

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
 Data File : BG059871.D
 Acq On : 24 Nov 2023 23:45
 Operator : MA/JU
 Sample : 05408-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 710-ELIZABETH-AVE

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: BG059871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.808	404	412	421	rBV	360322	590945	18.27%	4.595%
2	7.441	681	690	700	rBV	375581	667435	20.63%	5.190%
3	8.317	831	839	849	rVB2	136015	237806	7.35%	1.849%
4	9.515	1036	1043	1053	rVB2	251121	466894	14.43%	3.630%
5	11.166	1317	1324	1333	rBV2	182216	344053	10.63%	2.675%
6	13.570	1725	1733	1741	rBV	1237475	1851654	57.23%	14.398%
7	13.769	1761	1767	1773	rBV4	19801	34171	1.06%	0.266%
8	14.950	1960	1968	1978	rBV2	433848	696419	21.53%	5.415%
9	16.431	2213	2220	2229	rBV	1136925	1737054	53.69%	13.507%
10	17.700	2429	2436	2442	rBV	570819	895929	27.69%	6.967%
11	18.511	2569	2574	2578	rBV2	79539	109784	3.39%	0.854%
12	19.727	2778	2781	2785	rBV2	36419	53552	1.66%	0.416%
13	19.774	2786	2789	2793	rVB5	30287	34956	1.08%	0.272%
14	20.097	2840	2844	2850	rVB2	38700	59710	1.85%	0.464%
15	20.273	2868	2874	2879	rBV	2619299	3235269	100.00%	25.157%
16	21.554	3089	3092	3097	rVB7	61606	85552	2.64%	0.665%
17	22.018	3164	3171	3178	rBV2	408893	713245	22.05%	5.546%
18	22.524	3253	3257	3260	rVB6	42642	56385	1.74%	0.438%
19	23.417	3401	3409	3416	rVB7	52603	139208	4.30%	1.082%
20	25.585	3767	3778	3788	rBV2	231634	726645	22.46%	5.650%
21	25.790	3809	3813	3822	rVB10	50499	123827	3.83%	0.963%

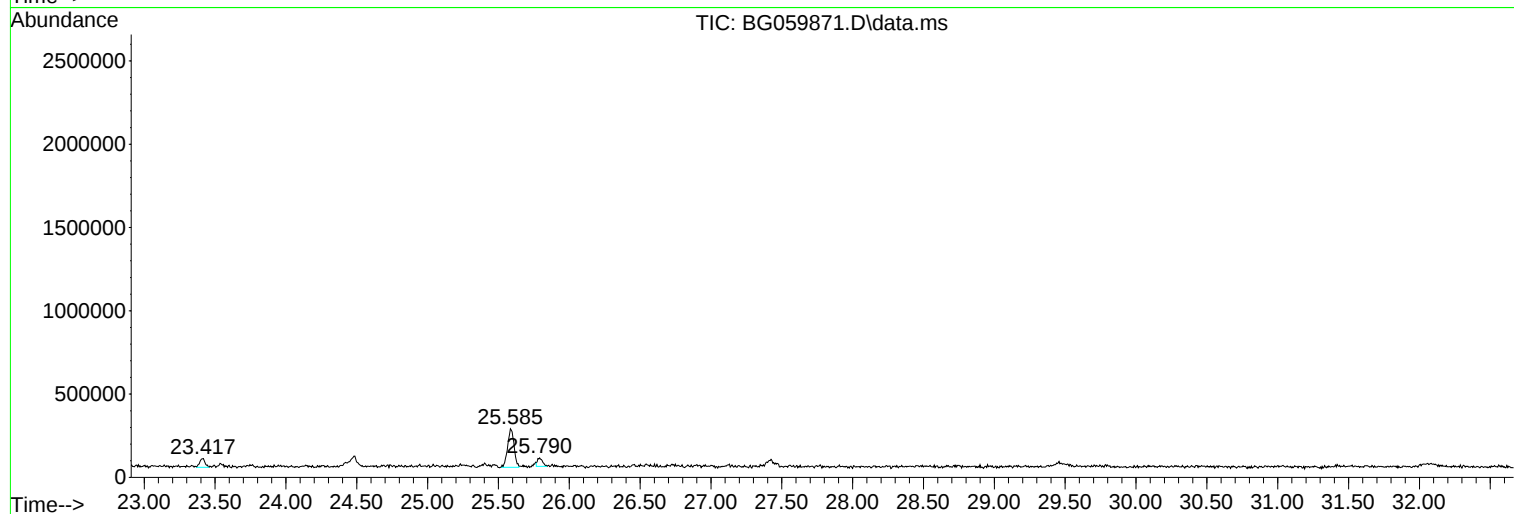
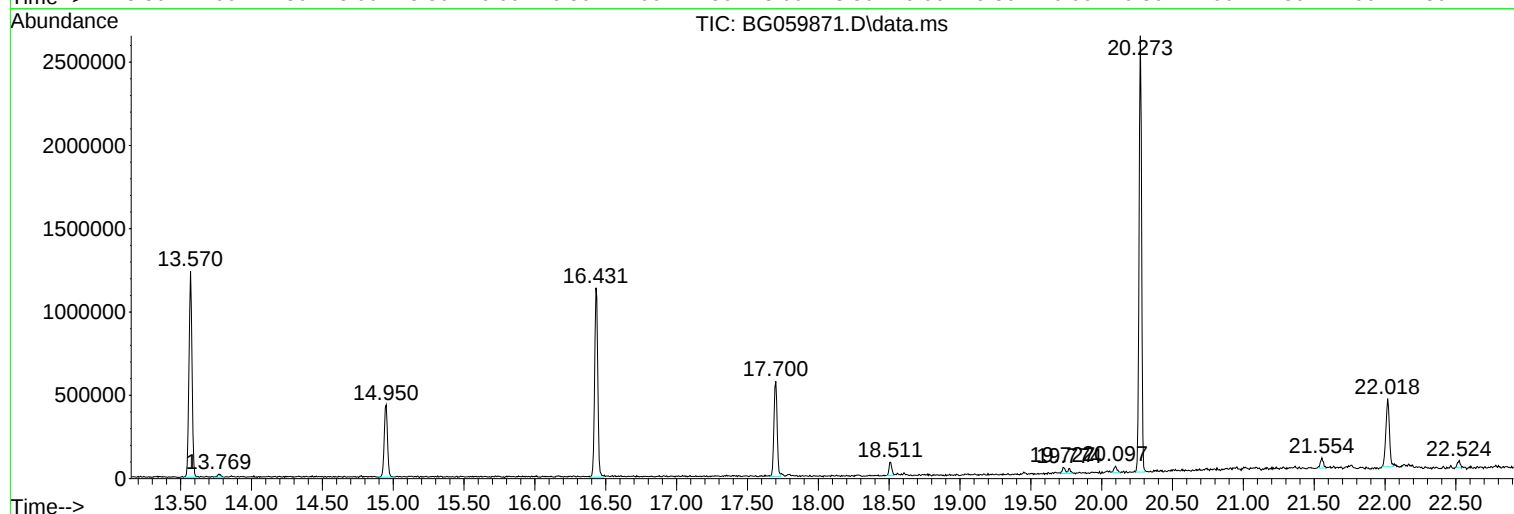
