

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
 Data File : BG054962.D
 Acq On : 15 Sep 2022 18:58
 Operator : CG/JU
 Sample : N4644-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-6-091422

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_G\Methods\8270-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054962.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.669	397	405	416	rBV	521905	862415	4.67%	2.029%
2	7.285	672	680	693	rBV	520396	925276	5.01%	2.177%
3	8.125	816	823	831	rBV	150370	252644	1.37%	0.594%
4	9.306	1016	1024	1043	rBV	317111	590906	3.20%	1.390%
5	10.951	1297	1304	1312	rBV	201584	369343	2.00%	0.869%
6	13.390	1712	1719	1729	rVB	987045	1508442	8.17%	3.549%
7	14.765	1945	1953	1960	rVB	320062	509912	2.76%	1.200%
8	16.257	2200	2207	2225	rBV	550643	911703	4.94%	2.145%
9	17.514	2415	2421	2426	rBV	375939	578320	3.13%	1.361%
10	18.161	2523	2531	2536	rBV	4965807	7348008	39.81%	17.287%
11	19.312	2716	2727	2729	rBV3	7255775	18456357	100.00%	43.422%
12	19.412	2741	2744	2746	rVB	190098	194356	1.05%	0.457%
13	19.453	2746	2751	2756	rVB	3703750	4605612	24.95%	10.835%
