

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
 Data File : BP008105.D
 Acq On : 23 Nov 2021 20:10
 Operator : CG/JU
 Sample : M4796-01 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 EO-03-111921

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_P\Methods\8270E-BP111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	28	rVB	102436	188344	3.24%	0.408%
2	5.411	406	412	423	rVB	462499	709167	12.21%	1.535%
3	7.005	674	683	697	rBV	460785	780234	13.44%	1.689%
4	7.822	815	822	830	rVB	564784	894633	15.41%	1.937%
5	8.981	1013	1019	1026	rBV	293126	480085	8.27%	1.039%
6	10.622	1288	1298	1304	rBV	733680	1299481	22.38%	2.813%
7	12.057	1536	1542	1547	rBV	35981	59841	1.03%	0.130%
8	13.087	1710	1717	1726	rBV	803239	1158464	19.95%	2.508%
9	13.298	1748	1753	1760	rVB	66256	97045	1.67%	0.210%
10	14.187	1898	1904	1910	rBV	269757	417174	7.18%	0.903%
11	14.375	1931	1936	1942	rVB	93340	120342	2.07%	0.261%
12	14.463	1945	1951	1958	rVV	1178595	1765189	30.40%	3.822%
13	14.869	2016	2020	2027	rVB3	45824	77532	1.34%	0.168%