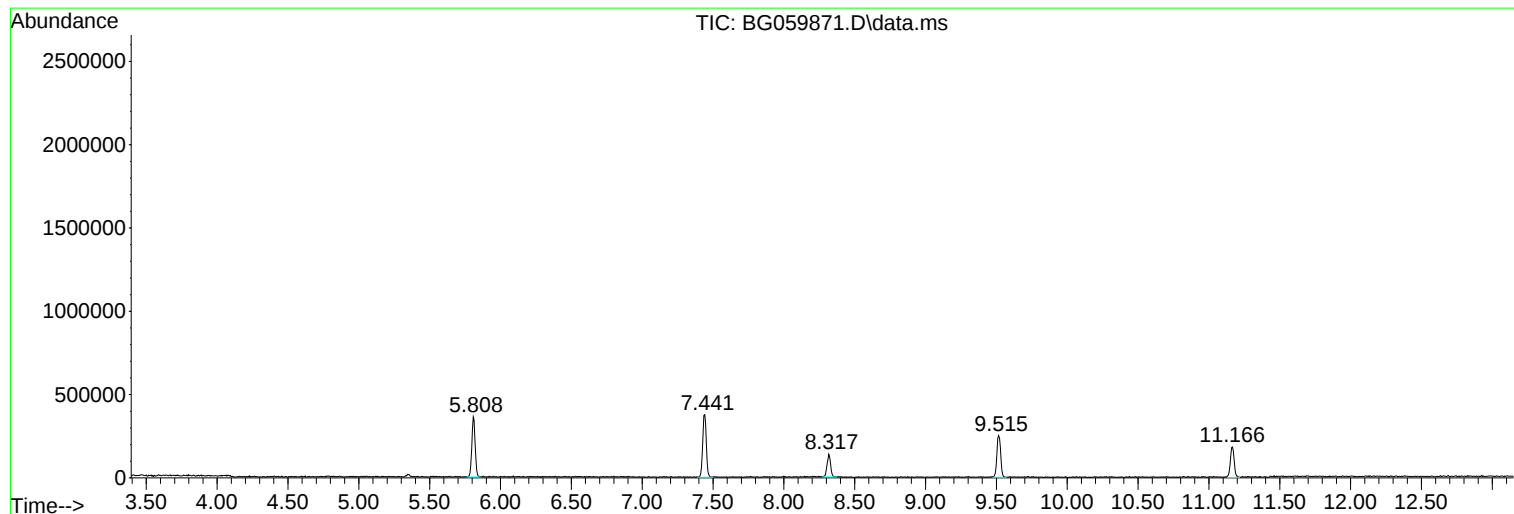
Sum of corrected areas: 12860493

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

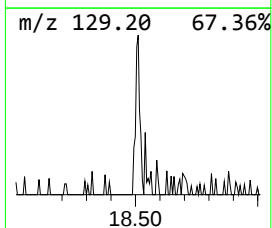
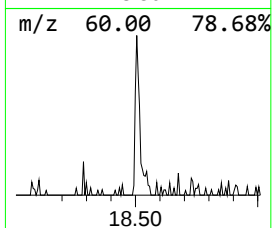
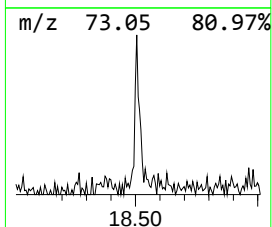
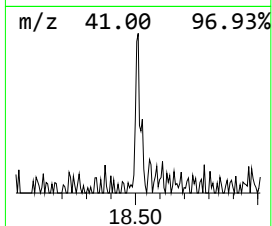
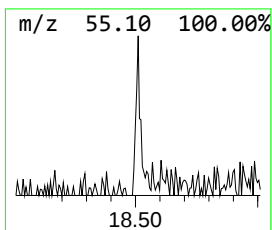
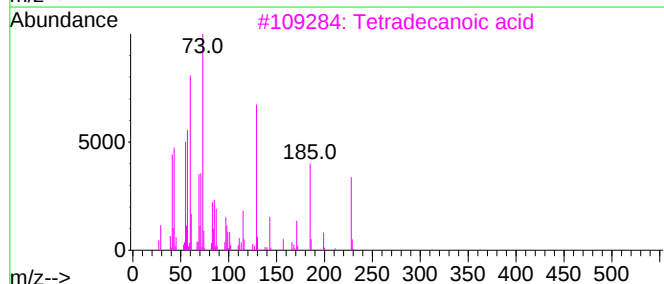
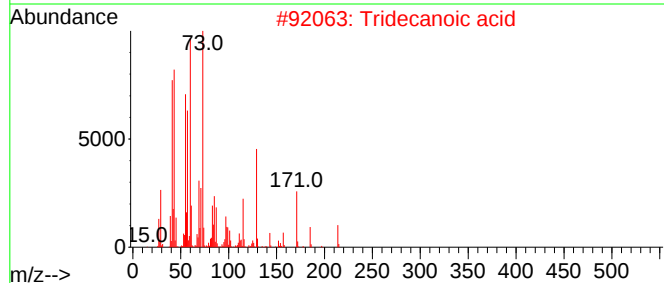
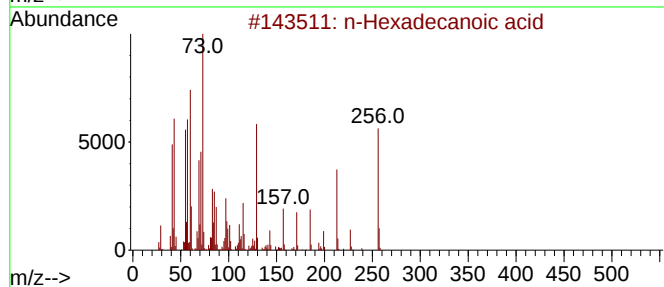
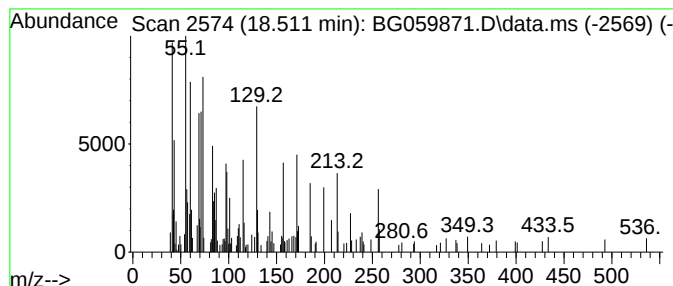
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	2.45 ng	109784	Phenanthrene-d10	17.700

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
2			Tridecanoic acid	214	C13H26O2	000638-53-9	43
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
