

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
 Data File : BG055135.D
 Acq On : 11 Oct 2022 20:48
 Operator : CG/JU
 Sample : N5080-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-6-101022

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.853	429	436	446	rBV	623694	1041957	1.70%	0.729%
2	7.463	702	710	722	rBV	653022	1158552	1.89%	0.811%
3	9.501	1050	1057	1064	rBV	392548	721276	1.17%	0.505%
4	13.567	1742	1749	1759	rVB	1073467	1650537	2.69%	1.155%
5	16.411	2228	2233	2241	rVB	781359	1212287	1.97%	0.848%
6	18.332	2550	2560	2564	rBV	12139673	21150310	34.41%	14.799%
7	18.585	2591	2603	2613	rBV2	2112742	4213522	6.86%	2.948%
8	18.743	2622	2630	2638	rBV3	273862	662371	1.08%	0.463%
9	18.849	2644	2648	2659	rVB2	447359	730880	1.19%	0.511%
10	19.460	2741	2752	2760	rBV3	14117409	61459034	100.00%	43.003%
11	19.548	2765	2767	2770	rVB2	14460464	12784561	20.80%	8.945%
12	19.619	2774	2779	2783	rVB	10383077	13302419	21.64%	9.308%
13	19.689	2783	2791	2794	rBV	4933975	11015585	17.92%	7.708%
14	20.077	2850	2857	2865	rVB	426806	1147681	1.87%	0.803%
15	20.265	2884	2889	2893	rVB	1660260	2051046	3.34%	1.435%
16	20.565	2937	2940	2947	rVB	986086	1351193	2.20%	0.945%
17	20.671	2954	2958	2962	rBV	1109289	1243754	2.02%	0.870%
18	20.718	2962	2966	2971	rBV2	523575	832906	1.36%	0.583%
19	20.923	2994	3001	3007	rVV3	394083	815147	1.33%	0.570%
20	20.982	3007	3011	3017	rVB2	747991	1165640	1.90%	0.816%
21	21.335	3065	3071	3077	rVB3	410014	887454	1.44%	0.621%
