

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071222\
 Data File : BG054259.D
 Acq On : 12 Jul 2022 16:55
 Operator : CG/JU
 Sample : N3649-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A-2-LC

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-BG071222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.611	371	378	389	rVB	187533	317216	22.49%	5.291%
2	7.209	642	650	659	rBV	193363	344598	24.43%	5.748%
3	8.043	786	792	799	rBV2	47742	84128	5.96%	1.403%
4	9.201	982	989	1000	rVB	114728	212315	15.05%	3.541%
5	10.852	1261	1270	1279	rBV	66583	120177	8.52%	2.005%
6	13.296	1677	1686	1693	rBV	347666	575329	40.78%	9.596%
7	14.671	1914	1920	1927	rBV2	117888	187592	13.30%	3.129%
8	16.157	2166	2173	2184	rBV3	447892	710576	50.37%	11.852%
9	17.415	2380	2387	2394	rBV	193954	304067	21.55%	5.072%
10	18.302	2532	2538	2543	rBV3	22882	37033	2.63%	0.618%
11	19.242	2691	2698	2702	rBV5	13173	19777	1.40%	0.330%
12	19.307	2702	2709	2716	rBV5	11128	29786	2.11%	0.497%
13	19.571	2749	2754	2764	rBV5	11546	23344	1.65%	0.389%
14	19.689	2764	2774	2782	rVV2	10525	30912	2.19%	0.516%
