

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
 Data File : BG054225.D
 Acq On : 7 Jul 2022 14:48
 Operator : CG/JU
 Sample : N3595-16
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20220493-FIELD-BLANK

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-BG061322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054225.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.637	376	383	392	rVB	134622	236817	10.27%	2.090%
2	7.230	648	654	663	rVB	88258	154711	6.71%	1.366%
3	8.064	789	796	805	rVB	74533	129759	5.63%	1.145%
4	9.227	985	994	1003	rBV	216727	411923	17.86%	3.636%
5	10.872	1267	1274	1283	rVB	98349	182105	7.90%	1.607%
6	12.271	1495	1512	1513	rBV6	8930	29964	1.30%	0.264%
7	13.317	1682	1690	1697	rBV	636019	1042557	45.21%	9.202%
8	14.692	1916	1924	1930	rBV	176316	280481	12.16%	2.476%
9	16.178	2170	2177	2191	rBV3	684115	1106598	47.98%	9.767%
10	17.435	2385	2391	2398	rBV	258694	397664	17.24%	3.510%
11	18.187	2510	2519	2525	rBV8	16463	61175	2.65%	0.540%
12	19.321	2707	2712	2720	rBV2	28134	73450	3.18%	0.648%
13	19.580	2750	2756	2769	rVB5	72560	219077	9.50%	1.934%
14	19.703	2769	2777	2780	rVV2	68549	155423	6.74%	1.372%
15	19.739	2780	2783	2788	rVB	67927	88524	3.84%	0.781%
16	20.044	2828	2835	2841	rBV	1633077	2306242	100.00%	20.356%
17	20.191	2853	2860	2869	rBV2	54915	107898	4.68%	0.952%
18	20.720	2942	2950	2962	rBV	879265	1343931	58.27%	11.862%
19	20.826	2964	2968	2974	rVB	27984	40496	1.76%	0.357%
20	20.920	2979	2984	2995	rVB	78609	132272	5.74%	1.167%
21	21.319	3045	3052	3059	rBV5	28395	74692	3.24%	0.659%
22	21.707	3110	3118	3128	rVB2	324258	647813	28.09%	5.718%
23	21.889	3142	3149	3156	rVB3	23434	56010	2.43%	0.494%
24	22.565	3258	3264	3273	rVB	54716	134759	5.84%	1.189%
25	23.187	3362	3370	3388	rBV	520900	1159499	50.28%	10.234%
26	23.575	3428	3436	3443	rVB3	39329	104115	4.51%	0.919%
27	24.774	3633	3640	3650	rVB3	37848	109860	4.76%	0.970%
28	24.968	3663	3673	3684	rBV2	186968	541700	23.49%	4.781%

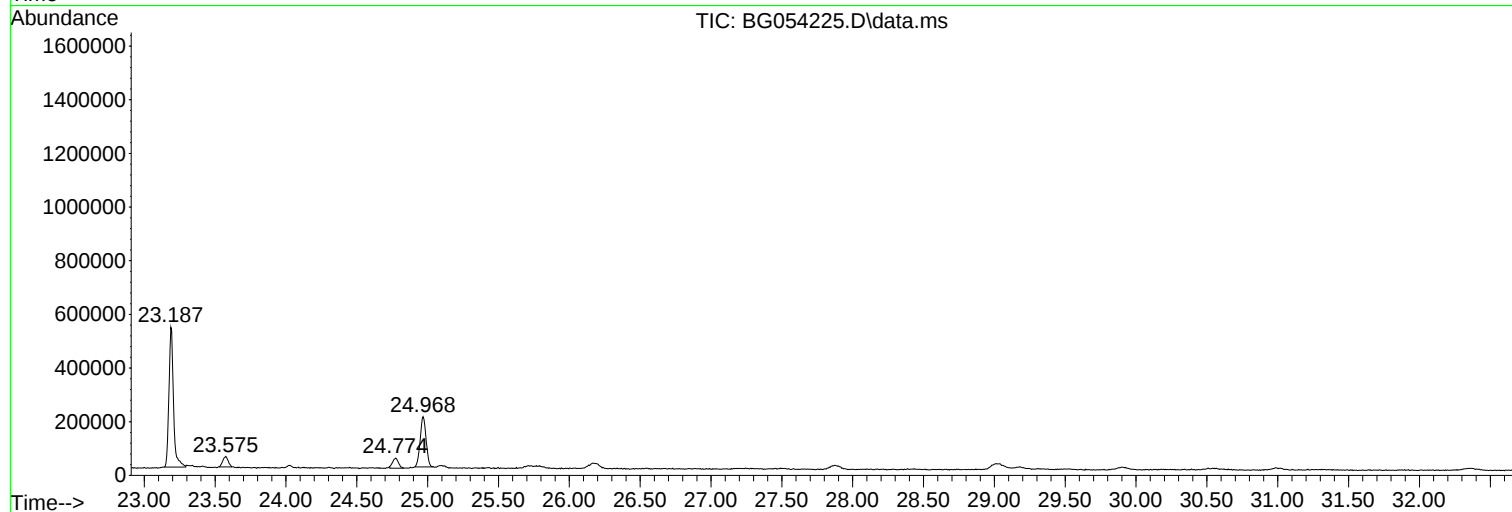
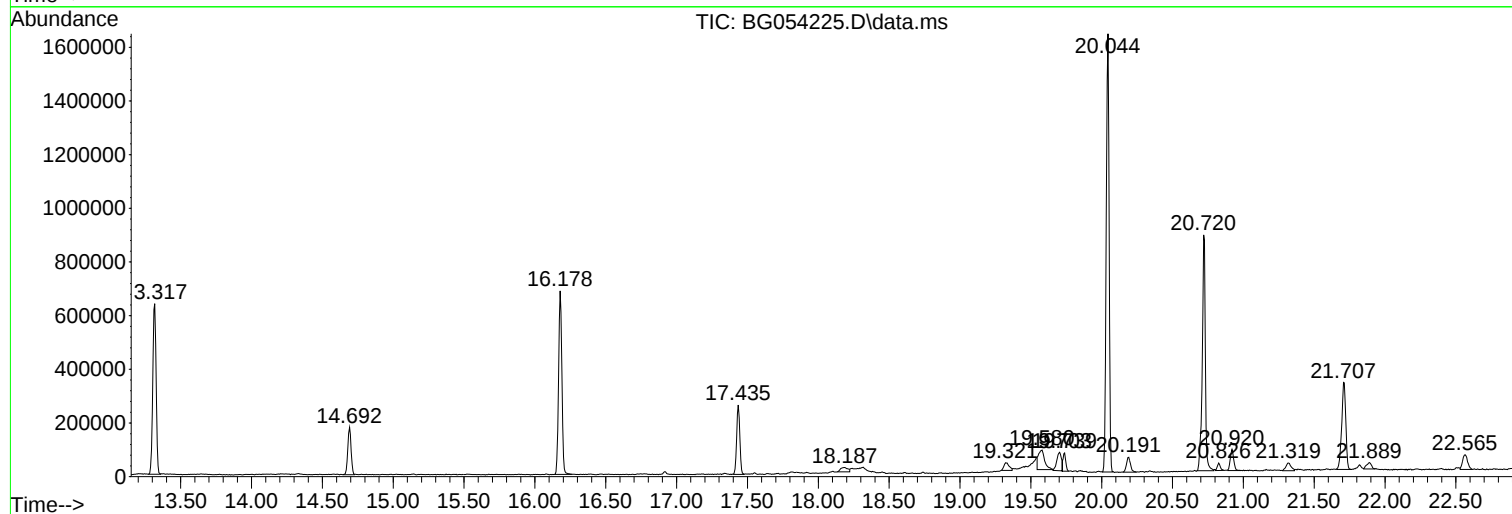
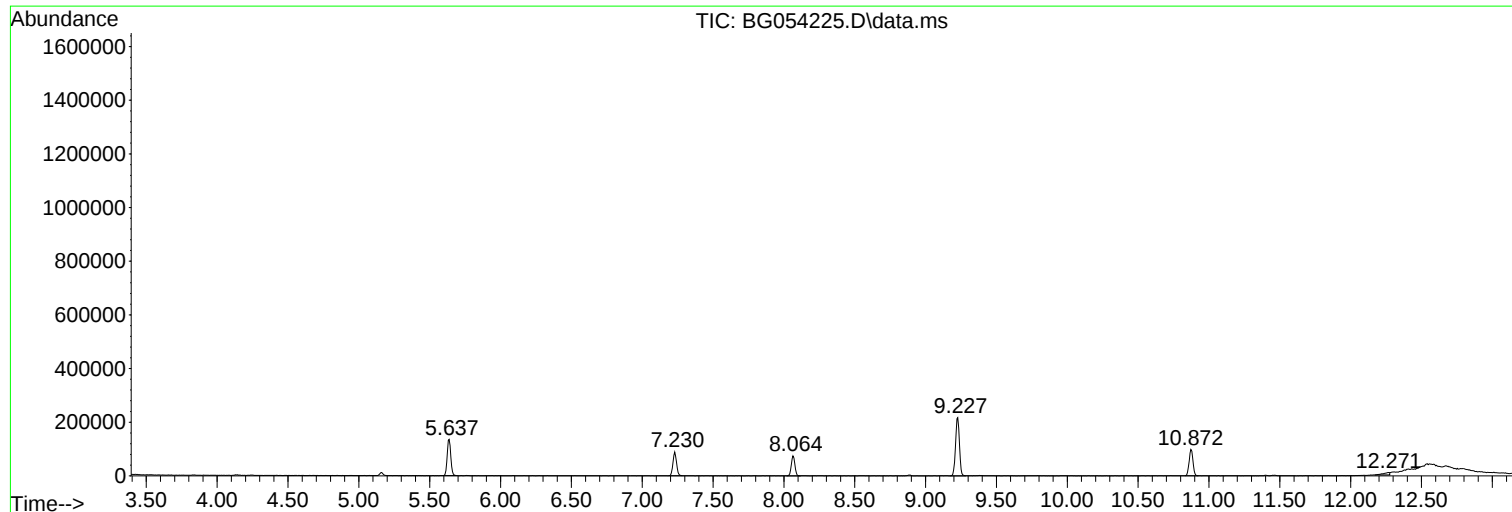
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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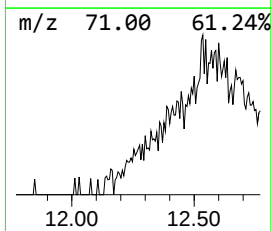
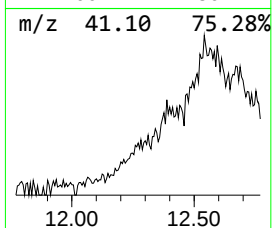
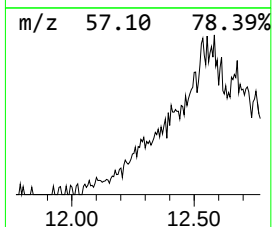
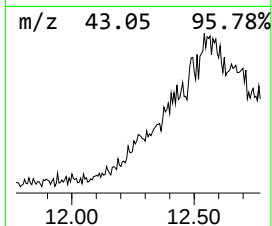
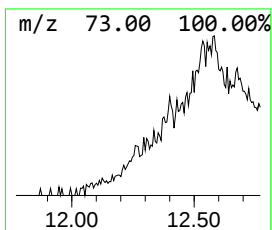
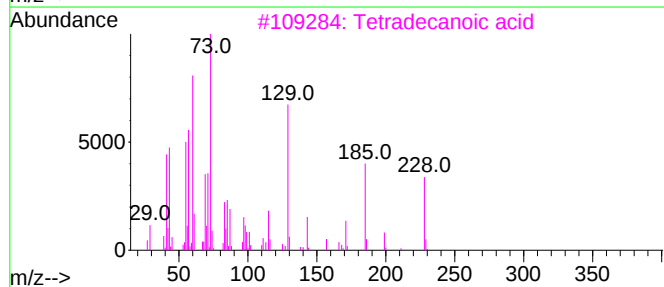
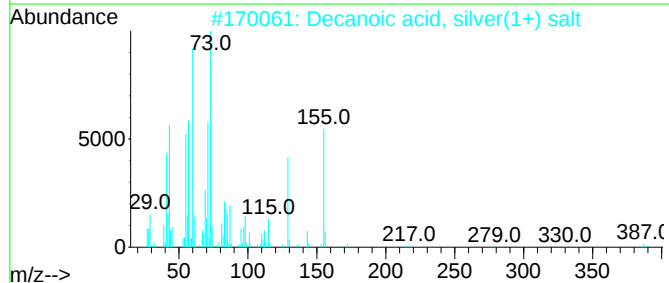
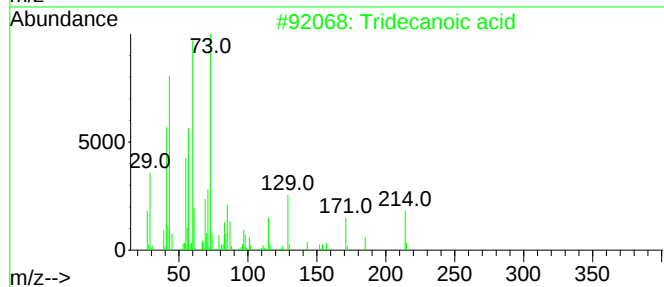
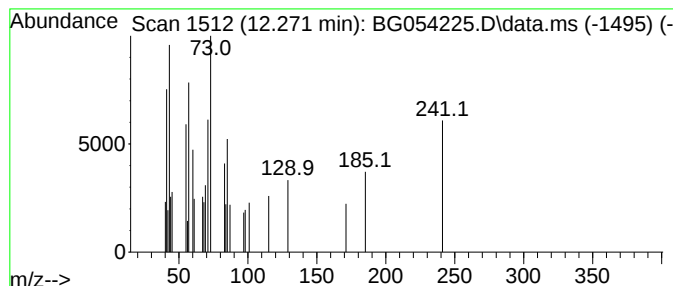
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown12.271 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.271	3.29 ng	29964	Naphthalene-d8	10.873

