

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022924\
 Data File : BP019949.D
 Acq On : 29 Feb 2024 21:54
 Operator : MA/JU
 Sample : P1622-01 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 HD-02-022824

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-BP022624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	398	404	414	rBV	217410	371272	23.37%	2.257%
2	7.069	670	677	688	rBV	216700	392710	24.72%	2.387%
3	7.893	810	817	827	rVB	248339	405172	25.50%	2.463%
4	9.069	1009	1017	1031	rBV	141092	270771	17.04%	1.646%
5	10.699	1280	1294	1309	rBV	311941	594288	37.40%	3.612%
6	12.581	1608	1614	1620	rBV2	11722	21753	1.37%	0.132%
7	13.163	1705	1713	1724	rBV	443450	683317	43.00%	4.153%
8	13.363	1743	1747	1755	rVB3	14552	25765	1.62%	0.157%
9	13.863	1827	1832	1837	rBV2	17715	32831	2.07%	0.200%
10	13.922	1837	1842	1850	rVB5	11677	24248	1.53%	0.147%
11	14.269	1896	1901	1907	rVB	18854	30849	1.94%	0.188%
12	14.440	1924	1930	1937	rBV2	26833	41490	2.61%	0.252%
13	14.540	1940	1947	1954	rVV	563829	868769	54.68%	5.281%
14	14.604	1954	1958	1965	rVB2	21508	36304	2.28%	0.221%
