

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
 Data File : BG057922.D
 Acq On : 30 Jun 2023 16:57
 Operator : CG/JU
 Sample : 03376-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-2

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.633	256	263	272	rBV	344980	561838	17.02%	3.277%
2	5.014	323	328	334	rBV2	25733	39406	1.19%	0.230%
3	5.490	401	409	417	rBV	390986	621647	18.83%	3.626%
4	7.077	671	679	687	rBV	247968	420466	12.74%	2.453%
5	7.911	813	821	829	rBV	153129	255532	7.74%	1.491%
6	9.074	1011	1019	1027	rBV	519686	909109	27.54%	5.303%
7	10.714	1291	1298	1306	rBV	221940	396153	12.00%	2.311%
8	13.175	1709	1717	1726	rVB	1336177	2124875	64.37%	12.394%
9	14.550	1945	1951	1960	rVB	405193	640017	19.39%	3.733%
10	14.826	1979	1998	1999	rBV8	17948	63179	1.91%	0.369%
11	15.385	2067	2093	2116	rBV4	335719	2444737	74.06%	14.260%
12	16.037	2197	2204	2213	rBV	1263146	1942284	58.84%	11.329%
13	17.294	2411	2418	2424	rBV	542772	800718	24.26%	4.671%
14	18.176	2559	2568	2578	rBV5	84519	196703	5.96%	1.147%
15	18.728	2655	2662	2669	rBV5	19589	57196	1.73%	0.334%
16	19.456	2782	2786	2794	rVB3	50965	86040	2.61%	0.502%
17	19.727	2829	2832	2839	rVB	35317	56712	1.72%	0.331%
18	19.909	2857	2863	2872	rBV	2468499	3301238	100.00%	19.256%
19	20.015	2876	2881	2886	rVB	70128	116387	3.53%	0.679%
20	20.449	2951	2955	2959	rBV2	22035	36072	1.09%	0.210%
21	21.137	3069	3072	3079	rVB5	29895	50913	1.54%	0.297%
22	21.542	3135	3141	3148	rVB2	503720	794626	24.07%	4.635%
23	21.883	3196	3199	3206	rVB2	38602	67554	2.05%	0.394%
24	22.077	3226	3232	3242	rVB2	97075	211199	6.40%	1.232%
25	22.329	3272	3275	3282	rVB	36649	54571	1.65%	0.318%