15	20.024	2824	2831	2837	rBV	1046749	1410765	100.00%	23.531%
16	20.194	2853	2860	2871	rBV2	19802	43327	3.07%	0.723%
17	20.776	2956	2959	2962	rBV	21473	24174	1.71%	0.403%
18	20.934	2981	2986	2996	rBV	25223	51901	3.68%	0.866%
19	21.322	3047	3052	3063	rBV4	33868	73397	5.20%	1.224%
20	21.686	3105	3114	3128	rBV	261357	488033	34.59%	8.140%
21	22.609	3265	3271	3279	rBV3	23681	53063	3.76%	0.885%
22	23.155	3358	3364	3375	rVB5	21647	46899	3.32%	0.782%
23	23.349	3393	3397	3405	rVB7	11403	24866	1.76%	0.415%
24	23.631	3439	3445	3454	rVB3	18749	46366	3.29%	0.773%
25	24.418	3571	3579	3585	rBV7	17898	51324	3.64%	0.856%
26	24.818	3643	3647	3649	rBV5	10972	16940	1.20%	0.283%
27	24.930	3656	3666	3677	rVB2	151800	437921	31.04%	7.304%
28	25.141	3694	3702	3704	rBV8	16832	37327	2.65%	0.623%
29	25.717	3797	3800	3809	rVB7	10748	27470	1.95%	0.458%
30	27.356	4071	4079	4081	rBV8	11562	29069	2.06%	0.485%
31	29.037	4355	4365	4380	rBV8	30559	135564	9.61%	2.261%

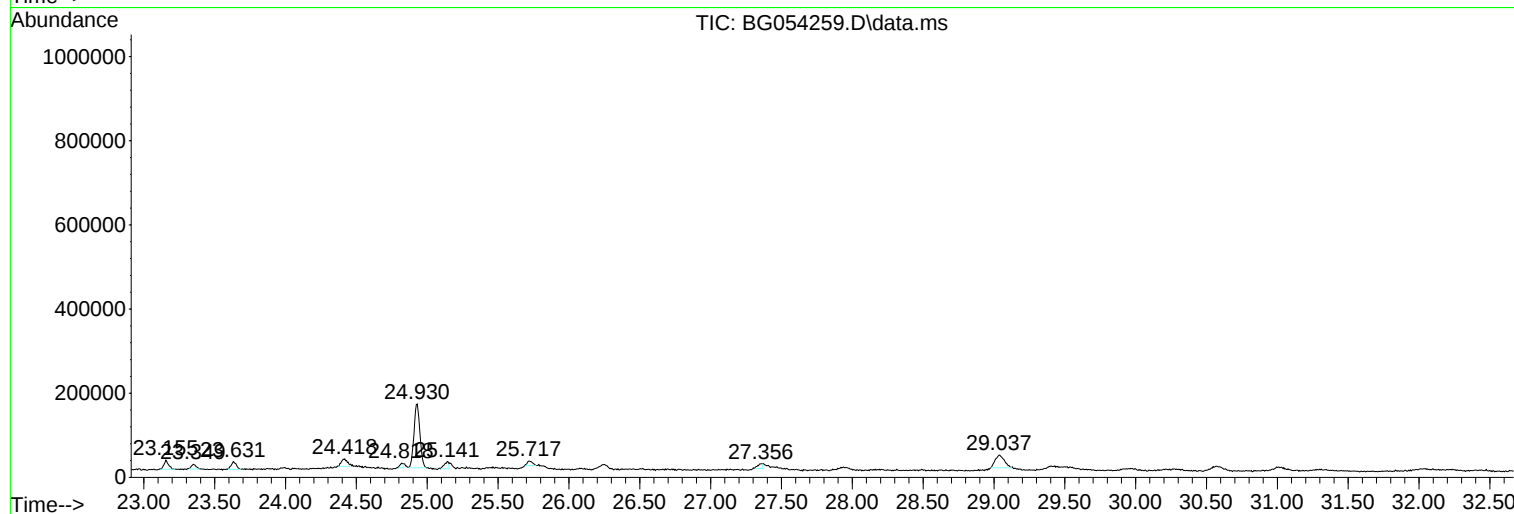
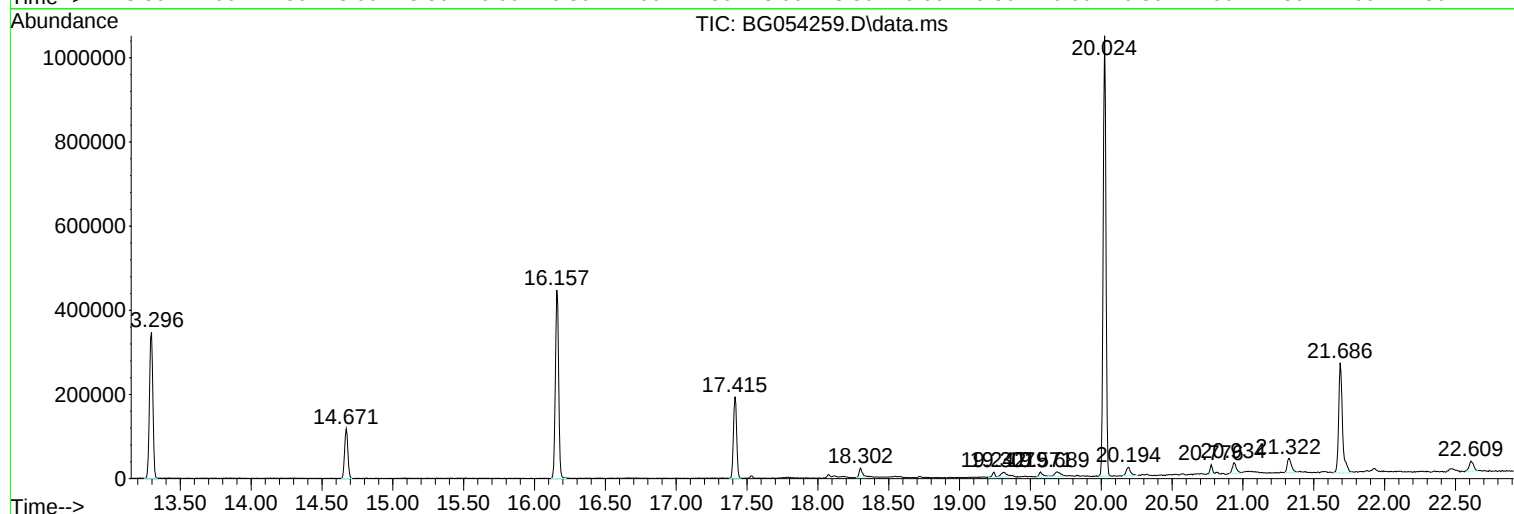
