

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053707.D
 Acq On : 25 May 2022 23:46
 Operator : CG/JU
 Sample : N2895-10
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P030-SS002-0006-01

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053707.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.100	14	19	33	rVB	204050	336495	2.15%	1.140%
2	5.555	430	437	450	rBV	398259	649179	4.15%	2.200%
3	7.165	704	711	723	rBV	431711	758772	4.85%	2.571%
4	9.150	1040	1049	1060	rBV	273789	491186	3.14%	1.664%
5	10.795	1323	1329	1338	rBV	124440	215504	1.38%	0.730%
6	13.245	1739	1746	1755	rVB	787739	1184150	7.57%	4.013%
7	14.625	1971	1981	1988	rVB	214539	325356	2.08%	1.102%
8	16.117	2228	2235	2250	rBV	623363	968654	6.20%	3.282%
9	17.369	2443	2448	2455	rVB	253993	384011	2.46%	1.301%
10	18.262	2595	2600	2615	rBV	304940	494385	3.16%	1.675%
11	19.413	2793	2796	2808	rVV3	92678	236869	1.51%	0.803%
12	19.531	2811	2816	2831	rVB	154679	270700	1.73%	0.917%
13	19.977	2886	2892	2899	rVB	1277297	1674733	10.71%	5.675%
14	21.263	3107	3111	3123	rBV	242218	366844	2.35%	1.243%
15	21.540	3148	3158	3162	rVB	8921158	15635038	100.00%	52.980%
16	21.639	3169	3175	3184	rBV	247889	427235	2.73%	1.448%
17	22.427	3302	3309	3318	rBV4	70687	208293	1.33%	0.706%
18	23.954	3563	3569	3579	rVB3	97915	241496	1.54%	0.818%
19	24.841	3711	3720	3729	rVB2	142506	411939	2.63%	1.396%
20	25.340	3797	3805	3815	rVB3	85382	237874	1.52%	0.806%
21	26.075	3919	3930	3947	rBV3	271182	1017380	6.51%	3.447%
22	28.066	4256	4269	4282	rBV3	322581	1266458	8.10%	4.291%
23	29.123	4441	4449	4464	rVB5	80468	344700	2.20%	1.168%
24	30.099	4604	4615	4639	rVB8	121516	664555	4.25%	2.252%
25	30.569	4681	4695	4697	rBV8	133189	396594	2.54%	1.344%
26	32.031	4928	4944	4957	rBV6	54574	302948	1.94%	1.027%

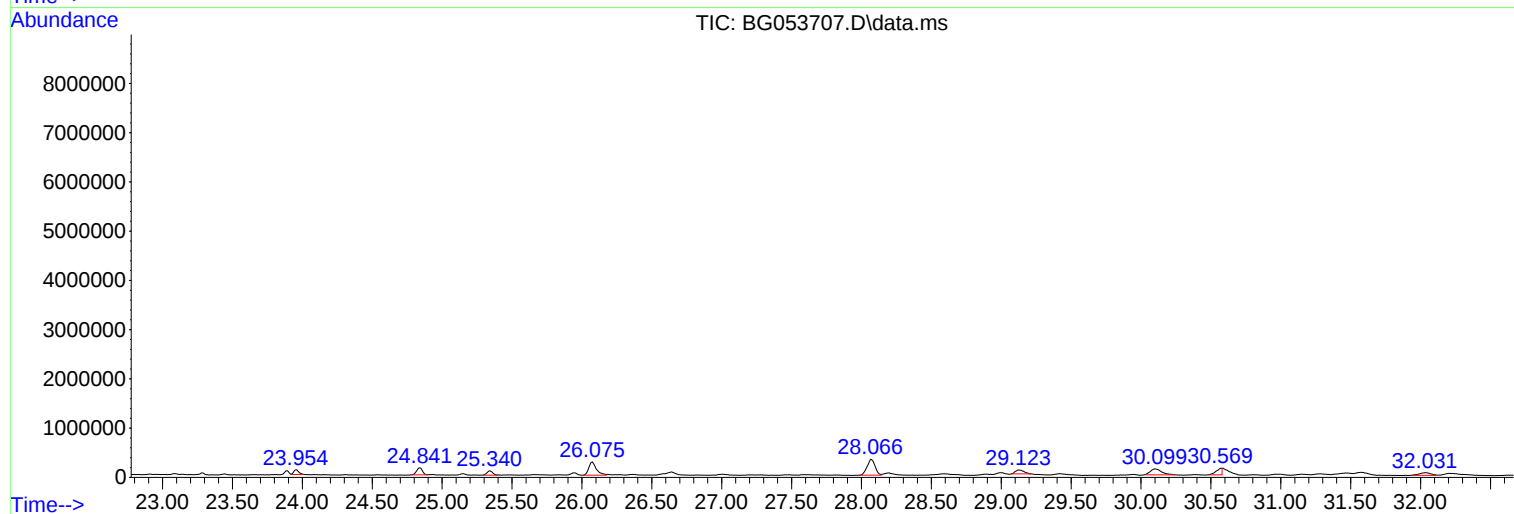
