

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
 Data File : BG054338.D
 Acq On : 20 Jul 2022 22:21
 Operator : CG/JU
 Sample : N3778-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-03-071922

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-BG071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.576	365	372	384	rVB	264217	462059	7.74%	1.721%
2	7.181	636	645	653	rBV	280629	507568	8.50%	1.891%
3	7.997	777	784	792	rBV	73899	129713	2.17%	0.483%
4	9.161	973	982	993	rVB	176640	328358	5.50%	1.223%
5	10.806	1255	1262	1270	rBV	94735	181051	3.03%	0.674%
6	13.256	1672	1679	1688	rVB	550855	894269	14.97%	3.331%
7	14.636	1904	1914	1920	rBV	171992	273729	4.58%	1.020%
8	16.123	2161	2167	2177	rBV3	520448	826187	13.83%	3.078%
9	17.380	2375	2381	2386	rBV	212915	338591	5.67%	1.261%
10	18.044	2485	2494	2499	rBV	561667	780085	13.06%	2.906%
11	18.315	2528	2540	2551	rBV	1504283	3418000	57.22%	12.732%
12	18.432	2556	2560	2567	rVV4	45483	71546	1.20%	0.267%
13	19.190	2682	2689	2692	rBV	4005500	5973282	100.00%	22.250%
14	19.219	2692	2694	2702	rVV2	2835532	3397832	56.88%	12.657%
15	19.284	2702	2705	2710	rVB2	73711	99184	1.66%	0.369%
16	19.343	2711	2715	2720	rBV	439900	527070	8.82%	1.963%
17	19.419	2720	2728	2730	rBV	764542	1458315	24.41%	5.432%
18	19.443	2730	2732	2745	rVV2	723820	1197878	20.05%	4.462%
19	19.560	2746	2752	2763	rVV	935378	1378190	23.07%	5.134%
20	19.801	2789	2793	2801	rVB	86818	150253	2.52%	0.560%
21	19.995	2821	2826	2831	rBV	1052965	1322617	22.14%	4.927%
22	20.535	2914	2918	2923	rBV3	120828	163270	2.73%	0.608%
23	20.624	2929	2933	2941	rVB2	388258	530842	8.89%	1.977%
24	20.759	2953	2956	2969	rVB5	147951	268367	4.49%	1.000%
25	21.282	3041	3045	3050	rBV3	129333	211778	3.55%	0.789%
26	21.652	3103	3108	3114	rVB	281484	461431	7.72%	1.719%
27	23.937	3491	3497	3503	rVB	331245	684493	11.46%	2.550%
28	26.011	3844	3850	3862	rVB	280804	810035	13.56%	3.017%

