

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030323\
 Data File : BF132624.D
 Acq On : 03 Mar 2023 12:39
 Operator : CG\JU
 Sample : PB151155BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB151155BL

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132624.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.640	345	349	356	rBV	218702	239797	3.08%	0.508%
2	5.245	445	452	464	rBV	2358854	3510305	45.16%	7.430%
3	5.634	513	518	521	rBV	4953749	5222662	67.18%	11.054%
4	6.016	579	583	589	rBV	180145	147148	1.89%	0.311%
5	6.628	681	687	690	rBV	4604546	5282201	67.95%	11.180%
6	6.998	746	750	754	rBV	1626088	1284424	16.52%	2.719%
7	7.569	841	847	850	rBV	3503620	3616383	46.52%	7.654%
8	8.286	965	969	972	rBV	2061705	1680328	21.62%	3.557%
9	9.363	1147	1152	1155	rBV	6795421	6323778	81.35%	13.385%
10	10.045	1264	1268	1272	rBV	2375661	2030774	26.12%	4.298%
11	10.845	1399	1404	1407	rBV	4637826	4455199	57.31%	9.430%
12	11.545	1519	1523	1526	rBV	2639724	2235166	28.75%	4.731%
13	13.139	1789	1794	1797	rBV	7037782	7773771	100.00%	16.454%
14	14.204	1971	1975	1980	rBV	2137654	1921629	24.72%	4.067%
15	15.757	2233	2239	2247	rBV2	1163520	1522951	19.59%	3.223%

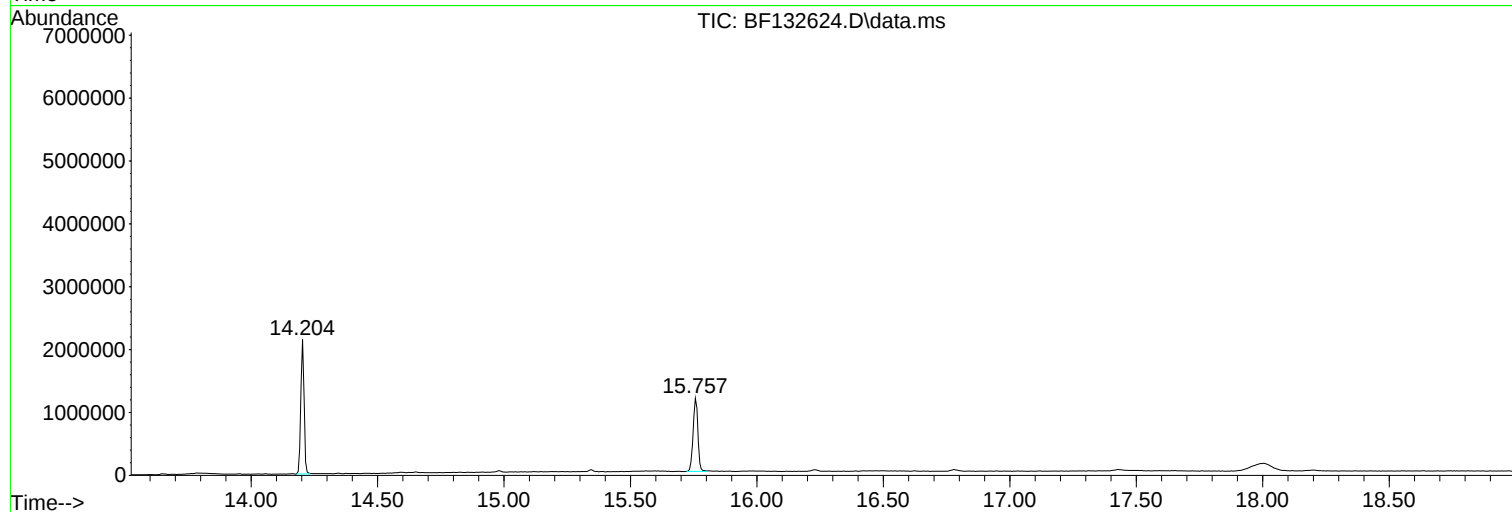
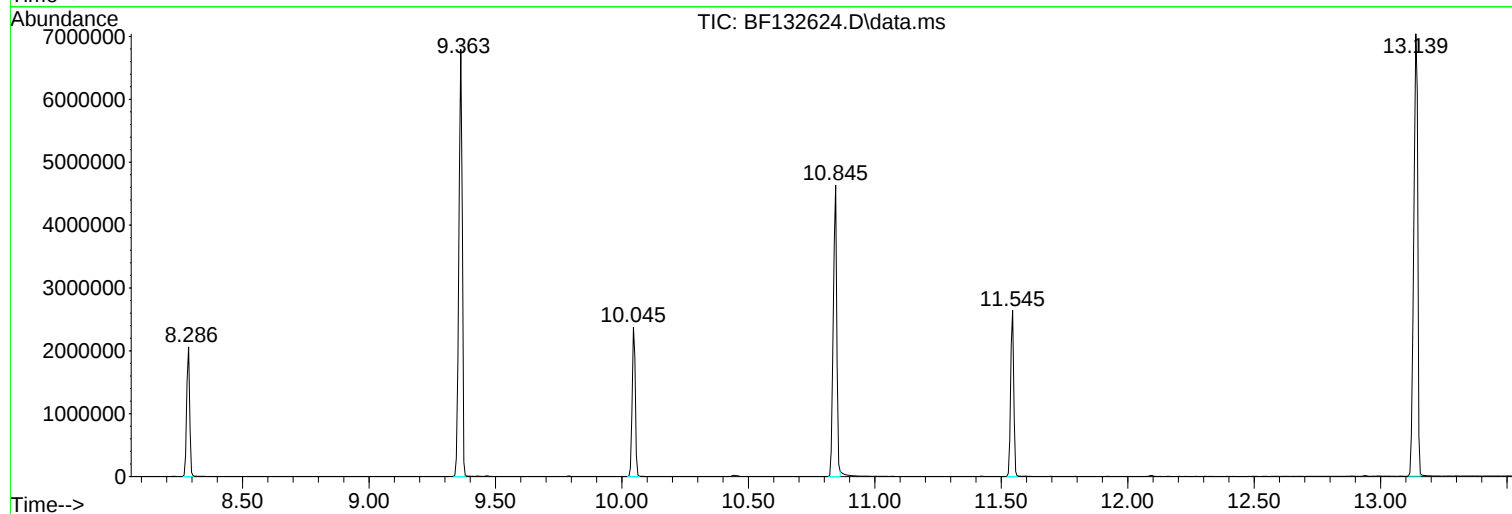
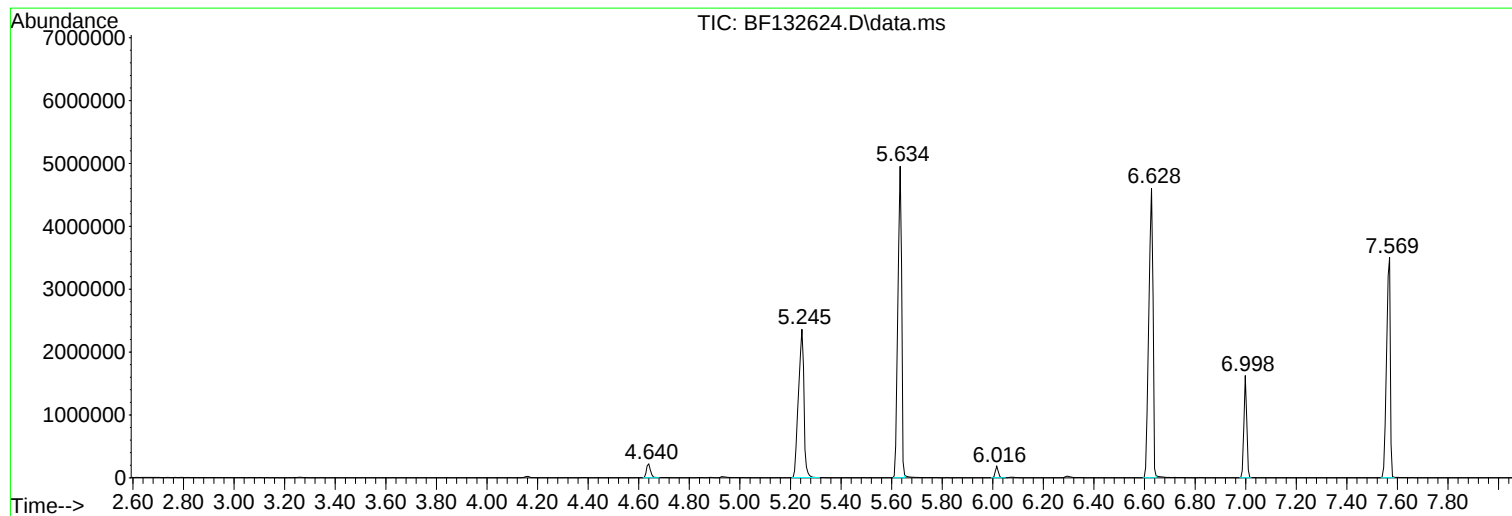