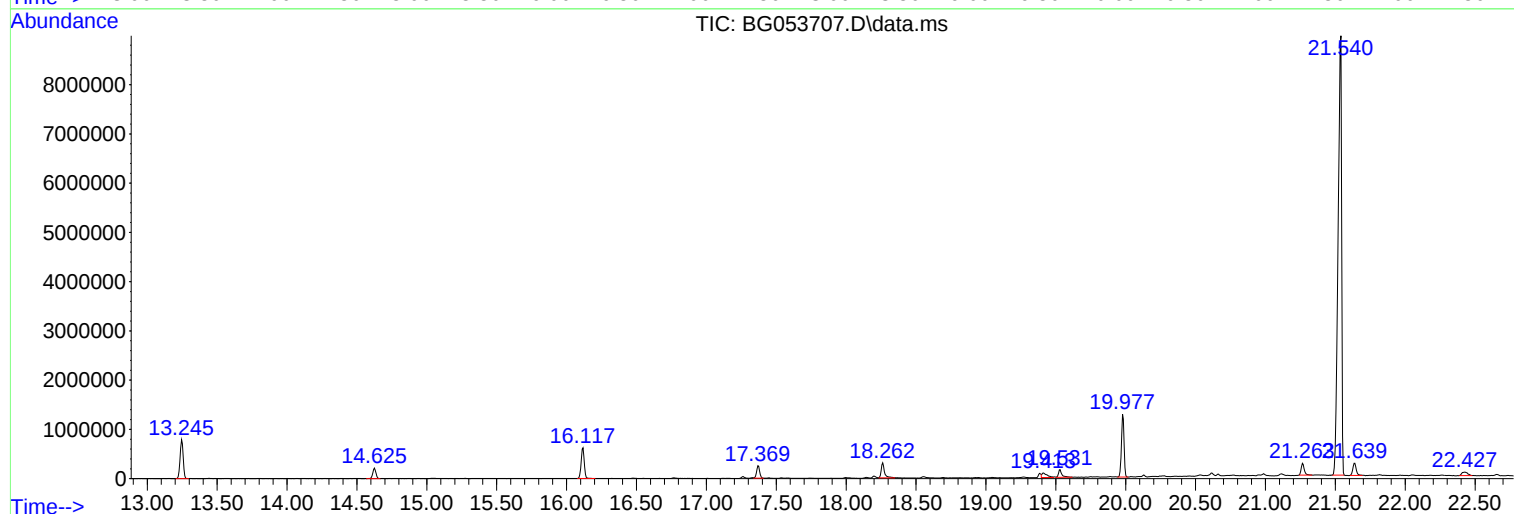
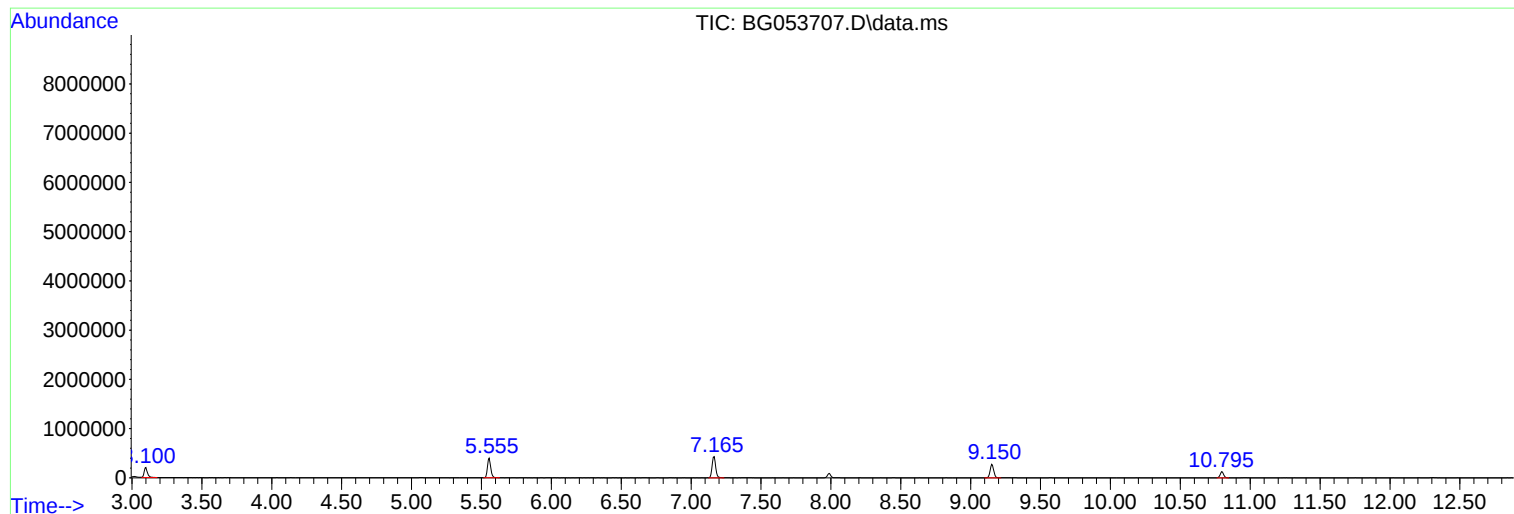
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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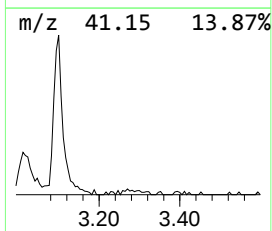
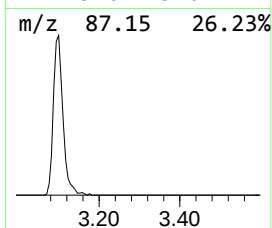
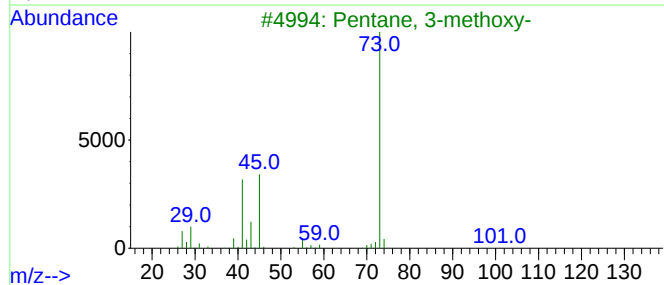
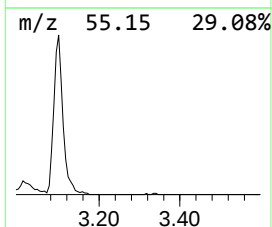
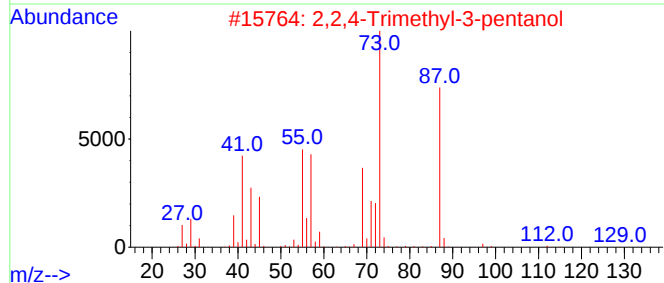
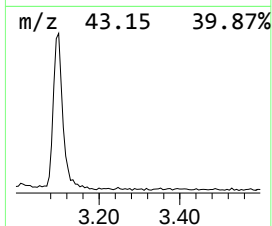
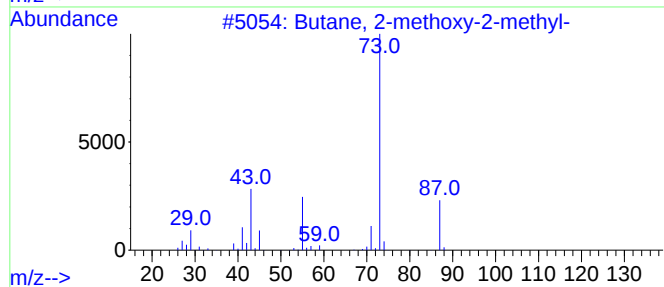
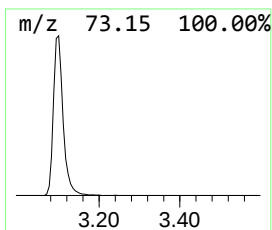
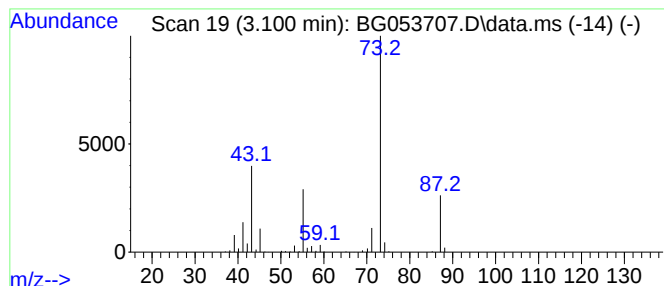
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.100	8.87 ng	336495	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



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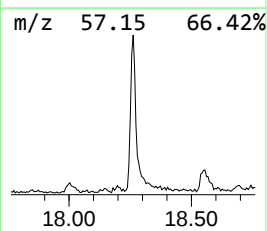
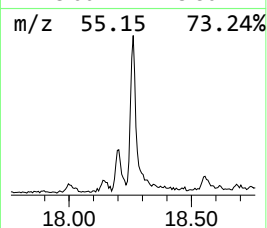
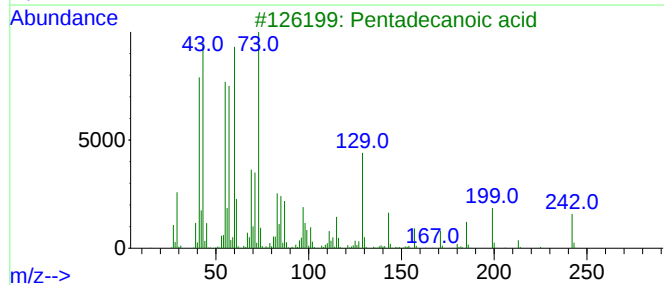
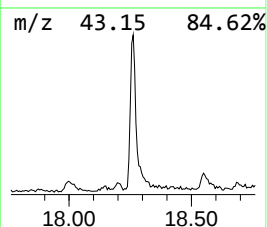
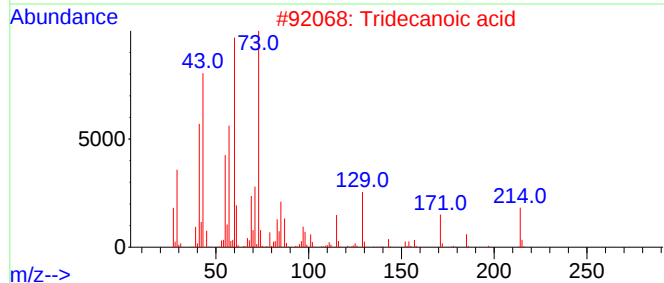
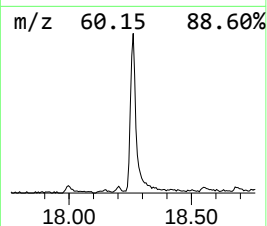
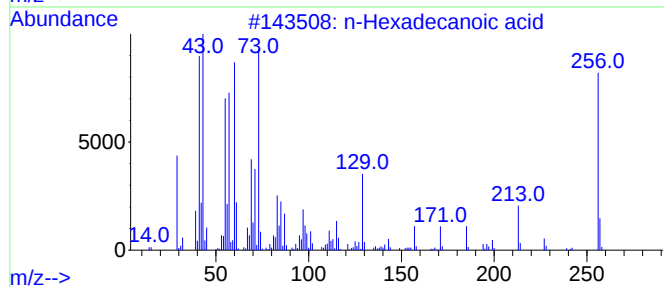
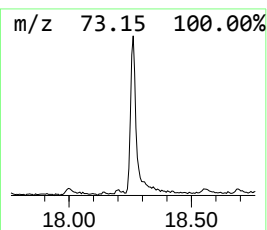
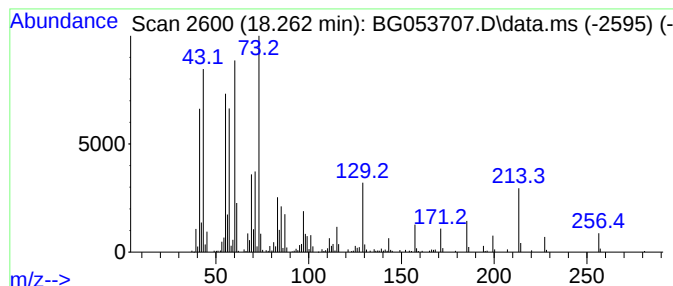
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.262	25.75 ng	494385	Phenanthrene-d10	17.369

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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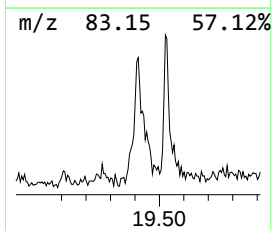
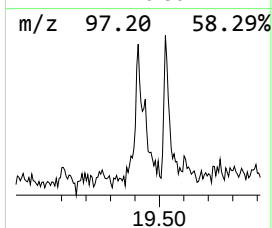
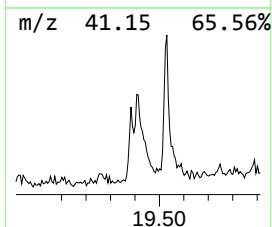
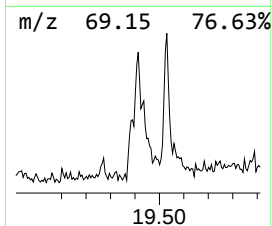
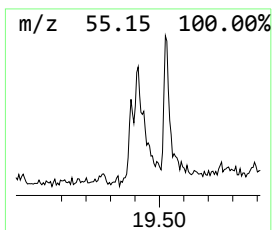
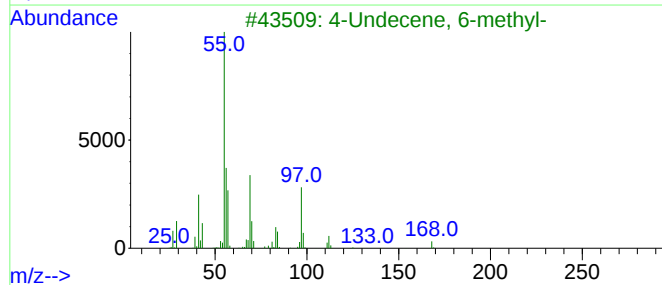
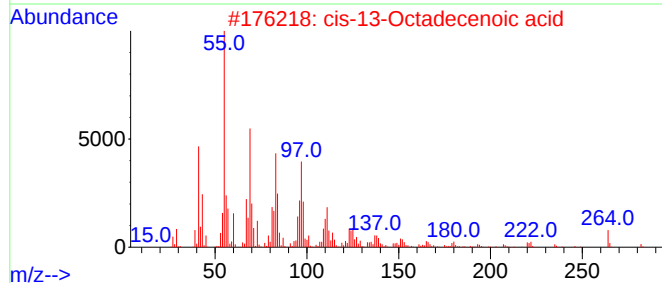
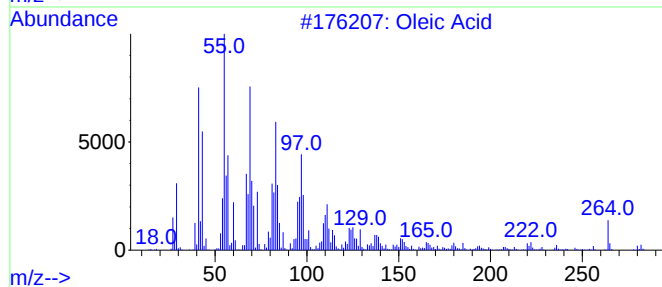
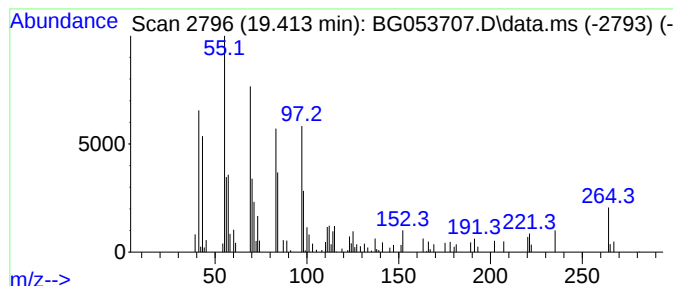
