

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042122\
 Data File : BG053246.D
 Acq On : 21 Apr 2022 18:11
 Operator : CG/JU
 Sample : N2448-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E14ST-B6-041522-GW-DUP

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-BG040822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.678	383	390	399	rBV	292600	477133	16.62%	3.462%
2	7.270	654	661	671	rBV2	183059	323557	11.27%	2.348%
3	8.110	797	804	811	rBV	232521	410069	14.28%	2.975%
4	9.273	995	1002	1014	rVB	474359	861082	29.99%	6.248%
5	10.924	1275	1283	1297	rVB	313912	584545	20.36%	4.241%
6	13.362	1690	1698	1706	rBV	1281945	2016281	70.23%	14.629%
7	14.737	1925	1932	1940	rVB	544018	854152	29.75%	6.197%
8	16.223	2177	2185	2199	rBV	1074582	1690544	58.88%	12.266%
9	17.480	2392	2399	2408	rVB	678488	1080650	37.64%	7.841%
10	18.132	2506	2510	2515	rVB3	23350	30283	1.05%	0.220%
11	19.001	2654	2658	2664	rVB	130054	157705	5.49%	1.144%
12	19.260	2699	2702	2708	rVB2	36238	47345	1.65%	0.344%
13	19.513	2741	2745	2749	rBV	89039	111451	3.88%	0.809%
14	19.759	2782	2787	2791	rVB	110353	139779	4.87%	1.014%
15	20.082	2836	2842	2849	rVB	2036702	2870930	100.00%	20.830%
16	21.768	3122	3129	3135	rBV2	603981	1049210	36.55%	7.613%
17	25.070	3680	3691	3702	rVB2	364182	1077986	37.55%	7.821%

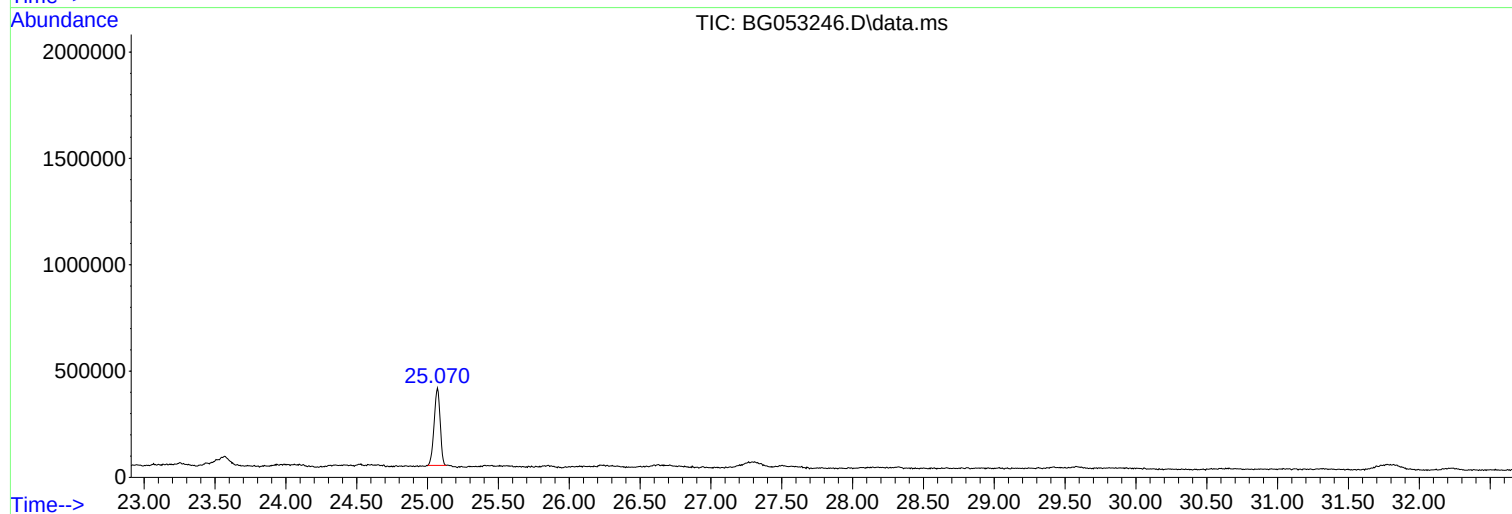
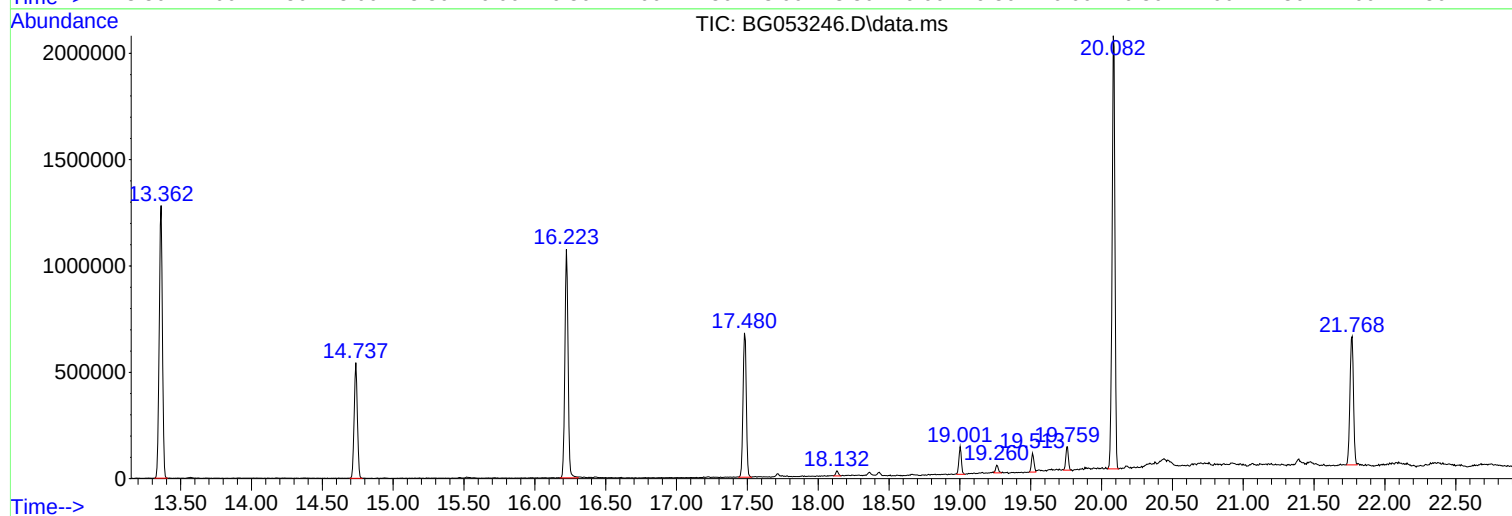
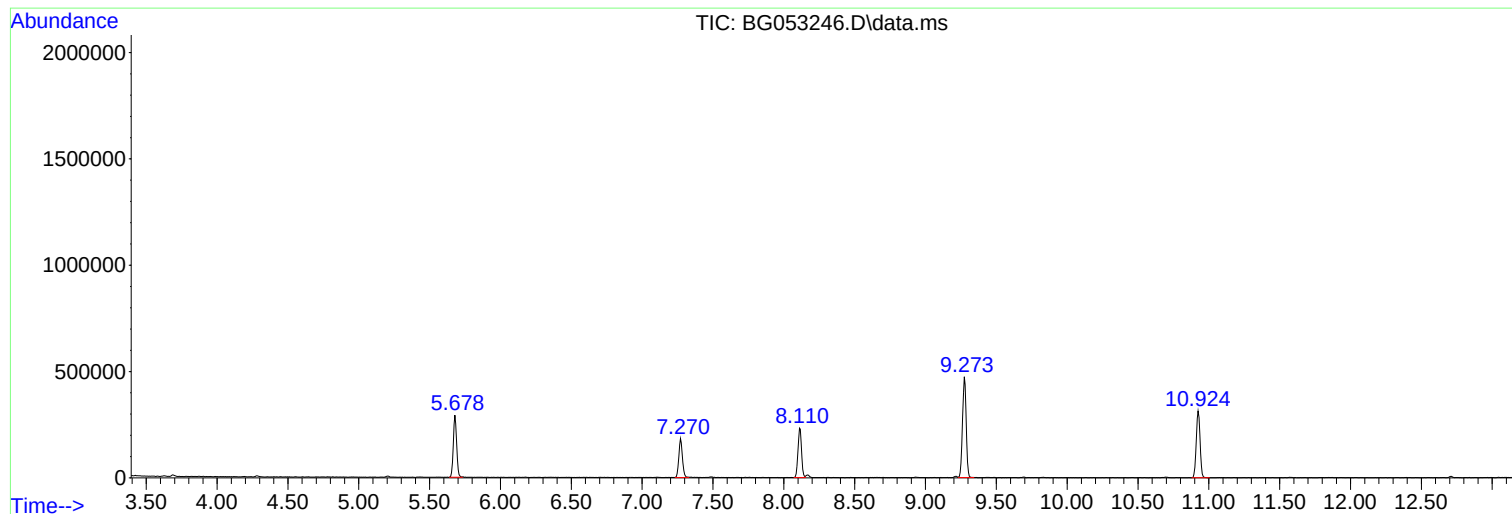
Sum of corrected areas: 13782702

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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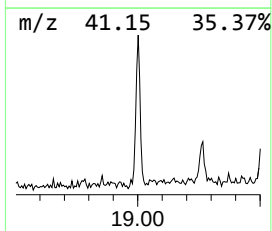
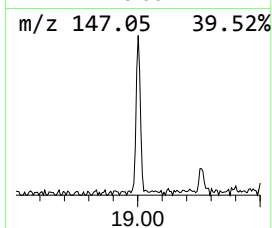
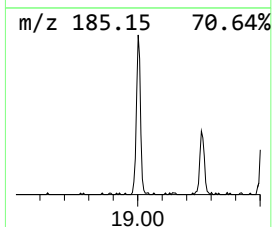
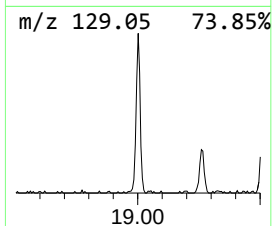
