

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
 Data File : BF132062.D
 Acq On : 13 Jan 2023 16:43
 Operator : CG\JU
 Sample : 01132-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-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_F\Methods\8270-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.651	91	96	105	rVB	78409	112995	4.49%	0.715%
2	4.987	487	493	507	rVB	749124	915458	36.39%	5.789%
3	5.404	560	564	578	rBV	1857440	1848578	73.48%	11.690%
4	6.422	733	737	752	rBV	1679675	1730520	68.79%	10.943%
5	6.769	793	796	800	rBV	592139	479648	19.07%	3.033%
6	7.345	889	894	897	rBV	1424933	1330137	52.87%	8.411%
7	8.063	1011	1016	1019	rBV	676552	609653	24.23%	3.855%
8	9.139	1194	1199	1202	rBV	2604499	2515791	100.00%	15.909%
9	9.822	1311	1315	1318	rVB	913118	726027	28.86%	4.591%
10	10.616	1446	1450	1453	rBV	1875711	1586374	63.06%	10.032%
11	11.310	1565	1568	1572	rBV	838116	741212	29.46%	4.687%
12	12.904	1834	1839	1842	rBV	2606957	2173732	86.40%	13.746%
13	13.798	1987	1991	2002	rVB2	118909	166583	6.62%	1.053%
14	13.963	2015	2019	2022	rBV	476896	410867	16.33%	2.598%
15	15.421	2262	2267	2273	rVB	390323	466125	18.53%	2.948%

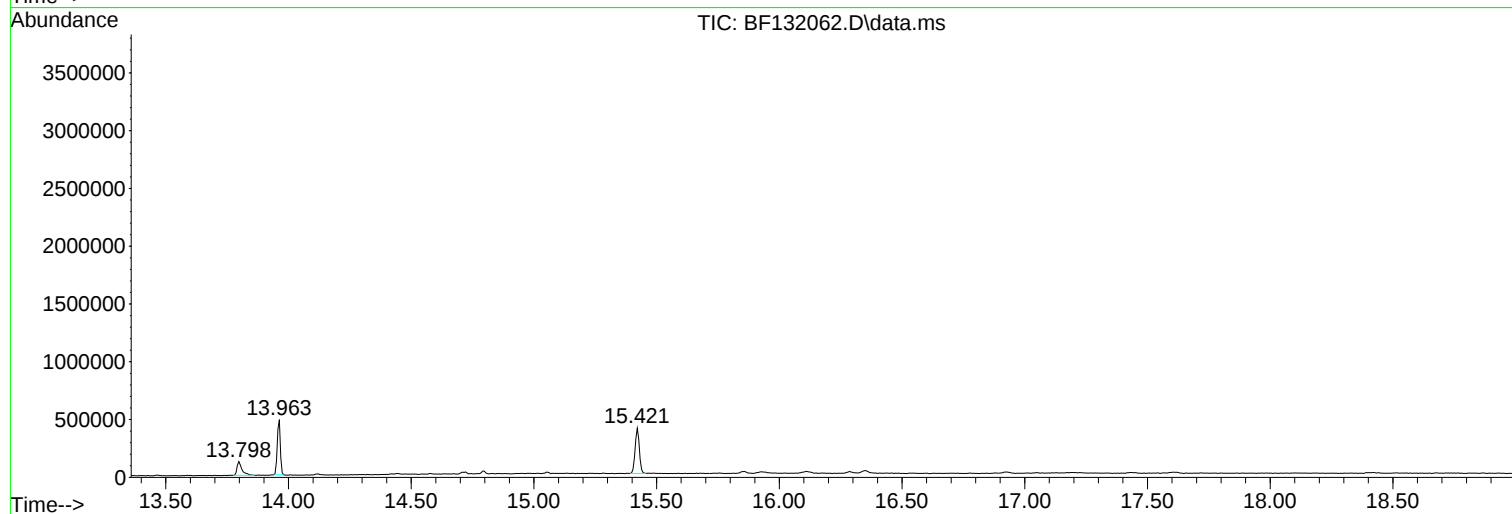
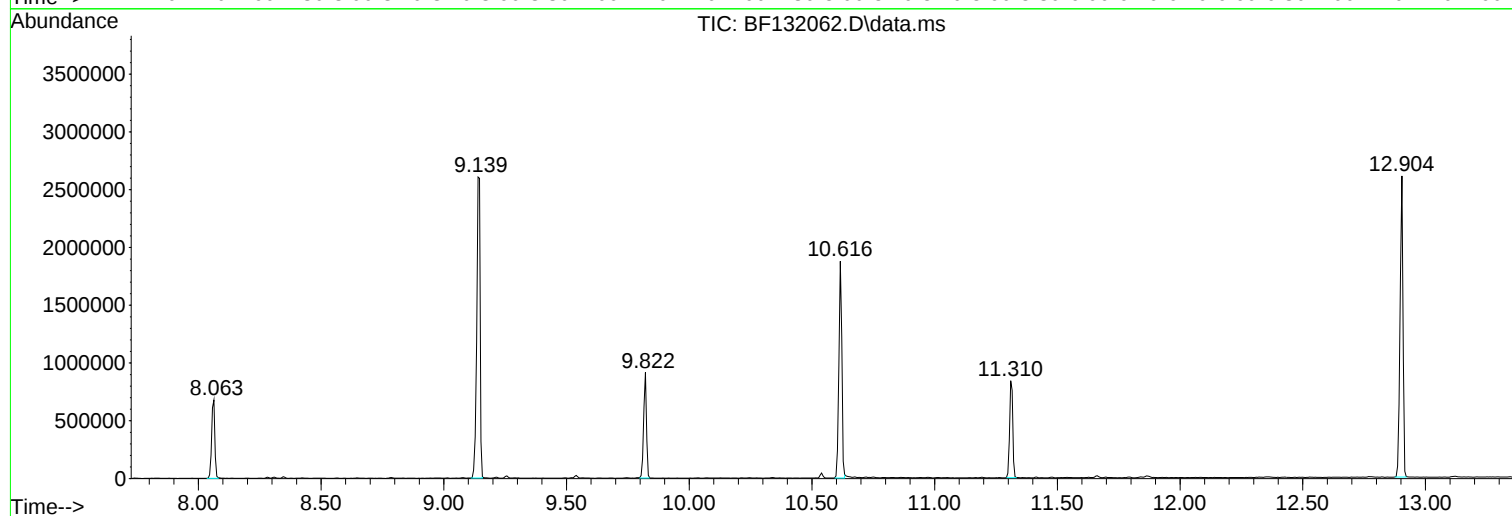
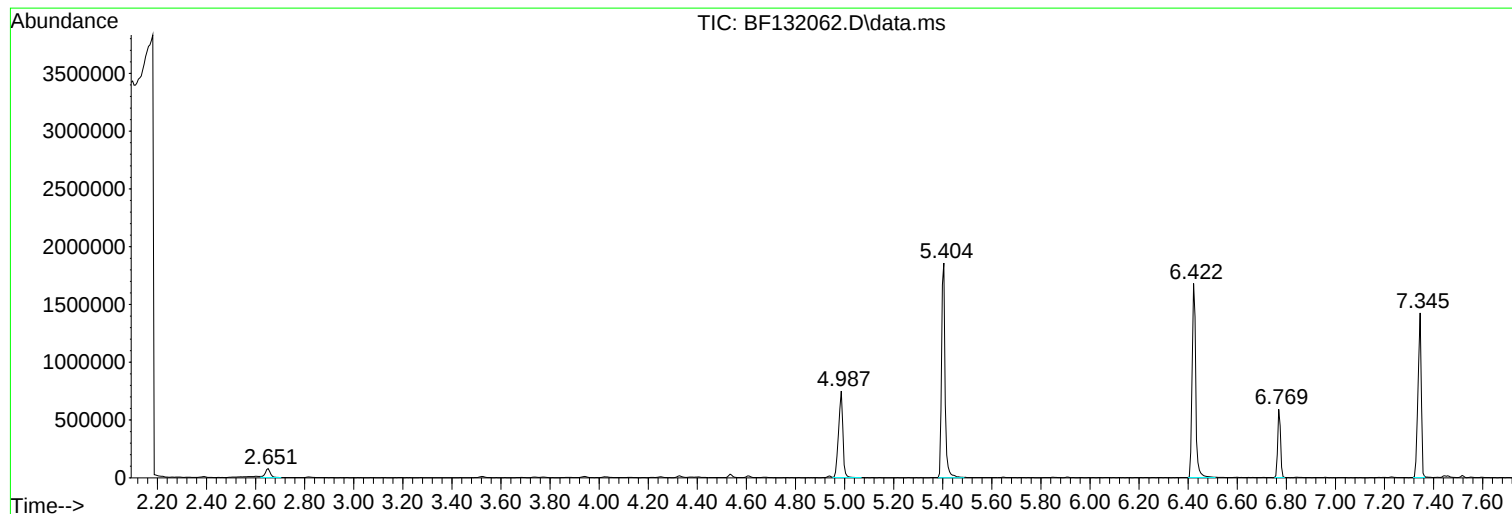
Sum of corrected areas: 15813700

