

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
 Data File : BG055105.D
 Acq On : 7 Oct 2022 19:03
 Operator : CG/JU
 Sample : N5033-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 596C-1

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_G\Methods\8270-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.372	9	14	37	rVB	496800	766647	28.96%	7.021%
2	4.765	246	251	258	rVB	19078	30143	1.14%	0.276%
3	5.387	349	357	370	rBV	807293	1236903	46.72%	11.327%
4	5.857	429	437	450	rBV	97762	202223	7.64%	1.852%
5	7.461	702	710	719	rBV	50466	91229	3.45%	0.835%
6	8.337	852	859	869	rVB	69770	119708	4.52%	1.096%
7	9.506	1050	1058	1067	rVB	237307	423607	16.00%	3.879%
8	11.163	1333	1340	1348	rBV	97606	177460	6.70%	1.625%
9	13.572	1743	1750	1757	rBV	714948	1120769	42.34%	10.264%
10	14.941	1976	1983	1990	rVB	190804	294635	11.13%	2.698%
11	16.421	2229	2235	2243	rBV3	39131	101164	3.82%	0.926%
12	17.673	2439	2448	2454	rBV	299784	450164	17.00%	4.122%
13	18.613	2601	2608	2613	rBV	1991020	2647299	100.00%	24.243%
14	20.246	2880	2886	2892	rBV	1676948	2186750	82.60%	20.025%
15	21.962	3170	3178	3186	rBV	308638	518984	19.60%	4.753%
16	25.405	3753	3764	3778	rBV2	178464	552258	20.86%	5.057%

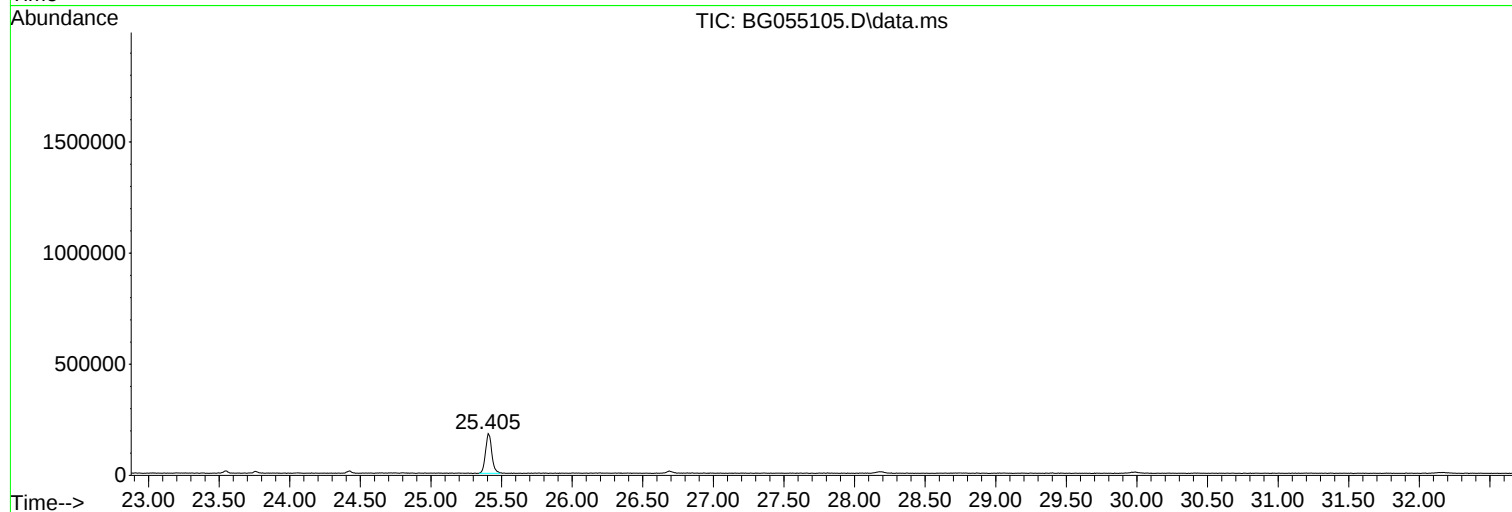
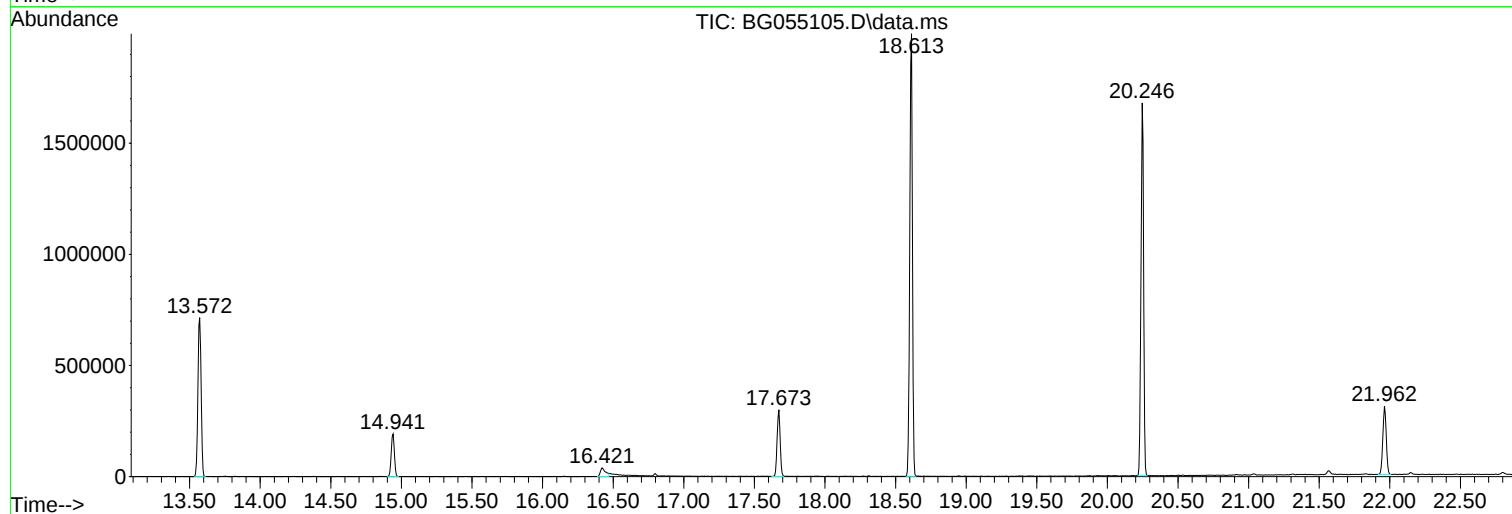
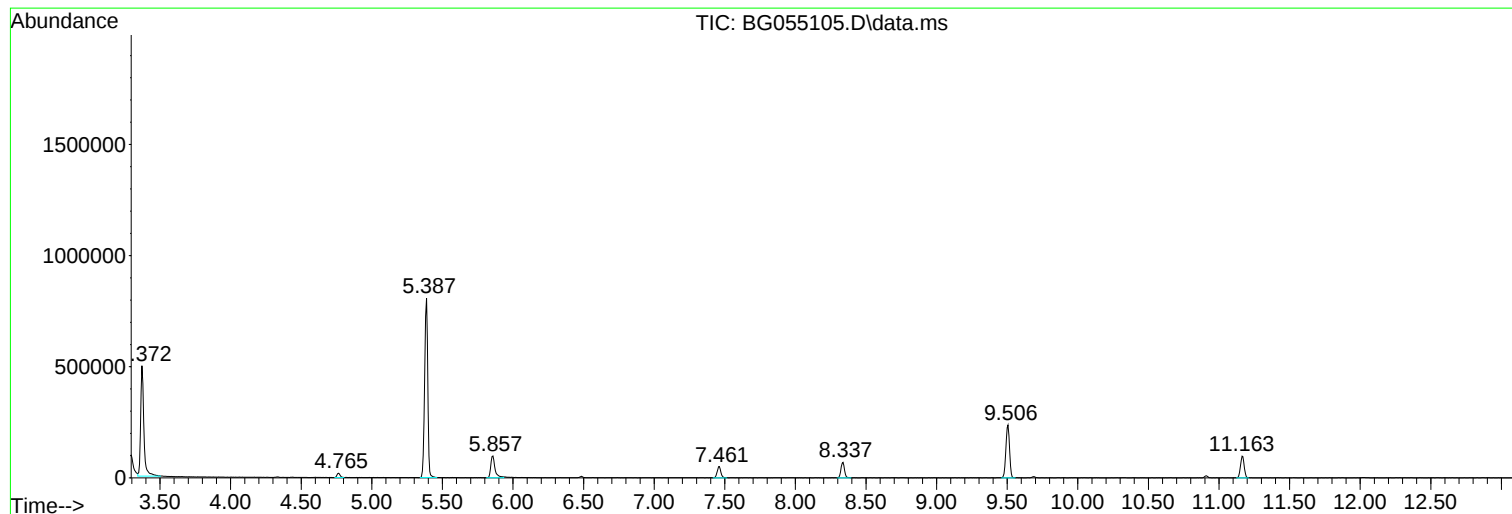
Sum of corrected areas: 10919943