14	19.565	2763	2770	2778	rBV	116126	259075	1.40%	0.610%
15	20.123	2859	2865	2870	rBV	1469534	1939954	10.51%	4.564%
16	20.429	2908	2917	2926	rVB3	275126	596857	3.23%	1.404%
17	20.534	2931	2935	2939	rBV	391355	433473	2.35%	1.020%
18	20.587	2939	2944	2950	rBV7	96262	201850	1.09%	0.475%
19	21.192	3041	3047	3052	rVB2	123297	247408	1.34%	0.582%
20	21.568	3106	3111	3120	rVB	335300	479466	2.60%	1.128%
21	21.809	3146	3152	3157	rBV	344699	590048	3.20%	1.388%
22	25.182	3718	3726	3738	rVB3	210119	643542	3.49%	1.514%

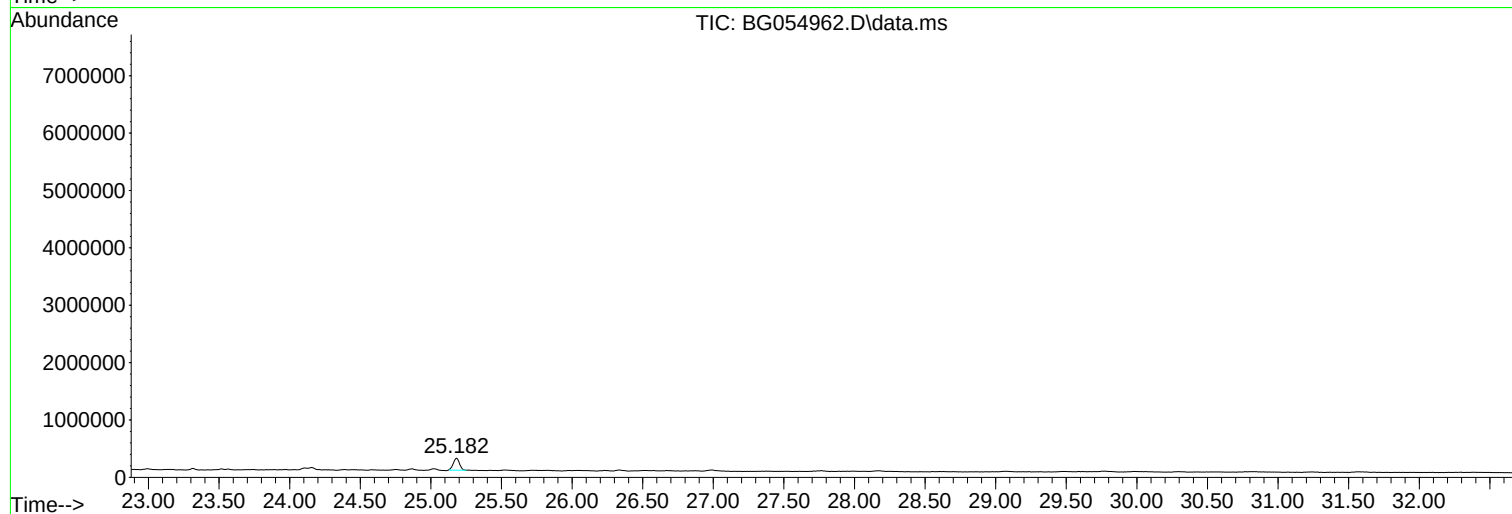
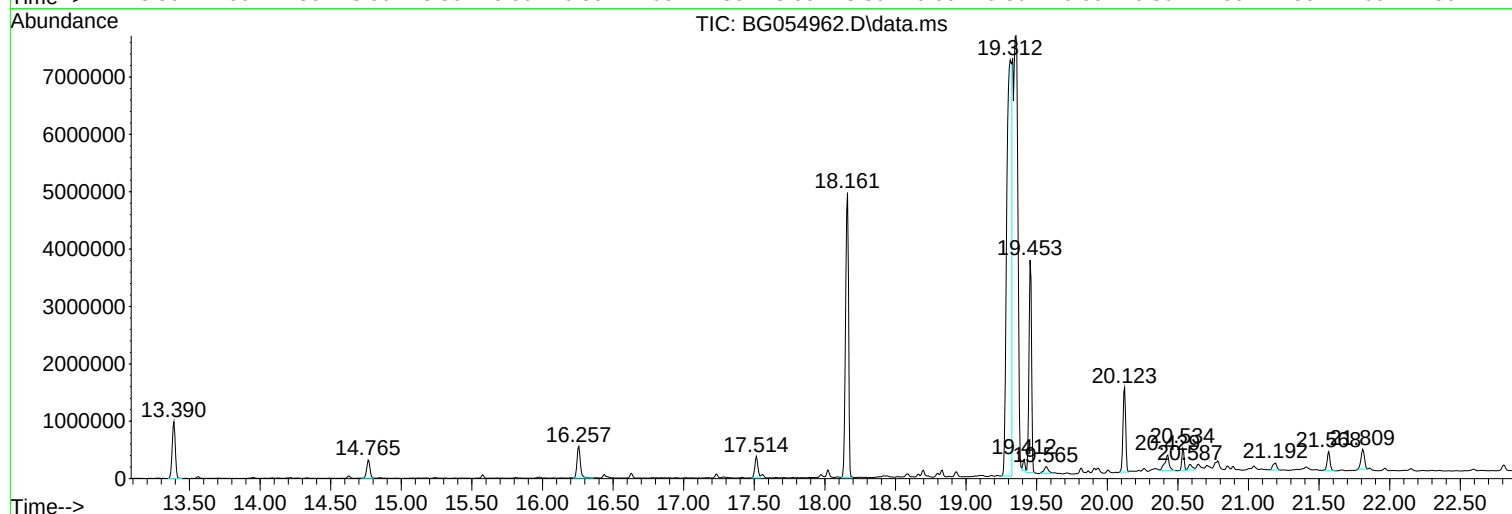
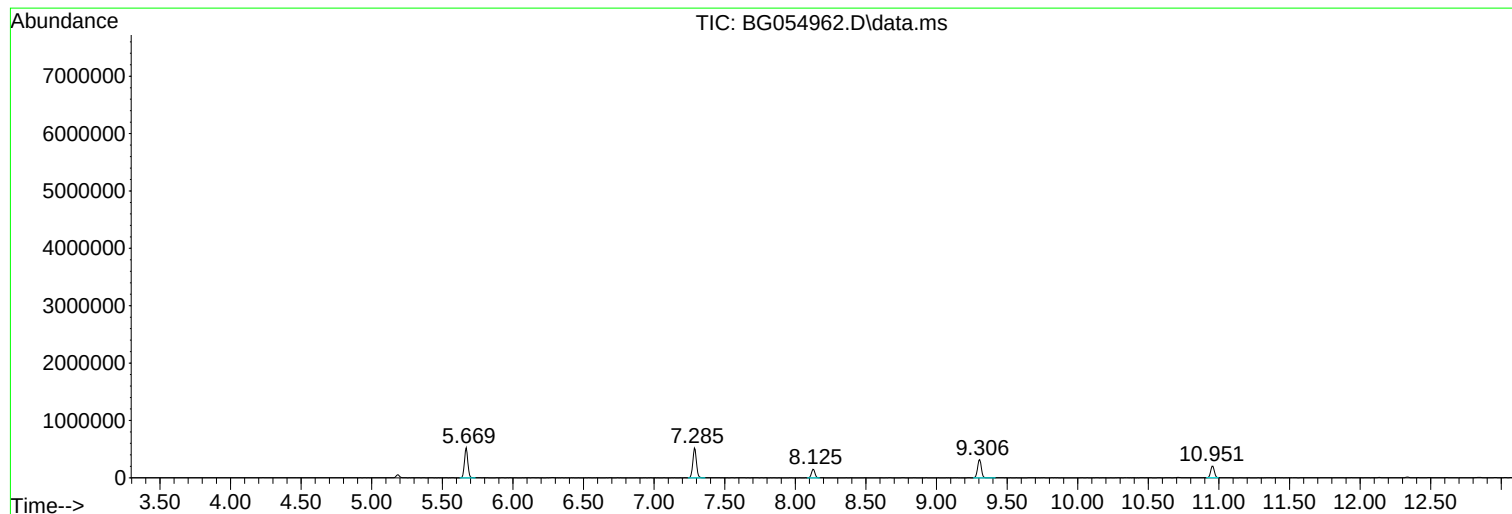
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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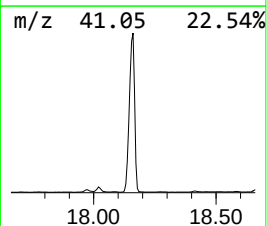
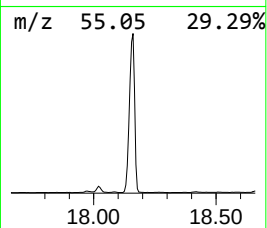
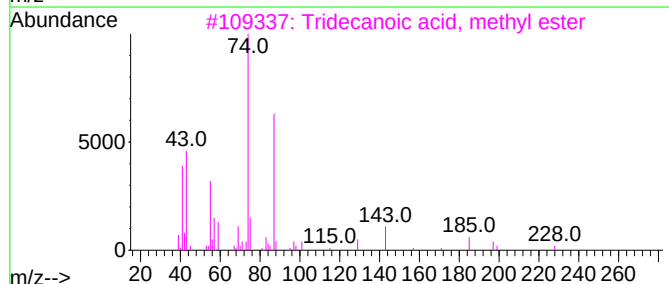
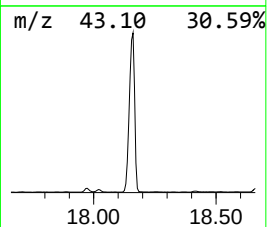
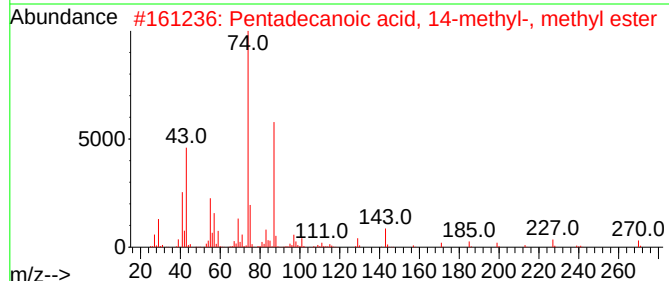
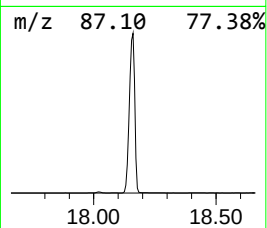
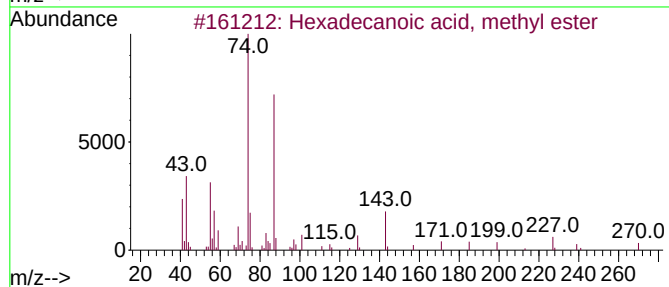
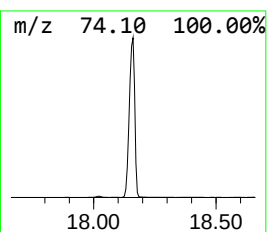
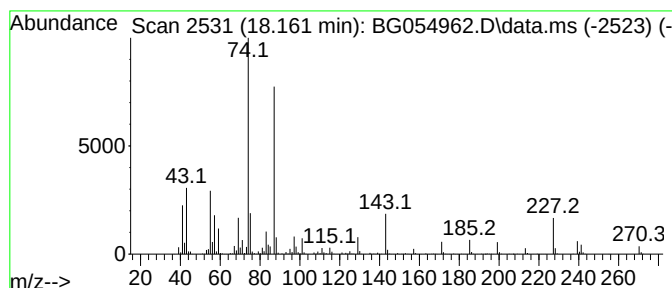
