

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
 Data File : BP005267.D
 Acq On : 12 Apr 2021 15:43
 Operator : CG/JU
 Sample : M1992-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 AU-05-040921

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-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.281	367	373	381	rVB	719479	1036071	67.51%	9.013%
2	6.863	636	642	654	rVB	622345	967680	63.05%	8.418%
3	7.681	775	781	787	rVB	137467	214118	13.95%	1.863%
4	8.840	971	978	991	rBV	356517	565191	36.83%	4.917%
5	10.469	1246	1255	1262	rBV	154625	254287	16.57%	2.212%
6	12.951	1668	1677	1694	rBV	710869	999128	65.10%	8.692%
7	14.340	1906	1913	1920	rBV2	224447	320736	20.90%	2.790%
8	15.839	2161	2168	2179	rBV	551299	770827	50.22%	6.706%
9	17.104	2374	2383	2388	rBV	270131	382114	24.90%	3.324%
10	17.145	2388	2390	2394	rVB	18575	20159	1.31%	0.175%
11	17.786	2494	2499	2505	rBV	122460	146499	9.55%	1.274%
12	18.004	2529	2536	2545	rBV2	88881	145041	9.45%	1.262%
13	18.892	2680	2687	2690	rBV	859948	938318	61.14%	8.163%
14	18.928	2690	2693	2702	rVB2	532914	698818	45.53%	6.079%
15	19.051	2711	2714	2720	rVB	79072	88751	5.78%	0.772%
16	19.127	2720	2727	2733	rBV	87154	128091	8.35%	1.114%
17	19.245	2743	2747	2755	rBV3	49063	71459	4.66%	0.622%
