

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
 Data File : BG048406.D
 Acq On : 17 Mar 2021 20:30
 Operator : CG/JU
 Sample : M1692-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FK-GF-02-069-A

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-BG031621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.421	9	14	24	rVB3	19057	40776	1.17%	0.175%
2	5.195	309	316	323	rVB	43846	69563	2.00%	0.299%
3	5.665	388	396	407	rVB	1098608	1807114	51.95%	7.770%
4	7.258	658	667	677	rBV	1201410	2095358	60.24%	9.009%
5	8.116	806	813	820	rBV	282715	459424	13.21%	1.975%
6	9.279	1002	1011	1019	rBV	751917	1346440	38.71%	5.789%
7	10.936	1282	1293	1300	rBV	368580	644158	18.52%	2.770%
8	13.380	1702	1709	1716	rVB	1727373	2766964	79.54%	11.896%
9	14.197	1841	1848	1854	rBV	104165	152657	4.39%	0.656%
10	14.755	1936	1943	1950	rVB	562376	878687	25.26%	3.778%
11	16.241	2188	2196	2203	rBV	1495813	2317971	66.64%	9.966%
12	17.234	2360	2365	2370	rBV9	20934	39952	1.15%	0.172%
13	17.505	2404	2411	2415	rBV	665670	1018390	29.28%	4.379%
14	17.546	2415	2418	2425	rVV	125774	186600	5.36%	0.802%
15	17.634	2427	2433	2438	rVB	39506	80414	2.31%	0.346%
16	18.380	2555	2560	2566	rBV	242982	355993	10.23%	1.531%
17	18.427	2566	2568	2573	rVB2	45026	56168	1.61%	0.241%
18	18.580	2587	2594	2597	rBV4	50811	105466	3.03%	0.453%
19	18.991	2660	2664	2669	rVB2	43757	63014	1.81%	0.271%
20	19.156	2689	2692	2698	rVB3	64823	88898	2.56%	0.382%
21	19.555	2754	2760	2765	rBV	456382	656746	18.88%	2.824%
22	19.649	2773	2776	2780	rBV4	67721	97212	2.79%	0.418%
23	19.884	2812	2816	2817	rBV	62160	76573	2.20%	0.329%
24	19.913	2817	2821	2828	rVB	344446	482154	13.86%	2.073%