22	21.734	3134	3139	3147	rVB	924061	1333275	2.17%	0.933%
23	21.969	3172	3179	3184	rBV2	362138	985349	1.60%	0.689%

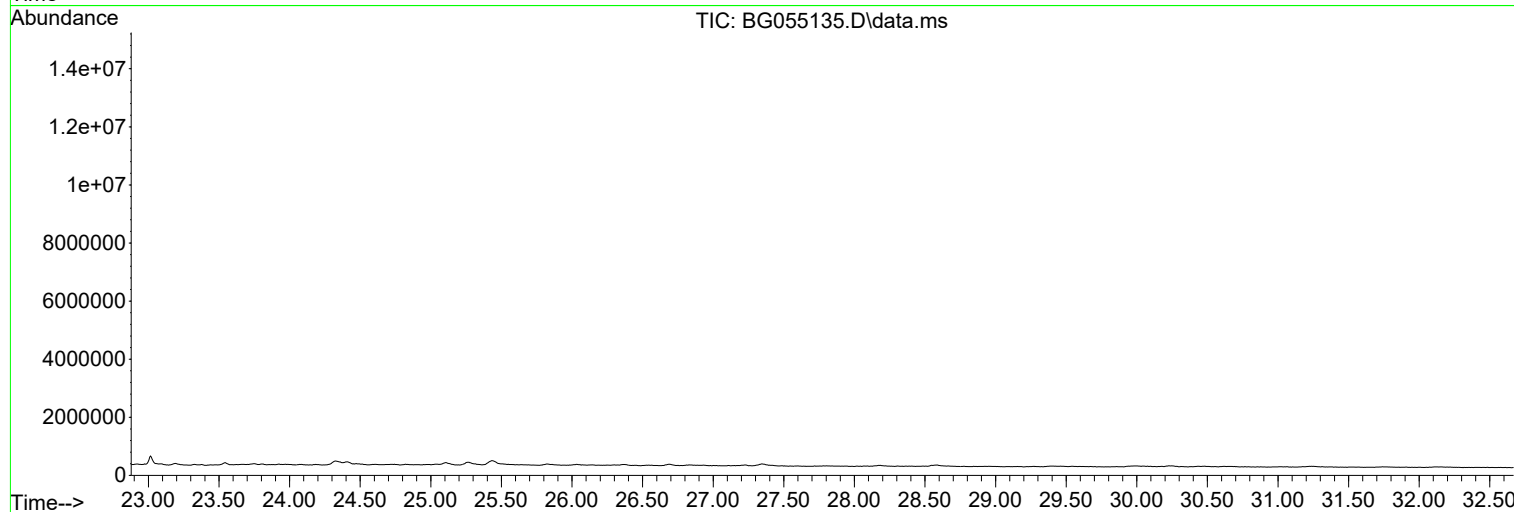
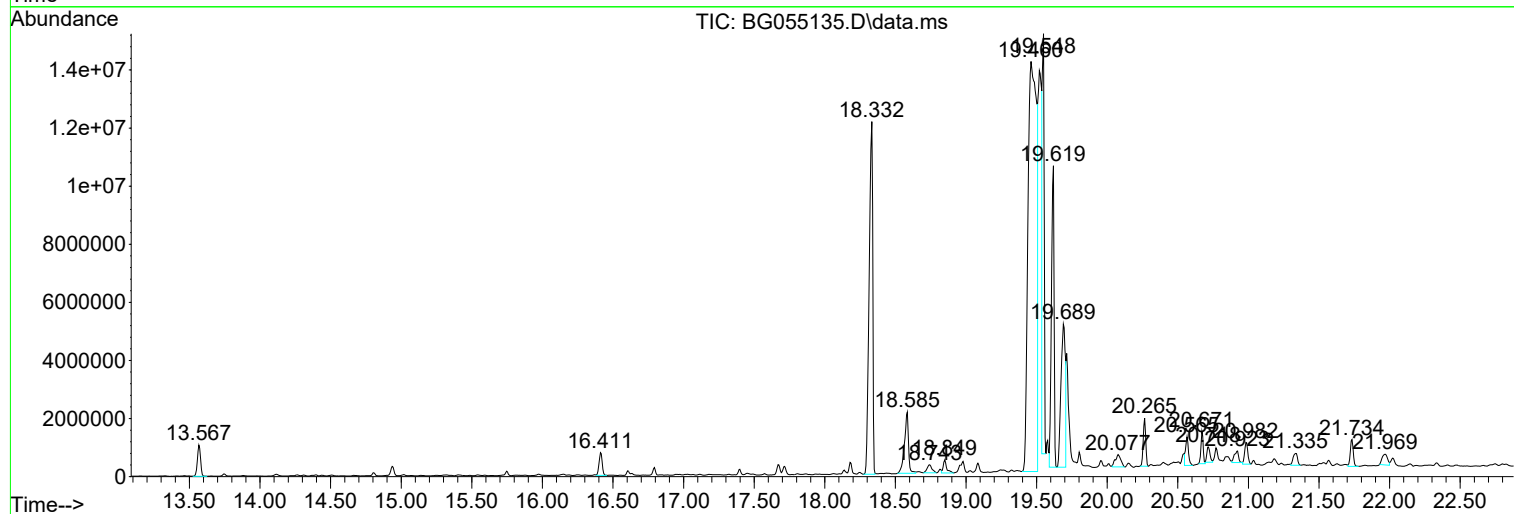
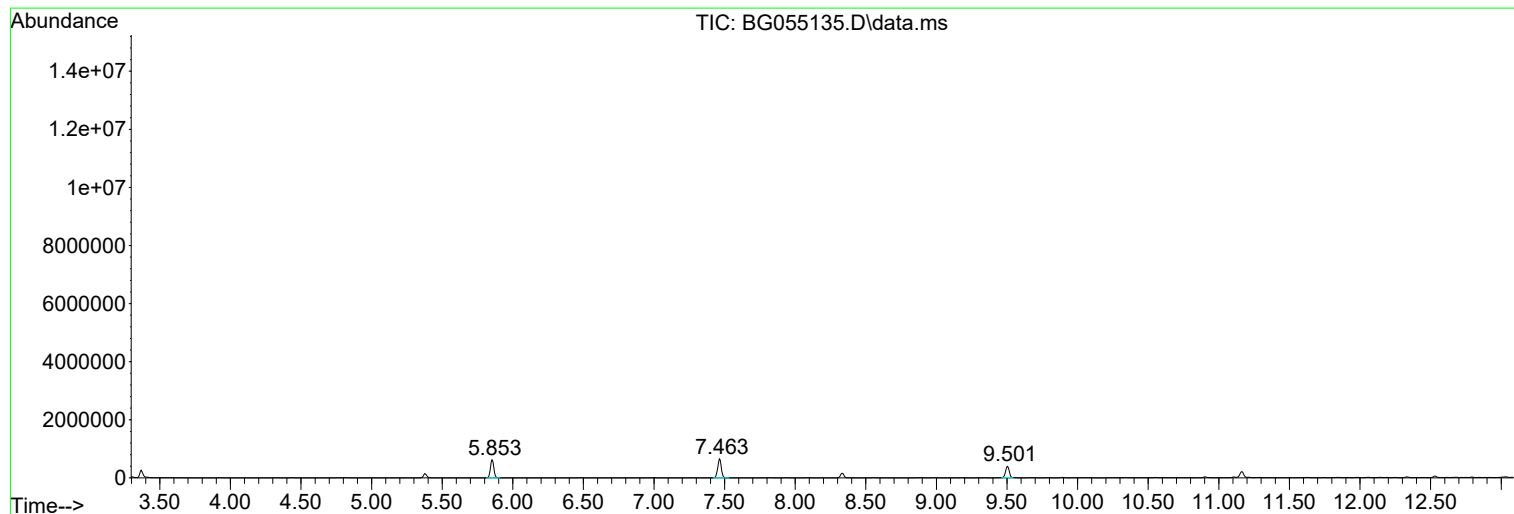
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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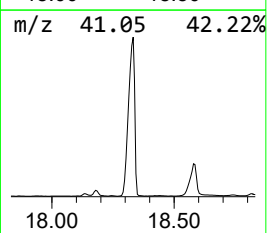
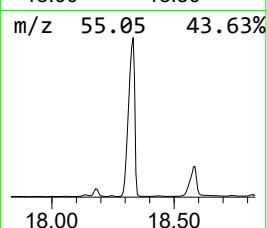
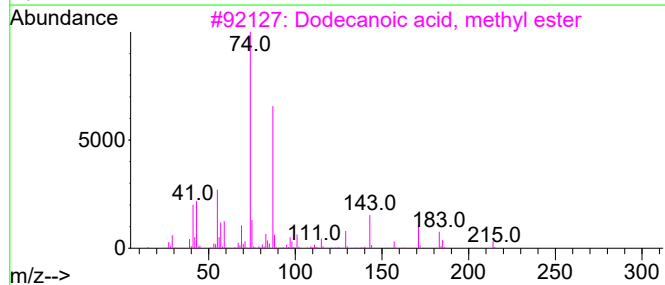
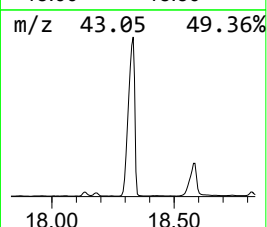
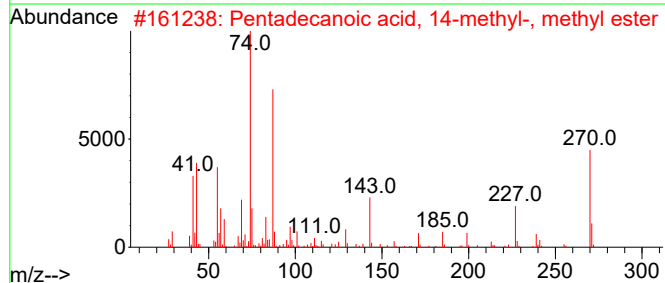
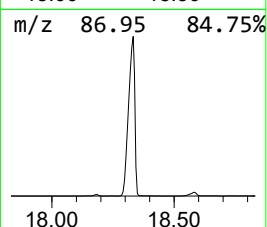
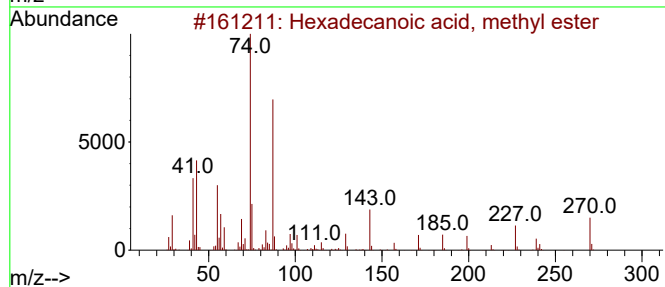
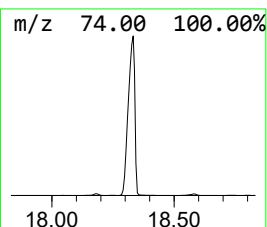
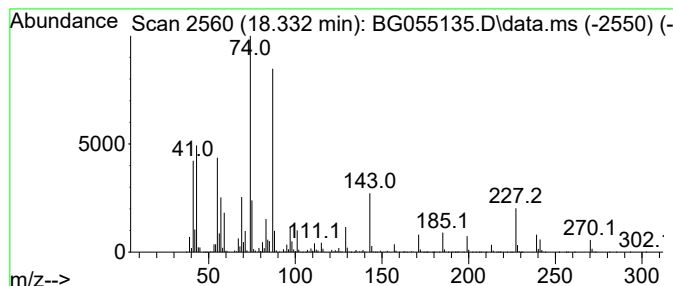
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
18.332	20.00 ng	21150300	Phenanthrene-d10	17.668

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	94
3			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87
4			Silane, methylvinyl(trans-2-meth...	270	C15H30O2Si	1000421-08-5	86
5			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	81



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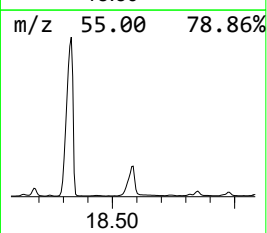
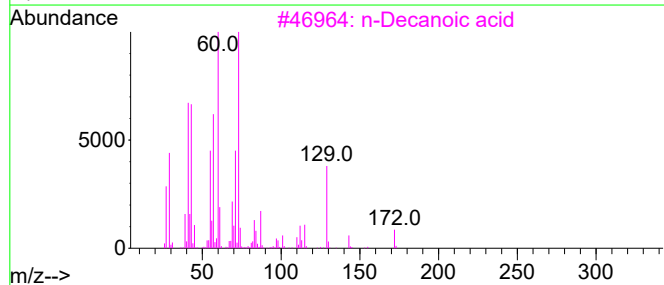
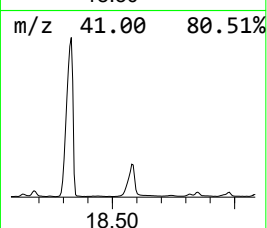
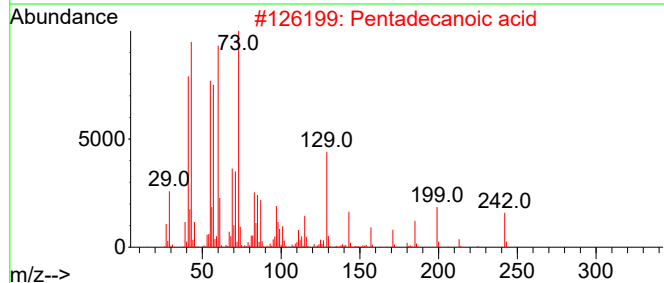
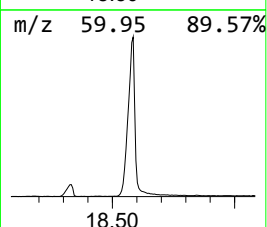
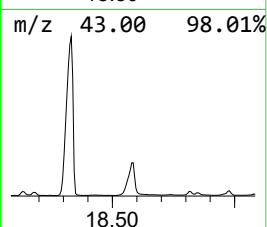
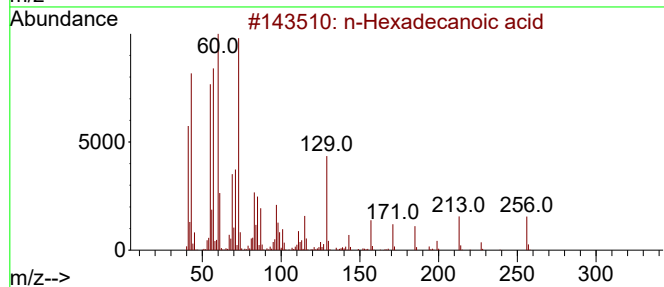
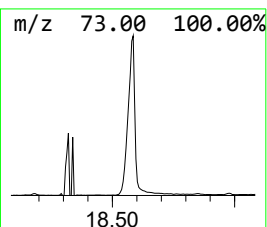
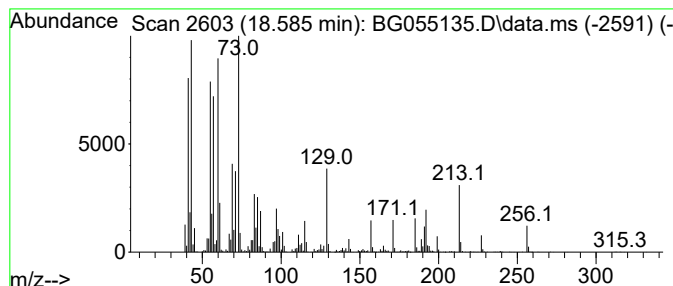