15	14.763	1978	1985	1990	rBV6	14146	33439	2.10%	0.203%
16	14.940	2012	2015	2023	rVB3	19395	33696	2.12%	0.205%
17	15.157	2049	2052	2058	rBV6	11715	22045	1.39%	0.134%
18	15.334	2076	2082	2085	rBV7	10830	21575	1.36%	0.131%
19	15.393	2085	2092	2097	rVV3	33201	60785	3.83%	0.369%
20	15.598	2122	2127	2131	rBV2	28604	42472	2.67%	0.258%
21	15.804	2158	2162	2166	rVB3	19656	23389	1.47%	0.142%
22	15.898	2173	2178	2184	rVB8	12737	27505	1.73%	0.167%
23	16.040	2196	2202	2210	rBV	433907	678541	42.70%	4.124%
24	16.263	2236	2240	2249	rVB4	45567	101125	6.36%	0.615%
25	16.657	2304	2307	2311	rVB3	14976	21150	1.33%	0.129%
26	16.751	2321	2323	2329	rVB6	15203	19781	1.24%	0.120%
27	17.063	2372	2376	2380	rVV3	38085	49115	3.09%	0.299%
28	17.116	2382	2385	2394	rVB2	34268	69189	4.35%	0.421%
29	17.304	2411	2417	2421	rBV	798024	1173447	73.85%	7.133%
30	17.345	2421	2424	2430	rVB	257309	369080	23.23%	2.243%
31	17.439	2436	2440	2445	rVB	91283	121249	7.63%	0.737%
32	17.810	2499	2503	2509	rBV3	35282	64517	4.06%	0.392%
33	17.981	2528	2532	2537	rVB	160057	196150	12.34%	1.192%
34	18.175	2561	2565	2566	rBV	84511	100811	6.34%	0.613%
