

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
 Data File : BM042526.D
 Acq On : 01 Nov 2023 00:24
 Operator : MA/JU
 Sample : 04938-07 10X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A-4(0-2)

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-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	307	311	316	rVB	14567	20915	1.28%	0.146%
2	5.463	381	387	398	rBV	127655	194183	11.91%	1.360%
3	5.875	451	457	465	rBV	63333	95985	5.89%	0.672%
4	7.087	658	663	673	rBV	127277	219127	13.44%	1.535%
5	7.922	798	805	814	rBV	300120	465536	28.55%	3.260%
6	8.193	846	851	861	rBV4	9621	21837	1.34%	0.153%
7	8.998	983	988	993	rBV	17197	27329	1.68%	0.191%
8	9.122	1000	1009	1015	rBV	71610	123793	7.59%	0.867%
9	9.522	1070	1077	1083	rBV2	14180	22520	1.38%	0.158%
10	9.581	1083	1087	1094	rVB	28917	44349	2.72%	0.311%
11	10.110	1172	1177	1182	rBV	14372	22285	1.37%	0.156%
12	10.622	1258	1264	1271	rBV3	18410	36117	2.21%	0.253%
13	10.739	1278	1284	1290	rBV	350874	577067	35.39%	4.042%
14	10.792	1290	1293	1301	rVB2	16537	25538	1.57%	0.179%
15	12.575	1587	1596	1609	rBV2	24060	77950	4.78%	0.546%
16	13.192	1696	1701	1708	rVB	149810	209916	12.87%	1.470%
