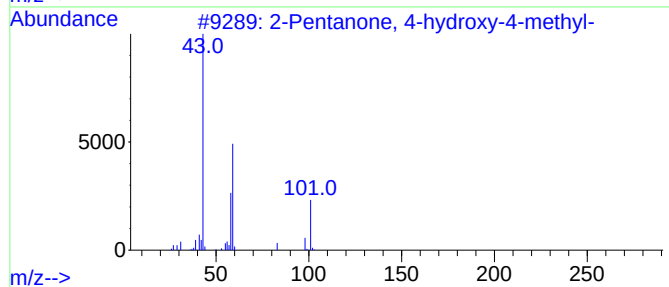
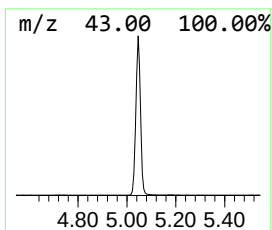
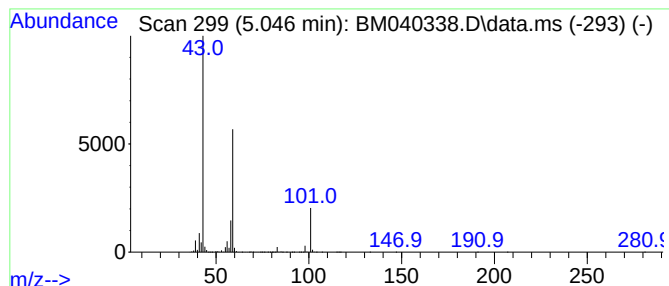
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	72.59 ng	5592170	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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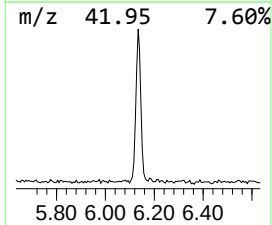
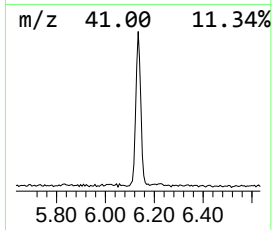
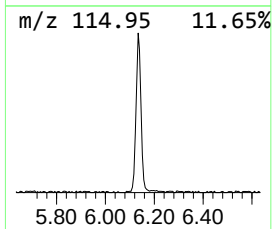
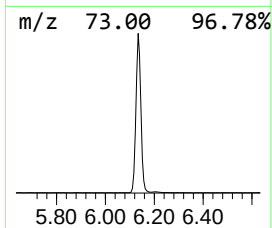
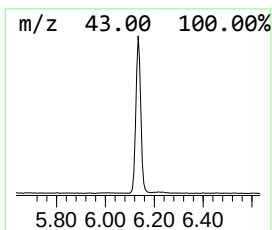
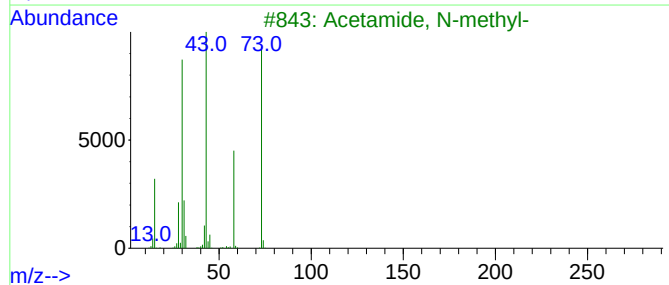
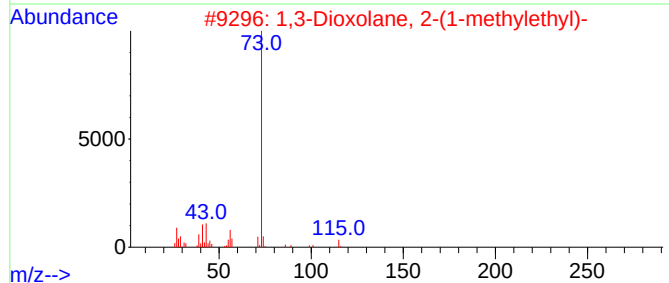
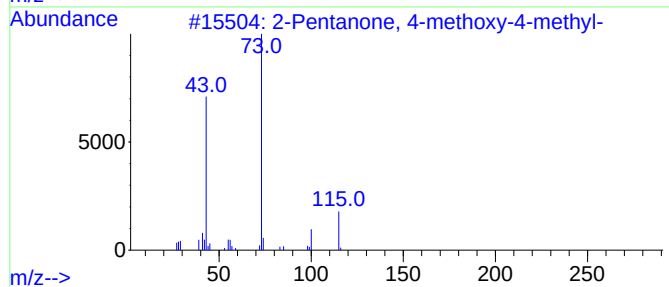
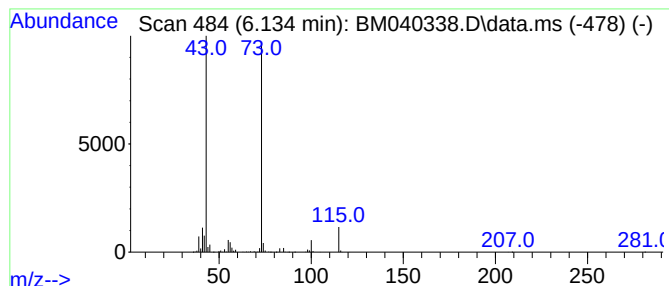
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.134	11.82 ng	910431	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.434	33.9	ng	2614480	1	7.957	1540660	20.0
2-Pentanone, 4-...	5.046	72.6	ng	5592170	1	7.957	1540660	20.0
2-Pentanone, 4-...	6.134	11.8	ng	910431	1	7.957	1540660	20.0