35	18.198	2566	2569	2579	rVV2	219790	468863	29.51%	2.850%
36	18.298	2583	2586	2590	rVV	54654	75443	4.75%	0.459%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.363	2592	2597	2601	rVV2	145946	279747	17.61%	1.700%
38	18.398	2601	2603	2608	rVB	83493	99417	6.26%	0.604%
39	18.481	2614	2617	2621	rBV	44716	58487	3.68%	0.356%
40	19.086	2713	2720	2723	rBV3	569861	821070	51.67%	4.991%
41	19.122	2723	2726	2729	rVB2	429151	499513	31.44%	3.036%
42	19.251	2745	2748	2752	rVB	103920	120038	7.55%	0.730%
43	19.322	2755	2760	2766	rVB	665981	932899	58.71%	5.671%
44	19.675	2812	2820	2828	rBV	638831	1083680	68.20%	6.587%
45	19.875	2849	2854	2858	rBV	978120	1171383	73.72%	7.120%
46	20.628	2978	2982	2986	rBV	1121311	1277264	80.38%	7.764%
47	21.410	3109	3115	3119	rBV2	924269	1588948	100.00%	9.658%
48	23.845	3524	3529	3536	rVB	486728	946440	59.56%	5.753%

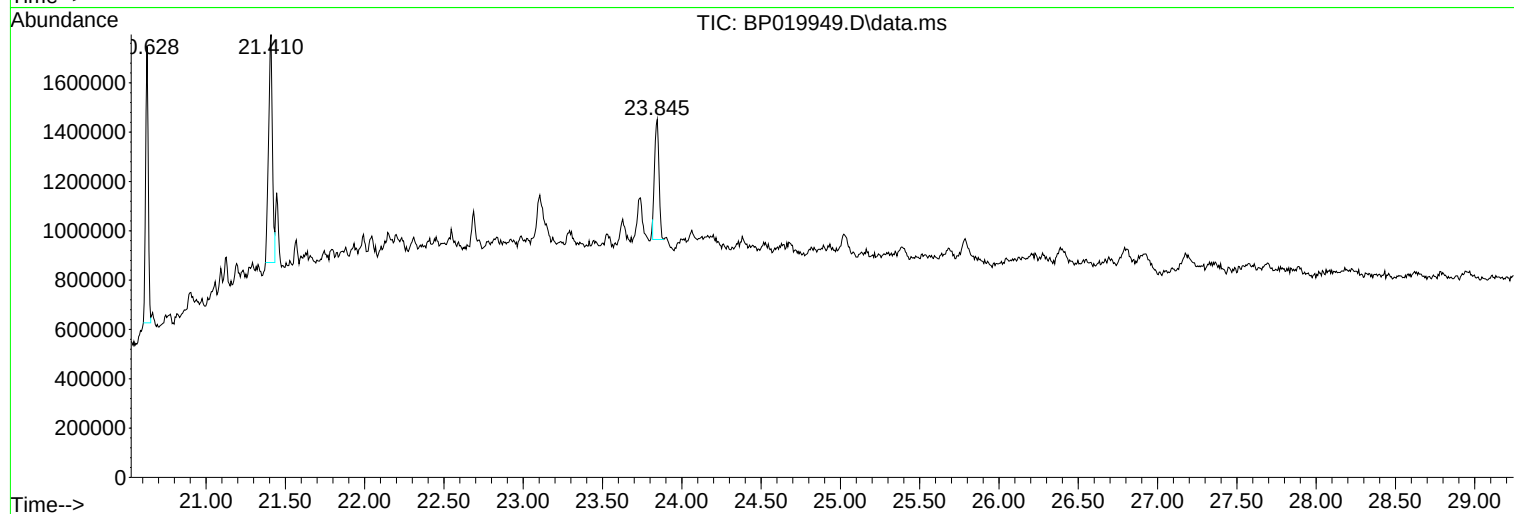
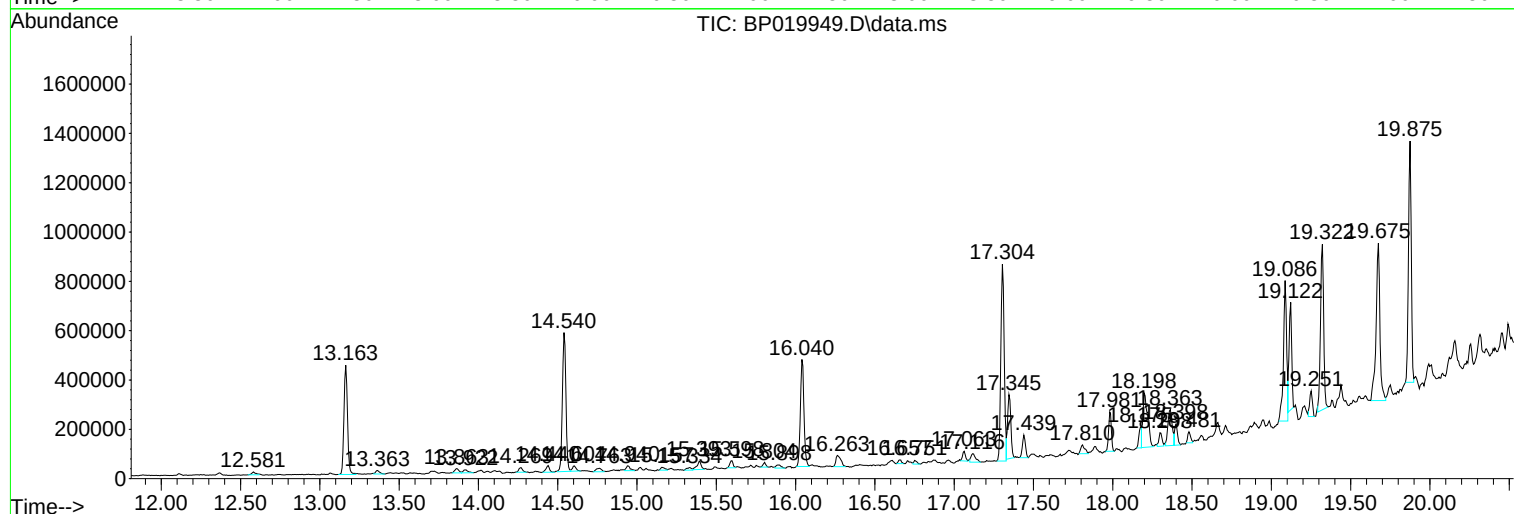
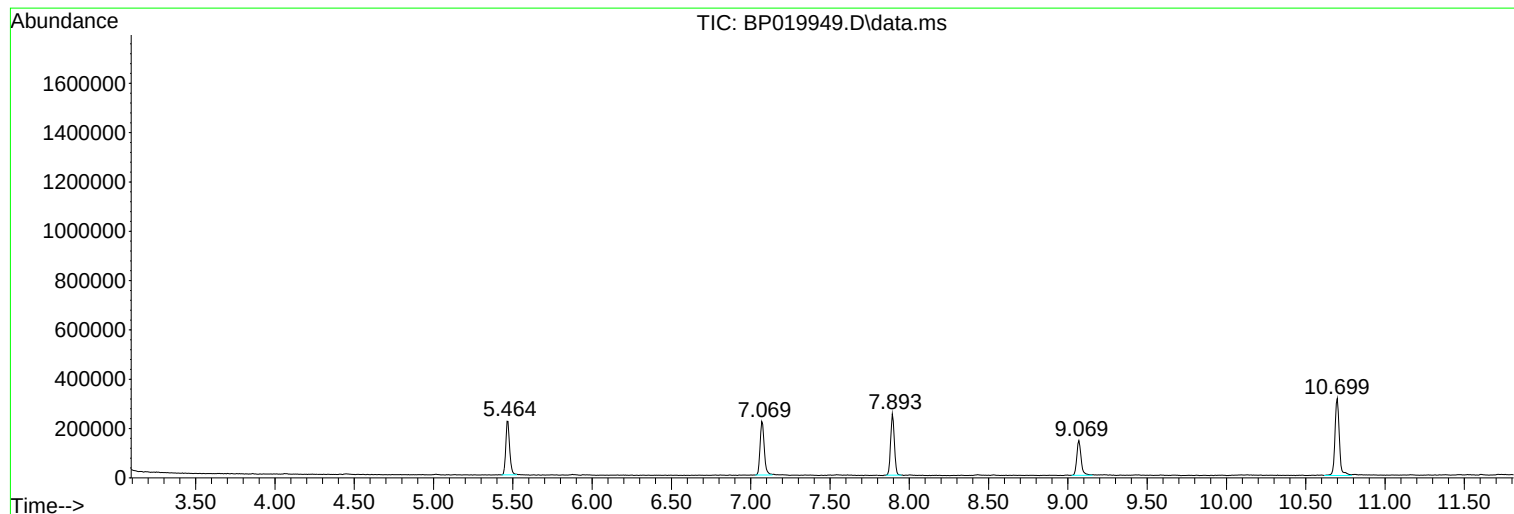
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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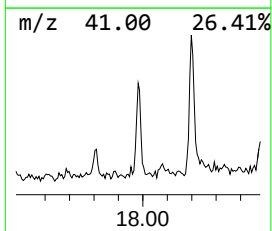
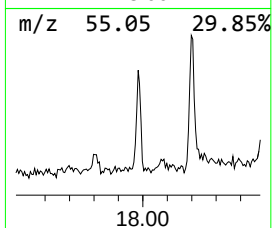