18	19.480	2779	2787	2789	rBV2	72464	117970	7.69%	1.026%
19	19.504	2789	2791	2798	rVB	67479	94589	6.16%	0.823%
20	19.680	2816	2821	2832	rVB	1319352	1534776	100.00%	13.351%
21	19.963	2865	2869	2876	rVB7	12406	30442	1.98%	0.265%
22	20.122	2893	2896	2899	rVB4	16109	16421	1.07%	0.143%
23	20.357	2934	2936	2940	rVB	22724	21444	1.40%	0.187%
24	20.886	3021	3026	3029	rBV	66898	104843	6.83%	0.912%
25	20.933	3029	3034	3039	rVV2	141009	260101	16.95%	2.263%
26	20.986	3039	3043	3050	rVV	292298	366417	23.87%	3.188%
27	21.204	3074	3080	3084	rBV2	429220	594471	38.73%	5.171%
28	21.239	3084	3086	3093	rVB	68347	73749	4.81%	0.642%
29	22.786	3345	3349	3354	rBV	50883	105937	6.90%	0.922%
30	23.480	3461	3467	3473	rVB	235888	426928	27.82%	3.714%

Sum of corrected areas: 11495376

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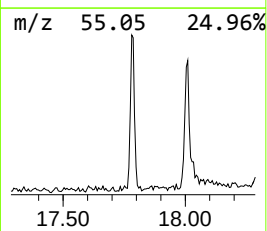
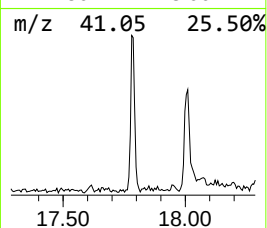
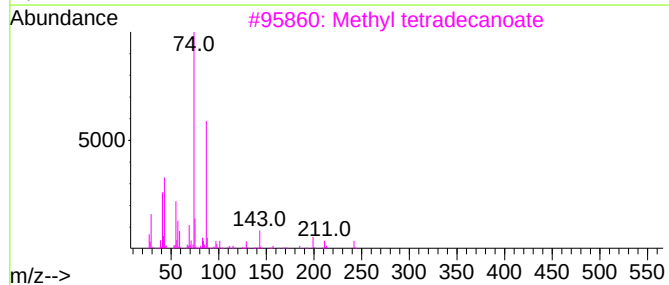
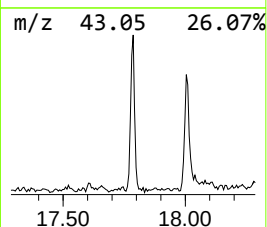
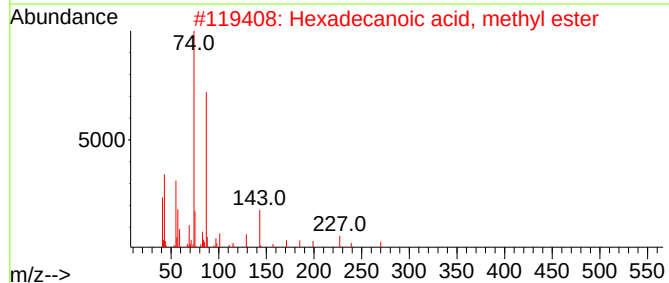
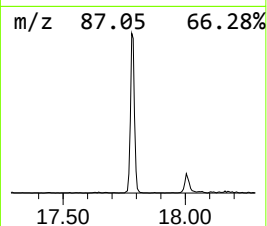
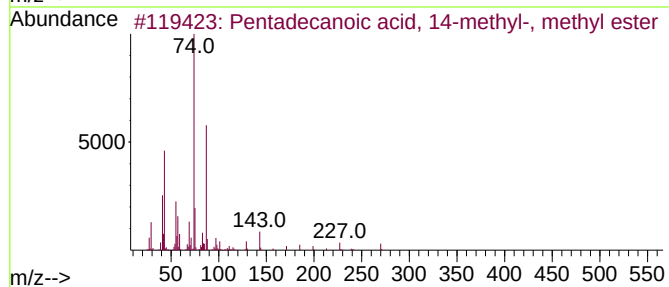
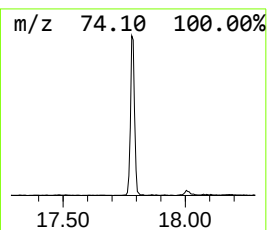
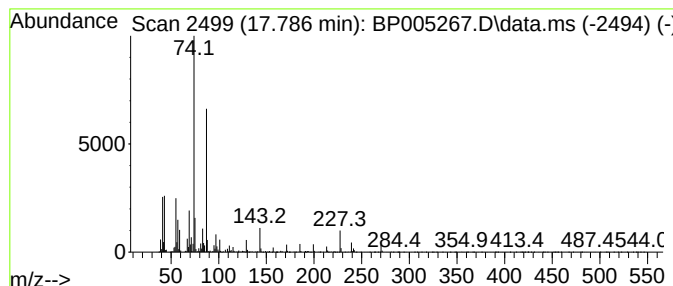
Instrument :
