

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
 Data File : BP007072.D
 Acq On : 21 Sep 2021 03:38
 Operator : CG/JU
 Sample : M3757-01 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 AU-06-091521

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-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	400	407	416	rBV	2445915	3572852	12.10%	2.991%
2	7.069	670	677	690	rBV	2274939	3618730	12.26%	3.030%
3	7.905	812	819	828	rBV	1396371	2214138	7.50%	1.854%
4	9.063	1009	1016	1026	rBV	1330122	2245922	7.61%	1.880%
5	10.487	1253	1258	1269	rBV2	154469	299863	1.02%	0.251%
6	10.705	1285	1295	1306	rBV	1880169	3142226	10.64%	2.631%
7	13.157	1705	1712	1724	rBV	3359354	5043567	17.08%	4.223%
8	14.534	1937	1946	1955	rBV	2706903	4064125	13.77%	3.403%
9	16.016	2192	2198	2207	rBV	2661476	3863542	13.09%	3.235%
10	17.281	2407	2413	2418	rBV	3240937	4488756	15.20%	3.758%
11	17.951	2522	2527	2533	rBV	3530627	4018014	13.61%	3.364%
12	18.175	2559	2565	2579	rBV	1951038	2879850	9.75%	2.411%
13	19.057	2709	2715	2718	rBV	19828889	29524928	100.00%	24.720%