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Oleic Acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.413	12.34 ng	236869	Phenanthrene-d10	17.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid			282	C18H34O2	000112-80-1	86
2	cis-13-Octadecenoic acid			282	C18H34O2	013126-39-1	47
3	4-Undecene, 6-methyl-			168	C12H24	1000061-85-4	47
4	cis-Vaccenic acid			282	C18H34O2	000506-17-2	43
5	2(5H)-Furanone, 5,5-dimethyl-			112	C6H8O2	020019-64-1	35



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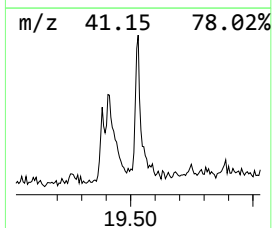
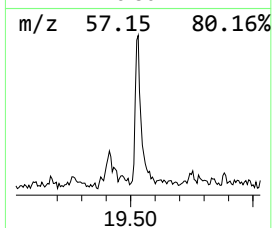
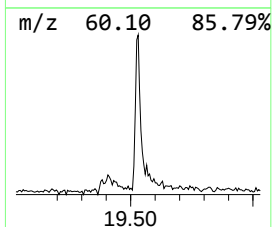
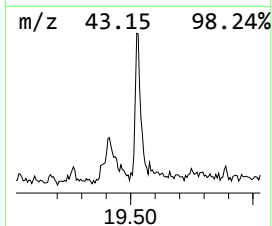
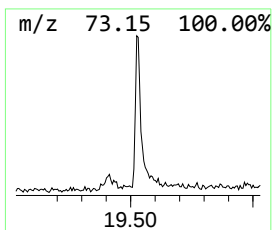
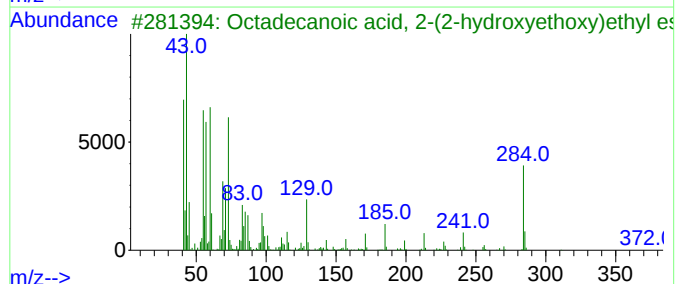
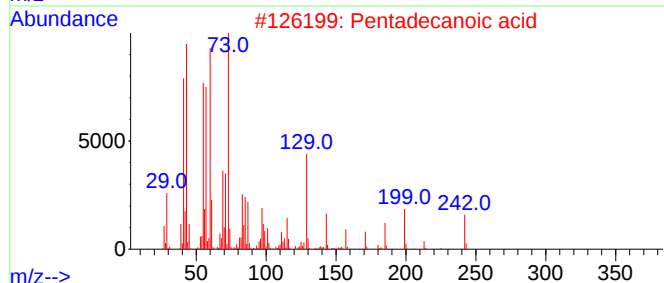
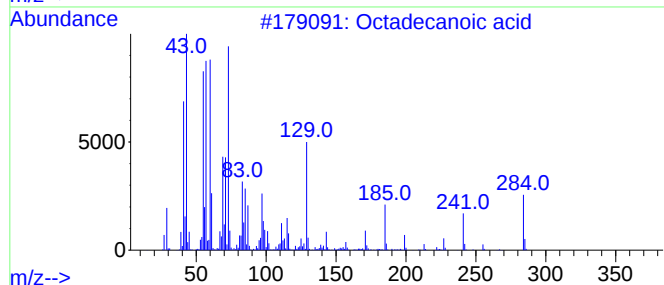
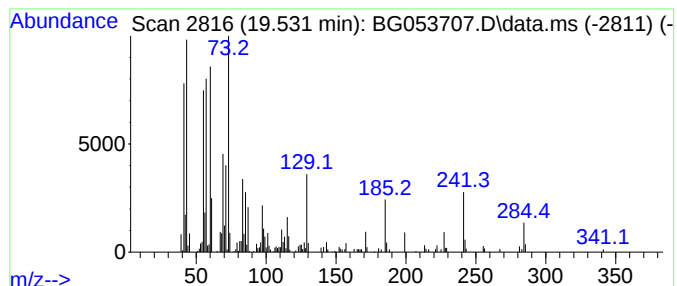
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.531	12.67 ng	270700	Chrysene-d12	21.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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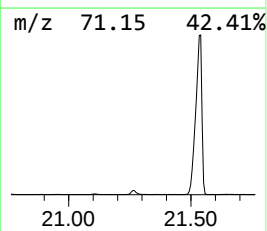
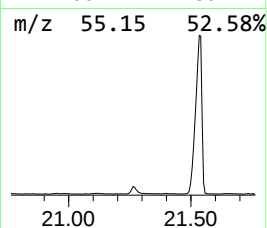
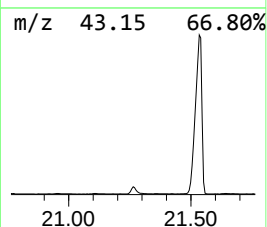
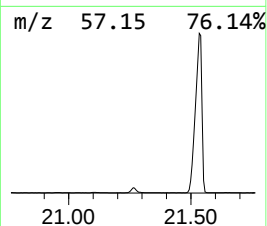
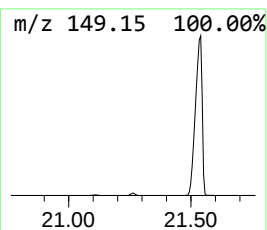
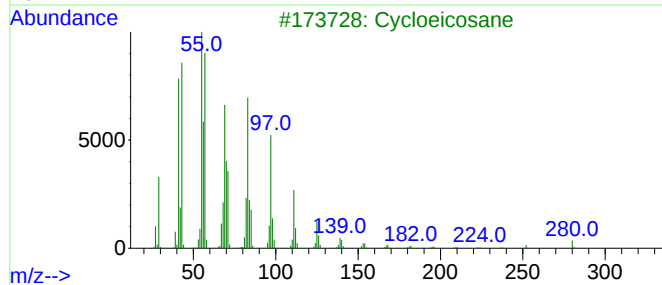
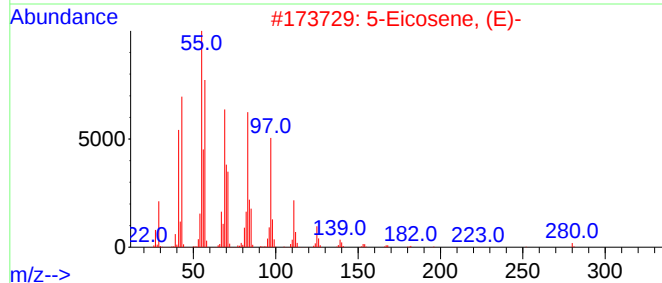
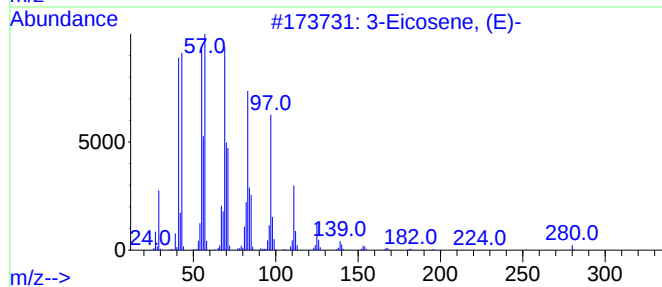
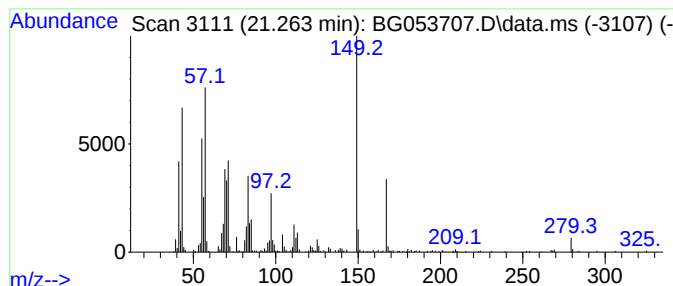
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.264	17.17 ng	366844	Chrysene-d12	21.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	92
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	92
3			Cycloeicosane	280	C20H40	000296-56-0	91
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	72
5			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	46



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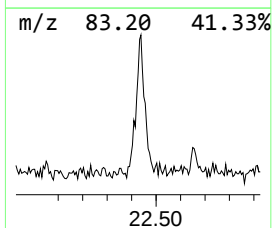