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	38
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	32
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	27
4			Lactose	342	C12H22O11	000063-42-3	14
5			Butanoic acid, 3-oxo-, propyl ester	144	C7H12O3	001779-60-8	14



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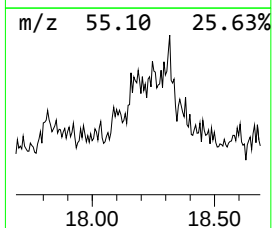
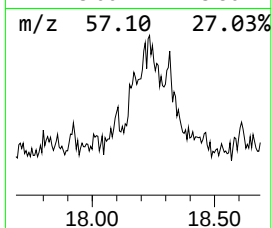
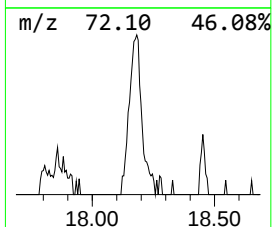
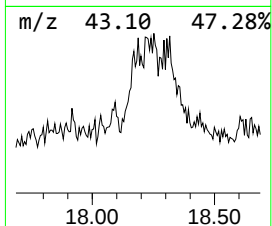
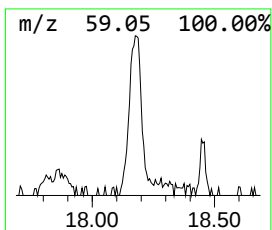
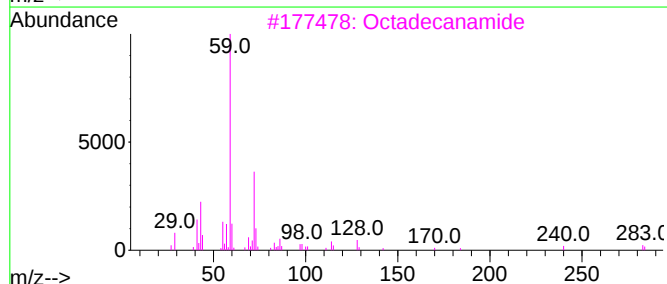
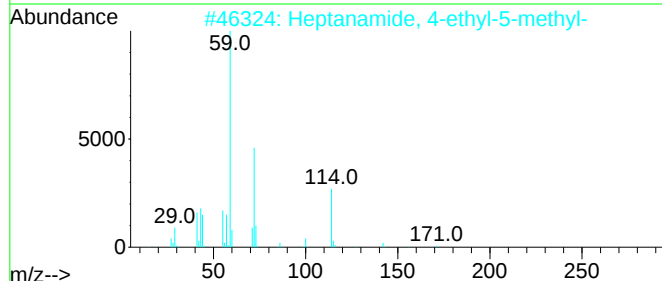
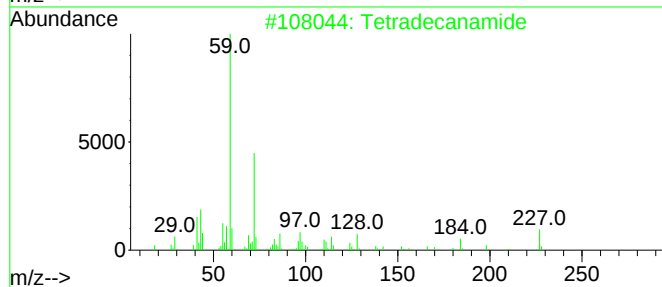
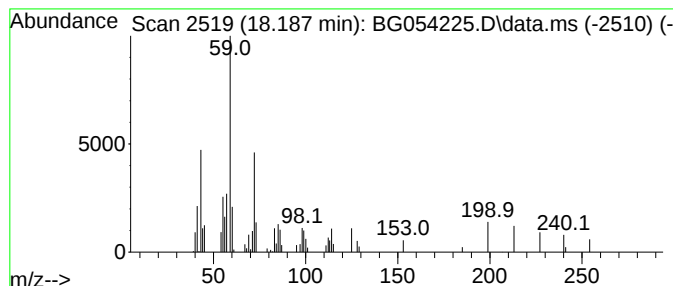
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tetradecanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.187	3.08 ng	61175	Phenanthrene-d10	17.435