17	13.298	1715	1719	1724	rBV2	27990	42720	2.62%	0.299%
18	14.039	1839	1845	1852	rBV	125079	181131	11.11%	1.269%
19	14.492	1917	1922	1929	rBV	23321	52705	3.23%	0.369%
20	14.569	1929	1935	1942	rVV	485613	723637	44.38%	5.068%
21	14.633	1942	1946	1954	rVB	32501	47212	2.90%	0.331%
22	14.969	1995	2003	2008	rBV3	12204	22630	1.39%	0.158%
23	15.310	2056	2061	2065	rBV	128651	172053	10.55%	1.205%
24	15.622	2108	2114	2118	rBV	25741	39871	2.45%	0.279%
25	16.063	2182	2189	2199	rBV	131142	212915	13.06%	1.491%
26	16.280	2222	2226	2238	rVB	49024	87049	5.34%	0.610%
27	16.680	2286	2294	2299	rBV8	19613	34066	2.09%	0.239%
28	16.986	2341	2346	2349	rBV	13383	22143	1.36%	0.155%
29	17.145	2368	2373	2376	rBV	19032	28727	1.76%	0.201%
30	17.321	2397	2403	2407	rBV	573918	842123	51.64%	5.898%
31	17.368	2407	2411	2418	rVV	410443	574314	35.22%	4.022%
32	17.457	2419	2426	2432	rVV	81394	130718	8.02%	0.915%
33	17.533	2435	2439	2444	rVB4	18069	31999	1.96%	0.224%
34	17.586	2444	2448	2452	rBV6	9955	17691	1.08%	0.124%
35	17.751	2467	2476	2481	rBV	48756	94150	5.77%	0.659%
36	17.810	2482	2486	2491	rBV	40757	62064	3.81%	0.435%

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37	18.051	2523	2527	2531	rBV6	20117	35357	2.17%	0.248%