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.161	254.12 ng	7348010	Phenanthrene-d10	17.514

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			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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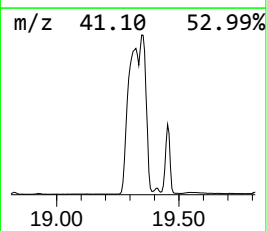
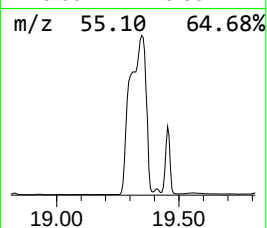
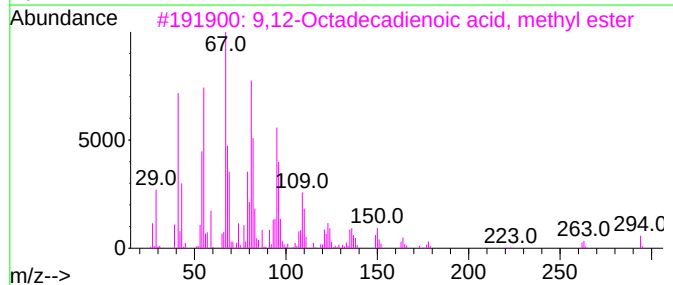
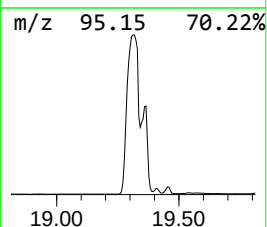
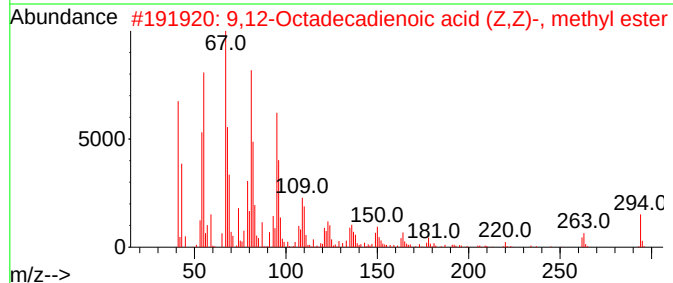
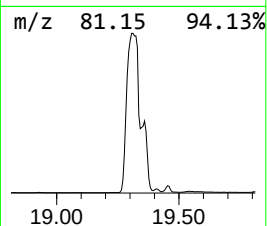
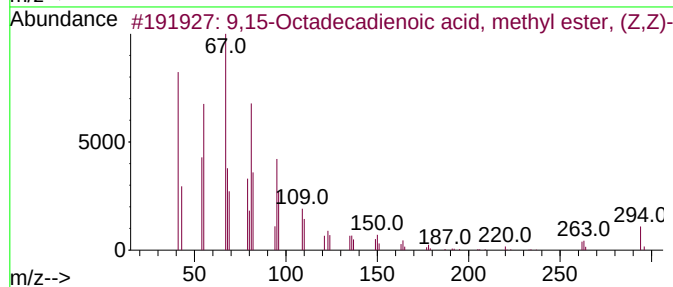
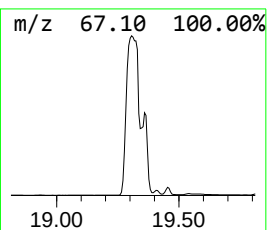
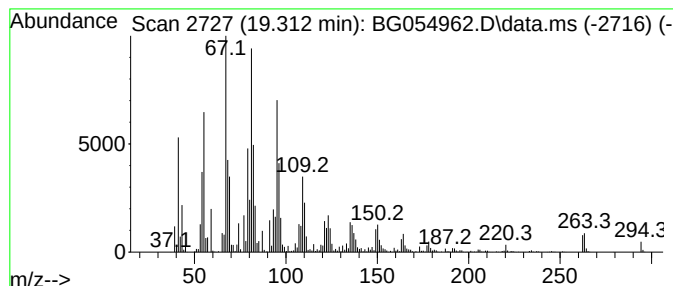
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 9,15-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.312	638.27 ng	18456400	Phenanthrene-d10	17.514	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99



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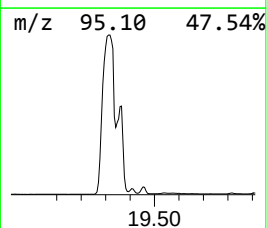
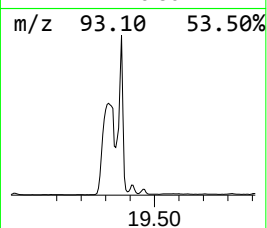
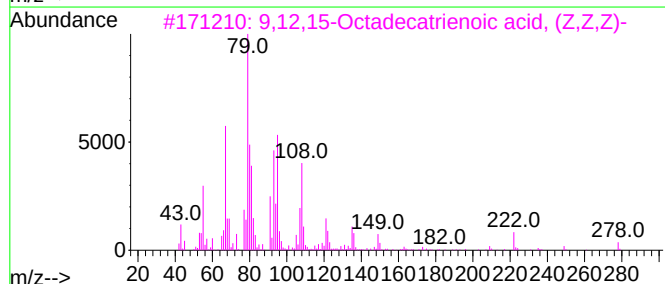
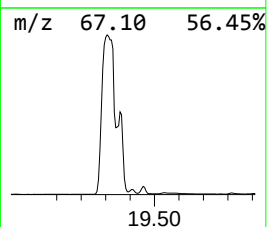
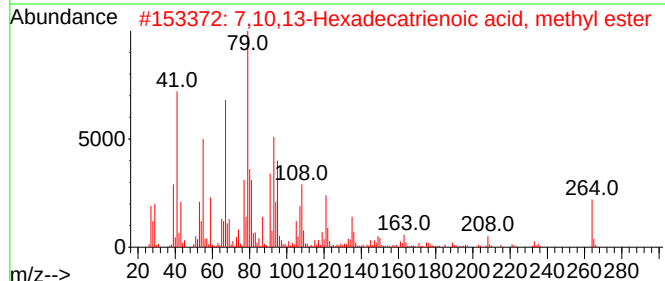