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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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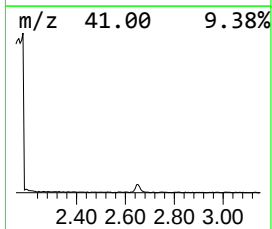
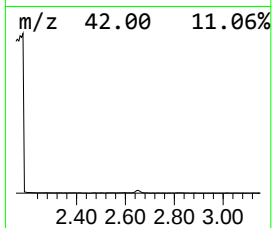
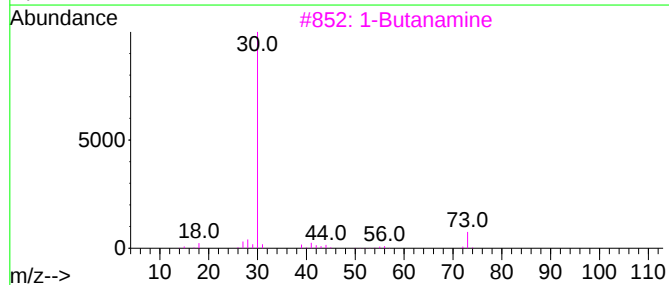
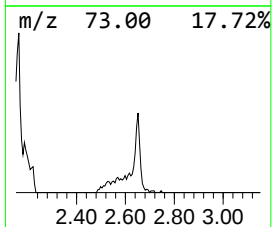
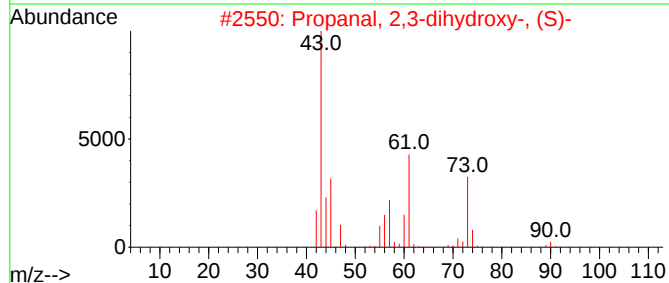
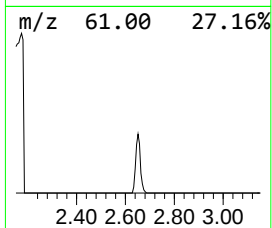
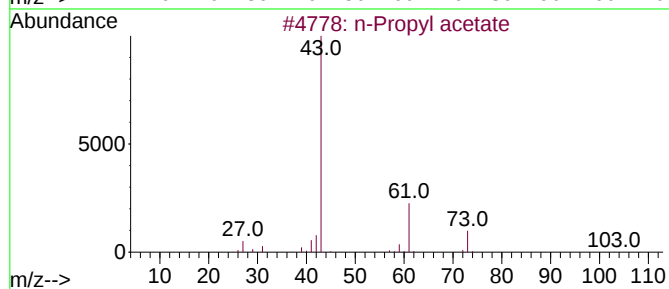
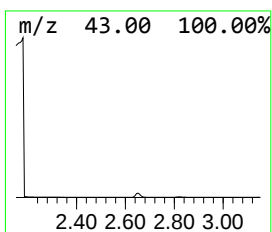
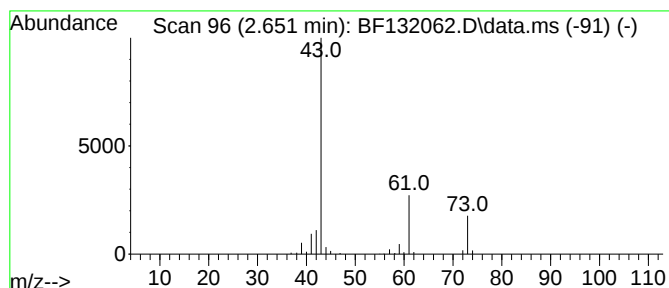
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.651	4.71 ng	112995	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	78