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	53
2			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50
3			Octadecanamide	283	C18H37NO	000124-26-5	50
4			Hexadecanamide	255	C16H33NO	000629-54-9	50
5			7-Nonenamide	155	C9H17NO	090949-53-4	47



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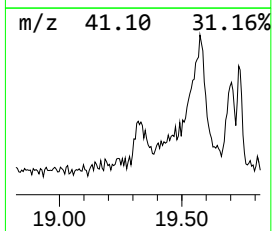
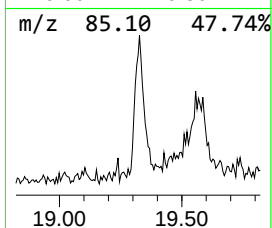
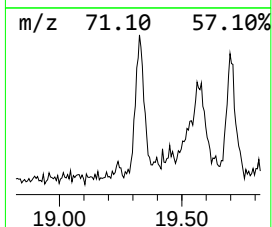
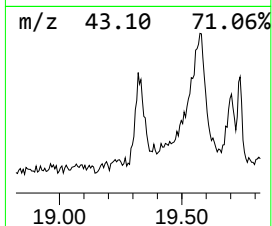
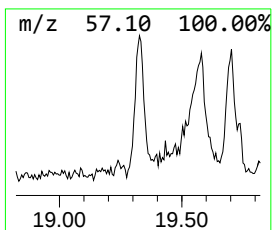
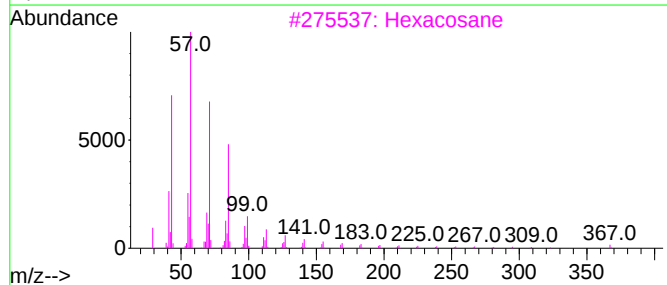
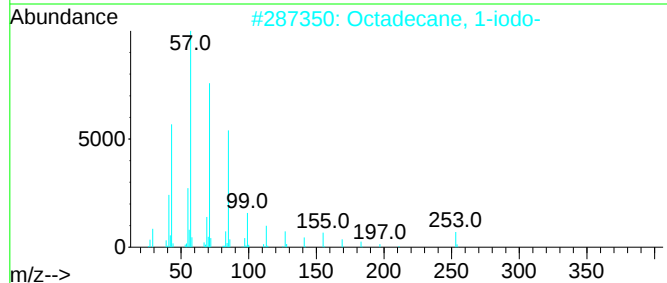
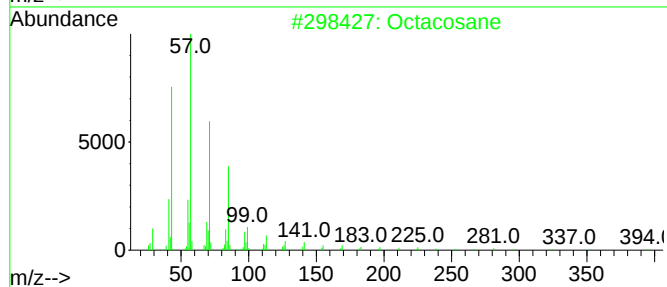
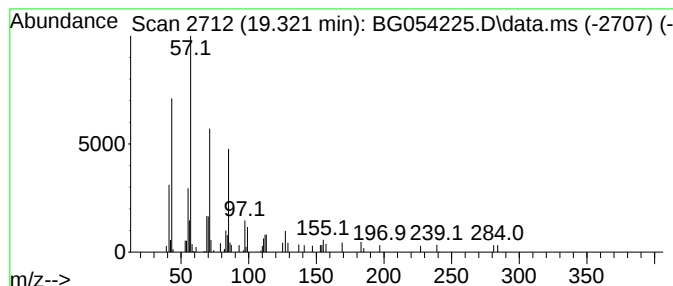
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	3.69 ng	73450	Phenanthrene-d10	17.435

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3			Hexacosane	366	C26H54	000630-01-3	86
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80



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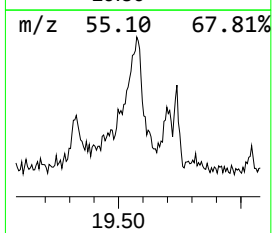
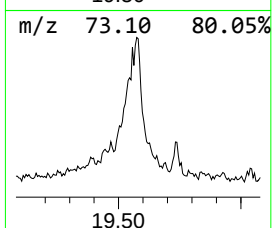
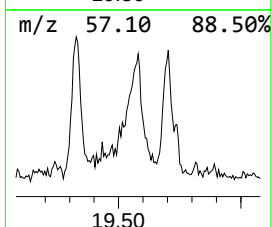
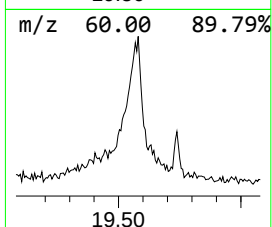
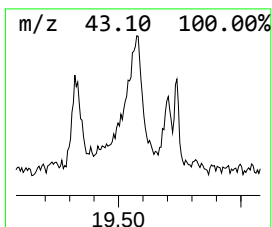
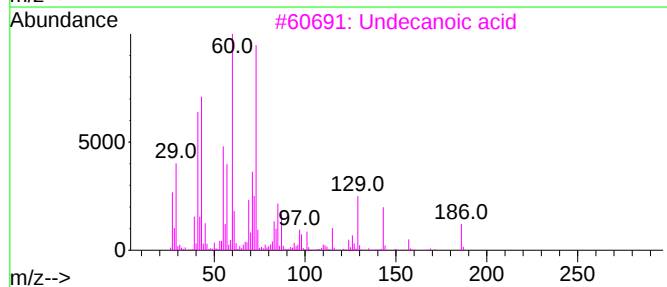
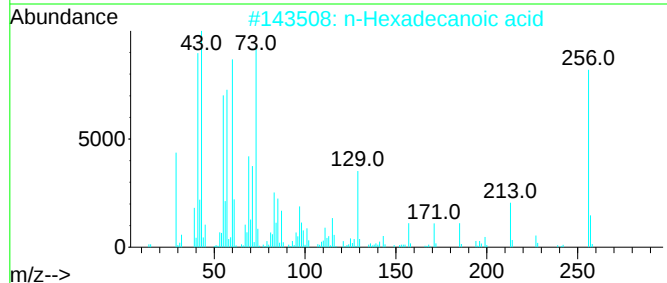
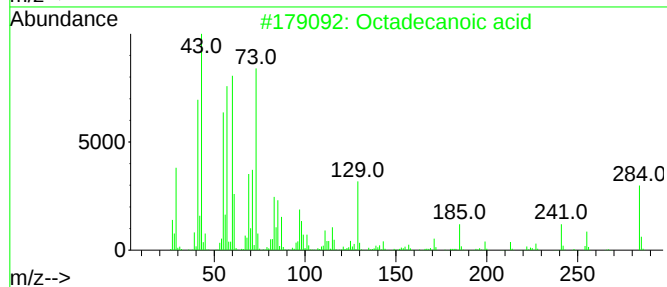
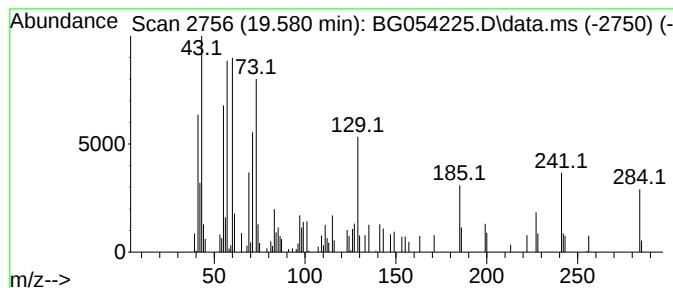
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.580	6.76 ng	219077	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	83
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3			Undecanoic acid	186	C11H22O2	000112-37-8	55
4			Dodecanoic acid	200	C12H24O2	000143-07-7	45
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38