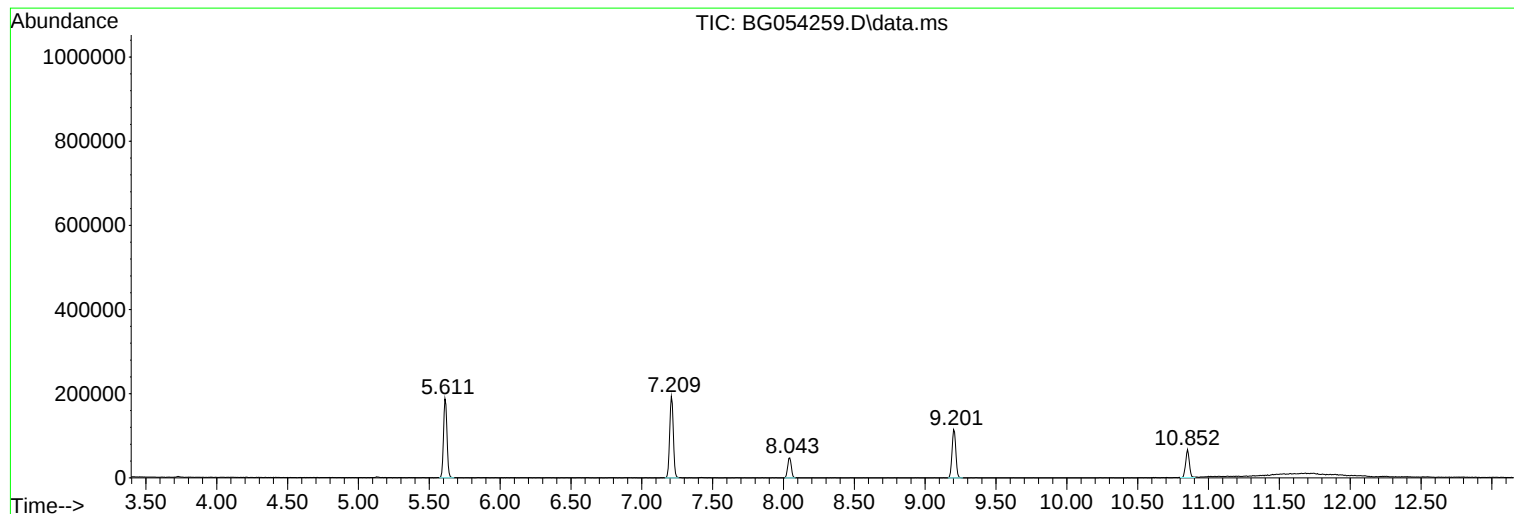
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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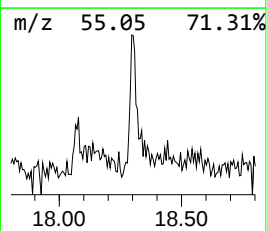
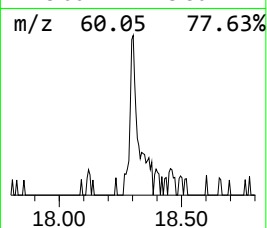
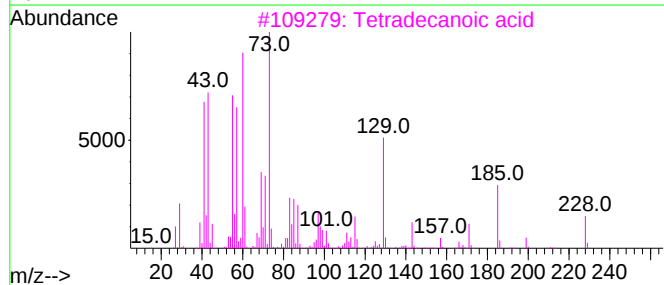
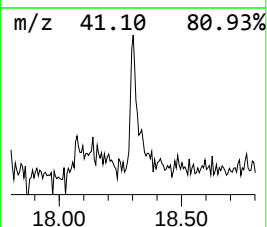
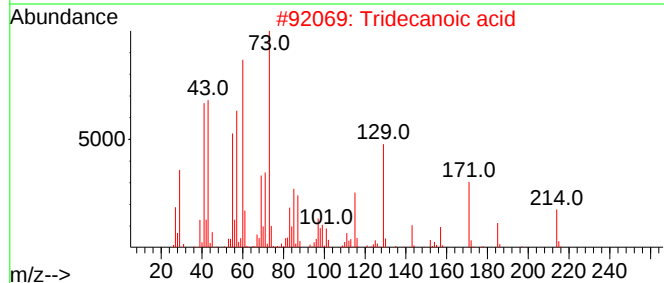
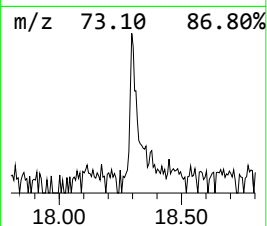
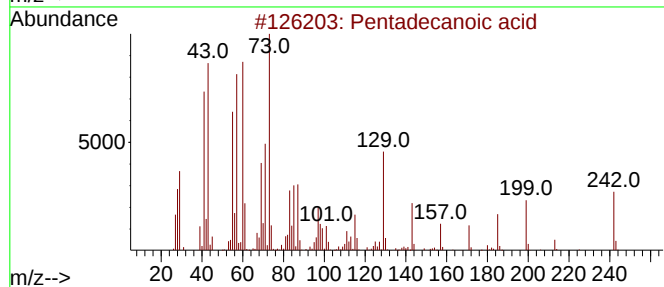
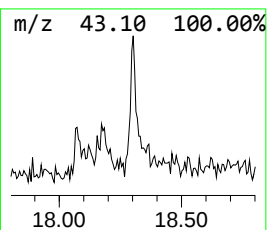
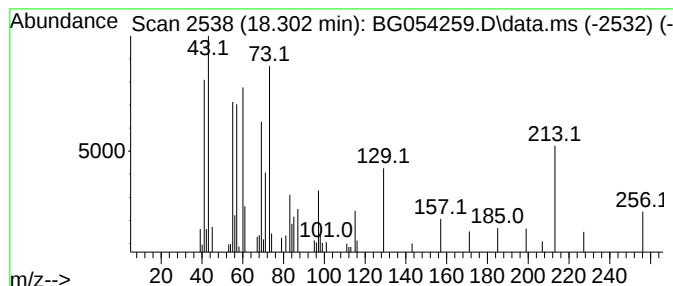
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.302	2.44 ng	37033	Phenanthrene-d10	17.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
2			Tridecanoic acid	214	C13H26O2	000638-53-9	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43



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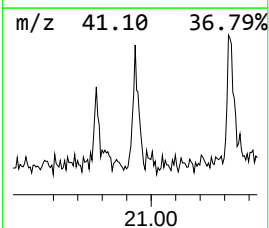
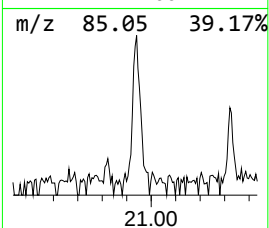
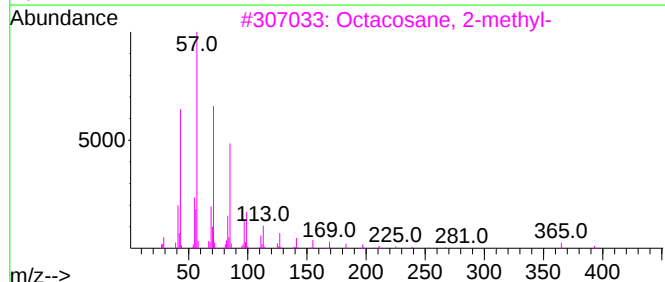
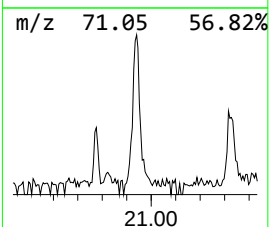
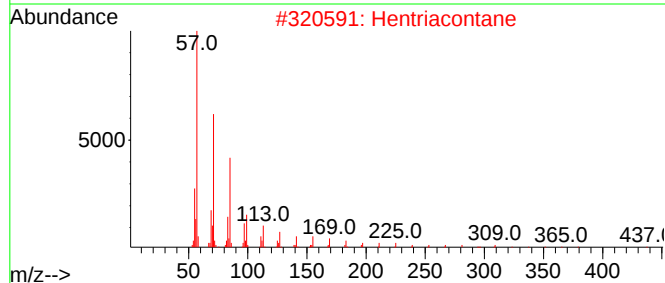
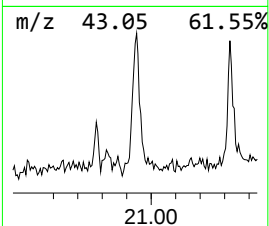