BNA_P
ClientSampleId :
AU-05-040921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentadecanoic acid, 14-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.786	7.67 ng	146499	Phenanthrene-d10	17.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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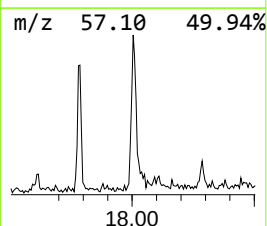
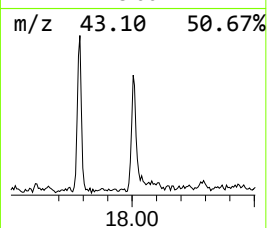
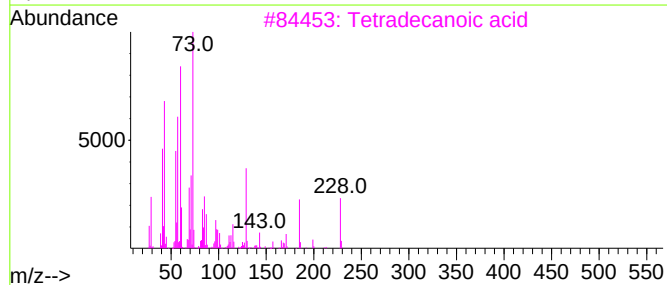
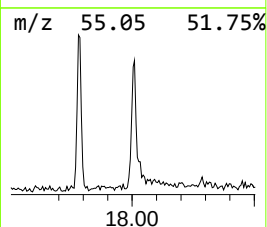
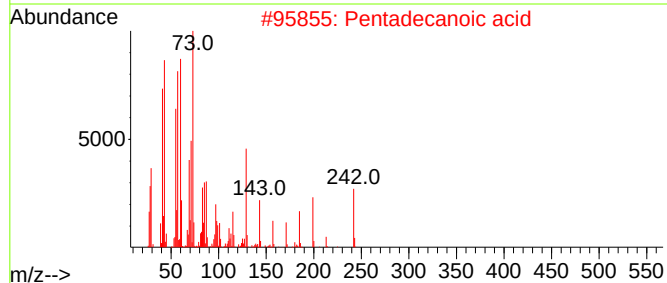
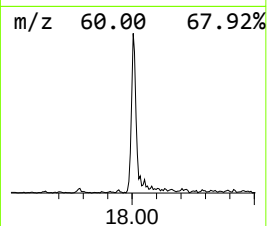
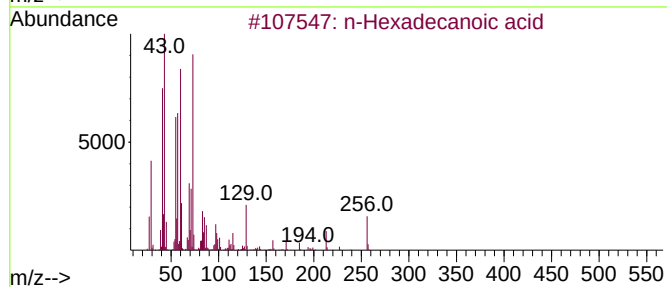
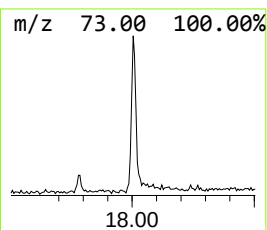
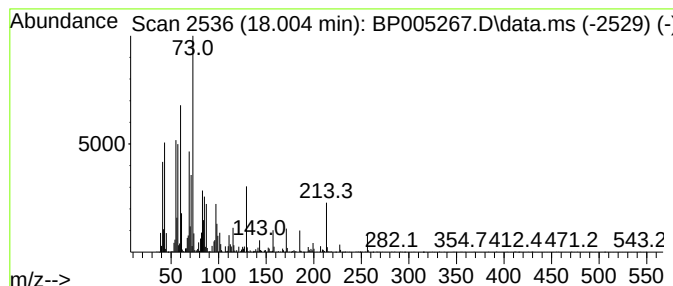
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	7.59 ng	145041	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Octadecanoic acid	284	C18H36O2	000057-11-4	49
5			Tridecanoic acid	214	C13H26O2	000638-53-9	43



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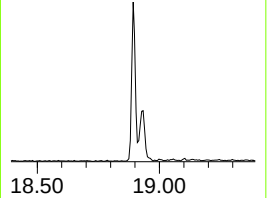
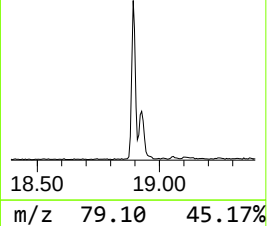
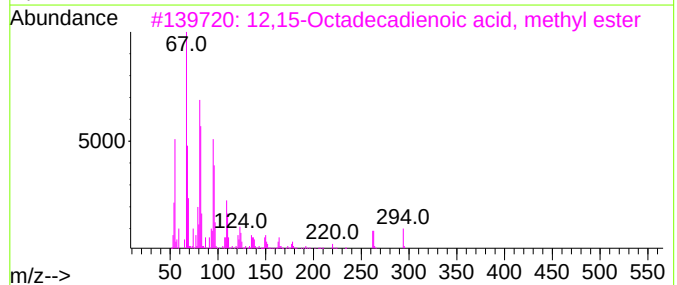
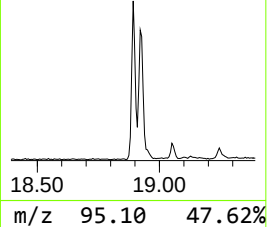
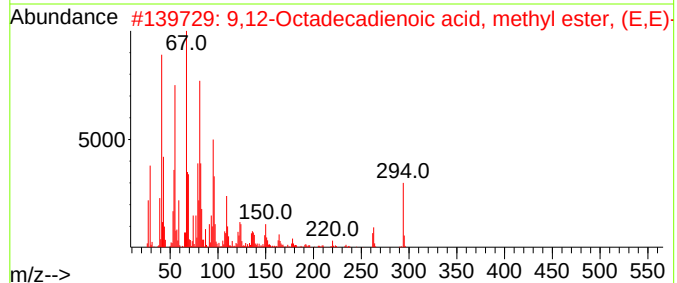
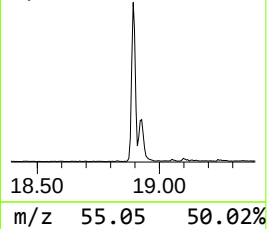
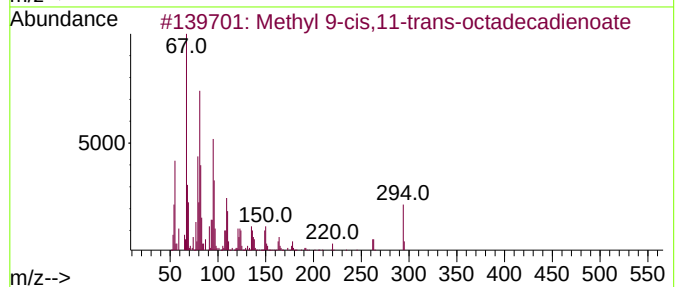