14	19.086	2718	2720	2730	rVB2	16535930	20743286	70.26%	17.368%
15	19.210	2737	2741	2745	rBV	3178345	3546561	12.01%	2.969%
16	19.263	2745	2750	2752	rBV	2568511	3240506	10.98%	2.713%
17	19.286	2752	2754	2769	rVV2	2735205	4589152	15.54%	3.842%
18	19.398	2770	2773	2782	rVB	580477	830664	2.81%	0.695%
19	19.639	2811	2814	2823	rVB	343833	554673	1.88%	0.464%
20	19.833	2842	2847	2852	rBV	5073549	6055627	20.51%	5.070%
21	20.275	2918	2922	2925	rBV	398990	479519	1.62%	0.401%
22	21.069	3055	3057	3063	rVB3	255203	304344	1.03%	0.255%
23	21.204	3077	3080	3083	rBV	354511	436528	1.48%	0.365%
24	21.357	3101	3106	3111	rBV	3594774	4832155	16.37%	4.046%
25	23.774	3511	3517	3525	rVB2	2386103	4845664	16.41%	4.057%

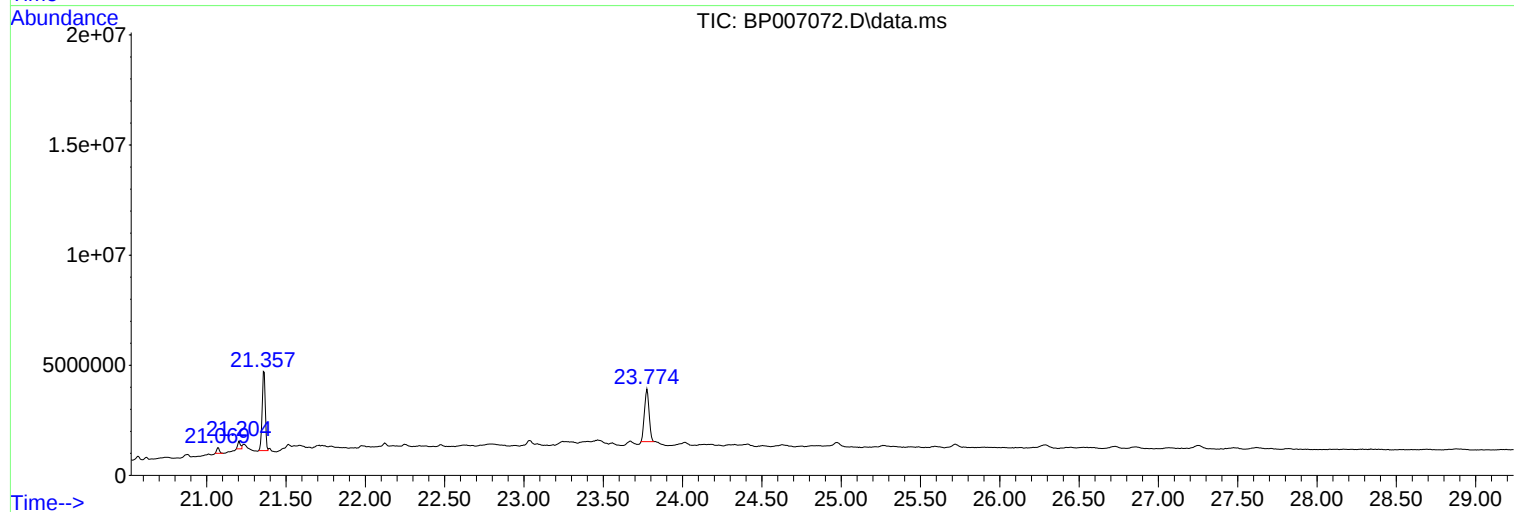
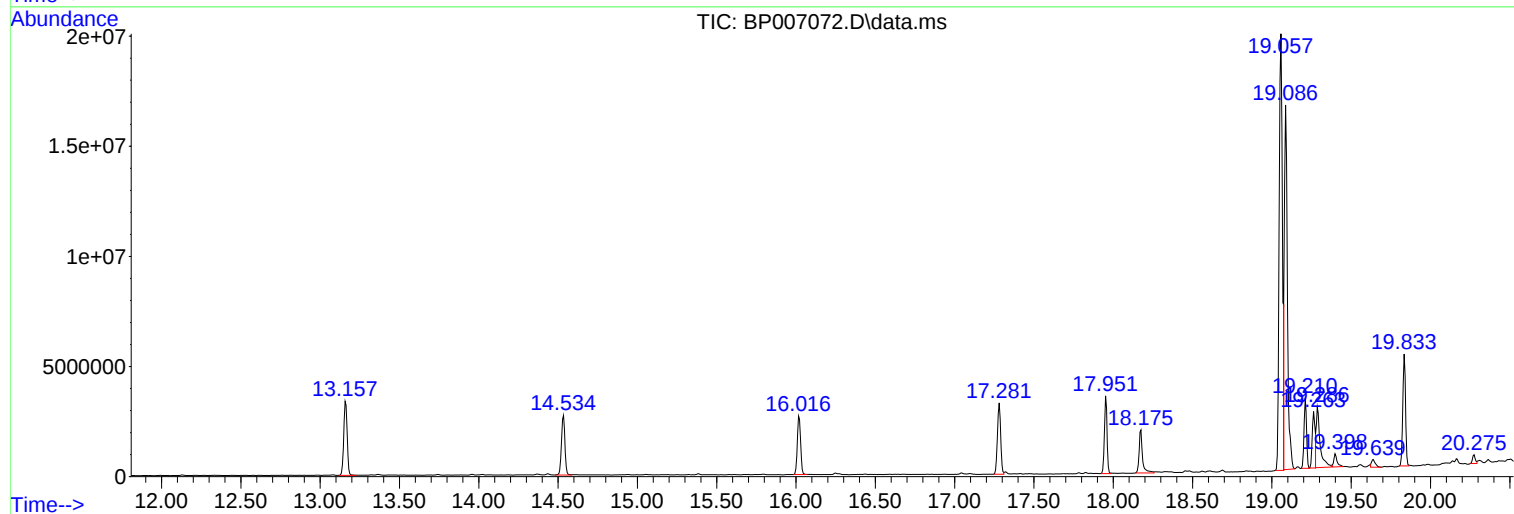
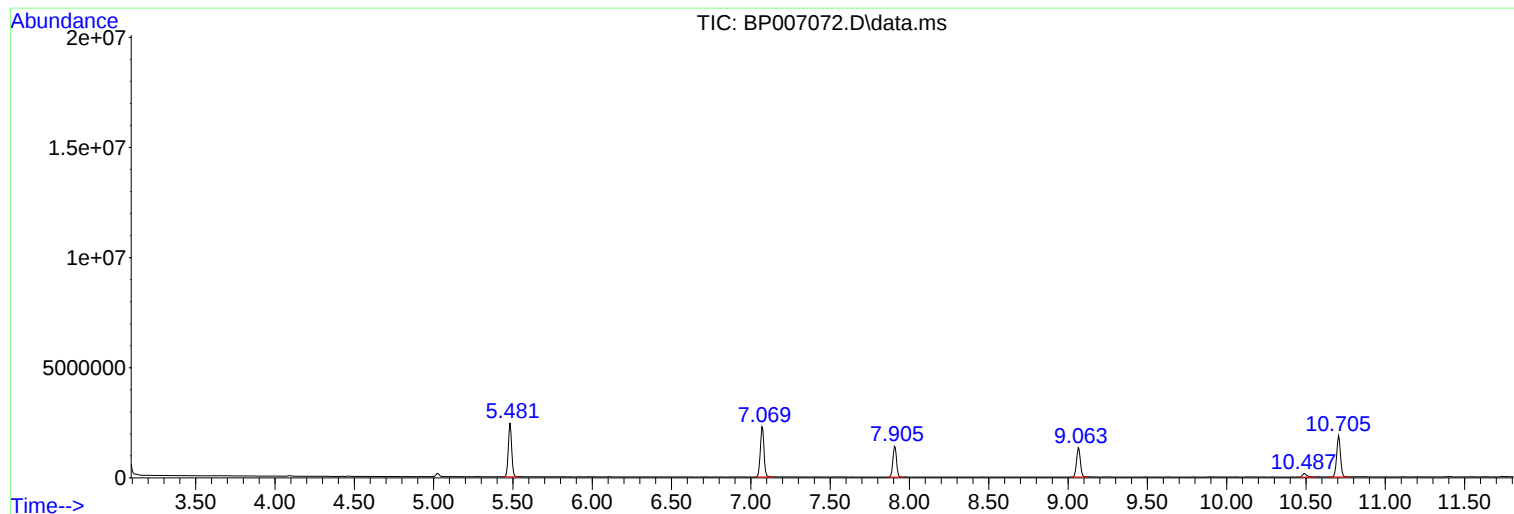
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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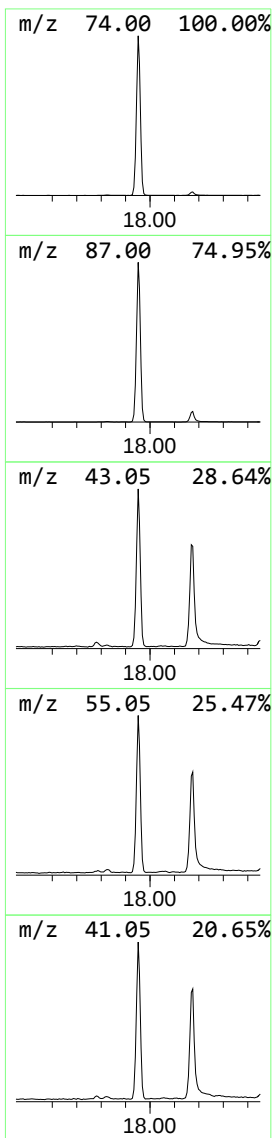
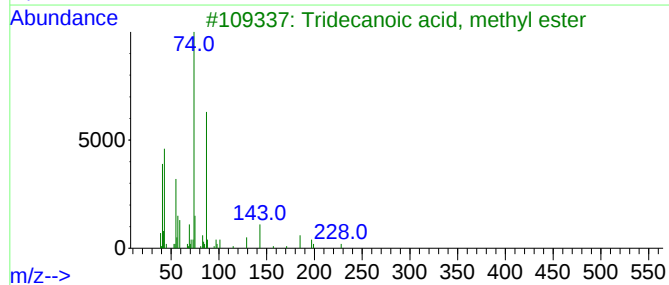