25	20.113	2848	2855	2860	rBV	2741802	3478585	100.00%	14.956%
26	20.225	2872	2874	2876	rBV3	30087	37351	1.07%	0.161%
27	20.501	2918	2921	2925	rBV	44922	58186	1.67%	0.250%
28	21.423	3074	3078	3088	rVB6	225666	416057	11.96%	1.789%
29	21.512	3089	3093	3098	rVB	131474	191292	5.50%	0.822%
30	21.794	3133	3141	3146	rBV2	662850	1445339	41.55%	6.214%
31	21.841	3146	3149	3158	rVB	178423	311219	8.95%	1.338%
32	24.067	3523	3528	3538	rBV	131823	448083	12.88%	1.927%
33	25.143	3702	3711	3719	rBV3	340656	985985	28.34%	4.239%

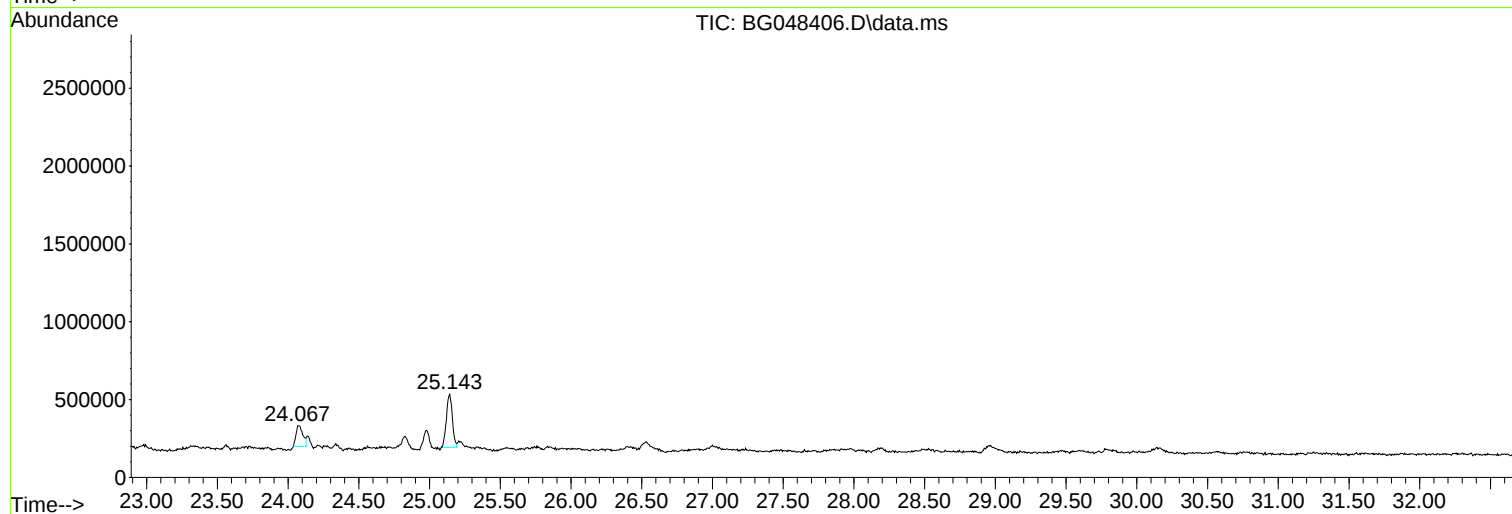
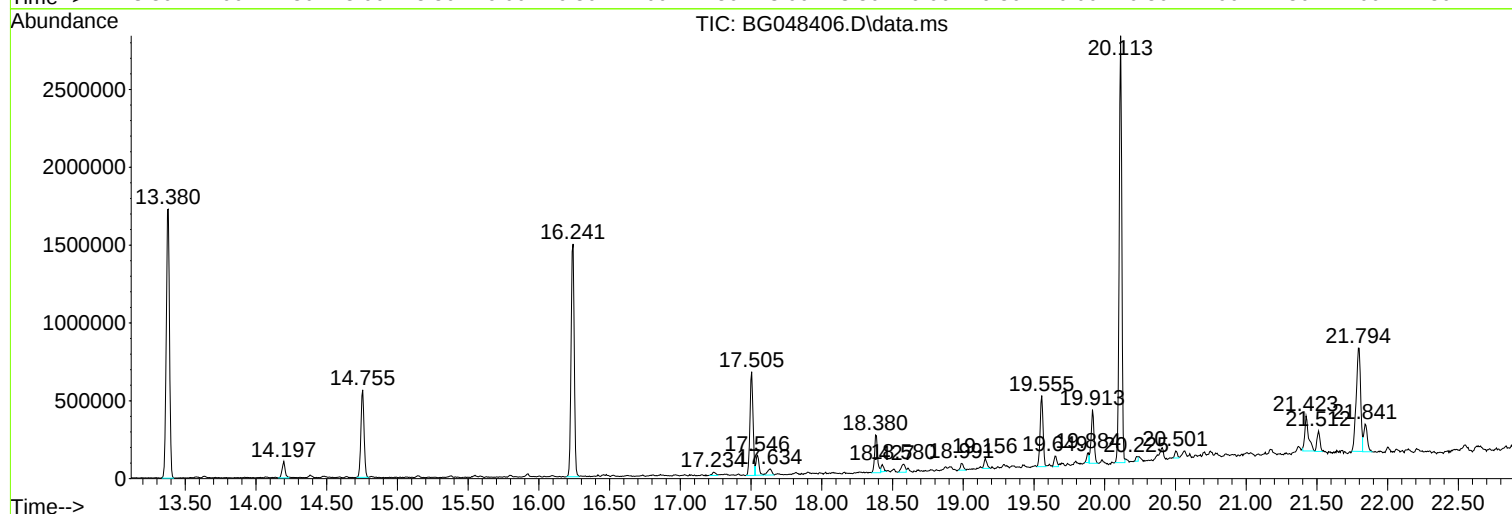
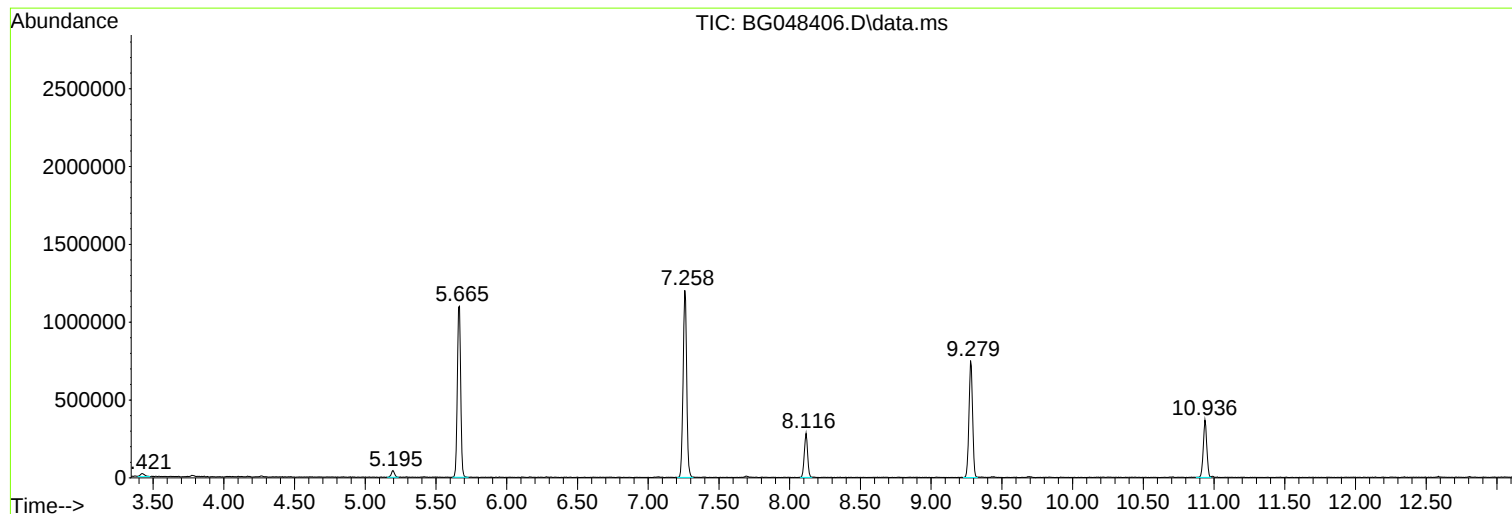
Sum of corrected areas: 23258789

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

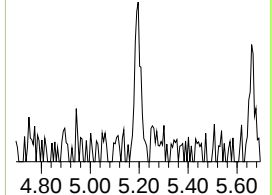
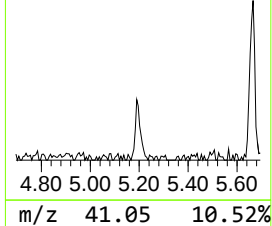
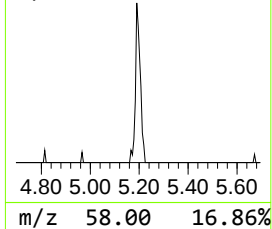