2			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			Pentane	72	C5H12	000109-66-0	5



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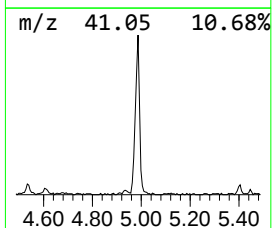
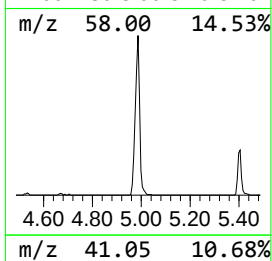
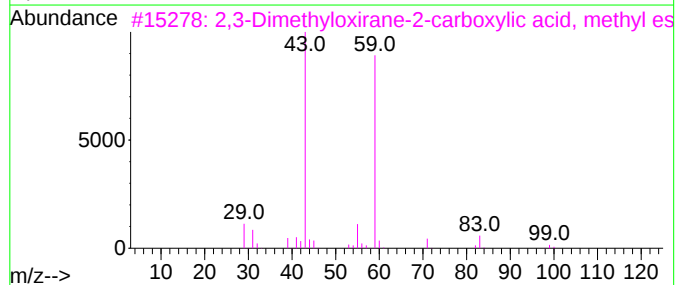
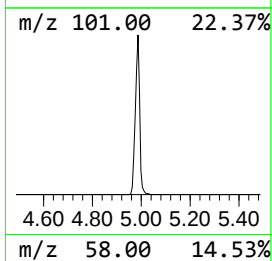
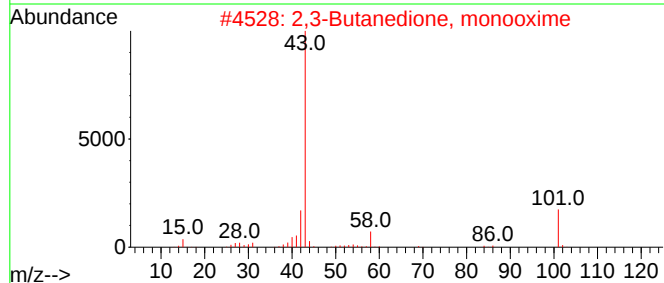
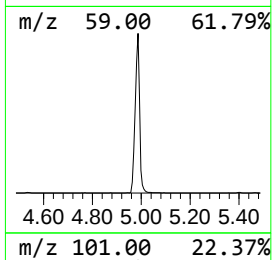
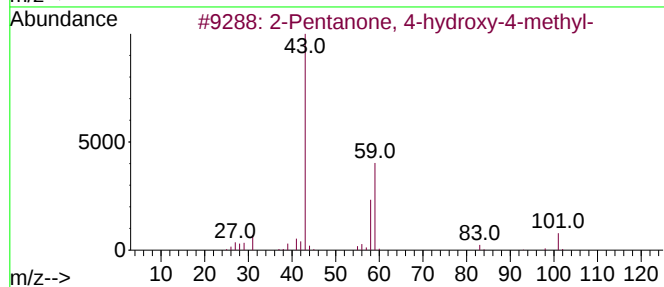
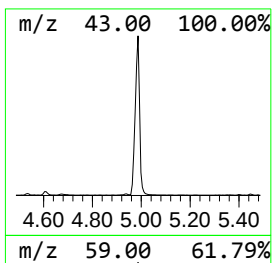
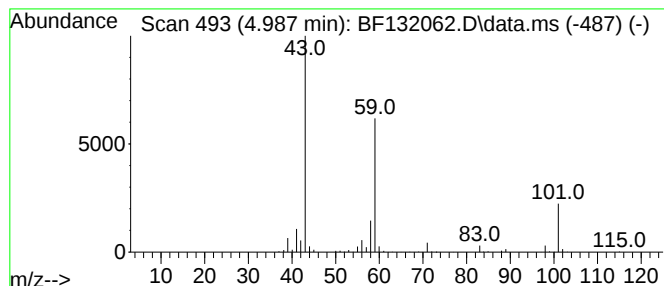
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	38.17 ng	915458	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Hexanamide	115	C6H13NO	000628-02-4	16