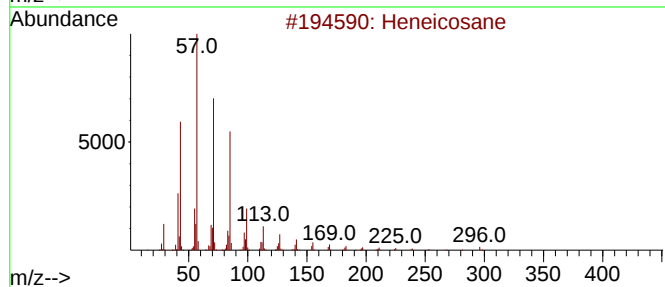
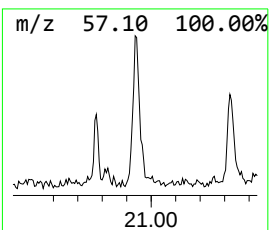
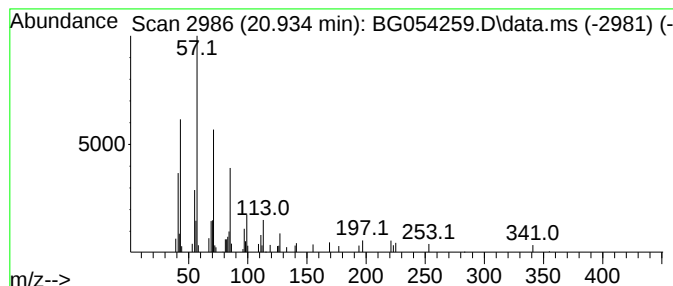
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.934	2.13 ng	51901	Chrysene-d12	21.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	86



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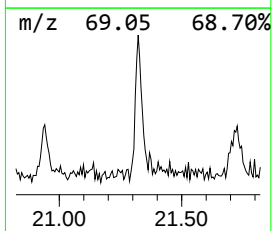
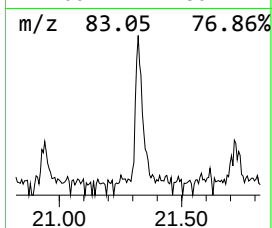
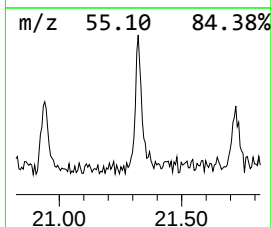
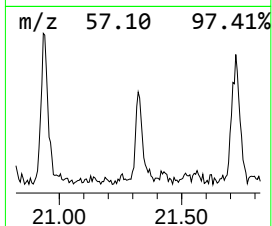
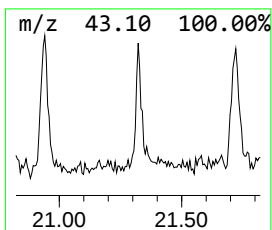
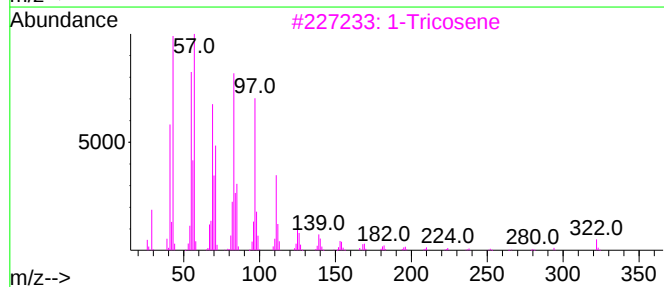
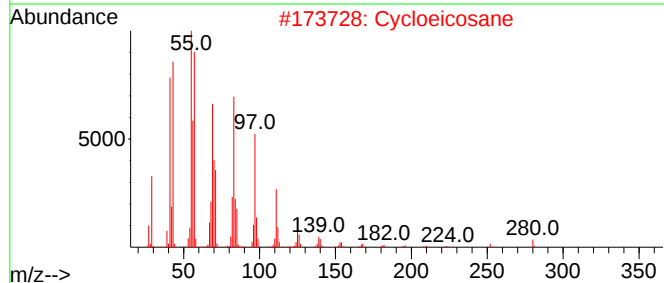
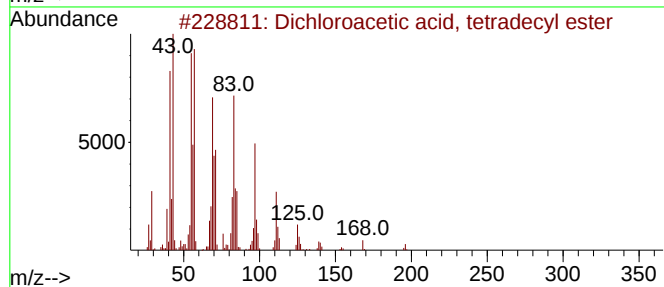
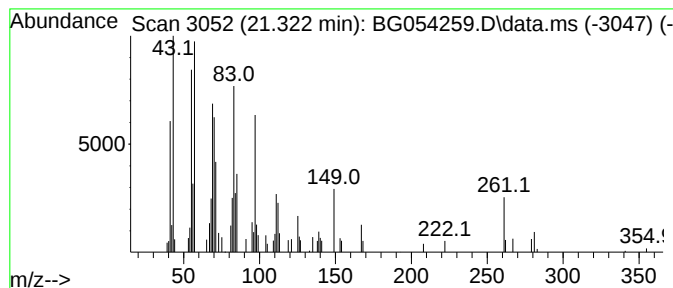
Instrument :
BNA_G
ClientSampleId :
A-2-LC

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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 3 Dichloroacetic acid, tetrad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.322	3.01 ng	73397	Chrysene-d12		21.686	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, tetradecyl ...		324	C16H30Cl2O2	083005-02-1	74