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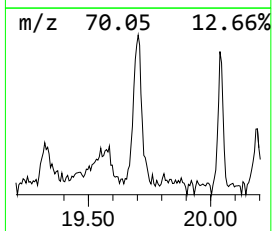
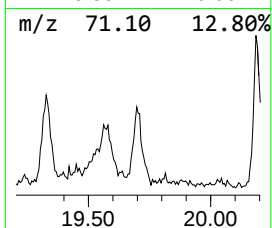
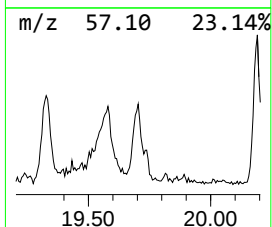
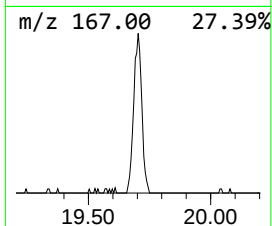
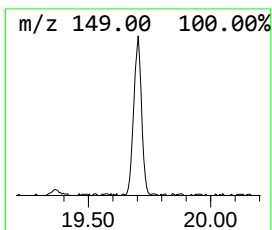
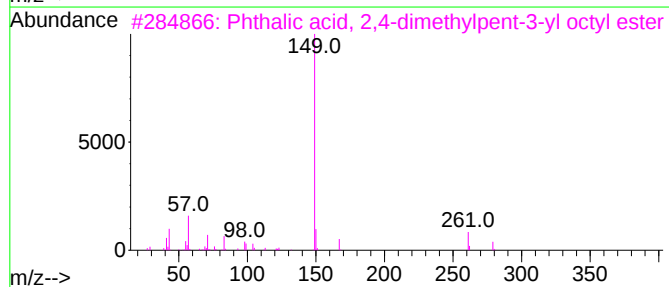
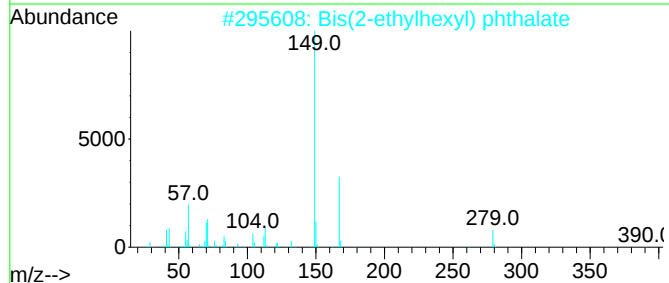
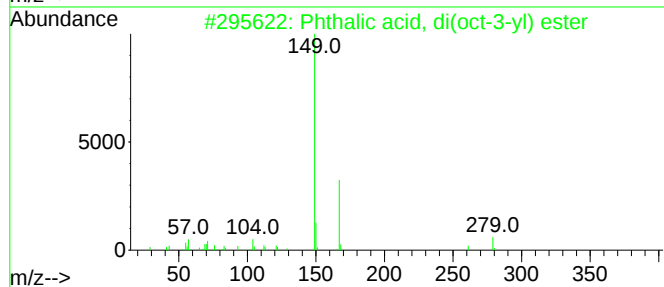
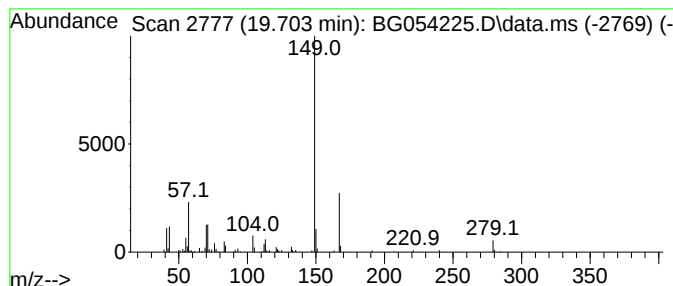
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Phthalic acid, di(oct-3-yl)... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.703	4.80 ng	155423	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, di(oct-3-yl) ester	390	C24H38O4	1000377-72-3	86
2			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	70
3			Phthalic acid, 2,4-dimethylpent-...	376	C23H36O4	1000356-84-7	64
4			Phthalic acid, octyl 2,4,4-trime...	390	C24H38O4	1010377-77-4	64
5			Phthalic acid, isohexyl 4-methyl...	334	C20H30O4	1010356-87-5	64



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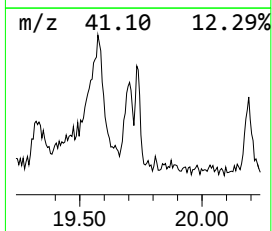
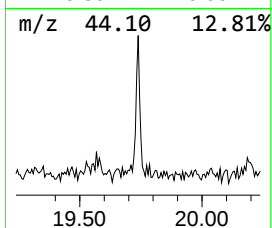
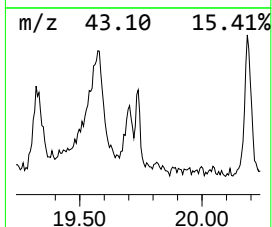
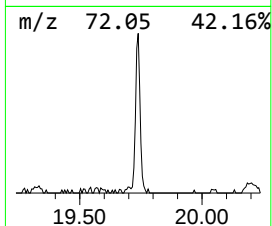
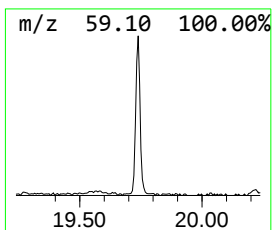
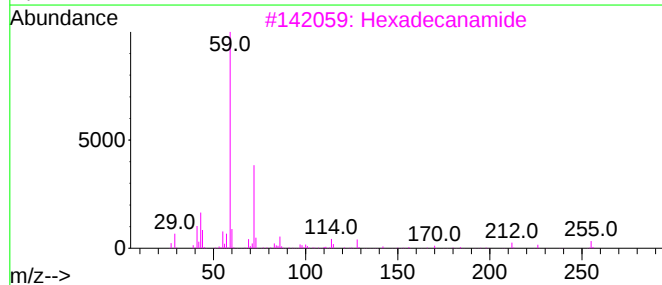
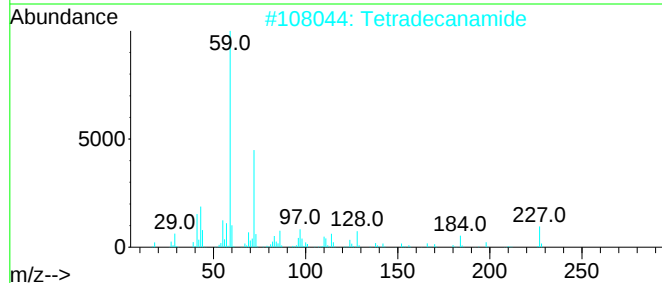
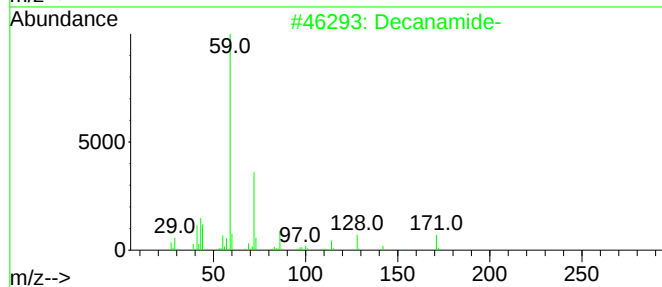
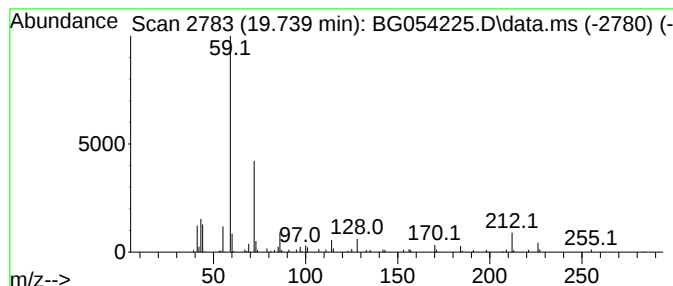
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decanamide- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.738	2.73 ng	88524	Chrysene-d12	21.713	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanamide-	171	C10H21NO	002319-29-1	83
2	Tetradecanamide	227	C14H29NO	000638-58-4	80
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Dodecanamide	199	C12H25NO	001120-16-7	72
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