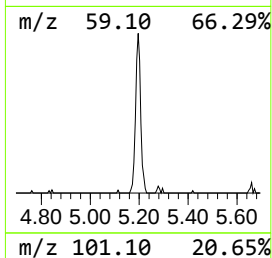
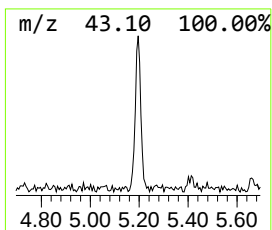
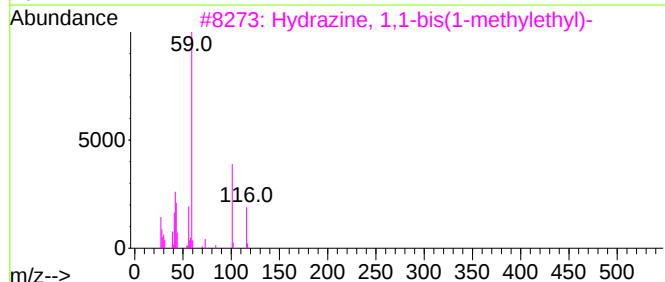
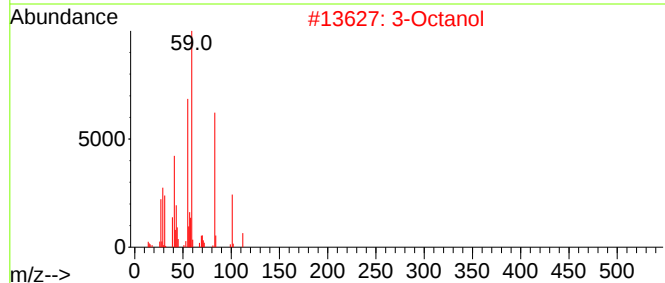
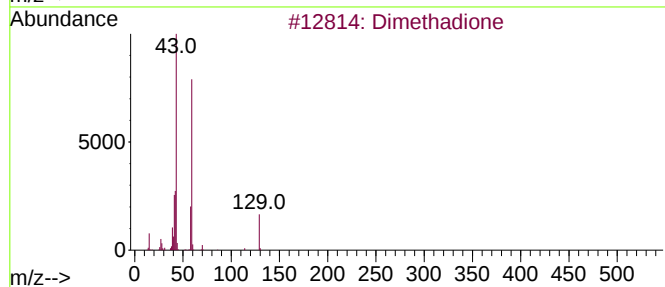
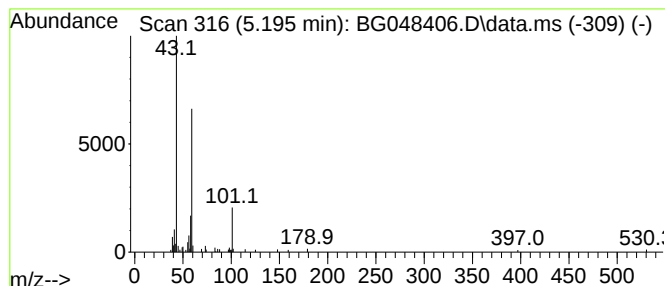
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.195 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	3.03 ng	69563	1,4-Dichlorobenzene-d4	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethadione	129	C5H7NO3	000695-53-4	36
2			3-Octanol	130	C8H18O	000589-98-0	33
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5			4,5-Dimethyl-3-heptanol	144	C9H20O	019549-76-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

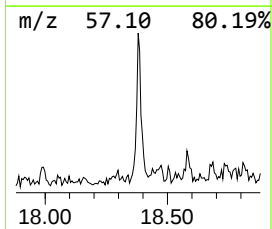
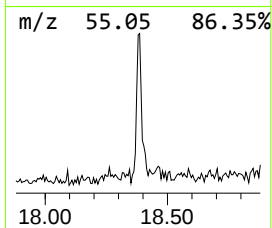
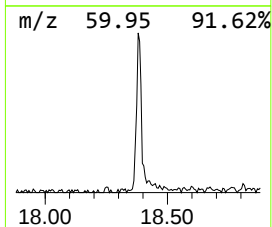
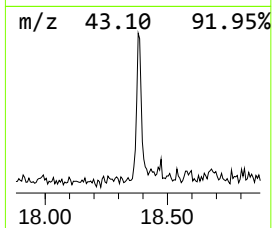