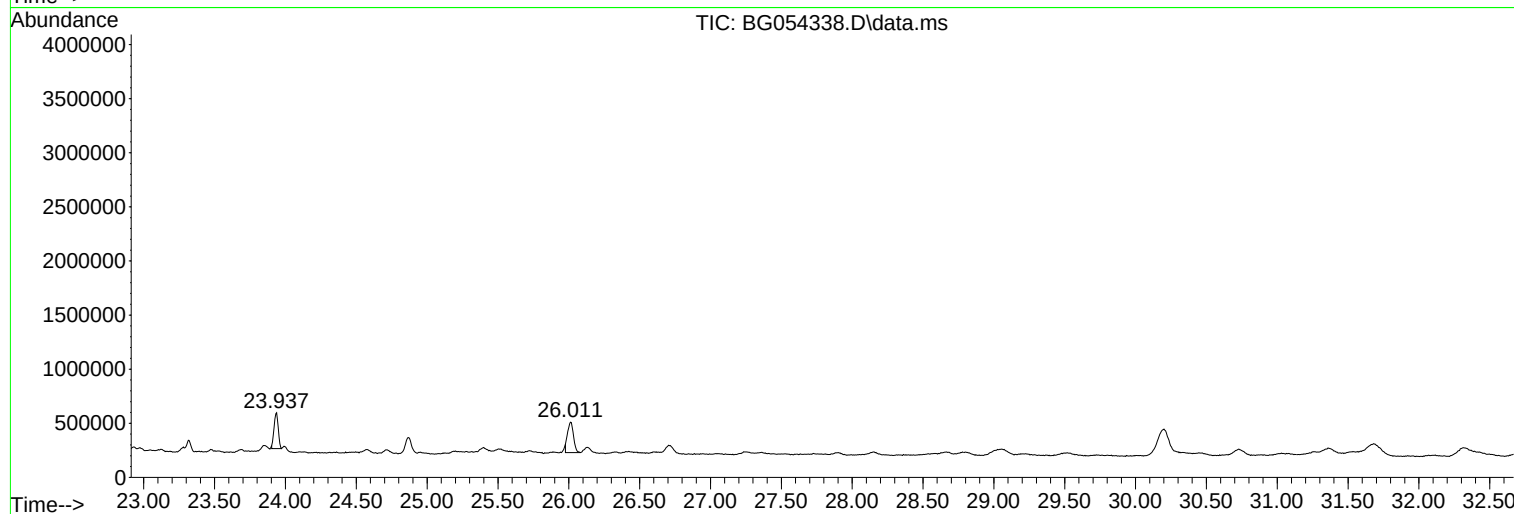
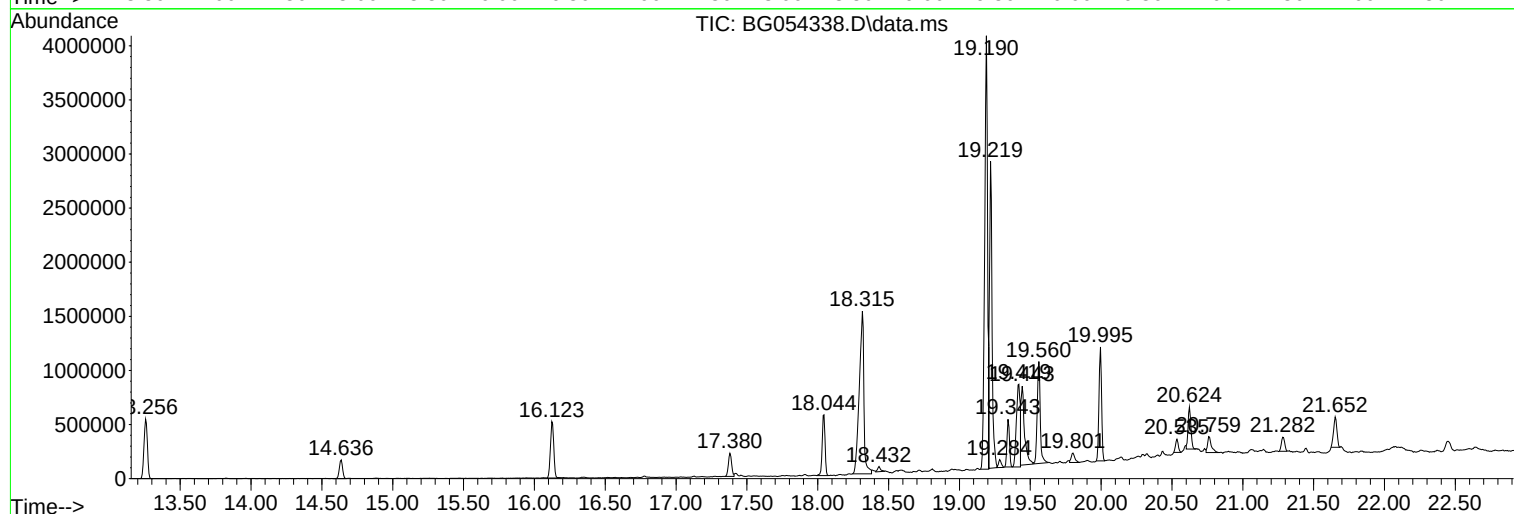
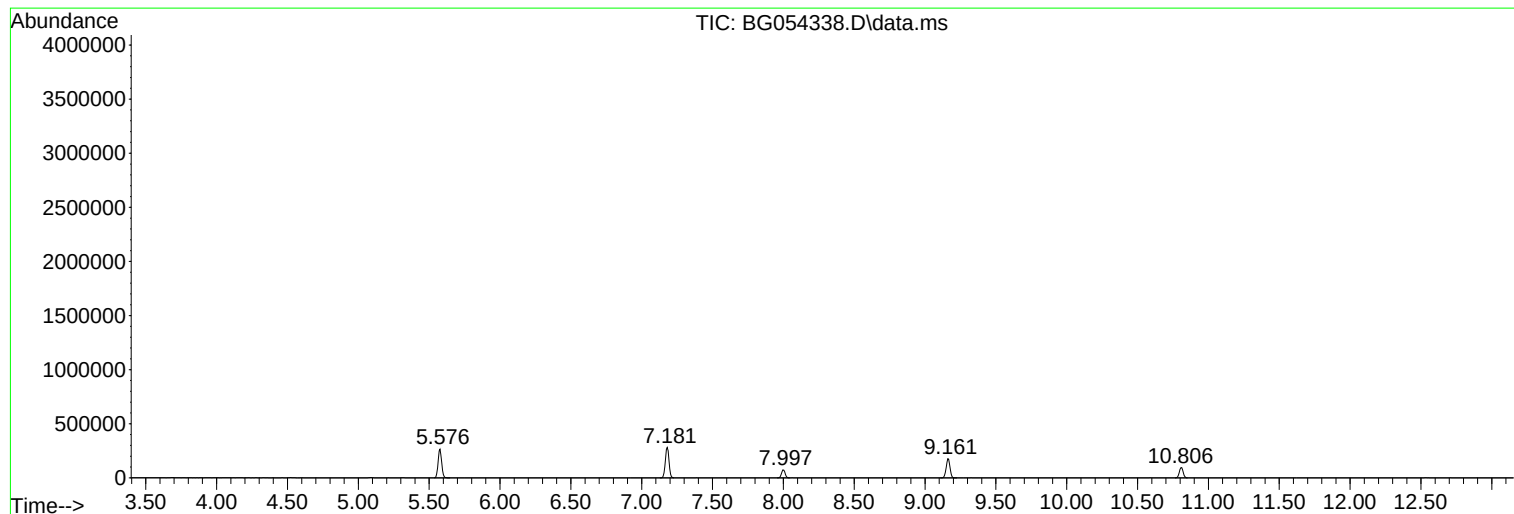
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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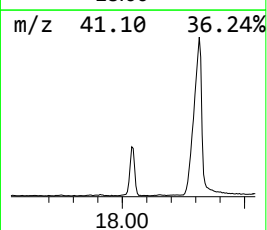
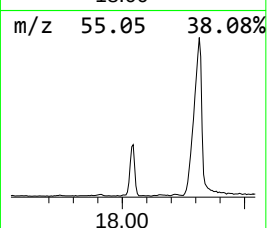
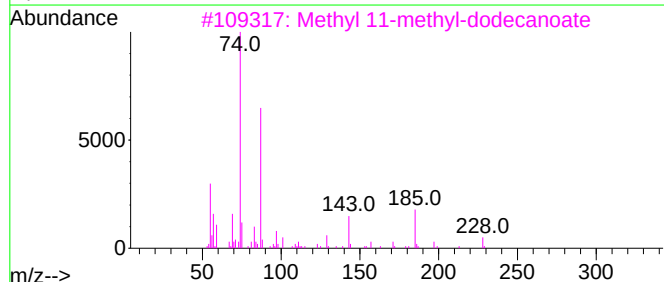
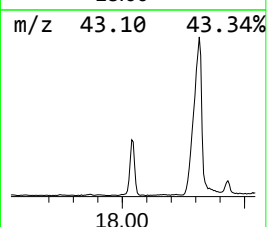
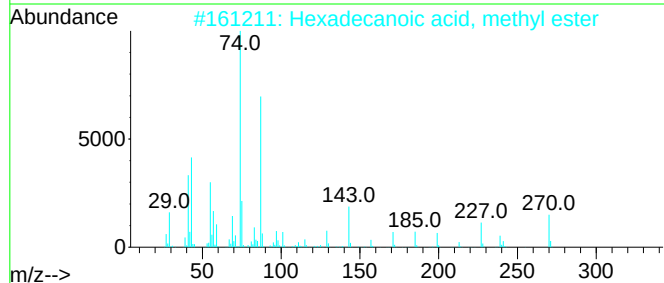
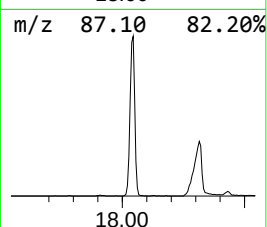
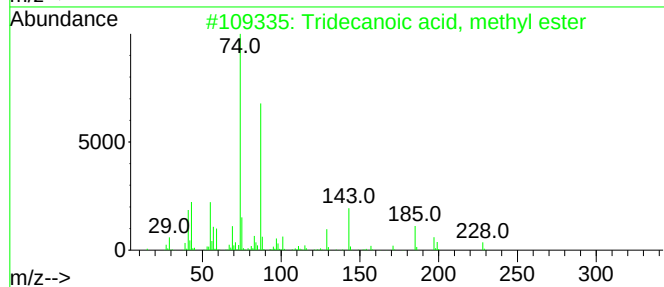
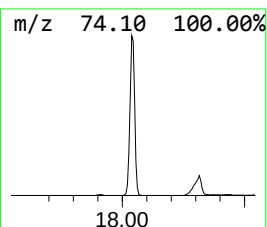
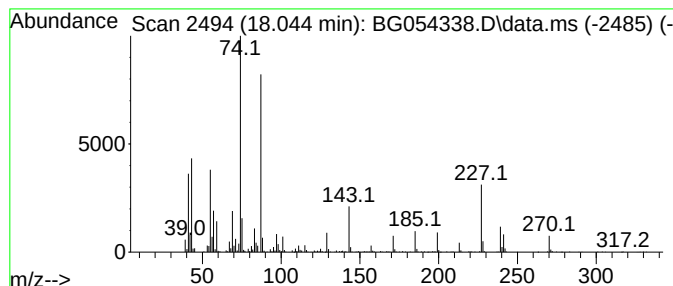
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.044	46.08 ng	780085	Phenanthrene-d10		17.380	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	96
2	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	95
3	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	93
4	Hexadecanoic acid, 2-methyl-		270	C17H34O2	027147-71-3	81
5	Methyl tetradecanoate		242	C15H30O2	000124-10-7	81



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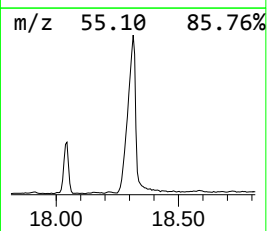
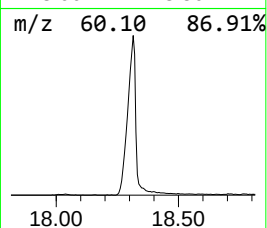
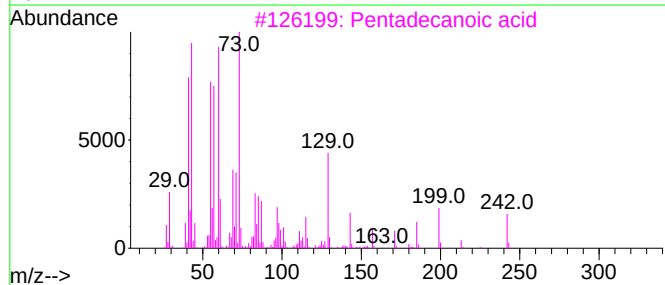
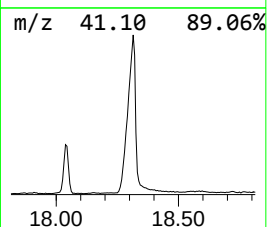
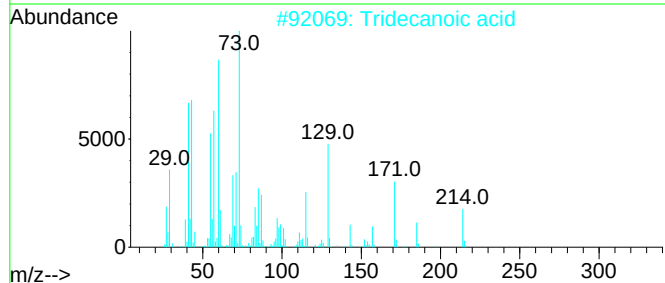
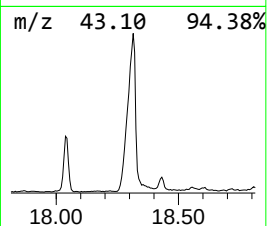
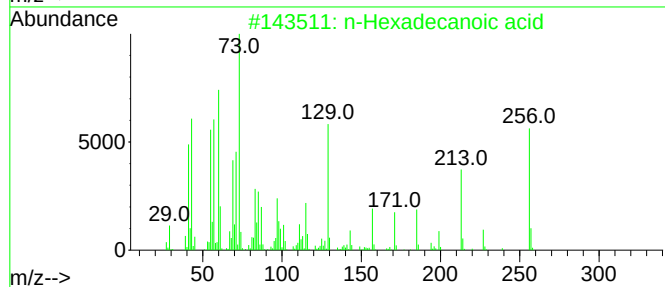
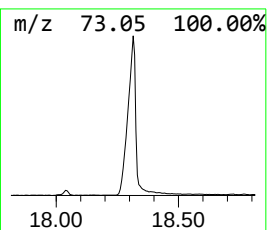
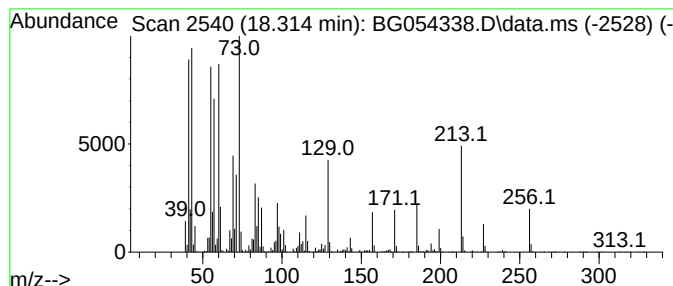
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.314	201.90 ng	3418000	Phenanthrene-d10	17.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Octadecanoic acid	284	C18H36O2	000057-11-4	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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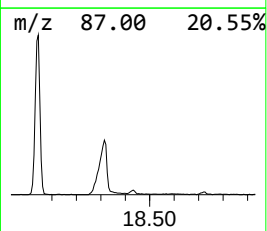
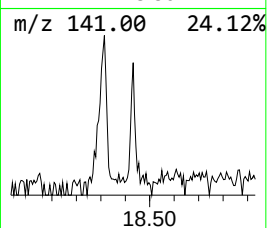
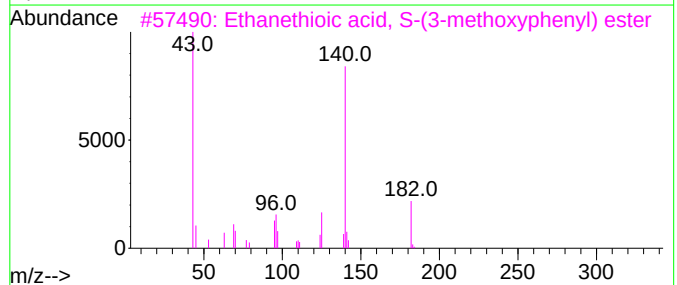
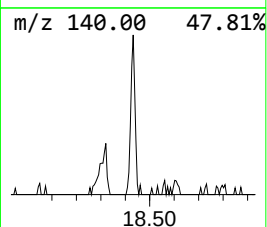
