

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059757.D
 Acq On : 18 Nov 2023 9:51
 Operator : MA/JU
 Sample : 05351-03
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 72-11985

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: BG059757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.833	410	416	423	rBV2	345670	550896	20.01%	4.497%
2	7.461	686	693	701	rBV	389013	682027	24.77%	5.568%
3	8.336	836	842	851	rBV2	99862	169675	6.16%	1.385%
4	9.541	1039	1047	1056	rVB	251354	451083	16.38%	3.683%
5	11.192	1318	1328	1335	rBV2	125739	239752	8.71%	1.957%
6	13.589	1729	1736	1744	rBV	911719	1404428	51.00%	11.466%
7	14.970	1965	1971	1979	rVB2	218504	360533	13.09%	2.943%
8	16.450	2217	2223	2229	rBV	874742	1305785	47.42%	10.660%
9	17.720	2431	2439	2444	rBV	432620	678535	24.64%	5.540%
10	17.767	2444	2447	2452	rVB2	23635	36253	1.32%	0.296%
11	18.530	2573	2577	2582	rBV4	141846	184955	6.72%	1.510%
12	19.752	2781	2785	2788	rBV	52729	65089	2.36%	0.531%
13	19.794	2788	2792	2797	rVB5	49721	68557	2.49%	0.560%
14	20.117	2842	2847	2850	rVB	44586	61716	2.24%	0.504%
