

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
 Data File : BM033402.D
 Acq On : 10 Dec 2021 19:50
 Operator : CG/JU
 Sample : M4965-31
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FLOORS-COMP

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-BM120821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033402.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.490	377	383	389	rBV	1228414	1797936	2.73%	1.391%
2	7.078	646	653	669	rVB	1461886	2358248	3.58%	1.824%
3	9.066	984	991	998	rBV	913628	1513631	2.30%	1.171%
4	10.701	1263	1269	1275	rVB	420764	731456	1.11%	0.566%
5	13.154	1677	1686	1698	rBV	1984758	3051862	4.63%	2.361%
6	14.530	1909	1920	1923	rBV	578482	950796	1.44%	0.736%
7	14.577	1923	1928	1949	rVB	3701739	5015687	7.62%	3.880%
8	16.013	2167	2172	2178	rVB	1068985	1535686	2.33%	1.188%
9	17.265	2380	2385	2390	rBV	728816	1153766	1.75%	0.893%
10	18.859	2647	2656	2660	rBV2	29206803	65850727	100.00%	50.942%
11	19.883	2826	2830	2836	rVB	2675421	3516316	5.34%	2.720%
12	21.336	3074	3077	3084	rVB	1577046	2070663	3.14%	1.602%
13	23.124	3377	3381	3391	rVB	2700784	4409817	6.70%	3.411%
14	25.259	3732	3744	3766	rVB	12722565	35308592	53.62%	27.315%

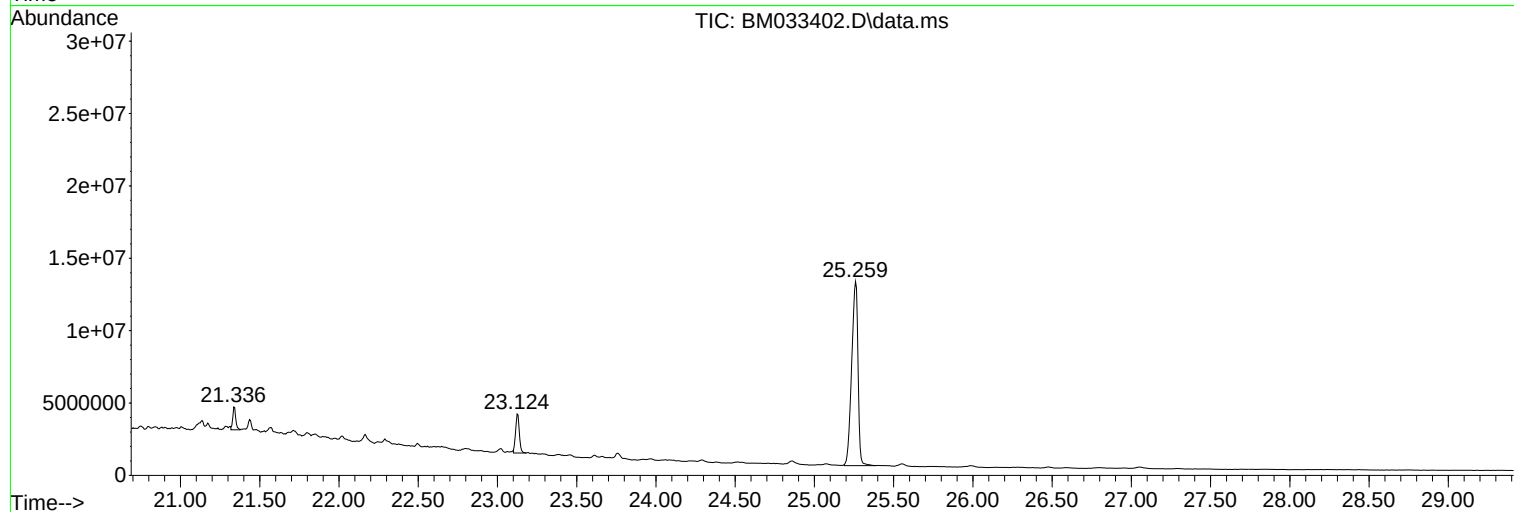
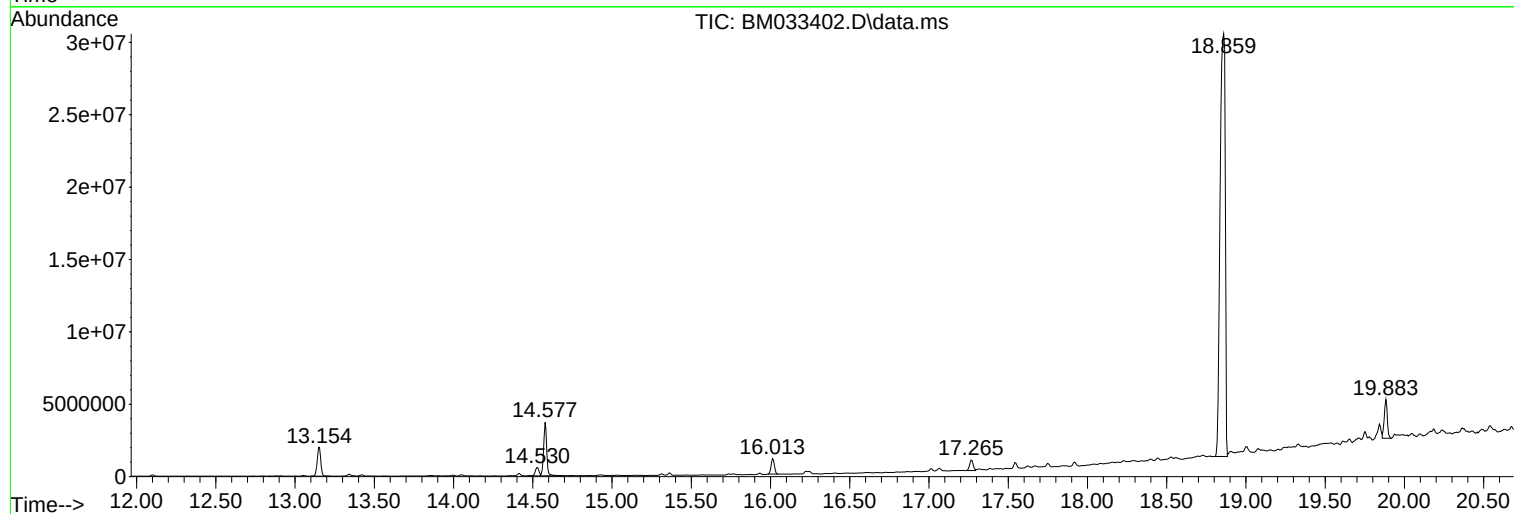
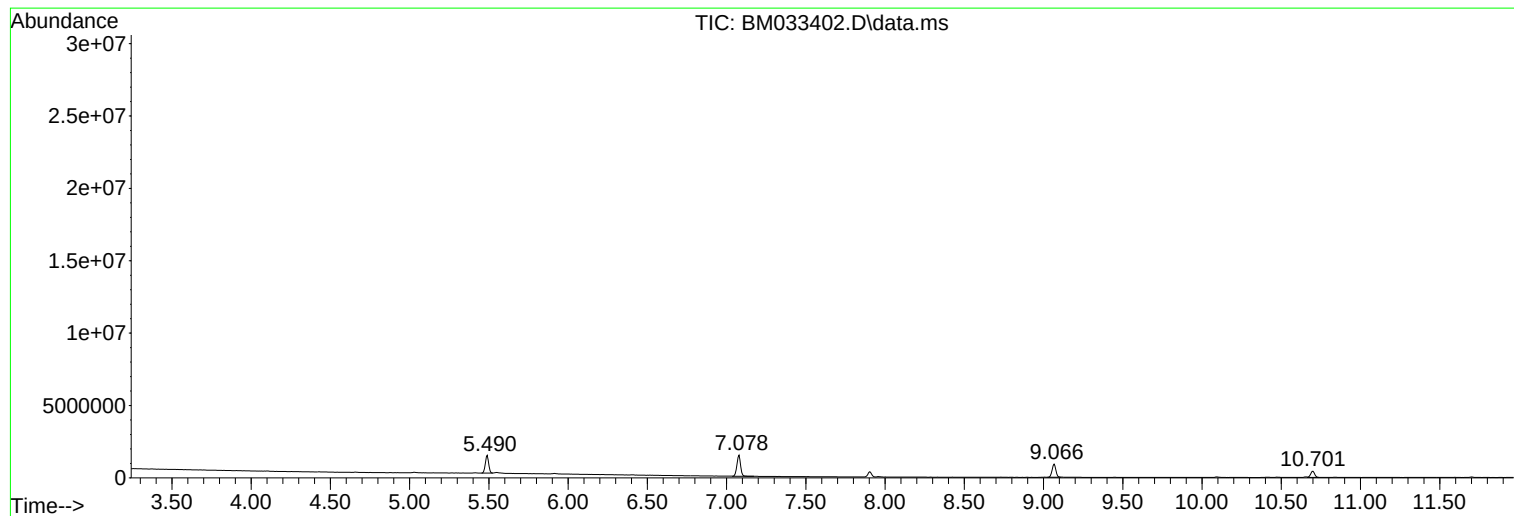
Sum of corrected areas: 129265183

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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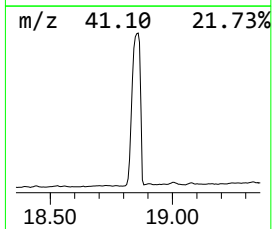
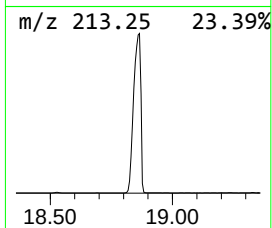
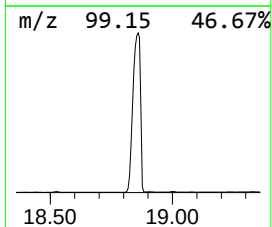
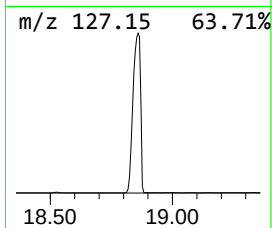
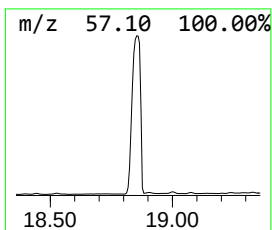
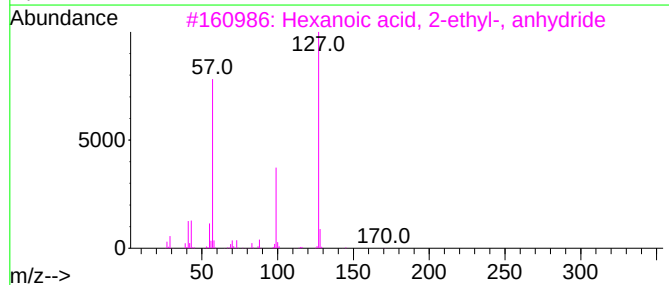
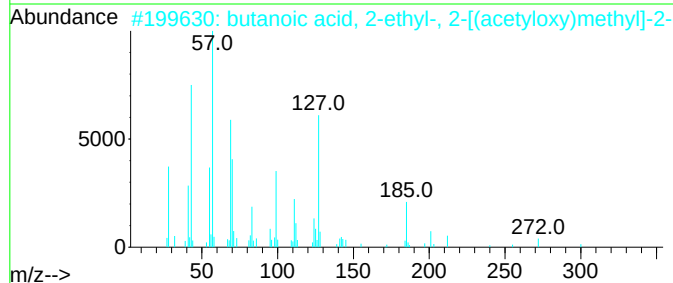
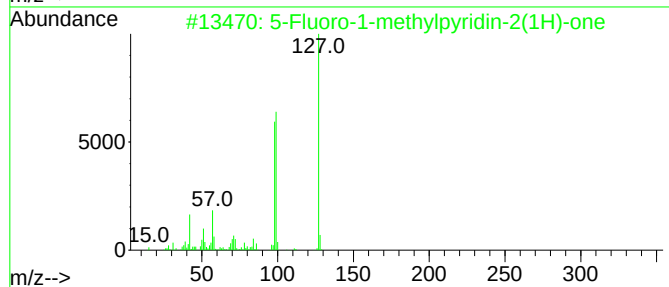