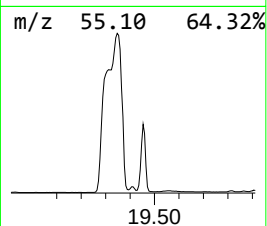
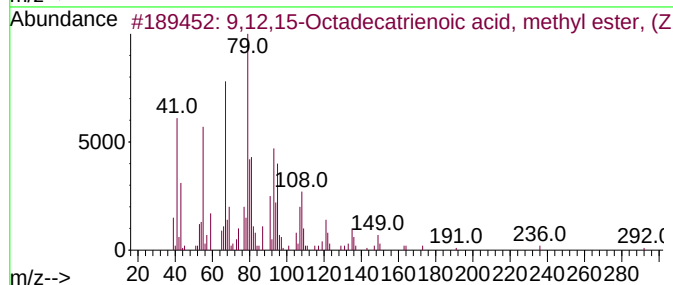
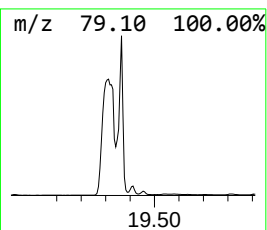
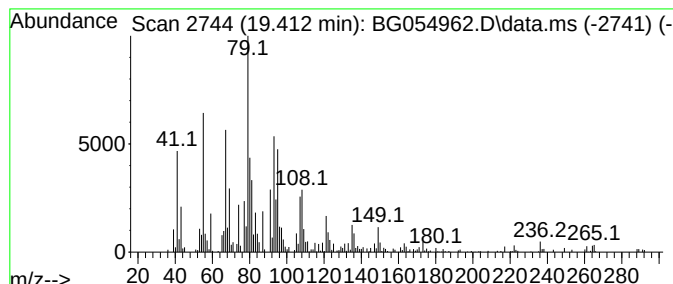
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Peak Number 3 9,12,15-Octadecatrienoic ac... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.412	6.72 ng	194356	Phenanthrene-d10	17.514	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	95
2	7,10,13-Hexadecatrienoic acid, m...	264	C17H28O2	056554-30-4	93
3	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	90
4	9,12,15-Octadecatrien-1-ol, (Z,Z...	264	C18H32O	000506-44-5	89
5	Methyl 8,11,14-heptadecatrienoate	278	C18H30O2	1000336-35-1	81



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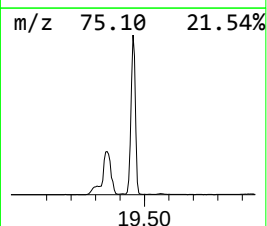
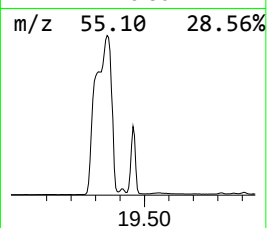
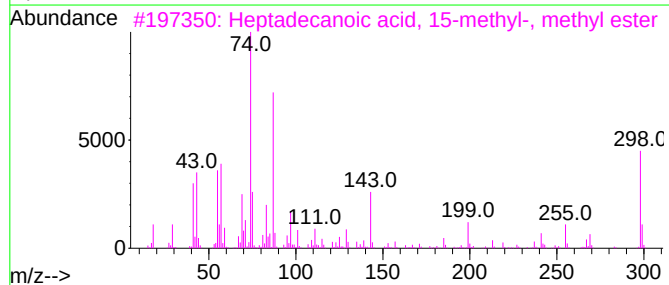
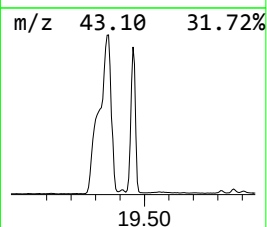
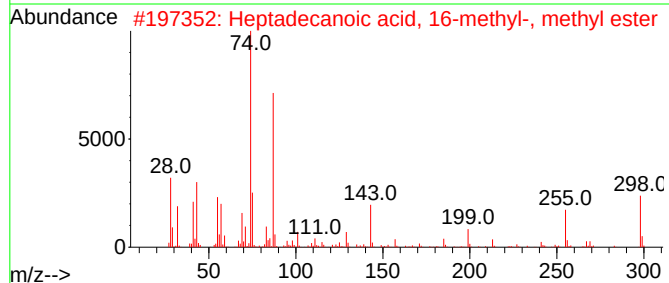
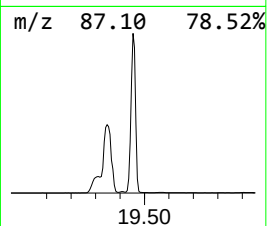
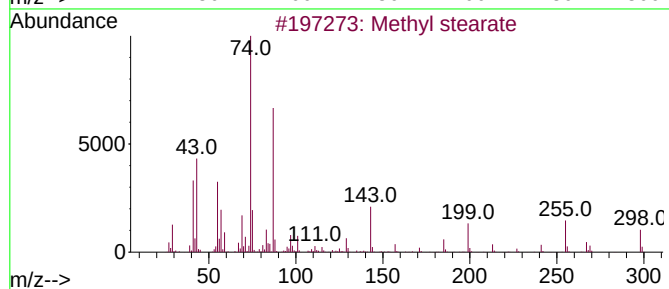
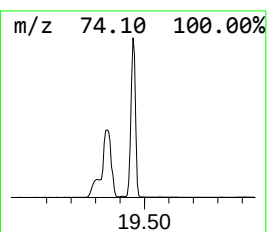
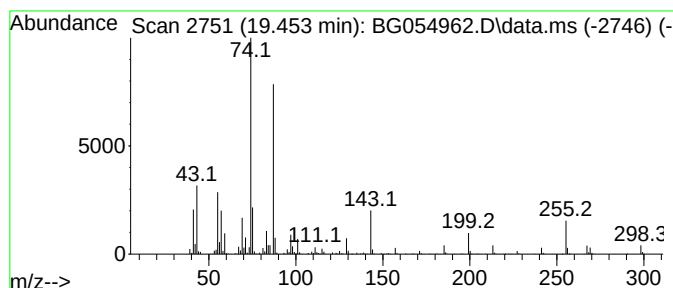
