

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
 Data File : BG048865.D
 Acq On : 23 Apr 2021 16:10
 Operator : CG/JU
 Sample : M2119-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 352

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048865.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.608	379	386	395	rVB	307526	496504	53.10%	7.044%
2	7.218	654	660	672	rVB	325800	564067	60.33%	8.002%
3	8.052	796	802	809	rBV2	107434	175282	18.75%	2.487%
4	9.227	995	1002	1012	rVB	208000	373924	39.99%	5.305%
5	10.878	1275	1283	1292	rBV	136848	243270	26.02%	3.451%
6	13.076	1650	1657	1659	rBV7	9412	16509	1.77%	0.234%
7	13.158	1666	1671	1675	rBV7	11315	17833	1.91%	0.253%
8	13.334	1692	1701	1708	rBV	483878	772927	82.66%	10.965%
9	13.493	1720	1728	1736	rBV	24224	73917	7.91%	1.049%
10	13.587	1743	1744	1749	rBV5	10127	11443	1.22%	0.162%
11	14.022	1816	1818	1822	rBV5	11108	16942	1.81%	0.240%
12	14.133	1833	1837	1842	rBV5	61353	122522	13.10%	1.738%
13	14.233	1851	1854	1860	rBV7	21801	37178	3.98%	0.527%
14	14.451	1887	1891	1897	rBV6	48524	98050	10.49%	1.391%
15	14.545	1902	1907	1912	rVB2	121977	203938	21.81%	2.893%
16	14.621	1913	1920	1924	rBV10	24657	68133	7.29%	0.967%
17	14.686	1924	1931	1932	rBV5	60213	118336	12.66%	1.679%
18	14.715	1932	1936	1942	rVB3	217811	392400	41.97%	5.567%
19	15.220	2018	2022	2026	rBV5	52900	84383	9.02%	1.197%
20	15.426	2055	2057	2063	rVB7	46393	71891	7.69%	1.020%
21	15.502	2065	2070	2074	rBV5	126110	211035	22.57%	2.994%