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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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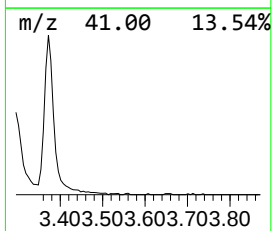
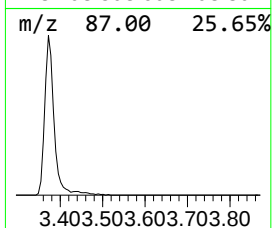
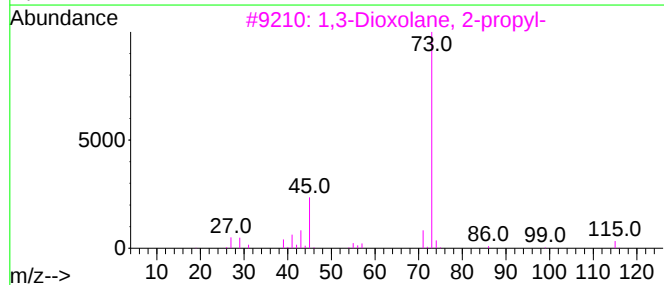
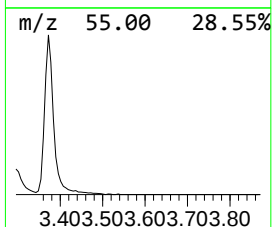
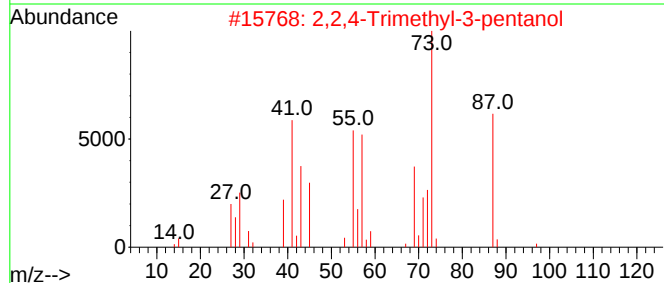
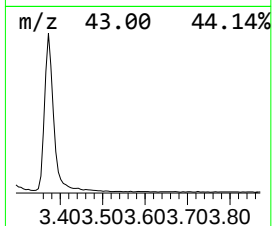
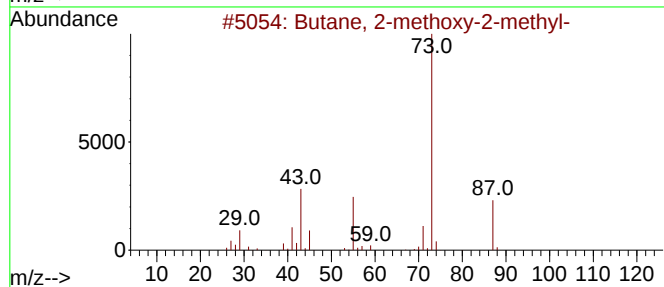
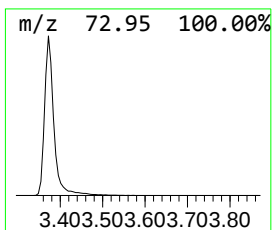
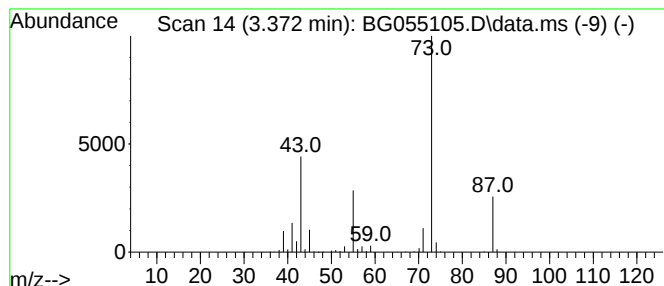
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.372	128.09 ng	766647	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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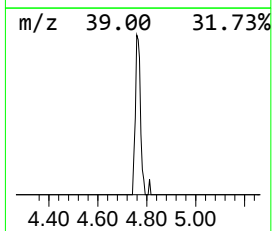