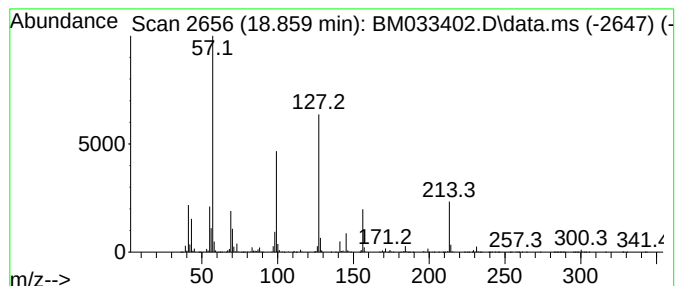
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown18.860 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.860	1141.49 ng	65850700	Phenanthrene-d10	17.265	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-1-methylpyridin-2(1H)-one	127	C6H6FN0	051173-06-9	43
2	butanoic acid, 2-ethyl-, 2-[(ace...	300	C17H32O4	1000397-51-4	38
3	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	38
4	4-(2-Hydroxyethyl)piperazin-2-on...	172	C8H16N2O2	1894458-43-5	35
5	5,6-Dihydro-4H-1,3-oxazin-2-ylam...	196	C6H7F3N2O2	1000509-76-9	32



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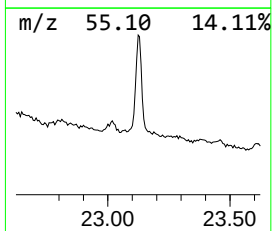
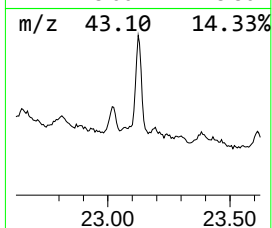
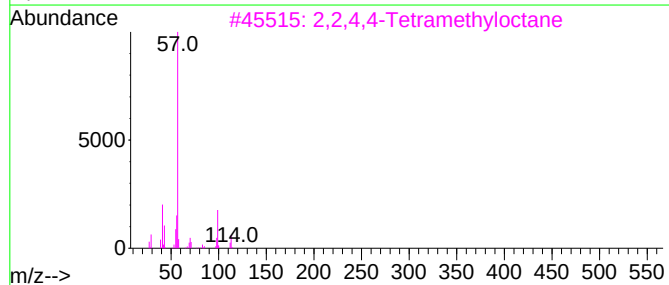
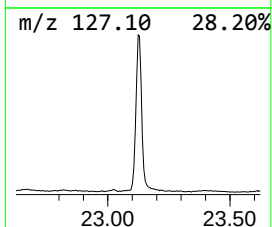
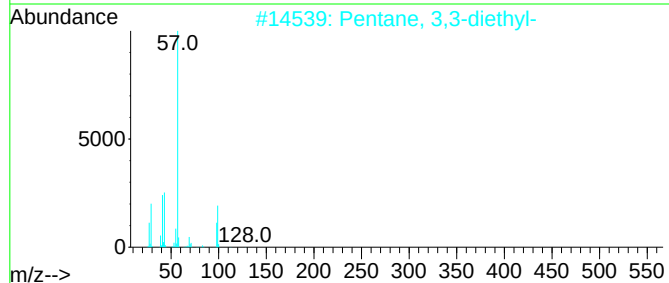
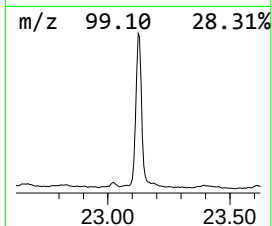
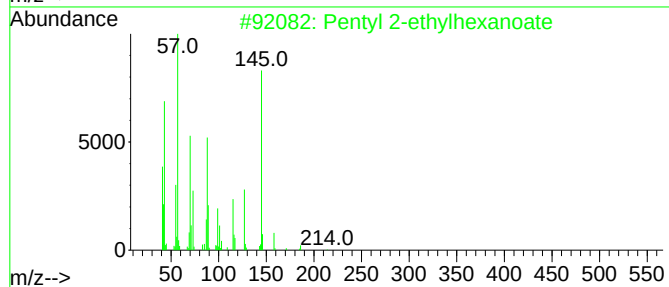