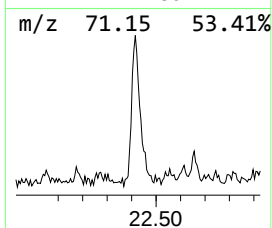
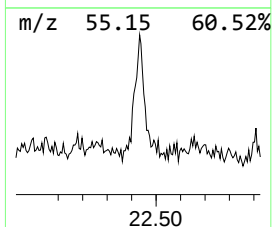
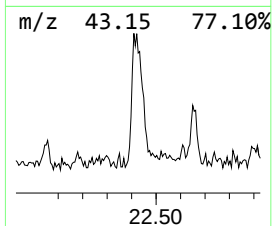
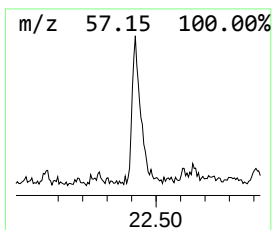
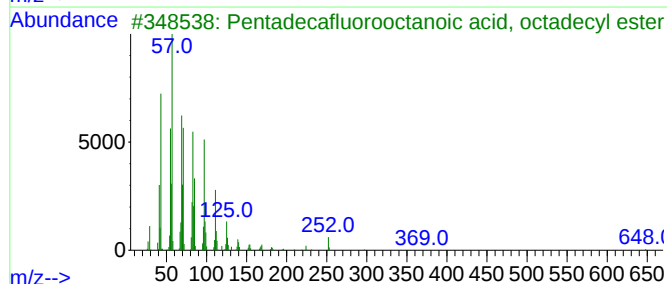
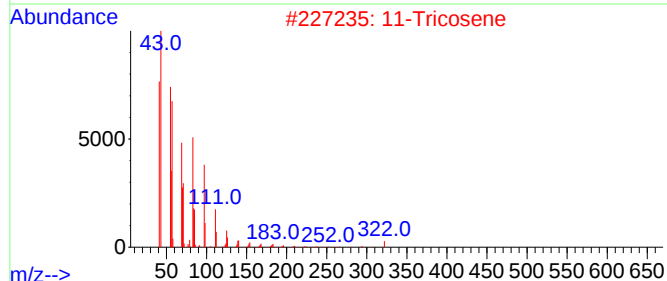
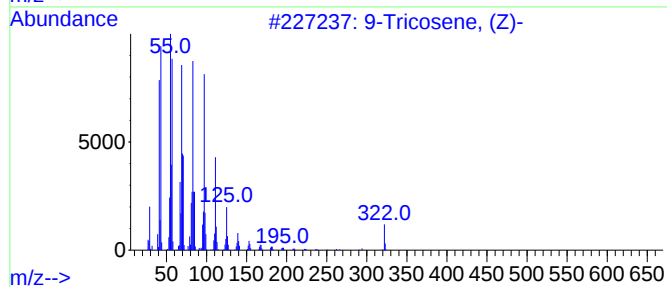
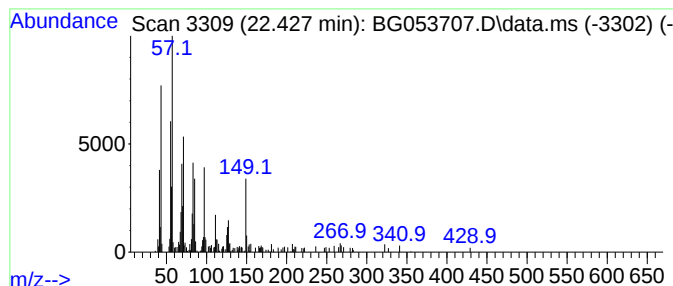
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Tricosene, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	9.75 ng	208293	Chrysene-d12	21.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
2			11-Tricosene	322	C23H46	052078-56-5	83
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	68
4			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	64
5			Heptyl octacosyl ether	509	C35H72O	1000406-40-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053707.D
Acq On : 25 May 2022 23:46
Operator : CG/JU
Sample : N2895-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P030-SS002-0006-01

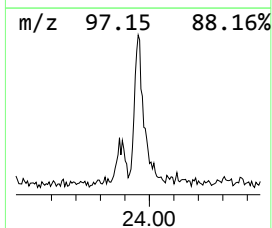
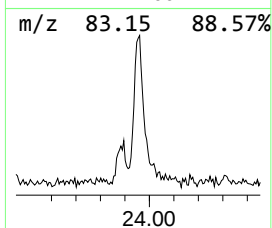
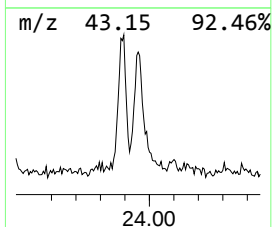
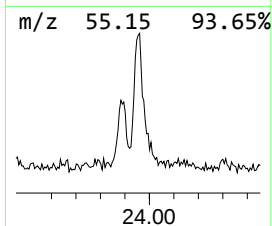
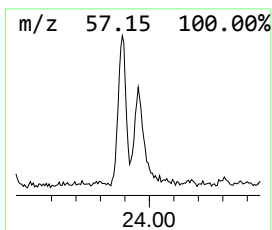
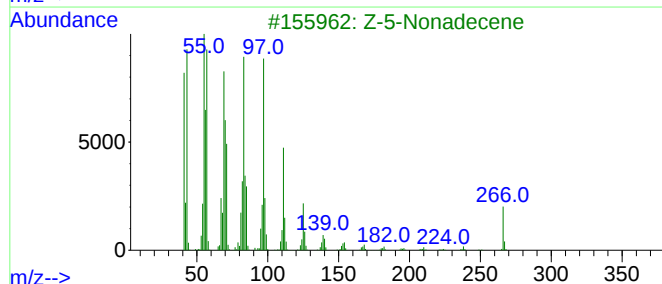
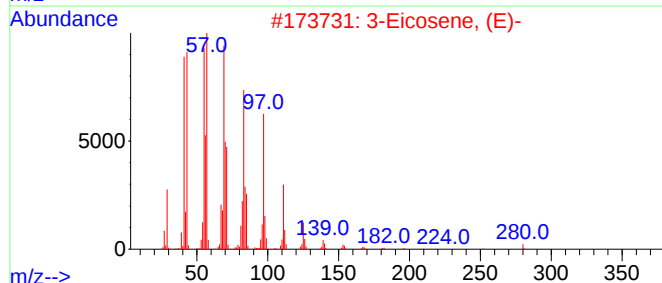
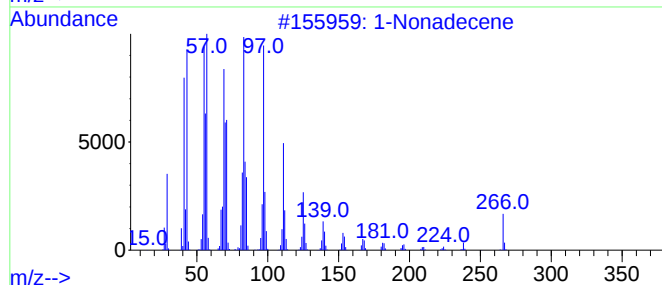
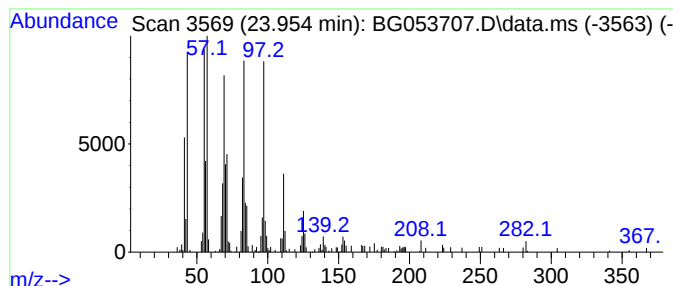
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.954	11.72 ng	241496	Perylene-d12	24.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	97
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	95
4			Behenic alcohol	326	C22H46O	000661-19-8	95
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053707.D
Acq On : 25 May 2022 23:46
Operator : CG/JU
Sample : N2895-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P030-SS002-0006-01

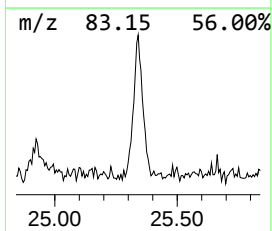