15	20.293	2869	2877	2883	rBV	2210429	2753520	100.00%	22.480%
16	21.574	3091	3095	3096	rBV4	52463	47856	1.74%	0.391%
17	22.044	3168	3175	3182	rBV	364935	662916	24.08%	5.412%
18	22.496	3240	3252	3262	rBV9	166929	646910	23.49%	5.281%
19	23.254	3374	3381	3391	rBV3	254742	475918	17.28%	3.885%
20	23.466	3413	3417	3418	rBV2	62683	69426	2.52%	0.567%
21	24.547	3595	3601	3612	rVB8	83757	237863	8.64%	1.942%
22	25.446	3751	3754	3759	rBV2	23463	40070	1.46%	0.327%
23	25.640	3775	3787	3796	rBV4	201239	632421	22.97%	5.163%
24	25.881	3819	3828	3835	rBV5	73153	205209	7.45%	1.675%
25	27.543	4102	4111	4112	rBV8	57839	131387	4.77%	1.073%
26	29.600	4457	4461	4462	rBV4	35125	38780	1.41%	0.317%
27	32.255	4907	4913	4915	rBV7	24673	47404	1.72%	0.387%

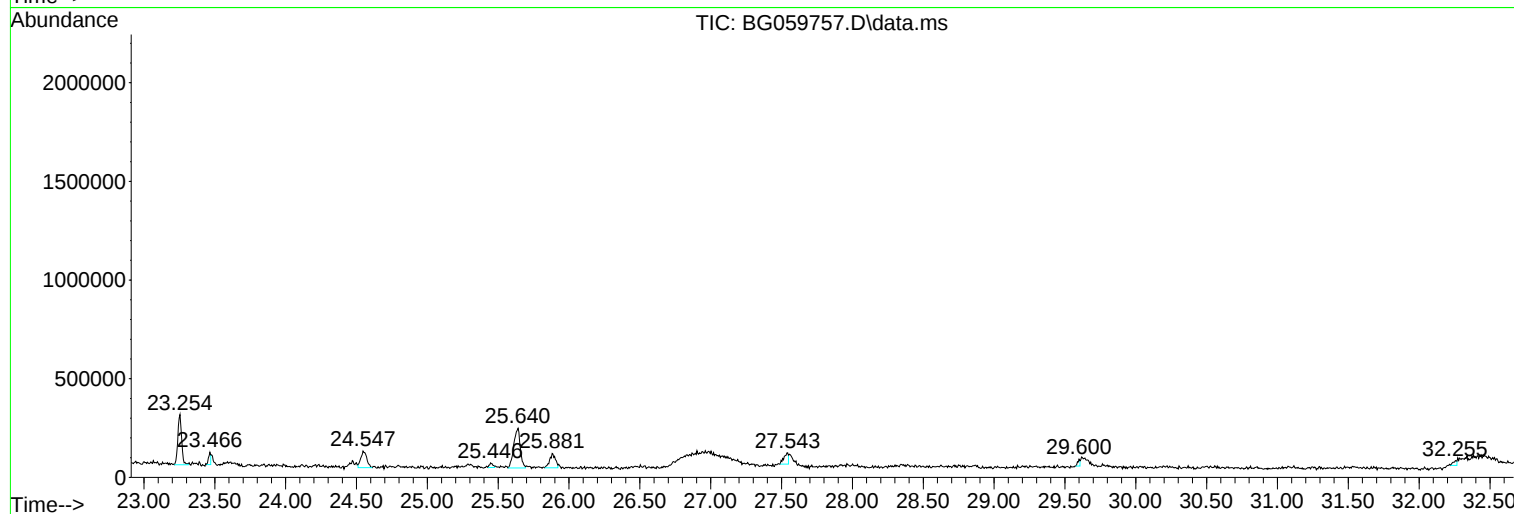
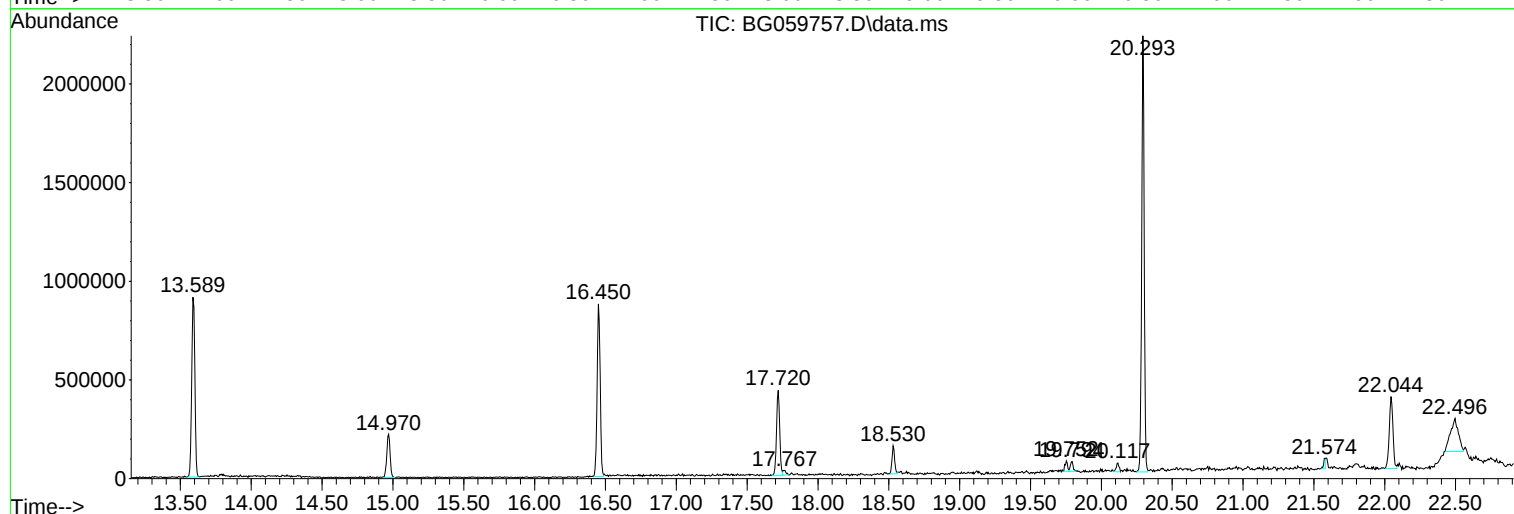
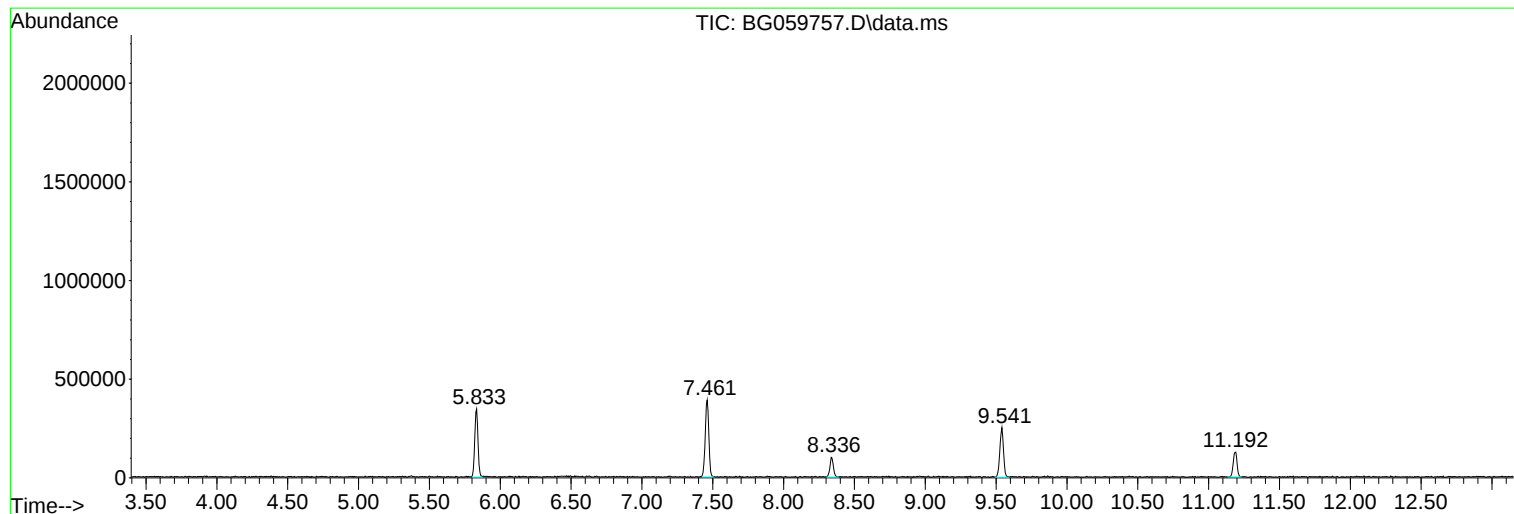
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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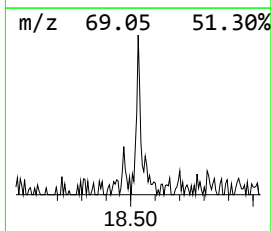
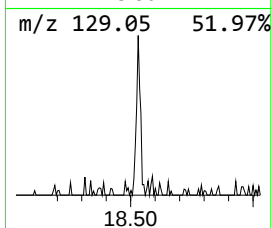
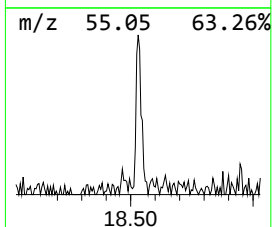