38	18.180	2543	2549	2557	rBV2	534805	821153	50.36%	5.751%
39	18.245	2557	2560	2567	rVB2	32581	65363	4.01%	0.458%
40	18.392	2581	2585	2589	rBV2	58634	92358	5.66%	0.647%
41	18.757	2644	2647	2652	rVB2	50077	64852	3.98%	0.454%
42	19.033	2691	2694	2699	rBV3	46821	60728	3.72%	0.425%
43	19.380	2748	2753	2759	rVB	947771	1213379	74.41%	8.498%
44	19.451	2759	2765	2775	rBV5	287721	710293	43.56%	4.975%
45	19.704	2805	2808	2811	rBV2	110217	171866	10.54%	1.204%
46	19.745	2811	2815	2823	rVB	775719	1037417	63.62%	7.266%
47	19.933	2844	2847	2854	rVB	262451	366177	22.46%	2.565%
48	21.503	3108	3114	3118	rBV2	894259	1630689	100.00%	11.421%
49	21.545	3118	3121	3127	rVB	360267	451036	27.66%	3.159%
50	23.180	3395	3399	3404	rBV	294031	579347	35.53%	4.058%
51	23.815	3503	3507	3513	rBV	274489	526870	32.31%	3.690%
52	23.927	3521	3526	3531	rVB	477105	847162	51.95%	5.933%

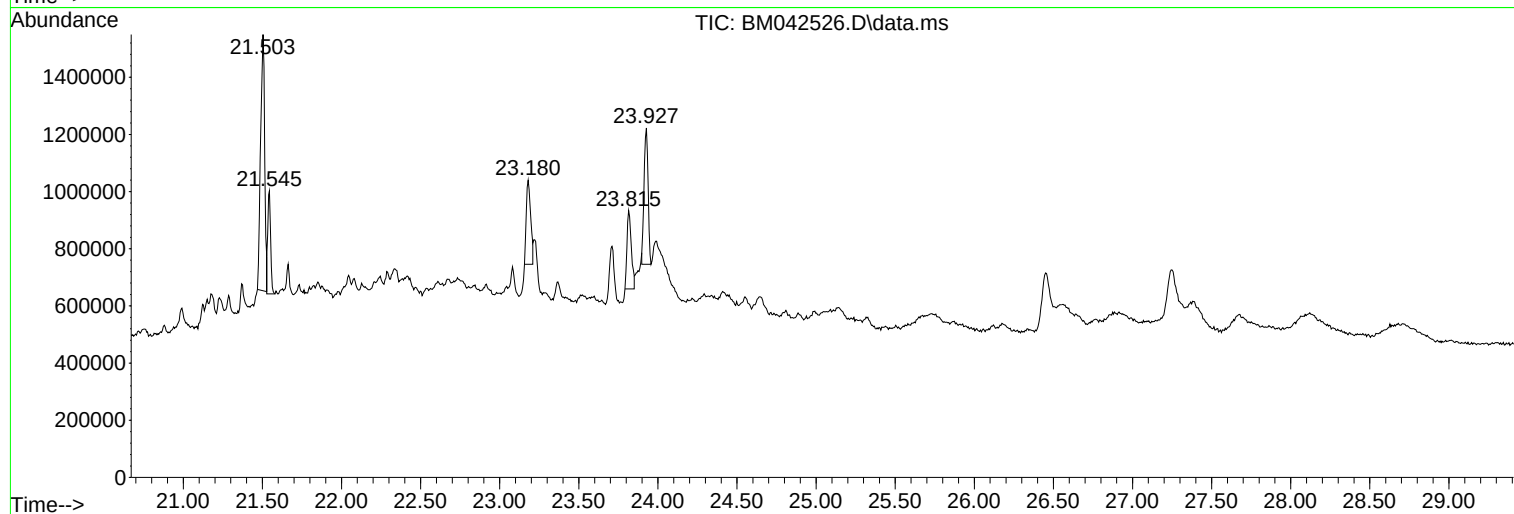
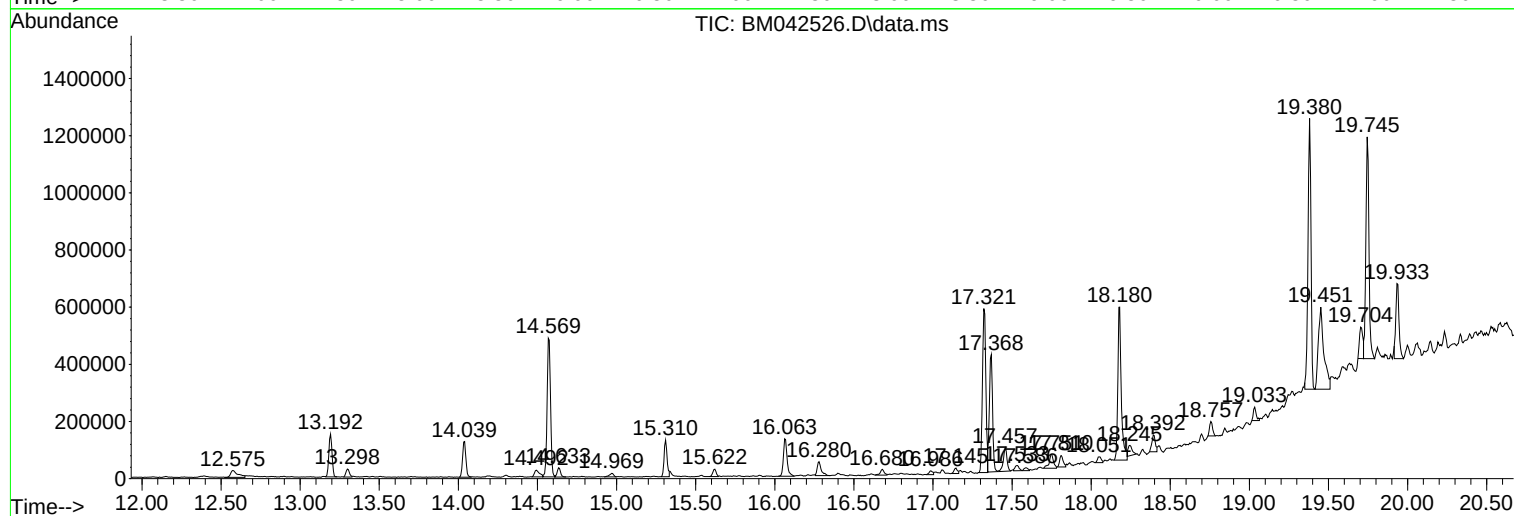
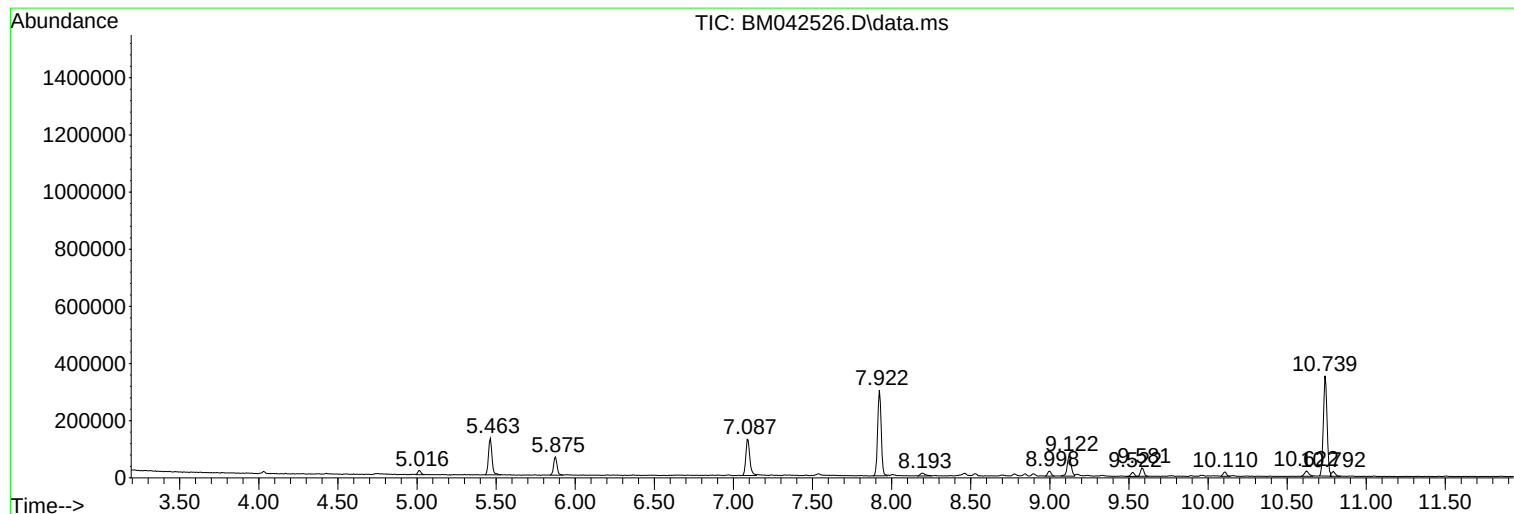
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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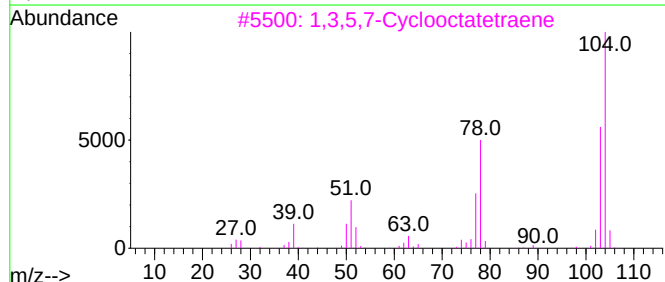