26	24.691	3668	3677	3688	rVB	320775	894554	27.10%	5.218%

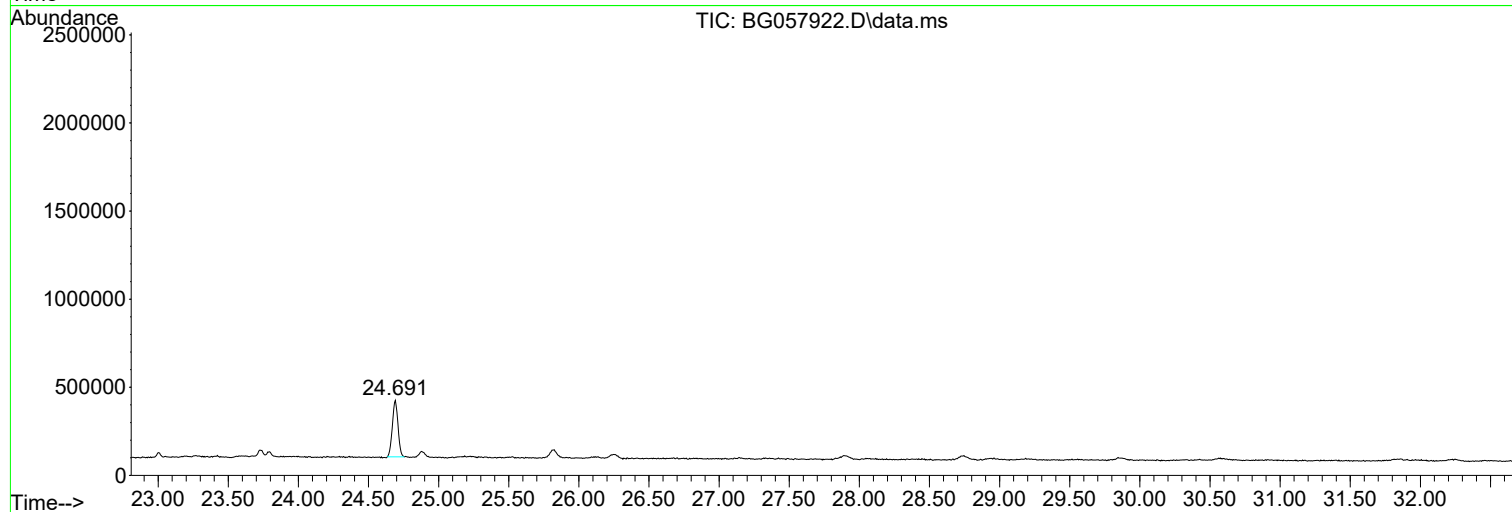
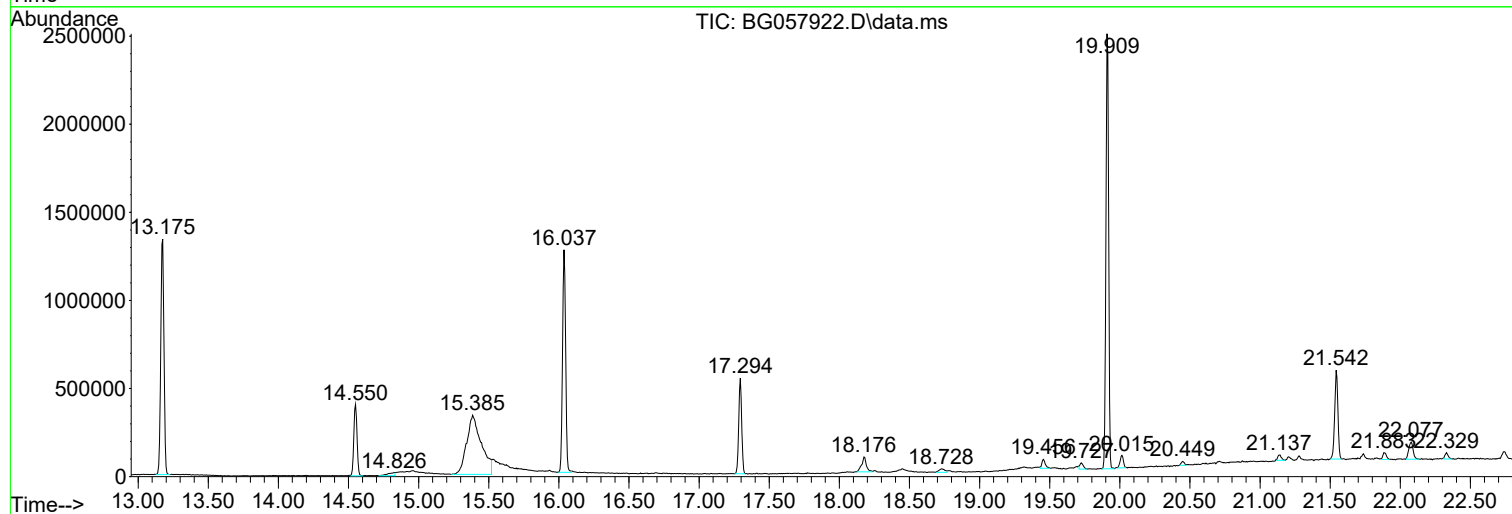
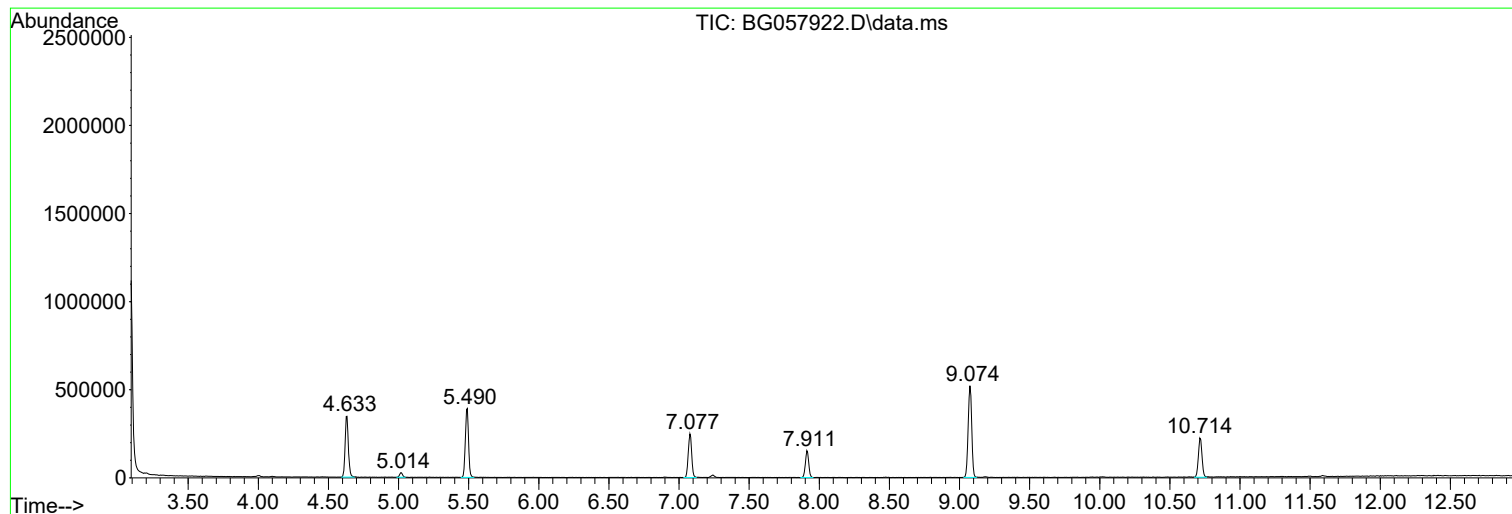
Sum of corrected areas: 17143726

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

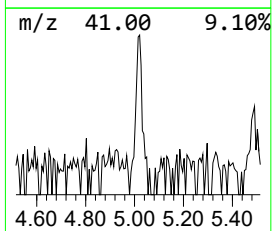
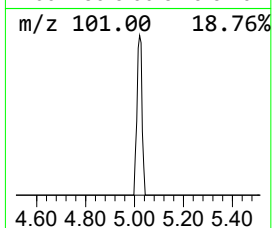
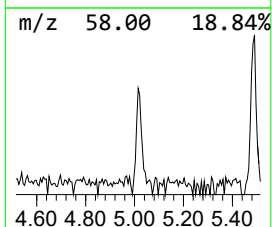
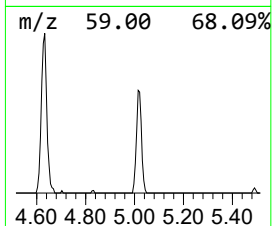
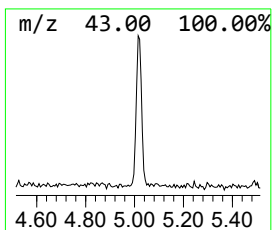
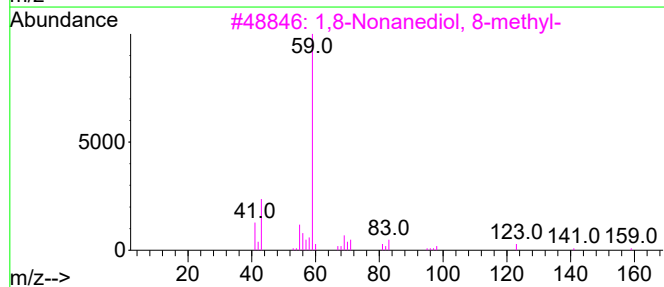
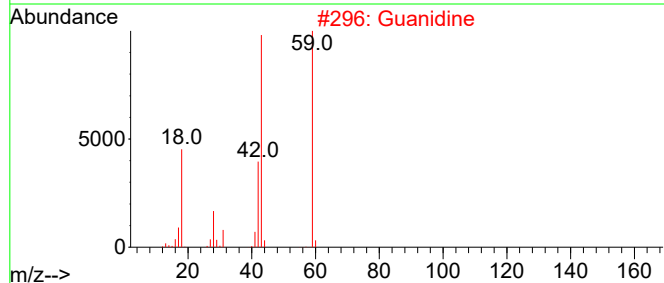
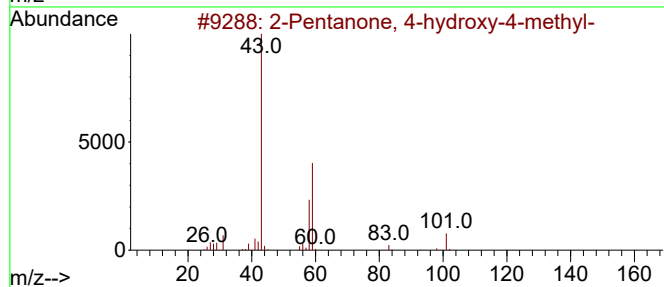
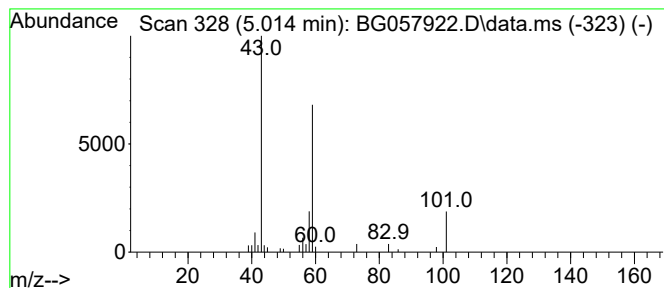
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.014	3.08 ng	39406	1,4-Dichlorobenzene-d4	7.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Guanidine	59	CH5N3	000113-00-8	47		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37		