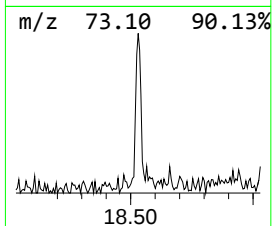
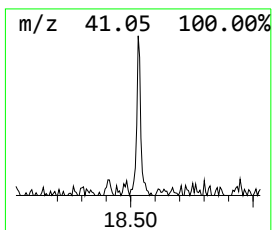
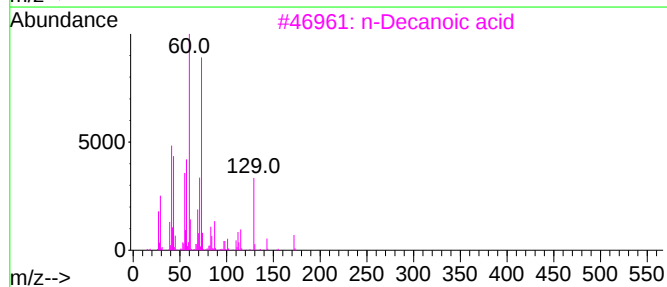
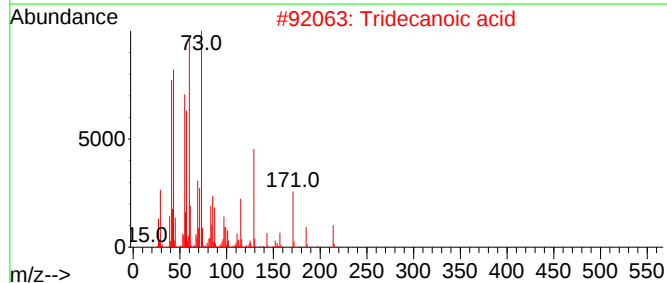
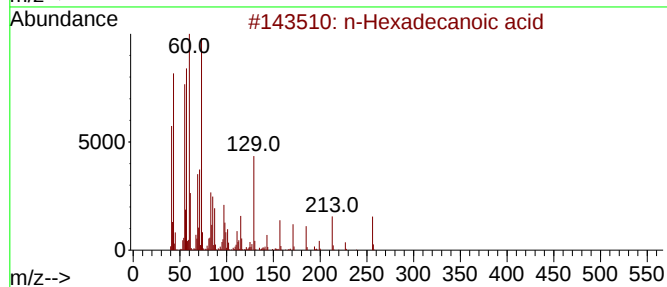
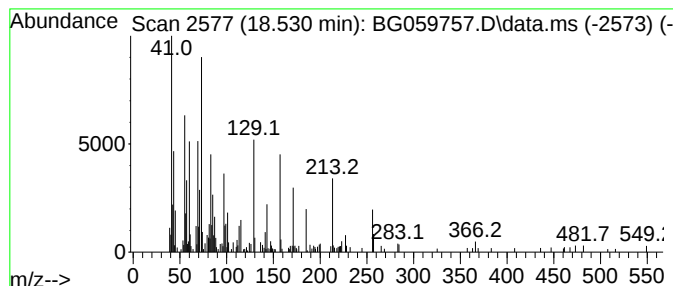
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.530	5.45 ng	184955	Phenanthrene-d10	17.720

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2			Tridecanoic acid	214	C13H26O2	000638-53-9	50
3			n-Decanoic acid	172	C10H20O2	000334-48-5	38
4			3,7-Dimethyl-8-oxo-1,5-dioxaspi...	256	C13H20O5	1000193-79-8	15
5			Cyclohexanebutanoic acid	170	C10H18O2	004441-63-8	11



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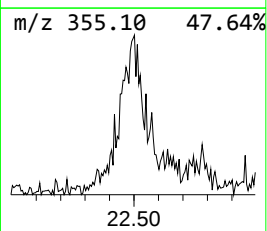
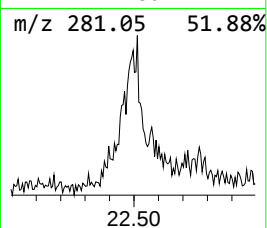
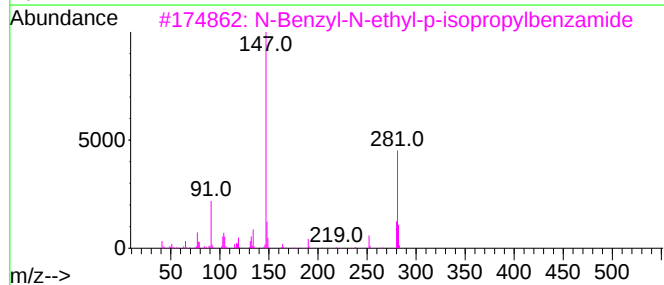
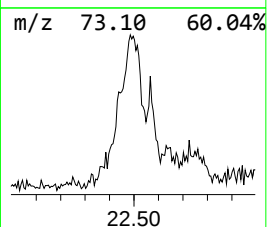
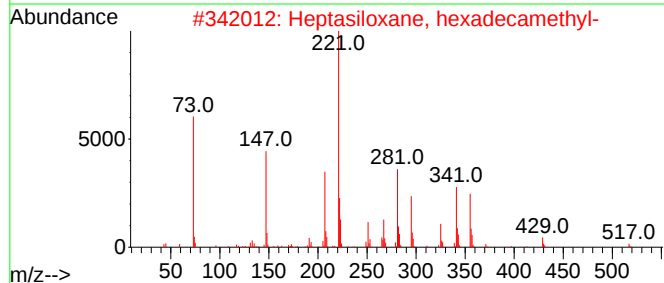
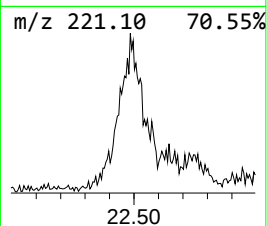
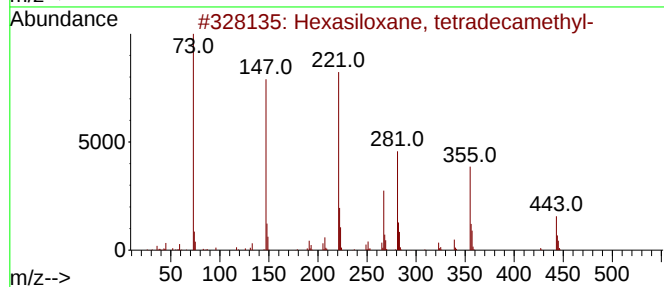
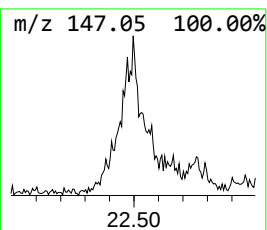
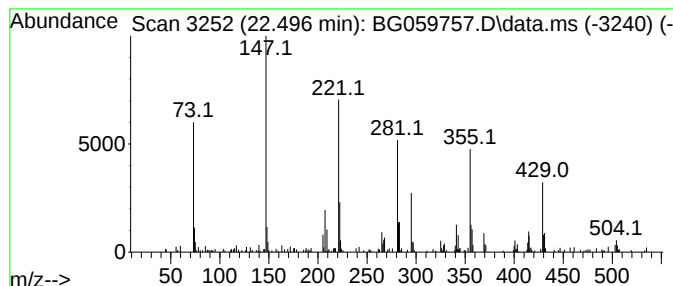