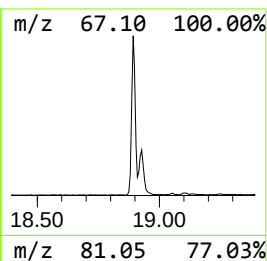
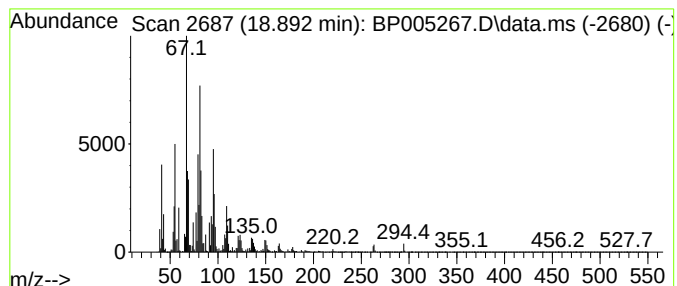
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.892	49.11 ng	938318	Phenanthrene-d10	17.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93
3	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	89
4	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	83
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	83



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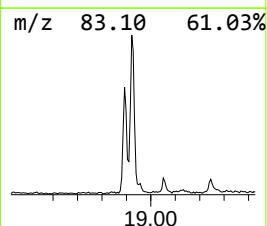
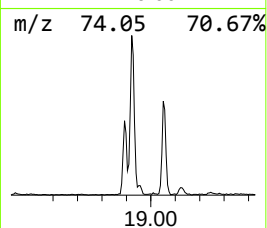
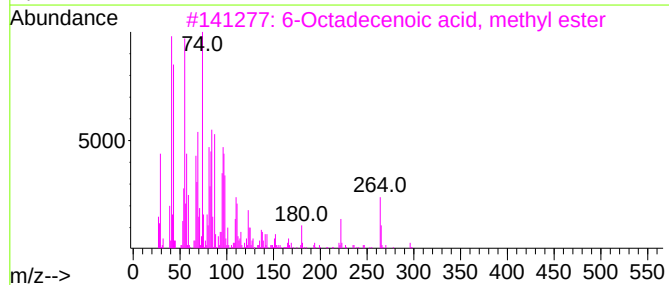
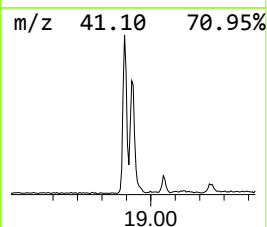
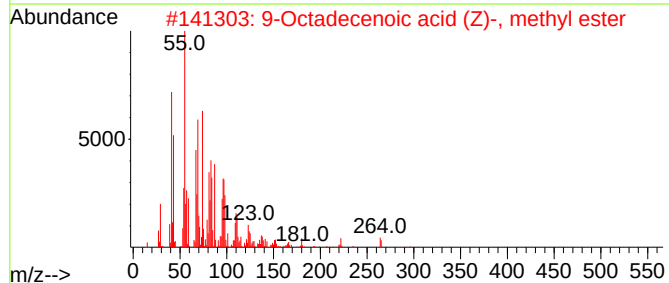
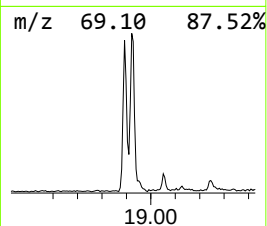
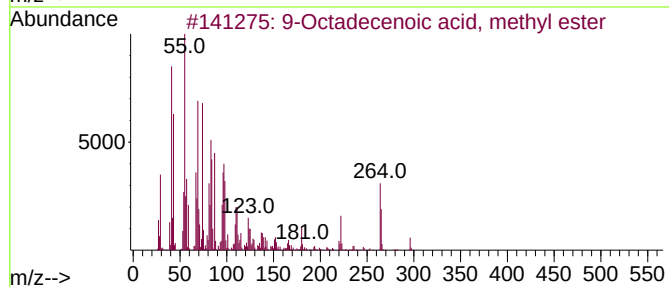
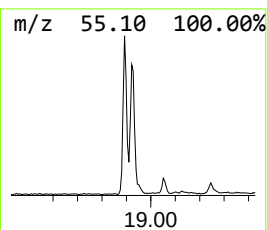
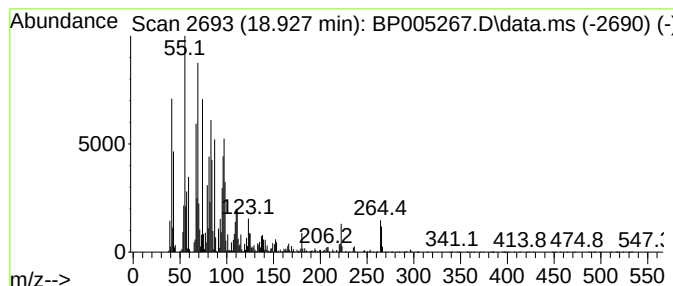
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.927	36.58 ng	698818	Phenanthrene-d10		17.104	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester		296	C19H36O2	002462-84-2	99
2	9-Octadecenoic acid (Z)-, methyl...		296	C19H36O2	000112-62-9	99
3	6-Octadecenoic acid, methyl ester		296	C19H36O2	052355-31-4	99
4	8-Octadecenoic acid, methyl este...		296	C19H36O2	026528-50-7	98