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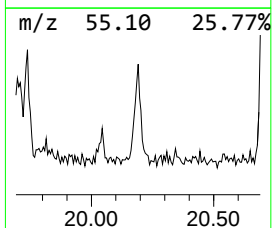
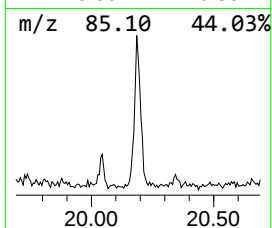
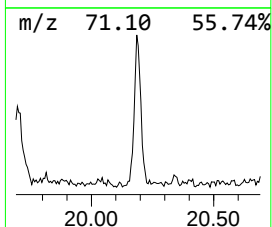
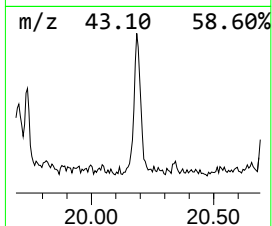
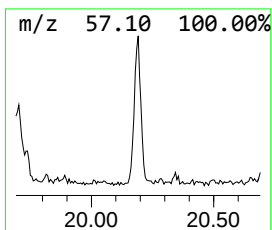
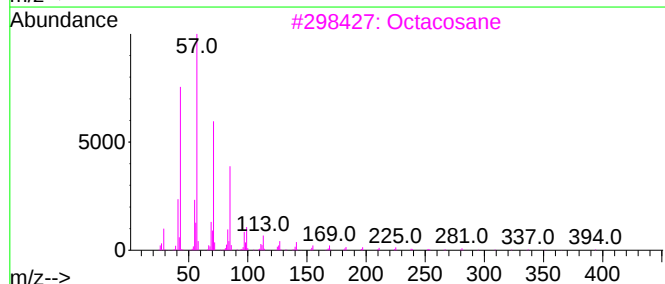
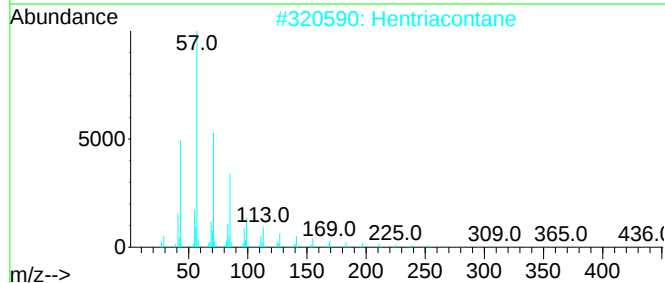
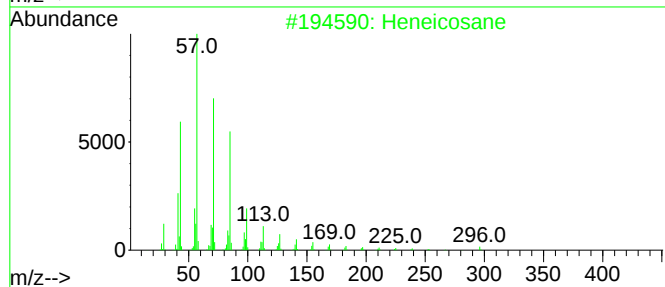
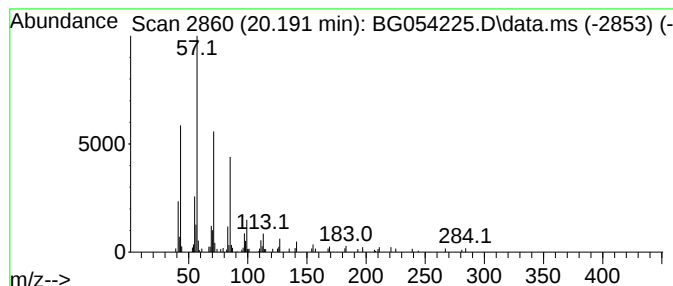
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.191	3.33 ng	107898	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Docosane	310	C22H46	000629-97-0	91
5			Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

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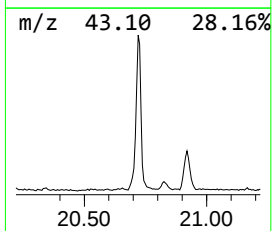
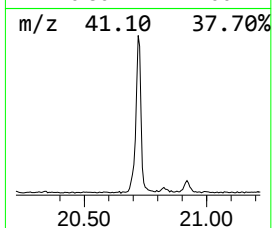
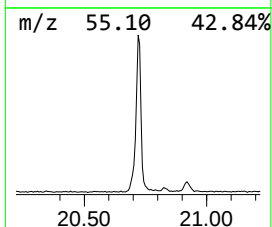
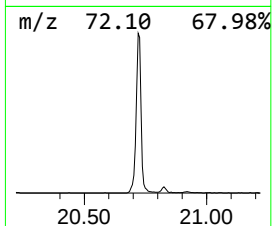
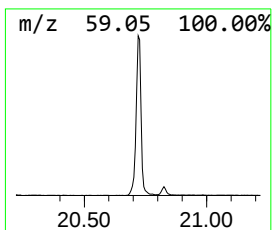
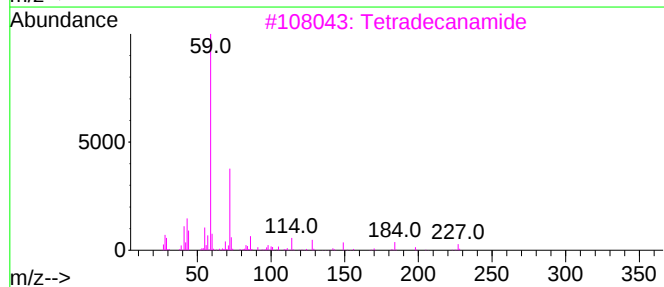
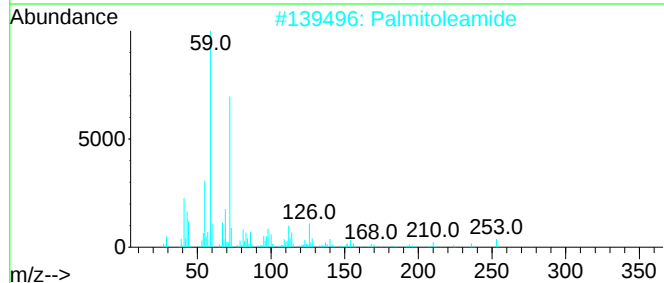
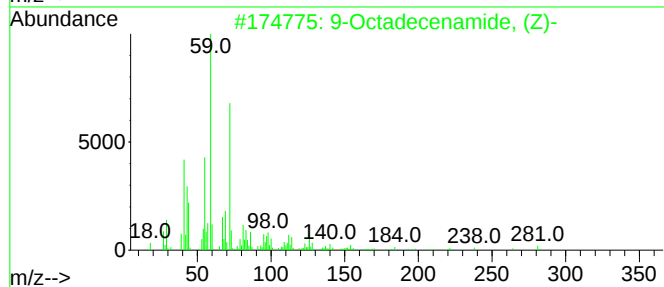
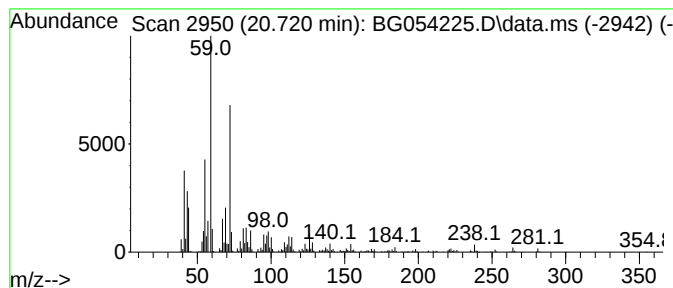
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.720	41.49 ng	1343930	Chrysene-d12	21.713