14	15.328	2094	2098	2106	rVB2	118367	172065	2.96%	0.373%
15	15.516	2126	2130	2143	rVB	90146	181997	3.13%	0.394%
16	15.739	2161	2168	2173	rBV4	48208	101684	1.75%	0.220%
17	15.816	2177	2181	2190	rVB5	25847	65175	1.12%	0.141%
18	15.963	2200	2206	2213	rVB	641360	963616	16.59%	2.086%
19	16.192	2241	2245	2249	rBV2	133249	203455	3.50%	0.440%
20	16.992	2377	2381	2385	rVV	109292	129296	2.23%	0.280%
21	17.045	2386	2390	2399	rVB2	86791	147799	2.55%	0.320%
22	17.228	2415	2421	2424	rBV	1492327	2170382	37.37%	4.699%
23	17.263	2424	2427	2434	rVB	624054	904205	15.57%	1.958%
24	17.357	2439	2443	2449	rVV	306215	426300	7.34%	0.923%
25	17.422	2449	2454	2460	rVV3	53471	98720	1.70%	0.214%
26	17.739	2504	2508	2511	rBV2	103774	141244	2.43%	0.306%
27	17.775	2511	2514	2518	rBV	119891	137872	2.37%	0.298%
28	17.904	2531	2536	2541	rBV	2158550	2506780	43.17%	5.427%
29	18.098	2564	2569	2570	rBV	132613	173534	2.99%	0.376%
30	18.122	2570	2573	2581	rVB2	260371	571846	9.85%	1.238%
31	18.222	2586	2590	2595	rVB	104325	135387	2.33%	0.293%
32	18.286	2596	2601	2604	rBV2	268370	446631	7.69%	0.967%