22	16.213	2186	2191	2195	rBV	335644	473299	50.62%	6.714%
23	16.436	2225	2229	2233	rVB2	185884	258656	27.66%	3.669%
24	17.476	2401	2406	2411	rBV	245112	409806	43.83%	5.814%
25	20.085	2846	2850	2857	rVB	706987	935041	100.00%	13.265%
26	21.384	3068	3071	3077	rVB7	64522	90677	9.70%	1.286%
27	21.771	3132	3137	3142	rVB	205895	336010	35.94%	4.767%
28	25.103	3696	3704	3714	rVB3	119801	352714	37.72%	5.004%
29	29.127	4386	4389	4390	rBV3	8051	9804	1.05%	0.139%
30	30.984	4702	4705	4707	rBV4	11622	12475	1.33%	0.177%

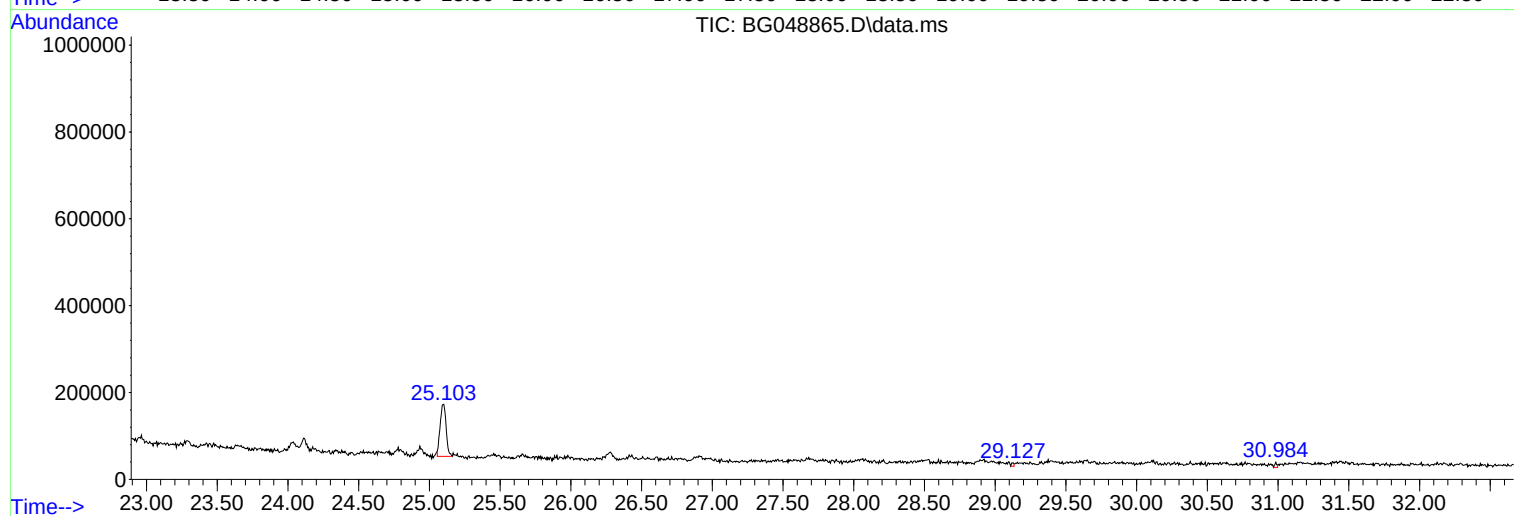
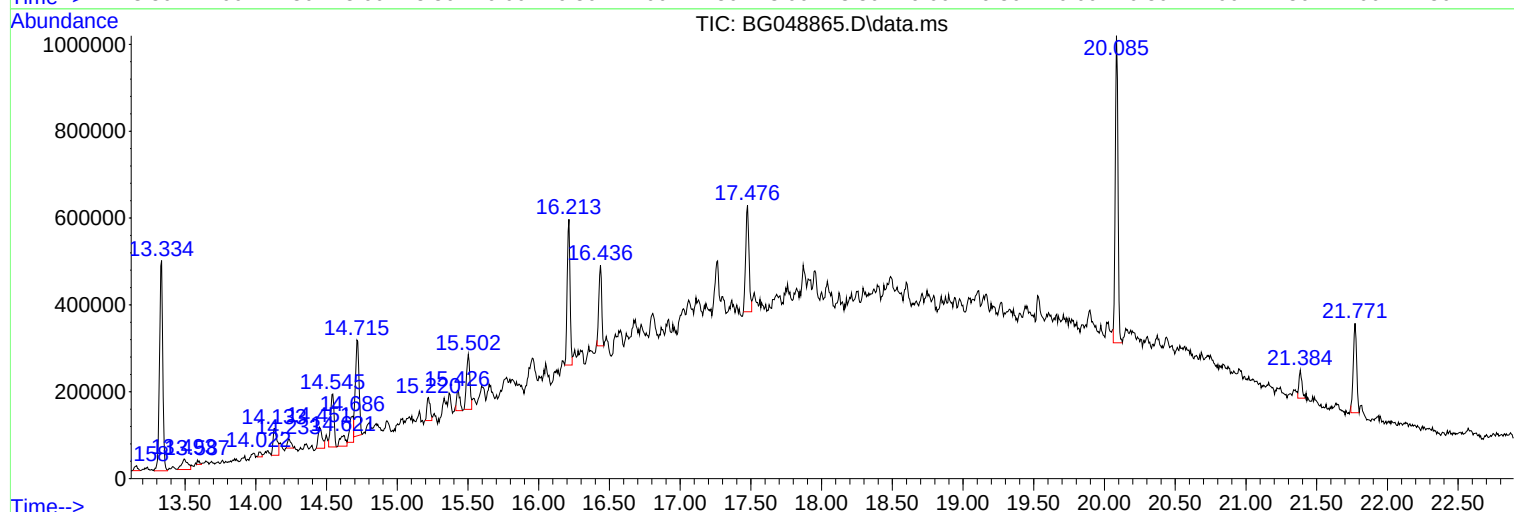
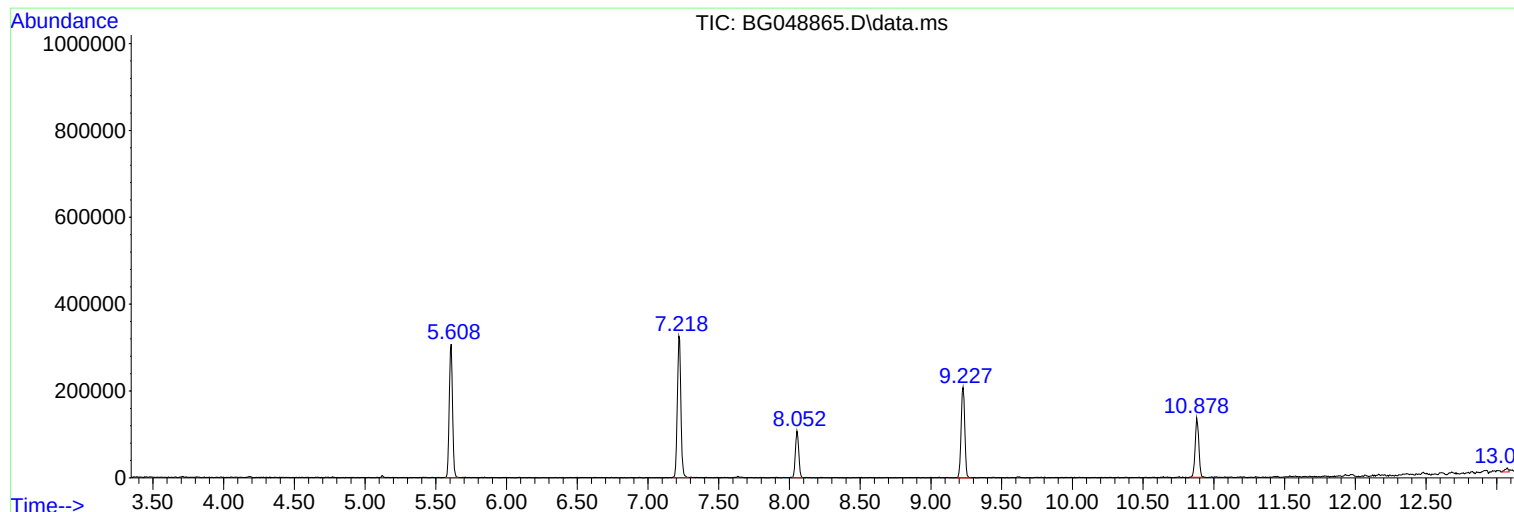
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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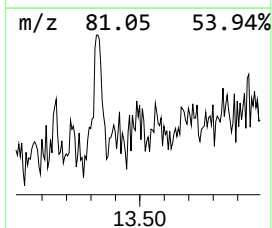