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.585	3.98 ng	4213520	Phenanthrene-d10	17.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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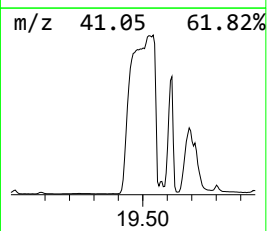
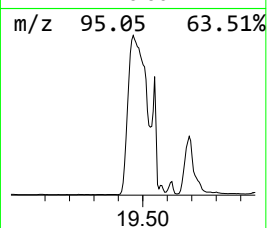
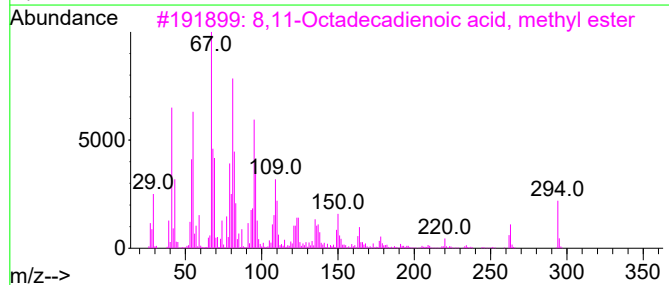
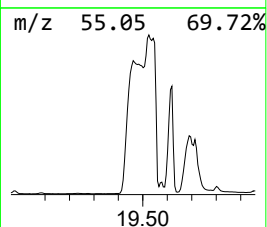
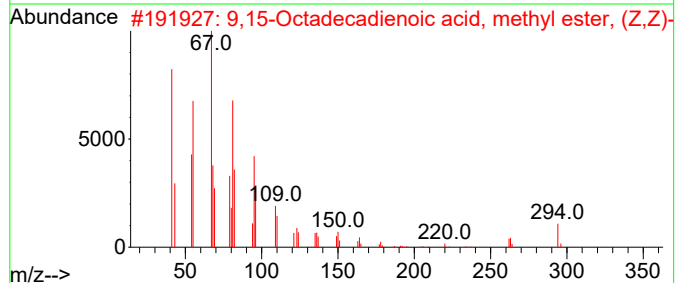
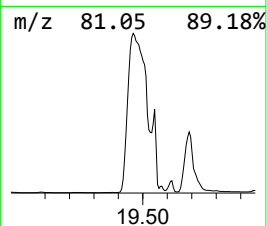
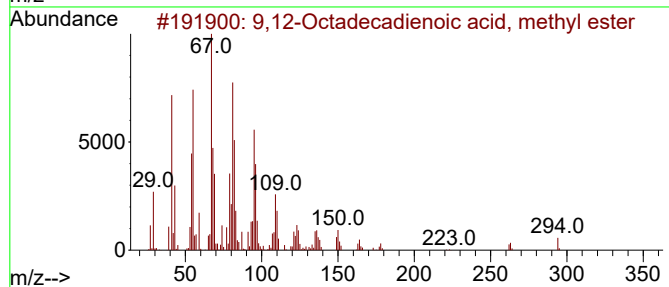
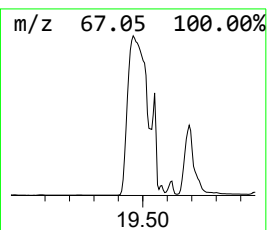
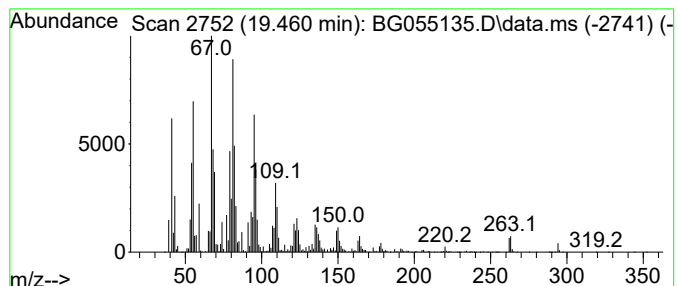
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.460	58.12 ng	61459000	Phenanthrene-d10	17.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98



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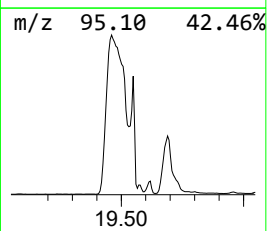
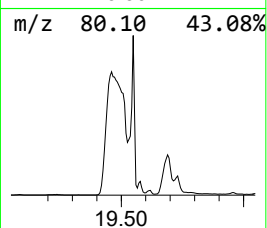
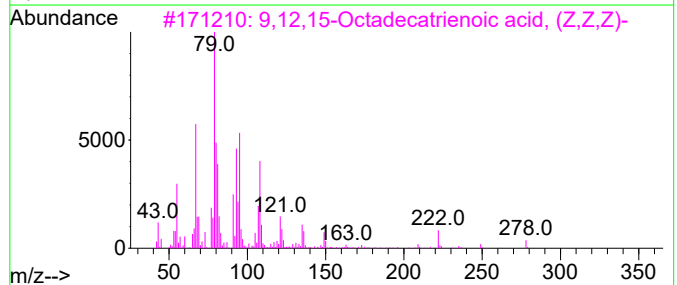
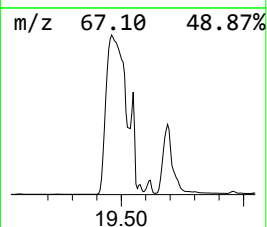
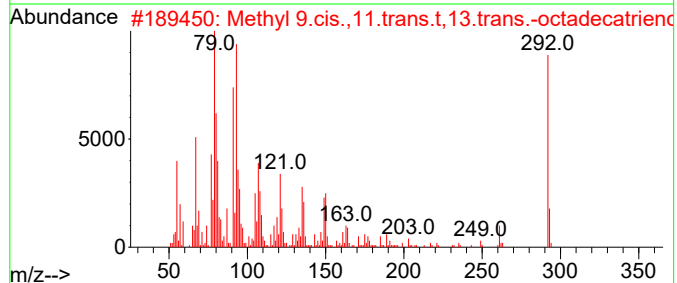
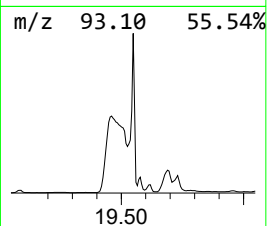
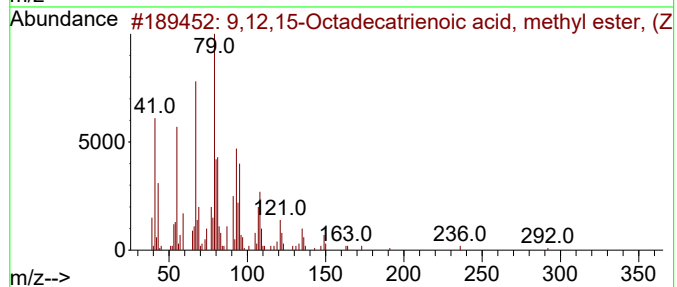
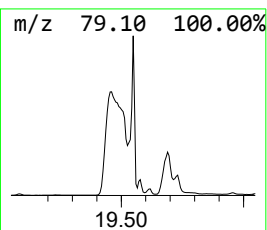
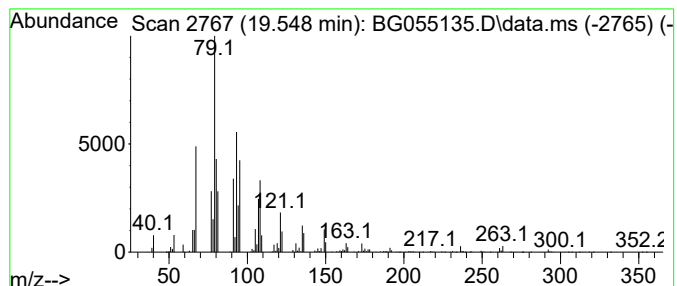
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9,12,15-Octadecatrienoic ac... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.548	12.09 ng	12784600	Phenanthrene-d10	17.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	91		
2	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	89		