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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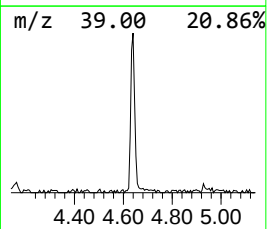
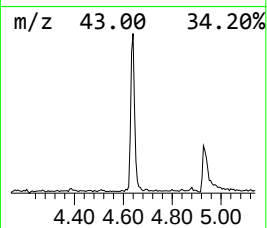
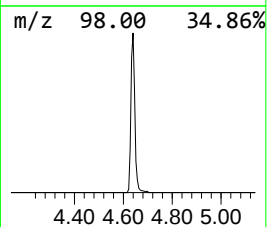
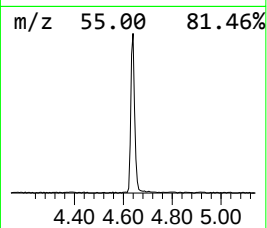
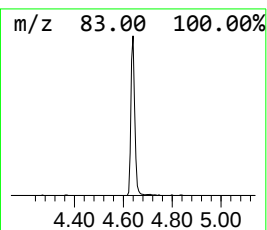
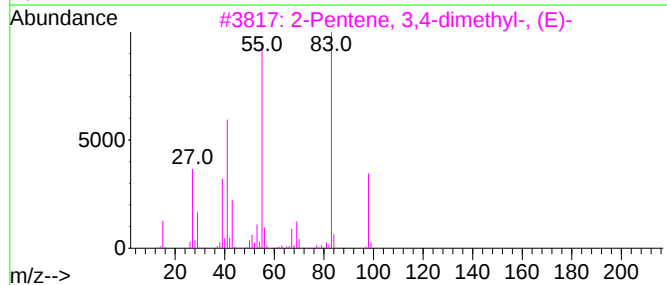
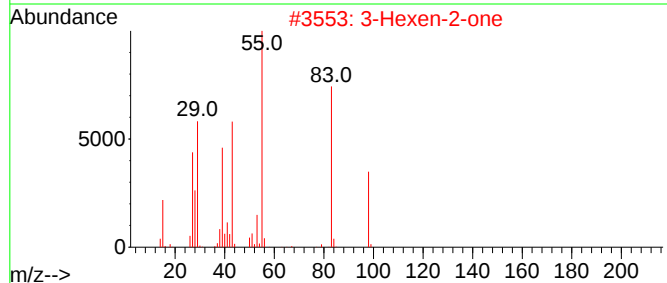
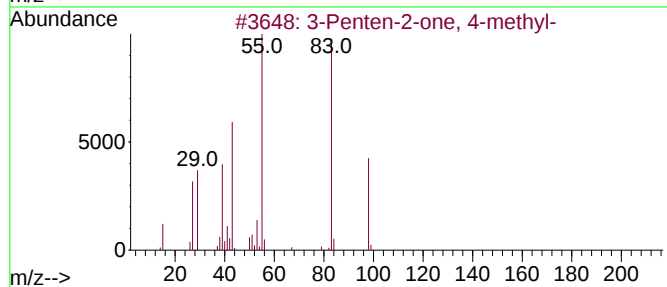
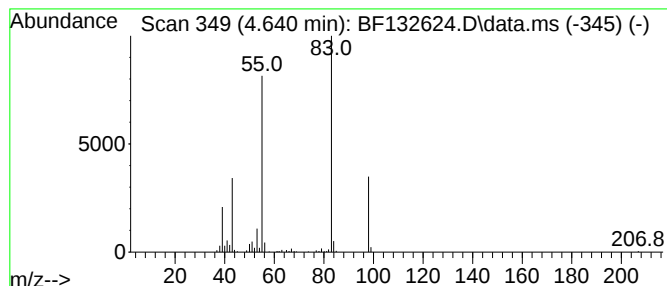
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.640	3.73 ng	239797	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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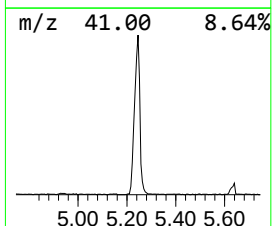