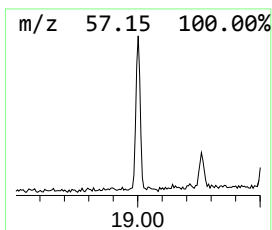
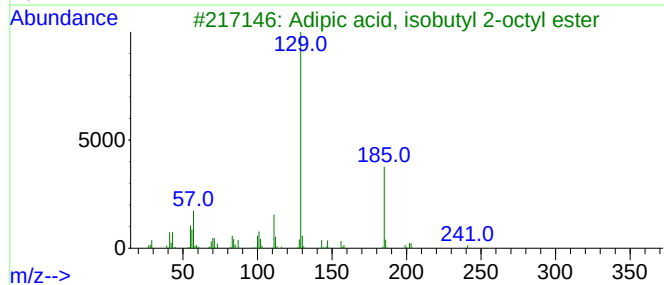
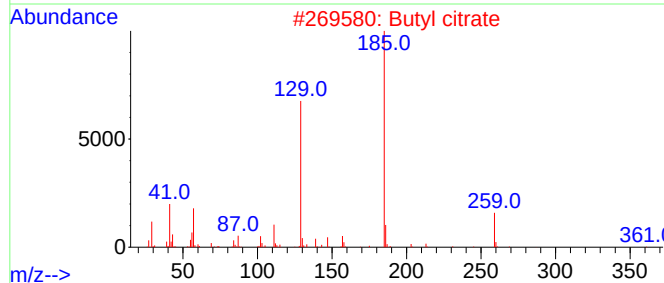
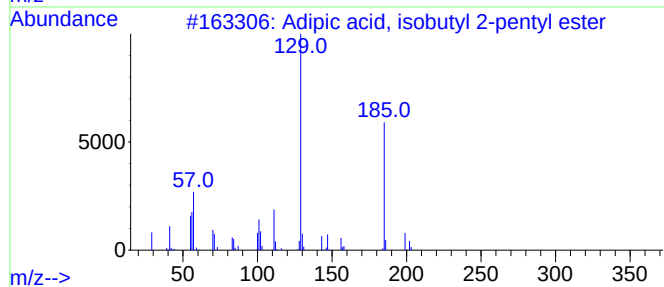
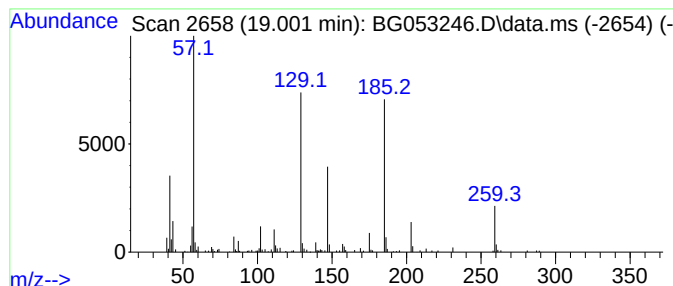
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown19.002 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.002	2.92 ng	157705	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	47
2			Butyl citrate	360	C18H32O7	000077-94-1	43
3			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	40
4			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	38
5			Adipic acid, cis-hex-3-enyl isob...	284	C16H28O4	1000353-97-1	38



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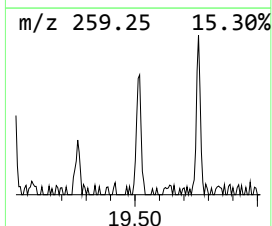
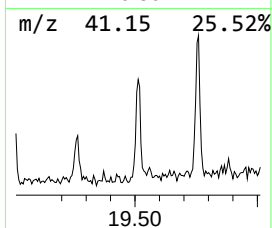
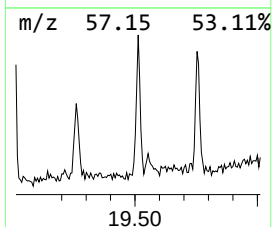
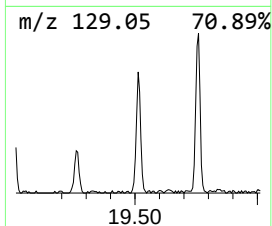