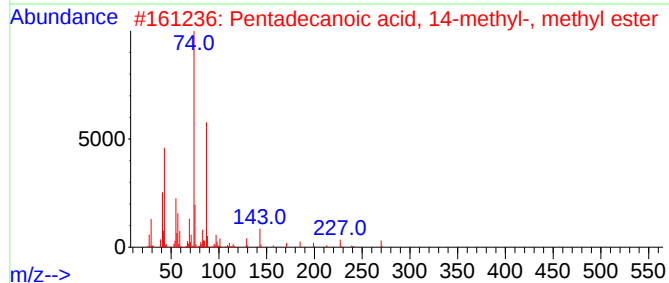
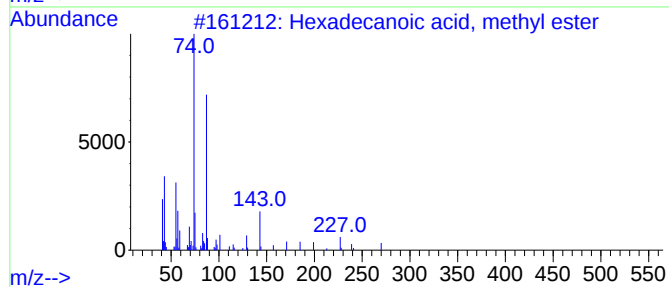
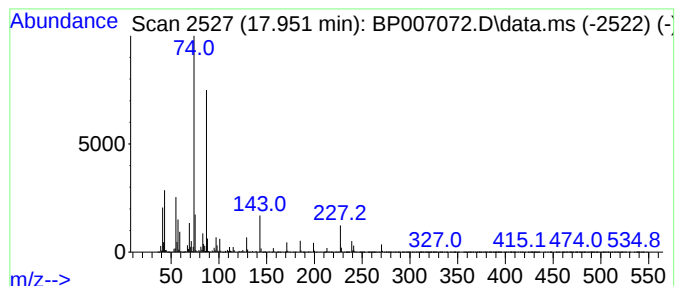
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Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.951	17.90 ng	4018010	Phenanthrene-d10		17.281	
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	95
3	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate		242	C15H30O2	000124-10-7	83



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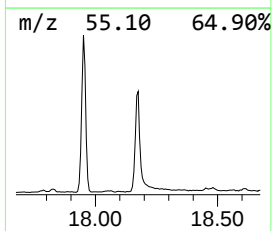
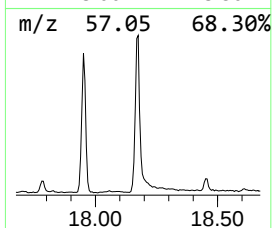
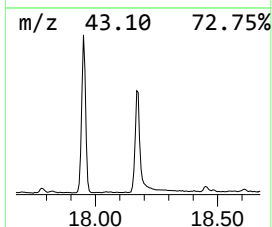
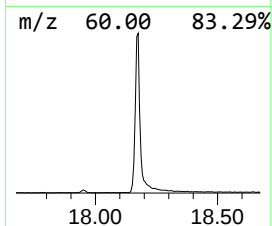
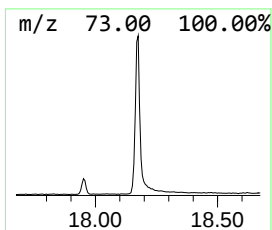
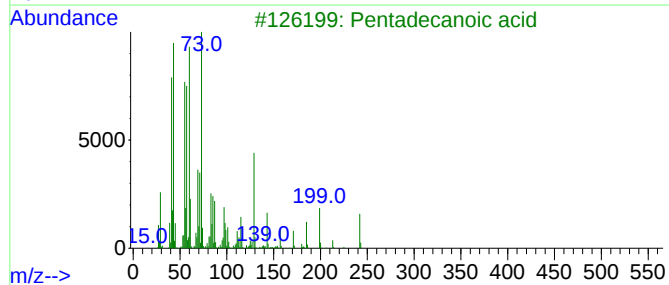
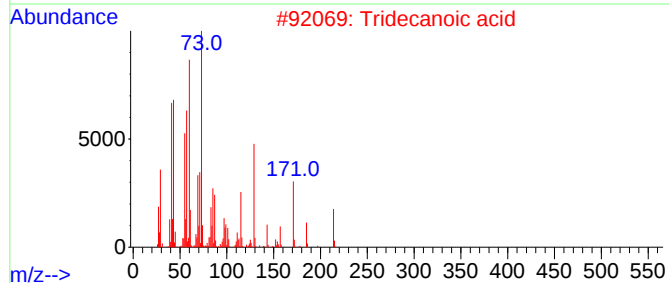
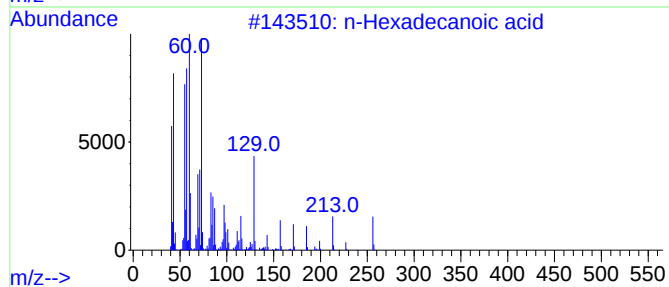
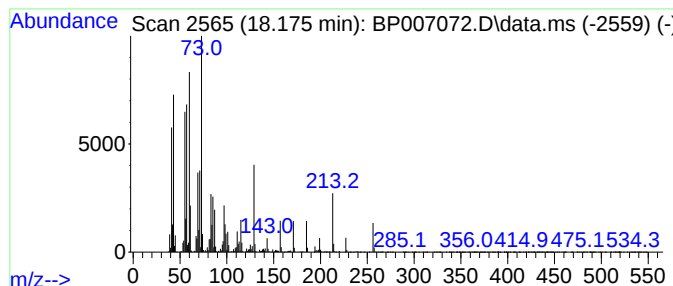
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	12.83 ng	2879850	Phenanthrene-d10	17.281