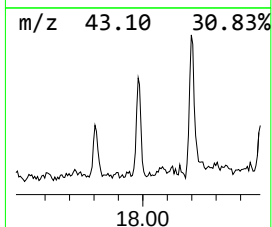
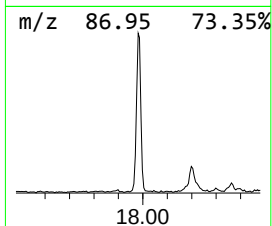
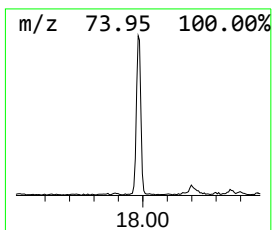
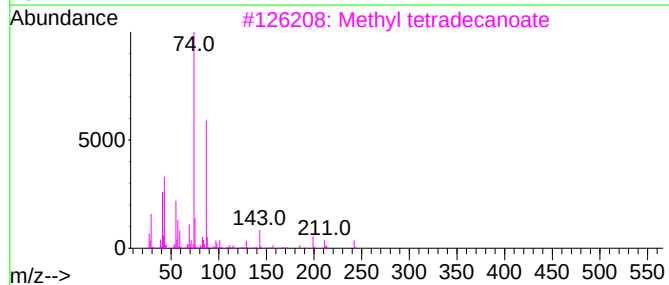
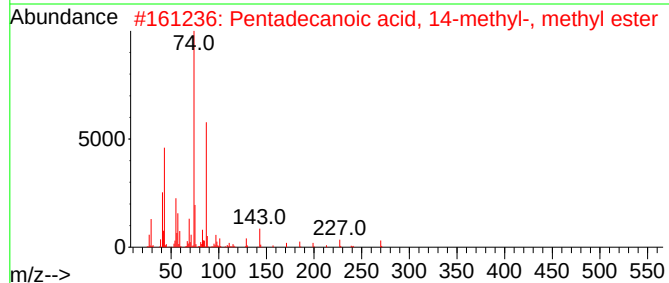
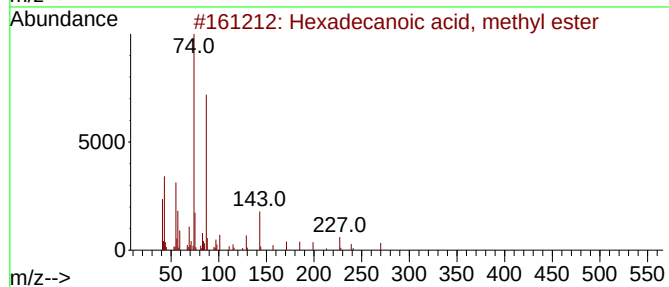
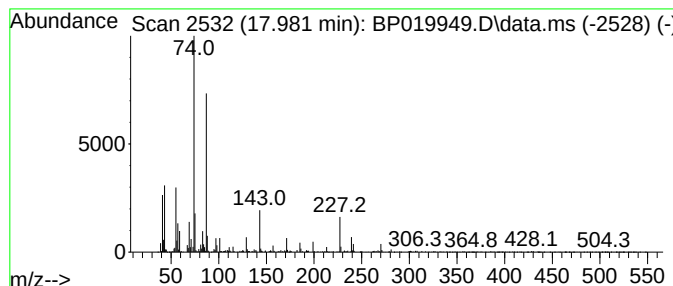
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.981	3.34 ng	196150	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	91
5			Methyl stearate	298	C19H38O2	000112-61-8	87



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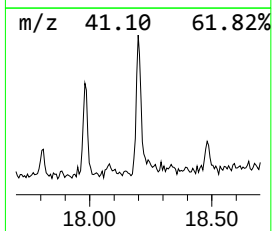
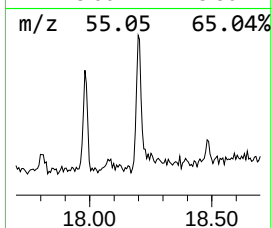
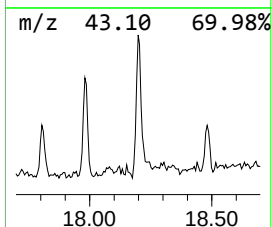
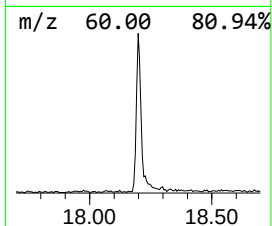
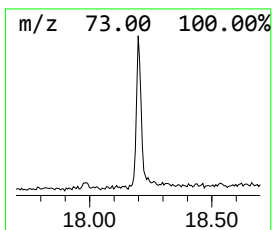
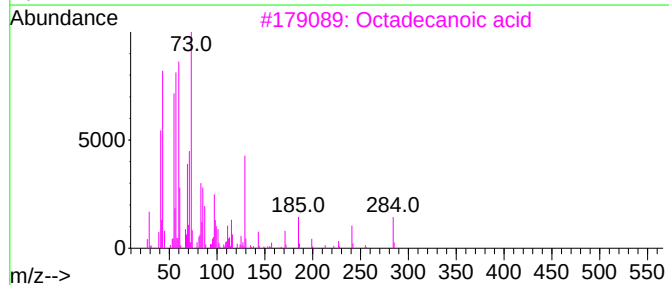
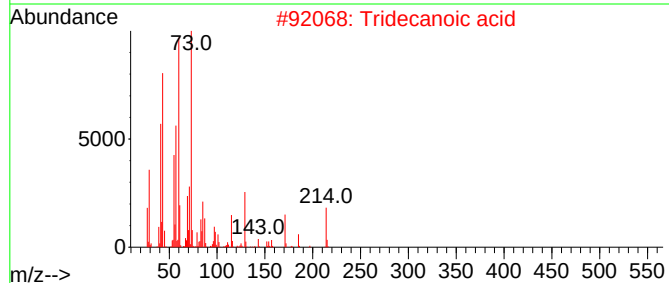
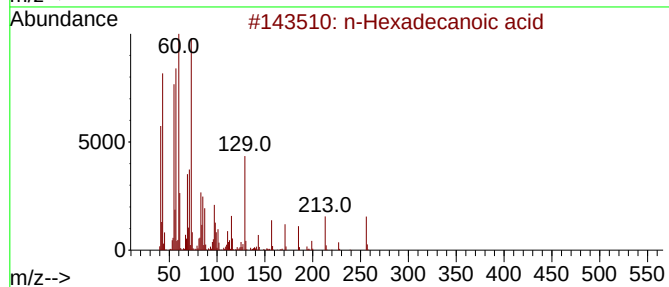
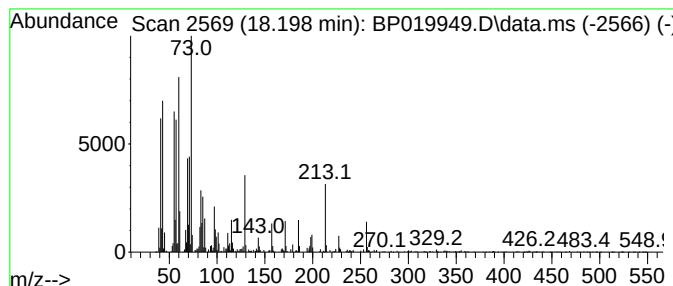
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	7.99 ng	468863	Phenanthrene-d10	17.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	83



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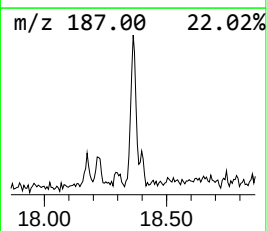