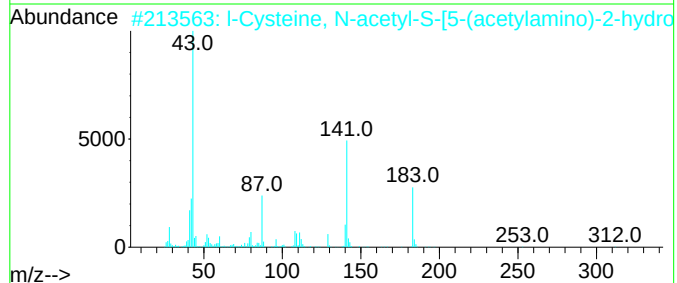
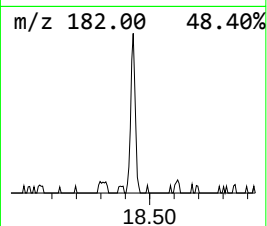
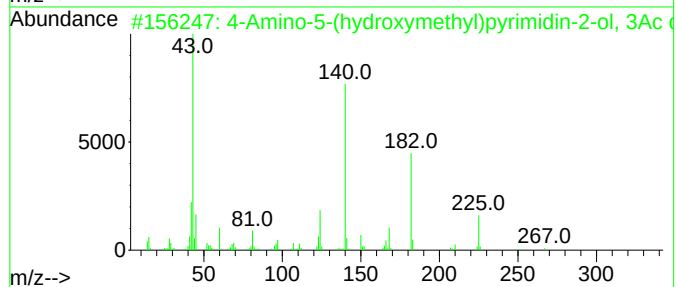
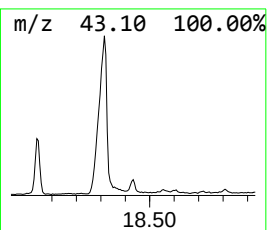
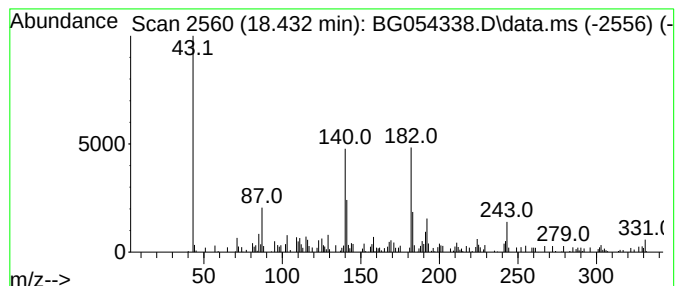
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown18.432 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.432	4.23 ng	71546	Phenanthrene-d10	17.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-5-(hydroxymethyl)pyrimidin...	267	C11H13N3O5	1000514-45-7	43		
2	l-Cysteine, N-acetyl-S-[5-(acety...	312	C13H16N2O5S	052372-86-8	10		
3	Ethanethioic acid, S-(3-methoxyp...	182	C9H10O2S	069746-44-7	9		
4	4-Acetamido-3-nitrobenzoic acid	224	C9H8N2O5	001539-06-6	9		
5	2,6-Dimethyl-4-thiopyrone	140	C7H8OS	001004-37-1	9		



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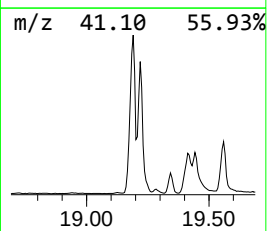
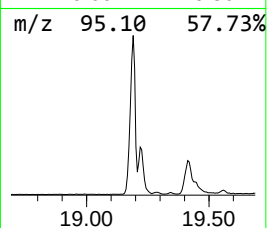
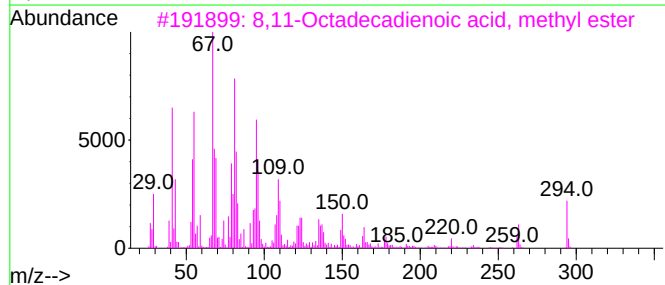
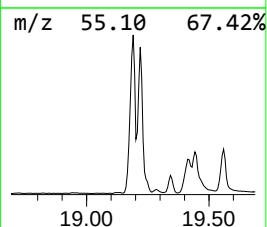
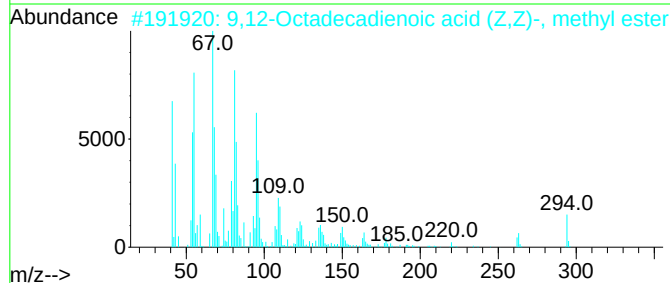
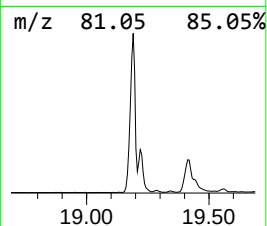
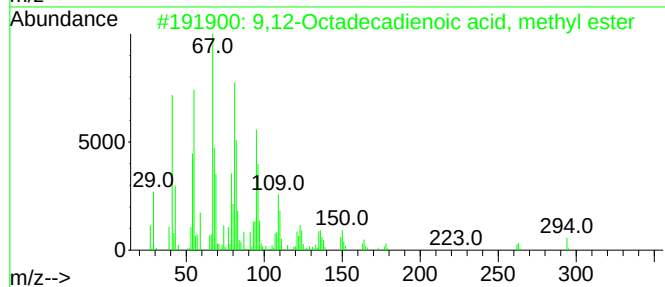
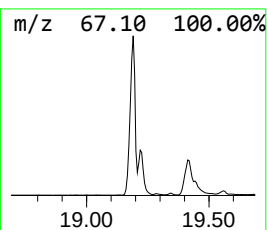
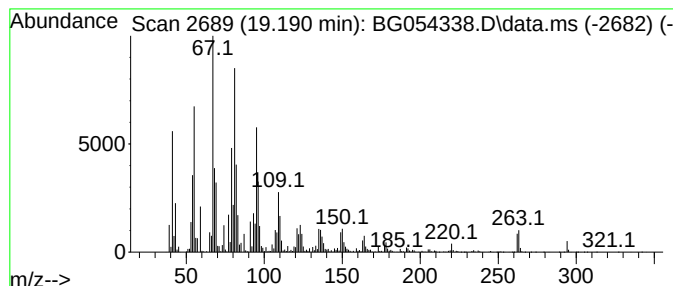
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.190	352.83 ng	5973280	Phenanthrene-d10	17.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99		
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98		
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98		
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98		



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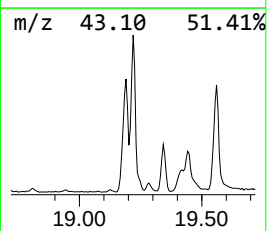
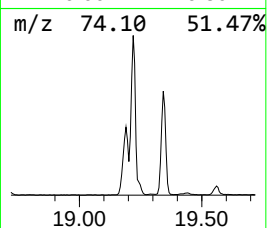
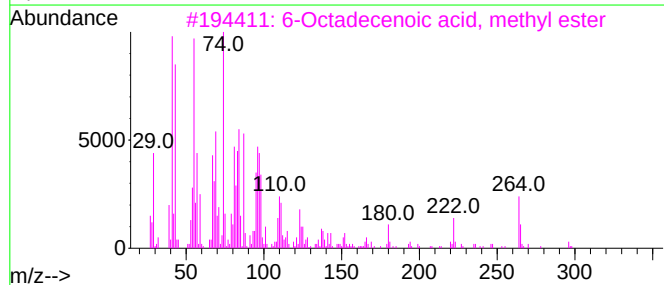
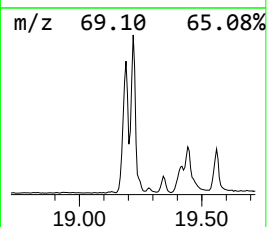
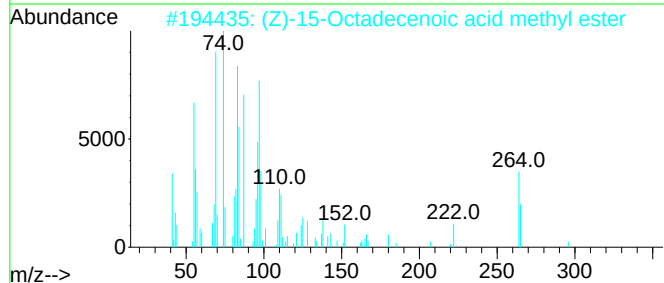
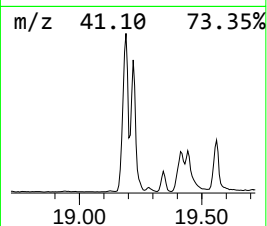
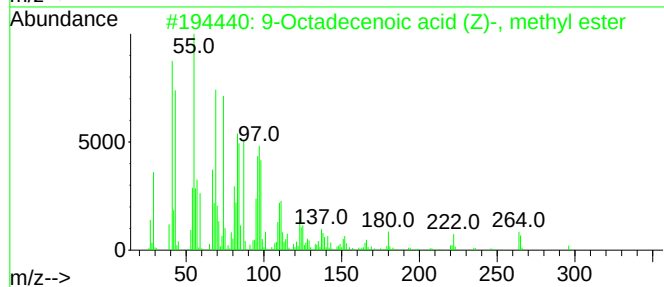
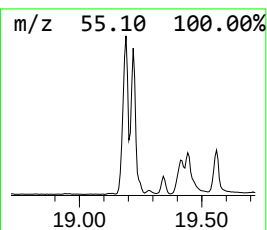