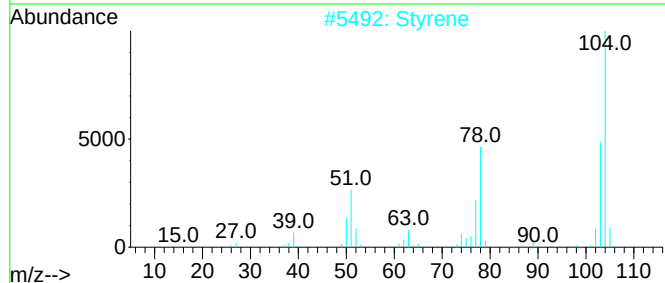
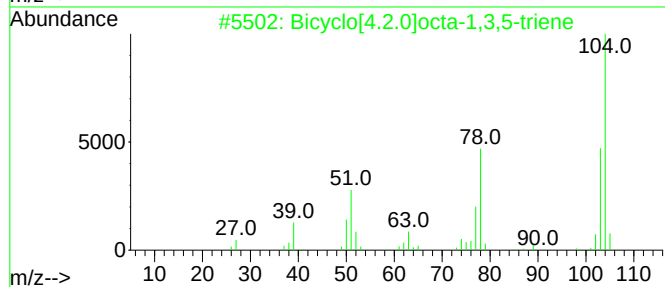
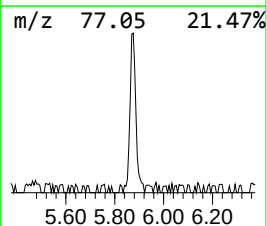
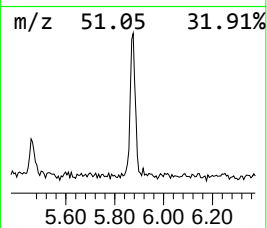
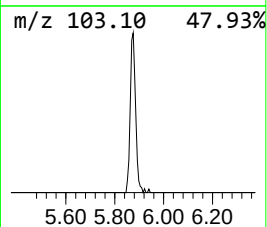
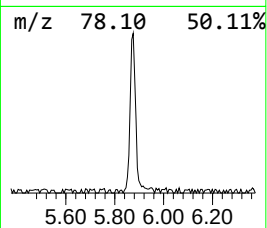
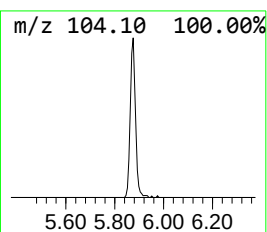
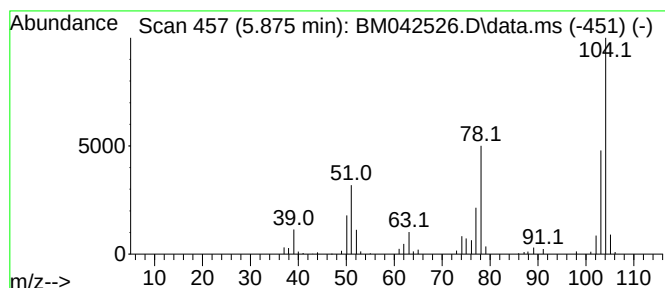
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	4.12 ng	95985	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
2			Styrene	104	C8H8	000100-42-5	96
3			1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	95
4			Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	64
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	58



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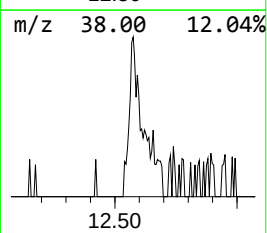
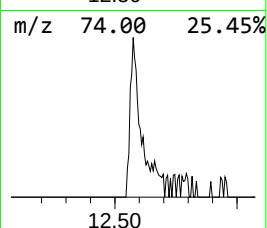
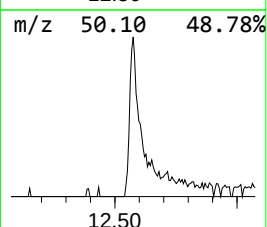
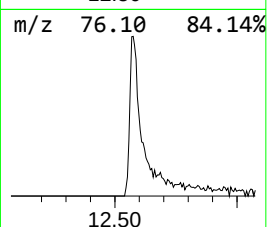
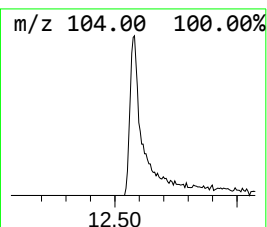
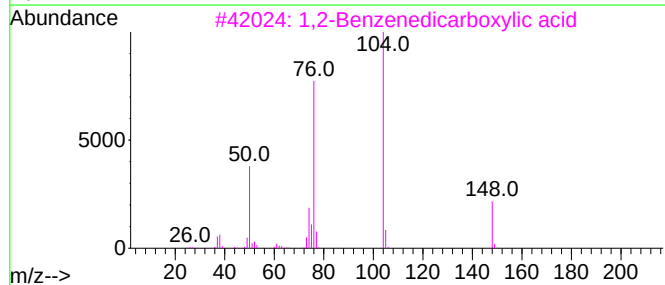
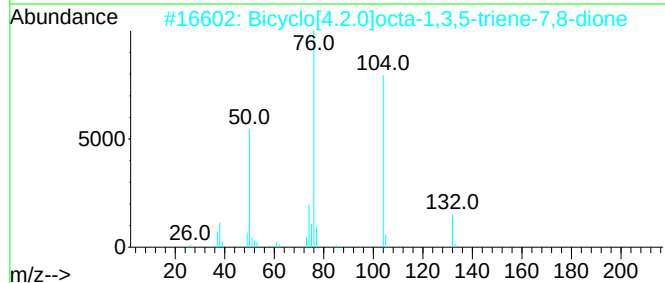
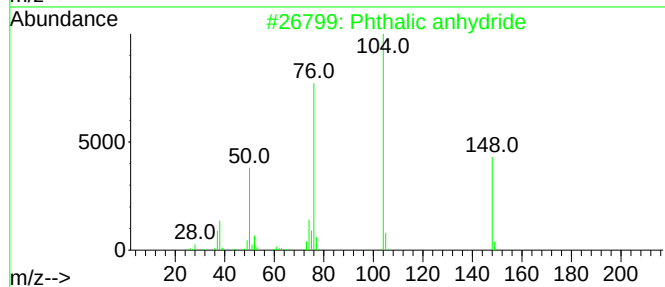
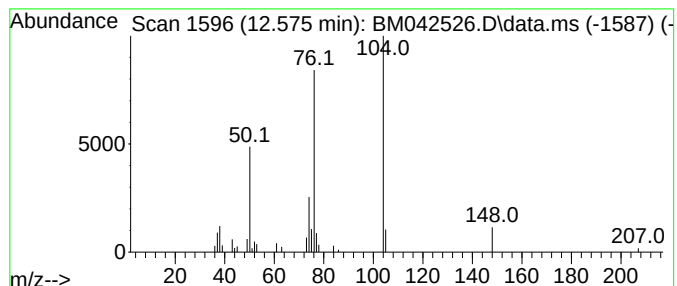
