

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059749.D
 Acq On : 18 Nov 2023 3:46
 Operator : MA/JU
 Sample : 05418-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 STONE-3

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-BG111623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059749.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.832	408	416	424	rVB	276402	446337	25.73%	5.768%
2	7.460	686	693	700	rBV	327239	553388	31.90%	7.151%
3	8.341	837	843	850	rBV2	94194	154737	8.92%	2.000%
4	9.539	1039	1047	1057	rVB	186145	331985	19.14%	4.290%
5	11.185	1320	1327	1335	rBV2	116767	218263	12.58%	2.820%
6	13.594	1728	1737	1742	rBV	599635	945460	54.51%	12.218%
7	13.787	1767	1770	1777	rBV2	9356	19568	1.13%	0.253%
8	14.968	1964	1971	1978	rBV2	205914	324832	18.73%	4.198%
9	16.449	2216	2223	2229	rBV2	596041	894187	51.55%	11.555%
10	17.718	2433	2439	2446	rVB	287191	432402	24.93%	5.588%
11	18.529	2571	2577	2584	rBV3	66012	97992	5.65%	1.266%
12	19.792	2783	2792	2798	rVB8	36738	59206	3.41%	0.765%
13	20.292	2871	2877	2886	rVB	1393742	1734500	100.00%	22.414%
14	21.578	3090	3096	3100	rBV4	45700	73085	4.21%	0.944%