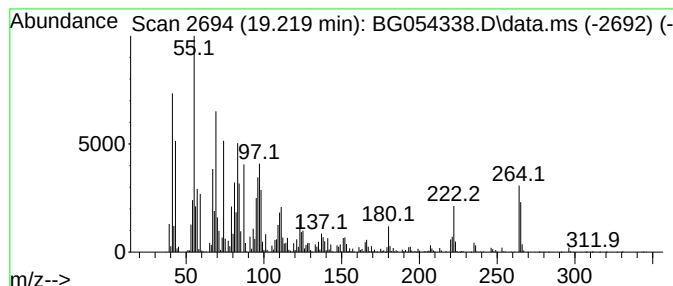
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Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.219	200.70 ng	3397830	Phenanthrene-d10	17.380	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	93
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91



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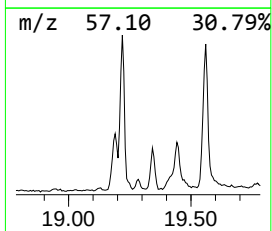
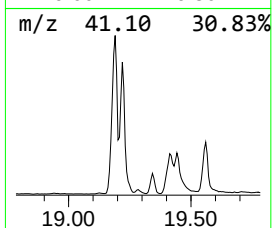
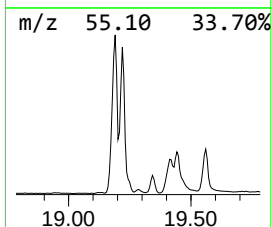
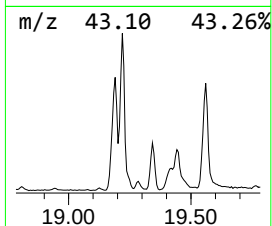
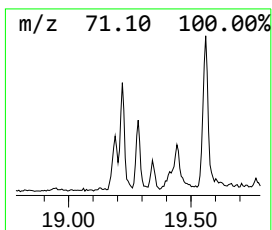
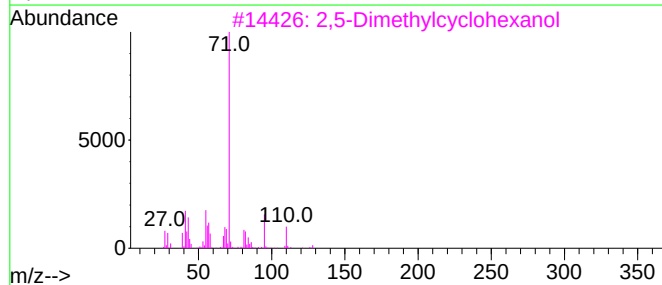
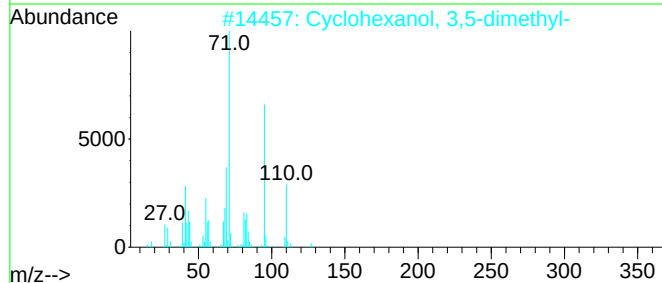
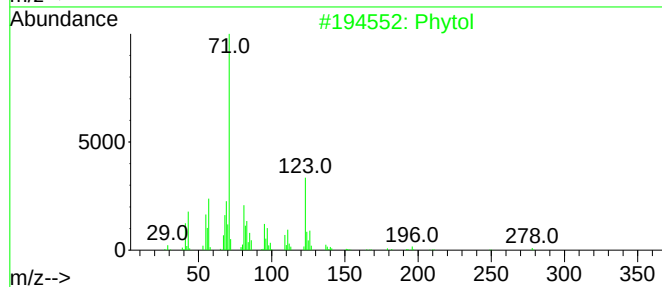
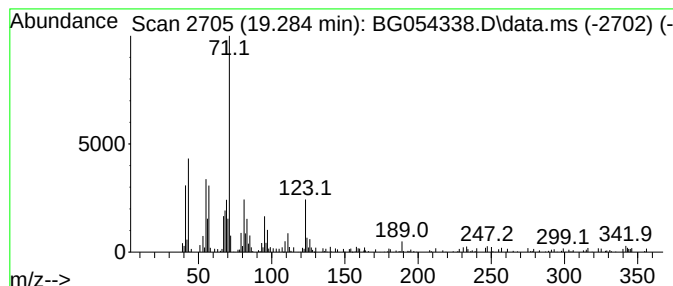
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phytol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.284	5.86 ng	99184	Phenanthrene-d10	17.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phytol	296	C20H40O	000150-86-7	86
2			Cyclohexanol, 3,5-dimethyl-	128	C8H16O	005441-52-1	52
3			2,5-Dimethylcyclohexanol	128	C8H16O	003809-32-3	47
4			Sulfurous acid, hexadecyl 2-pent...	376	C21H44O3S	1000309-16-5	47
5			Butyric acid, 3-tetradecyl ester	284	C18H36O2	1000280-57-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
Acq On : 20 Jul 2022 22:21
Operator : CG/JU
Sample : N3778-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-071922

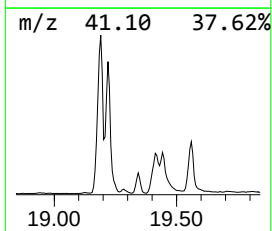
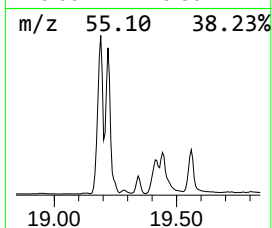
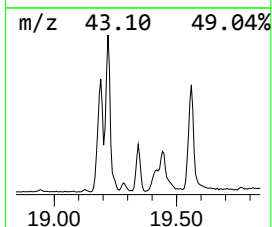
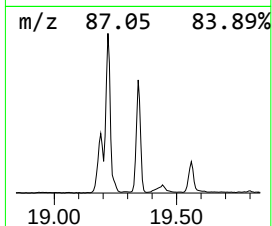
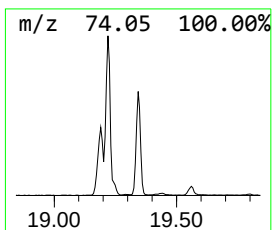
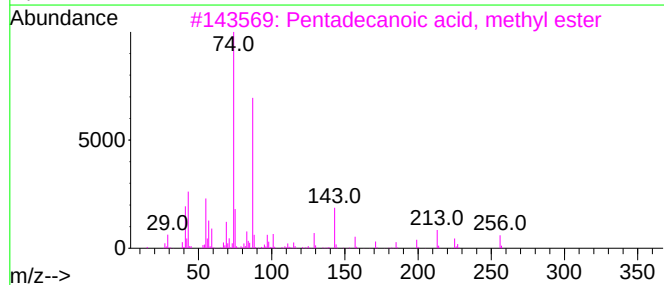
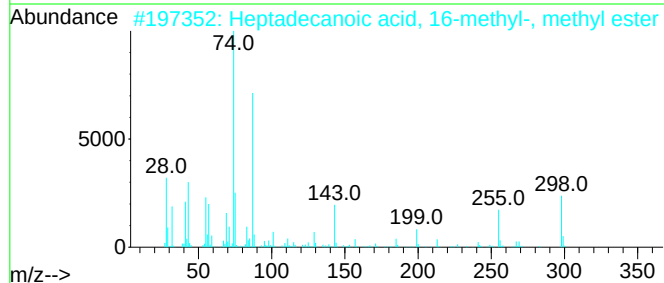
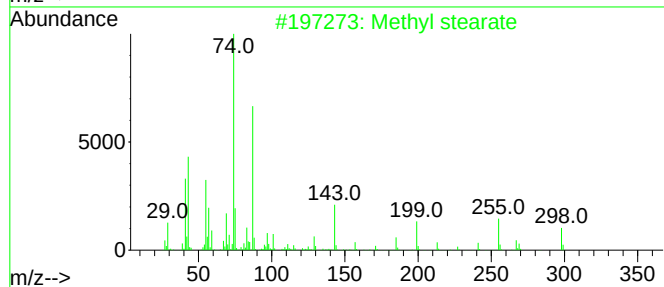
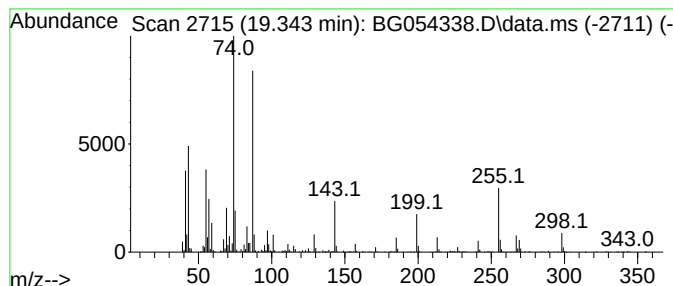
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.343	31.13 ng	527070	Phenanthrene-d10	17.380