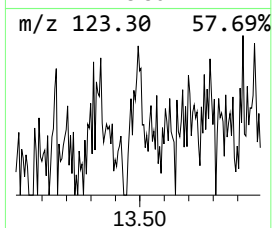
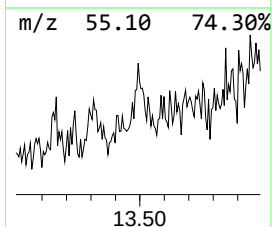
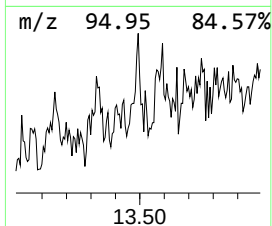
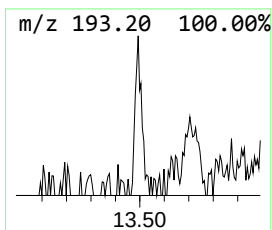
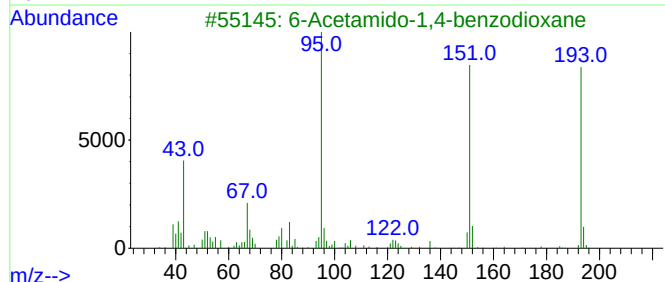
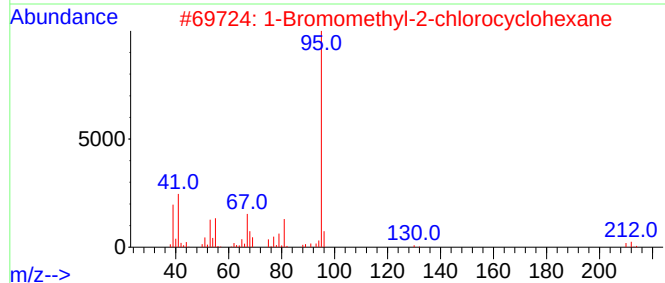
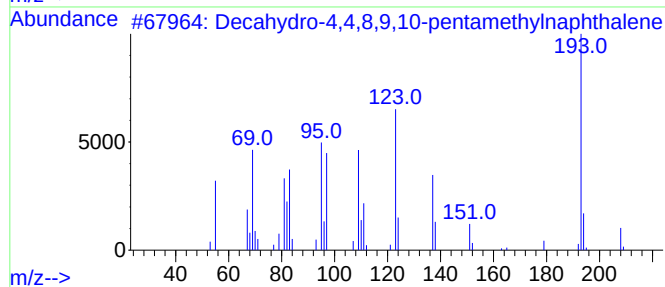
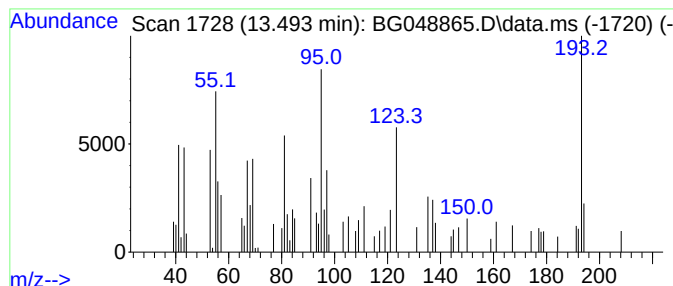
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown13.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.493	3.77 ng	73917	Acenaphthene-d10	14.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	46
2			1-Bromomethyl-2-chlorocyclohexane	210	C7H12BrCl	090009-23-7	38
3			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	25