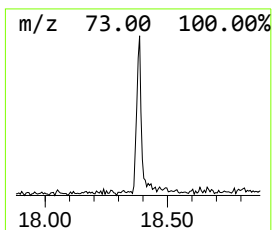
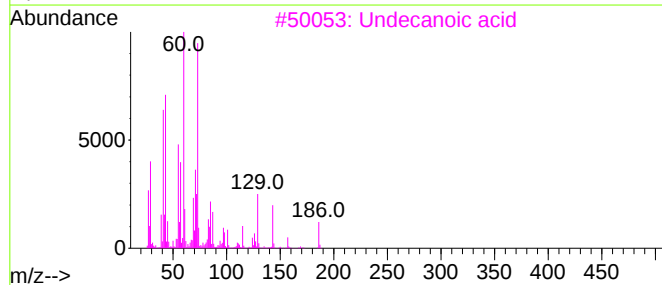
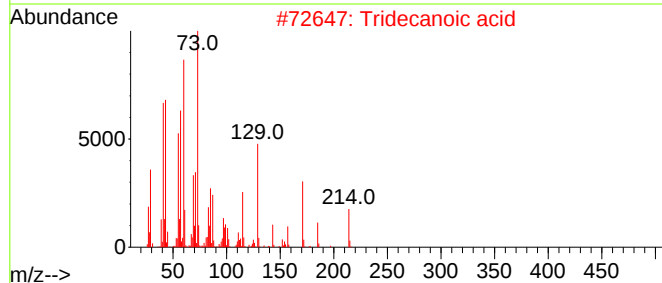
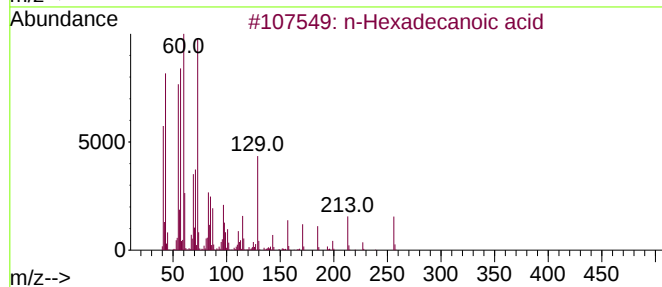
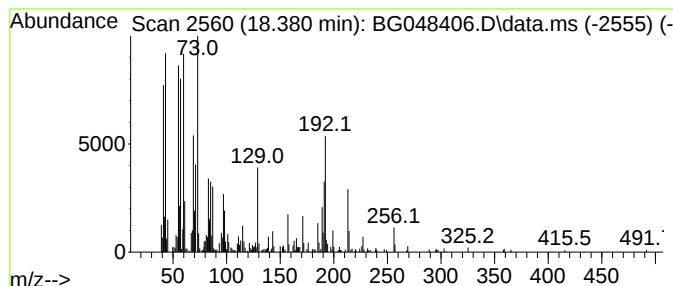
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	6.99 ng	355993	Phenanthrene-d10	17.505

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			Undecanoic acid	186	C11H22O2	000112-37-8	45
4			Octadecanoic acid	284	C18H36O2	000057-11-4	43
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

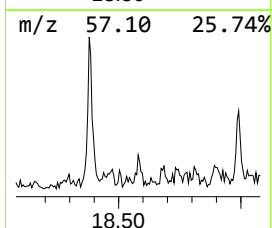
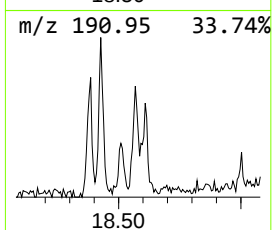
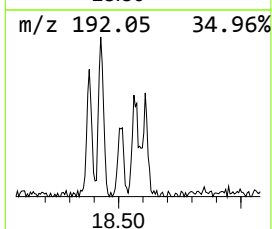
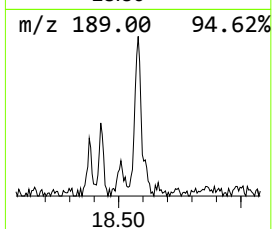
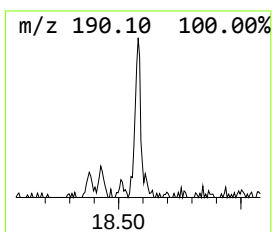
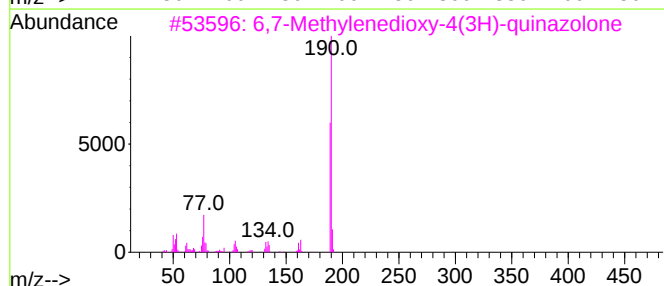
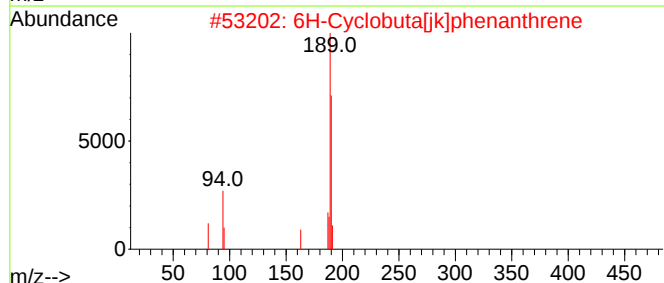
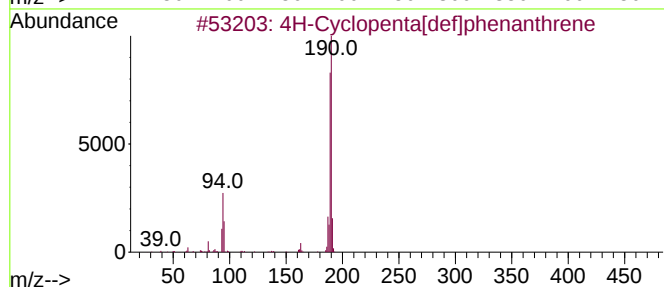