3	9,12,15-Octadecatrienoic acid, (...)	278	C18H30O2	000463-40-1	87		
4	11,14,17-Eicosatrienoic acid, me...	320	C21H36O2	055682-88-7	83		
5	3-Heptadecen-5-yne, (Z)-	234	C17H30	074744-55-1	83		



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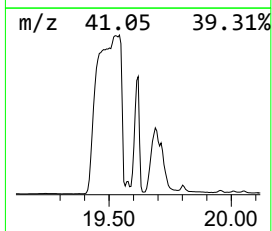
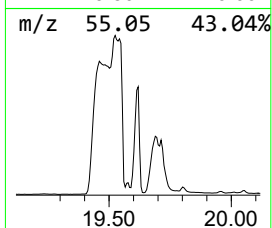
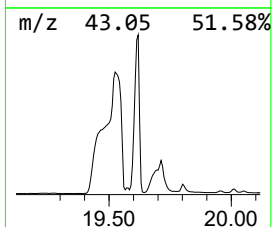
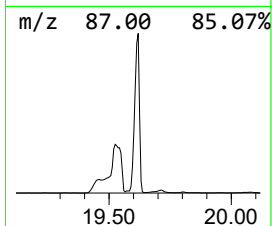
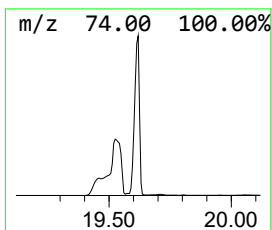
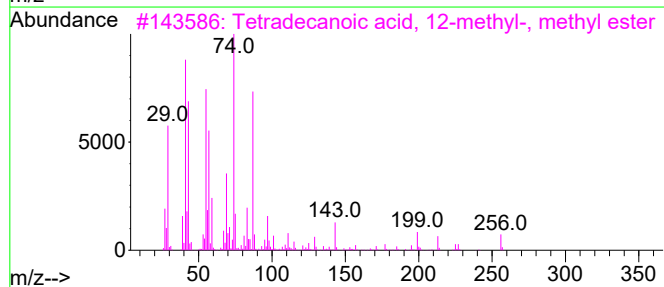
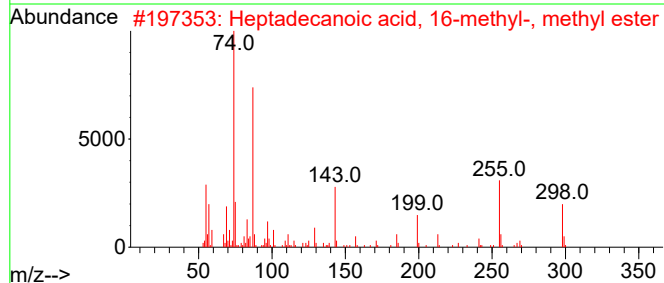
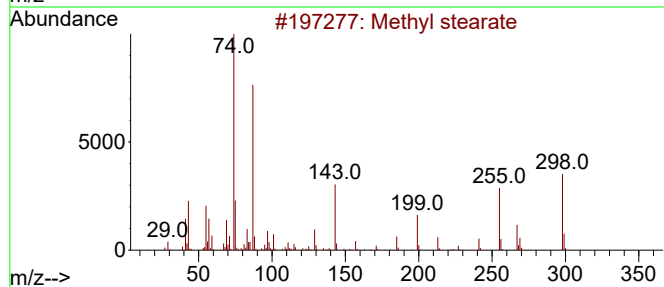
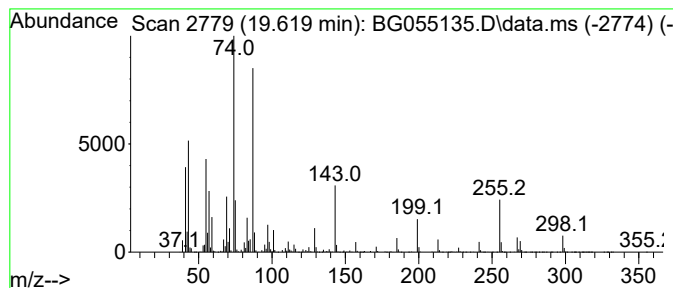
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.619	12.58 ng	13302400	Phenanthrene-d10	17.668

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	94
3			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	005129-66-8	86
4			Methyl 13-methyltetradecanoate	256	C16H32O2	1000424-50-7	86
5			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	83



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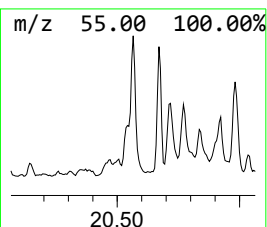
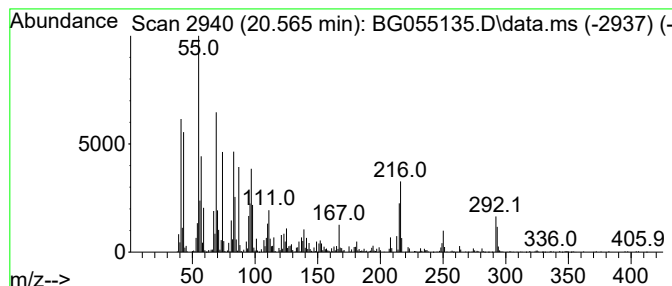
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Peak Number 6 cis-13-Eicosenoic acid, met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.565	27.43 ng	1351190	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	95
2			Oleic Acid	282	C18H34O2	000112-80-1	66
3			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	64
4			Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	64