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	93
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
4			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	83
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
Acq On : 20 Jul 2022 22:21
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Sample : N3778-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-071922

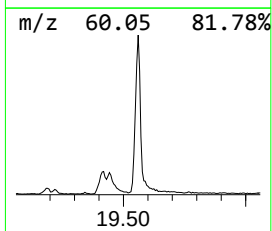
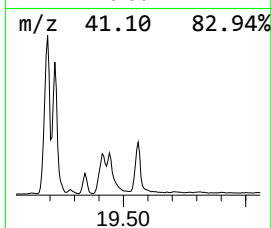
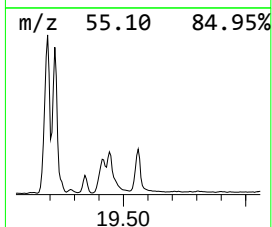
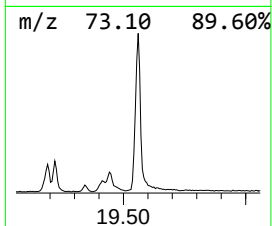
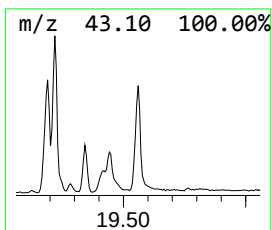
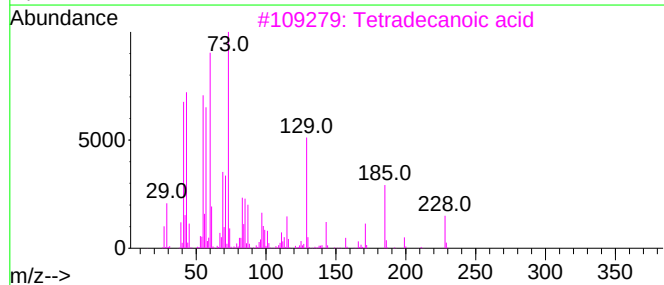
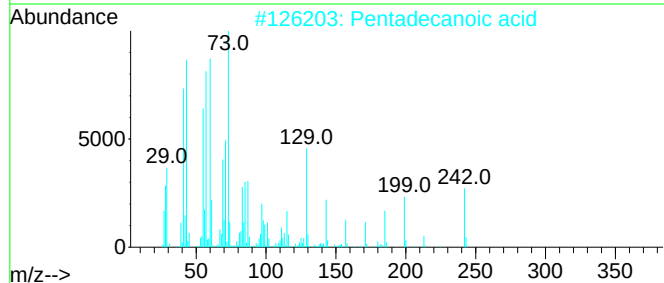
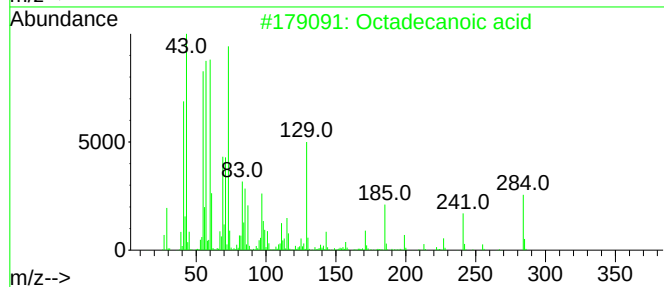
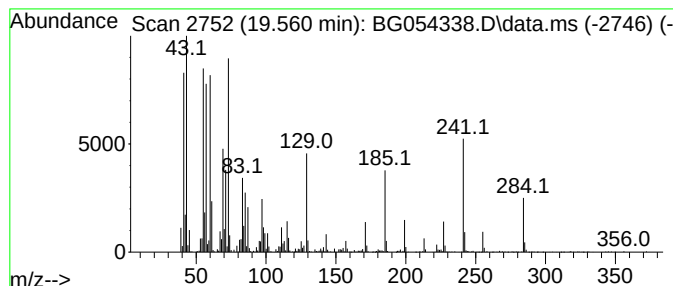
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.560	59.74 ng	1378190	Chrysene-d12	21.652

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	78
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
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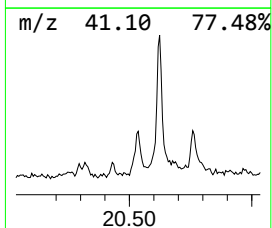
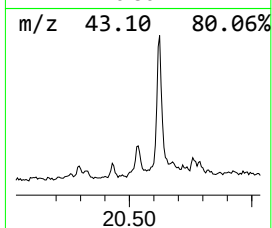
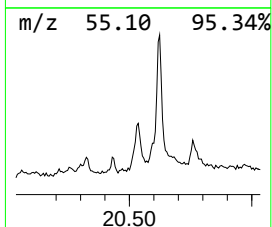
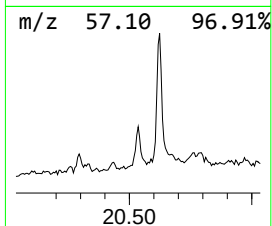
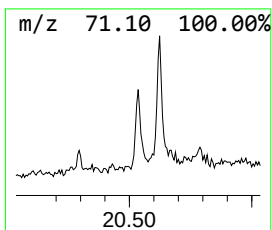
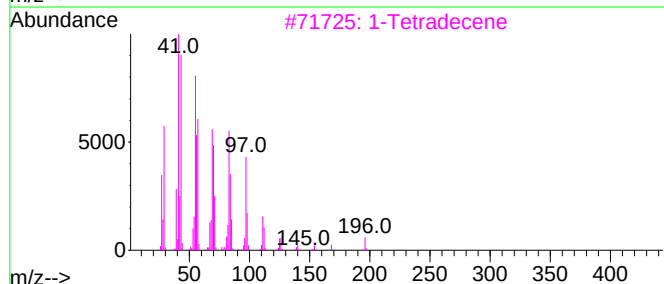
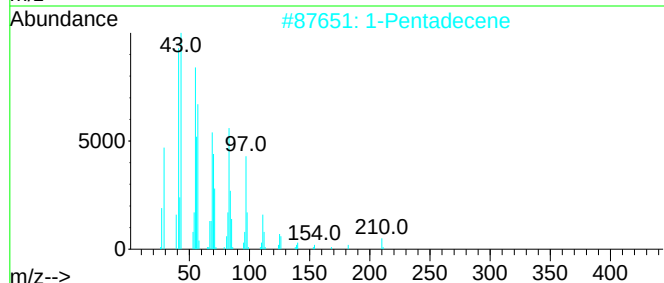
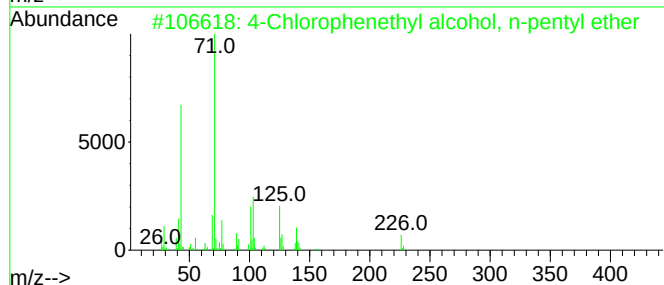
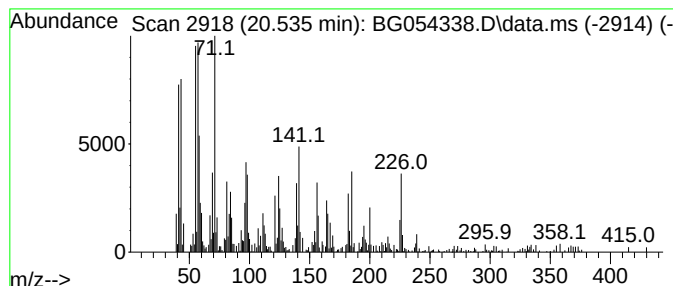
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.535 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.535	7.08 ng	163270	Chrysene-d12	21.652	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chlorophenethyl alcohol, n-pen...	226	C13H19ClO	1000394-99-2	25
2	1-Pentadecene	210	C15H30	013360-61-7	25
3	1-Tetradecene	196	C14H28	001120-36-1	25
4	Oct-3-enoylamide, N-(2-pentyl)-N...	225	C14H27NO	1000490-20-0	18
5	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