4			2-Furanmethanamine, N-(2-furanyl...	177	C10H11NO2	018240-50-1	22
5			Bicyclo[3.2.2]non-3-en-2-one, 6,...	150	C9H10O2	1000155-95-4	22



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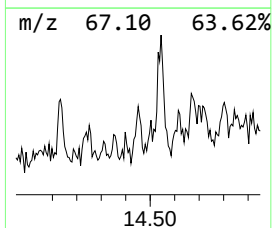
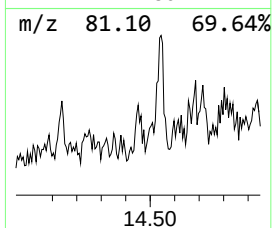
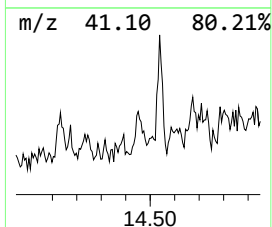
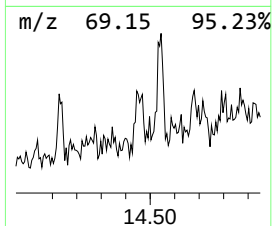
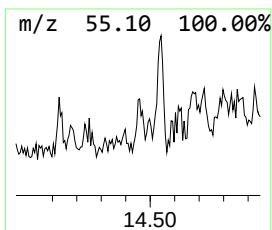
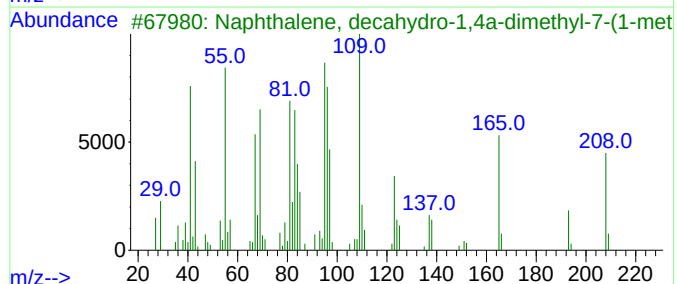
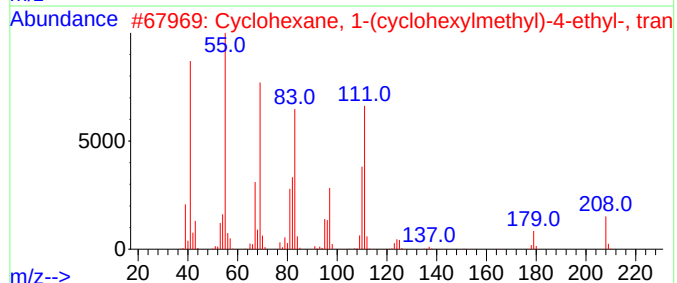
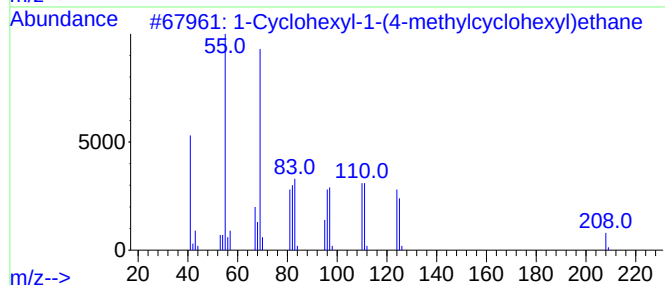
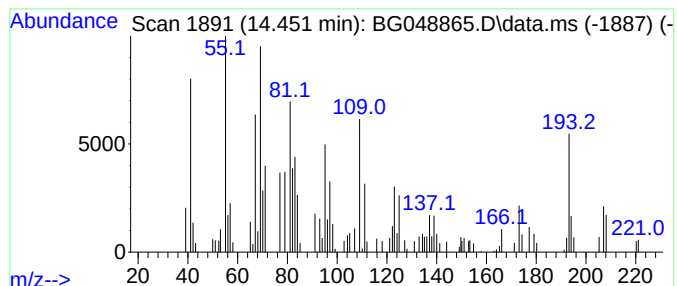
Instrument :
BNA_G
ClientSampleId :
352

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown14.45 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.			