15	21.796	3130	3133	3137	rVB5	15564	20753	1.20%	0.268%
16	21.854	3141	3143	3146	rVB3	19558	17359	1.00%	0.224%
17	22.042	3167	3175	3181	rBV2	218677	385121	22.20%	4.977%
18	22.166	3191	3196	3199	rBV6	10004	17374	1.00%	0.225%
19	22.471	3245	3248	3251	rBV5	16766	26941	1.55%	0.348%
20	23.470	3414	3418	3424	rVB6	19009	33939	1.96%	0.439%
21	24.551	3596	3602	3604	rBV6	27809	44006	2.54%	0.569%
22	25.626	3773	3785	3798	rVB2	131802	425081	24.51%	5.493%
23	25.879	3822	3828	3829	rBV6	21099	36806	2.12%	0.476%
24	27.542	4104	4111	4113	rBV7	38369	76447	4.41%	0.988%
25	27.941	4175	4179	4182	rBV5	9311	18189	1.05%	0.235%
26	28.958	4350	4352	4357	rVB6	11028	17945	1.03%	0.232%
27	29.634	4456	4467	4468	rBV8	66401	166685	9.61%	2.154%
28	30.186	4559	4561	4568	rVB8	14359	29802	1.72%	0.385%
29	32.254	4900	4913	4914	rBV10	60422	136085	7.85%	1.759%

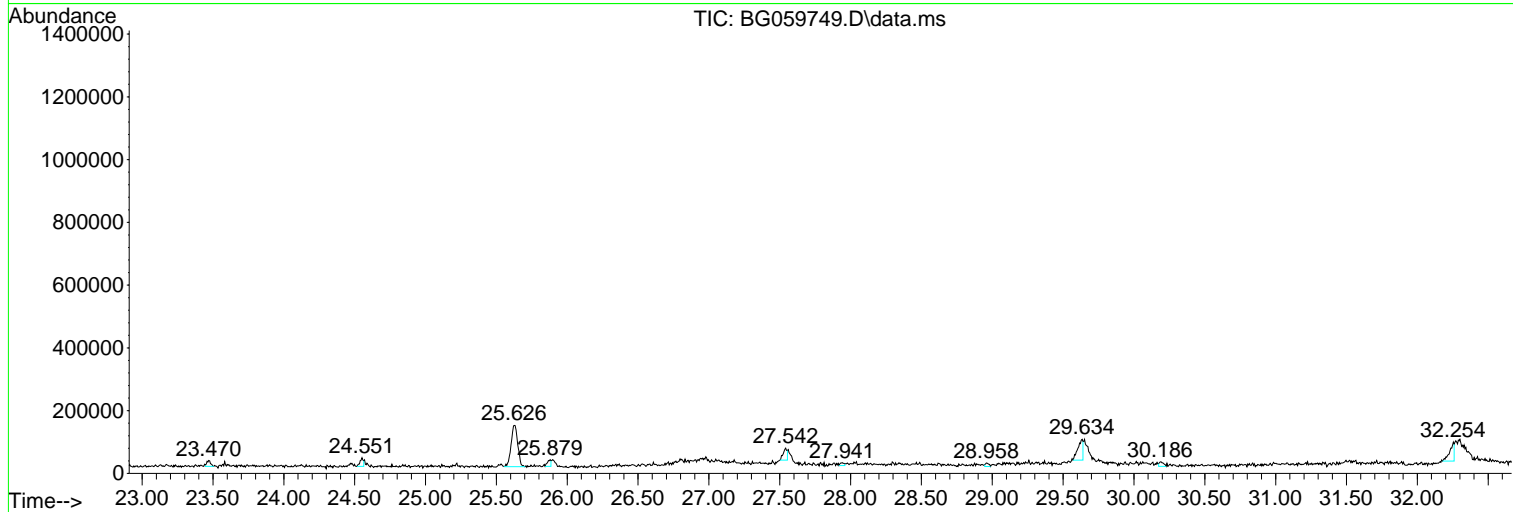
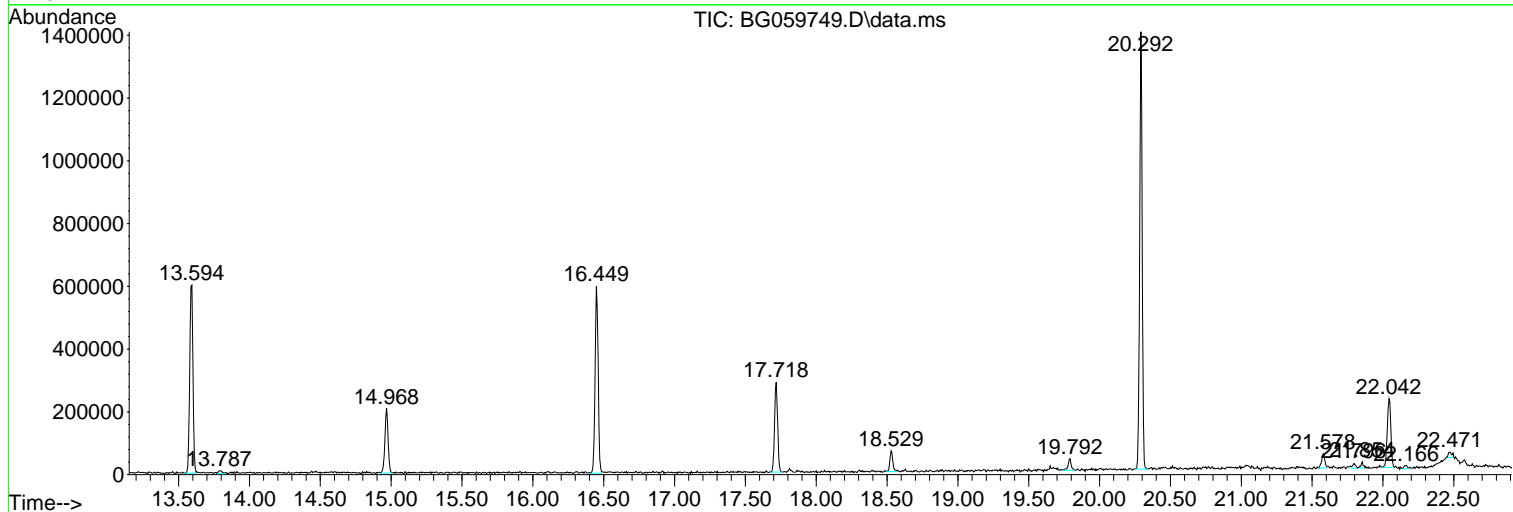
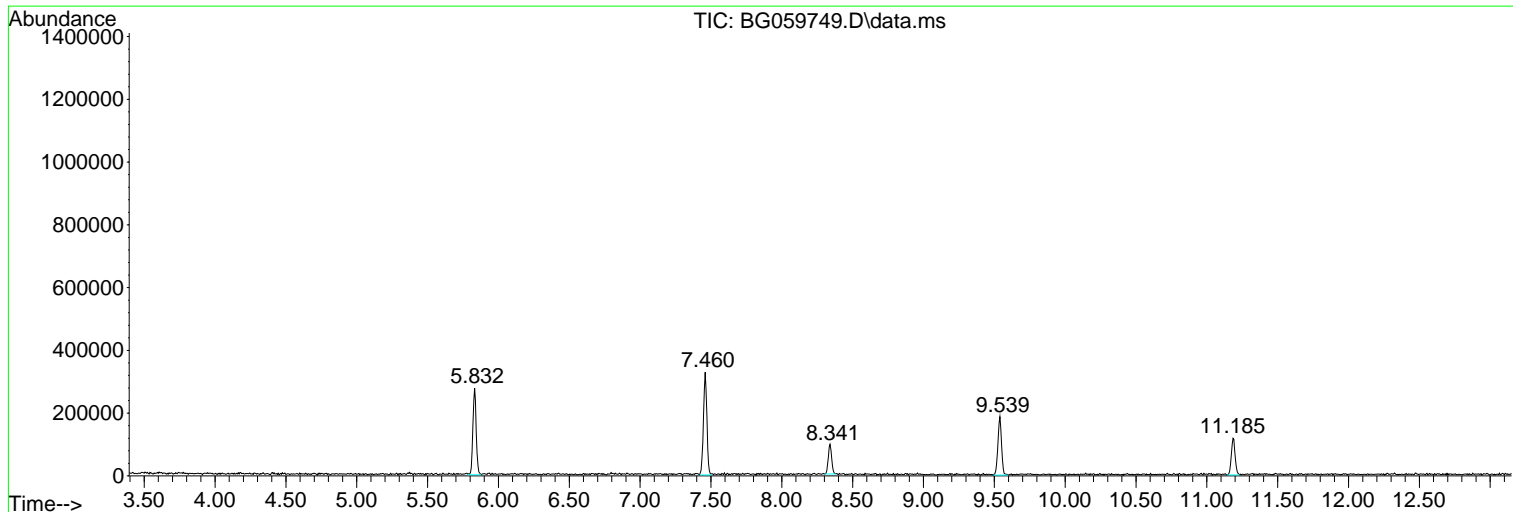
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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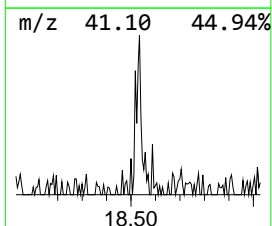
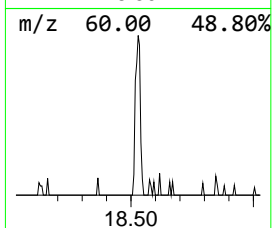
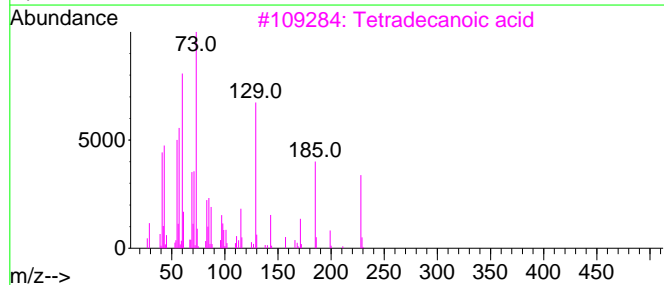