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Operator : CG/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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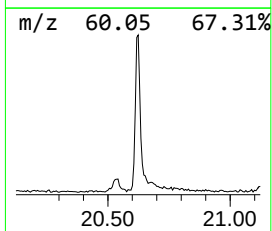
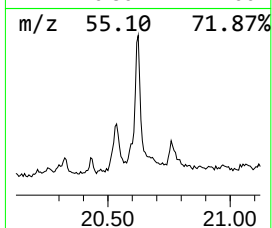
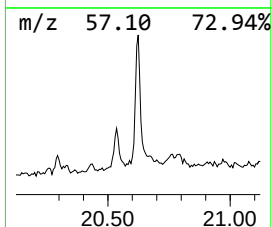
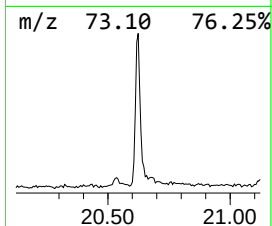
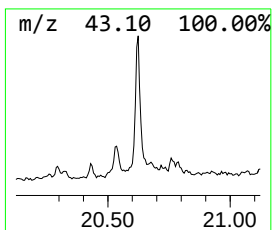
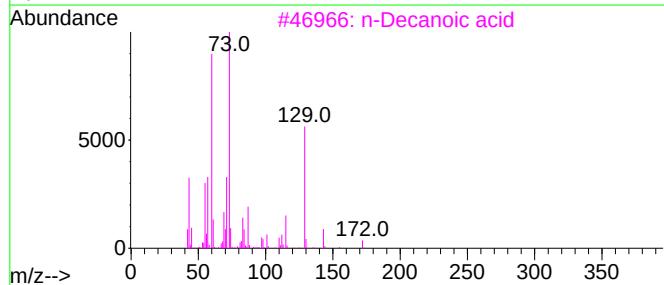
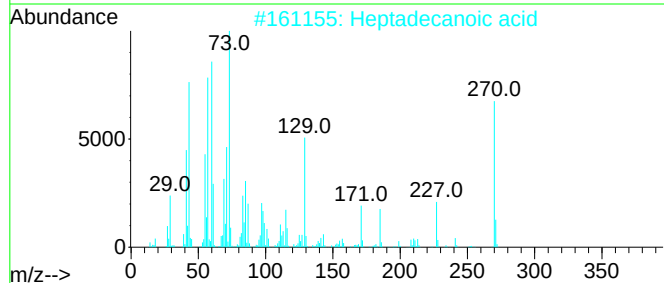
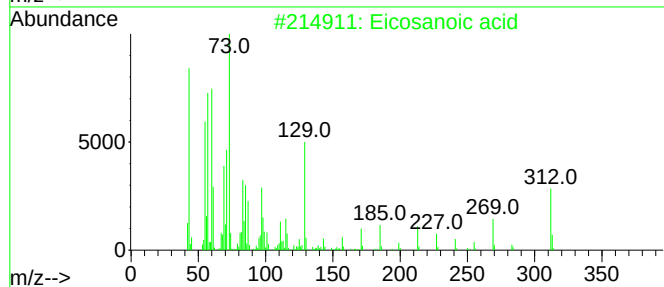
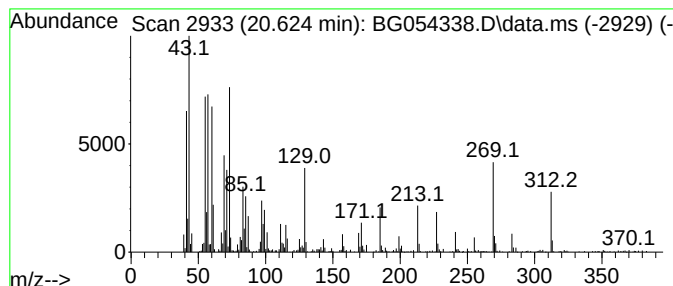
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.624	23.01 ng	530842	Chrysene-d12	21.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid	312	C20H40O2	000506-30-9	99
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	87
3			n-Decanoic acid	172	C10H20O2	000334-48-5	55
4			Octadecanoic acid	284	C18H36O2	000057-11-4	49
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
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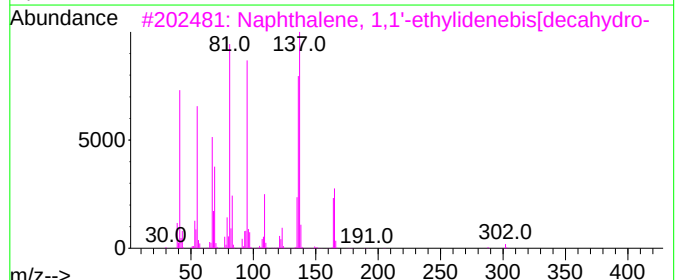
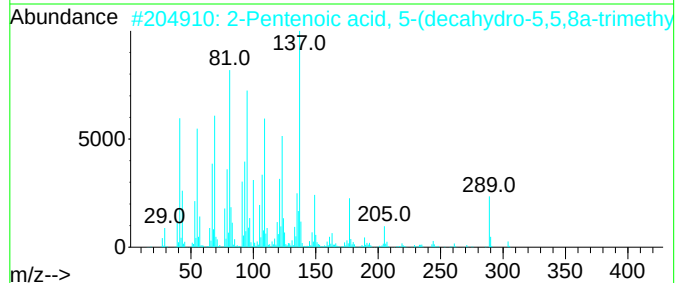
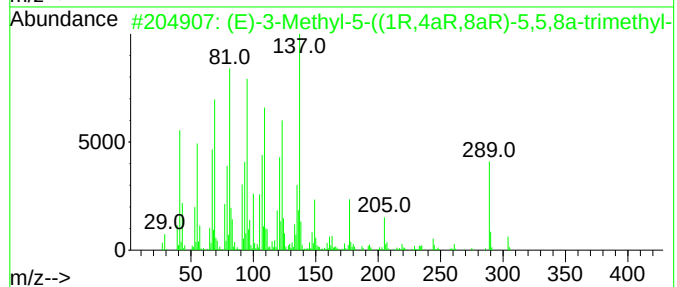
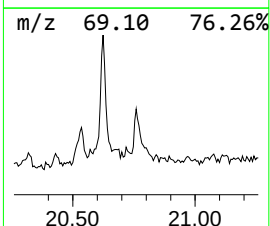
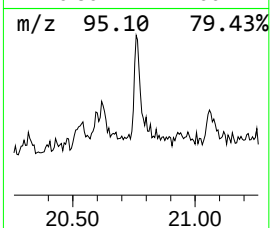
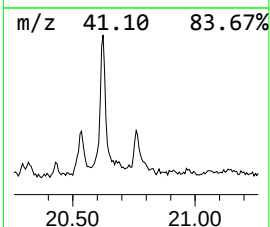
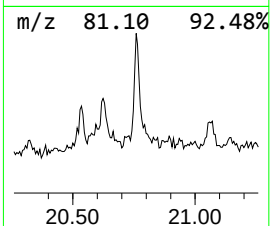
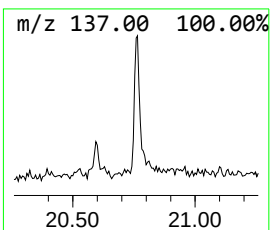
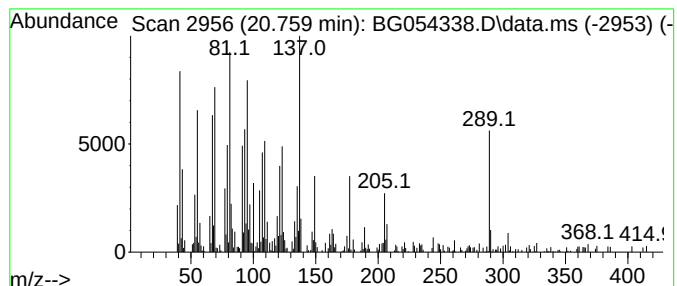
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 (E)-3-Methyl-5-((1R,4aR,8aR... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.759	11.63 ng	268367	Chrysene-d12		21.652	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5...		304	C20H32O2	020257-75-4	93
2	2-Pentenoic acid, 5-(decahydro-5...		304	C20H32O2	024470-48-2	70
3	Naphthalene, 1,1'-ethylidenebis[...		302	C22H38	054934-70-2	64
4	Acetic acid, 3-(5,5-dimethyl-spi...		250	C16H26O2	077143-33-0	38
5	2,5-Octadiene, 3,4,5,6-tetramethyl-		166	C12H22	247797-85-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