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
5	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

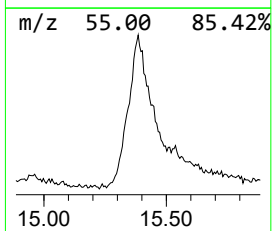
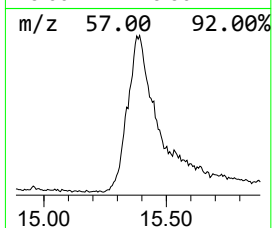
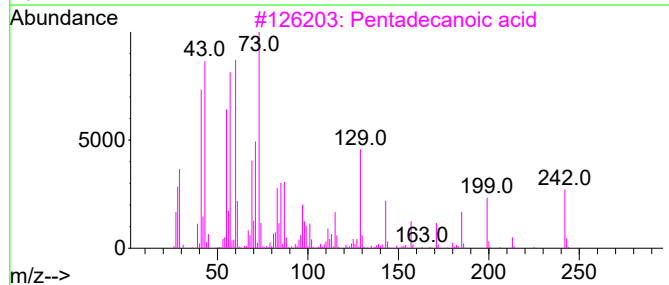
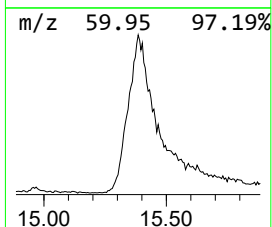
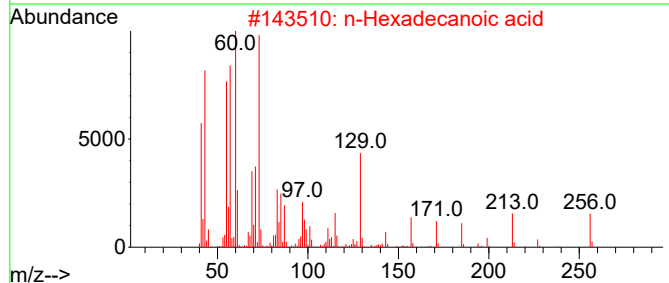
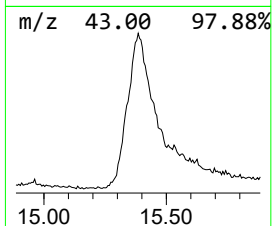
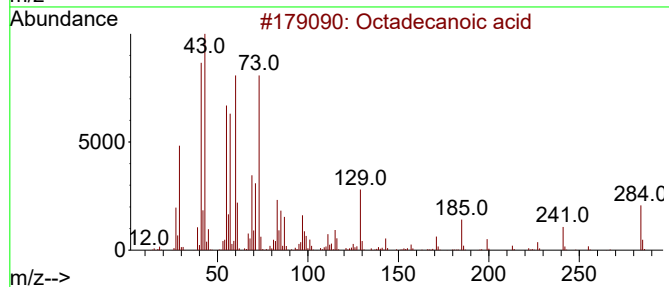
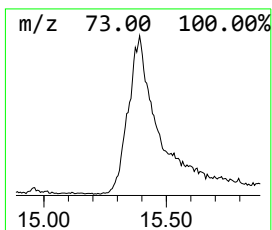
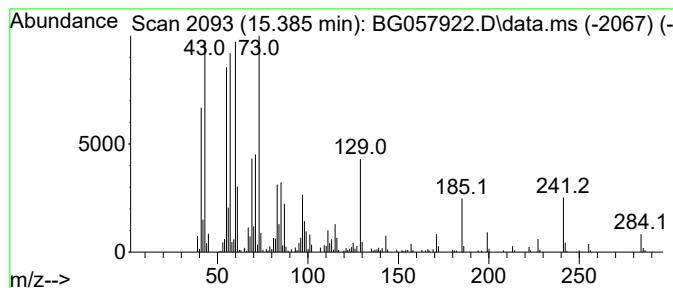
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.385	76.40 ng	2444740	Acenaphthene-d10	14.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

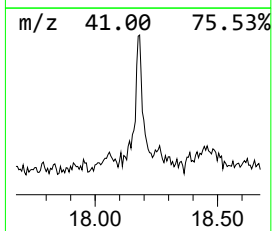
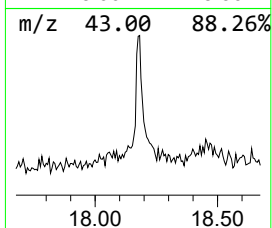
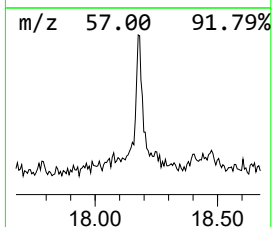
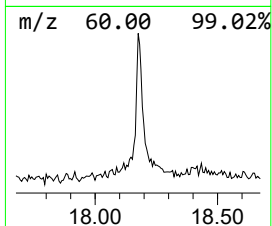