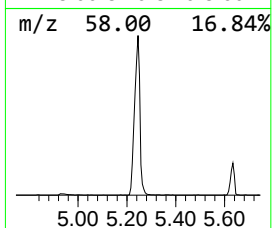
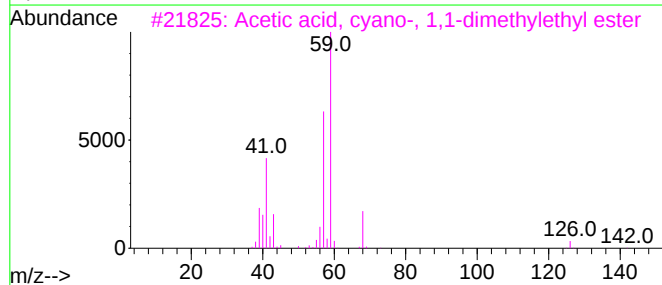
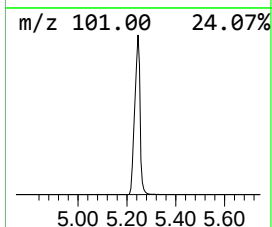
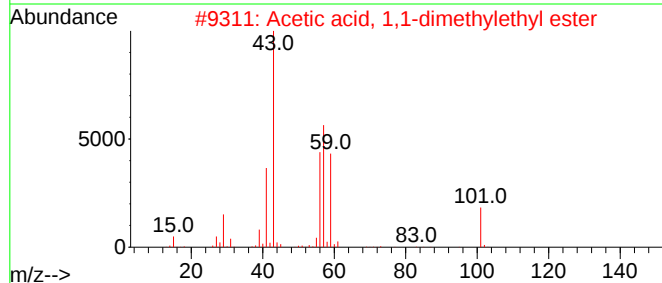
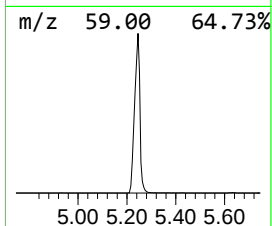
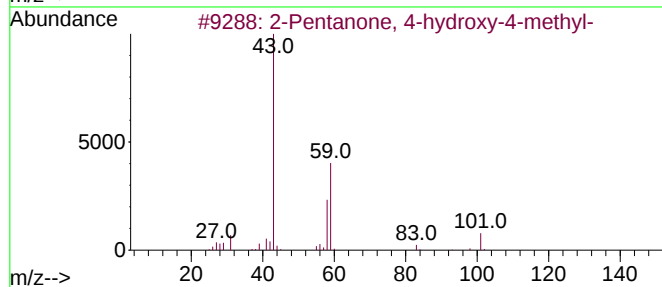
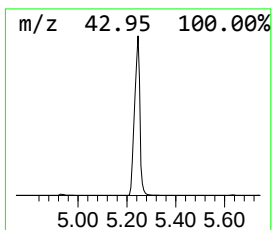
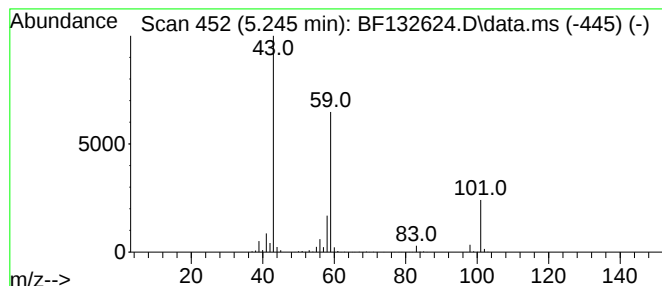
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.245	54.66 ng	3510310	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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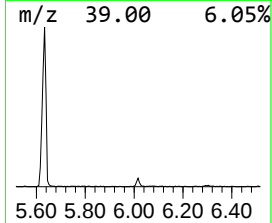
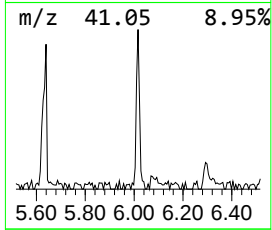
