

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050322\
 Data File : BG053414.D
 Acq On : 3 May 2022 13:00
 Operator : CG/JU
 Sample : N2619-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SS01-1-2-FT

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053414.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.668	381	388	399	rBV	480896	784549	28.74%	6.733%
2	7.266	652	660	673	rBV	483087	873664	32.01%	7.498%
3	8.100	795	802	809	rBV	78512	136159	4.99%	1.169%
4	9.263	992	1000	1009	rBV	302771	560057	20.52%	4.806%
5	10.908	1274	1280	1287	rVB	95734	179405	6.57%	1.540%
6	13.346	1688	1695	1703	rVB	802969	1219277	44.67%	10.464%
7	14.720	1924	1929	1936	rVB	157316	251590	9.22%	2.159%
8	16.212	2176	2183	2195	rBV	780927	1264288	46.32%	10.850%
9	17.470	2391	2397	2403	rBV	245223	380891	13.95%	3.269%
10	18.321	2536	2542	2544	rBV6	17180	37618	1.38%	0.323%
11	18.856	2614	2633	2651	rVB7	77932	455285	16.68%	3.907%
12	19.285	2701	2706	2716	rVB9	22939	63006	2.31%	0.541%
13	19.596	2751	2759	2760	rBV3	59004	119062	4.36%	1.022%
14	20.072	2834	2840	2846	rVB	2032765	2729691	100.00%	23.426%
15	20.242	2860	2869	2878	rBV2	159408	381342	13.97%	3.273%
16	21.264	3036	3043	3053	rVB2	138226	345801	12.67%	2.968%
17	21.370	3056	3061	3074	rBV2	51564	111493	4.08%	0.957%
18	21.752	3120	3126	3136	rVB2	310964	536492	19.65%	4.604%
19	22.457	3236	3246	3257	rVB4	88989	326523	11.96%	2.802%
20	23.832	3470	3480	3490	rVB2	82280	275597	10.10%	2.365%
21	25.042	3677	3686	3697	rVB2	188712	553448	20.28%	4.750%
22	26.710	3962	3970	3972	rBV9	30775	67043	2.46%	0.575%