5			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-101022

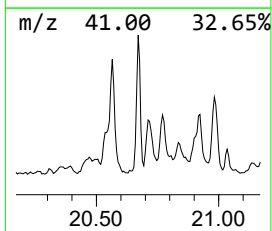
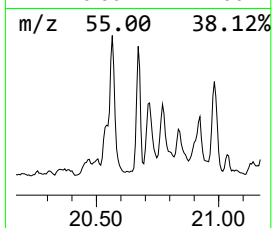
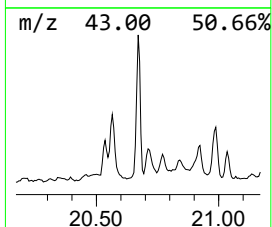
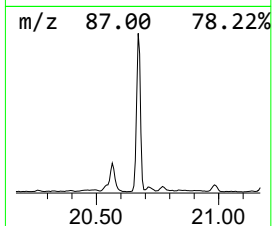
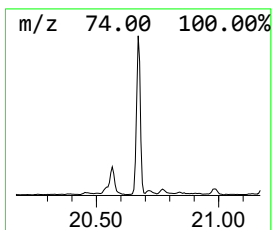
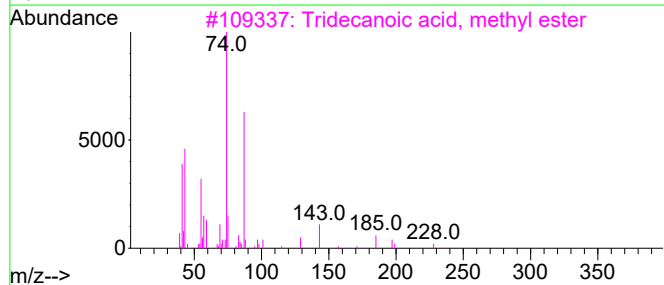
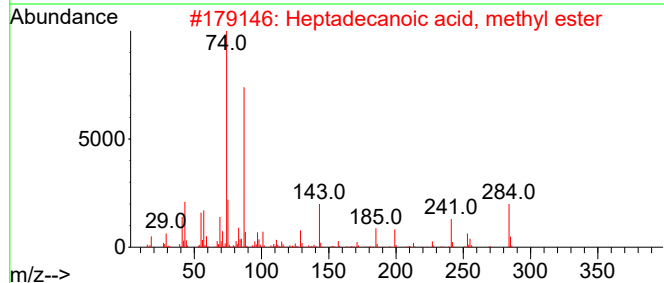
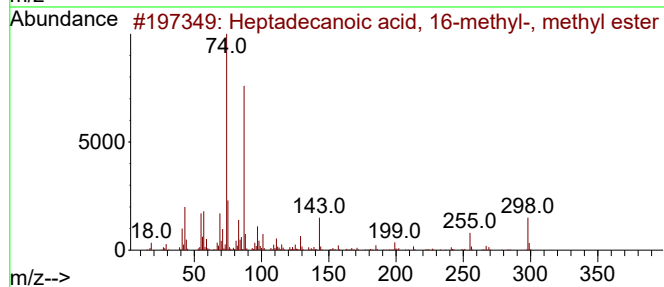
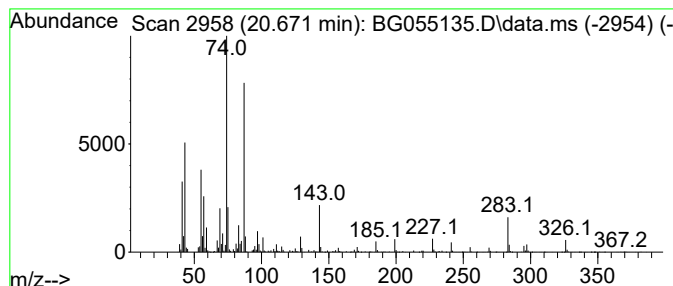
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecanoic acid, 16-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.671	25.24 ng	1243750	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
5			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-101022

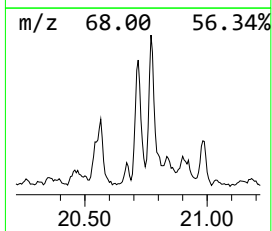
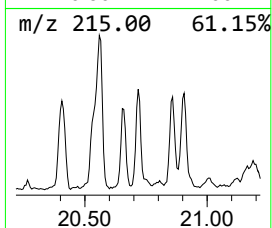
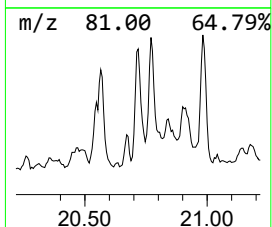
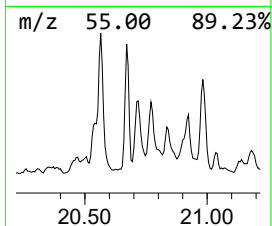
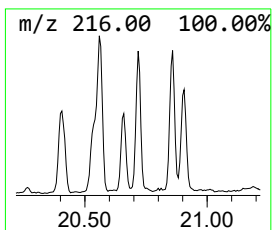
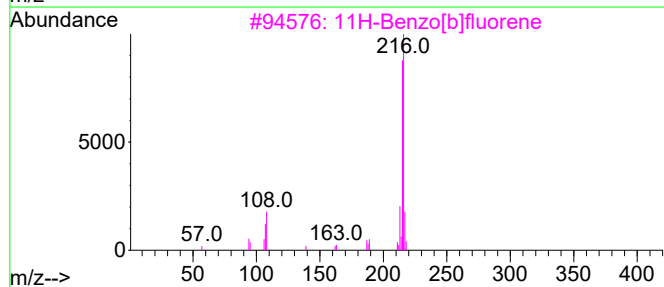
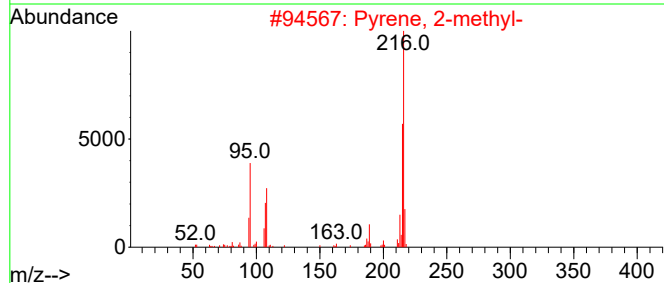
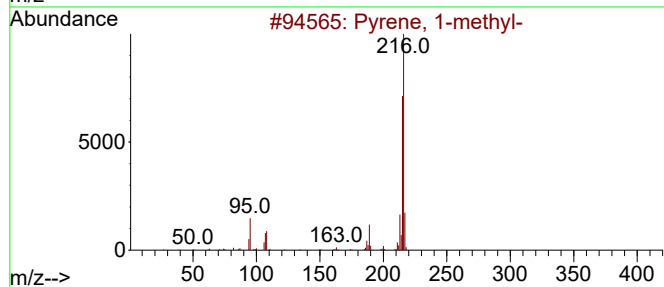
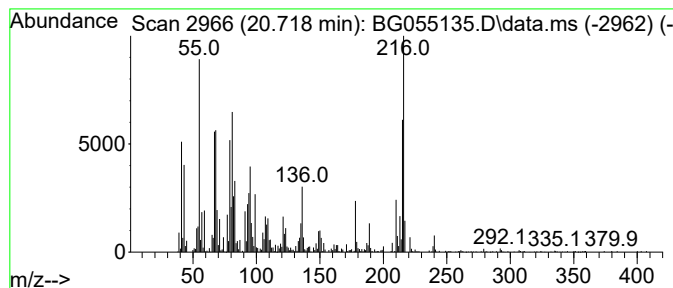
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.718	16.91 ng	832906	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2			Pyrene, 2-methyl-	216	C17H12	003442-78-2	86
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5			Pyrene, 4-methyl-	216	C17H12	003353-12-6	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-101022

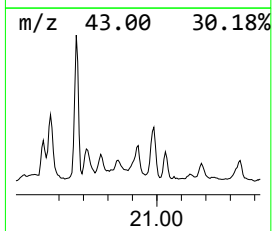