14.451	5.00 ng	98050	Acenaphthene-d10	14.715			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexyl-1-(4-methylcyclohexyl)ethane	208	C15H28	002027-12-5	38
2			Cyclohexane, 1-(cyclohexylmethyl)-4-ethyl-, trans	208	C15H28	054934-94-0	30
3			Naphthalene, decahydro-1,4a-dimethyl-7-(1-methyl-2-propenyl)-	208	C15H28	030824-81-8	25
4			2(1H)-Naphthalenone, octahydro-4-methyl-	166	C11H18O	000938-07-8	18
5			3-Aminomethyl-3,5,5-trimethylcyclohexane	171	C10H21NO	130343-30-5	18



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampled :
352

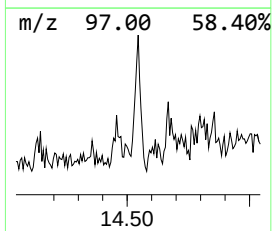
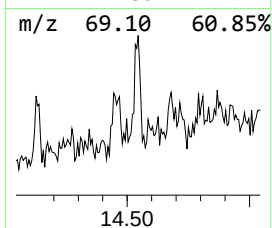
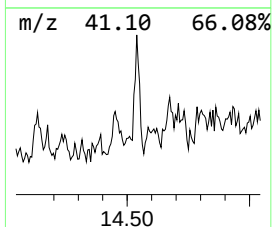
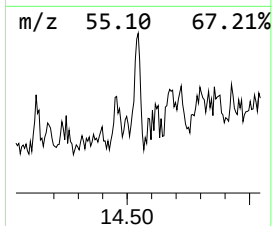
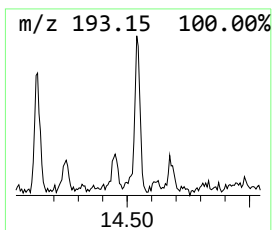
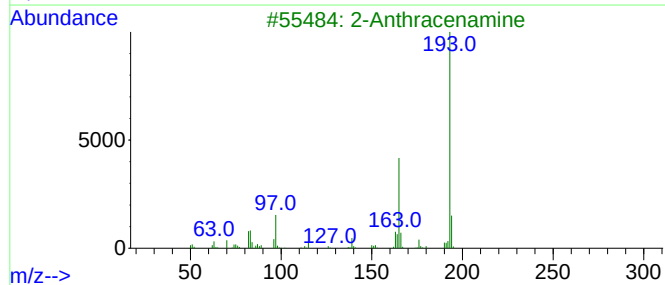
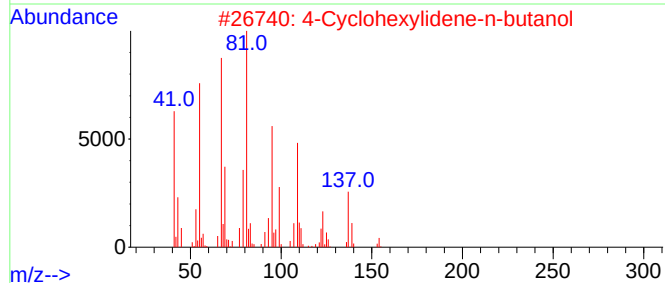
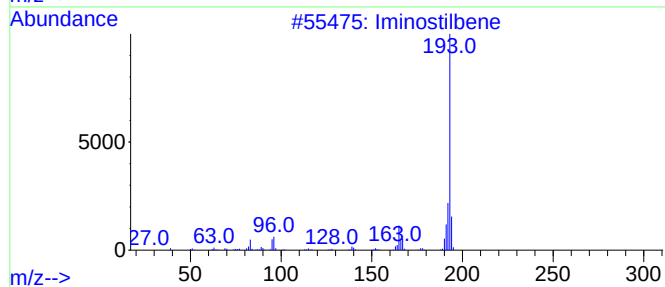
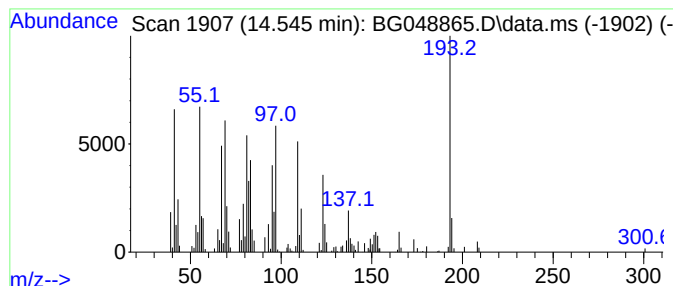