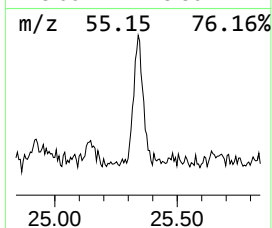
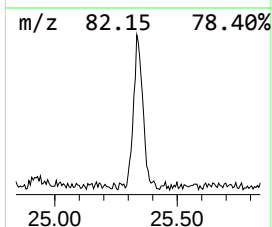
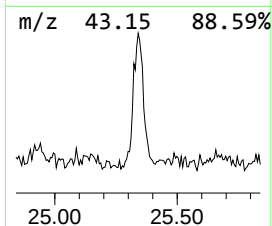
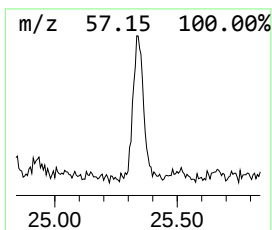
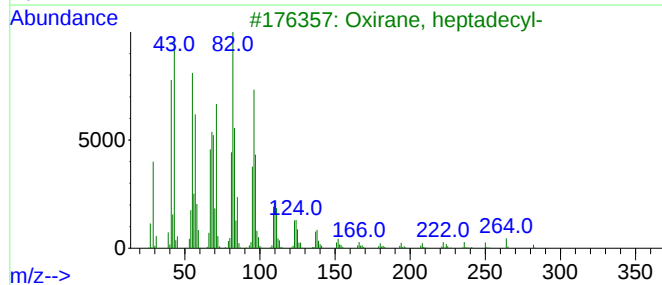
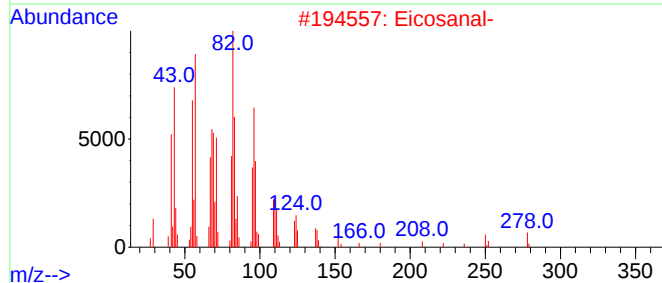
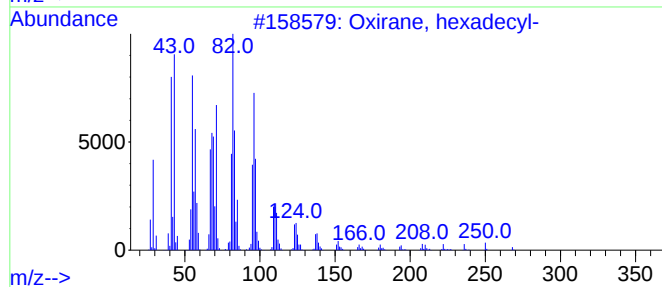
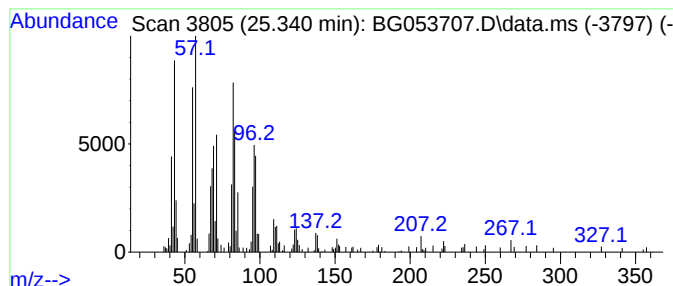
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanal- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.340	11.55 ng	237874	Perylene-d12	24.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	81	
2	Eicosanal-		296	C20H40O	002400-66-0	74	
3	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	74	
4	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	70	
5	Hexadecanal		240	C16H32O	000629-80-1	68	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
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Misc :
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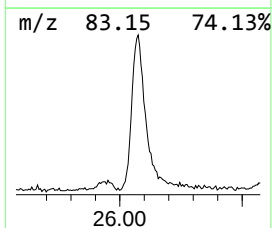
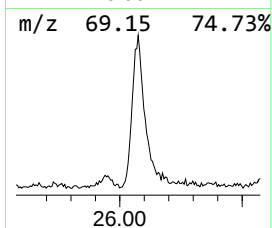
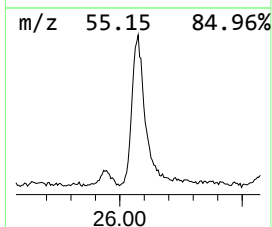
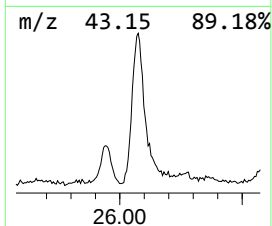
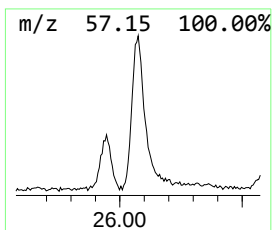
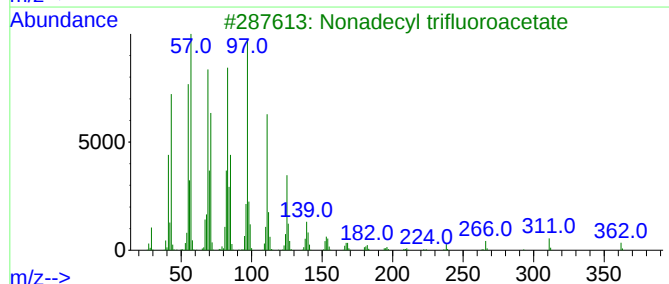
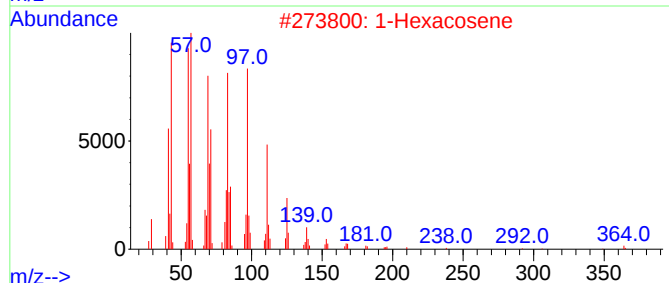
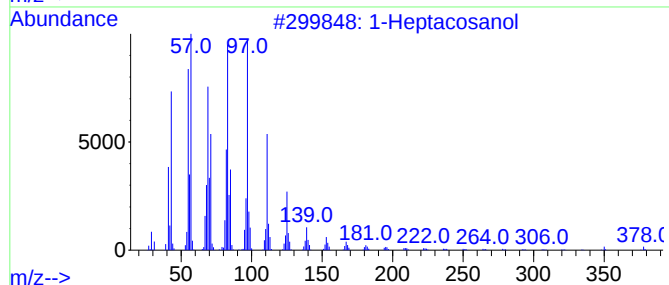
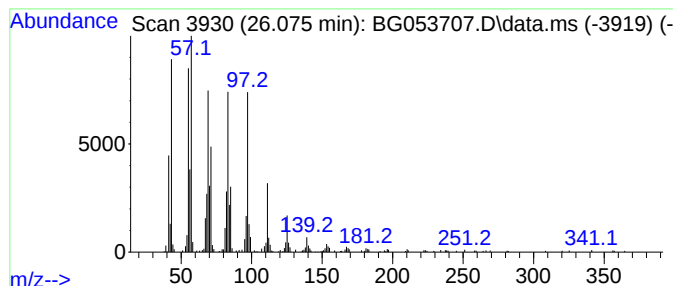
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.075	49.39 ng	1017380	Perylene-d12	24.841	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4	Octacosanol	410	C28H58O	000557-61-9	90
5	1-Tetracosene	336	C24H48	010192-32-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
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Sample : N2895-10
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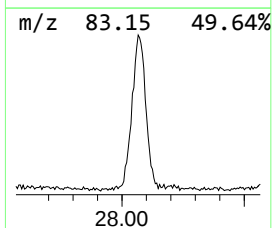
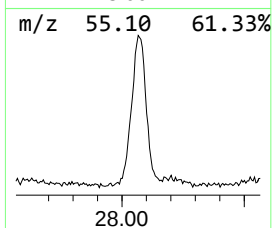
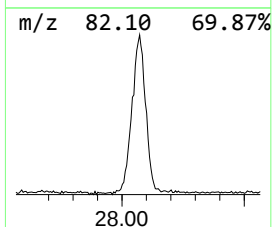