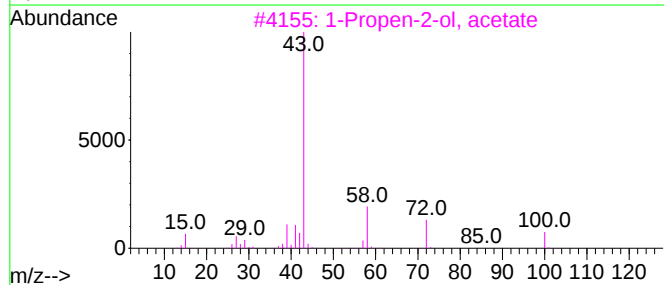
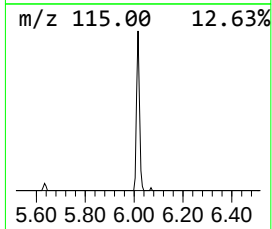
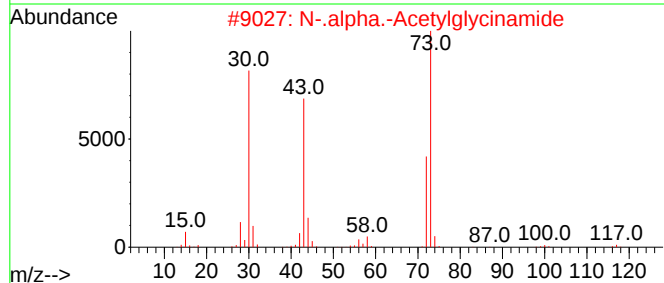
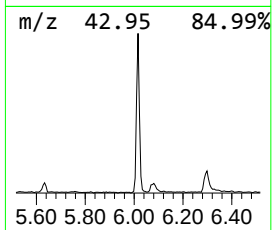
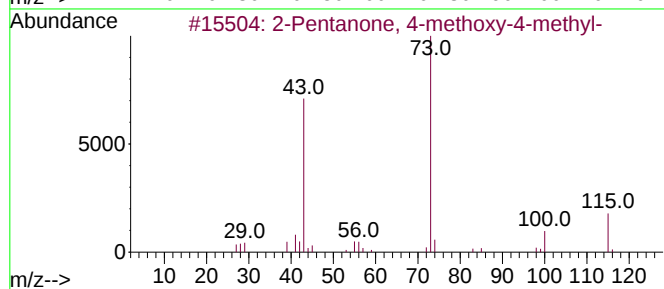
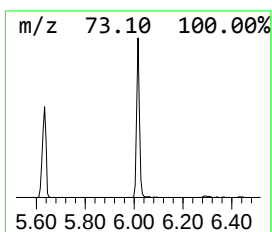
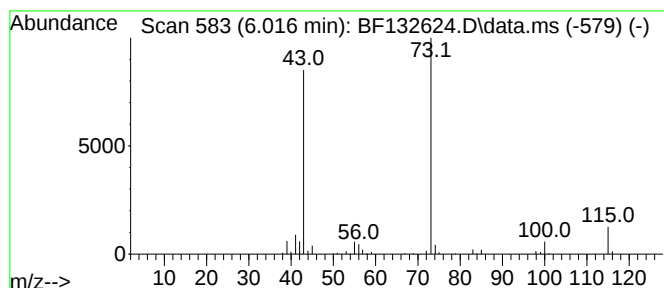
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.016	2.29 ng	147148	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9		



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.640	3.7	ng	239797	1	6.998	1284420	20.0
2-Pentanone, 4-...	5.245	54.7	ng	3510310	1	6.998	1284420	20.0
2-Pentanone, 4-...	6.016	2.3	ng	147148	1	6.998	1284420	20.0