2	Cycloeicosane		280	C20H40	000296-56-0	68
3	1-Tricosene		322	C23H46	018835-32-0	68
4	1-Hexacosene		364	C26H52	018835-33-1	62
5	Bromoacetic acid, octadecyl ester		390	C20H39BrO2	018992-03-5	62



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ClientSampleId :
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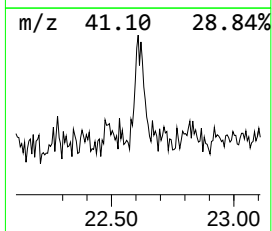
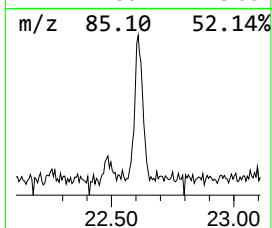
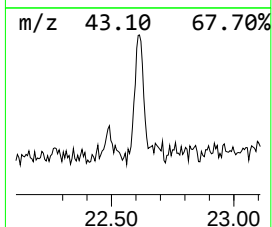
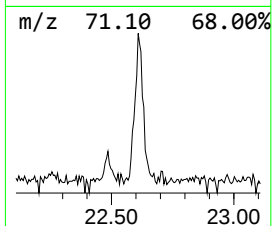
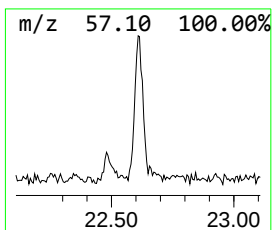
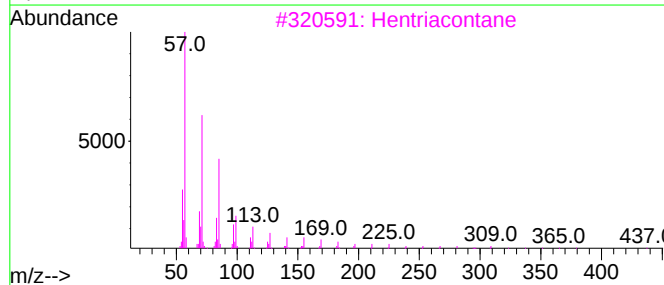
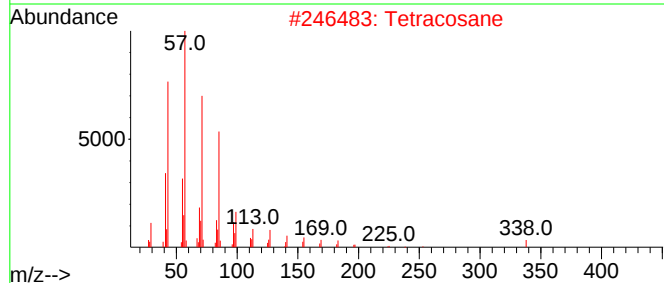
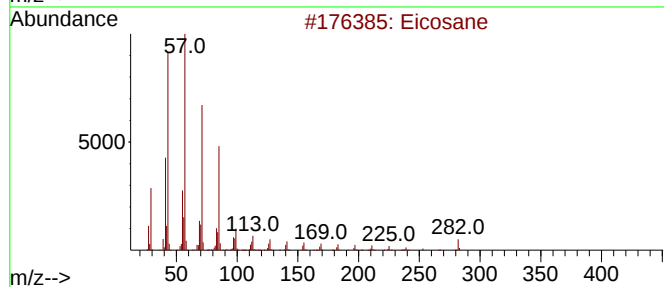
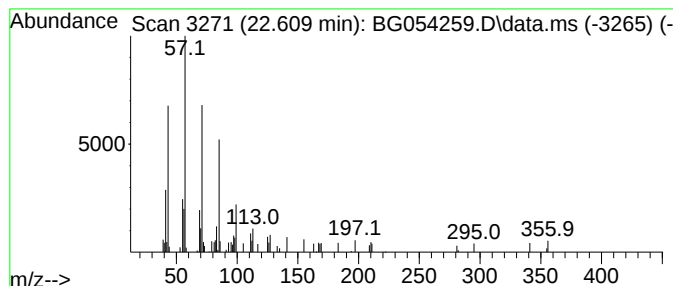
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Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.609	2.17 ng	53063	Chrysene-d12	21.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80



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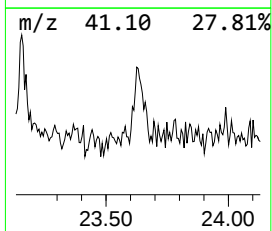
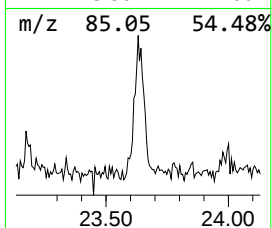
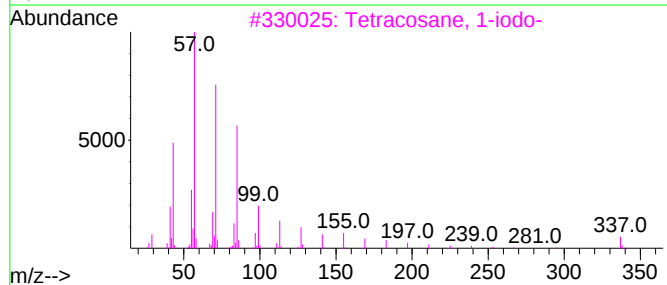