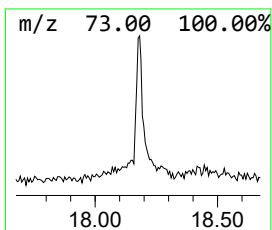
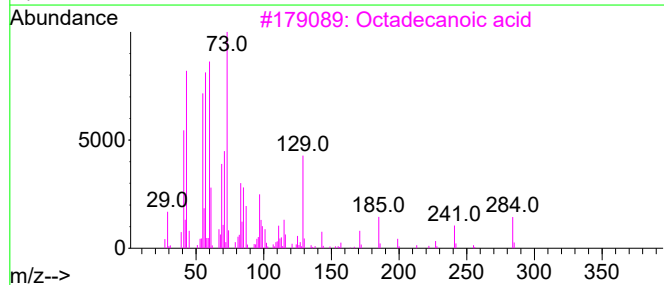
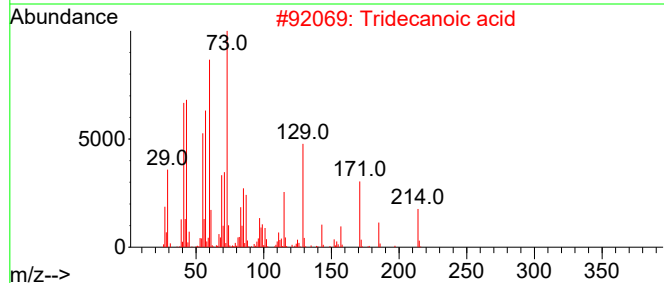
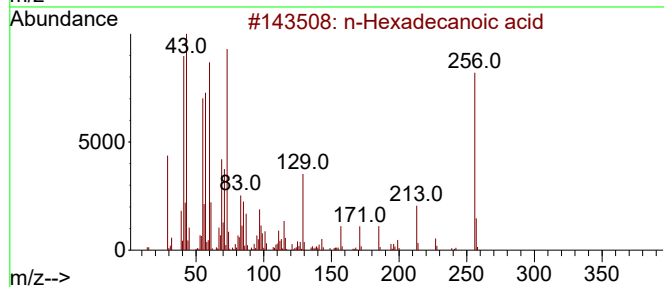
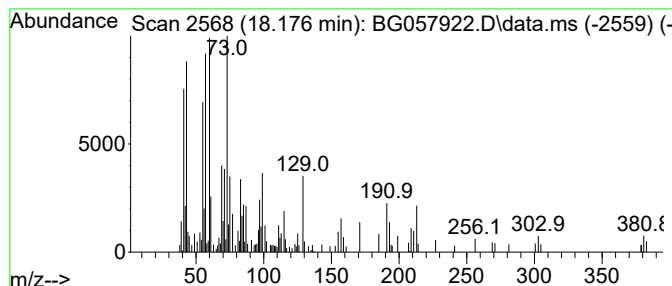
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.176	4.91 ng	196703	Phenanthrene-d10	17.294

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Octadecanoic acid	284	C18H36O2	000057-11-4	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

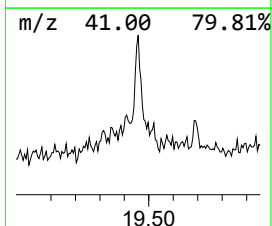
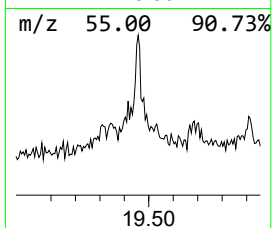
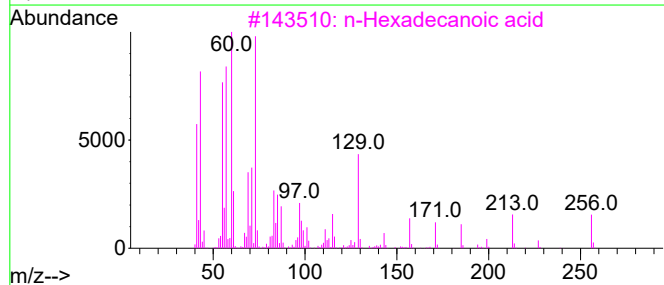
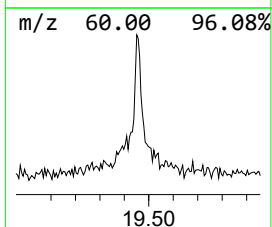
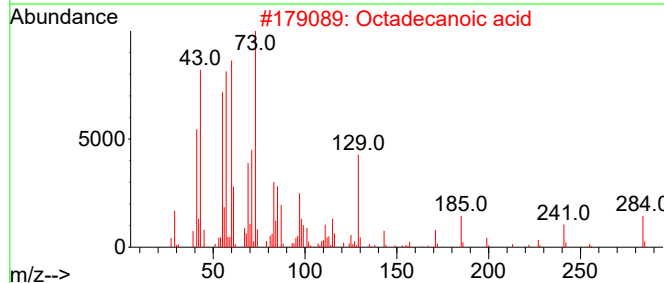
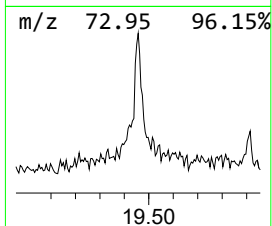
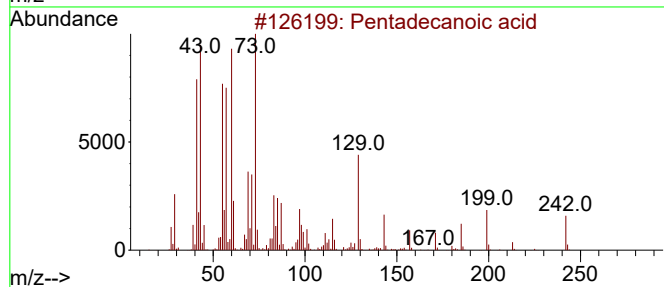
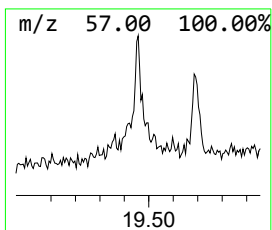
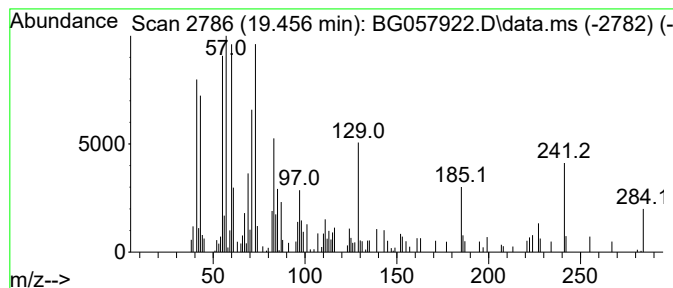