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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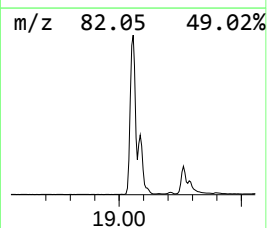
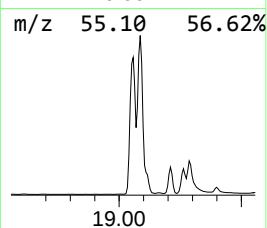
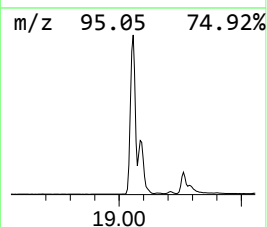
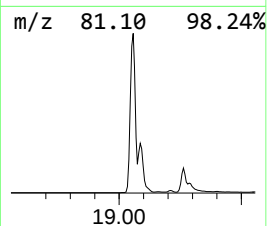
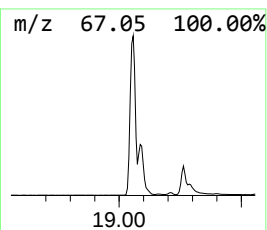
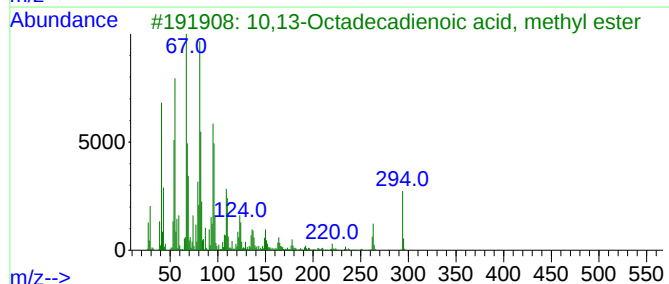
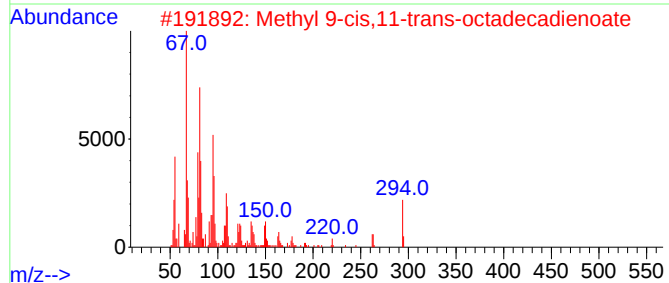
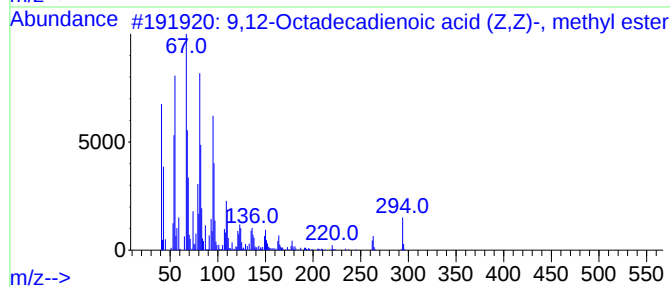
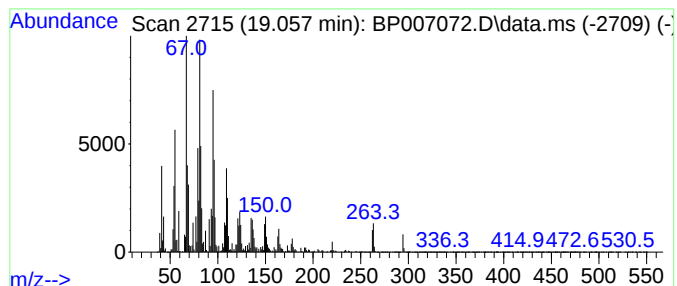
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Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	131.55 ng	29524900	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99



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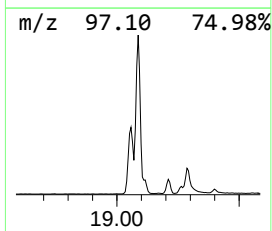
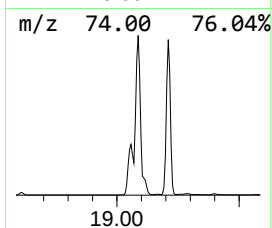
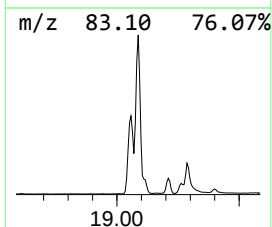
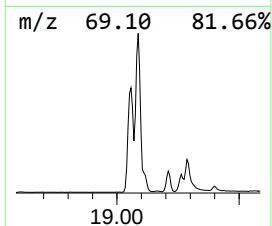
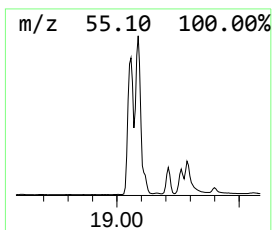
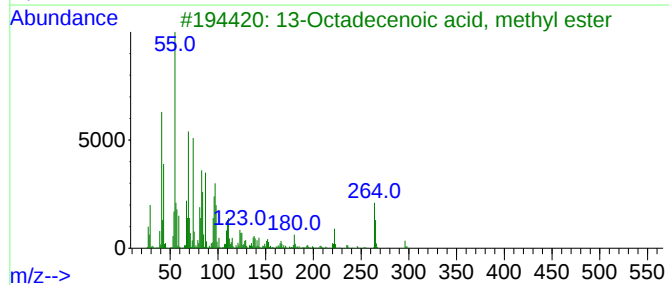
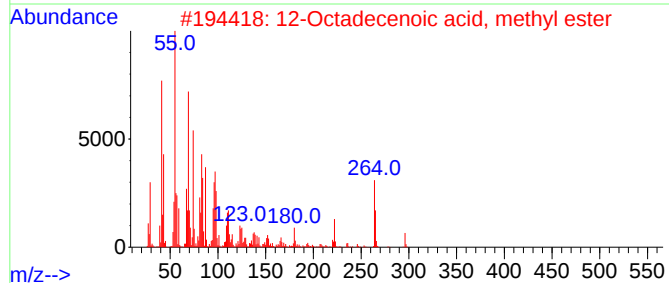
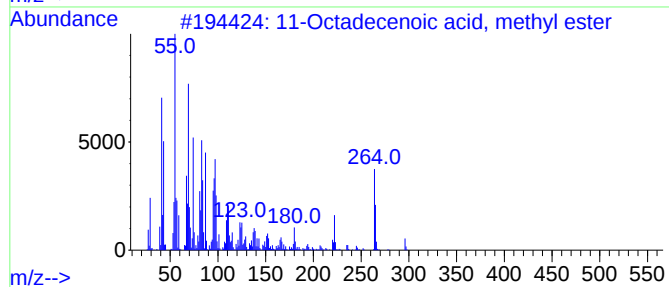
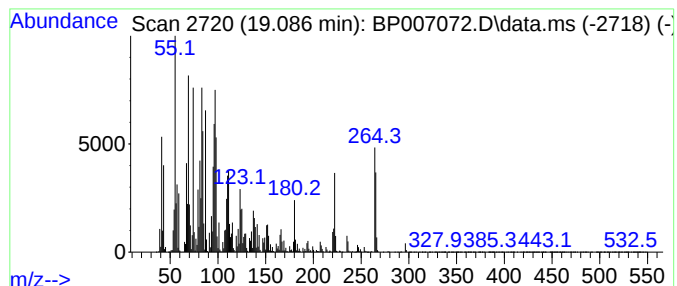