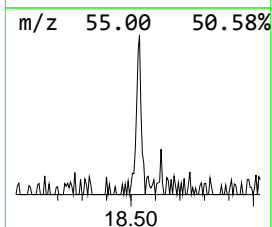
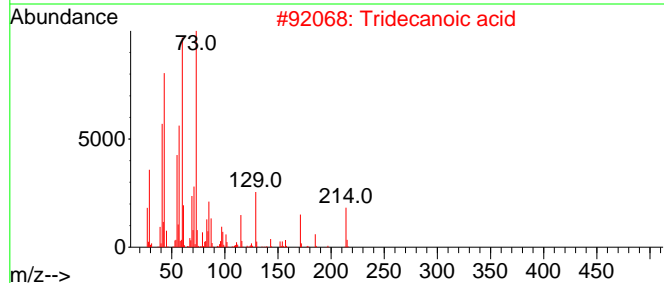
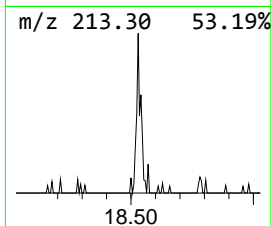
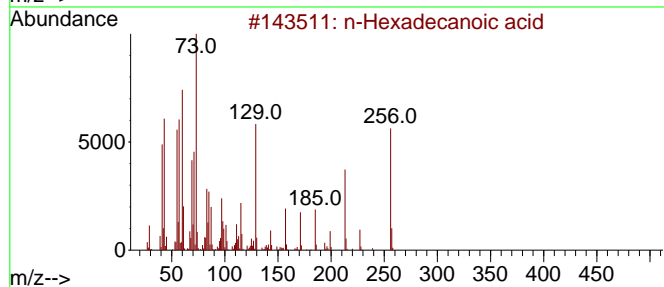
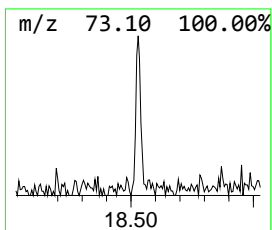
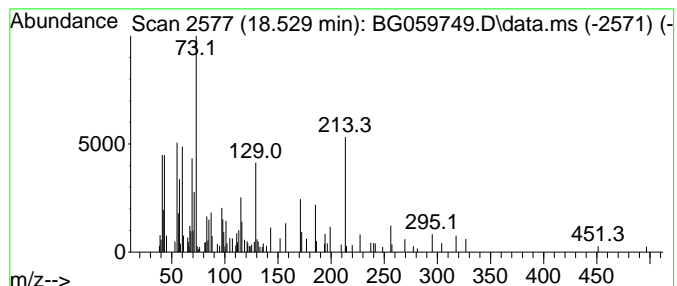
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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 Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.529	4.53 ng	97992	Phenanthrene-d10	17.718

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2		Tridecanoic acid	214	C13H26O2	000638-53-9	49
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4		n-Decanoic acid	172	C10H20O2	000334-48-5	27
5		Acetamide, N-nonyl-	185	C11H23NO	1000406-54-9	22



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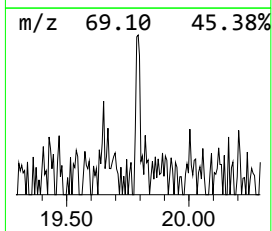
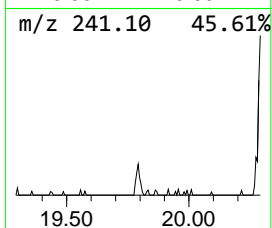
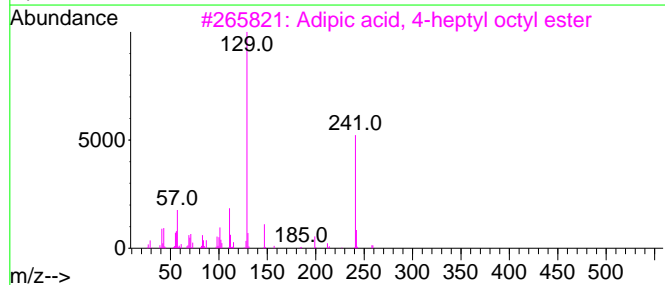
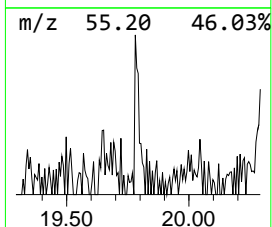
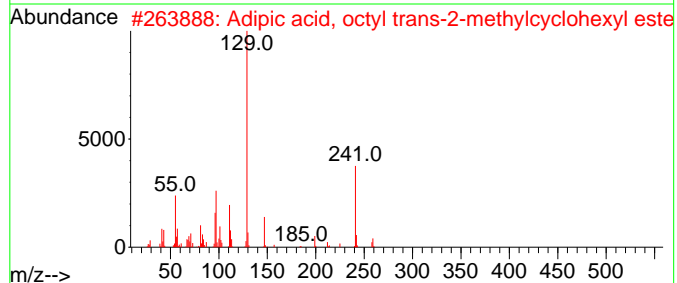
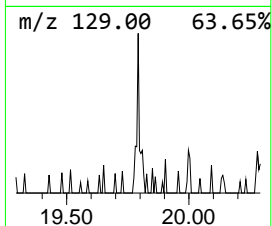
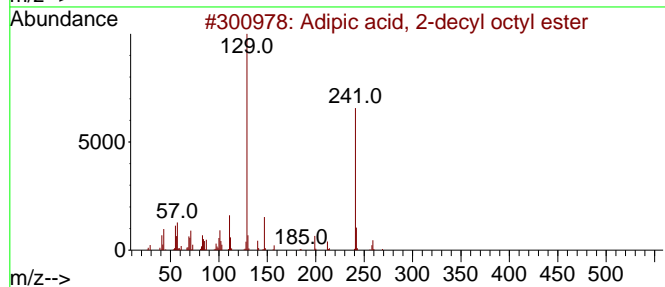
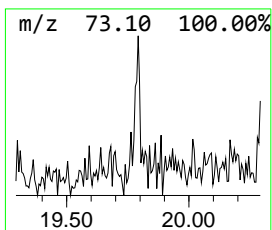
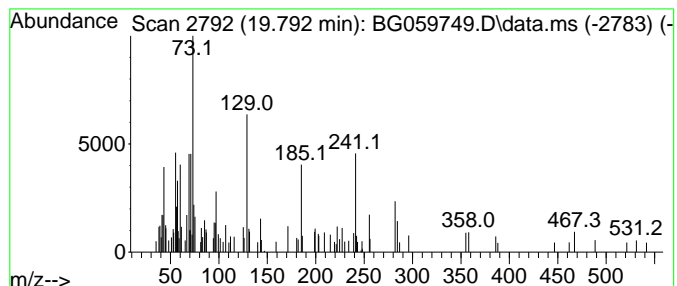