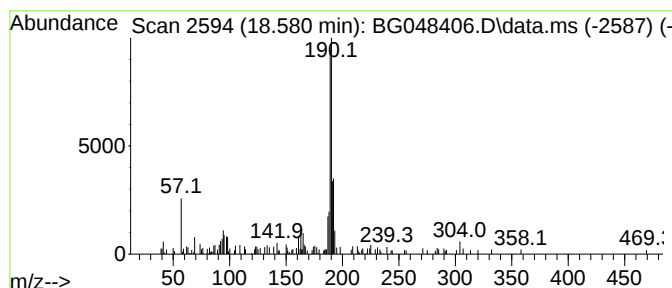
Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.580	2.07 ng	105466	Phenanthrene-d10		17.505	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	59
2	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	59
3	6,7-Methylenedioxy-4(3H)-quinazo...		190	C9H6N2O3	028310-11-4	43
4	4-(4-Methyl-piperidin-1-yl)-phen...		190	C12H18N2	342013-25-6	40
5	Pyrimidine, 2-chloro-5-phenyl-		190	C10H7ClN2	022536-62-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

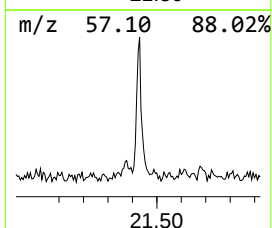
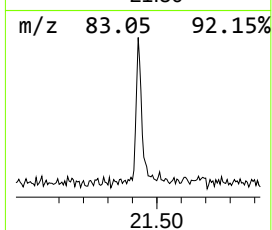
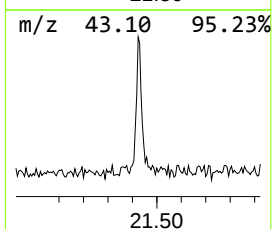
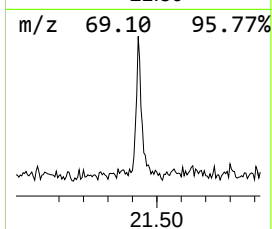
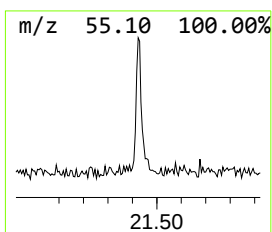
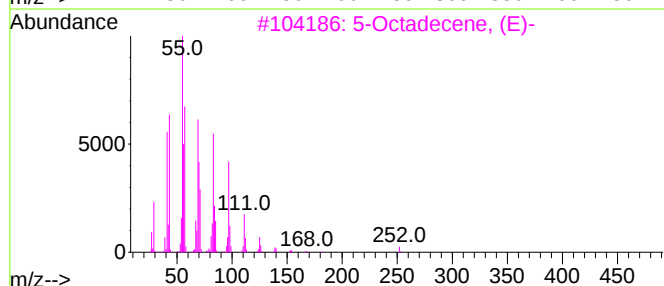
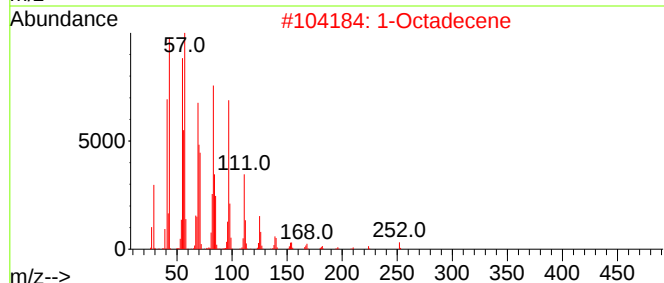
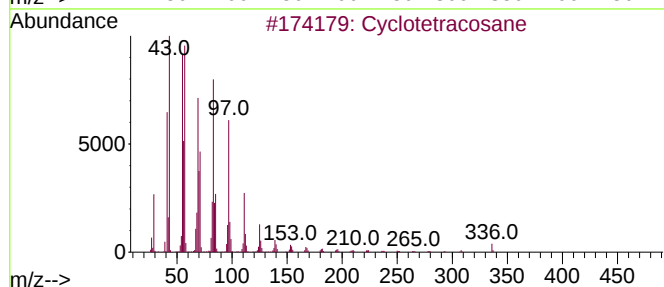