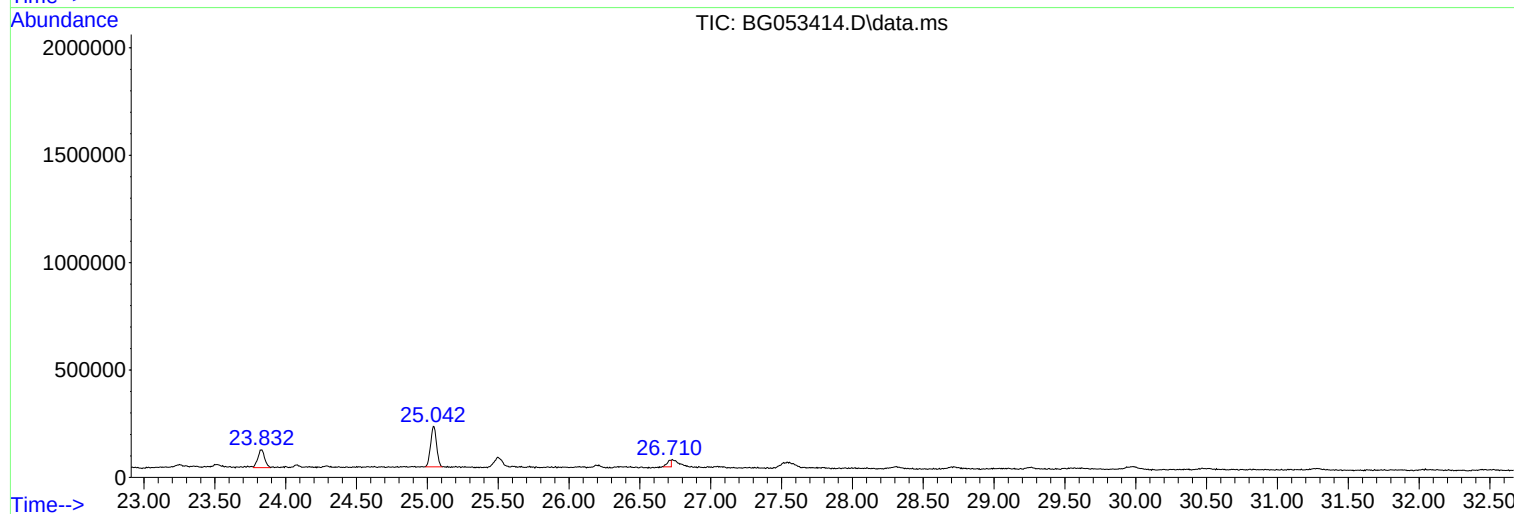
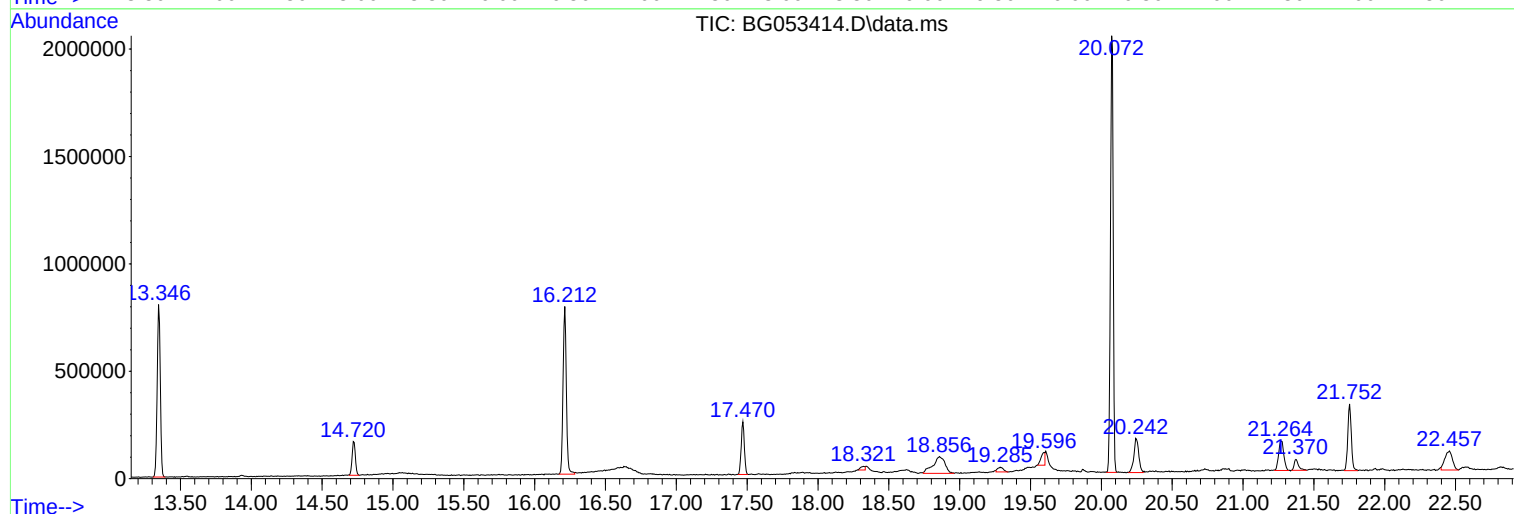
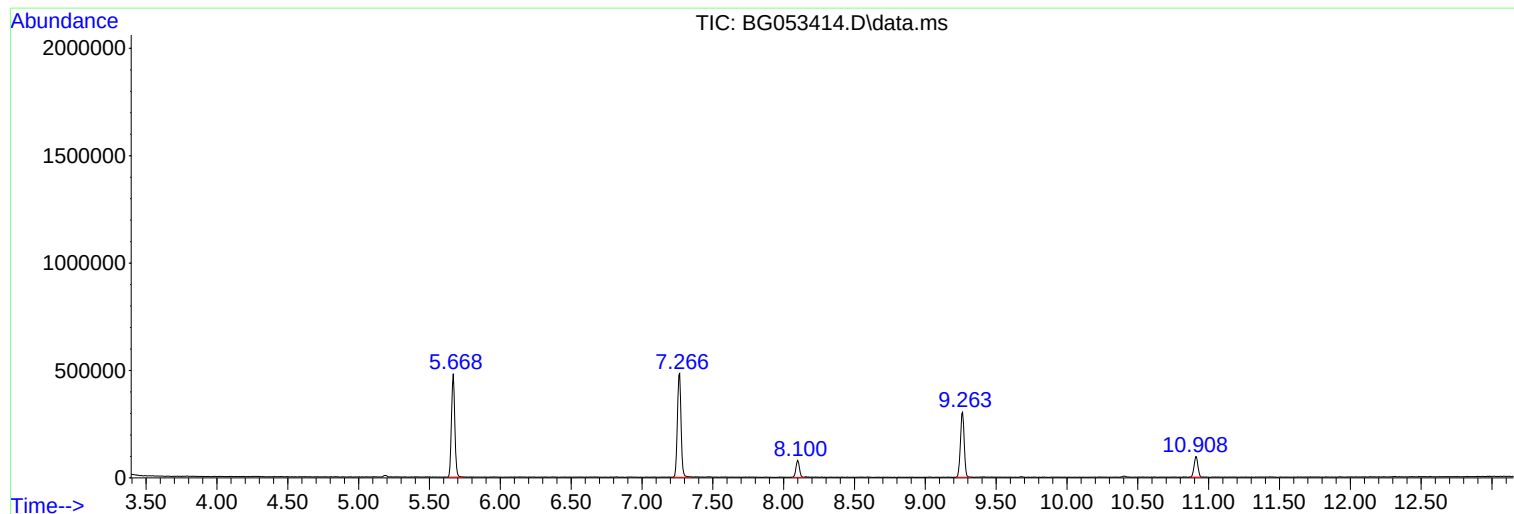
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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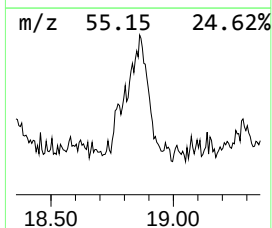
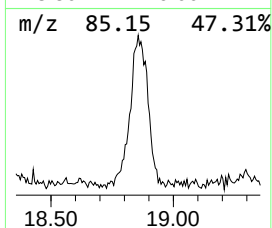
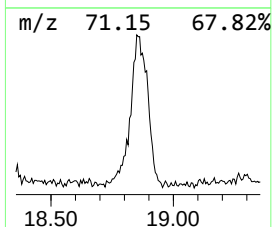
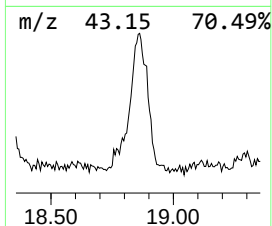
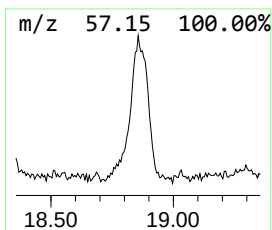
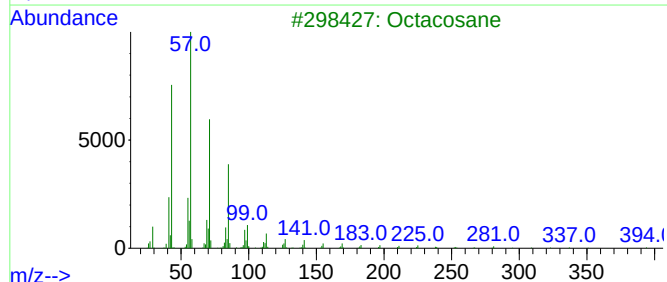
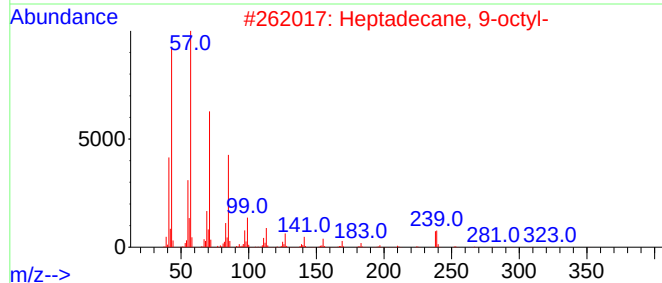
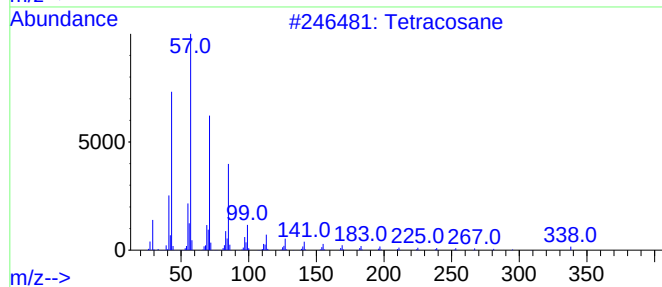
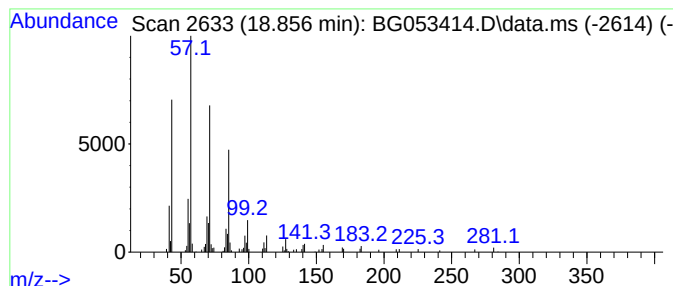
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.856	23.91 ng	455285	Phenanthrene-d10	17.470