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 unknown19.792 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.792	2.74 ng	59206	Phenanthrene-d10	17.718

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-decyl octyl ester	398	C24H46O4	1000353-60-2	22
2			Adipic acid, octyl trans-2-methy...	354	C21H38O4	1000324-75-1	22
3			Adipic acid, 4-heptyl octyl ester	356	C21H40O4	1000349-74-2	12
4			Adipic acid, butyl octyl ester	314	C18H34O4	1000324-46-9	12
5			Adipic acid, cyclohexyl octyl ester	340	C20H36O4	1000324-26-3	12



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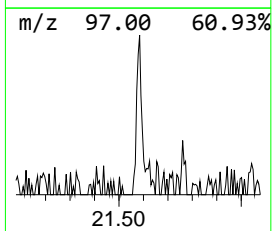
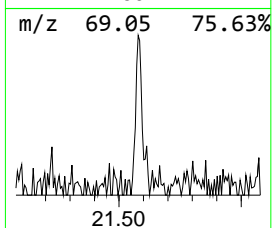
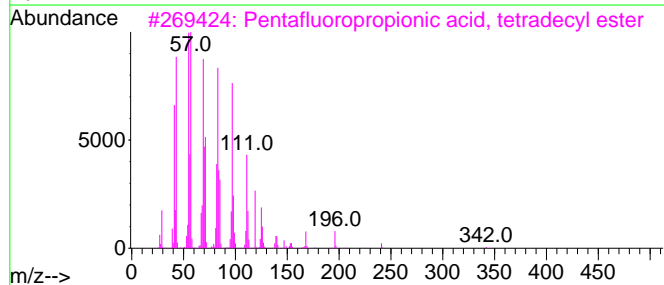
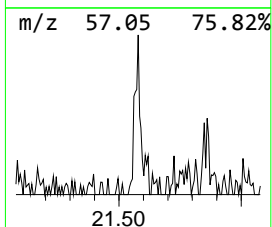
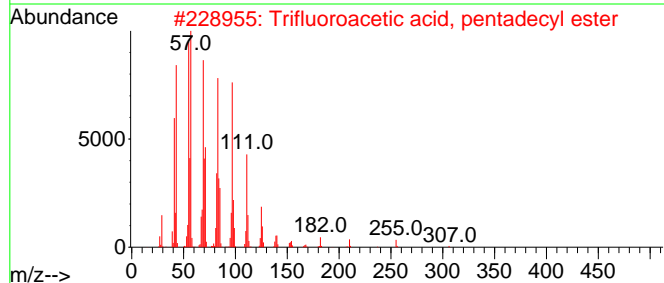
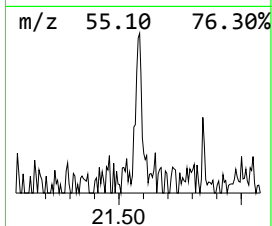
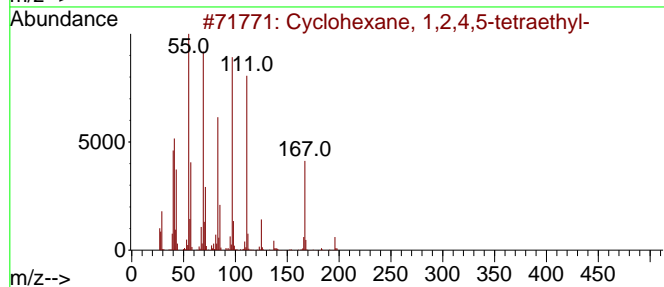
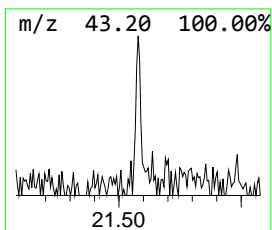
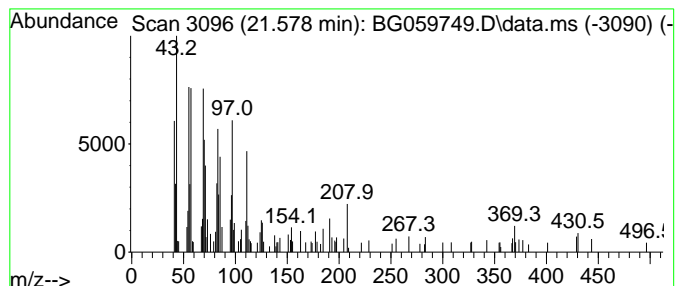
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TIC Library : C:\Database\NIST20.L