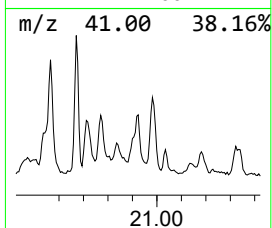
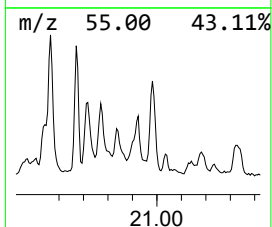
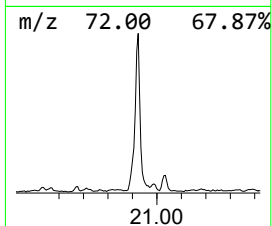
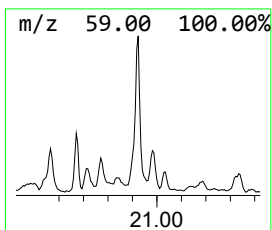
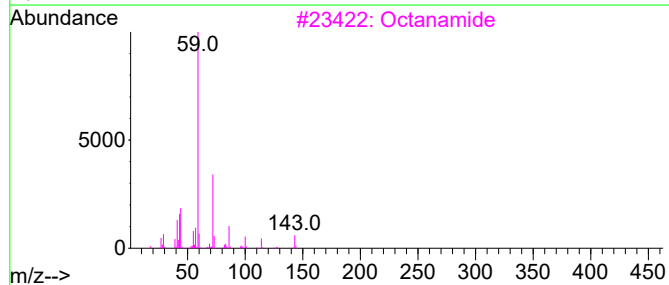
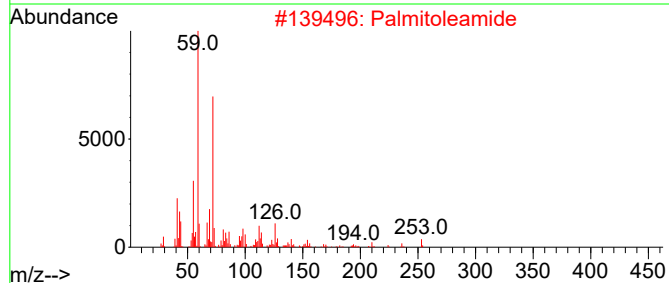
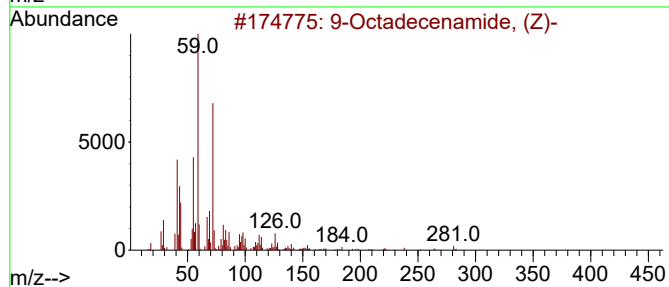
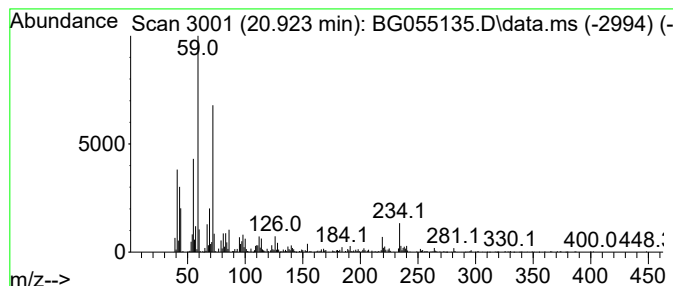
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.923	16.55 ng	815147	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Palmitoleamide	253	C16H31NO	106010-22-4	86
3			Octanamide	143	C8H17NO	000629-01-6	64
4			Dodecanamide	199	C12H25NO	001120-16-7	53
5			Octadecanamide	283	C18H37NO	000124-26-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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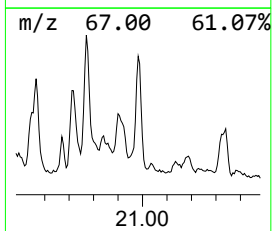
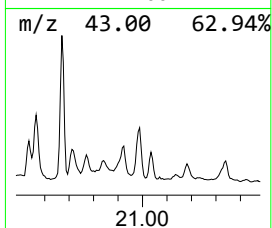
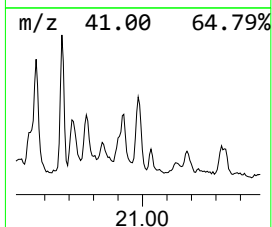
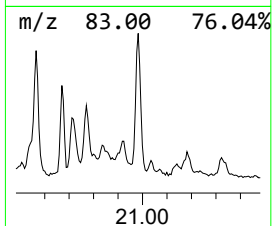
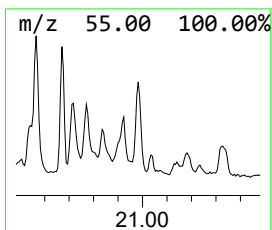
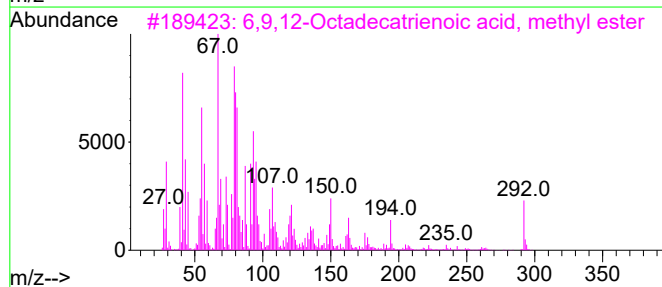
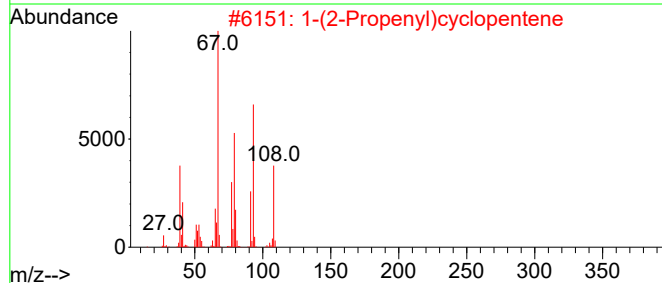
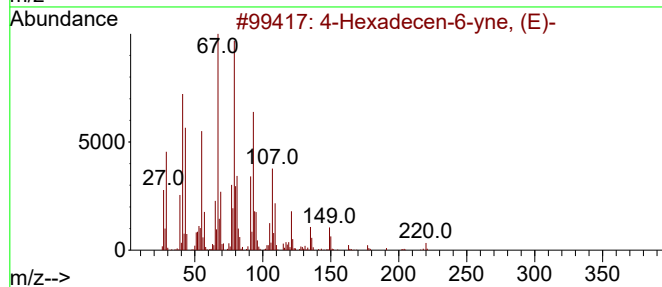
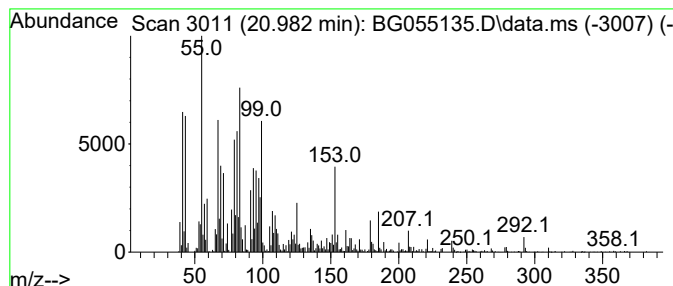
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4-Hexadecen-6-yne, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.982	23.66 ng	1165640	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Hexadecen-6-yne, (E)-	220	C16H28	074744-51-7	92
2			1-(2-Propenyl)cyclopentene	108	C8H12	037689-19-3	35
3			6,9,12-Octadecatrienoic acid, me...	292	C19H32O2	002676-41-7	30