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Dodecane	170	C12H26	000112-40-3	91
5			Hexacosane	366	C26H54	000630-01-3	91



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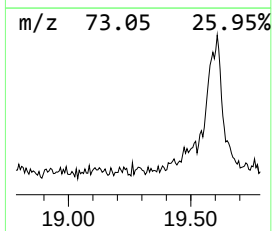
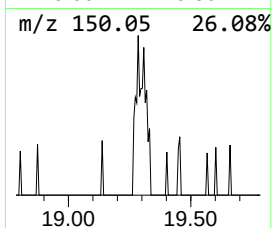
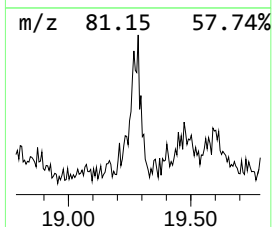
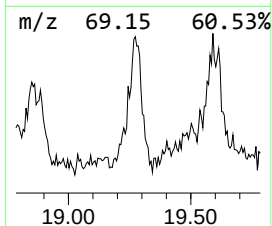
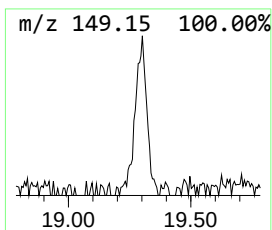
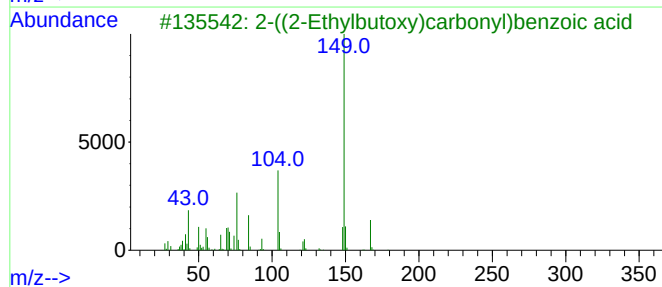
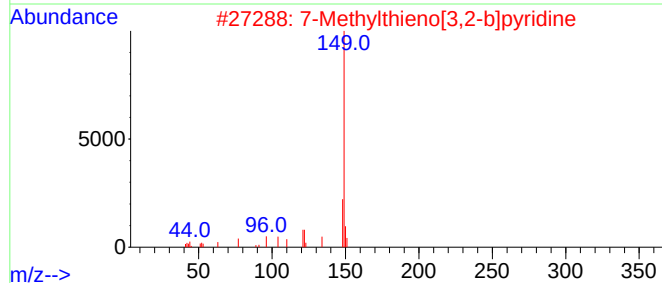
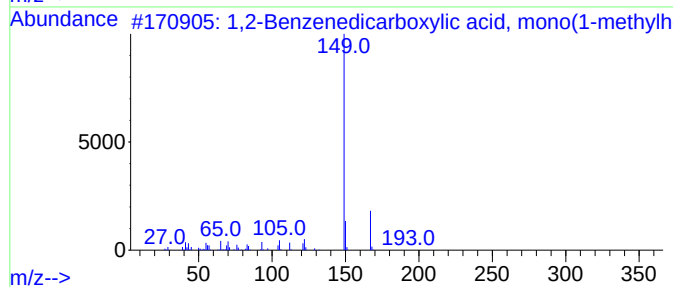
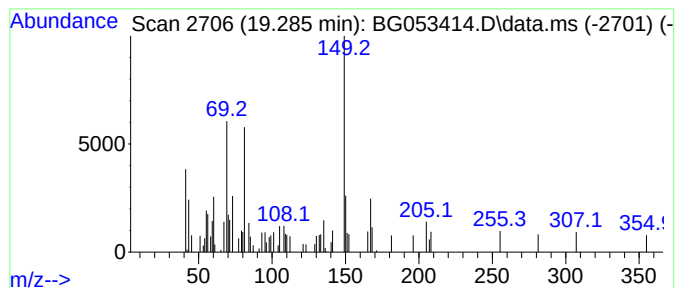
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown19.285 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.285	3.31 ng	63006	Phenanthrene-d10	17.470