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phthalic anhydride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	2.70 ng	77950	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	91
2			Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	90
3			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
4			Indan-1,2,3-trione	160	C9H4O3	000938-24-9	90
5			[2,2'-Bi-1H-indene]-1,1'-dione, ...	358	C18H14O8	005950-69-6	90



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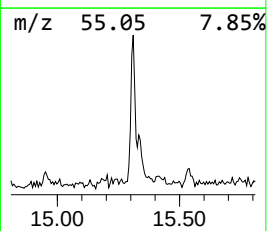
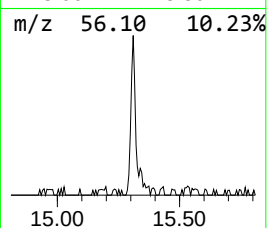
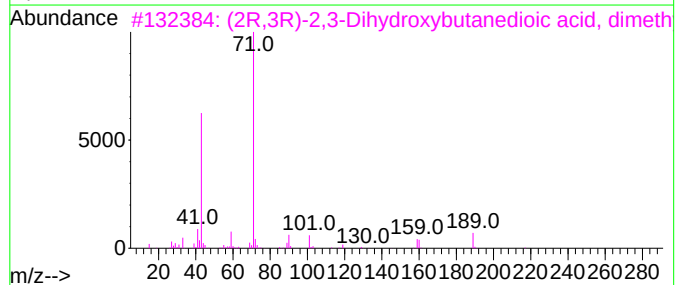
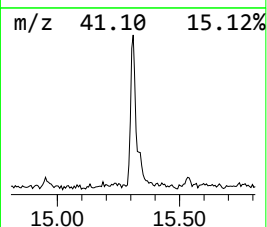
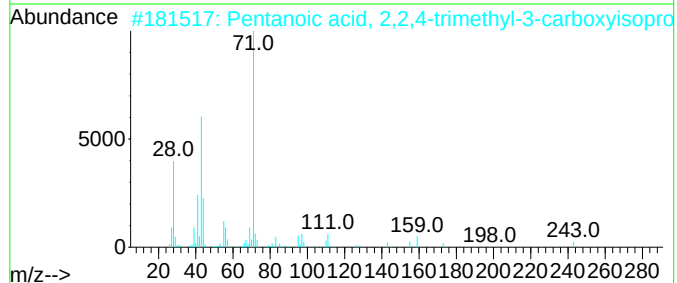
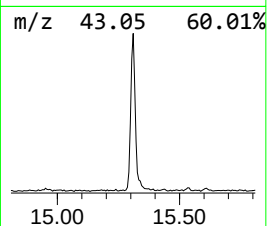
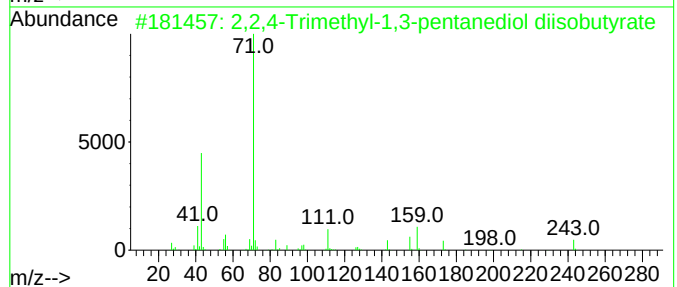
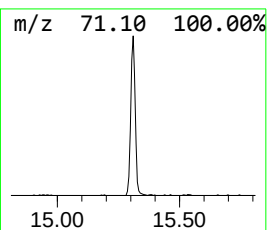
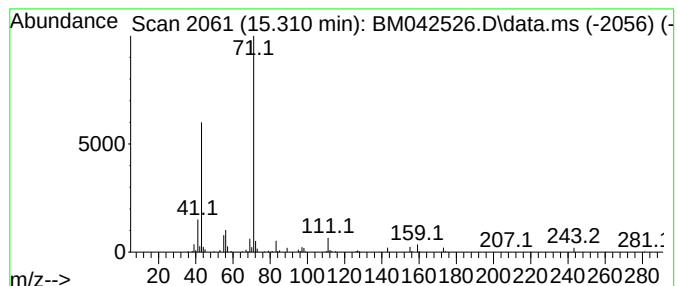
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	4.76 ng	172053	Acenaphthene-d10	14.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83		
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64		
3	(2R,3R)-2,3-Dihydroxybutanedioic...	248	C10H16O7	1000462-99-8	59		
4	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50		
5	Succinic acid, 2,2-dichloroethyl...	298	C11H16Cl2O5	1000390-71-6	45		