5	8-Octadecenoic acid, methyl ester		296	C19H36O2	002345-29-1	97



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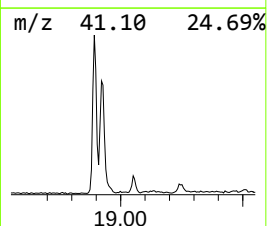
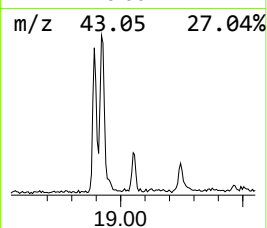
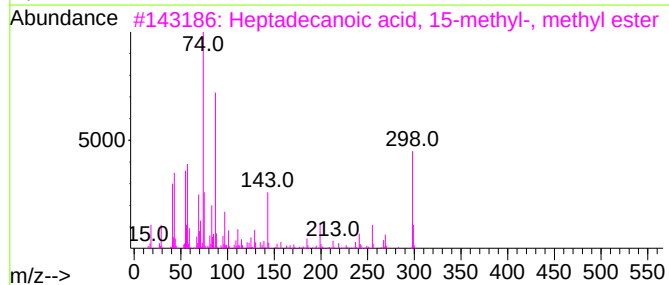
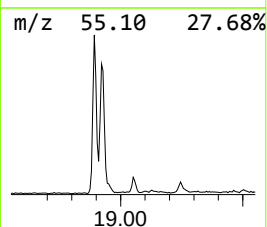
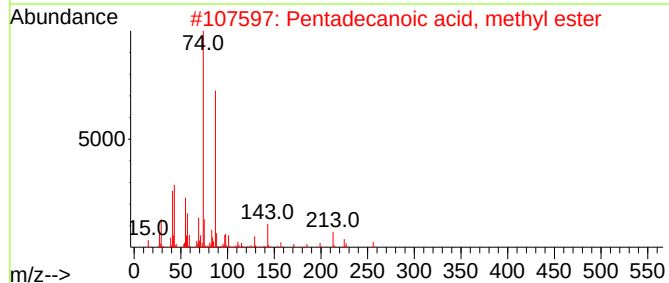
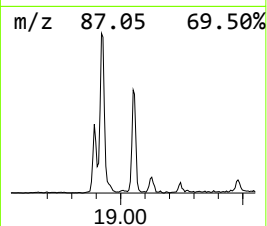
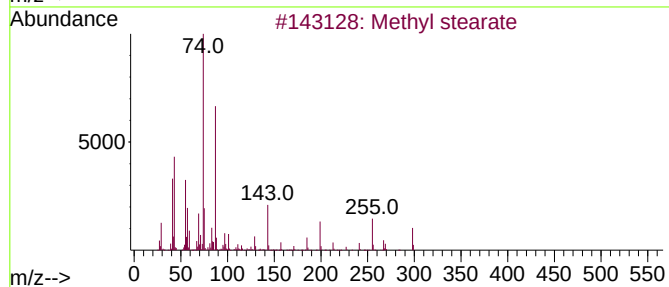
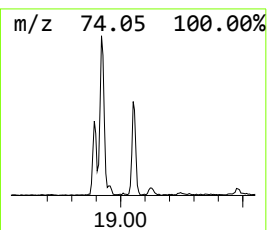
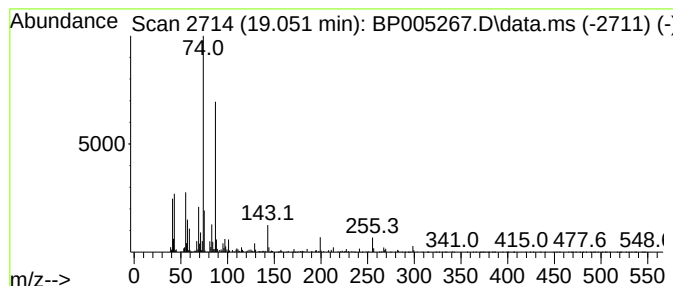
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.051	4.65 ng	88751	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	94
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5			Methyl 13-methyltetradecanoate	256	C16H32O2	1000336-31-4	90



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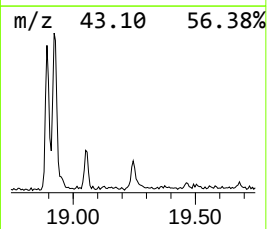
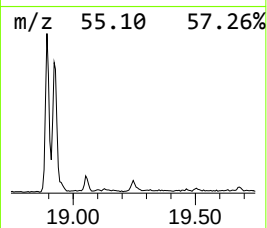
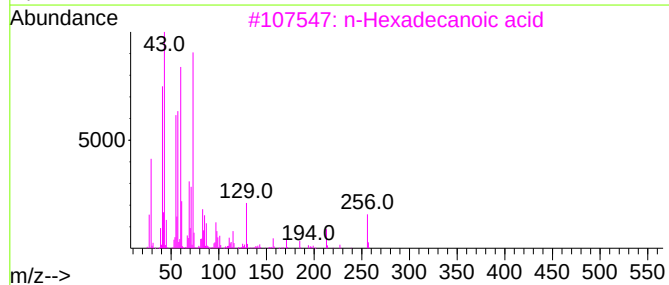
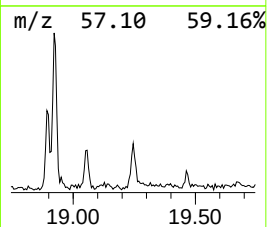
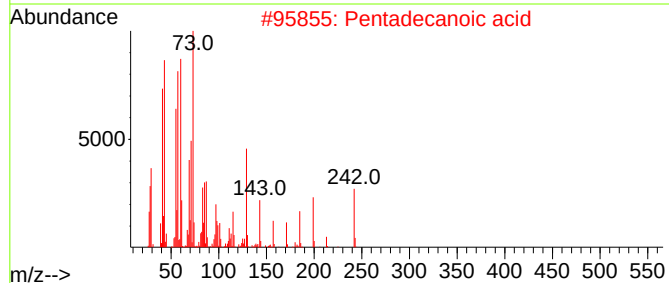
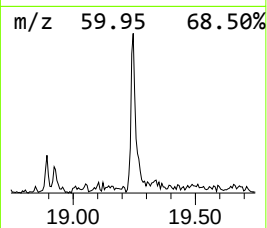
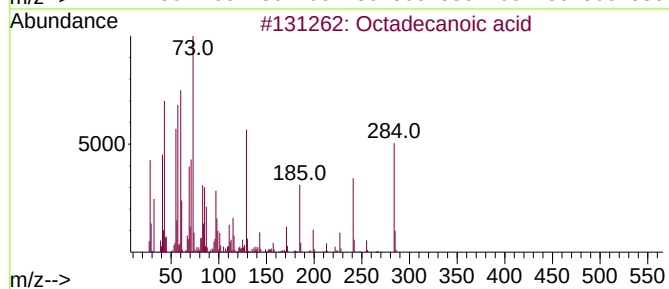
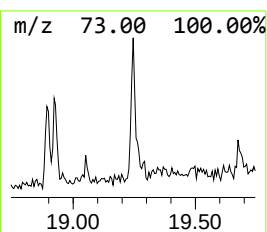
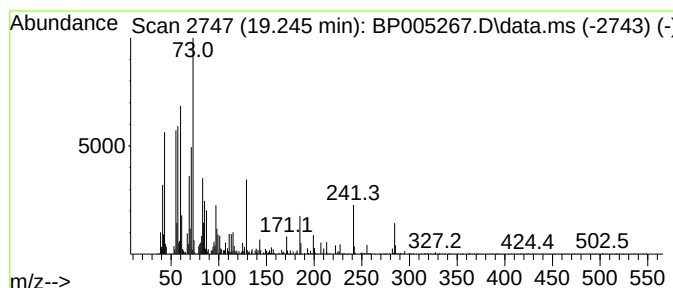
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	2.40 ng	71459	Chrysene-d12	21.204