33	18.404	2618	2621	2625	rBV	96211	121082	2.09%	0.262%
34	18.580	2647	2651	2655	rVB	110686	143737	2.48%	0.311%
35	19.010	2716	2724	2727	rBV	4214764	5807155	100.00%	12.572%
36	19.039	2727	2729	2733	rVB2	3944888	4484235	77.22%	9.708%

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37	19.122	2740	2743	2747	rBV2	107355	155139	2.67%	0.336%
38	19.169	2747	2751	2756	rVB	823286	881377	15.18%	1.908%
39	19.239	2756	2763	2770	rBV	2046585	3067284	52.82%	6.641%
40	19.386	2786	2788	2792	rVB	156687	176534	3.04%	0.382%
41	19.563	2815	2818	2819	rBV	212851	225497	3.88%	0.488%
42	19.592	2819	2823	2831	rVB	1567119	2225465	38.32%	4.818%
43	19.792	2853	2857	2861	rVB	1341540	1589935	27.38%	3.442%
44	20.074	2903	2905	2912	rVB2	259037	338818	5.83%	0.734%
45	20.180	2919	2923	2926	rBV	226661	276795	4.77%	0.599%
46	20.233	2930	2932	2936	rVB	246156	292255	5.03%	0.633%
47	21.321	3111	3117	3121	rBV2	1811700	3423362	58.95%	7.411%
48	21.363	3121	3124	3134	rVB	827227	1153612	19.87%	2.498%
49	22.998	3398	3402	3407	rBV	635063	1280713	22.05%	2.773%
50	23.621	3504	3508	3517	rVB	657095	1265220	21.79%	2.739%