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	95
3			Tetradecanamide	227	C14H29NO	000638-58-4	64
4			Octanamide	143	C8H17NO	000629-01-6	64
5			2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

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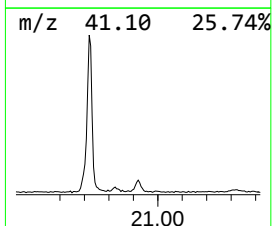
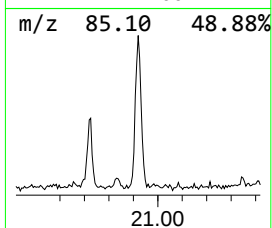
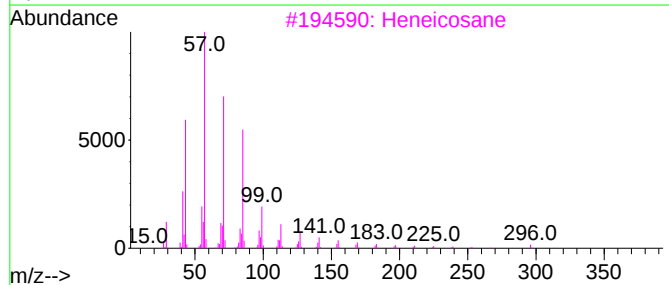
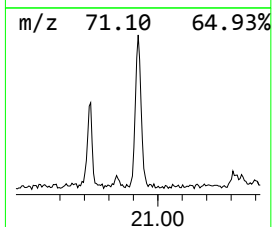
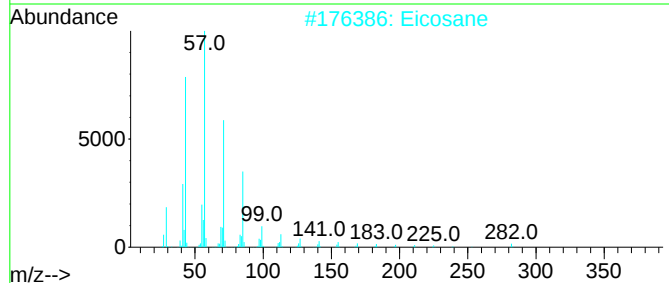
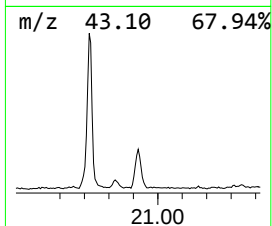
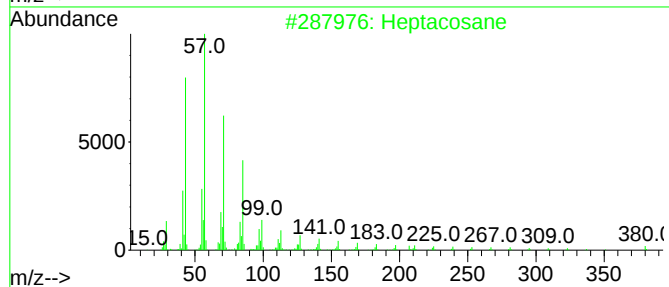
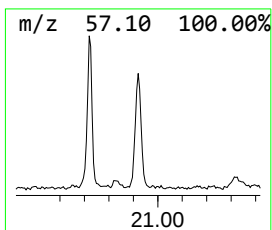
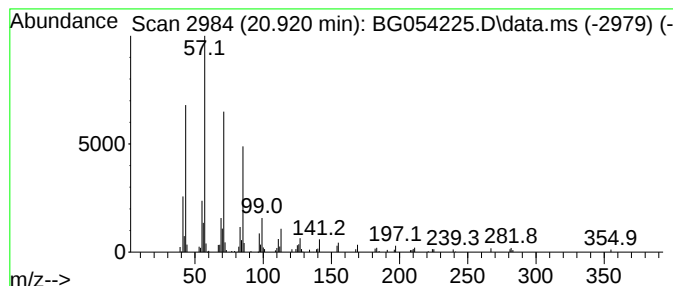
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.919	4.08 ng	132272	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	94
2			Eicosane	282	C20H42	000112-95-8	93
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
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Instrument :
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ClientSampleId :
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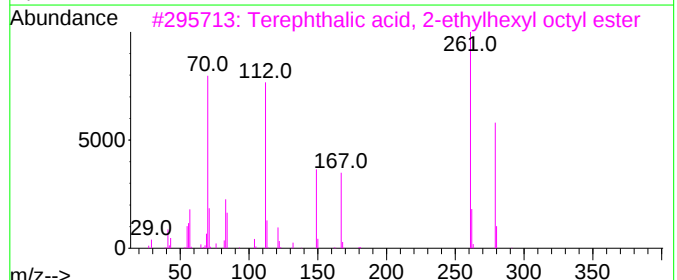
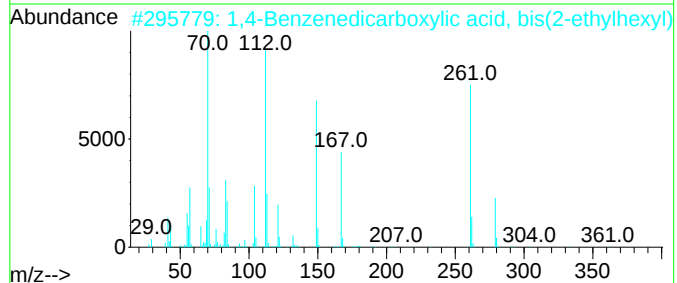
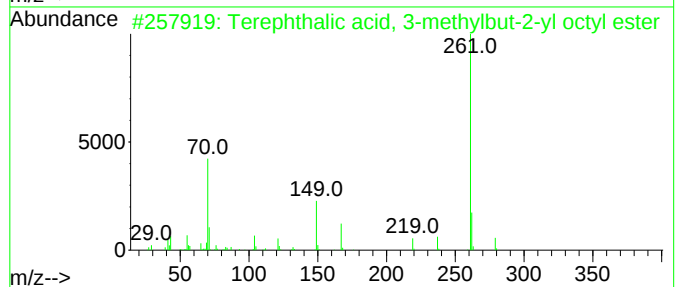
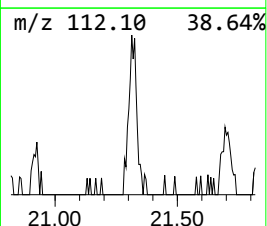
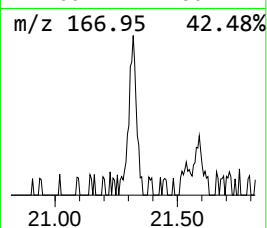
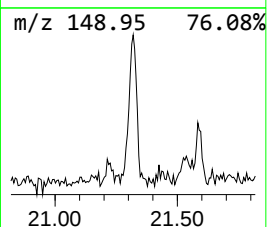
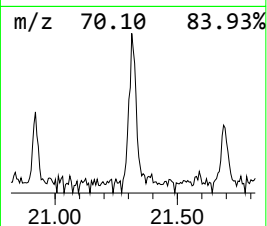
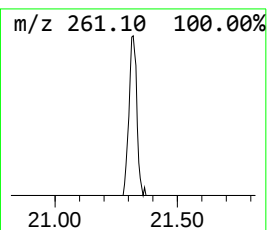
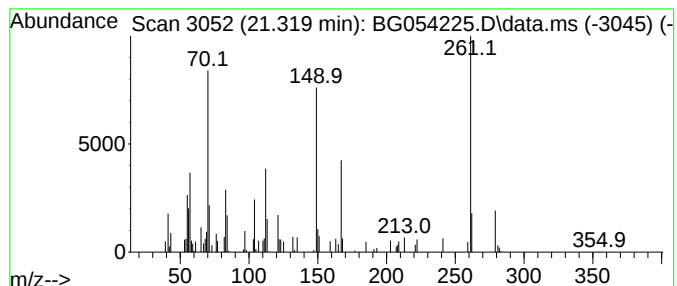
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Terephthalic acid, 3-methyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.319	2.31 ng	74692	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	47
4			Terephthalic acid, 2-fluoro-3-tr...	440	C23H24F4O4	1010415-81-5	38
5			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