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	068296-97-9	43
2			7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	38
3			2-((2-Ethylbutoxy)carbonyl)benzo...	250	C14H18O4	091401-46-6	38
4			Phthalic acid, hexyl 4-methyl-3-...	399	C22H25NO6	1000382-58-4	38
5			2,4,7,14-Tetramethyl-4-vinyl-tri...	290	C20H34O	1000193-31-2	38



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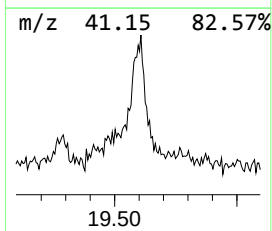
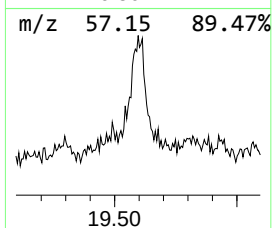
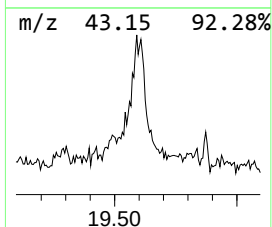
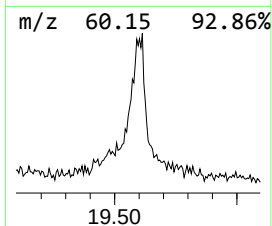
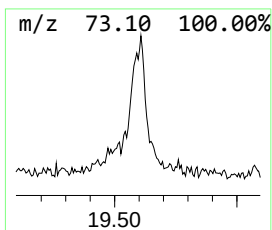
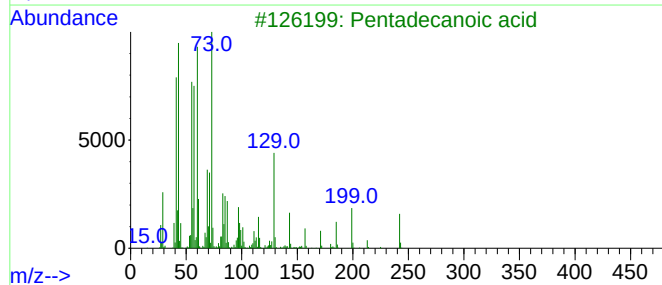
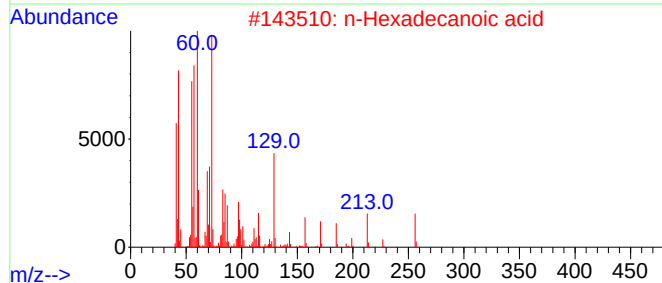
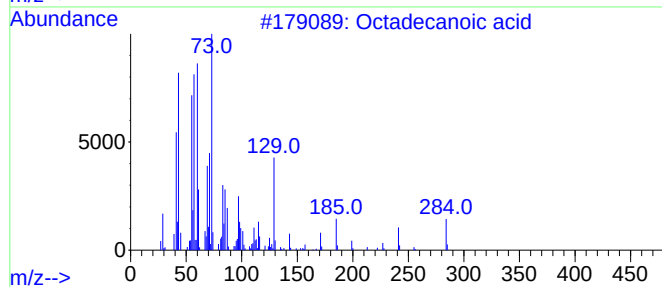
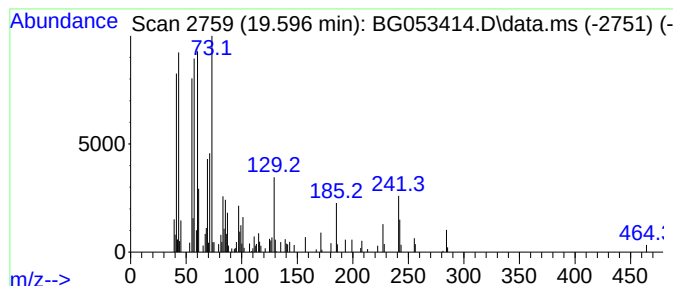
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.596	6.25 ng	119062	Phenanthrene-d10	17.470