51	23.727	3521	3526	3532	rVV2	795521	1556680	26.81%	3.370%

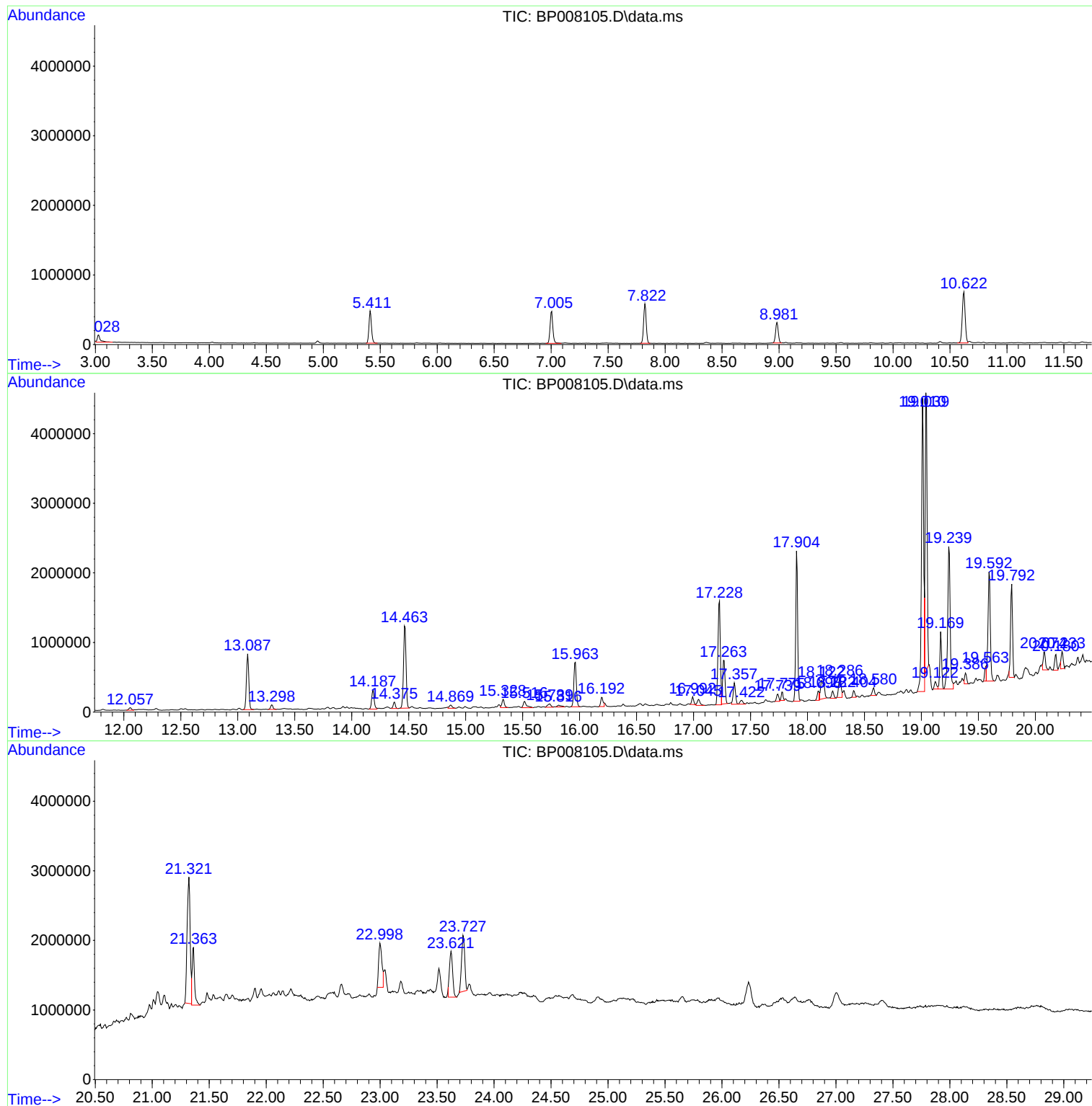
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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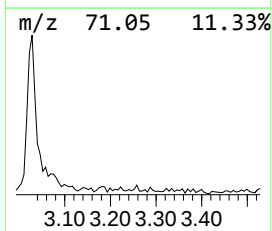
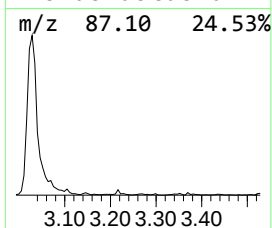
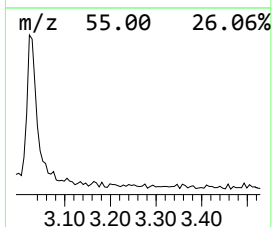
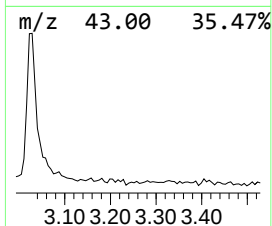
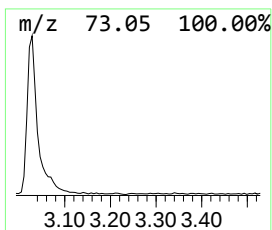
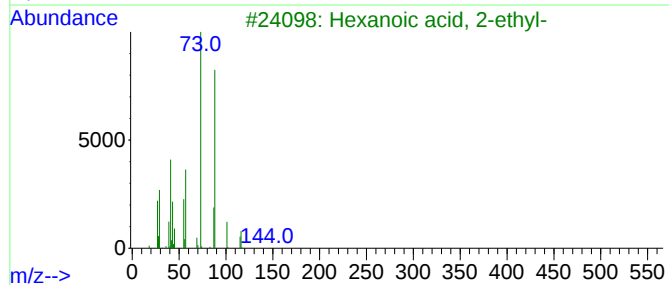
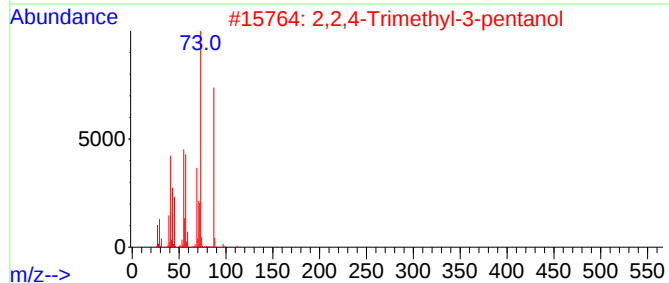
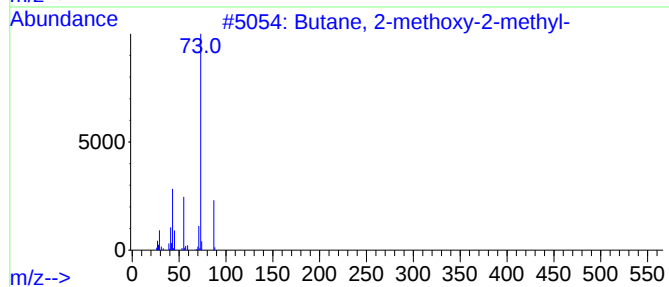
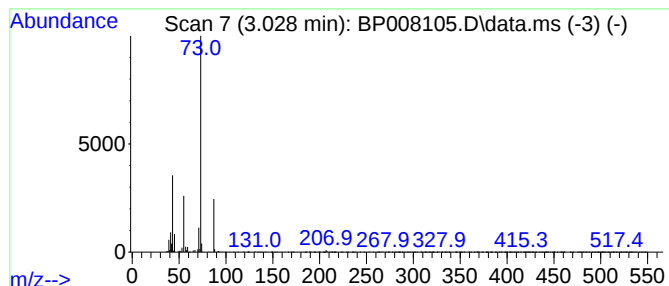
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	4.21 ng	188344	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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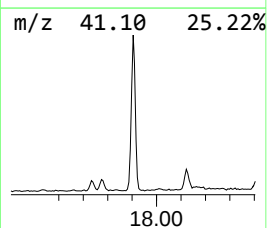
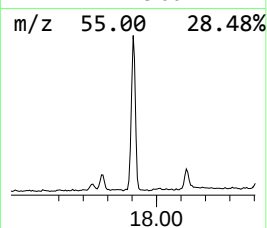
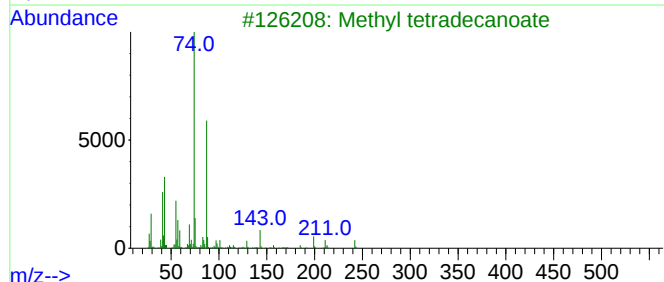
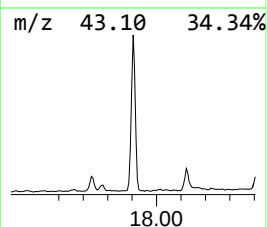
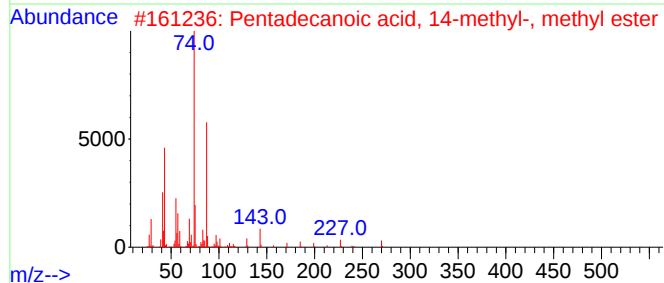
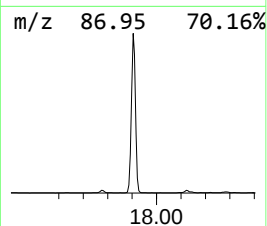
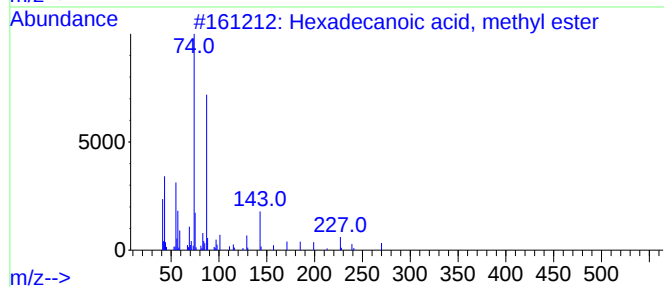