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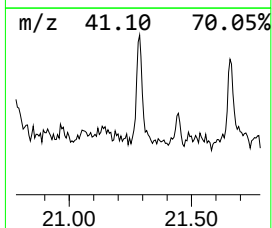
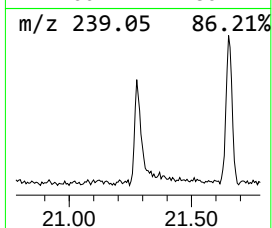
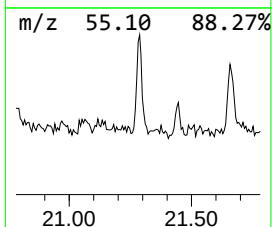
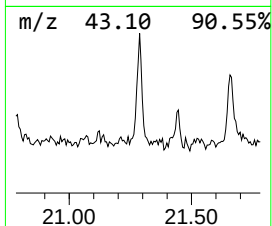
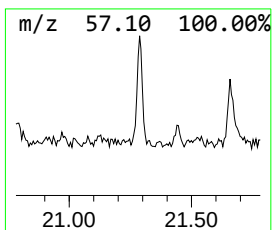
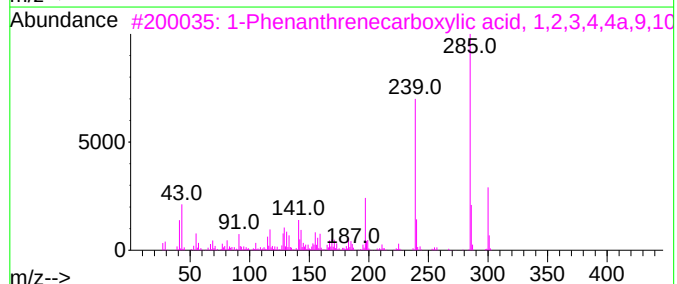
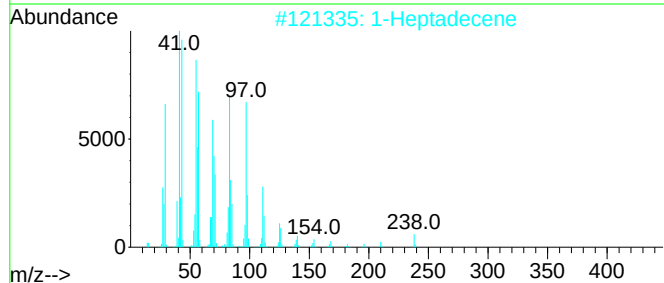
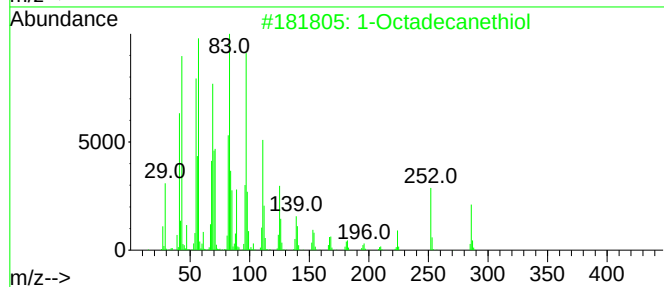
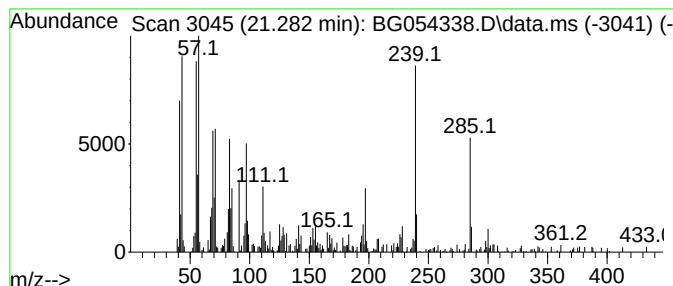
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Octadecanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.282	9.18 ng	211778	Chrysene-d12	21.652	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9	92
2	1-Heptadecene	238	C17H34	006765-39-5	91
3	1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	90
4	Cyclohexadecane	224	C16H32	000295-65-8	90
5	Dehydroabietic acid	300	C20H28O2	001740-19-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
Acq On : 20 Jul 2022 22:21
Operator : CG/JU
Sample : N3778-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

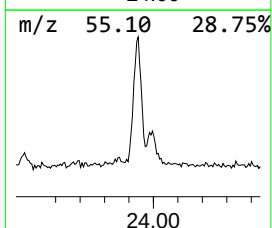
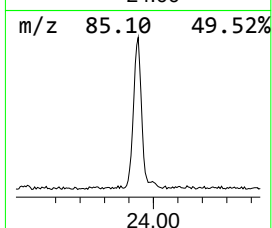
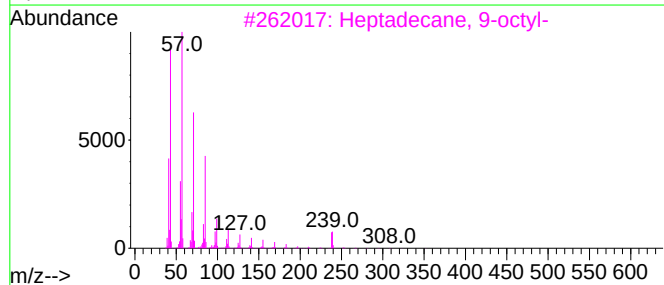
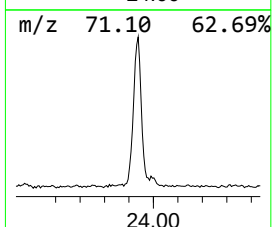
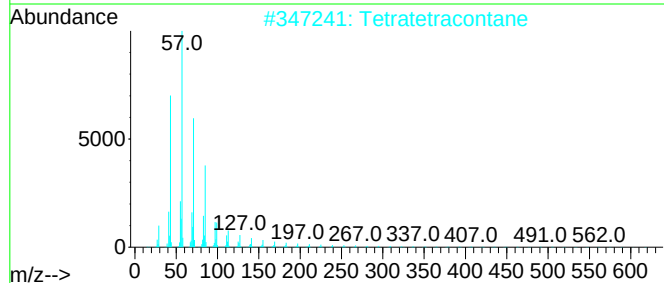
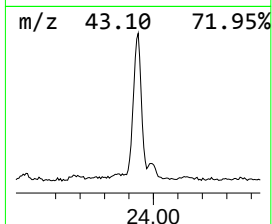
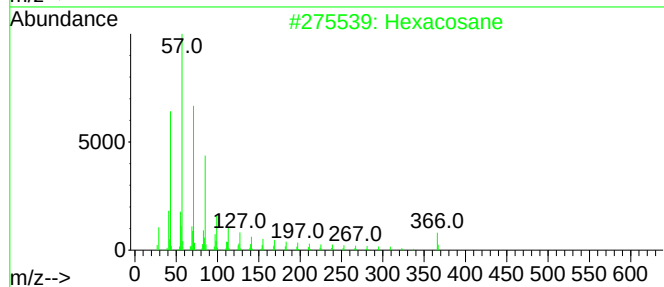
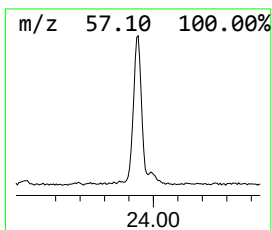
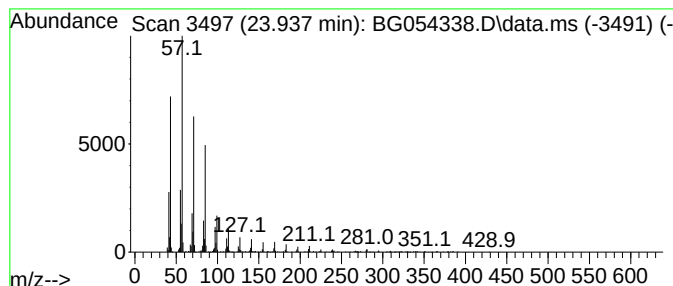
Instrument :
BNA_G
ClientSampleId :
BU-03-071922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.937	20.00 ng	684493	Perylene-d12	24.866	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	95
2	Tetratetracontane	619	C44H90	007098-22-8	95
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5	2-Methyltetracosane	352	C25H52	001560-78-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
Acq On : 20 Jul 2022 22:21
Operator : CG/JU