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.453	159.28 ng	4605610	Phenanthrene-d10	17.514

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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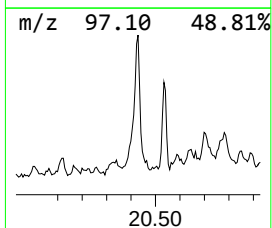
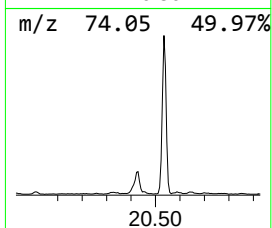
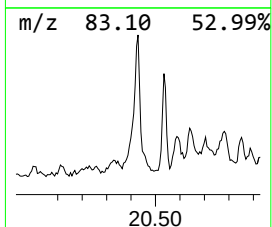
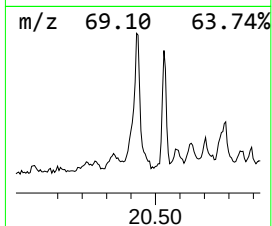
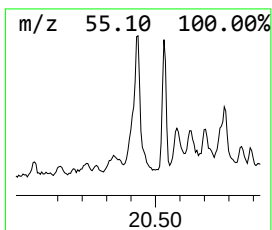
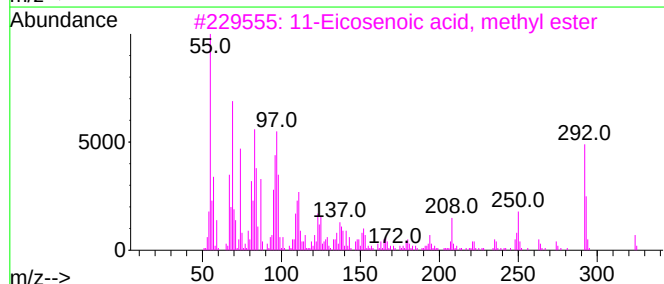
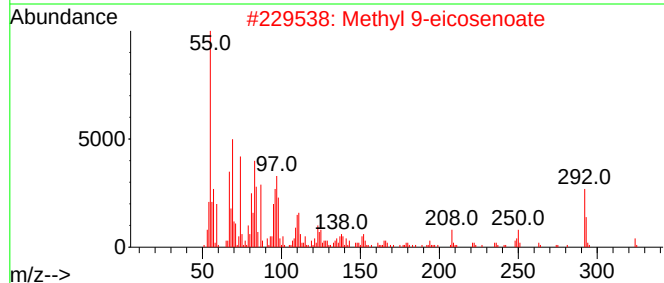
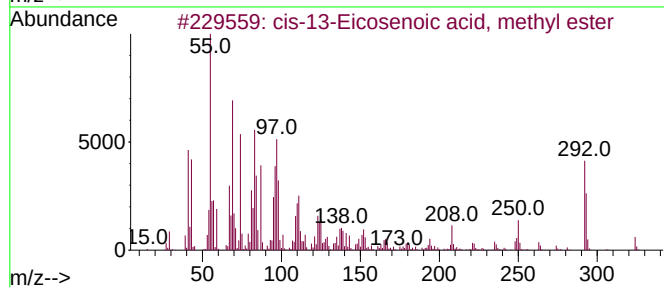
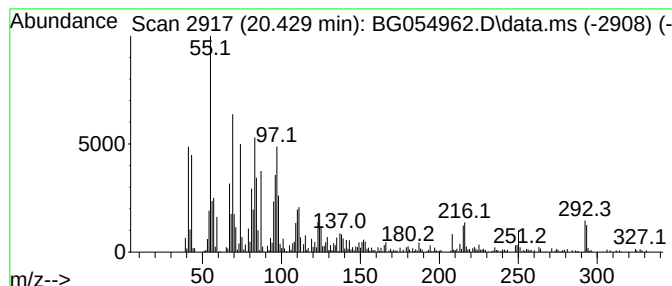
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TIC Integration Parameters: LSCINT.P

Peak Number 5 cis-13-Eicosenoic acid, met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.429	20.23 ng	596857	Chrysene-d12	21.809	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	99
2	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	99
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
4	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91
5	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	89