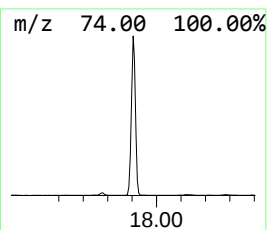
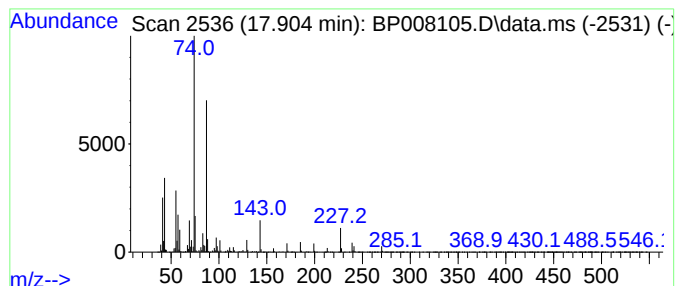
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.904	23.10 ng	2506780	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



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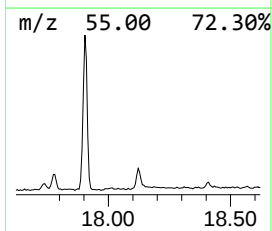
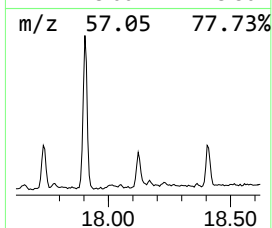
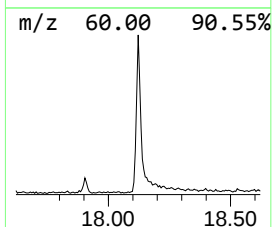
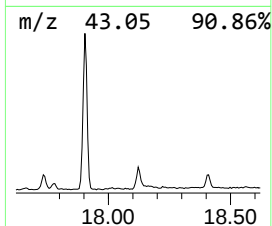
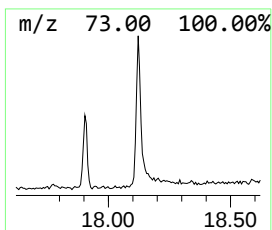
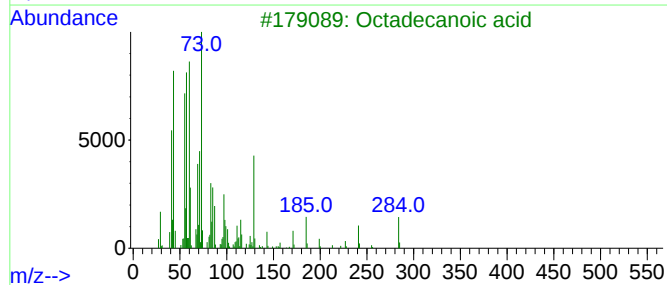
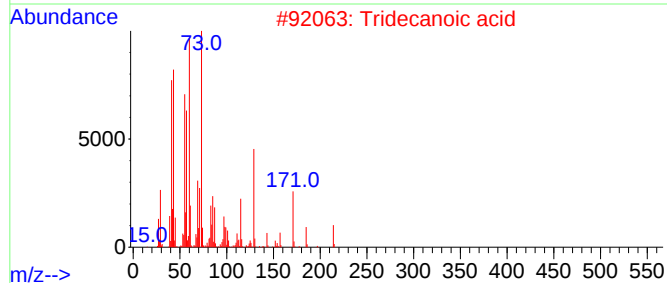
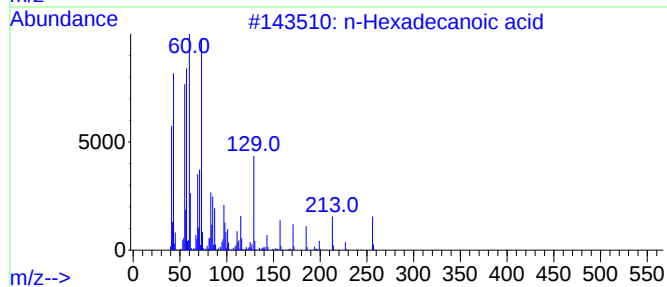
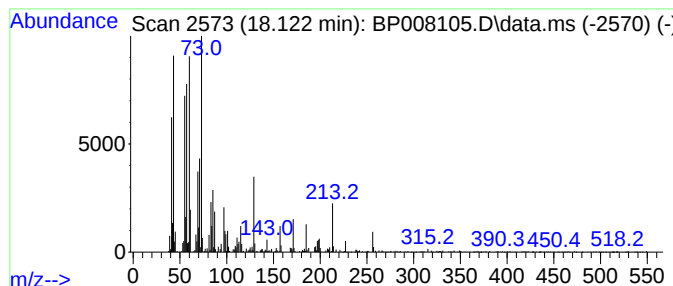
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	5.27 ng	571846	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			Dodecanoic acid	200	C12H24O2	000143-07-7	83



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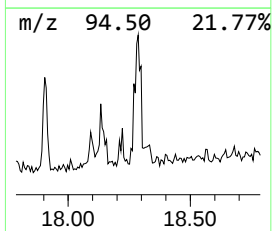
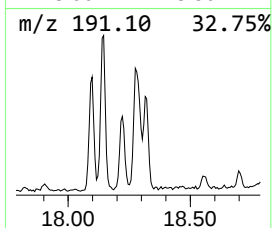
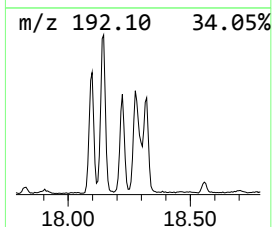
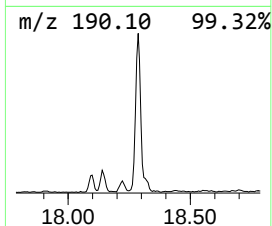
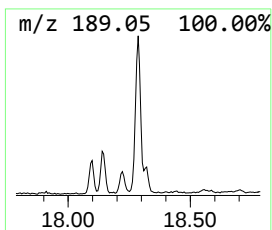