5			1,2-Benzisothiazole, 3-(hexahydr...	264	C13H16N2O2S	309735-29-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

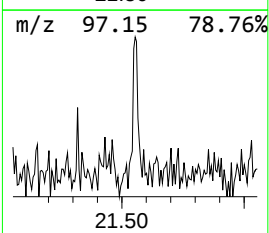
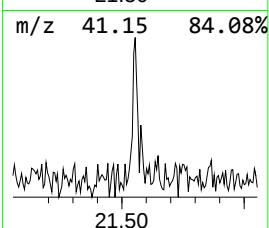
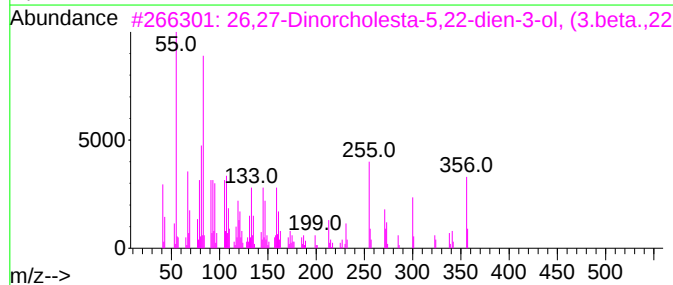
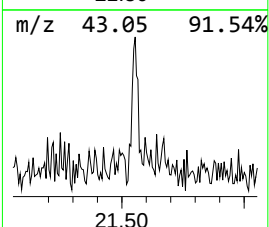
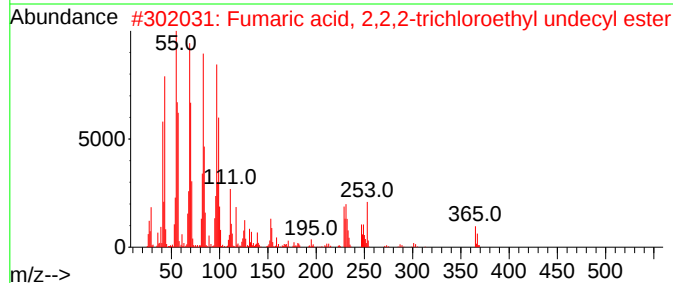
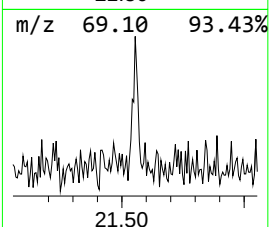
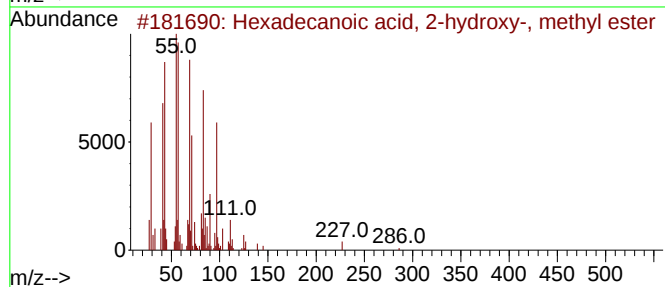
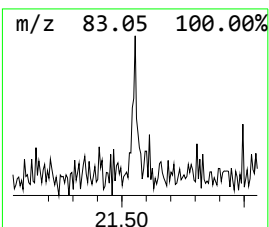
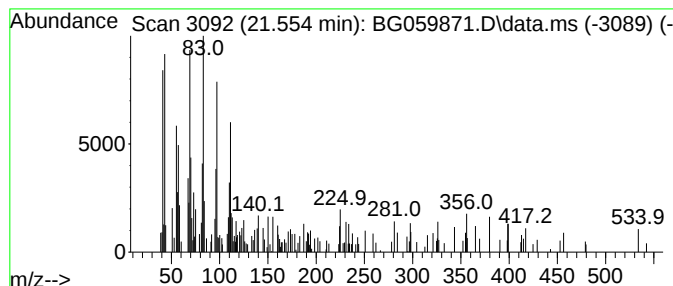
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown21.554 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.554	2.40 ng	85552	Chrysene-d12	22.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	23
2			Fumaric acid, 2,2,2-trichloroeth...	400	C17H27Cl3O4	1000348-50-8	13
3			26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	9