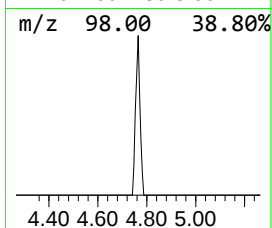
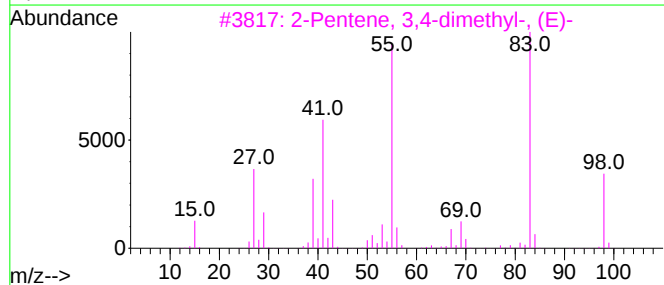
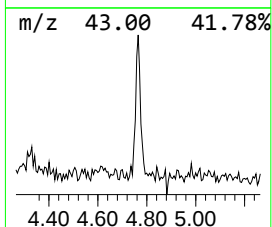
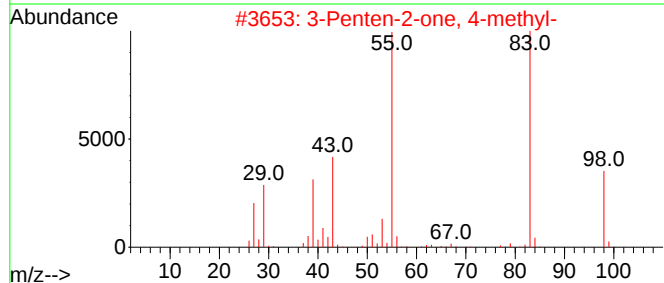
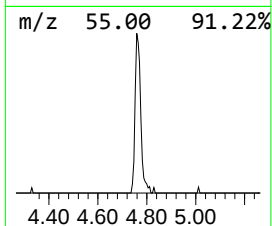
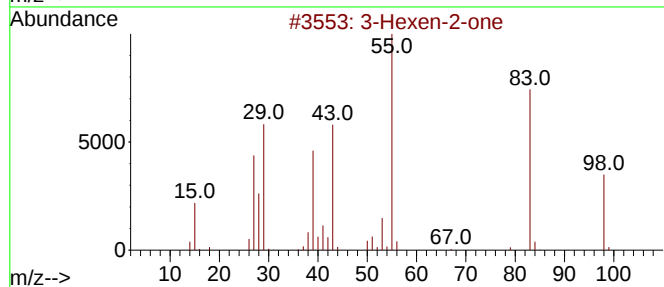
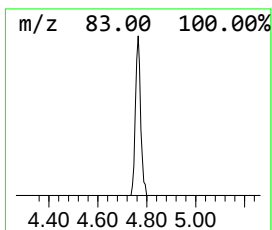
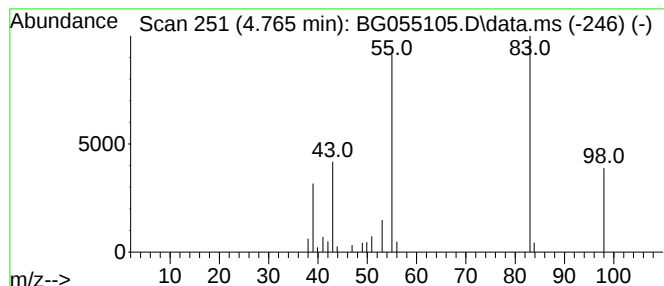
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Peak Number 2 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.765	5.04 ng	30143	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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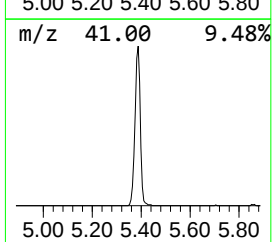