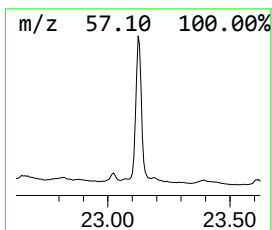
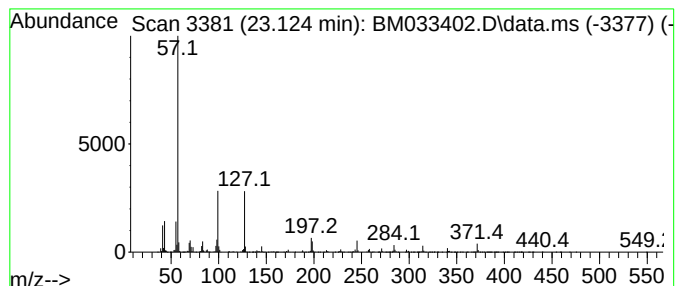
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Peak Number 2 unknown23.124 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.124	20.00 ng	4409820	Perylene-d12	23.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentyl 2-ethylhexanoate	214	C13H26O2	029660-71-7	36
2			Pentane, 3,3-diethyl-	128	C9H20	001067-20-5	35
3			2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	35
4			Heptane, 3-bromo-	178	C7H15Br	001974-05-6	25
5			2-Pentene, 5-butoxy-, (E)-	142	C9H18O	054004-23-8	25



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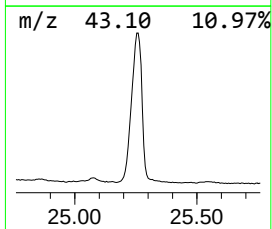
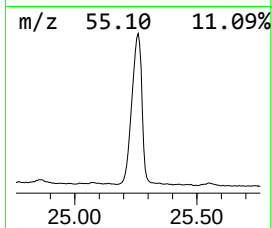
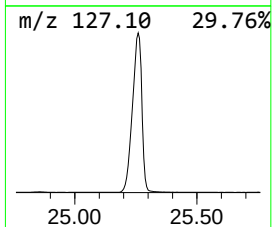
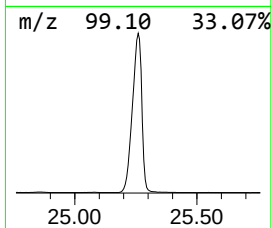
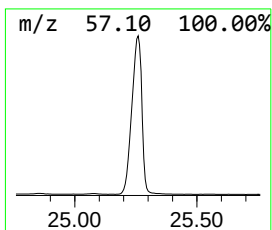
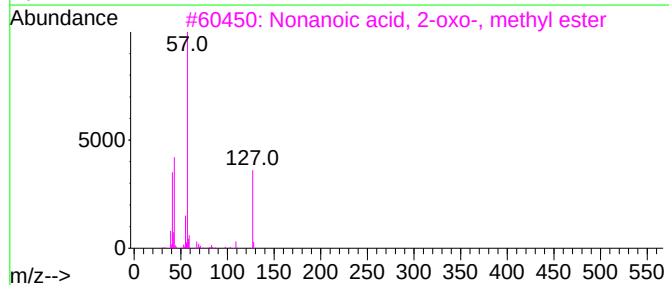