4			2-Bromo-1,1,1-trifluoroethane	162	C2H2BrF3	000421-06-7	9
5			1,1,1,3,3,4,4,4-Octafluoro-2-[3-...	414	C8HF15O2	1000461-21-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

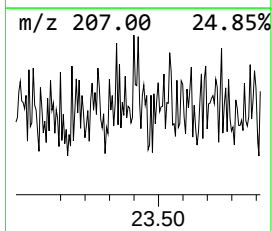
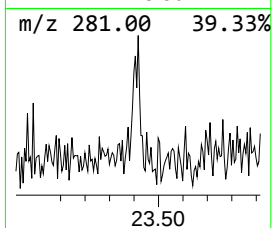
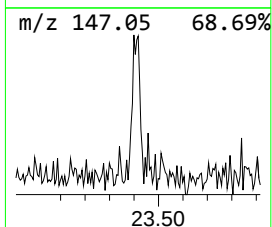
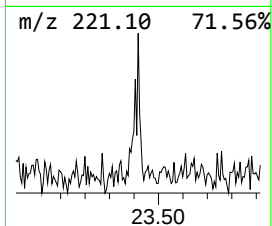
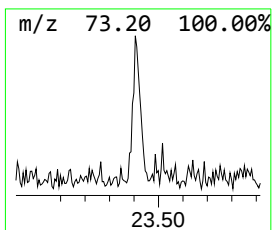
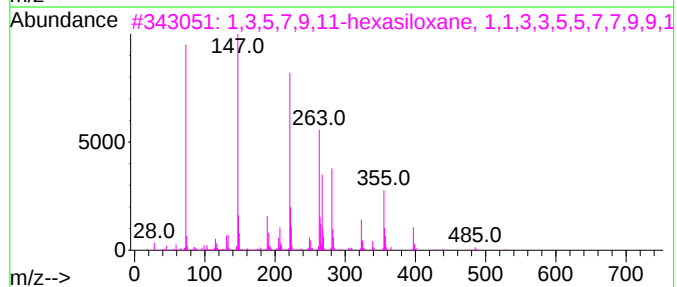
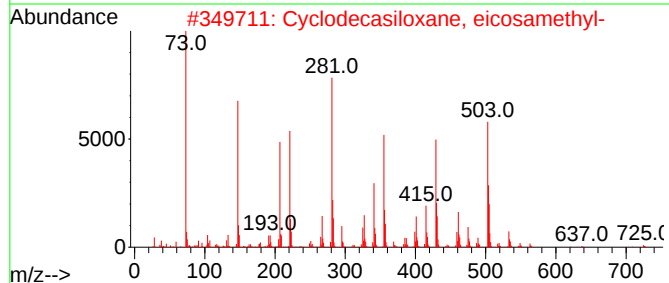
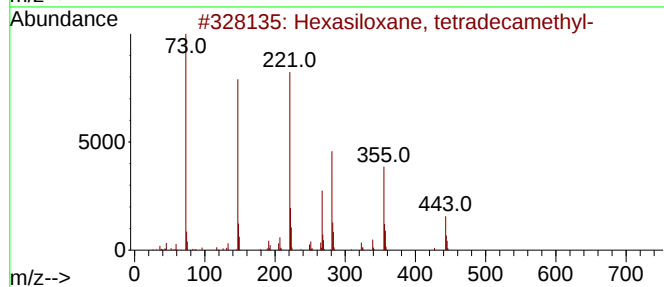
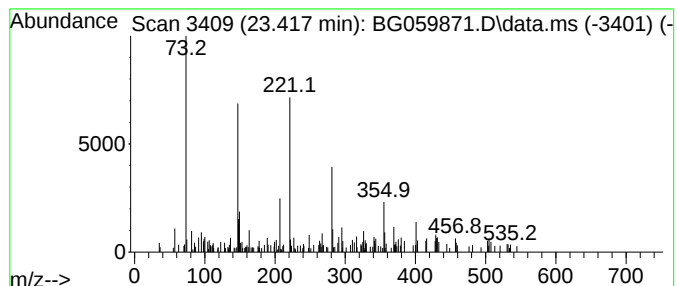
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown23.417 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.417	3.90 ng	139208	Chrysene-d12	22.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	42
2			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	38