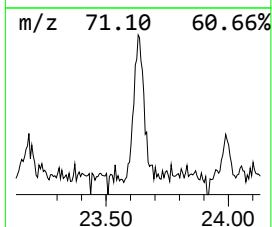
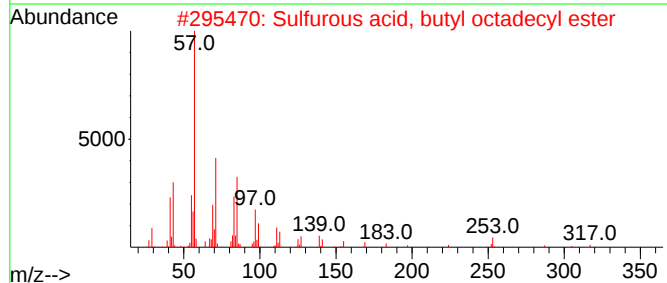
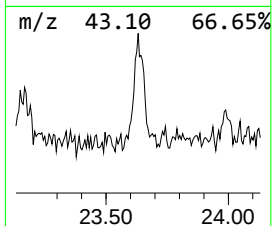
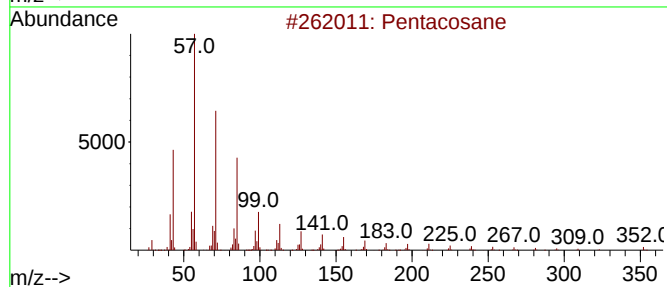
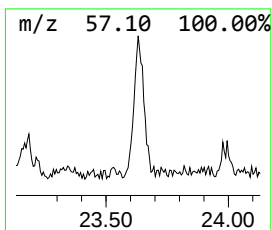
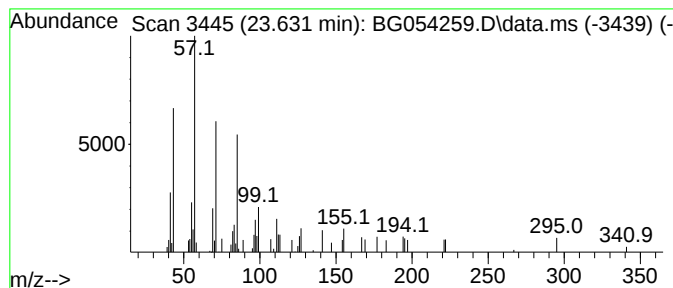
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.631	2.12 ng	46366	Perylene-d12	24.930

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	80
2			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	72
4			Tetratriacontane	479	C34H70	014167-59-0	64
5			Tricosane	324	C23H48	000638-67-5	64



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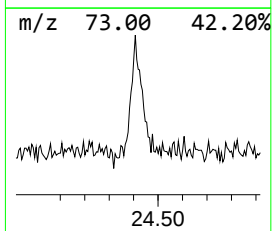
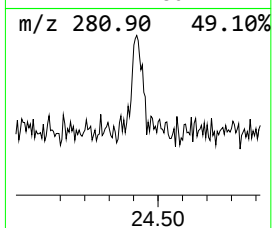
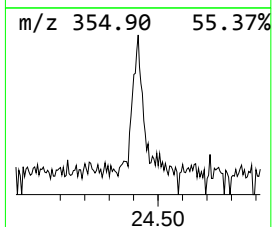
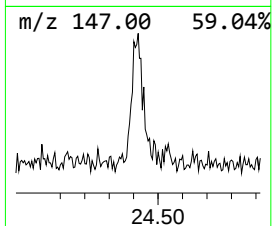
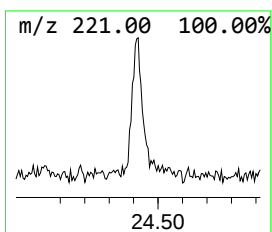
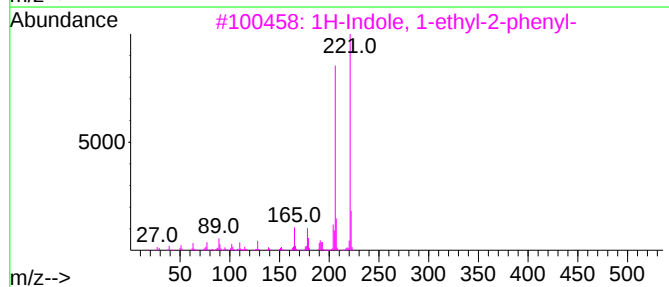
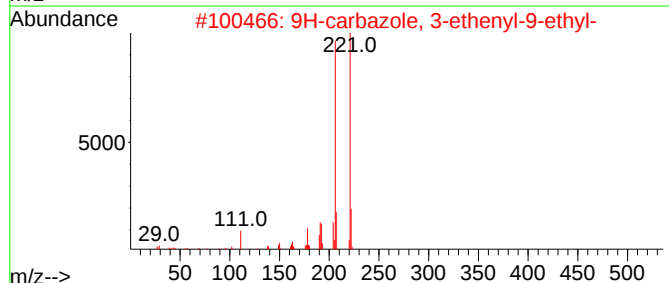
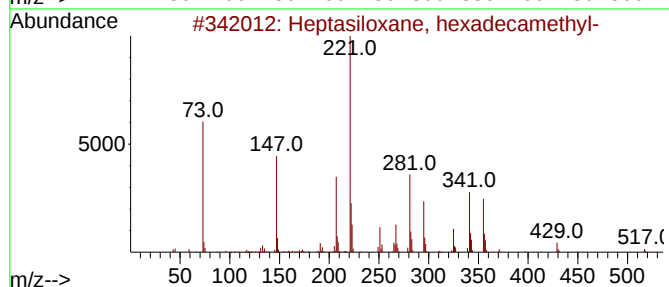
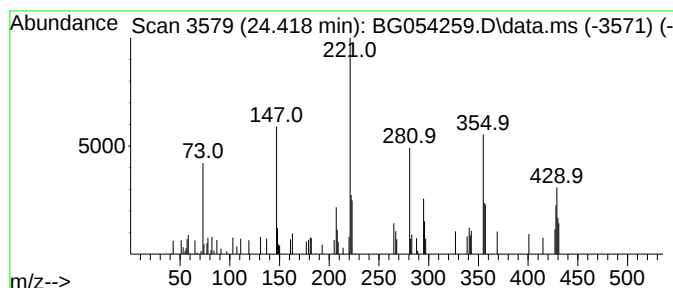
Instrument :
BNA_G
ClientSampleId :