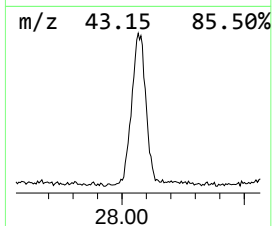
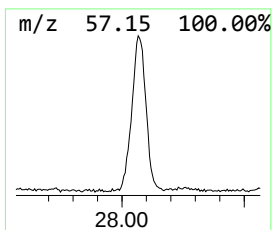
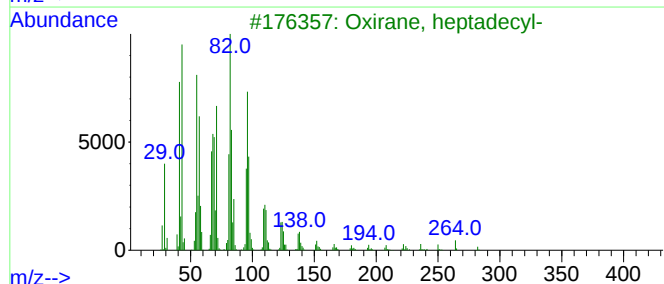
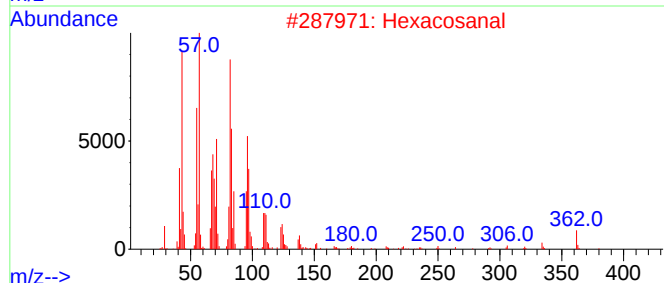
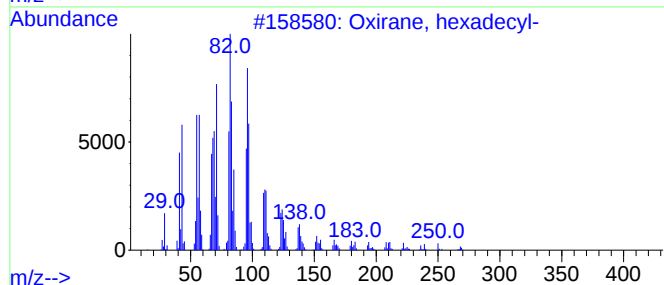
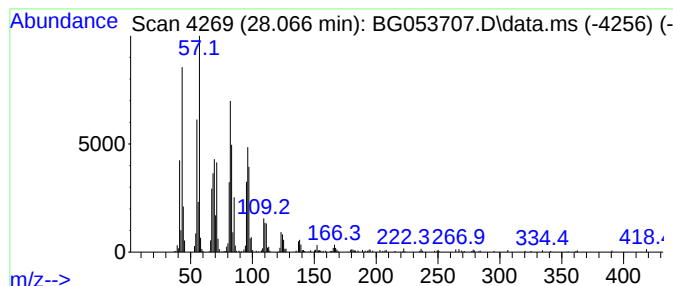
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, hexadecyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
28.066	61.49 ng	1266460	Perylene-d12		24.841	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
2	Hexacosanal		380	C26H52O	026627-85-0	91
3	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	91
4	Octadecanal		268	C18H36O	000638-66-4	90
5	Tetracosanal		352	C24H48O	057866-08-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053707.D
Acq On : 25 May 2022 23:46
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ALS Vial : 16 Sample Multiplier: 1

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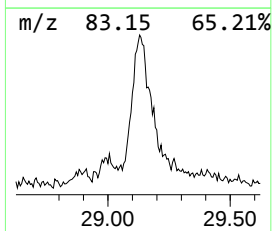
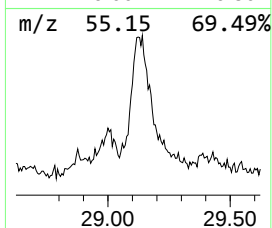
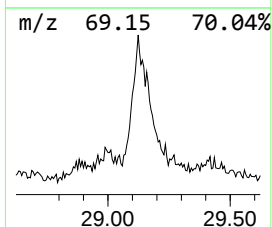
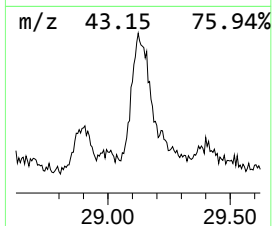
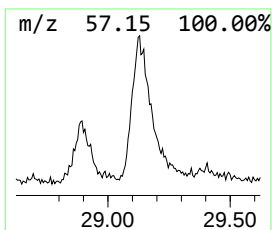
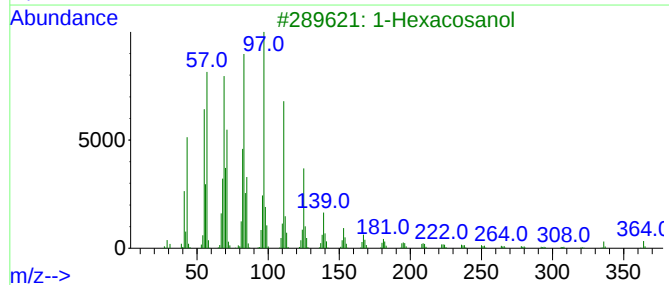
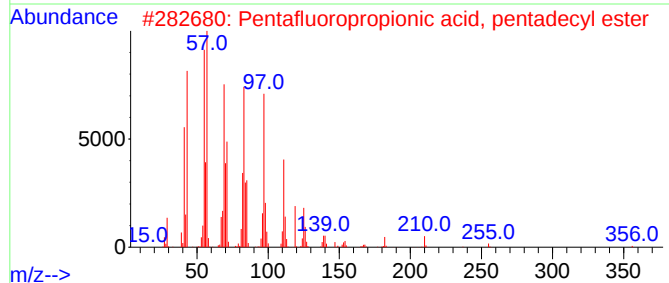
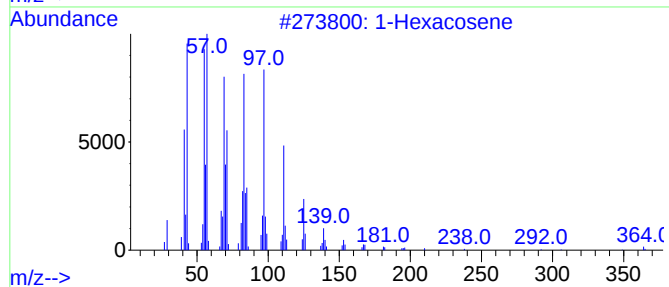
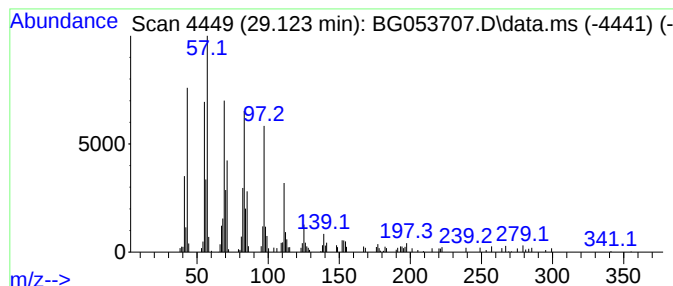
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexacosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.123	16.74 ng	344700	Perylene-d12	24.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
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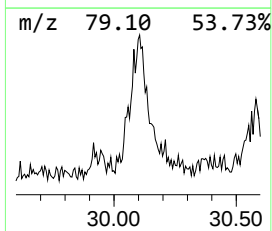
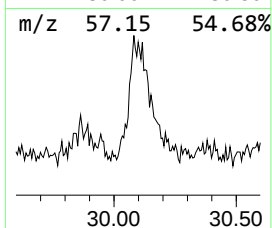
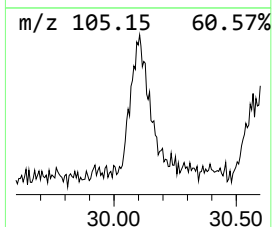
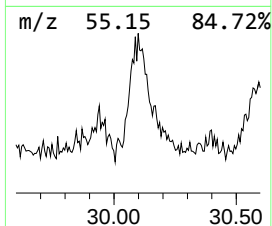
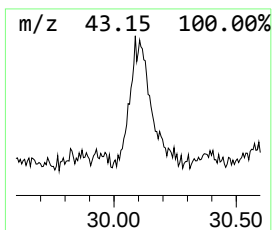
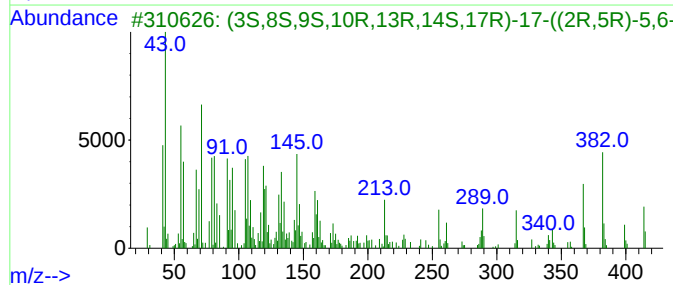
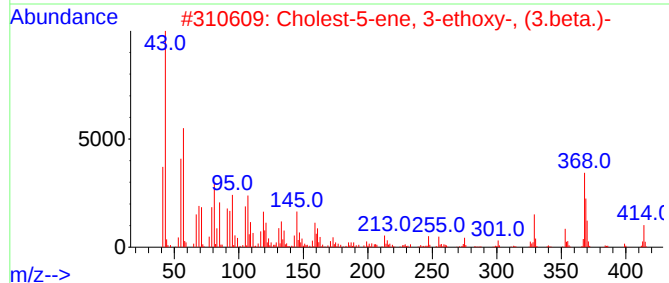