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	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5			Fumaric acid, nonyl pentadecyl e...	452	C28H52O4	1000339-28-8	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005267.D
Acq On : 12 Apr 2021 15:43
Operator : CG/JU
Sample : M1992-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-05-040921

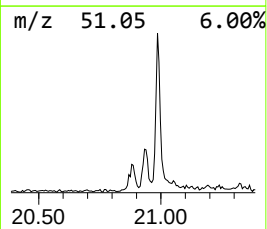
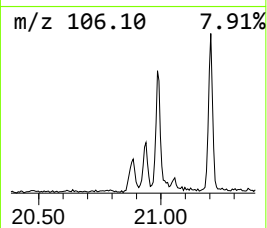
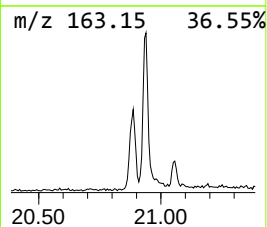
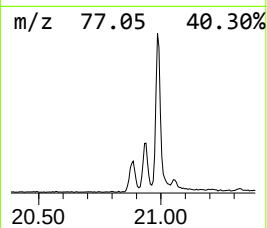
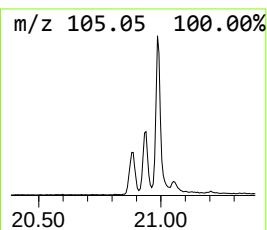
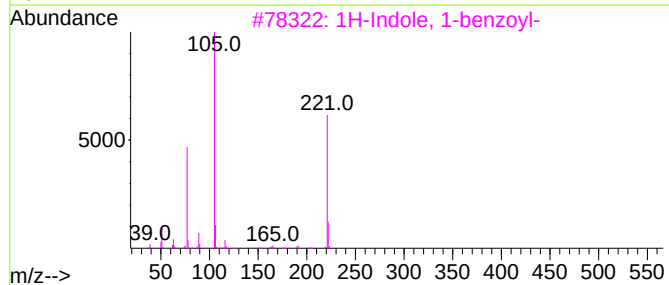
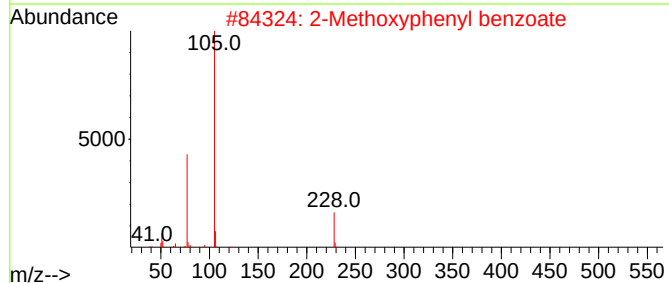
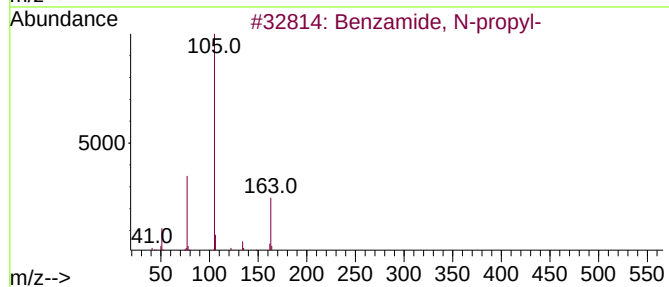
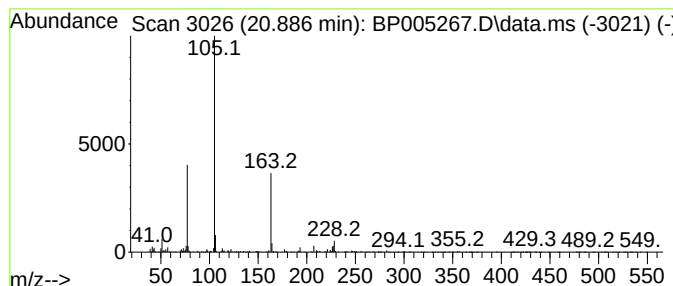
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzamide, N-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	3.53 ng	104843	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2			2-Methoxyphenyl benzoate	228	C14H12O3	000531-37-3	50
3			1H-Indole, 1-benzoyl-	221	C15H11NO	001496-76-0	47
4			Acetic acid, 1-(3-benzoyl-2-t-bu...	519	C29H33N3O6	1000189-67-6	47
5			Benzoic acid, 3-formylphenyl ester	226	C14H10O3	033696-06-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005267.D