Sample : N3778-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

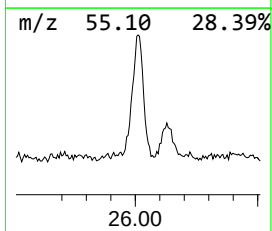
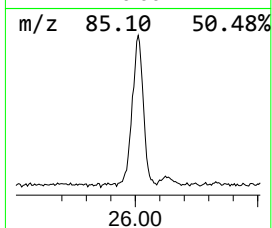
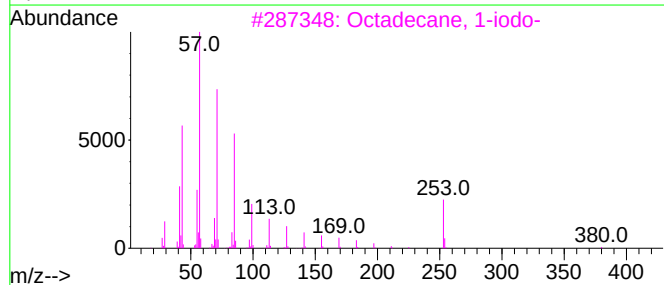
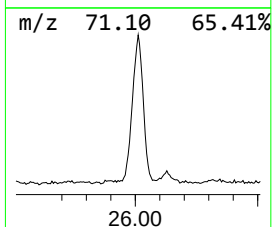
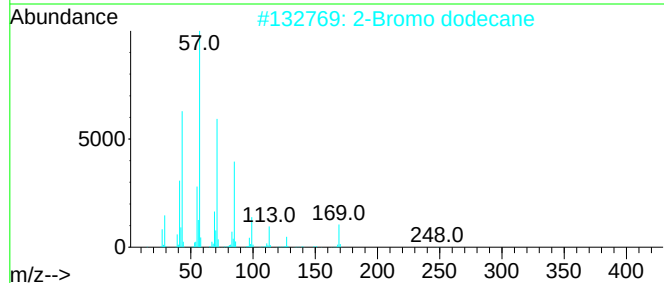
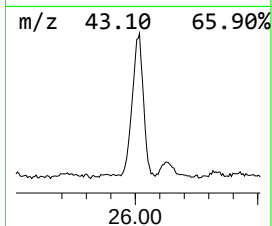
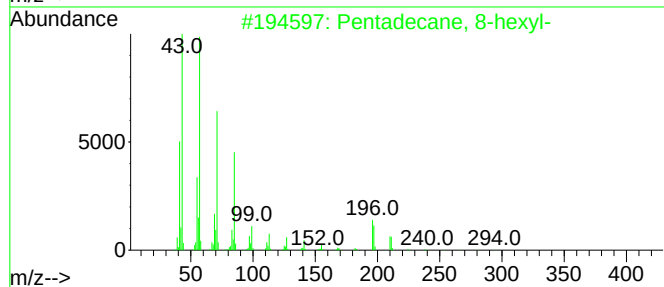
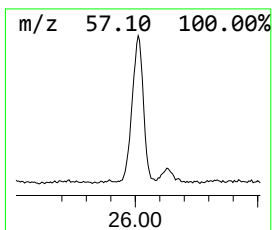
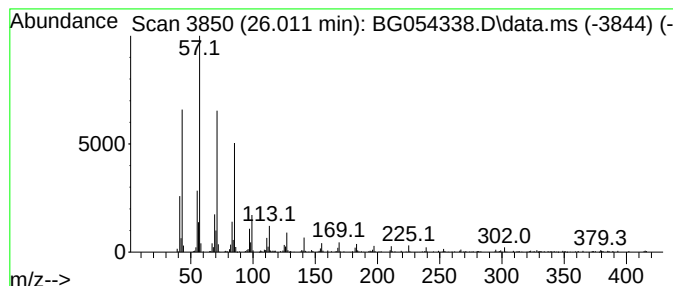
Instrument :
BNA_G
ClientSampleId :
BU-03-071922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
26.011	23.67 ng	810035	Perylene-d12		24.866	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	94
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	93
3	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	93
4	Heptadecane, 3-methyl-		254	C18H38	006418-44-6	91
5	Tetratetracontane		619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054338.D
Acq On : 20 Jul 2022 22:21
Operator : CG/JU
Sample : N3778-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-071922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Tridecanoic aci...	18.044	46.1	ng	780085	4	17.380	338591	20.0
n-Hexadecanoic ...	18.314	201.9	ng	3418000	4	17.380	338591	20.0
unknown18.432	18.432	4.2	ng	71546	4	17.380	338591	20.0
9,12-Octadecadi...	19.190	352.8	ng	5973280	4	17.380	338591	20.0
9-Octadecenoic ...	19.219	200.7	ng	3397830	4	17.380	338591	20.0
Phytol	19.284	5.9	ng	99184	4	17.380	338591	20.0
Methyl stearate	19.343	31.1	ng	527070	4	17.380	338591	20.0
Octadecanoic acid	19.560	59.7	ng	1378190	5	21.652	461431	20.0
unknown20.535	20.535	7.1	ng	163270	5	21.652	461431	20.0
Eicosanoic acid	20.624	23.0	ng	530842	5	21.652	461431	20.0
(E)-3-Methyl-5-...	20.759	11.6	ng	268367	5	21.652	461431	20.0
1-Octadecanethiol	21.282	9.2	ng	211778	5	21.652	461431	20.0
Hexacosane	23.937	20.0	ng	684493	6	24.866	684493	20.0
Pentadecane, 8-...	26.011	23.7	ng	810035	6	24.866	684493	20.0