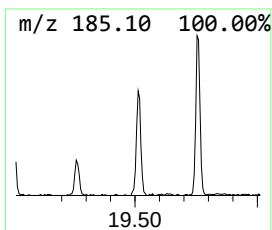
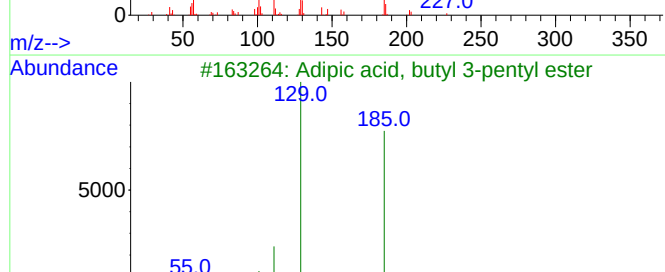
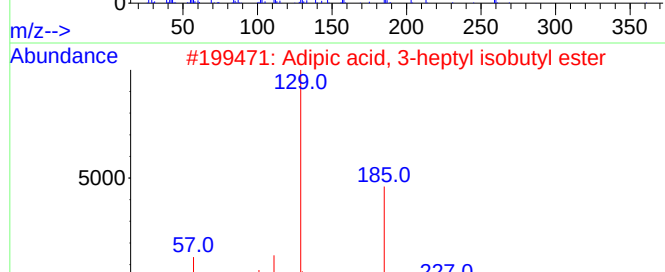
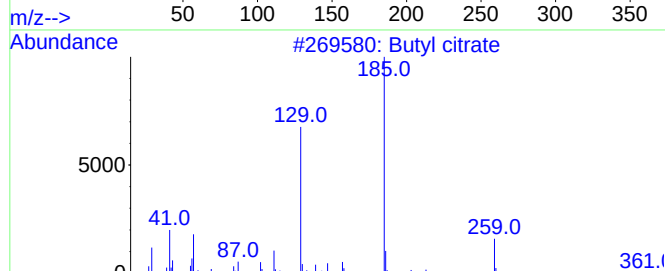
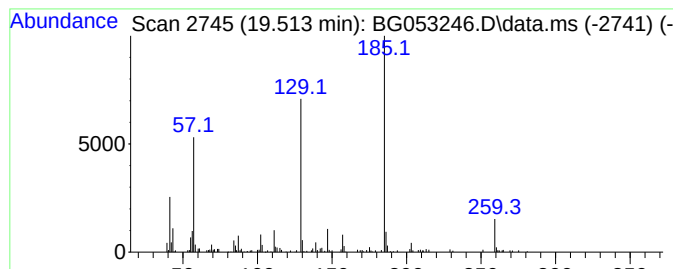
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Peak Number 2 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.512	2.06 ng	111451	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	90
2			Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	72
3			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	72
4			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	56
5			Adipic acid, butyl 3-heptyl ester	300	C17H32O4	1010353-64-9	50



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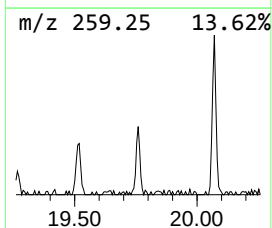
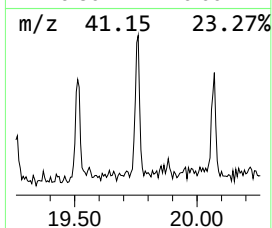
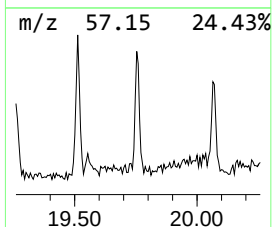
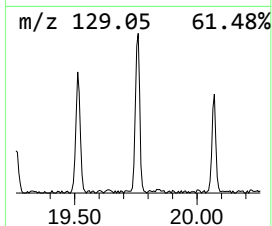