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
22.496	19.52 ng	646910	Chrysene-d12			22.044
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	64
2	Heptasiloxane, hexadecamethyl-		532	C16H48O6Si7	000541-01-5	38
3	N-Benzyl-N-ethyl-p-isopropylbenz...		281	C19H23NO	015089-22-2	30
4	Pentasiloxane, dodecamethyl-		384	C12H36O4Si5	000141-63-9	27
5	Phthalic acid, 2TMS derivative		310	C14H22O4Si2	002078-22-0	12



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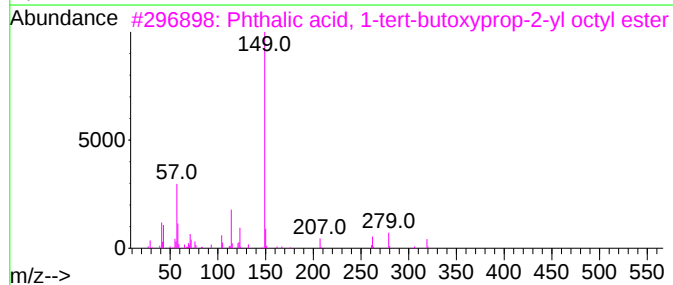
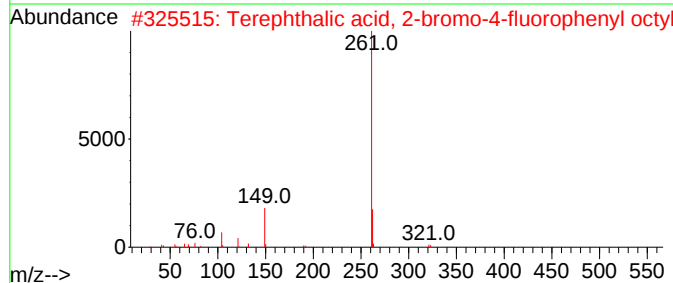
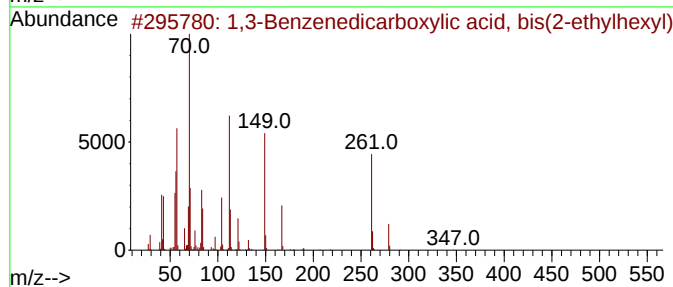
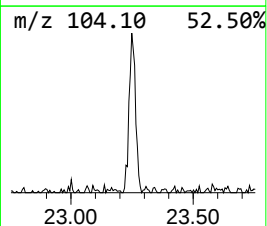
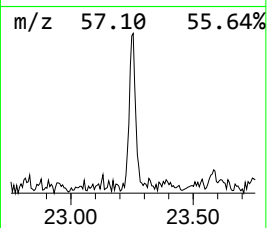
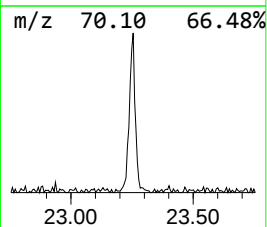
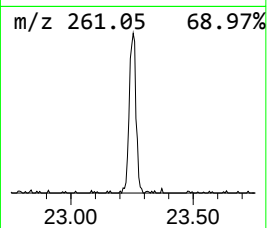
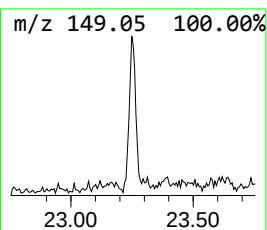
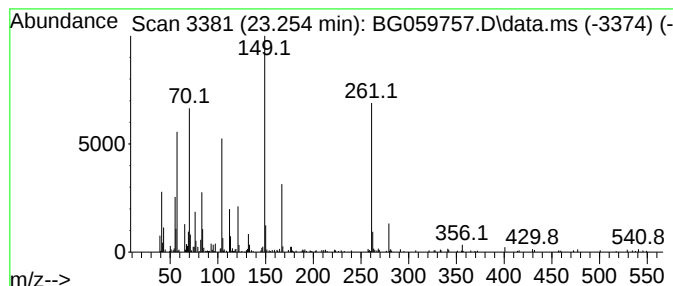
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown23.254 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.254	14.36 ng	475918	Chrysene-d12	22.044

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	38
2			Terephthalic acid, 2-bromo-4-flu...	450	C22H24BrFO4	1000323-71-2	38