Acq On : 12 Apr 2021 15:43
Operator : CG/JU
Sample : M1992-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-05-040921

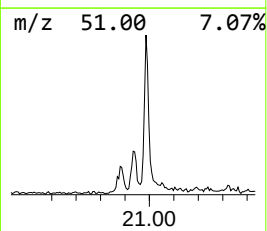
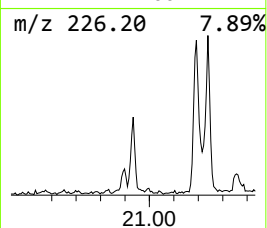
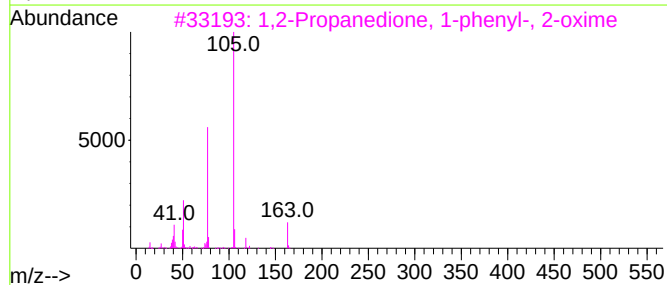
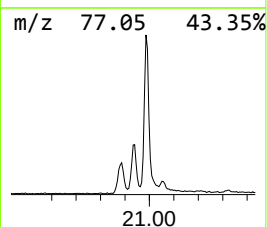
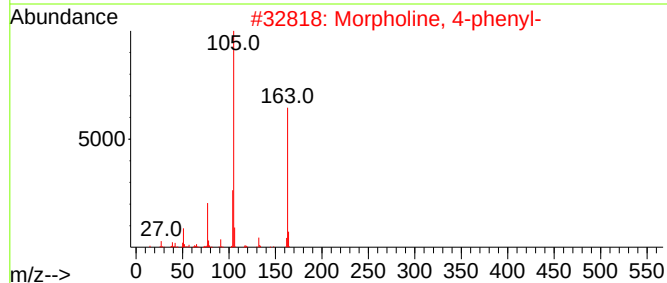
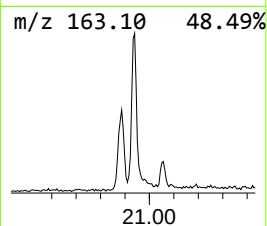
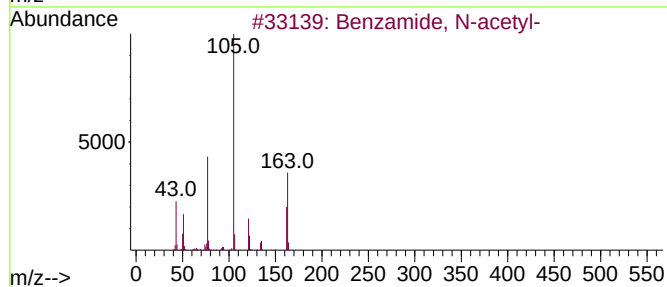
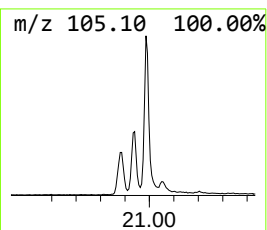
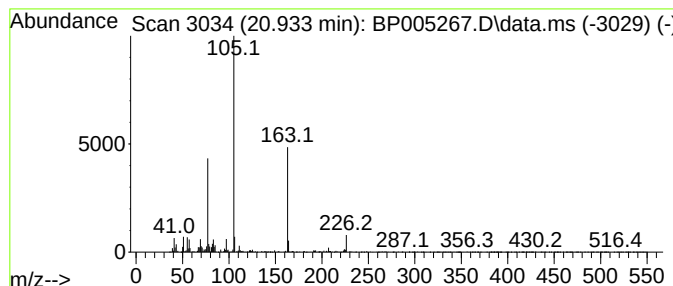
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzamide, N-acetyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	8.75 ng	260101	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	43
4			Acetic acid, 1-(3-benzoyl-2-t-bu...	519	C29H33N3O6	1000189-67-6	38
5			Oxazol-5(4H)-one, 4-(3,5-dibromo...	421	C16H9Br2NO3	113425-80-2	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005267.D
Acq On : 12 Apr 2021 15:43
Operator : CG/JU
Sample : M1992-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-05-040921

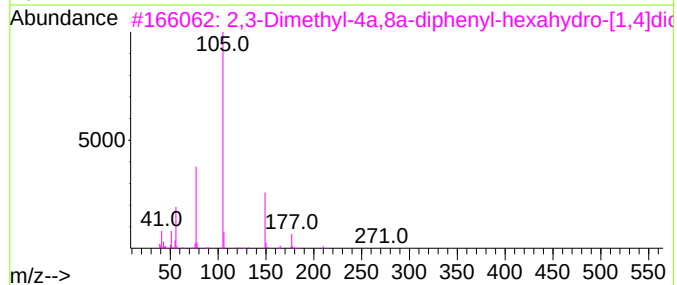
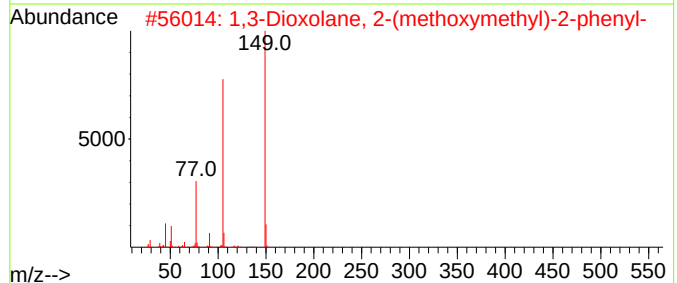
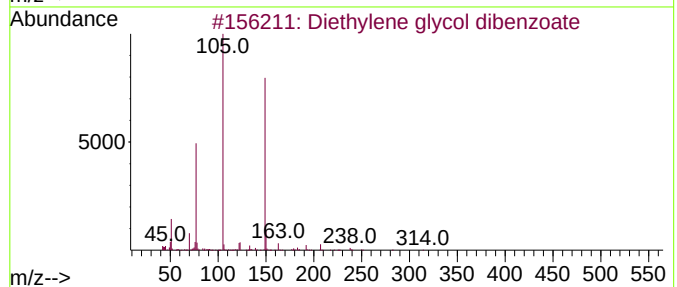
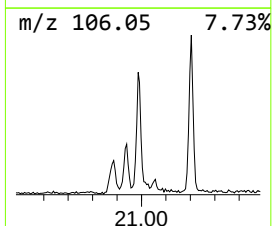