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 Peak Number 3 Cyclohexane, 1,2,4,5-tetrae... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	3.80 ng	73085	Chrysene-d12	22.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4,5-tetraethyl-	196	C14H28	061142-00-5	70
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	70
3			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	64
4			4-Trifluoroacetoxylhexadecane	338	C18H33F3O2	1000215-97-5	62
5			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	60



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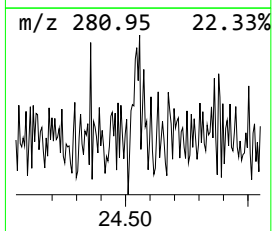
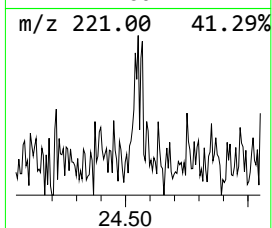
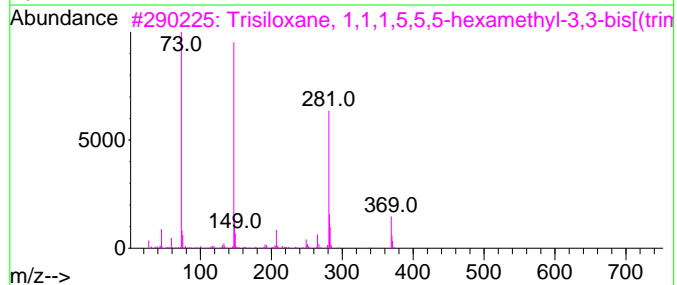
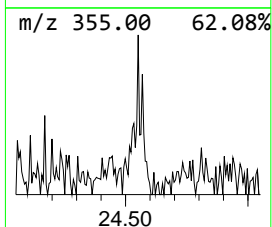
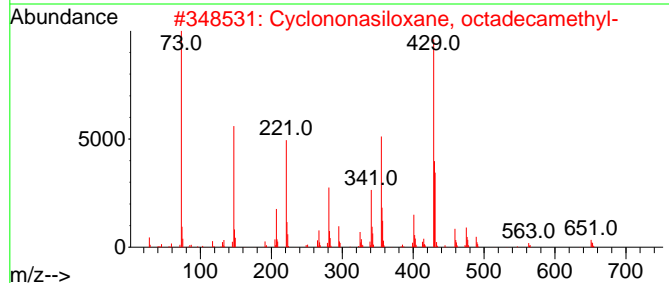
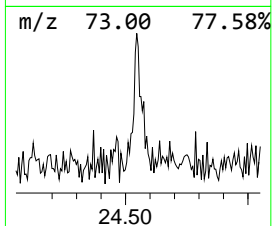
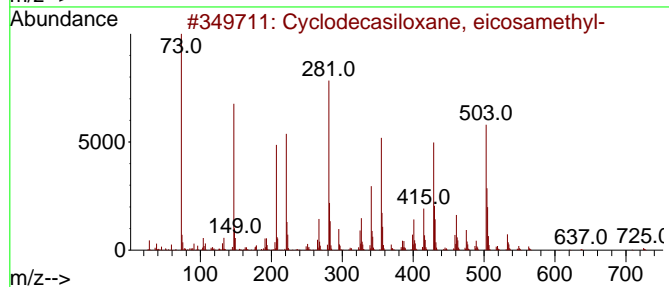
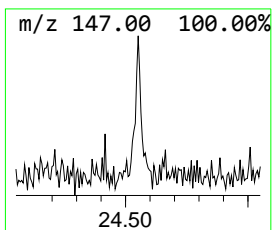
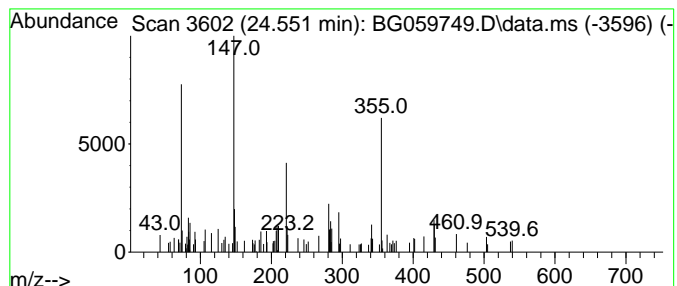
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 Peak Number 4 unknown24.551 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.551	2.07 ng	44006	Perylene-d12	25.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecasiloxane, eicosamethyl-	740	C20H60010Si10	018772-36-6	35
2			Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	32