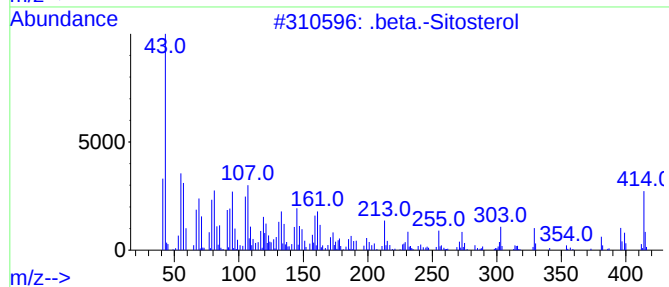
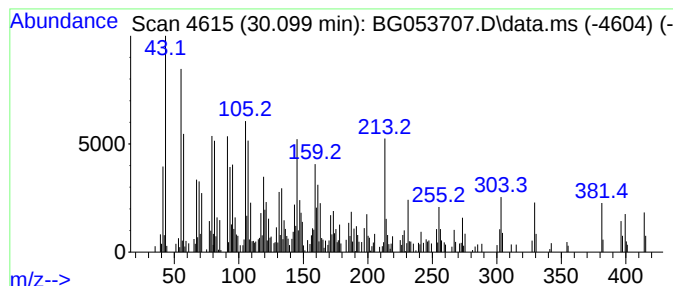
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.099	32.26 ng	664555	Perylene-d12	24.841
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 93
2		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 64
3		(3S,8S,9S,10R,13R,14S,17R)-17-((...	414 C29H50O	029365-29-5 58
4		.gamma.-Sitosterol	414 C29H50O	000083-47-6 49
5		Campesterol	400 C28H48O	000474-62-4 46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053707.D
Acq On : 25 May 2022 23:46
Operator : CG/JU
Sample : N2895-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P030-SS002-0006-01

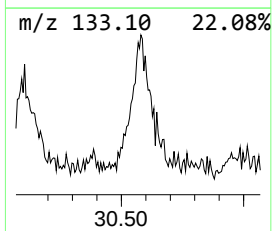
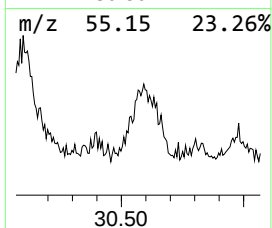
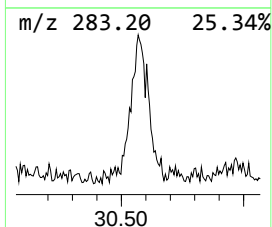
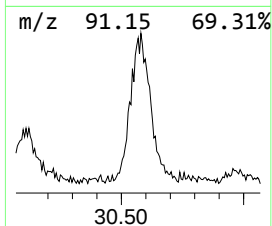
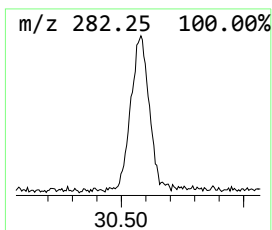
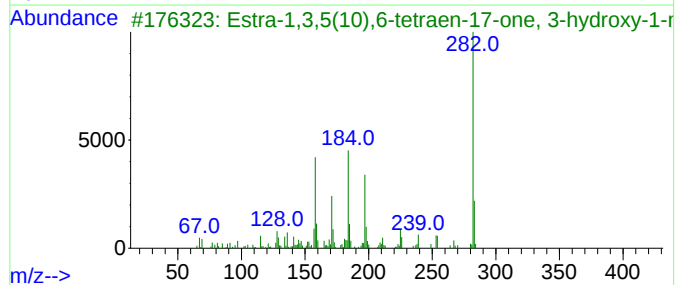
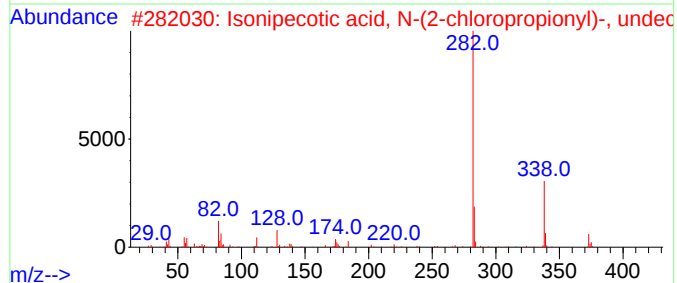
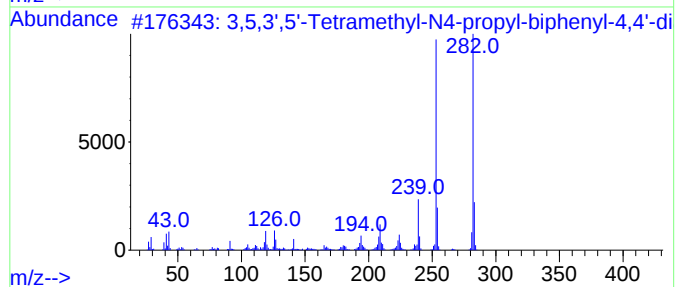
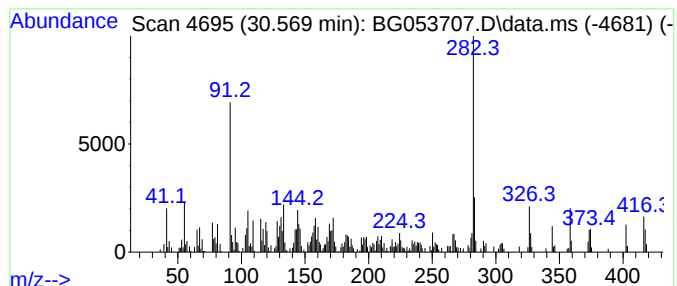
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown30.569 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.569	19.25 ng	396594	Perylene-d12	24.841

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,5,3',5'-Tetramethyl-N4-propyl-...	282	C19H26N2	1000193-02-0	46
2		Isonipecotic acid, N-(2-chloropr...	373	C20H36ClNO3	1000361-02-1	45
3		Estra-1,3,5(10),6-tetraen-17-one...	282	C19H22O2	003129-08-6	41
4		Thebaol, O-ethyl-	282	C18H18O3	1000449-91-2	41
5		6H-Benzofuro[3,2-c][1]benzopyran...	282	C17H14O4	001433-08-5	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053707.D
Acq On : 25 May 2022 23:46
Operator : CG/JU
Sample : N2895-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P030-SS002-0006-01

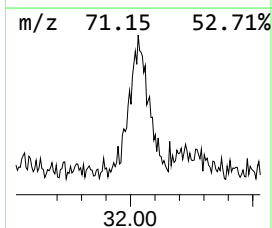
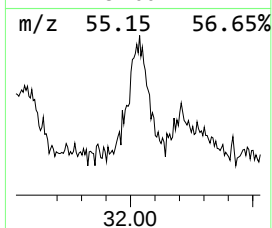