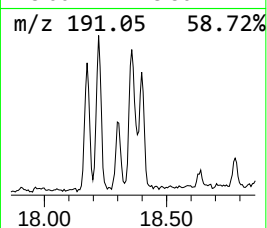
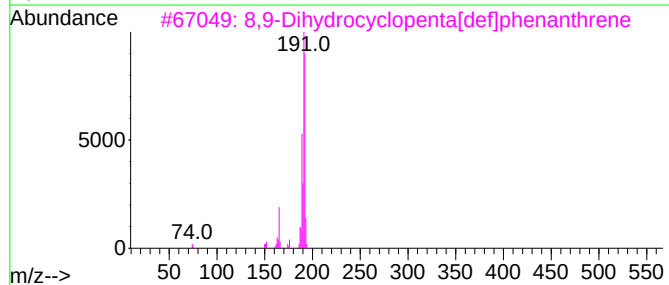
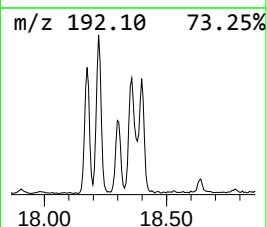
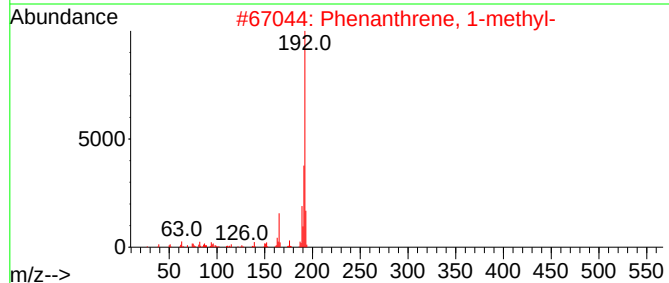
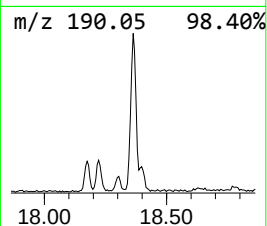
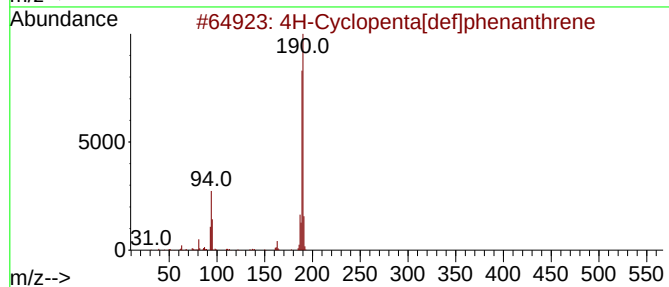
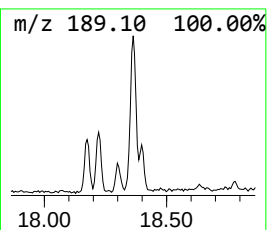
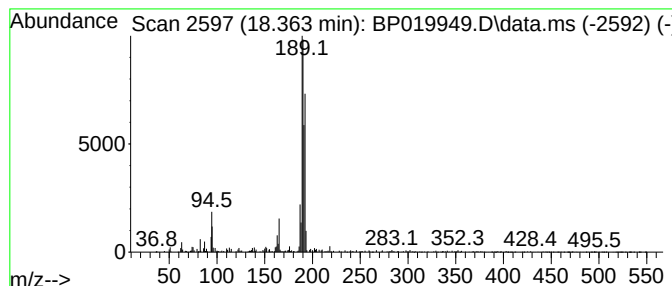
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.363	4.77 ng	279747	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
3			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
4			3-Bromo-2-furoic acid	190	C5H3BrO3	014903-90-3	35
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30



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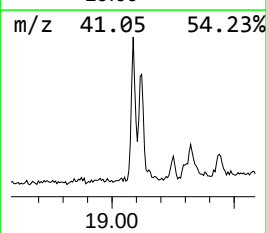
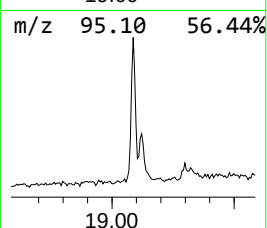
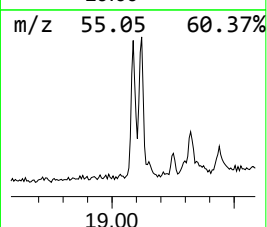
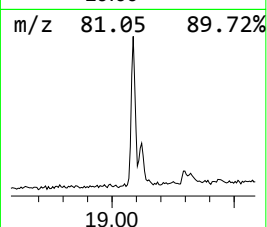
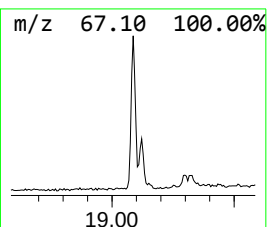
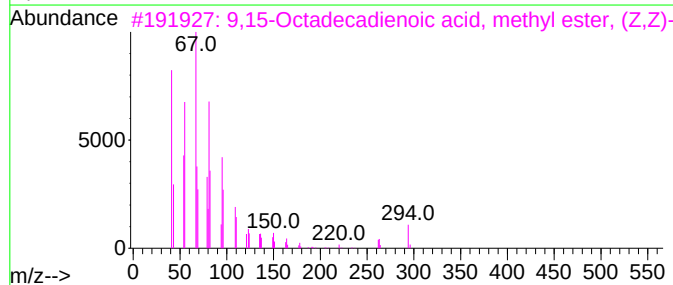
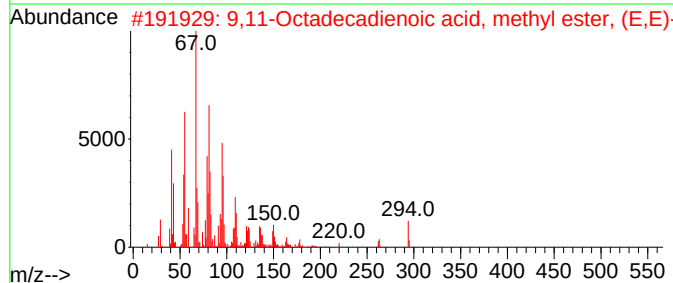
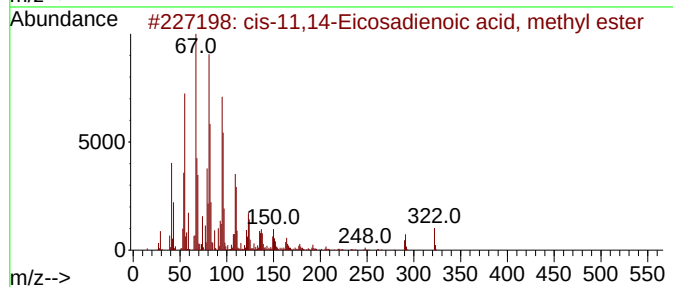
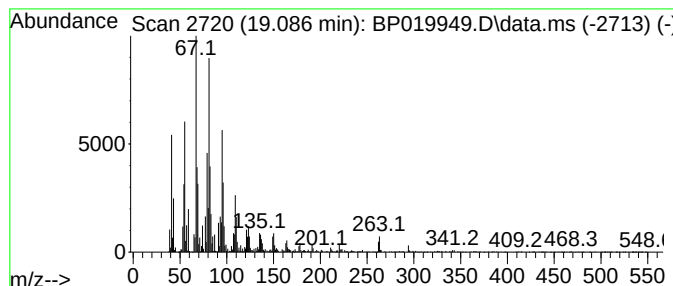