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	32
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H2002SSi2	006398-62-5	27
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N203SSi3	1000500-82-8	25



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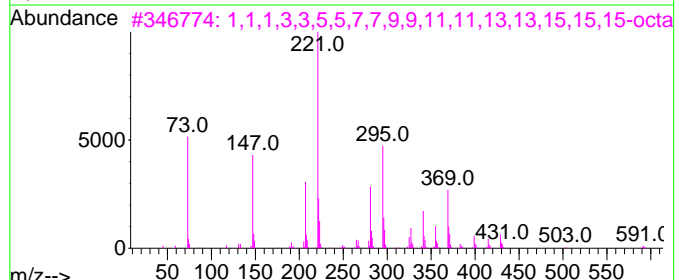
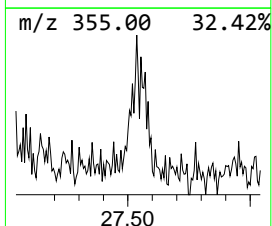
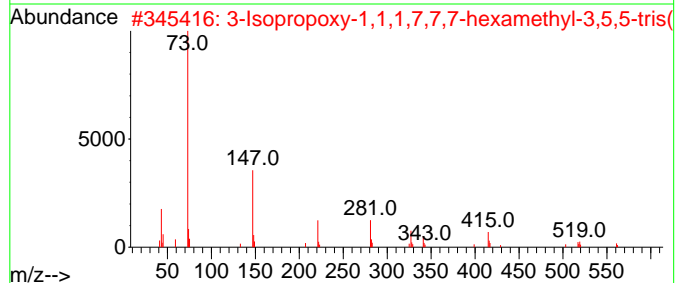
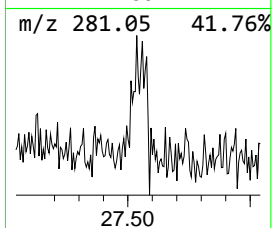
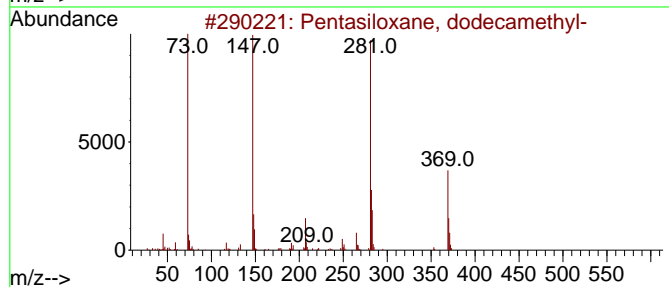
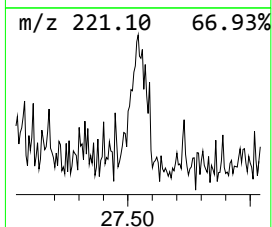
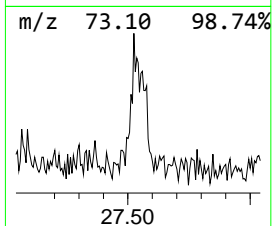
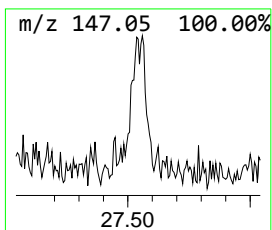
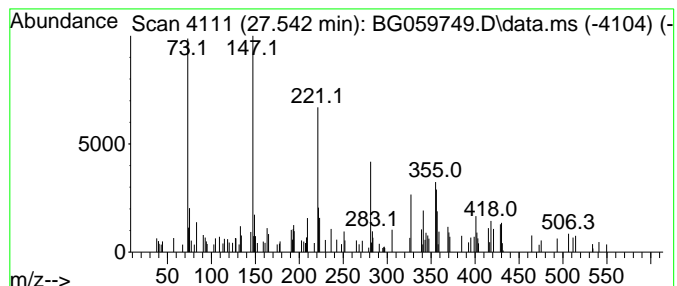
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 Peak Number 5 unknown27.542 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.542	3.60 ng	76447	Perylene-d12	25.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	42
2			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	42
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	37
4			Pyrido[2,3-d]pyrimidin-4(1H)-one	147	C7H5N3O	024410-19-3	35
5			N-(4-Nitrophenyl)-2-thiophenesul...	284	C10H8N2O4S2	053442-39-0	35



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 STONE-3