3			Phthalic acid, 1-tert-butoxyprop...	392	C23H36O5	1000371-01-3	27
4			Phthalic acid, isohexyl 4-methyl...	334	C20H30O4	1010356-87-5	27
5			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	22



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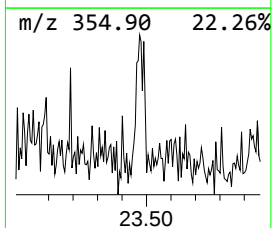
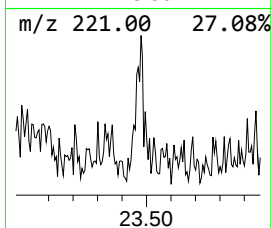
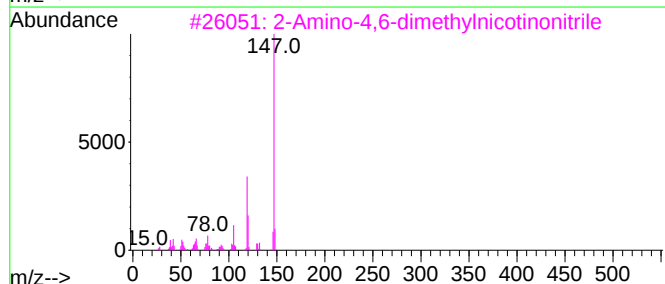
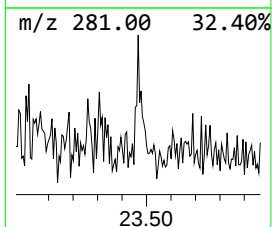
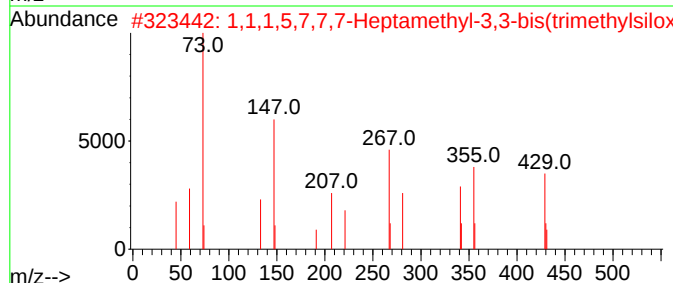
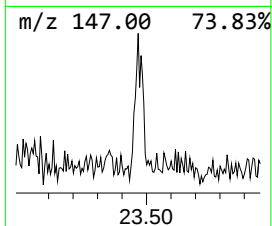
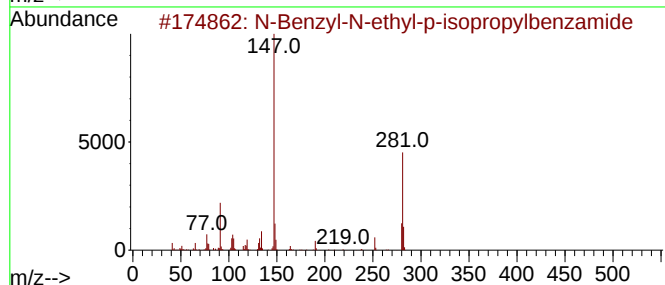
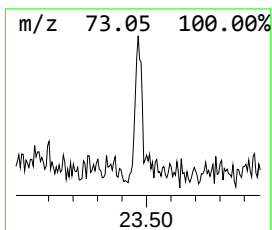
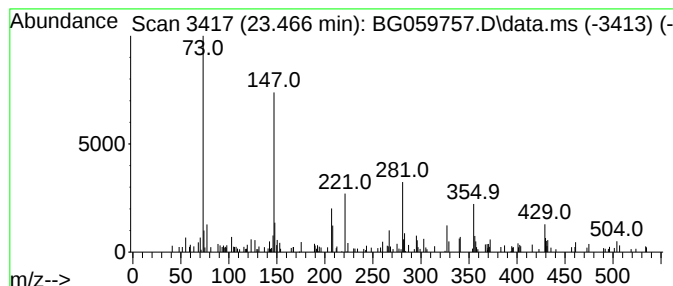
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Peak Number 4 N-Benzyl-N-ethyl-p-isopropy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.466	2.09 ng	69426	Chrysene-d12	22.044

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	58
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
3			2-Amino-4,6-dimethylnicotinonitrile	147	C8H9N3	005468-34-8	43
4			2-(Morpholin-4-yl)-2-sulfanylide...	277	C15H19NO2S	037167-44-5	38