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 cis-11,14-Eicosadienoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.086	13.99 ng	821070	Phenanthrene-d10	17.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-11,14-Eicosadienoic acid, me...	322	C21H38O2	1010333-61-8	99
2	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98



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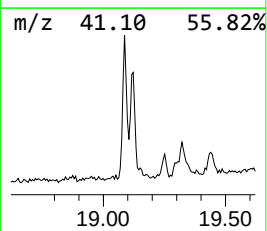
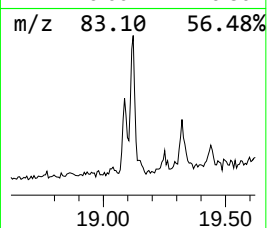
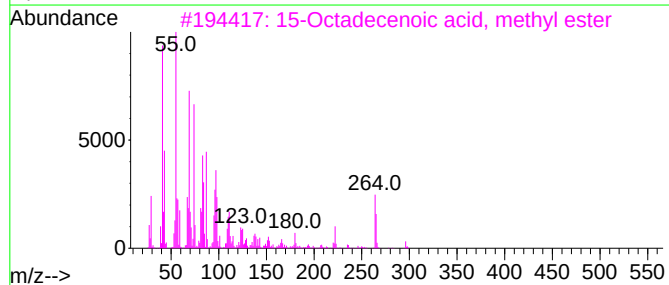
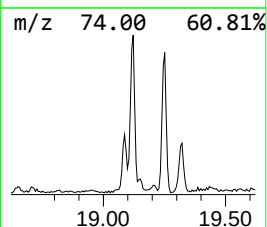
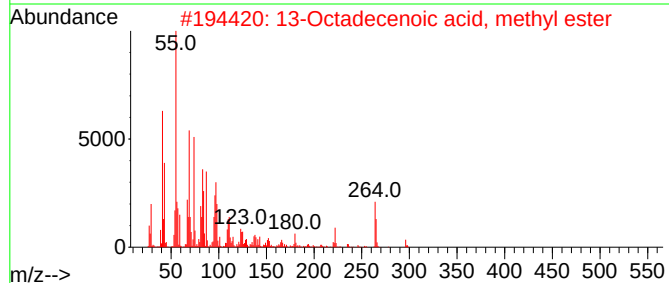
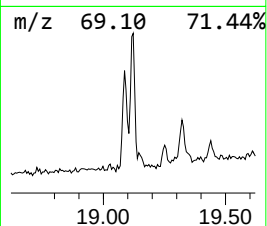
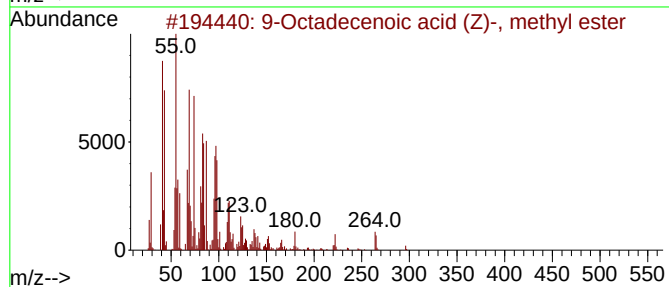
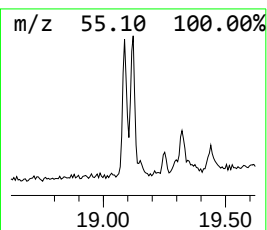
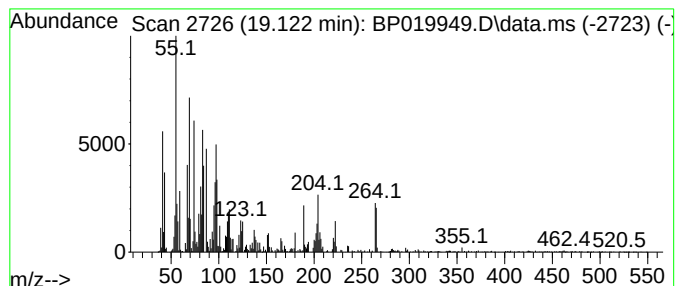
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ClientSampleId :
HD-02-022824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.122	8.51 ng	499513	Phenanthrene-d10	17.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022924\
Data File : BP019949.D
Acq On : 29 Feb 2024 21:54
Operator : MA/JU
Sample : P1622-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-022824