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.456	2.17 ng	86040	Chrysene-d12	21.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			Octadecanoic acid	284	C18H36O2	000057-11-4	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4			Tridecanoic acid	214	C13H26O2	000638-53-9	47
5			Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

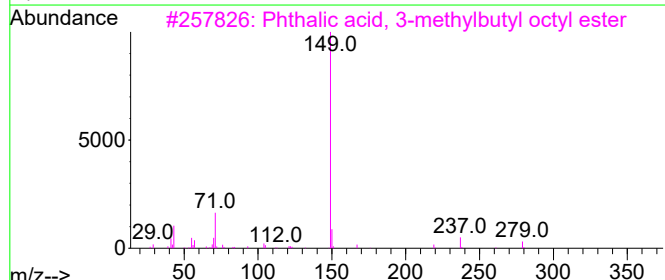
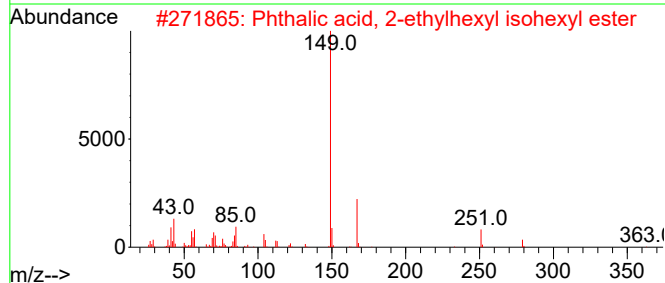
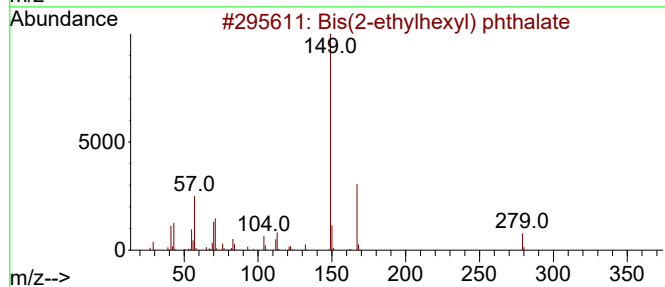
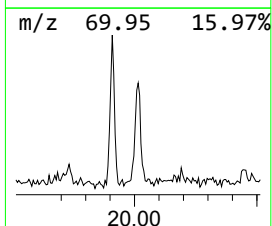
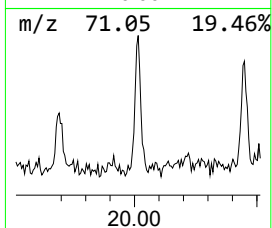
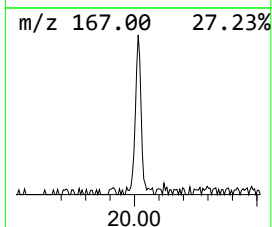
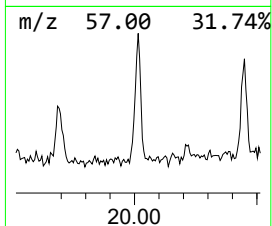
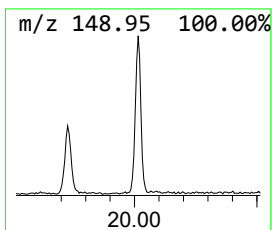
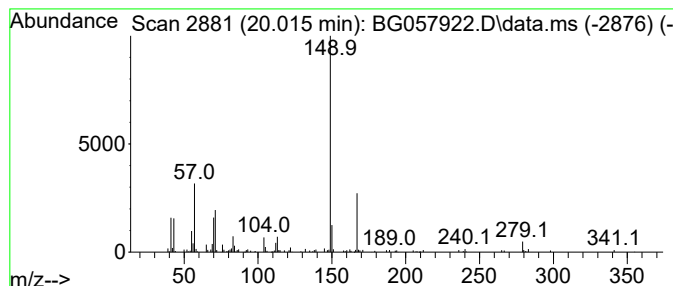
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phthalic acid, 2-ethylhexyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.015	2.93 ng	116387	Chrysene-d12	21.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	83