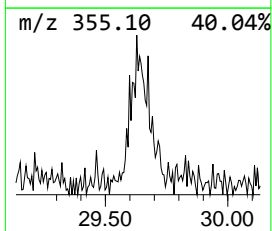
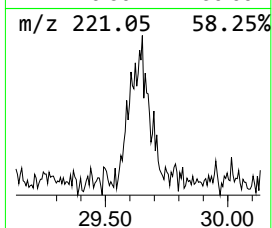
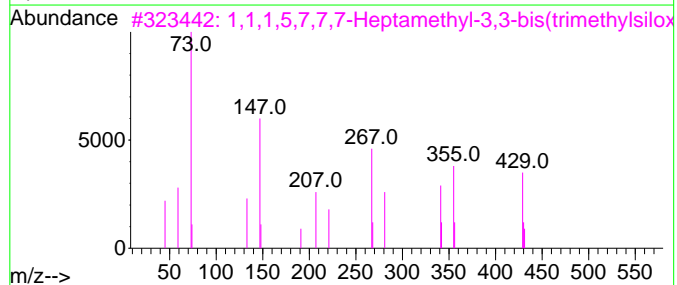
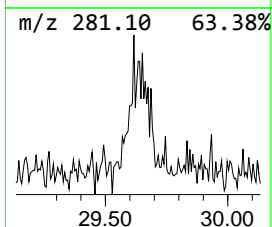
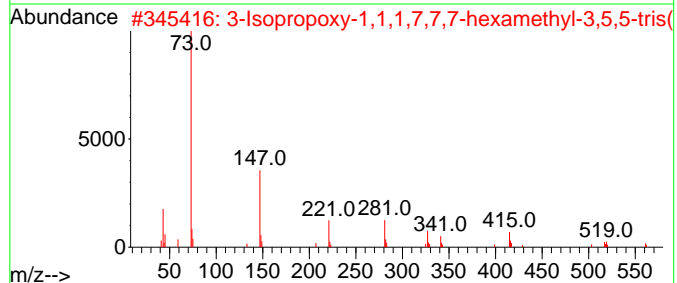
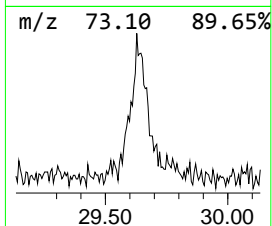
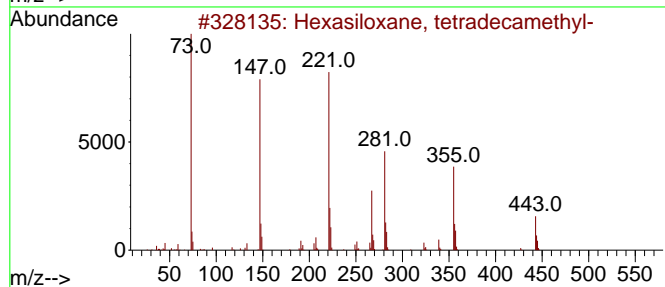
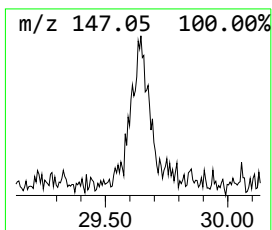
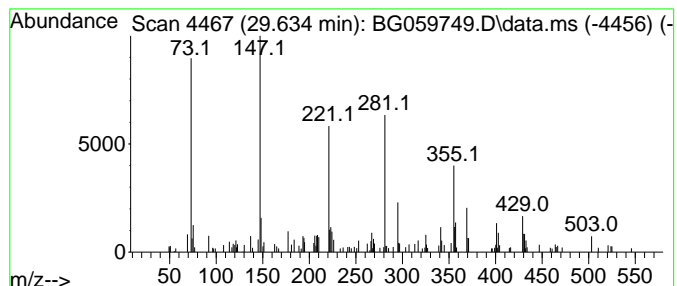
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 unknown29.634 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.634	7.84 ng	166685	Perylene-d12	25.627

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
2		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38
3		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
4		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35
5		1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059749.D
 Acq On : 18 Nov 2023 3:46
 Operator : MA/JU
 Sample : 05418-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 STONE-3

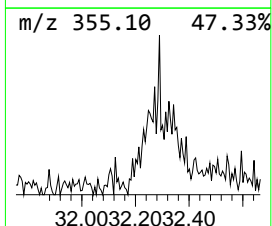
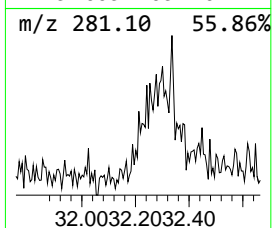
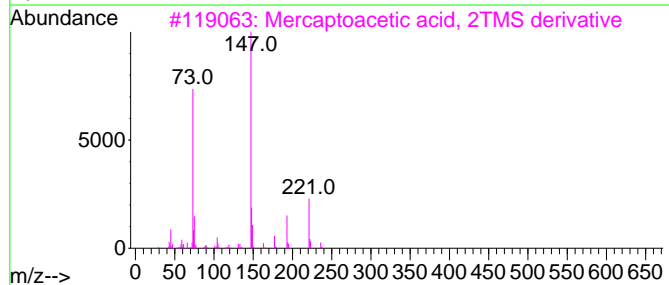
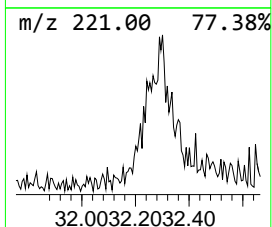