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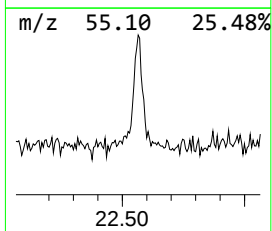
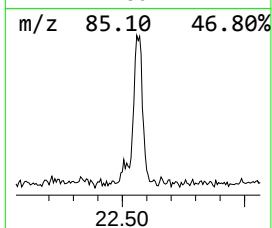
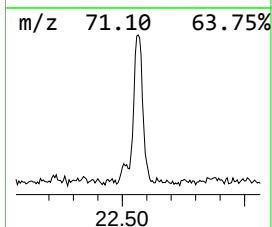
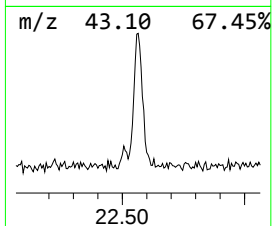
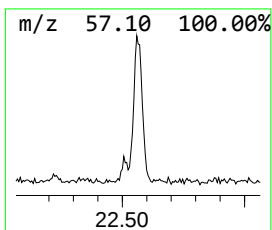
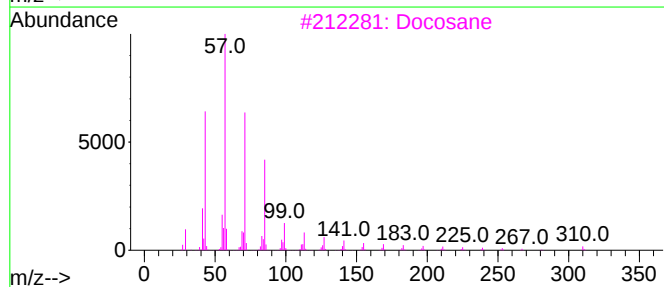
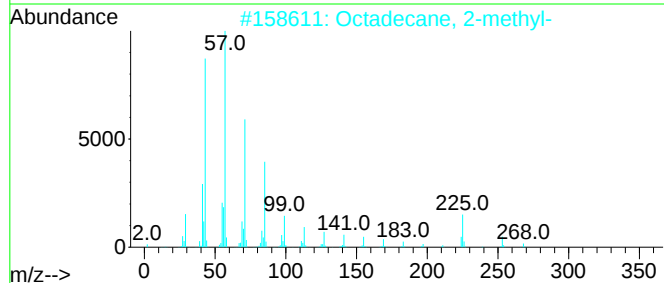
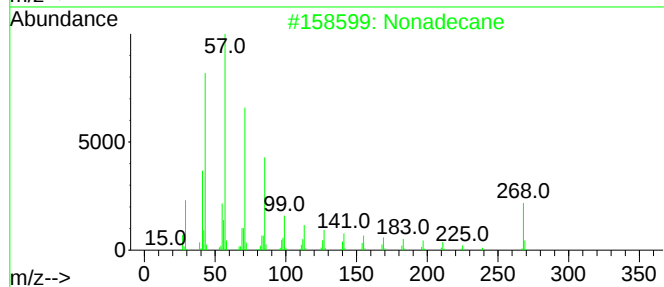
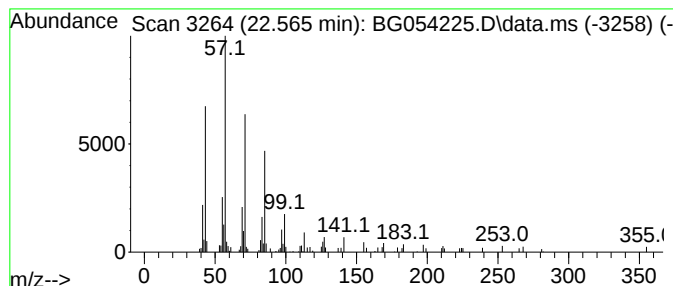
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.565	4.16 ng	134759	Chrysene-d12	21.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
3	Docosane	310	C22H46	000629-97-0	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

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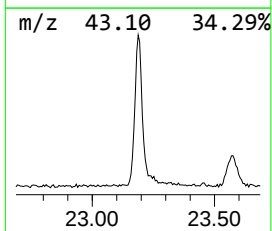
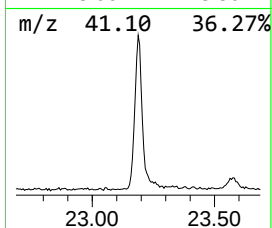
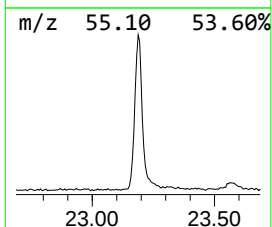
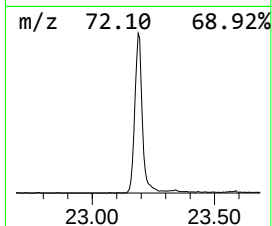
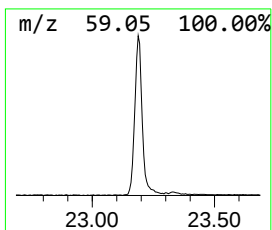
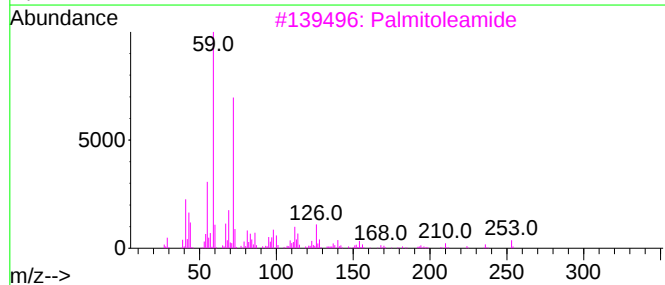
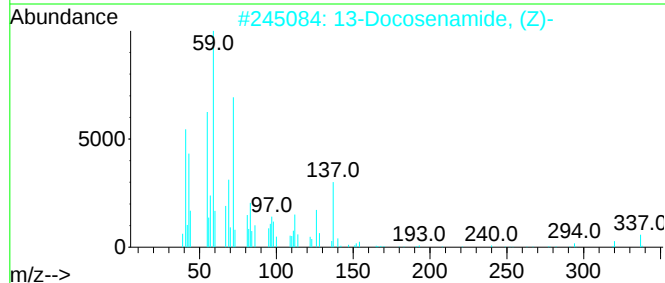
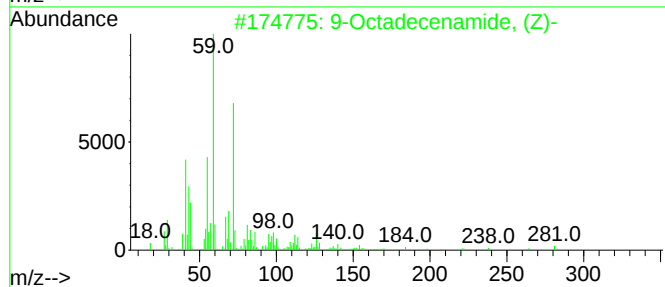
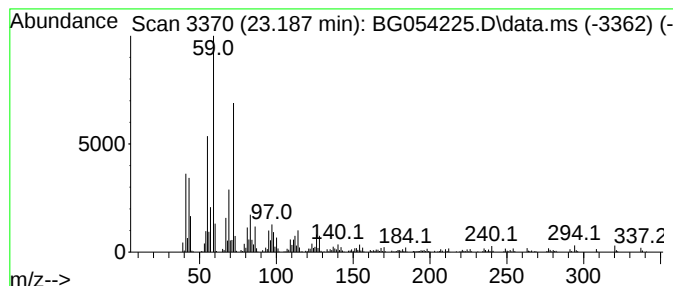
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.187	35.80 ng	1159500	Chrysene-d12	21.713

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3		Palmitoleamide	253	C16H31NO	106010-22-4	64
4		2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38
5		2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