A-2-LC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown24.418 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.418	2.34 ng	51324	Perylene-d12	24.930	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
2	9H-carbazole, 3-ethenyl-9-ethyl-	221	C16H15N	1000400-80-8	18
3	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	14
4	4-Fluoro-N-[4-(3-nitro-phenyl)-t...	343	C16H10FN3O3S	1000295-81-1	14
5	2-Methyl-6-tert-butylphenol, TBD...	278	C17H30O5Si	1000467-05-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071222\
Data File : BG054259.D
Acq On : 12 Jul 2022 16:55
Operator : CG/JU
Sample : N3649-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

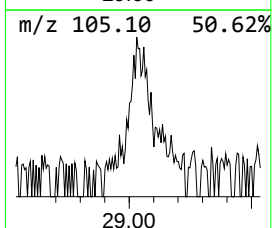
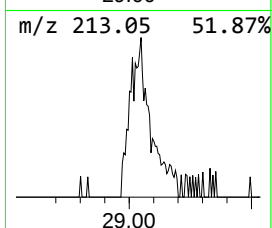
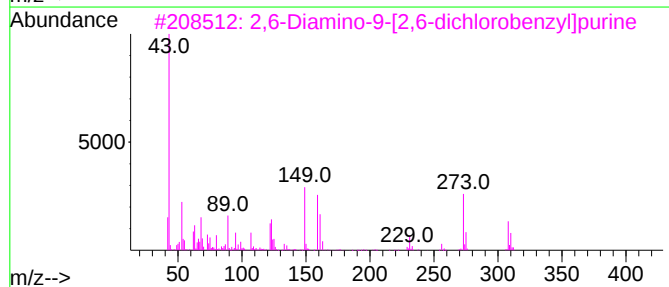
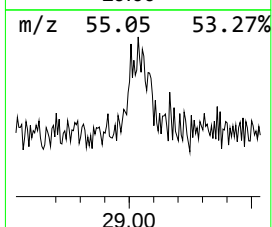
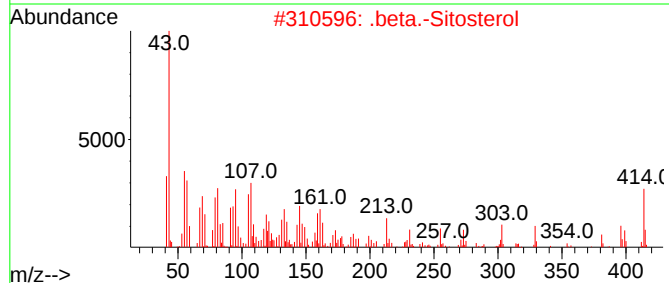
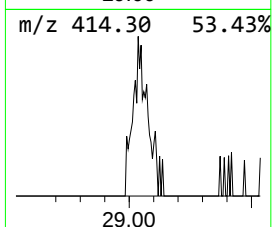
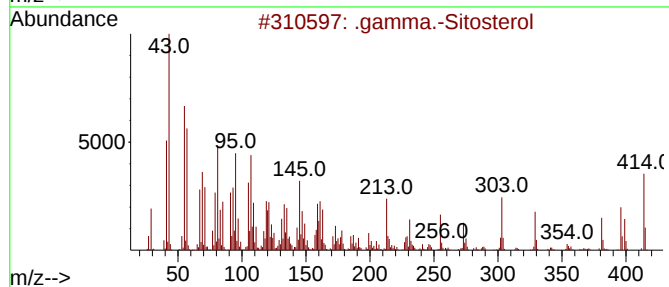
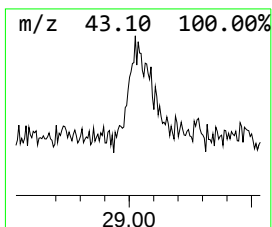
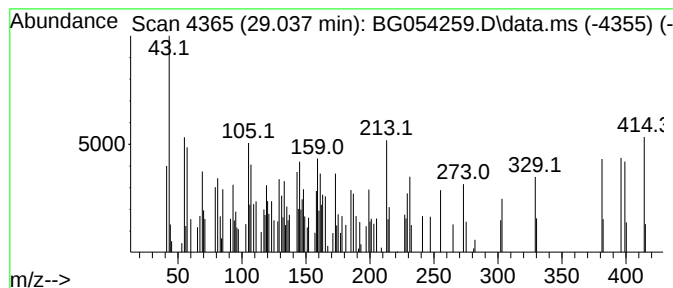
Instrument :
BNA_G
ClientSampleId :