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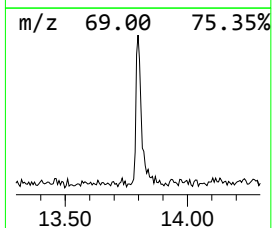
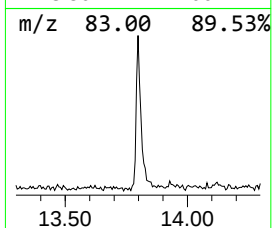
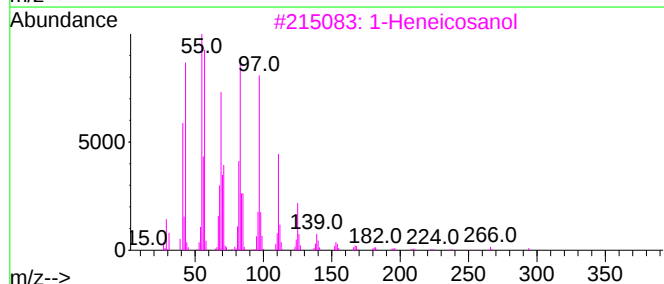
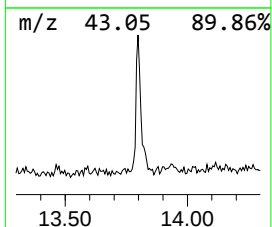
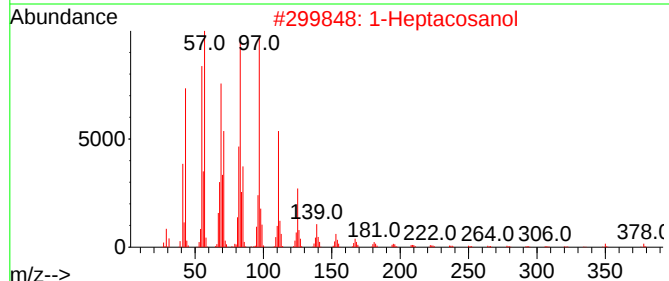
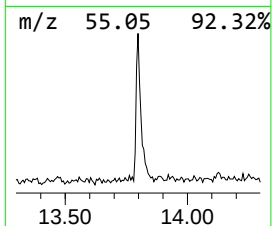
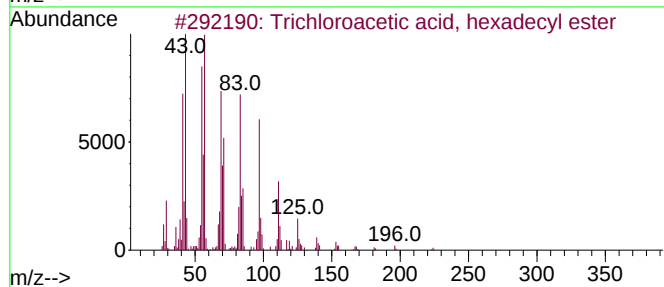
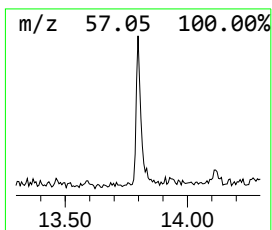
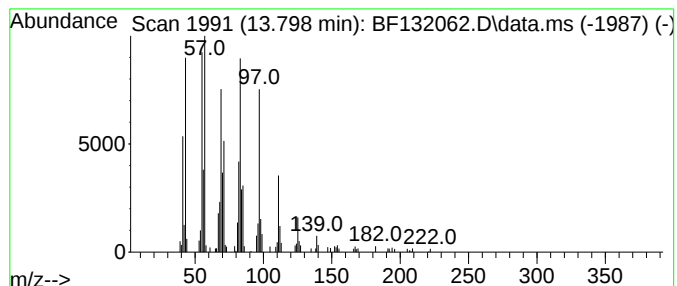
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.798	8.11 ng	166583	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.651	4.7	ng	112995	1	6.769	479648	20.0
2-Pentanone, 4-...	4.987	38.2	ng	915458	1	6.769	479648	20.0
Trichloroacetic...	13.798	8.1	ng	166583	5	13.963	410867	20.0