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Peak Number 4 11-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.087	92.42 ng	20743300	Phenanthrene-d10	17.281	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99



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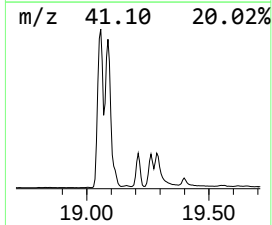
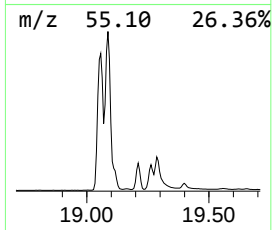
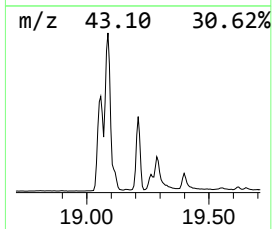
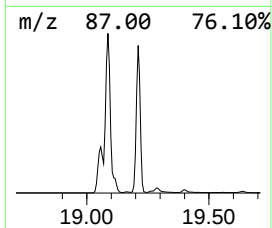
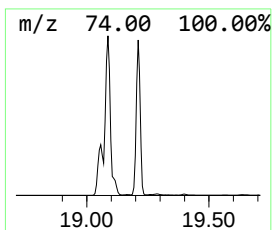
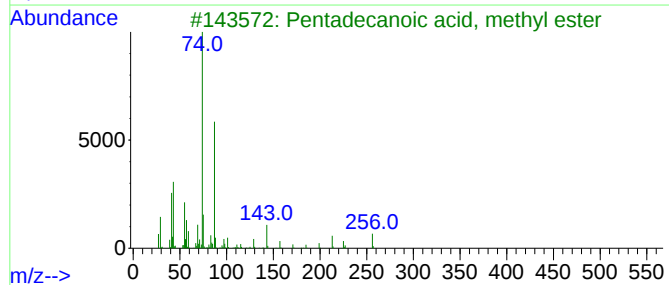
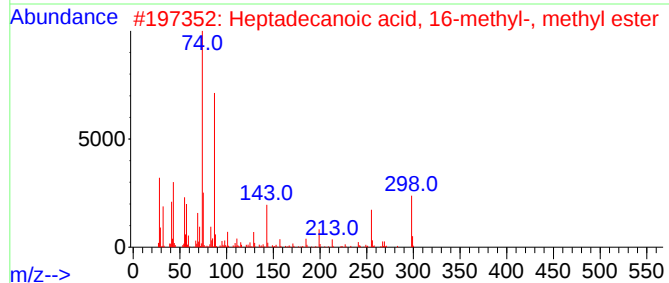
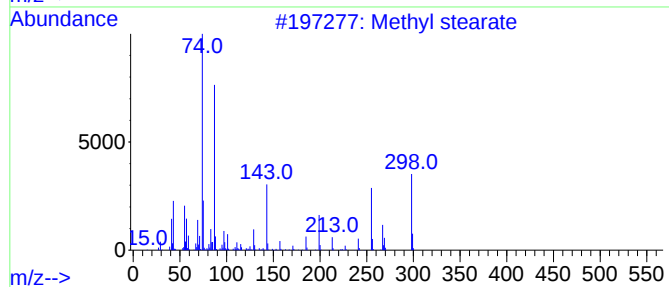
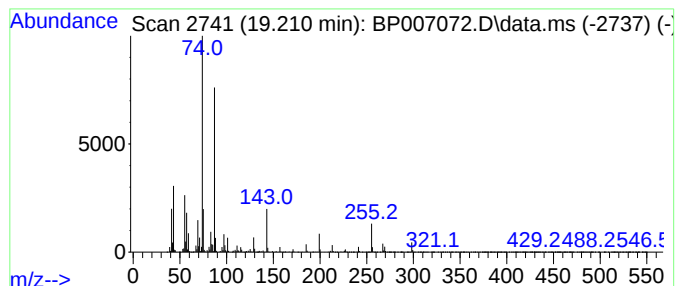
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Peak Number 5 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	15.80 ng	3546560	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	80



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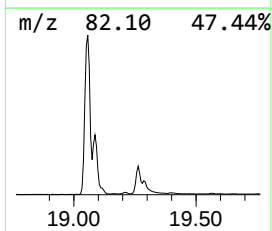
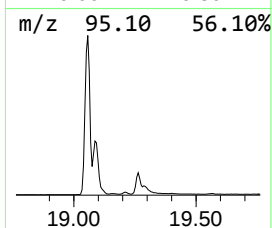
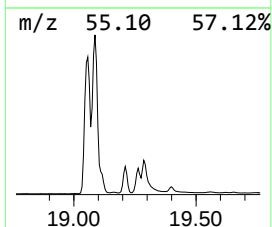