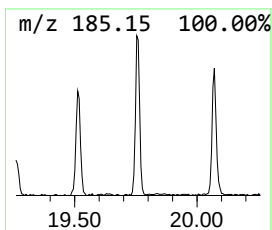
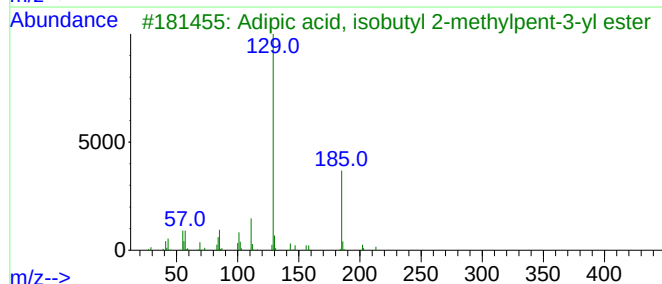
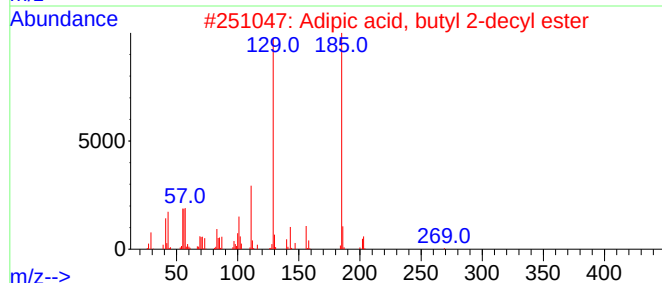
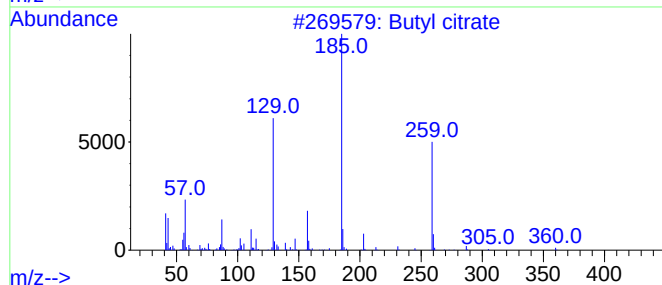
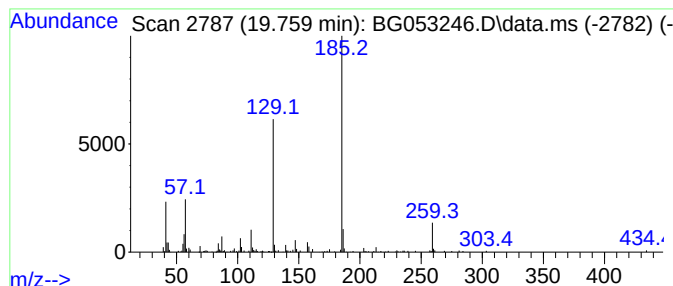
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Peak Number 3 Adipic acid, butyl 2-decyl ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.759	2.66 ng	139779	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	83
2			Adipic acid, butyl 2-decyl ester	342	C20H38O4	1000353-59-7	72
3			Adipic acid, isobutyl 2-methylpe...	286	C16H30O4	1000353-55-7	72
4			Adipic acid, butyl isobutyl ester	258	C14H26O4	1010324-09-3	64
5			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown19.002	19.002	2.9	ng	157705	4	17.480	1080650	20.0
Butyl citrate	19.512	2.1	ng	111451	4	17.480	1080650	20.0
Adipic acid, bu...	19.759	2.7	ng	139779	5	21.768	1049210	20.0