4			Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	25
5			9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-101022

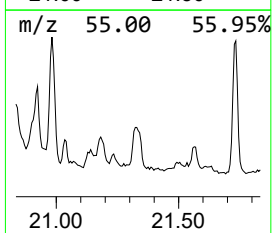
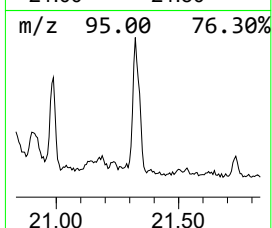
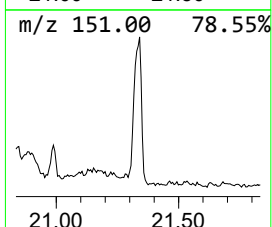
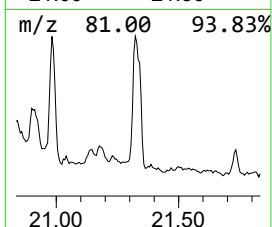
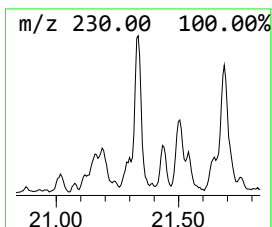
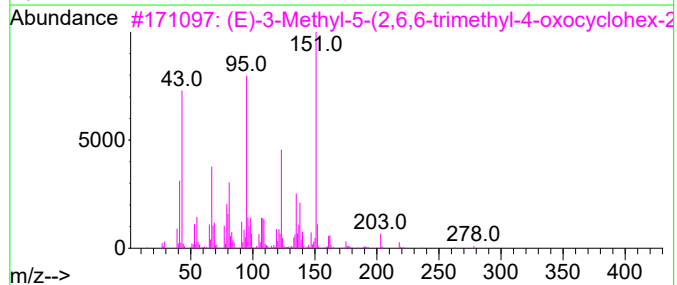
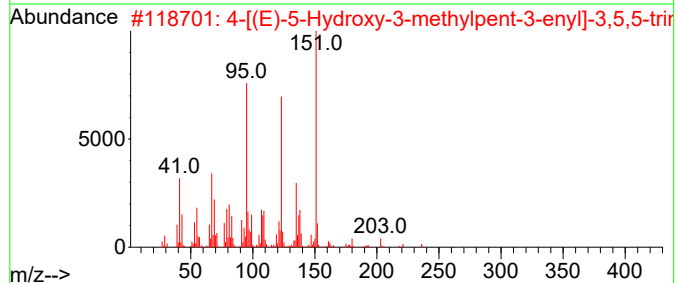
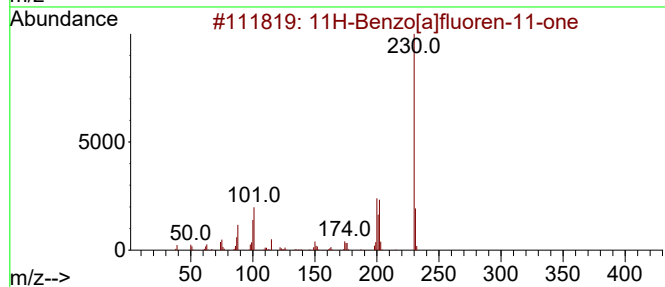
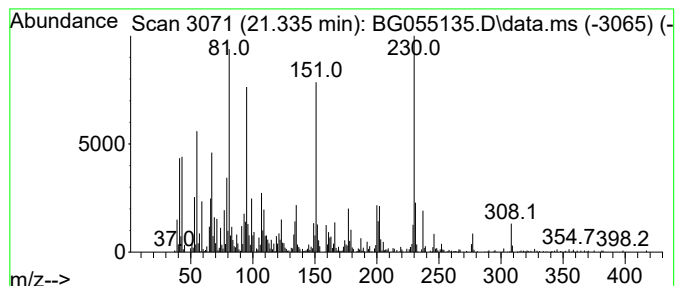
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown21.334 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.334	18.01 ng	887454	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	45
2			4-[(E)-5-Hydroxy-3-methylpent-3-enyl]-3,5,5-trimethyl-4-oxocyclohex-2-en-1-one	236	C15H24O2	1083195-46-3	35
3			(E)-3-Methyl-5-(2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl)-3,5,5-trimethyl-4-oxocyclohex-2-en-1-one	278	C17H26O3	1000495-80-8	25
4			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	25
5			Methyl 2-octylcyclopropene-1-oct-1-ylcarbamate	308	C20H36O2	003220-60-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
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Instrument :
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ClientSampleId :
TR-6-101022

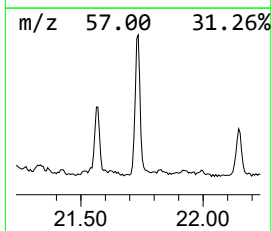
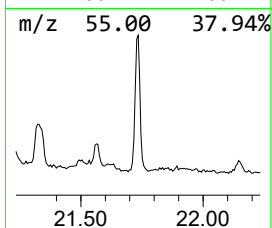
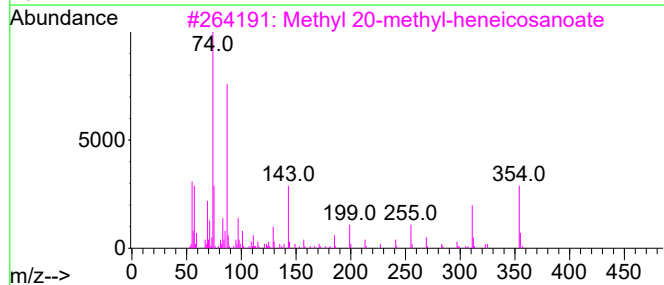
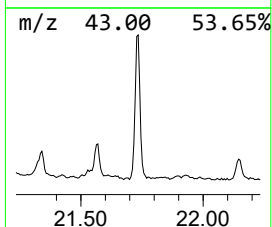