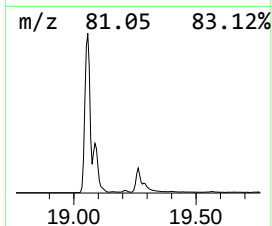
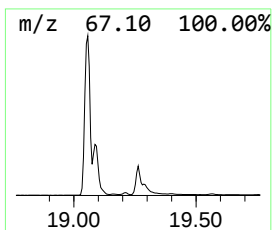
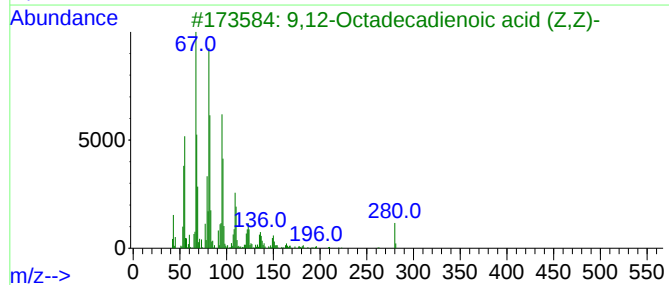
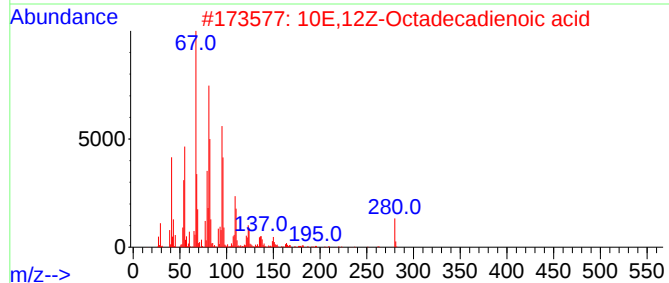
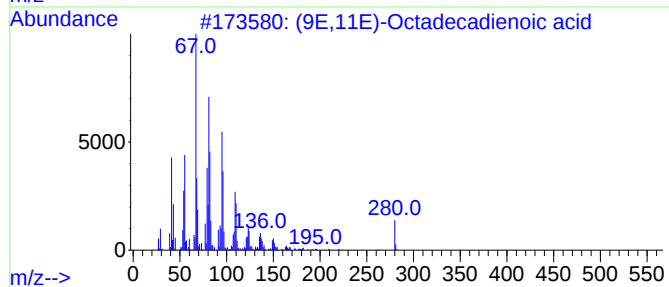
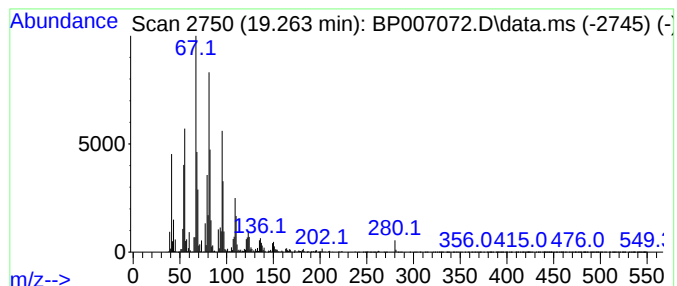
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ClientSampleId :
AU-06-091521

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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 (9E,11E)-Octadecadienoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.263	14.44 ng	3240510	Phenanthrene-d10	17.281	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	99
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	99
3	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
4	Linoleic acid	280	C18H32O2	000506-21-8	99
5	7-Hexadecyne	222	C16H30	074685-28-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007072.D
Acq On : 21 Sep 2021 03:38
Operator : CG/JU
Sample : M3757-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-06-091521

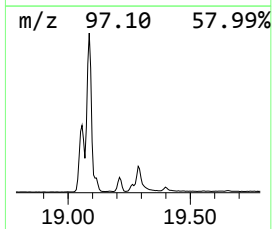