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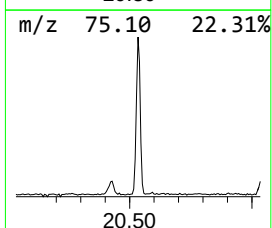
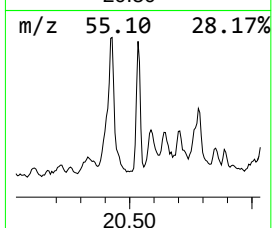
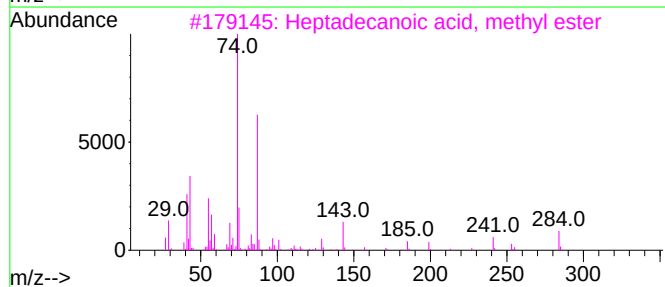
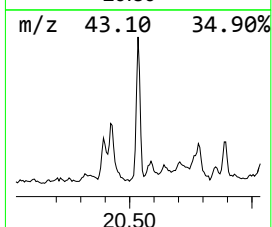
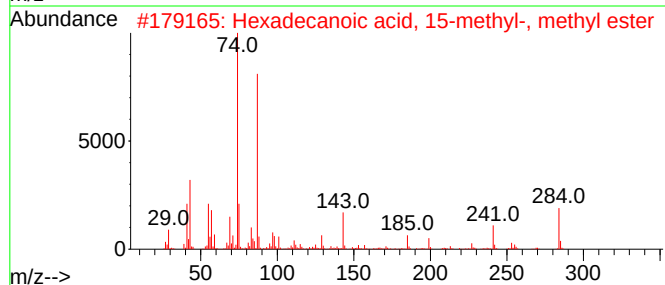
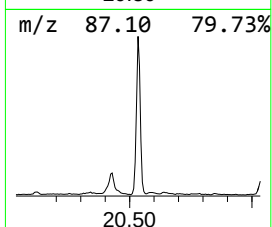
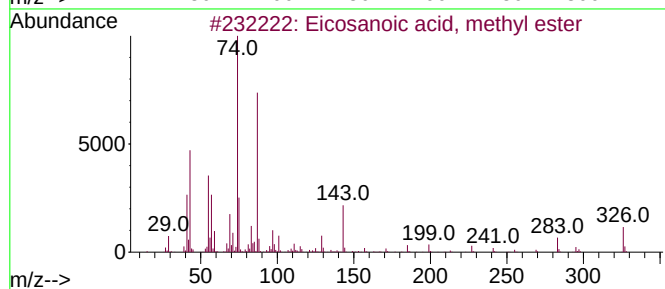
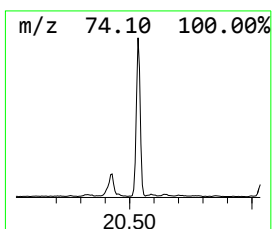
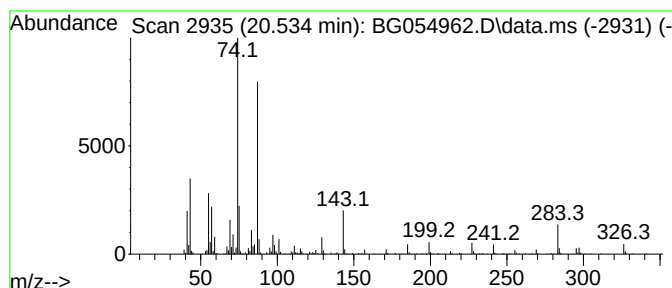
Instrument :
BNA_G
ClientSampleId :
TR-6-091422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.534	14.69 ng	433473	Chrysene-d12	21.809	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	96
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054962.D
Acq On : 15 Sep 2022 18:58
Operator : CG/JU
Sample : N4644-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-091422

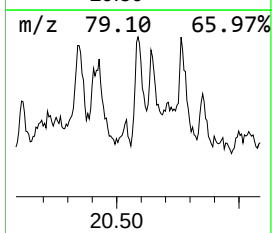
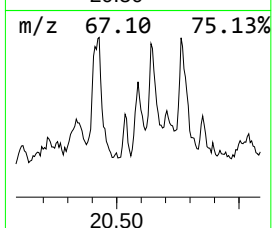
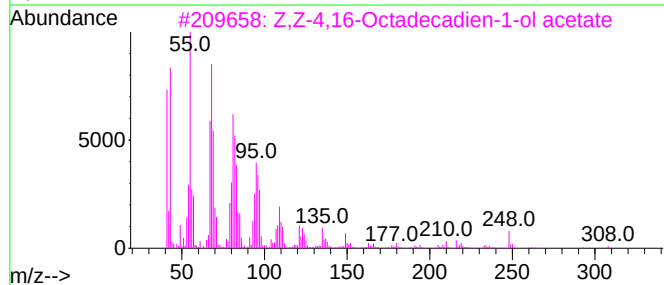
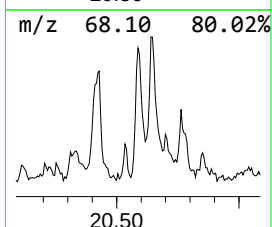
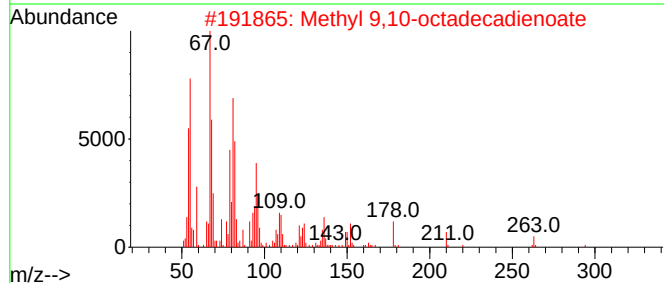
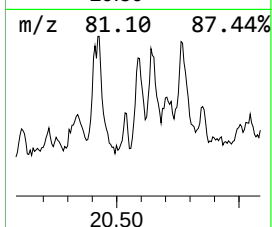
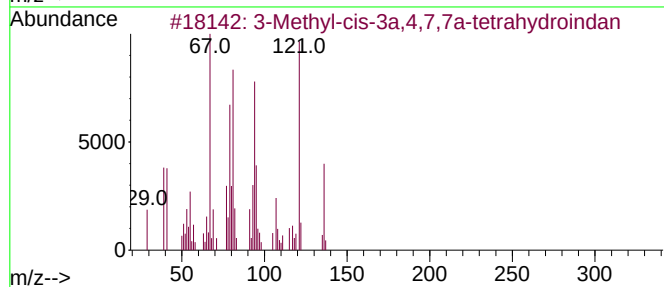
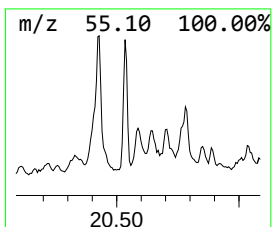
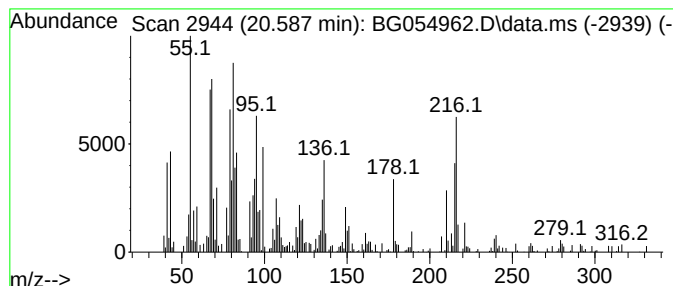