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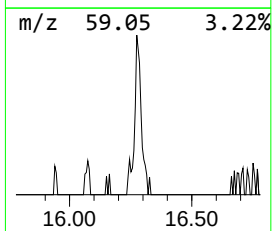
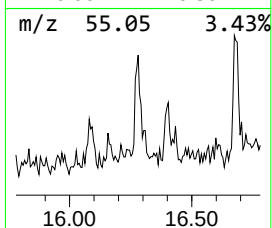
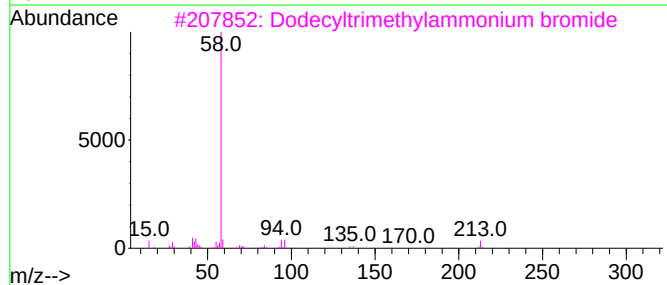
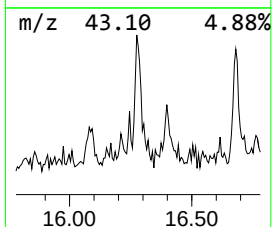
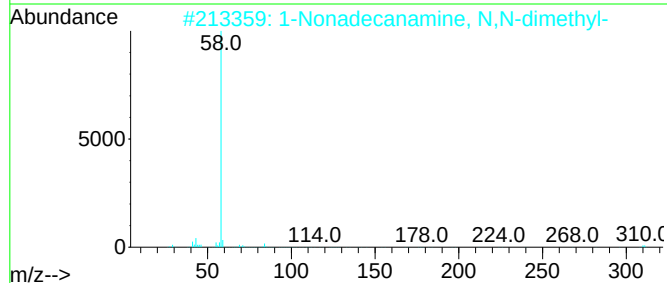
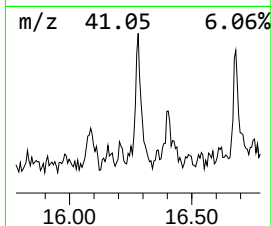
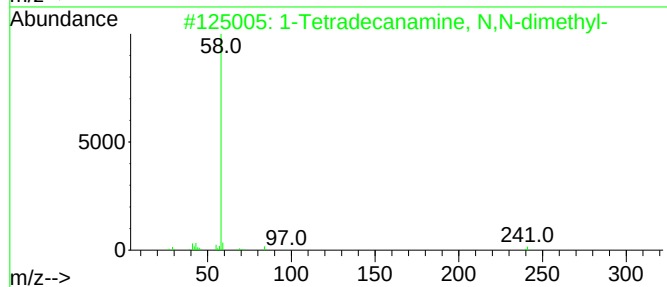
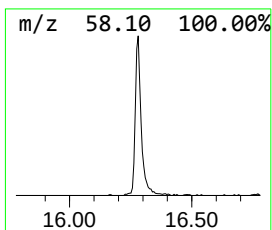
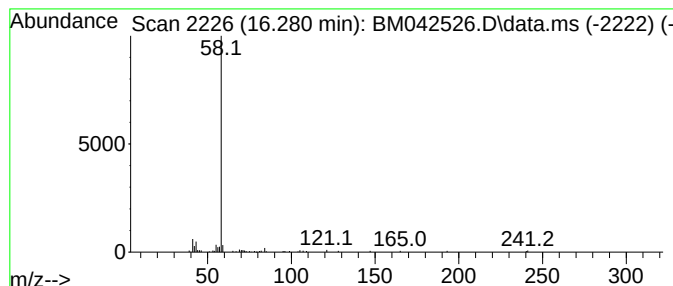
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Tetradecanamine, N,N-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	2.07 ng	87049	Phenanthrene-d10	17.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	78
2			1-Nonadecanamine, N,N-dimethyl-	311	C21H45N	049859-87-2	72
3			Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	72
4			Dimantine	297	C20H43N	000124-28-7	72
5			Dimethyl palmitamine	269	C18H39N	000112-69-6	72



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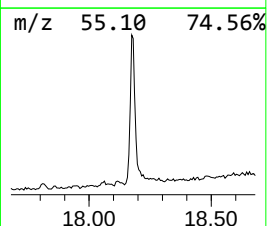
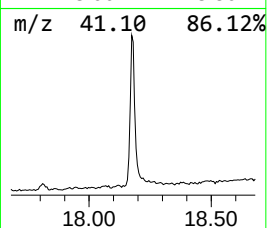
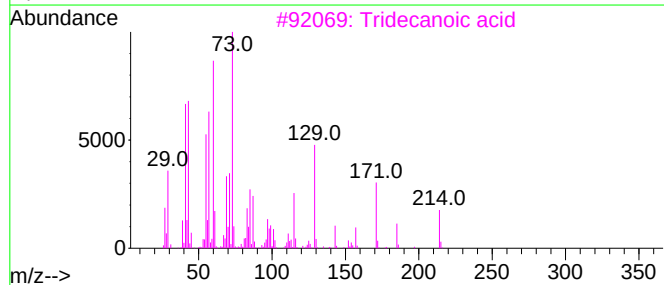
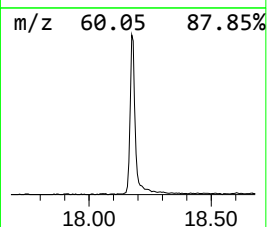
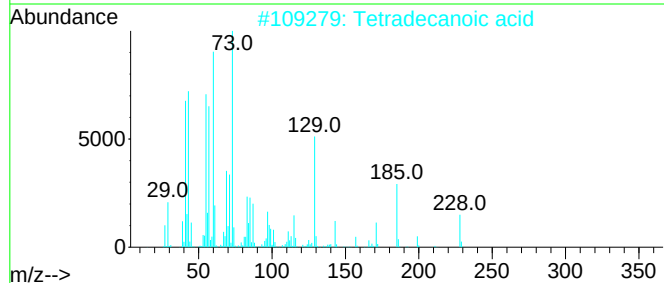
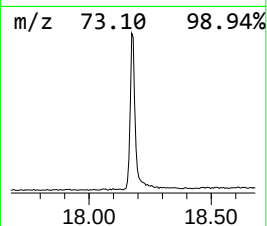