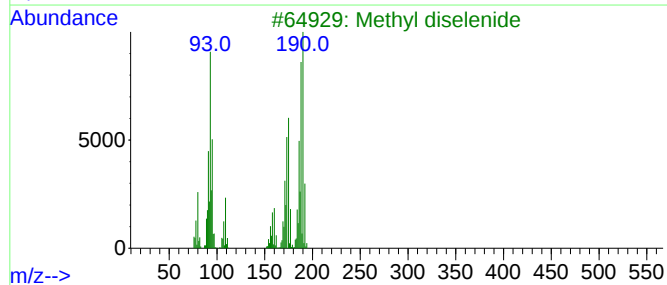
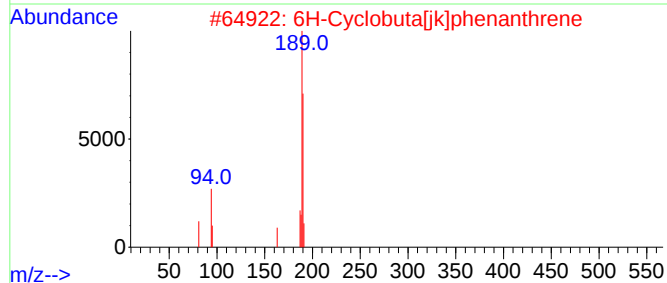
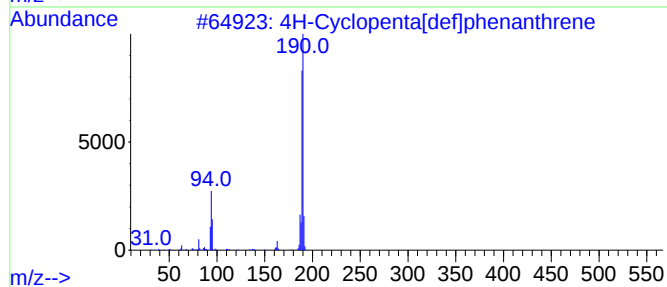
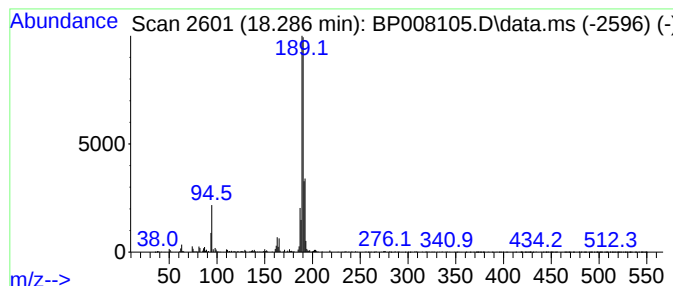
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	4.12 ng	446631	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			Methyl diselenide	190	C2H6Se2	007101-31-7	49
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5			Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	38



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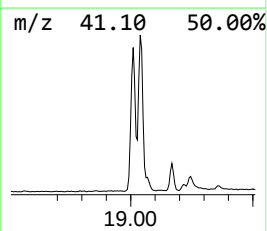
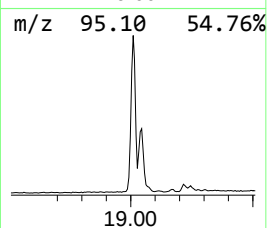
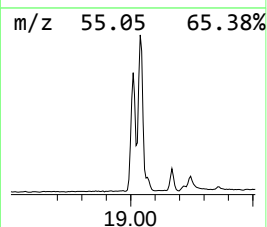
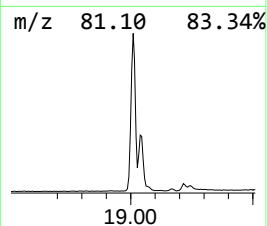
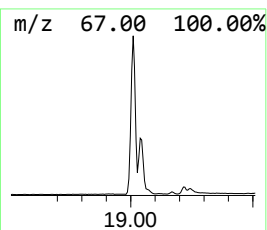
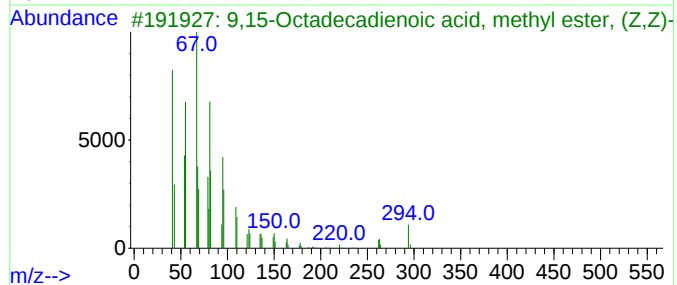
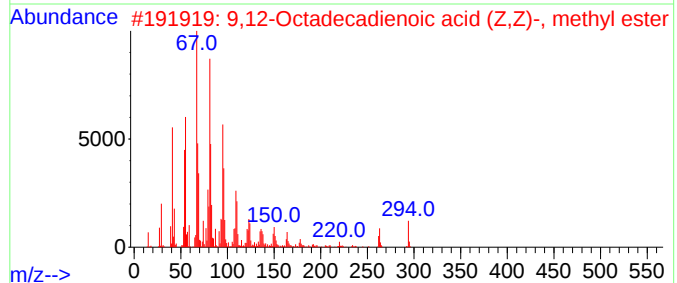
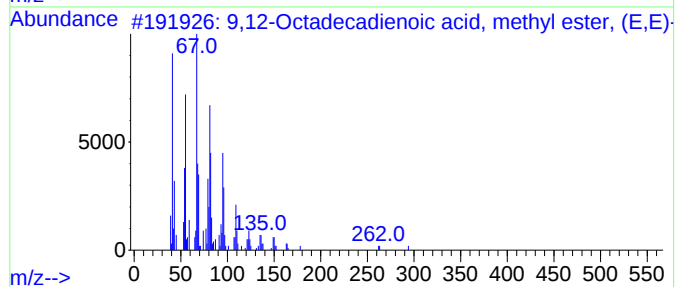
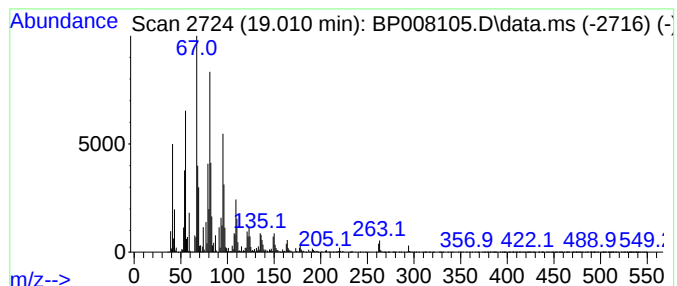
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.010	53.51 ng	5807160	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008105.D
Acq On : 23 Nov 2021 20:10
Operator : CG/JU