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.587 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.587	6.84 ng	201850	Chrysene-d12	21.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-cis-3a,4,7,7a-tetrahydr...	136	C10H16	1000144-04-4	46
2			Methyl 9,10-octadecadienoate	294	C19H34O2	1010336-45-7	42
3			Z,Z-4,16-Octadecadien-1-ol acetate	308	C20H36O2	1000130-95-7	42
4			1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	35
5			Undec-10-ynoic acid, tridec-2-yn...	360	C24H40O2	1000406-96-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054962.D
Acq On : 15 Sep 2022 18:58
Operator : CG/JU
Sample : N4644-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

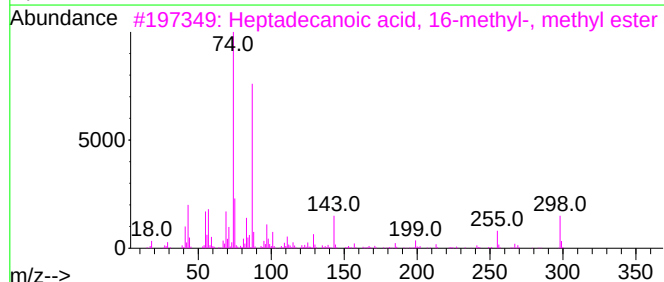
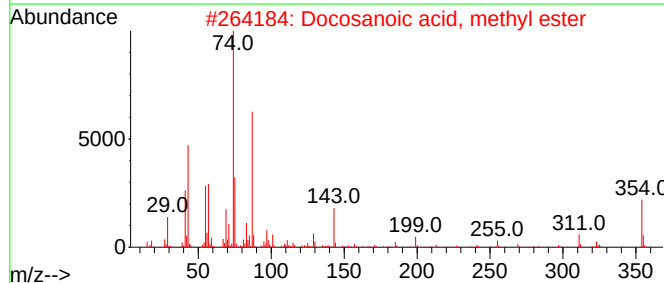
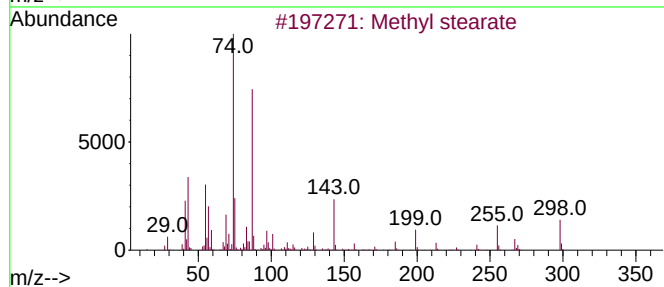
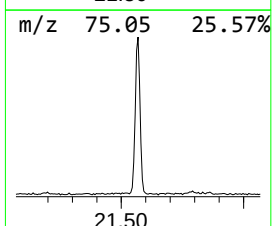
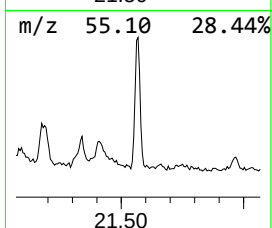
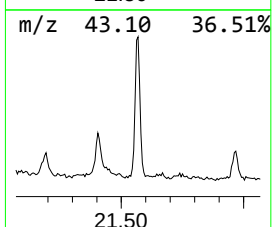
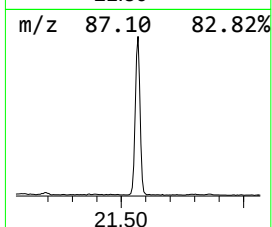
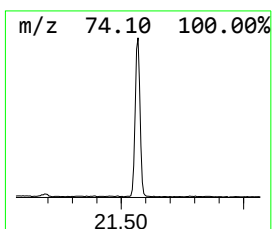
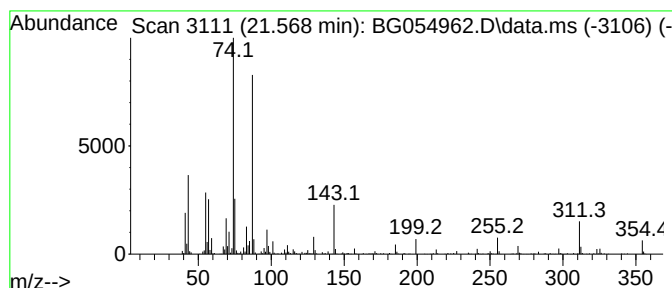
Instrument :
BNA_G
ClientSampleId :
TR-6-091422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.568	16.25 ng	479466	Chrysene-d12		21.809	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	98
2		Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	97
3		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	87
4		Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	87
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054962.D
Acq On : 15 Sep 2022 18:58
Operator : CG/JU
Sample : N4644-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-091422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	18.161	254.1	ng	7348010	4	17.514	578320	20.0
9,15-Octadecadi...	19.312	638.3	ng	18456400	4	17.514	578320	20.0
9,12,15-Octadec...	19.412	6.7	ng	194356	4	17.514	578320	20.0
Methyl stearate	19.453	159.3	ng	4605610	4	17.514	578320	20.0
cis-13-Eicoseno...	20.429	20.2	ng	596857	5	21.809	590048	20.0
Eicosanoic acid...	20.534	14.7	ng	433473	5	21.809	590048	20.0
unknown20.587	20.587	6.8	ng	201850	5	21.809	590048	20.0
4-[(E)-5-Hydrox...	21.192	8.4	ng	247408	5	21.809	590048	20.0
Docosanoic acid...	21.568	16.3	ng	479466	5	21.809	590048	20.0