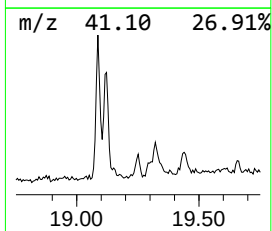
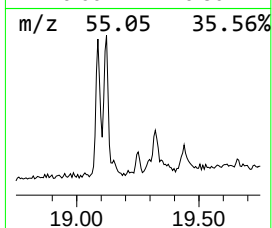
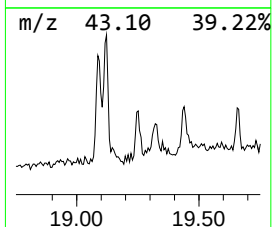
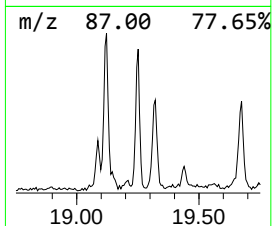
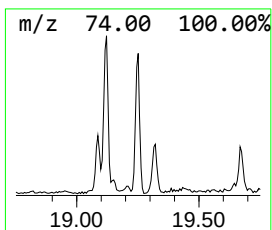
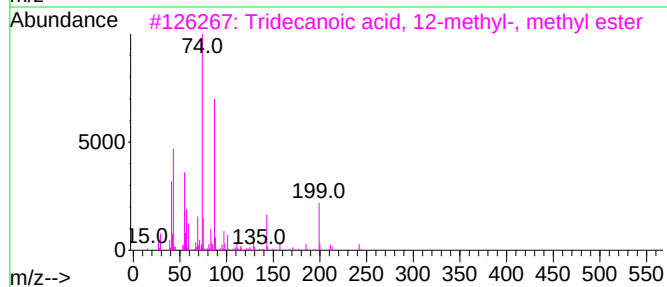
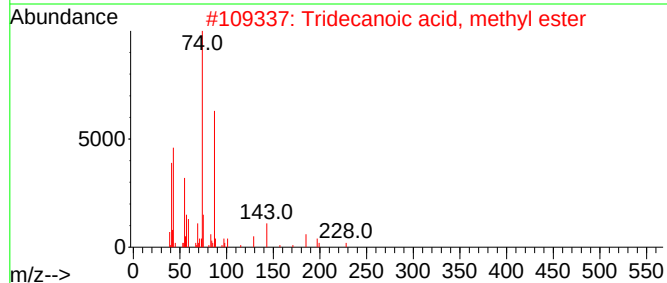
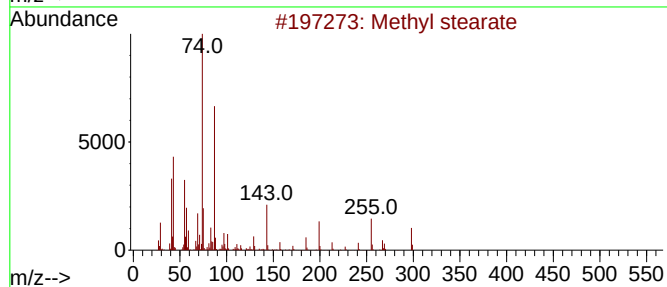
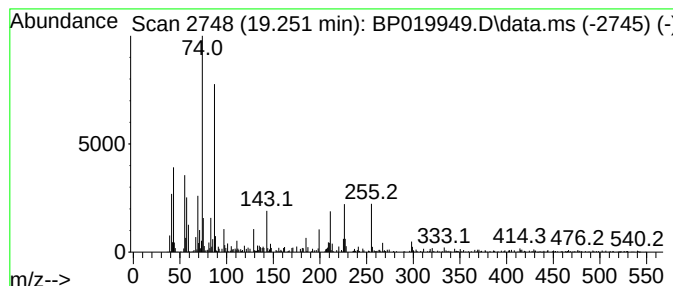
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	2.05 ng	120038	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	90
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	70
3			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	68
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	68
5			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022924\
Data File : BP019949.D
Acq On : 29 Feb 2024 21:54
Operator : MA/JU
Sample : P1622-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-022824

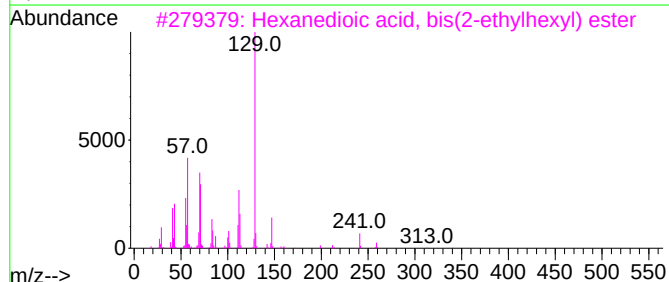
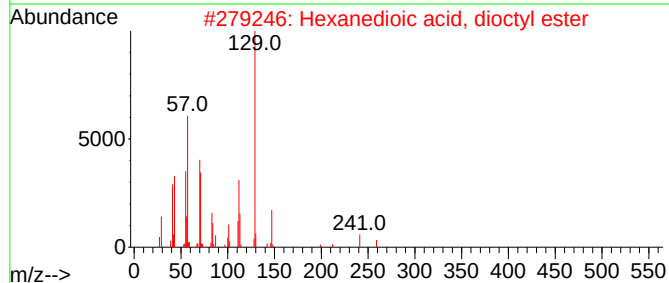
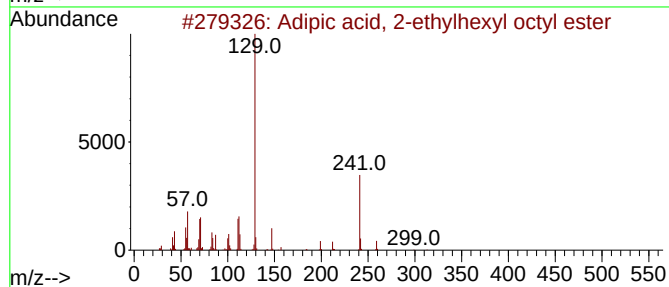
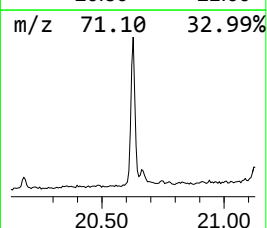
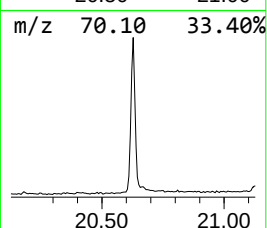
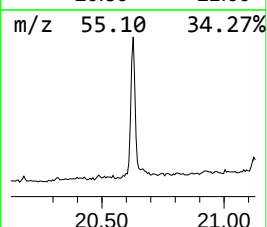