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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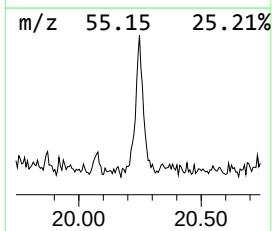
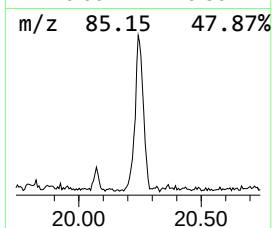
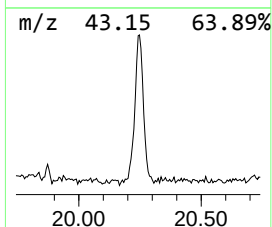
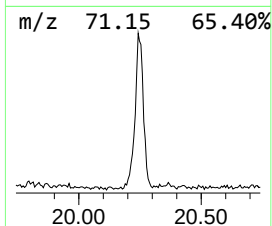
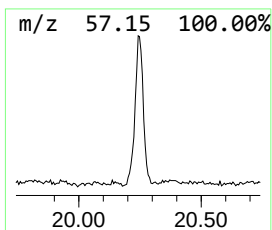
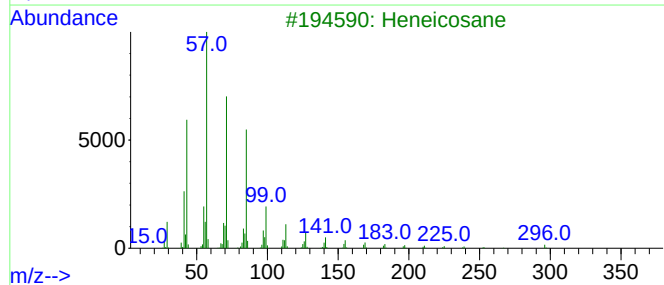
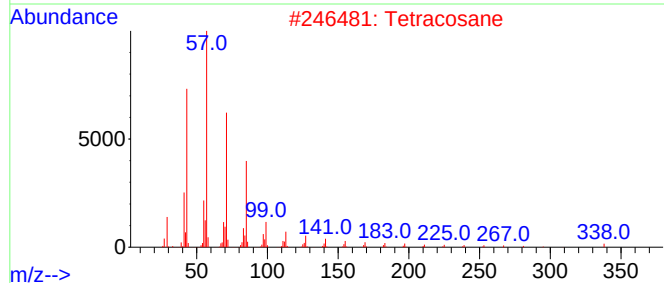
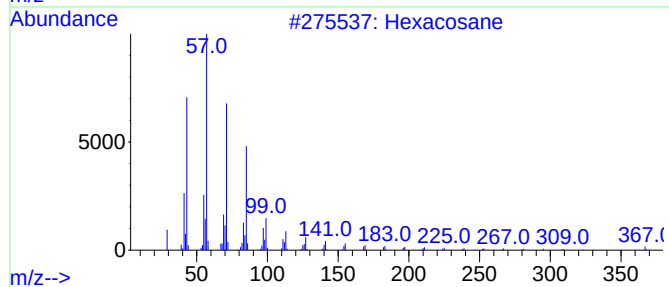
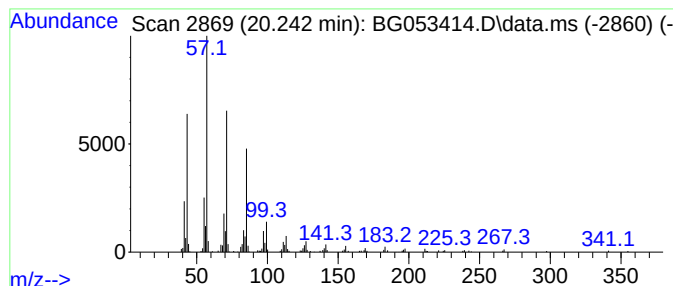
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Peak Number 4 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.242	14.22 ng	381342	Chrysene-d12	21.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Pentacosane	352	C25H52	000629-99-2	91



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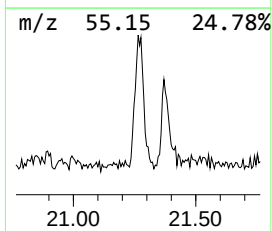
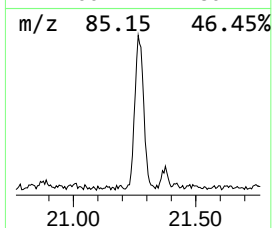
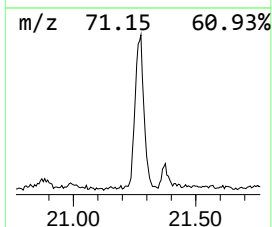
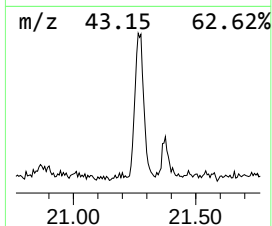
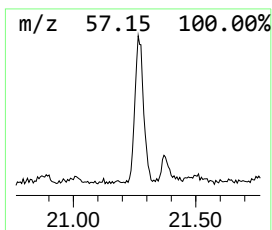
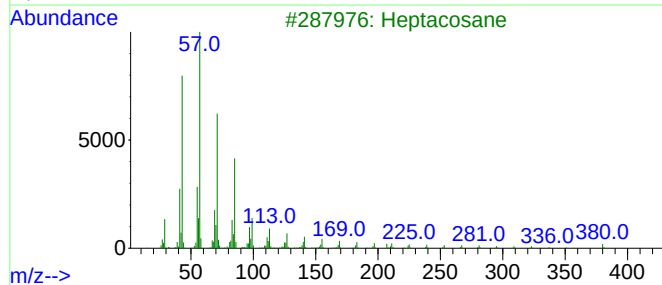
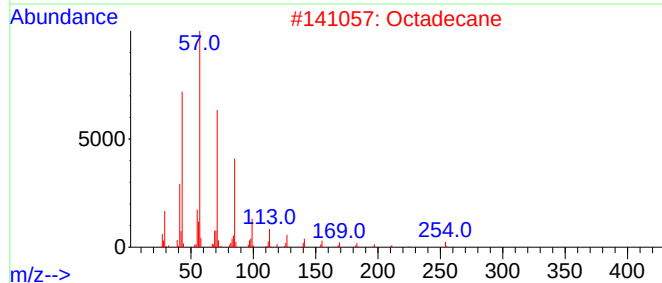
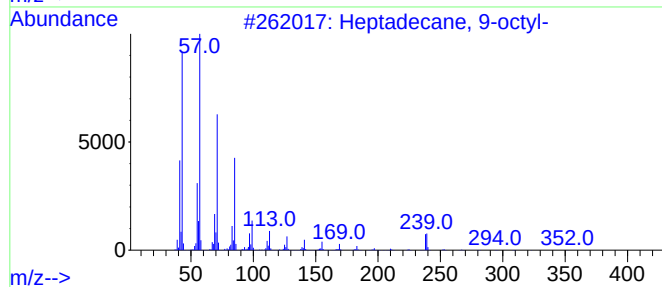
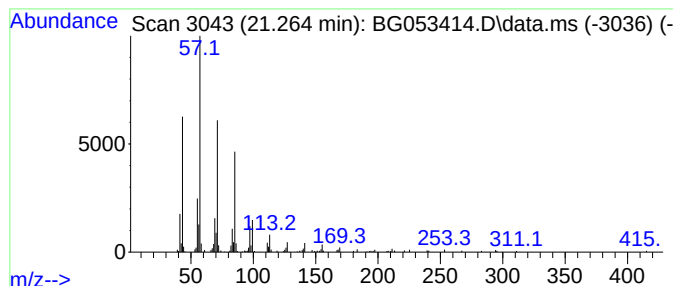
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.264	12.89 ng	345801	Chrysene-d12	21.752