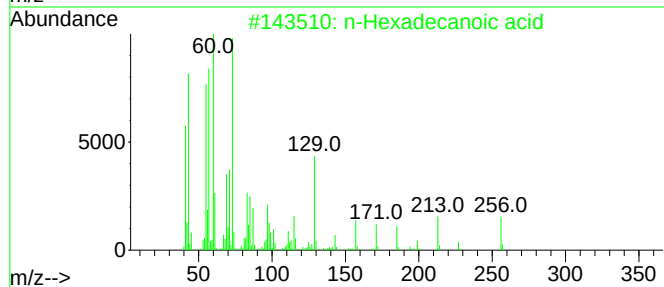
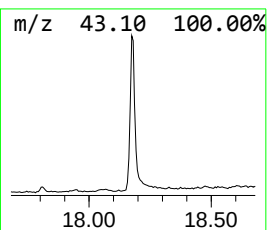
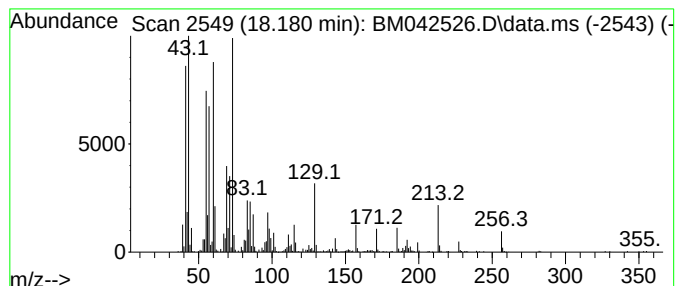
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.180	19.50 ng	821153	Phenanthrene-d10	17.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042526.D
Acq On : 01 Nov 2023 00:24
Operator : MA/JU
Sample : 04938-07 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

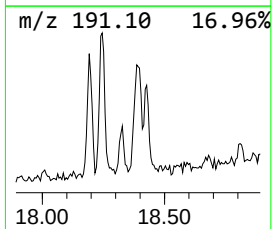
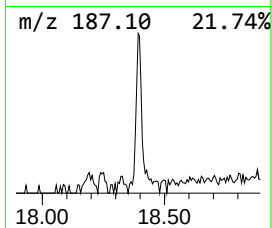
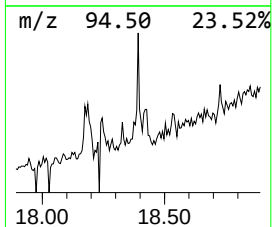
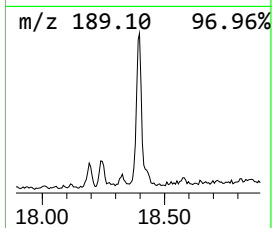
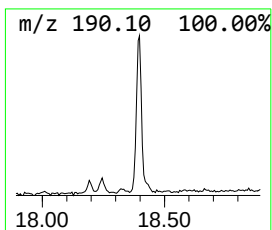
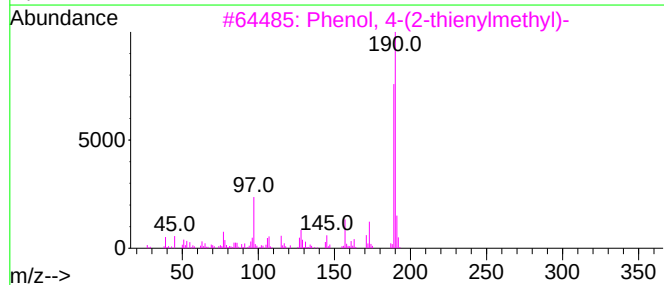
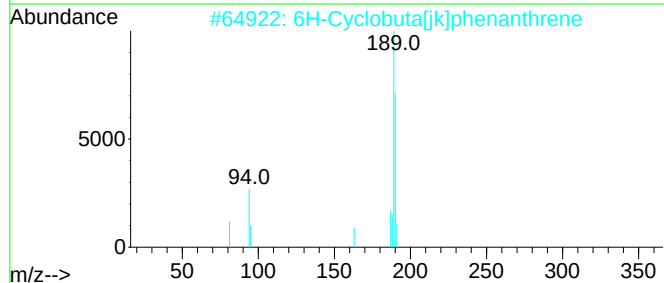
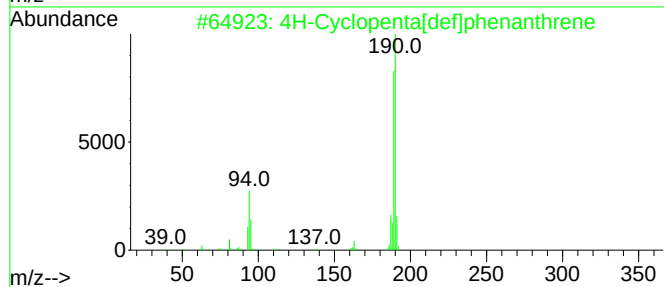
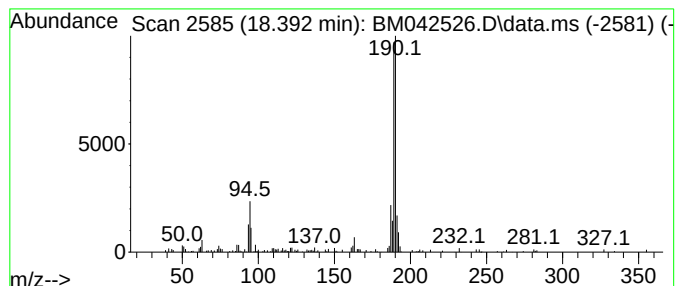
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.392	2.19 ng	92358	Phenanthrene-d10	17.321	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	95
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10O5	091680-55-6	45
4	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	42
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042526.D
Acq On : 01 Nov 2023 00:24
Operator : MA/JU