A-2-LC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
29.037	6.19 ng	135564	Perylene-d12		24.930	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol		414	C29H50O	000083-47-6	50
2	.beta.-Sitosterol		414	C29H50O	000083-46-5	50
3	2,6-Diamino-9-[2,6-dichlorobenzy...		308	C12H10Cl2N6	1000212-70-6	9
4	Dihydrosarsasapogenin-5,17(20)-dien		414	C27H42O3	096974-10-6	9
5	2-Amino-4-hydroxy-6,7-bis[3,4-di...		399	C24H25N5O	049647-32-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071222\
Data File : BG054259.D
Acq On : 12 Jul 2022 16:55
Operator : CG/JU
Sample : N3649-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A-2-LC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentadecanoic acid	18.302	2.4	ng	37033	4	17.415	304067	20.0
Heneicosane	20.934	2.1	ng	51901	5	21.686	488033	20.0
Dichloroacetic ...	21.322	3.0	ng	73397	5	21.686	488033	20.0
Eicosane	22.609	2.2	ng	53063	5	21.686	488033	20.0
Pentacosane	23.631	2.1	ng	46366	6	24.930	437921	20.0
unknown24.418	24.418	2.3	ng	51324	6	24.930	437921	20.0
.gamma.-Sitosterol	29.037	6.2	ng	135564	6	24.930	437921	20.0