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2		Octadecane	254	C18H38	000593-45-3	87
3		Heptacosane	380	C27H56	000593-49-7	86
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5		Heneicosane	296	C21H44	000629-94-7	83



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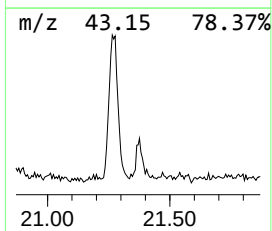
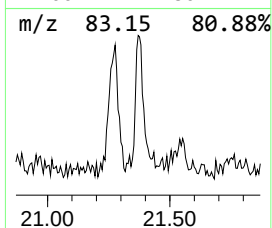
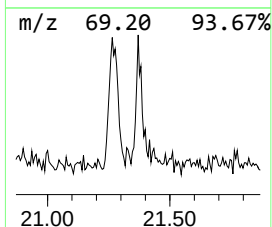
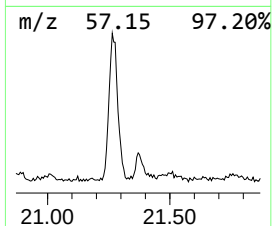
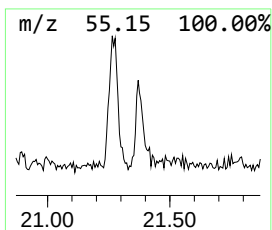
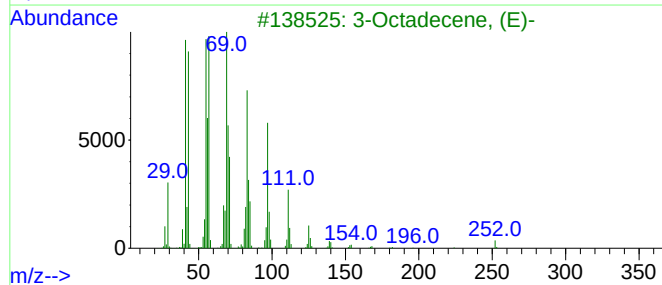
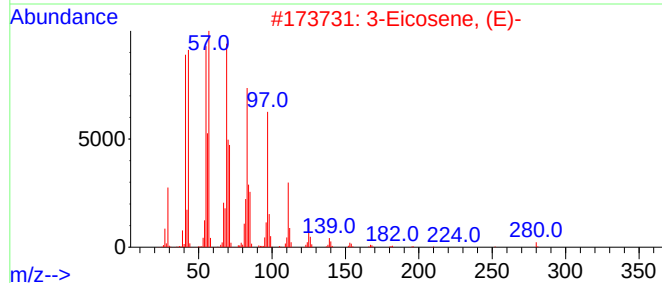
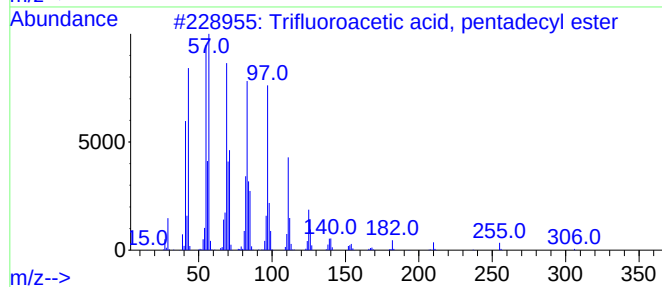
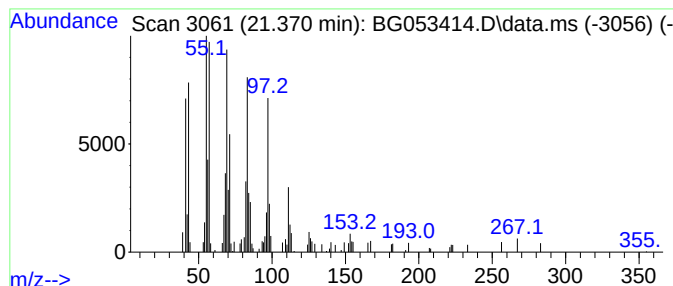
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.370	4.16 ng	111493	Chrysene-d12	21.752

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
3		3-Octadecene, (E)-	252	C18H36	007206-19-1	80
4		Cyclotridecane	182	C13H26	000295-02-3	78
5		Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050322\
Data File : BG053414.D
Acq On : 3 May 2022 13:00
Operator : CG/JU
Sample : N2619-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS01-1-2-FT