Sample : M4796-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

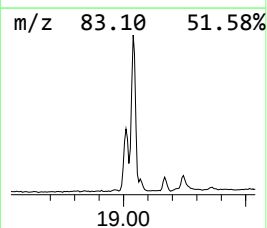
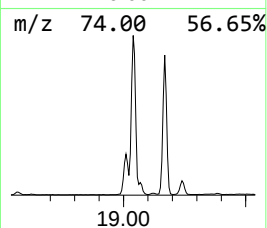
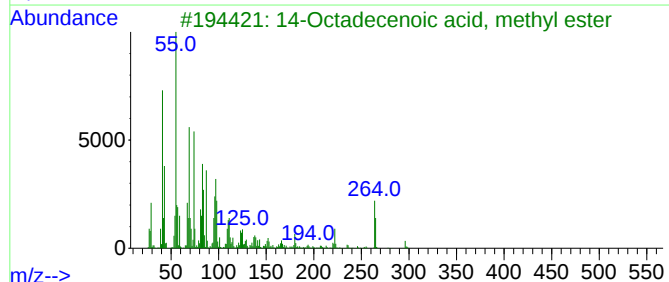
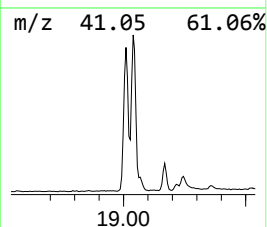
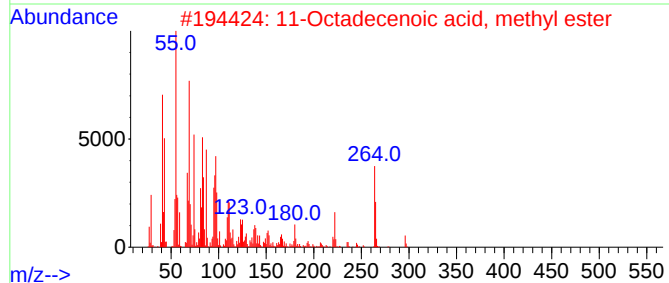
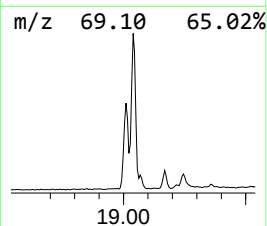
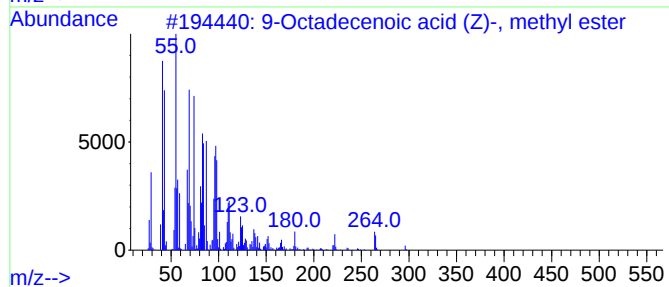
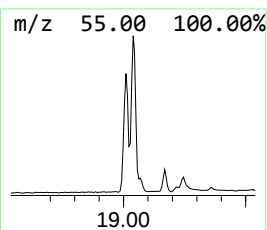
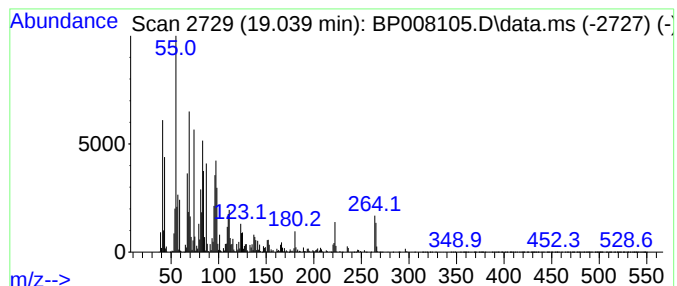
Instrument :
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ClientSampleId :
EO-03-111921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.039	41.32 ng	4484240	Phenanthrene-d10	17.227	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008105.D
Acq On : 23 Nov 2021 20:10
Operator : CG/JU
Sample : M4796-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EO-03-111921

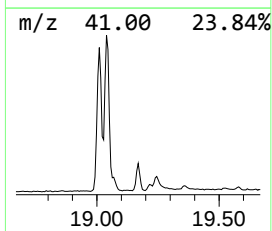
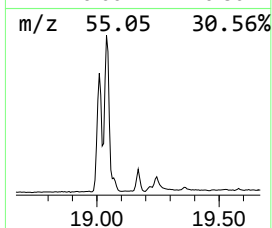
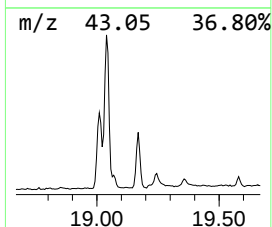
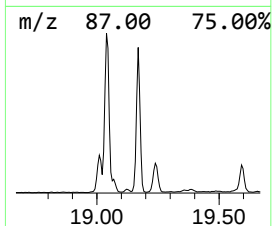
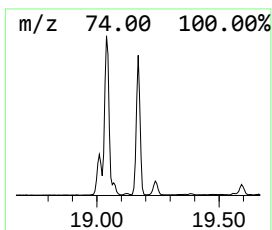
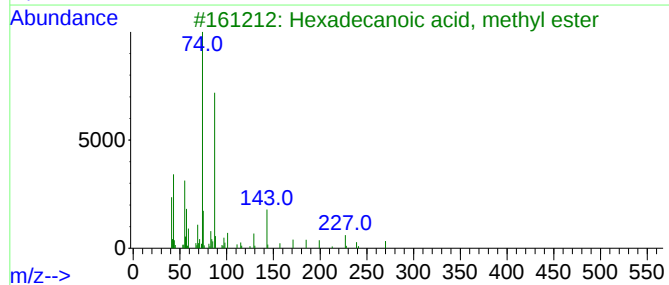