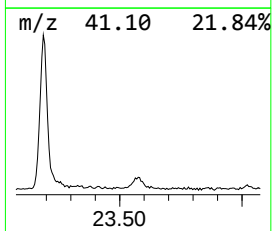
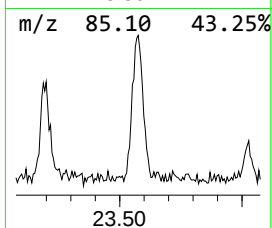
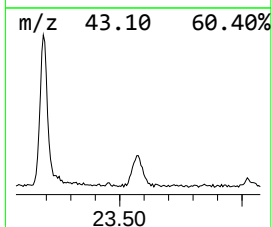
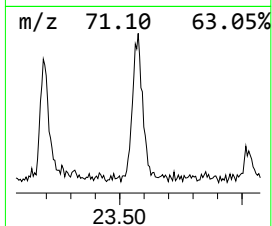
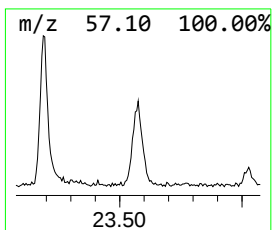
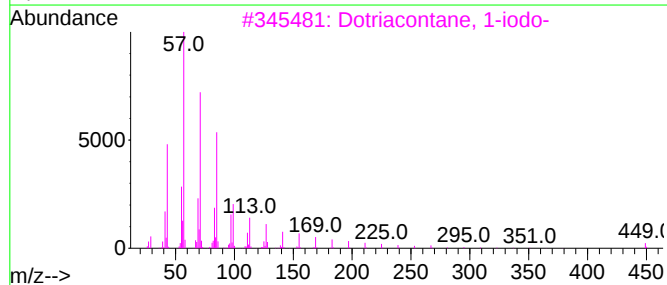
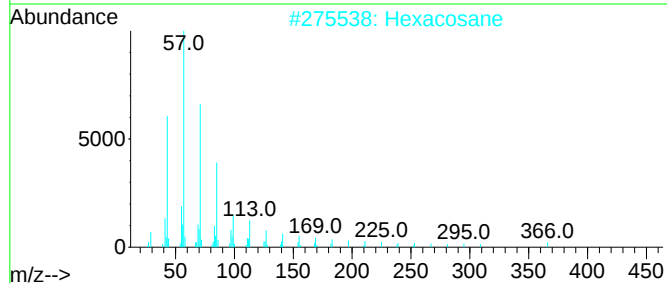
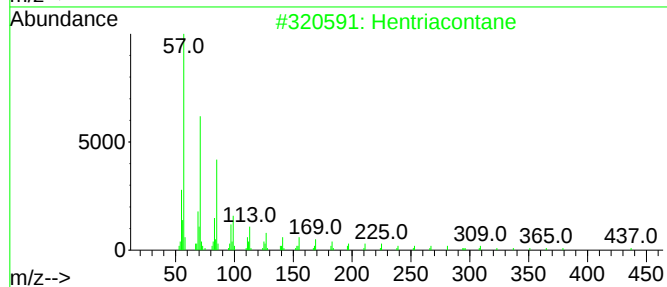
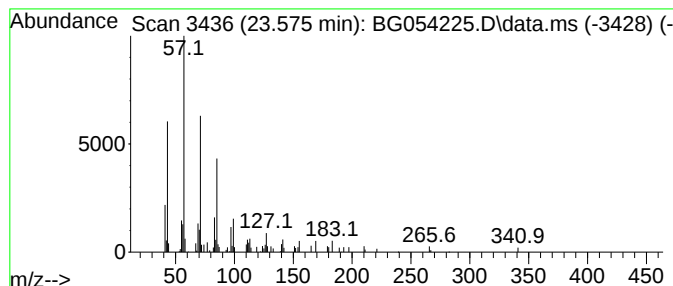
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.575	3.84 ng	104115	Perylene-d12	24.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220493-FIELD-BLANK

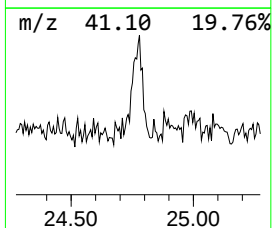
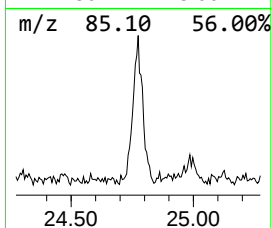
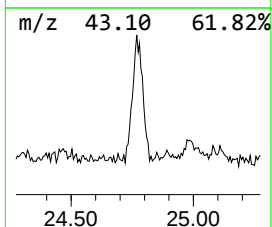
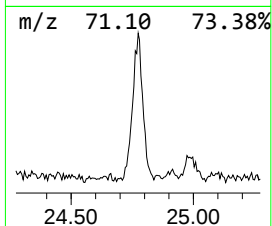
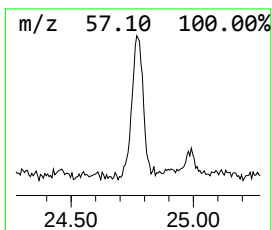
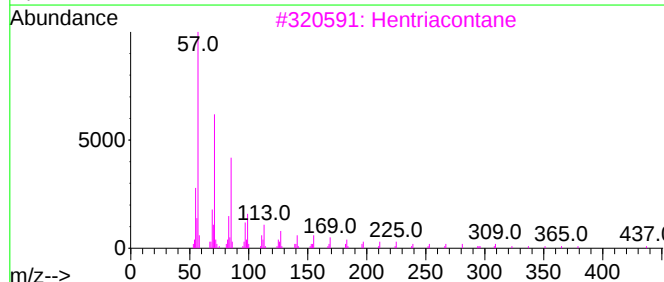
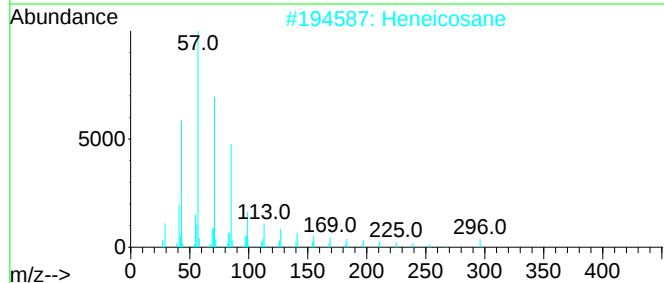
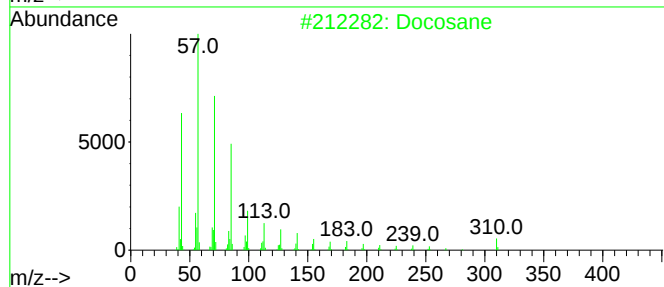
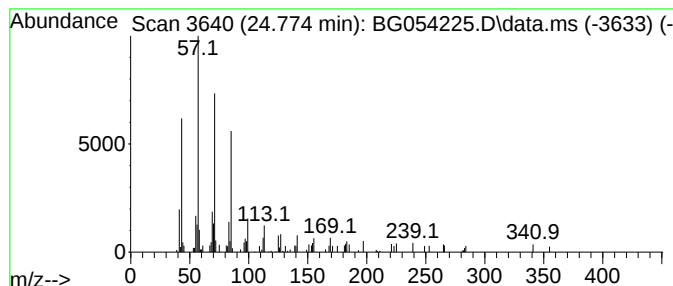
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.774	4.06 ng	109860	Perylene-d12	24.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane	310	C22H46	000629-97-0	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hentriacontane	437	C31H64	000630-04-6	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070722\
Data File : BG054225.D
Acq On : 7 Jul 2022 14:48
Operator : CG/JU
Sample : N3595-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220493-FIELD-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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
unknown12.271	12.271	3.3	ng	29964	2	10.873	182105	20.0
Tetradecanamide	18.187	3.1	ng	61175	4	17.435	397664	20.0
Octacosane	19.321	3.7	ng	73450	4	17.435	397664	20.0
Octadecanoic acid	19.580	6.8	ng	219077	5	21.713	647813	20.0
Phthalic acid, ...	19.703	4.8	ng	155423	5	21.713	647813	20.0
Decanamide-	19.738	2.7	ng	88524	5	21.713	647813	20.0
Heneicosane	20.191	3.3	ng	107898	5	21.713	647813	20.0
9-Octadecenamid...	20.720	41.5	ng	1343930	5	21.713	647813	20.0
Heptacosane	20.919	4.1	ng	132272	5	21.713	647813	20.0
Terephthalic ac...	21.319	2.3	ng	74692	5	21.713	647813	20.0
Nonadecane	22.565	4.2	ng	134759	5	21.713	647813	20.0
13-Docosenamide...	23.187	35.8	ng	1159500	5	21.713	647813	20.0
Hentriacontane	23.575	3.8	ng	104115	6	24.968	541700	20.0
Docosane	24.774	4.1	ng	109860	6	24.968	541700	20.0