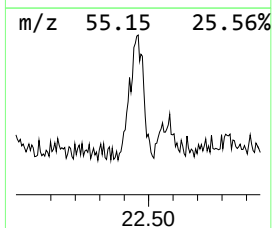
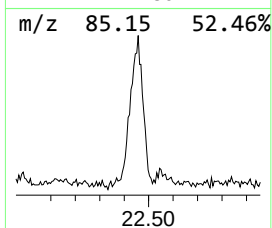
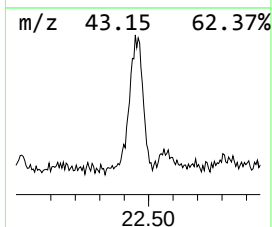
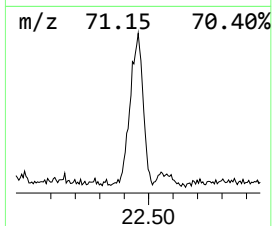
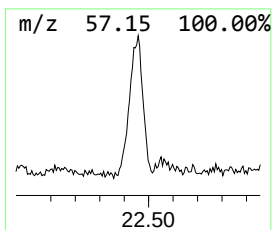
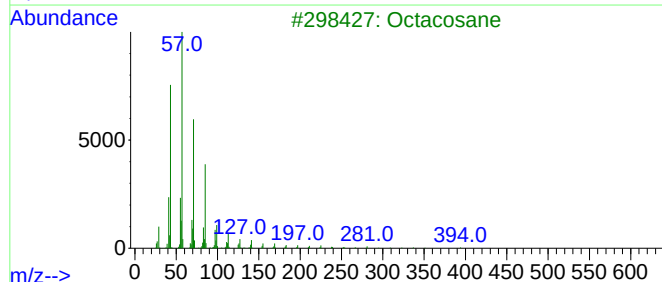
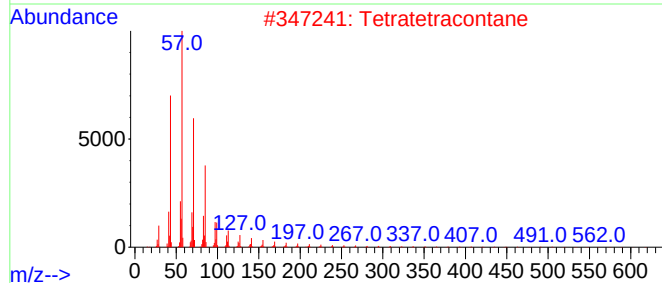
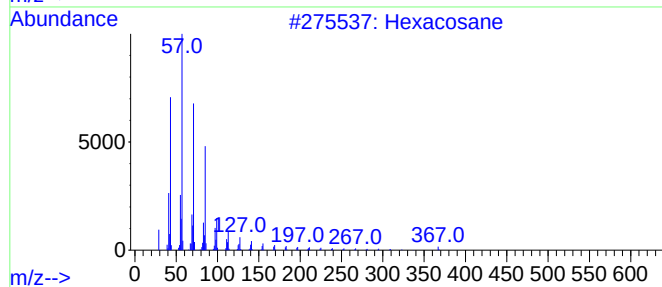
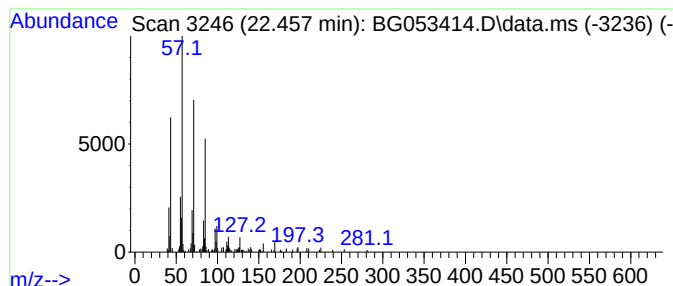
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.457	12.17 ng	326523	Chrysene-d12	21.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050322\
Data File : BG053414.D
Acq On : 3 May 2022 13:00
Operator : CG/JU
Sample : N2619-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS01-1-2-FT

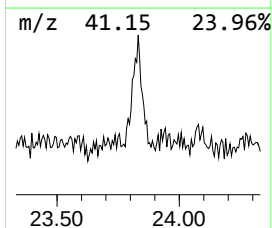
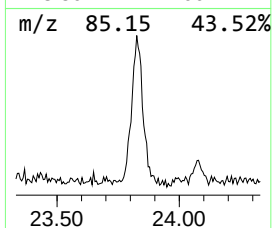
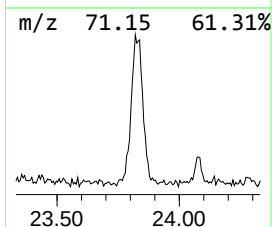
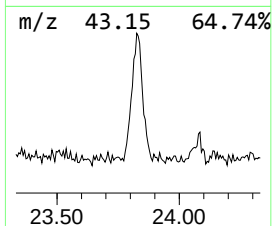
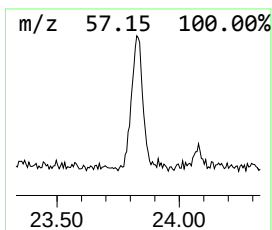
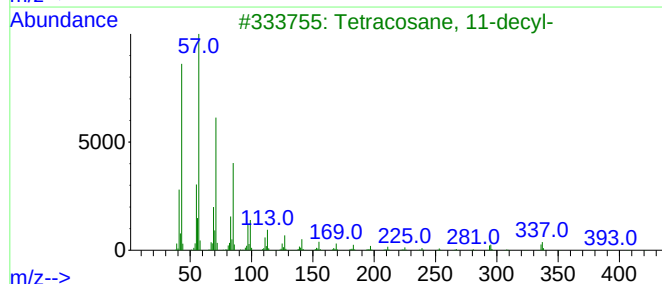
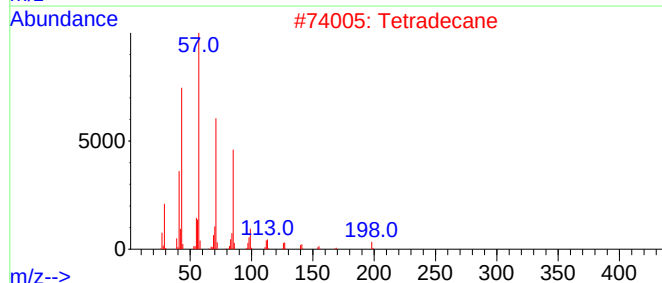
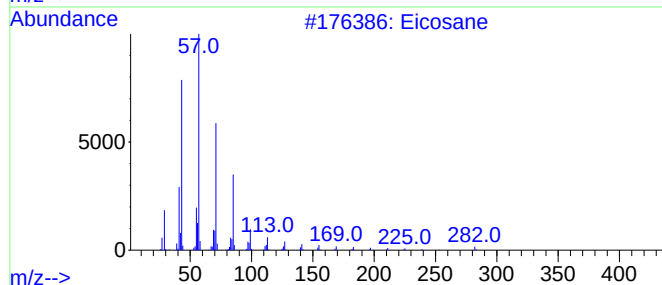
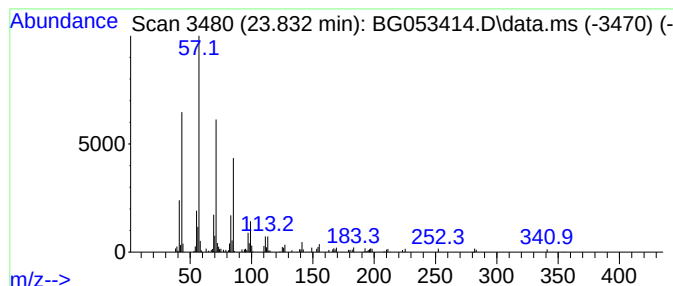
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.831	9.96 ng	275597	Perylene-d12	25.042