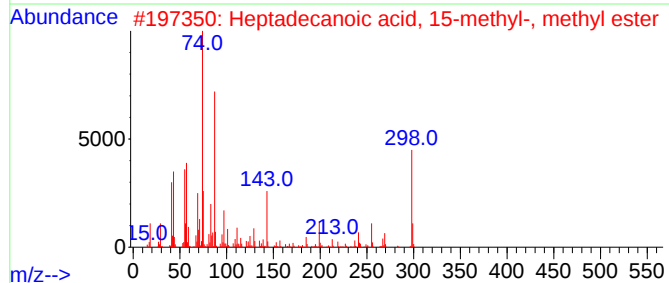
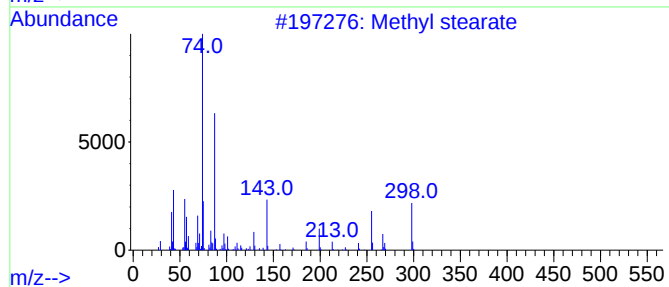
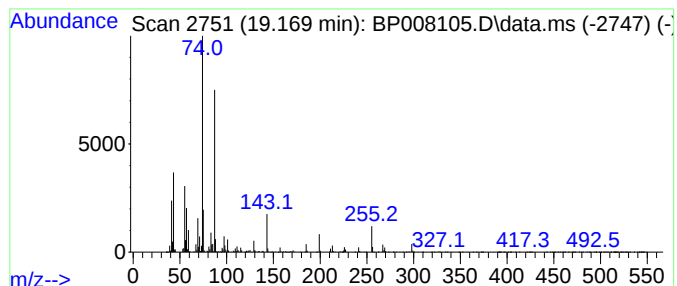
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.169	8.12 ng	881377	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	94
2			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	94
3			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008105.D
Acq On : 23 Nov 2021 20:10
Operator : CG/JU
Sample : M4796-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EO-03-111921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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
Butane, 2-metho...	3.028	4.2	ng	188344	1	7.822	894633	20.0
Hexadecanoic ac...	17.904	23.1	ng	2506780	4	17.227	2170380	20.0
n-Hexadecanoic ...	18.122	5.3	ng	571846	4	17.227	2170380	20.0
4H-Cyclopenta[d...	18.286	4.1	ng	446631	4	17.227	2170380	20.0
9,12-Octadecadi...	19.010	53.5	ng	5807160	4	17.227	2170380	20.0
9-Octadecenoic ...	19.039	41.3	ng	4484240	4	17.227	2170380	20.0
Methyl stearate	19.169	8.1	ng	881377	4	17.227	2170380	20.0