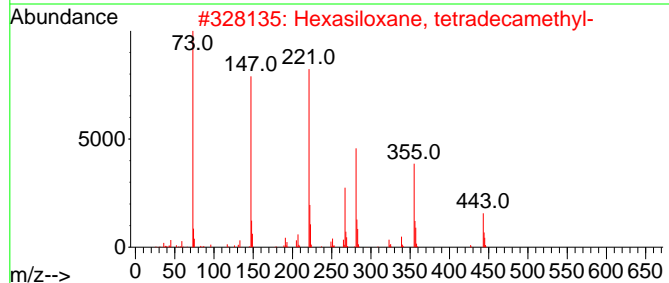
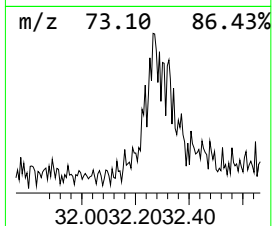
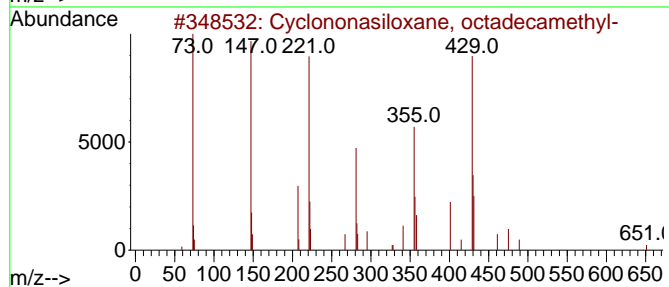
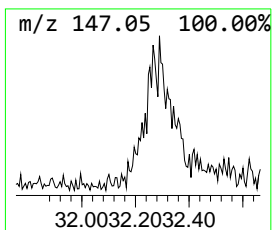
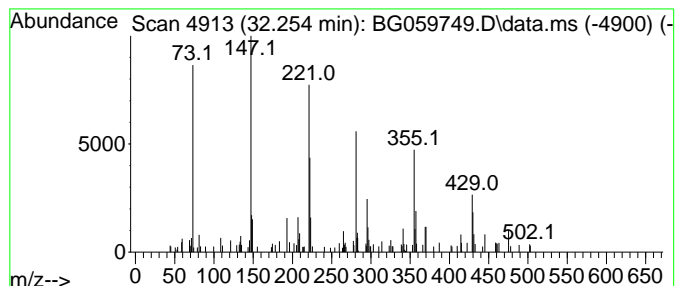
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.254	6.40 ng	136085	Perylene-d12	25.627

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	76
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
3		Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38
4		1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	35
5		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059749.D
 Acq On : 18 Nov 2023 3:46
 Operator : MA/JU
 Sample : 05418-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 STONE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
n-Hexadecanoic ...	18.529	4.5	ng	97992	4	17.718	432402	20.0
unknown19.792	19.792	2.7	ng	59206	4	17.718	432402	20.0
Cyclohexane, 1,...	21.578	3.8	ng	73085	5	22.048	385121	20.0
unknown24.551	24.551	2.1	ng	44006	6	25.627	425081	20.0
unknown27.542	27.542	3.6	ng	76447	6	25.627	425081	20.0
unknown29.634	29.634	7.8	ng	166685	6	25.627	425081	20.0
Cyclononasiloxa...	32.254	6.4	ng	136085	6	25.627	425081	20.0