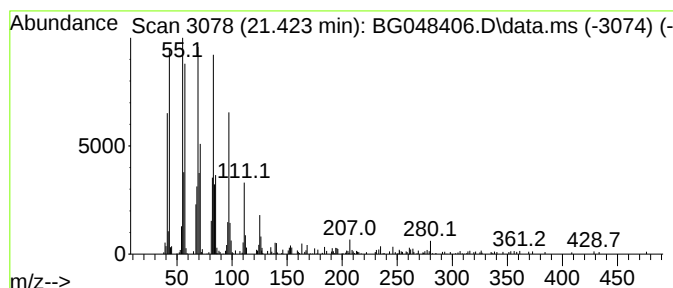
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.424	5.76 ng	416057	Chrysene-d12	21.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	98
2			1-Octadecene	252	C18H36	000112-88-9	94
3			5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4			3-Octadecene, (E)-	252	C18H36	007206-19-1	93
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

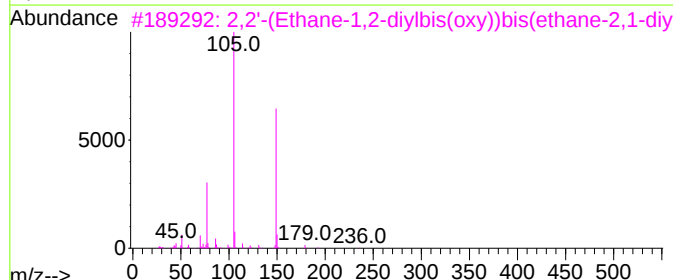
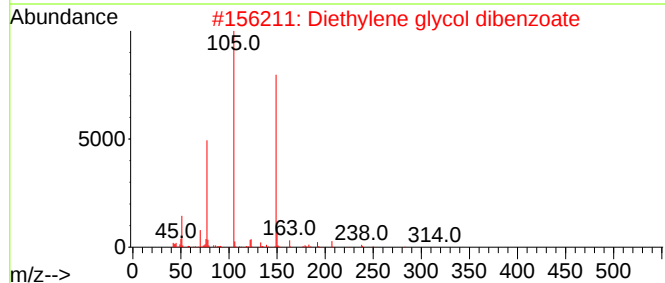
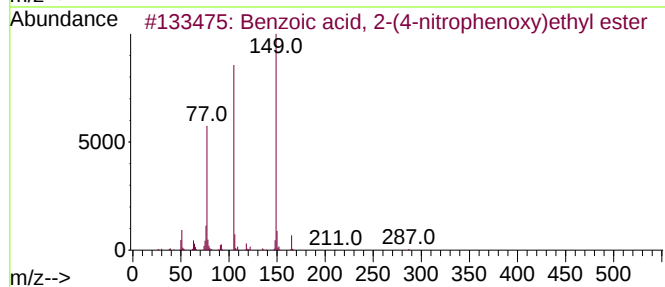
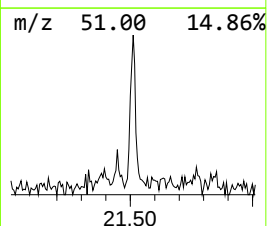
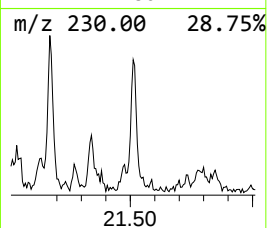
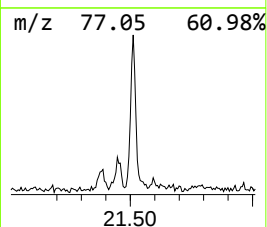
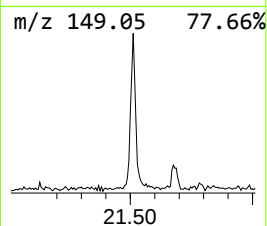
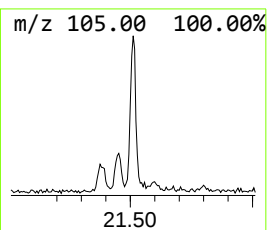
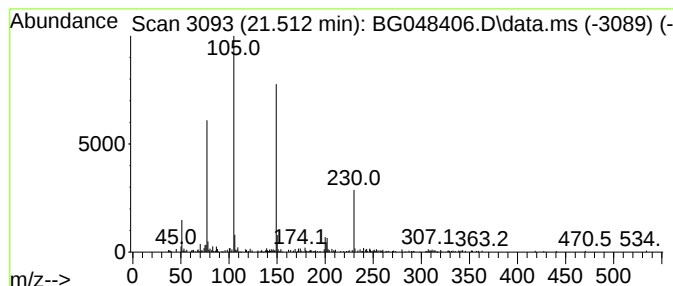
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzoic acid, 2-(4-nitrophe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.512	2.65 ng	191292	Chrysene-d12	21.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	76
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50
4			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
5			3-Benzoyl-2-t-butyl-4-methyl-4-v...	287	C17H21NO3	109918-61-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048406.D
Acq On : 17 Mar 2021 20:30
Operator : CG/JU
Sample : M1692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-069-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.195	5.195	3.0	ng	69563	1	8.116	459424	20.0
n-Hexadecanoic ...	18.380	7.0	ng	355993	4	17.505	1018390	20.0
4H-Cyclopenta[d...]	18.580	2.1	ng	105466	4	17.505	1018390	20.0
Cyclotetracosane	21.424	5.8	ng	416057	5	21.799	1445340	20.0
Benzoic acid, 2...	21.512	2.6	ng	191292	5	21.799	1445340	20.0