2			Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	72
3			Phthalic acid, 3-methylbutyl oct...	348	C21H32O4	1000356-80-9	64
4			1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	64
5			Phthalic acid, di(2-methylbutyl)...	306	C18H26O4	1000322-82-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

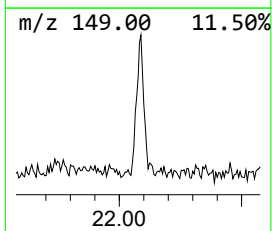
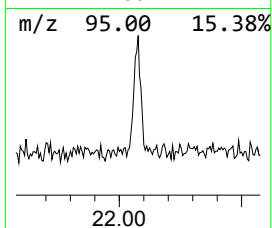
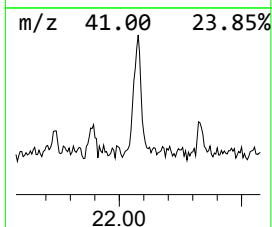
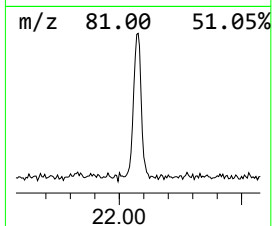
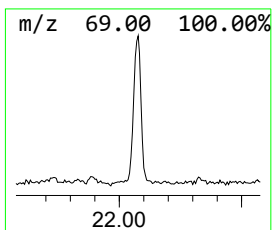
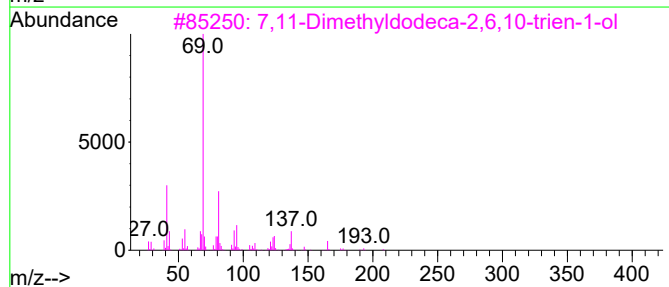
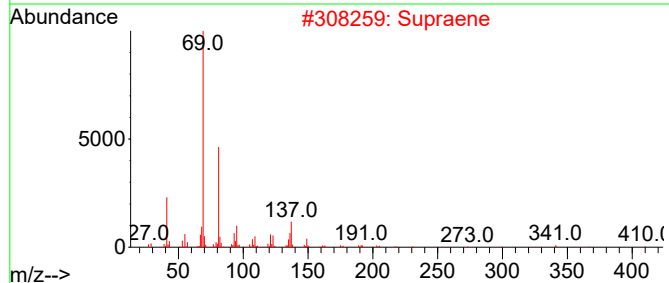
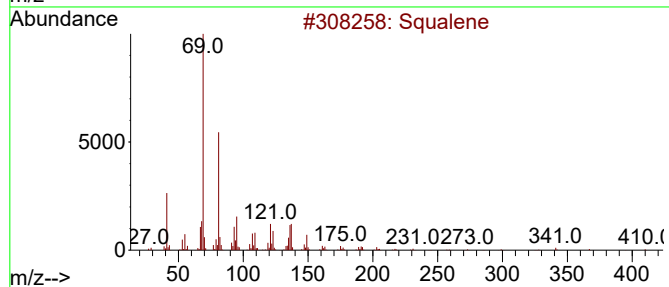
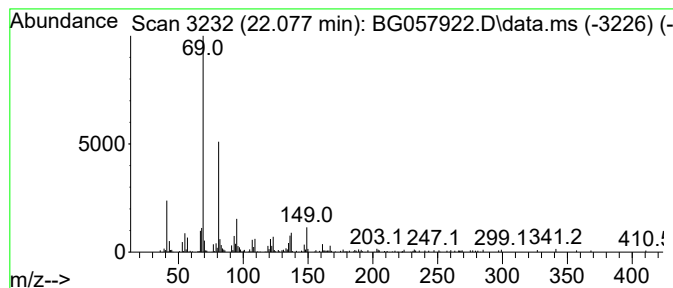
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.077	5.32 ng	211199	Chrysene-d12	21.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	94
2			Supraene	410	C30H50	007683-64-9	93
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
4			1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	53
5			Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057922.D
Acq On : 30 Jun 2023 16:57
Operator : CG/JU
Sample : 03376-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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
2-Pentanone, 4-...	5.014	3.1	ng	39406	1	7.911	255532	20.0
Octadecanoic acid	15.385	76.4	ng	2444740	3	14.550	640017	20.0
n-Hexadecanoic ...	18.176	4.9	ng	196703	4	17.294	800718	20.0
Pentadecanoic acid	19.456	2.2	ng	86040	5	21.542	794626	20.0
Phthalic acid, ...	20.015	2.9	ng	116387	5	21.542	794626	20.0
Squalene	22.077	5.3	ng	211199	5	21.542	794626	20.0