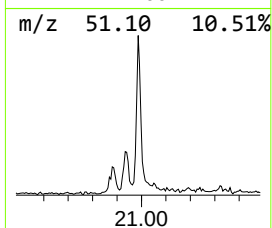
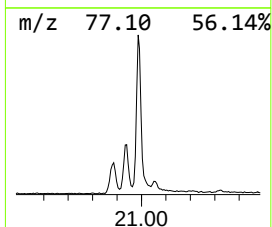
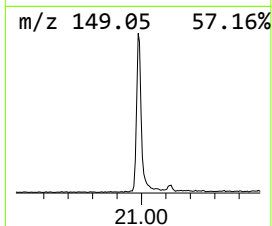
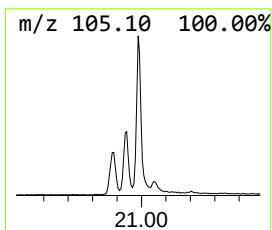
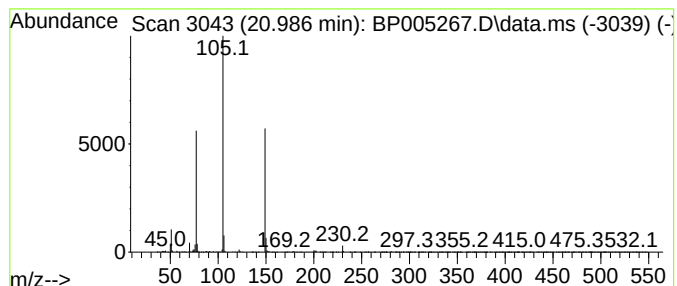
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	12.33 ng	366417	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3			2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59
4			Ethanone, 2-bromo-1,2-diphenyl-	274	C14H11BrO	001484-50-0	47
5			4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005267.D
Acq On : 12 Apr 2021 15:43
Operator : CG/JU
Sample : M1992-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-05-040921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentadecanoic a...	17.786	7.7	ng	146499	4	17.104	382114	20.0
n-Hexadecanoic ...	18.004	7.6	ng	145041	4	17.104	382114	20.0
Methyl 9-cis,11...	18.892	49.1	ng	938318	4	17.104	382114	20.0
9-Octadecenoic ...	18.927	36.6	ng	698818	4	17.104	382114	20.0
Methyl stearate	19.051	4.7	ng	88751	4	17.104	382114	20.0
Octadecanoic acid	19.245	2.4	ng	71459	5	21.204	594471	20.0
Benzamide, N-pr...	20.886	3.5	ng	104843	5	21.204	594471	20.0
Benzamide, N-ac...	20.933	8.8	ng	260101	5	21.204	594471	20.0
Diethylene glyc...	20.986	12.3	ng	366417	5	21.204	594471	20.0