Sample : 04938-07 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-4(0-2)

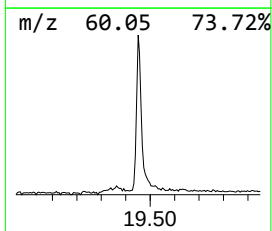
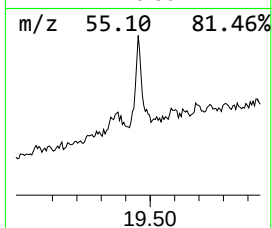
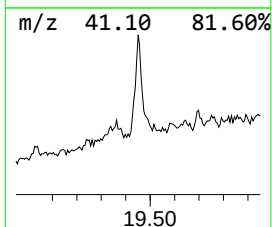
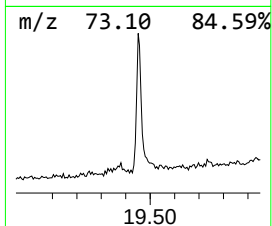
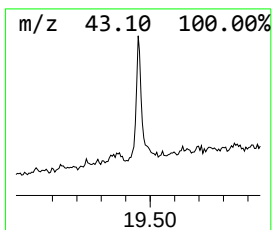
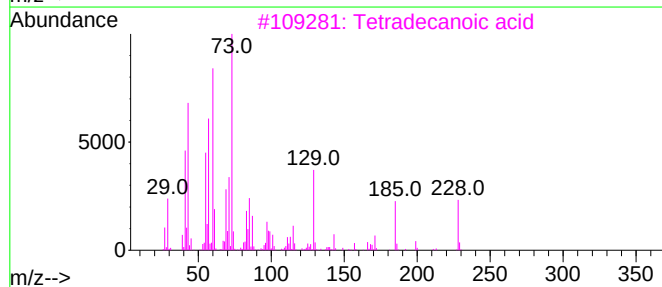
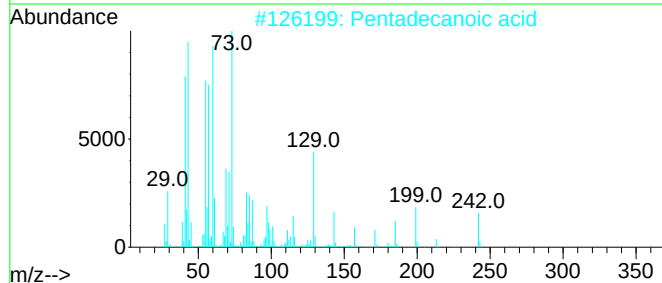
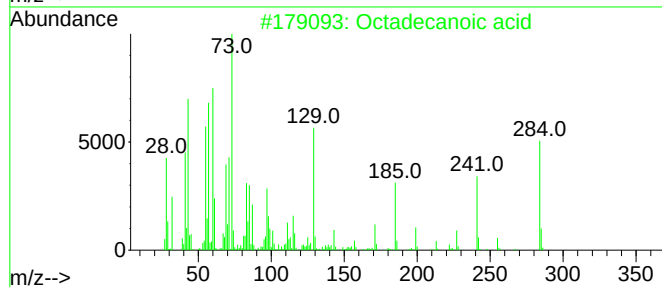
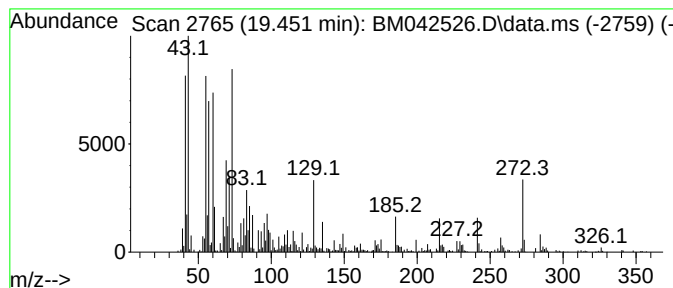
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	8.71 ng	710293	Chrysene-d12	21.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042526.D
Acq On : 01 Nov 2023 00:24
Operator : MA/JU
Sample : 04938-07 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-4(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bicyclo[4.2.0]o...	5.875	4.1	ng	95985	1	7.922	465536	20.0
Phthalic anhydride	12.575	2.7	ng	77950	2	10.740	577067	20.0
2,2,4-Trimethyl...	15.310	4.8	ng	172053	3	14.569	723637	20.0
1-Tetradecanami...	16.280	2.1	ng	87049	4	17.321	842123	20.0
n-Hexadecanoic ...	18.180	19.5	ng	821153	4	17.321	842123	20.0
4H-Cyclopenta[d...	18.392	2.2	ng	92358	4	17.321	842123	20.0
Octadecanoic acid	19.451	8.7	ng	710293	5	21.503	1630690	20.0