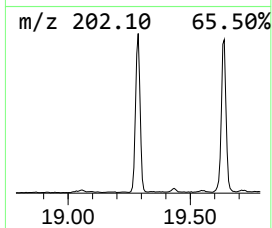
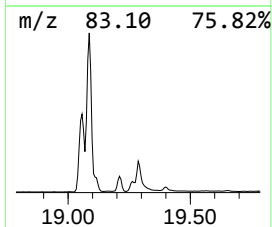
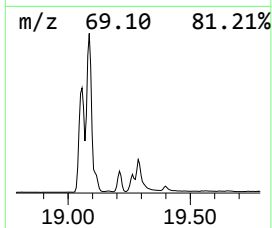
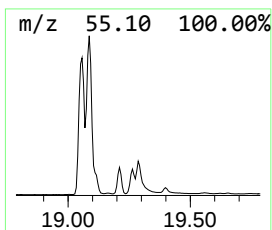
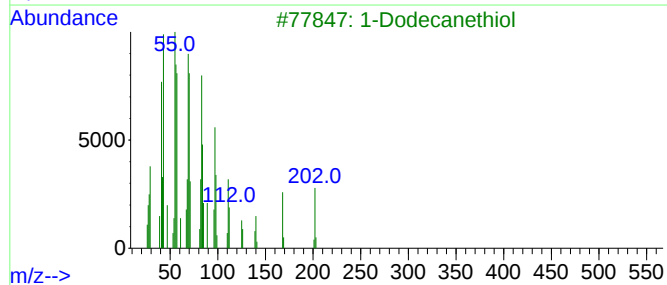
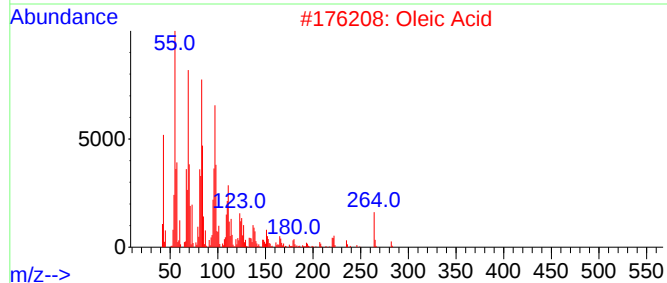
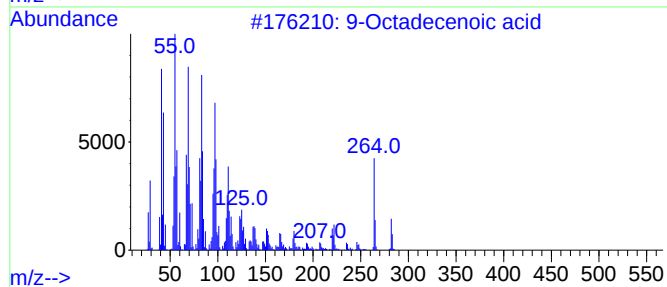
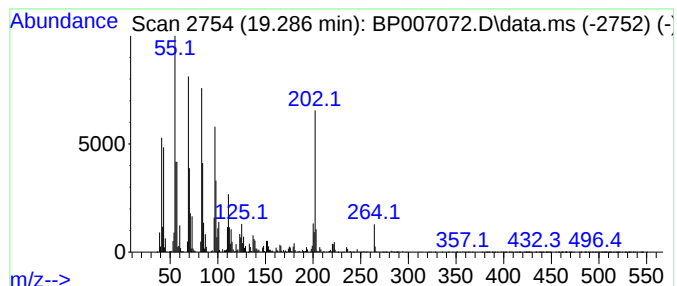
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.287	20.45 ng	4589150	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid	282	C18H34O2	002027-47-6	86
2			Oleic Acid	282	C18H34O2	000112-80-1	86
3			1-Dodecanethiol	202	C12H26S	000112-55-0	83
4			Cyclopentadecane	210	C15H30	000295-48-7	64
5			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007072.D
Acq On : 21 Sep 2021 03:38
Operator : CG/JU
Sample : M3757-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-06-091521

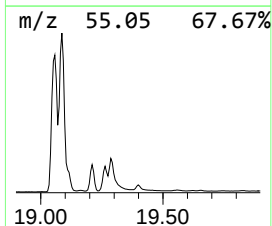
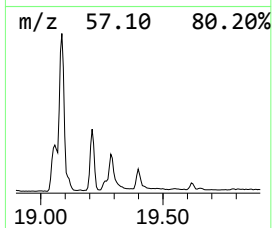
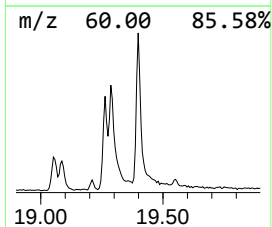
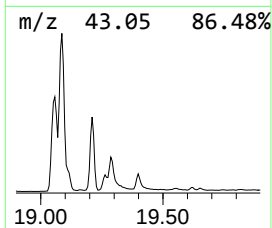
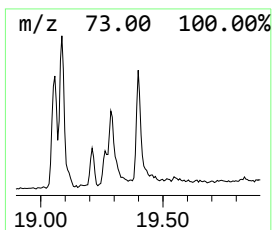