5			D-Xylulose, tetrakis(trimethylsi...	633	C24H44F5NO5Si4	1000394-61-3	38



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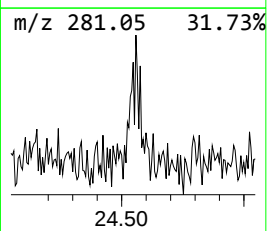
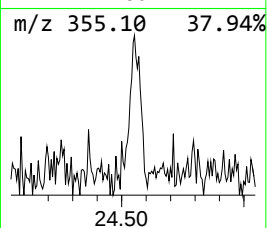
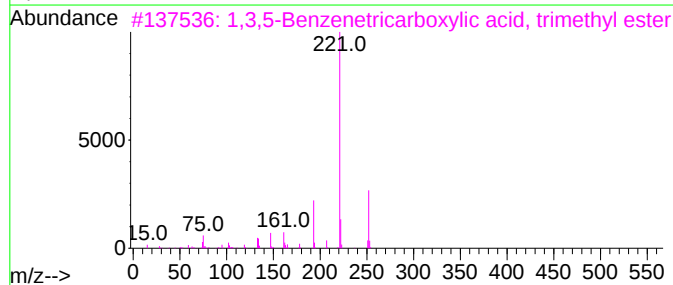
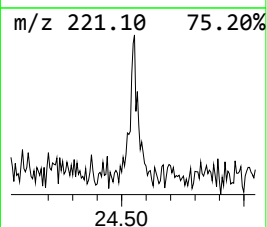
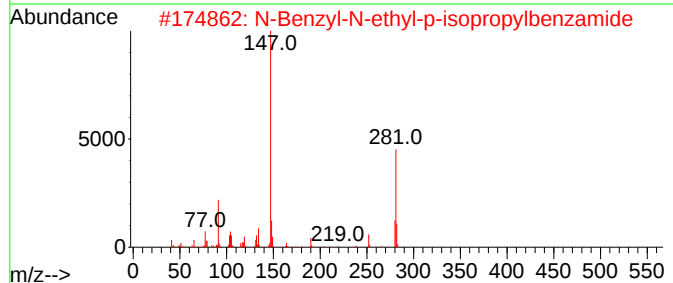
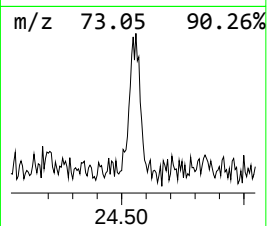
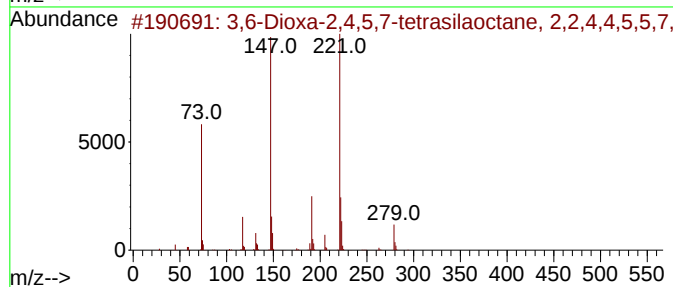
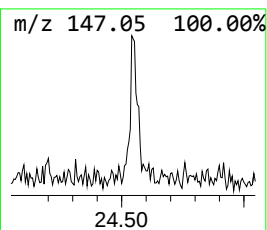
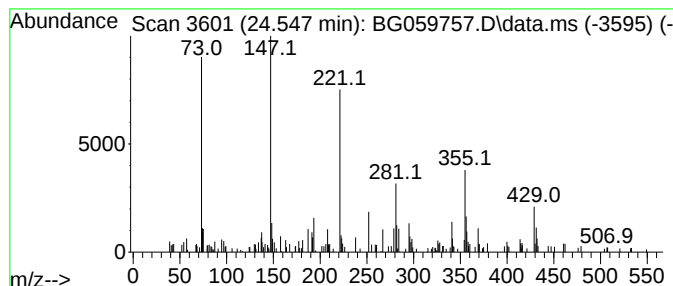
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Peak Number 5 unknown24.547 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.547	7.52 ng	237863	Perylene-d12	25.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
3			1,3,5-Benzenetricarboxylic acid,...	252	C12H12O6	002672-58-4	18
4			2-Amino-4-(4-nitrophenyl)thiazole	221	C9H7N3O2S	002104-09-8	18
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	16



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72-11985

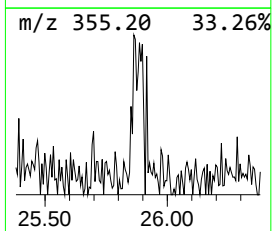
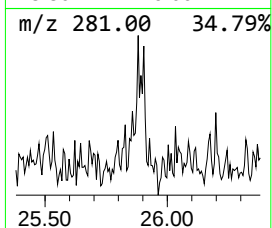