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Tetradecane	198	C14H30	000629-59-4	90
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050322\
Data File : BG053414.D
Acq On : 3 May 2022 13:00
Operator : CG/JU
Sample : N2619-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS01-1-2-FT

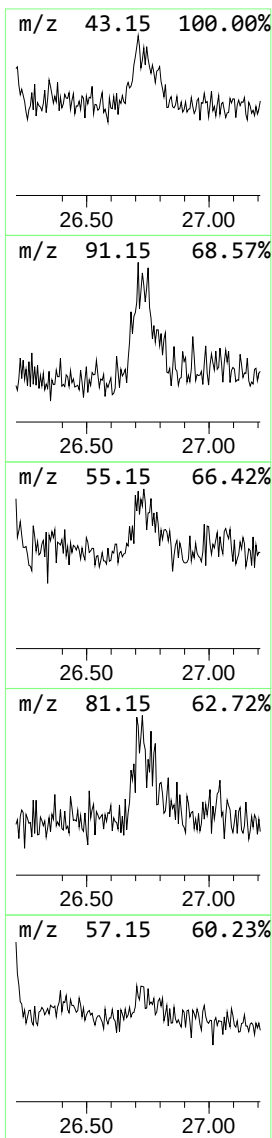
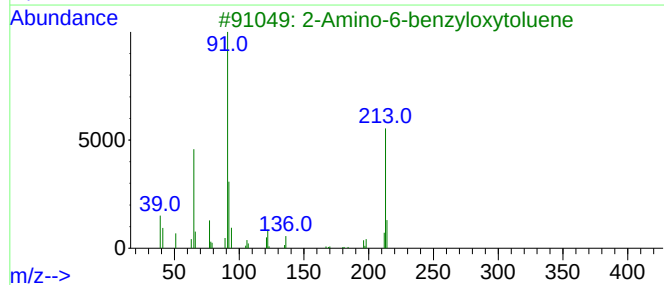
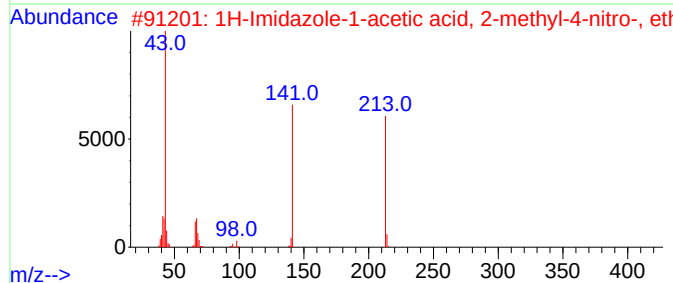
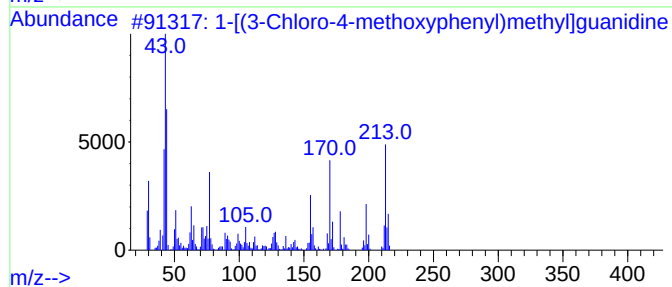
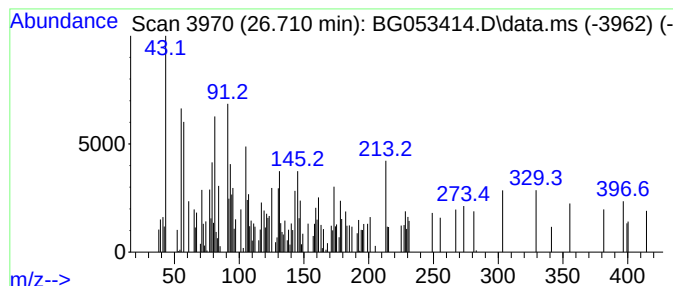
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown26.710 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.710	2.42 ng	67043	Perylene-d12	25.042

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	[(3-Chloro-4-methoxyphenyl)met...	213	C9H12ClN3O	048144-57-6	15	
2	1H-Imidazole-1-acetic acid, 2-me...	213	C8H11N3O4	013230-22-3	10		
3	2-Amino-6-benzoyloxytoluene	213	C14H15NO	065361-82-2	10		
4	N-Benzyl-p-anisidine	213	C14H15NO	017377-95-6	10		
5	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	213	C8H11N3O4	1000277-26-0	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050322\
Data File : BG053414.D
Acq On : 3 May 2022 13:00
Operator : CG/JU
Sample : N2619-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS01-1-2-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown19.285	19.285	3.3	ng	63006	4	17.470	380891	20.0
Octadecanoic acid	19.596	6.3	ng	119062	4	17.470	380891	20.0
Hexacosane	20.242	14.2	ng	381342	5	21.752	536492	20.0
Heptadecane, 9-...	21.264	12.9	ng	345801	5	21.752	536492	20.0
Trifluoroacetic...	21.370	4.2	ng	111493	5	21.752	536492	20.0
Tetratetracontane	22.457	12.2	ng	326523	5	21.752	536492	20.0
Eicosane	23.831	10.0	ng	275597	6	25.042	553448	20.0
unknown26.710	26.710	2.4	ng	67043	6	25.042	553448	20.0