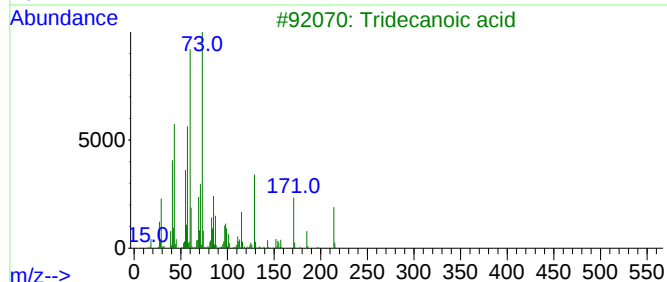
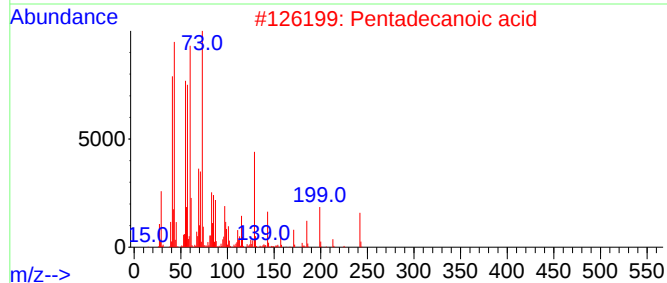
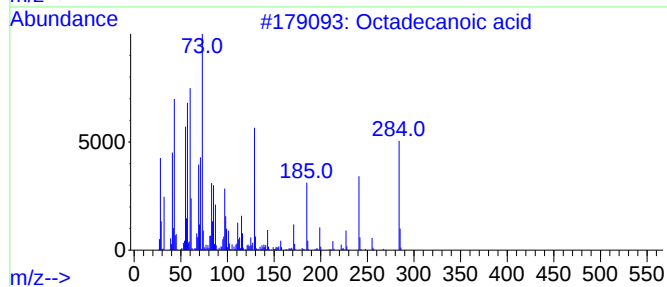
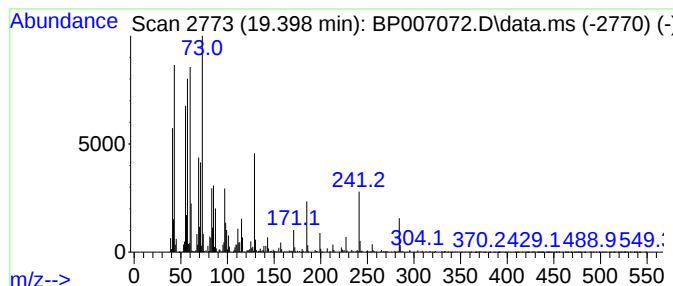
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	3.44 ng	830664	Chrysene-d12	21.363

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007072.D
Acq On : 21 Sep 2021 03:38
Operator : CG/JU
Sample : M3757-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AU-06-091521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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...	17.951	17.9	ng	4018010	4	17.281	4488760	20.0
n-Hexadecanoic ...	18.175	12.8	ng	2879850	4	17.281	4488760	20.0
9,12-Octadecadi...	19.057	131.6	ng	29524900	4	17.281	4488760	20.0
11-Octadecenoic...	19.087	92.4	ng	20743300	4	17.281	4488760	20.0
Methyl stearate	19.210	15.8	ng	3546560	4	17.281	4488760	20.0
(9E,11E)-Octade...	19.263	14.4	ng	3240510	4	17.281	4488760	20.0
9-Octadecenoic ...	19.287	20.4	ng	4589150	4	17.281	4488760	20.0
Octadecanoic acid	19.398	3.4	ng	830664	5	21.363	4832160	20.0