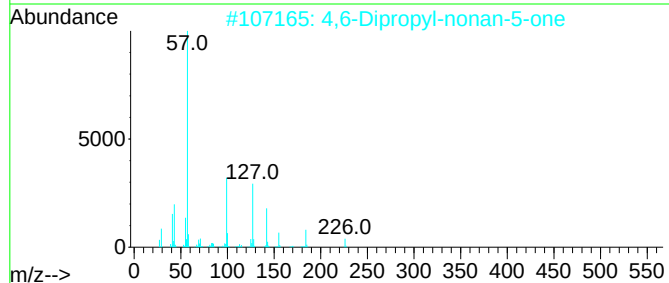
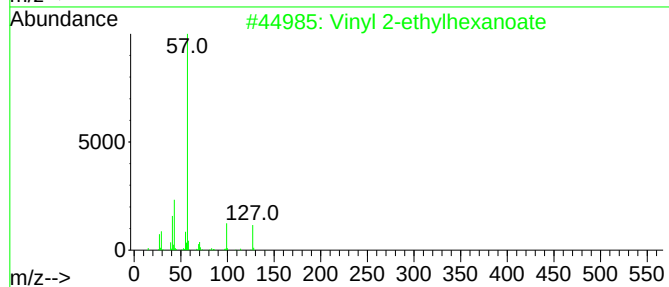
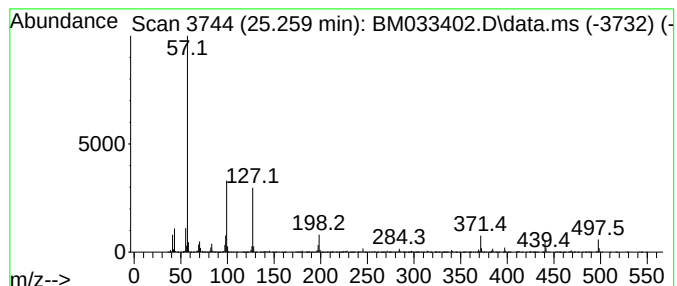
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Peak Number 3 Vinyl 2-ethylhexanoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.259	160.14 ng	35308600	Perylene-d12	23.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vinyl 2-ethylhexanoate	170	C10H18O2	000094-04-2	50
2			4,6-Dipropyl-nonan-5-one	226	C15H30O	1000190-93-3	40
3			Nonanoic acid, 2-oxo-, methyl ester	186	C10H18O3	056275-54-8	35
4			Heptane, 3-bromo-	178	C7H15Br	001974-05-6	25
5			3,5-Heptanedione, 4-bromo-2,2,6,...	262	C11H19BrO2	039516-78-4	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown18.860	18.860	1141.5	ng	65850700	4	17.265	1153770	20.0
unknown23.124	23.124	20.0	ng	4409820	6	23.759	4409820	20.0
Vinyl 2-ethylhe...	25.259	160.1	ng	35308600	6	23.759	4409820	20.0