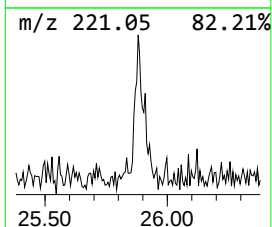
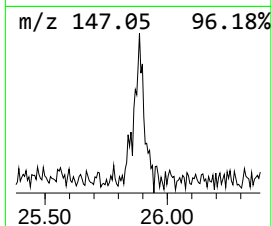
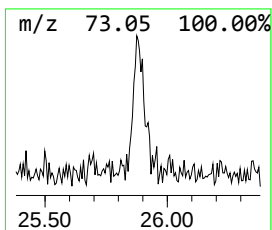
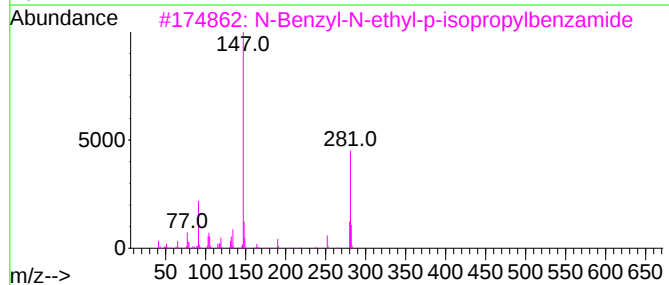
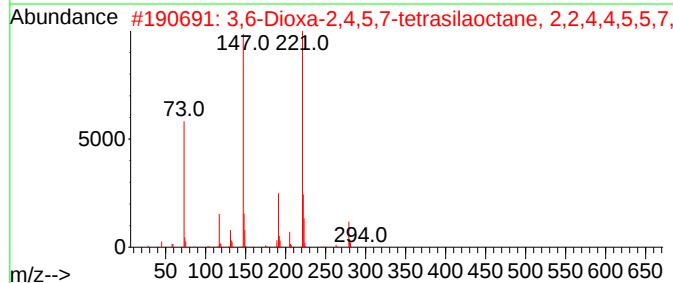
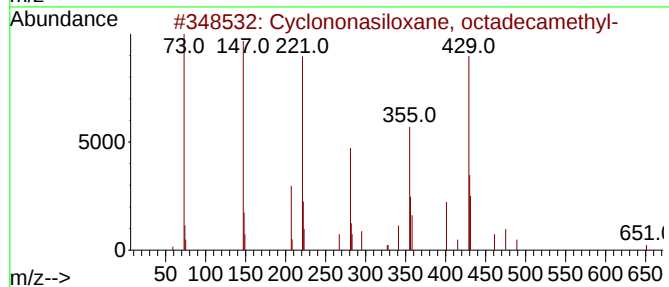
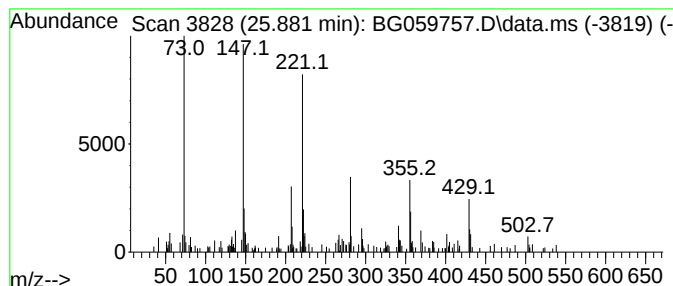
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.881	6.49 ng	205209	Perylene-d12	25.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
4			Benzophenone-2,4',5-tricarboxyli...	356	C19H16O7	345651-64-1	22
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059757.D
Acq On : 18 Nov 2023 9:51
Operator : MA/JU
Sample : 05351-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11985

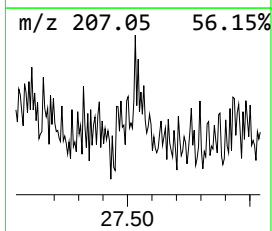
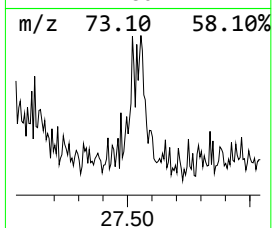
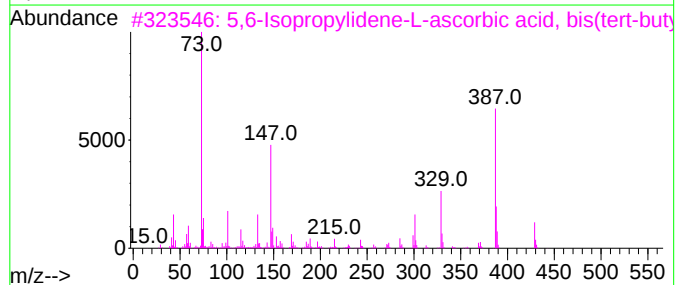
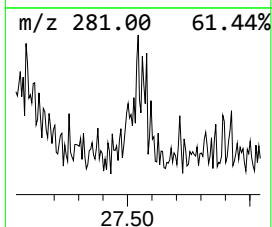
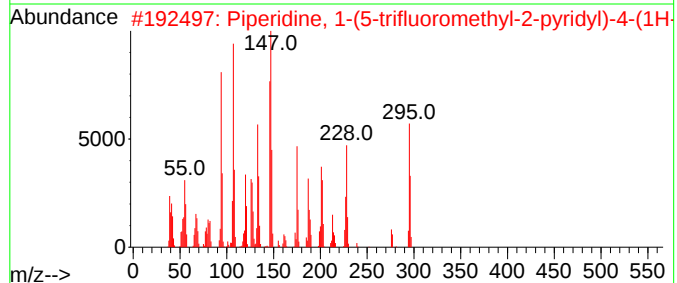
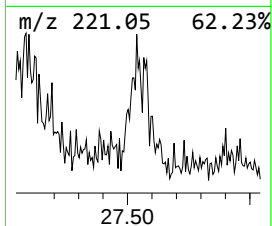
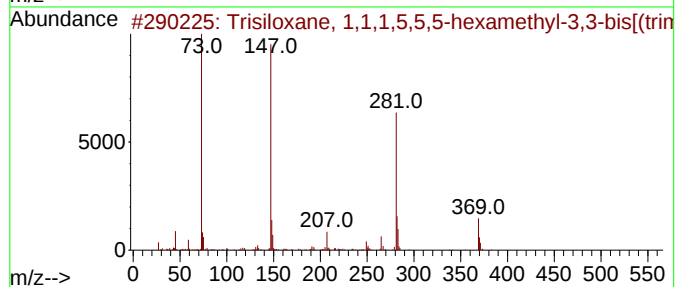
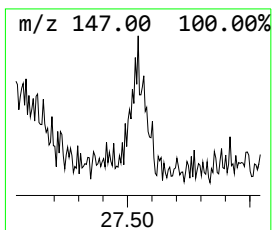
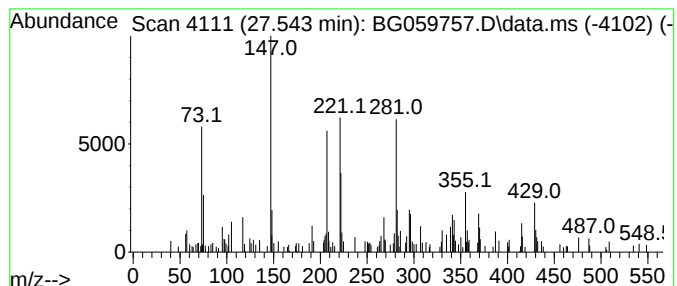
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown27.543 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.543	4.16 ng	131387	Perylene-d12	25.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	43
2			Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	27
3			5,6-Isopropylidene-L-ascorbic ac...	444	C21H40O6Si2	1000364-74-1	25
4			Heptasiloxane, 1,1,3,3,5,5,7,9...	504	C14H44O6Si7	019095-23-9	25
5			4-(2-Hydroxyethyl)benzenesulfona...	417	C17H35NO3SSi3	1000501-31-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059757.D
Acq On : 18 Nov 2023 9:51
Operator : MA/JU
Sample : 05351-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-11985

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 ...	18.530	5.5	ng	184955	4	17.720	678535	20.0
Hexasiloxane, t...	22.496	19.5	ng	646910	5	22.044	662916	20.0
unknown23.254	23.254	14.4	ng	475918	5	22.044	662916	20.0
N-Benzyl-N-ethy...	23.466	2.1	ng	69426	5	22.044	662916	20.0
unknown24.547	24.547	7.5	ng	237863	6	25.628	632421	20.0
Cyclononasiloxa...	25.881	6.5	ng	205209	6	25.628	632421	20.0
unknown27.543	27.543	4.2	ng	131387	6	25.628	632421	20.0