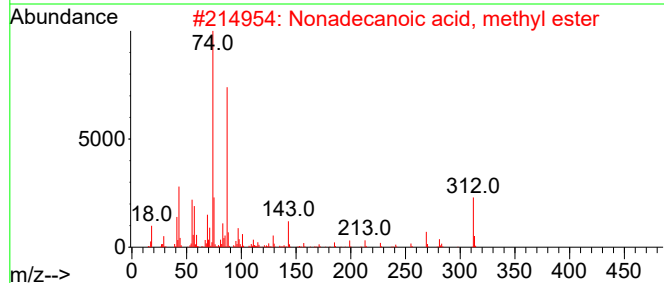
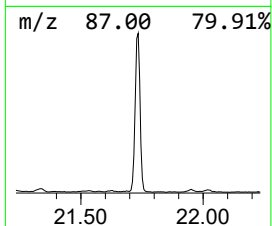
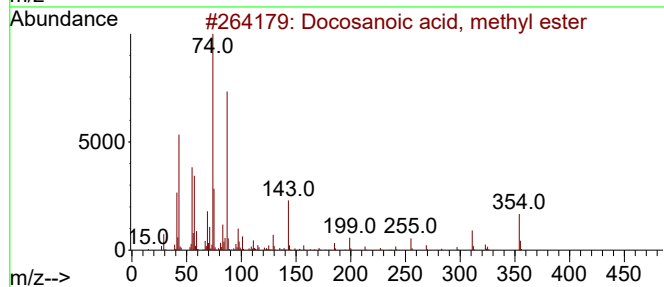
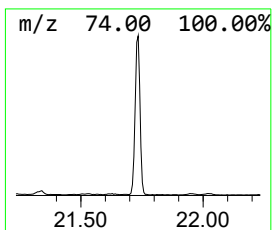
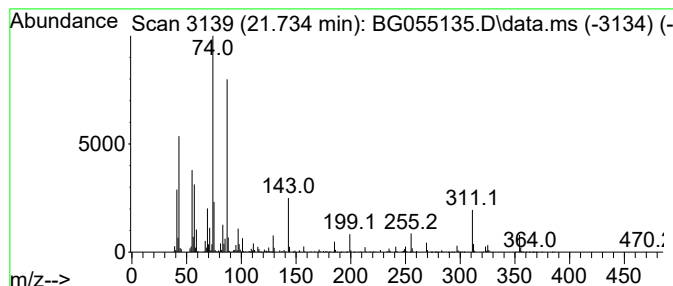
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.734	27.06 ng	1333280	Chrysene-d12	21.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	97
3			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
4			Methyl stearate	298	C19H38O2	000112-61-8	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055135.D
Acq On : 11 Oct 2022 20:48
Operator : CG/JU
Sample : N5080-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-6-101022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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
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n-Hexadecanoic ...	18.585	4.0	ng	4213520	4	17.668	21150300	20.0
9,12-Octadecadi...	19.460	58.1	ng	61459000	4	17.668	21150300	20.0
9,12,15-Octadec...	19.548	12.1	ng	12784600	4	17.668	21150300	20.0
Methyl stearate	19.619	12.6	ng	13302400	4	17.668	21150300	20.0
cis-13-Eicoseno...	20.565	27.4	ng	1351190	5	21.975	985349	20.0
Heptadecanoic a...	20.671	25.2	ng	1243750	5	21.975	985349	20.0
Pyrene, 1-methyl-	20.718	16.9	ng	832906	5	21.975	985349	20.0
9-Octadecenamid...	20.923	16.6	ng	815147	5	21.975	985349	20.0
4-Hexadecen-6-y...	20.982	23.7	ng	1165640	5	21.975	985349	20.0
unknown21.334	21.334	18.0	ng	887454	5	21.975	985349	20.0
Docosanoic acid...	21.734	27.1	ng	1333280	5	21.975	985349	20.0