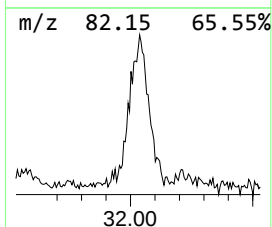
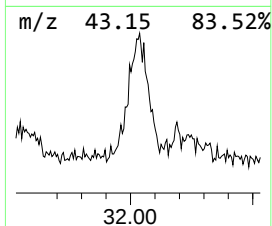
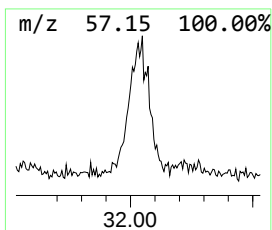
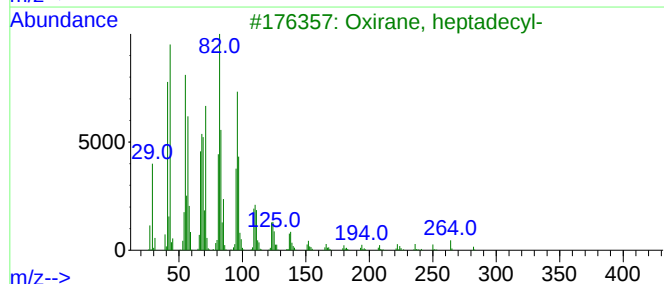
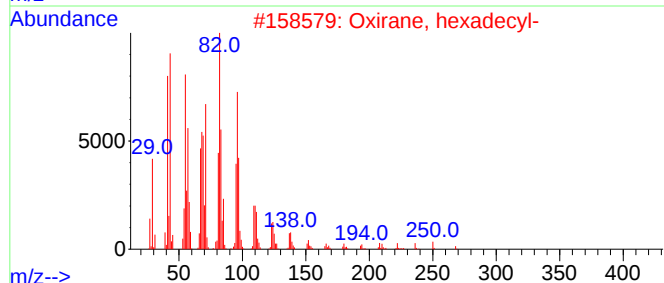
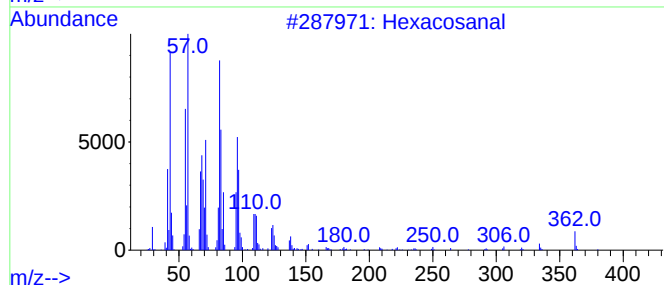
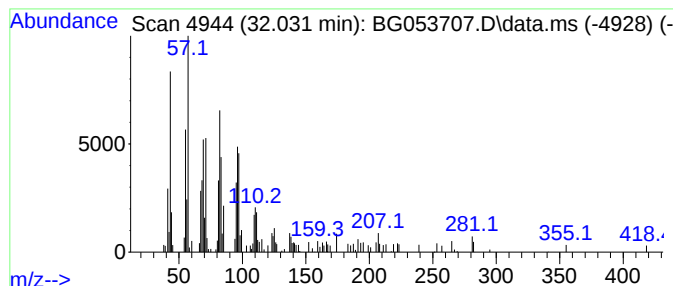
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexacosanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.031	14.71 ng	302948	Perylene-d12	24.841

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosanal	380	C26H52O	026627-85-0	83
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	72
4		1,19-Eicosadiene	278	C20H38	014811-95-1	68
5		Octadecanal	268	C18H36O	000638-66-4	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053707.D
 Acq On : 25 May 2022 23:46
 Operator : CG/JU
 Sample : N2895-10
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P030-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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
Butane, 2-metho...	3.100	8.9	ng	336495	1	7.987	758772	20.0
n-Hexadecanoic ...	18.262	25.8	ng	494385	4	17.369	384011	20.0
Oleic Acid	19.413	12.3	ng	236869	4	17.369	384011	20.0
Octadecanoic acid	19.531	12.7	ng	270700	5	21.634	427235	20.0
3-Eicosene, (E)-	21.264	17.2	ng	366844	5	21.634	427235	20.0
9-Tricosene, (Z)-	22.427	9.8	ng	208293	5	21.634	427235	20.0
1-Nonadecene	23.954	11.7	ng	241496	6	24.841	411939	20.0
Eicosanal-	25.340	11.6	ng	237874	6	24.841	411939	20.0
1-Heptacosanol	26.075	49.4	ng	1017380	6	24.841	411939	20.0
Oxirane, hexade...	28.066	61.5	ng	1266460	6	24.841	411939	20.0
1-Hexacosene	29.123	16.7	ng	344700	6	24.841	411939	20.0
.beta.-Sitosterol	30.099	32.3	ng	664555	6	24.841	411939	20.0
unknown30.569	30.569	19.3	ng	396594	6	24.841	411939	20.0
Hexacosanal	32.031	14.7	ng	302948	6	24.841	411939	20.0