3			1,3,5,7,9,11-hexasiloxane, 1,1,3...	542	C20H54O5Si6	1000458-50-7	37
4			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	25
5			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

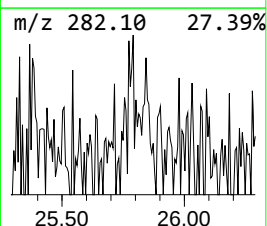
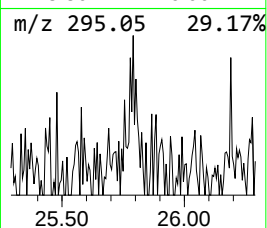
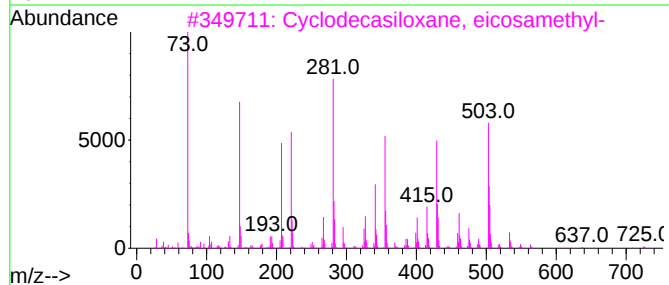
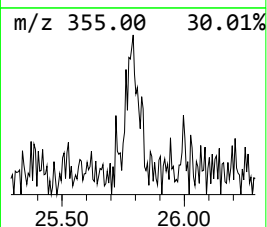
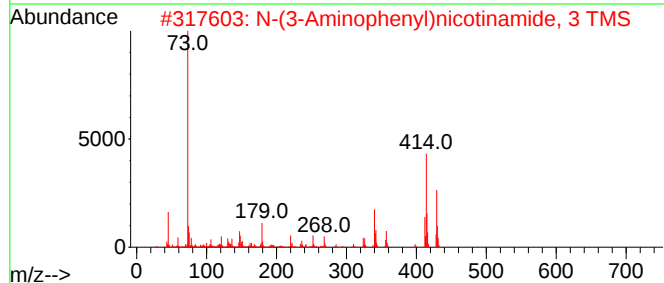
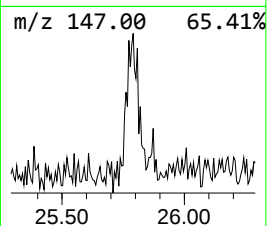
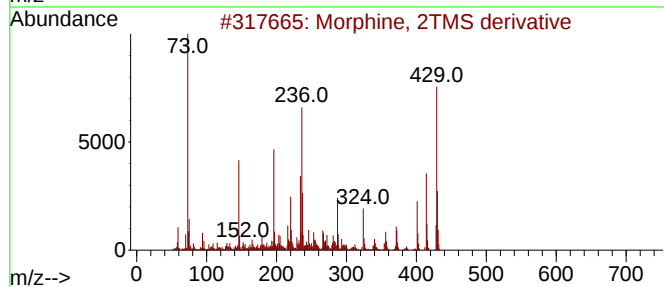
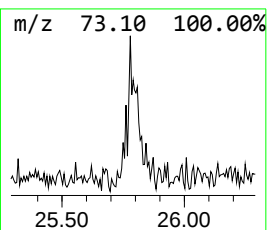
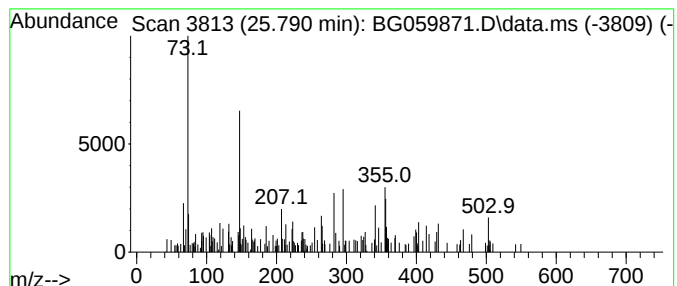
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown25.791 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.791	3.41 ng	123827	Perylene-d12	25.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morphine, 2TMS derivative	429	C23H35NO3Si2	055449-66-6	9
2			N-(3-Aminophenyl)nicotinamide, 3...	429	C21H35N3OSi3	1000470-77-2	9
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	9
4			2-(2-Chloro-acetylamino)-4-(2-ch...	429	C18H21ClN2O3SSi	1010507-75-4	9
5			3-Hydroxy-2,4,6-tribromobenzoic ...	516	C13H19Br3O3Si2	1000500-23-4	8



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059871.D
Acq On : 24 Nov 2023 23:45
Operator : MA/JU
Sample : 05408-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-ELIZABETH-AVE

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 ...	18.511	2.5	ng	109784	4	17.700	895929	20.0
unknown21.554	21.554	2.4	ng	85552	5	22.018	713245	20.0
unknown23.417	23.417	3.9	ng	139208	5	22.018	713245	20.0
unknown25.791	25.791	3.4	ng	123827	6	25.585	726645	20.0