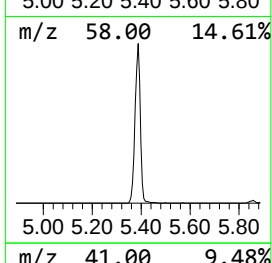
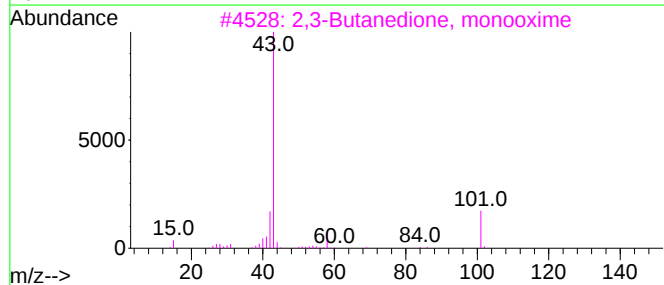
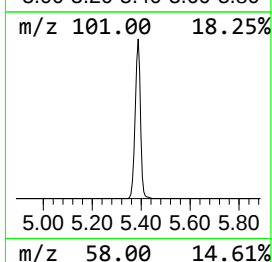
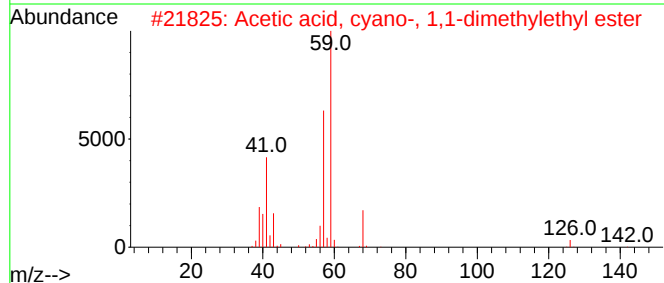
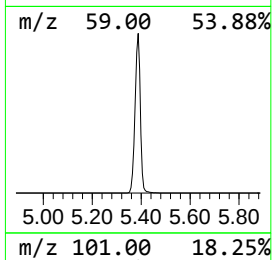
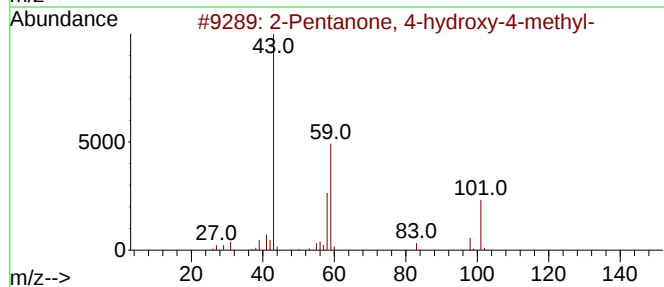
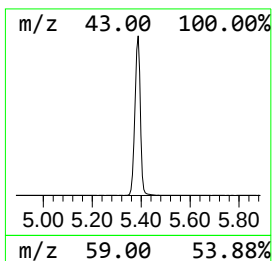
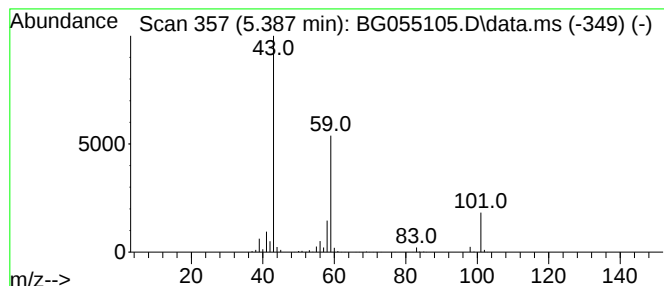
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.387	206.65 ng	1236900	1,4-Dichlorobenzene-d4	8.337

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.372	128.1	ng	766647	1	8.337	119708	20.0
3-Hexen-2-one	4.765	5.0	ng	30143	1	8.337	119708	20.0
2-Pentanone, 4-...	5.387	206.7	ng	1236900	1	8.337	119708	20.0