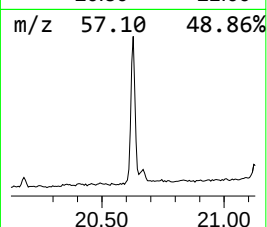
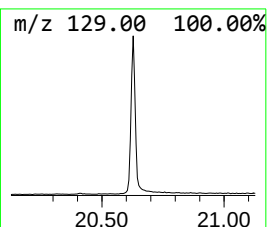
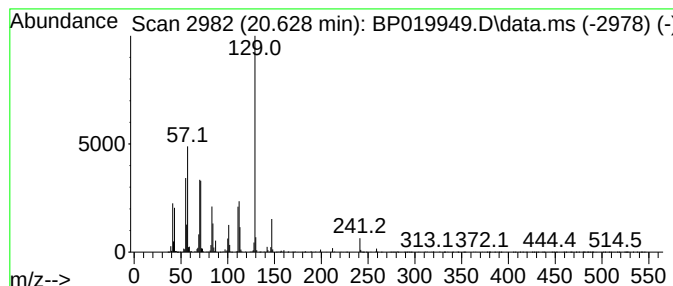
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Adipic acid, 2-ethylhexyl o... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.628	16.08 ng	1277260	Chrysene-d12	21.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
3			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022924\
Data File : BP019949.D
Acq On : 29 Feb 2024 21:54
Operator : MA/JU
Sample : P1622-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-022824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.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
Hexadecanoic ac...	17.981	3.3	ng	196150	4	17.304	1173450	20.0
n-Hexadecanoic ...	18.198	8.0	ng	468863	4	17.304	1173450	20.0
4H-Cyclopenta[d...	18.363	4.8	ng	279747	4	17.304	1173450	20.0
cis-11,14-Eicos...	19.086	14.0	ng	821070	4	17.304	1173450	20.0
9-Octadecenoic ...	19.122	8.5	ng	499513	4	17.304	1173450	20.0
Methyl stearate	19.251	2.0	ng	120038	4	17.304	1173450	20.0
Adipic acid, 2-...	20.628	16.1	ng	1277260	5	21.410	1588950	20.0