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.54 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	10.39 ng	203938	Acenaphthene-d10	14.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Iminostilbene	193	C14H11N	000256-96-2	41
2			4-Cyclohexylidene-n-butanol	154	C10H18O	004441-58-1	38
3			2-Anthracenamine	193	C14H11N	000613-13-8	38
4			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
5			6-Octenal, 3,7-dimethyl-, (R)-	154	C10H18O	002385-77-5	25



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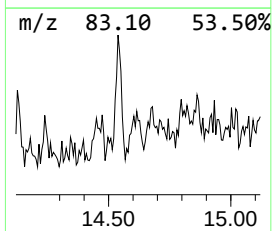
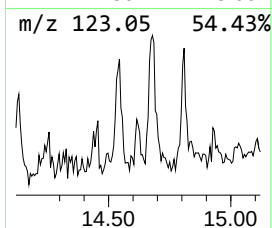
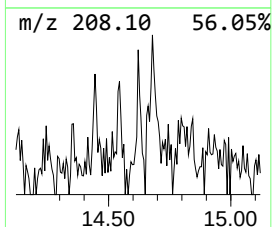
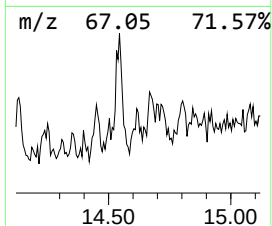
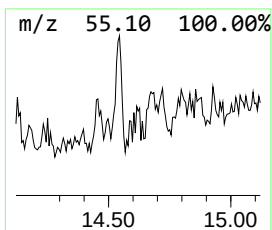
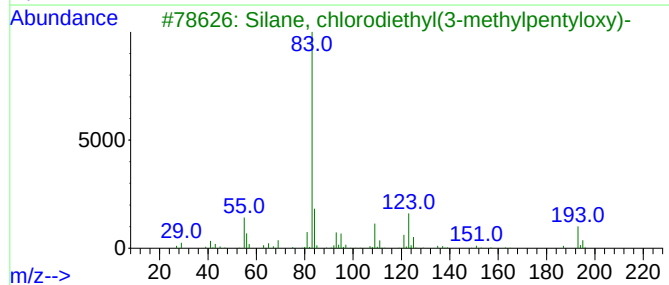
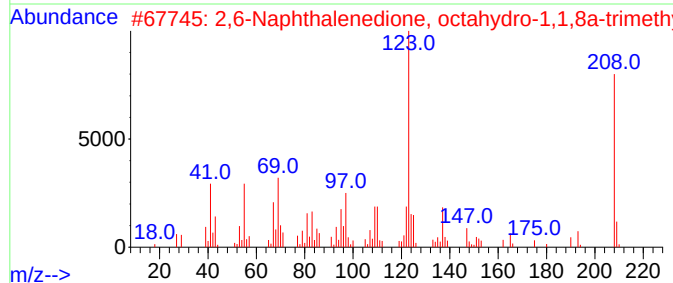
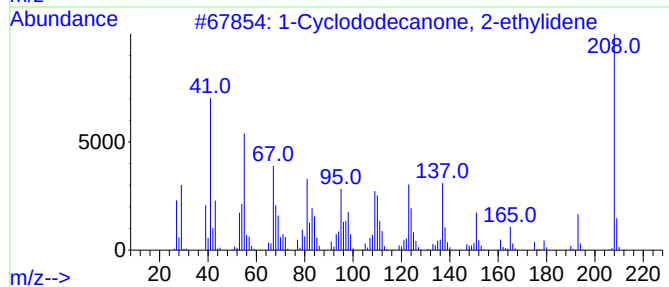
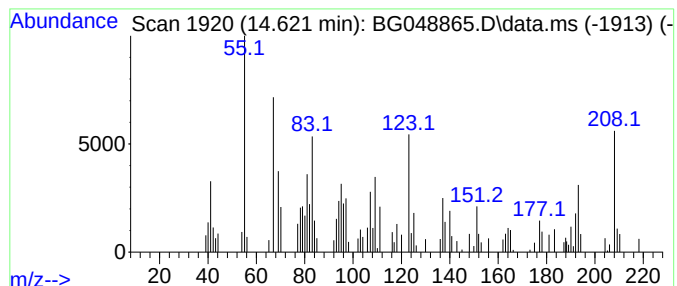
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown14.62 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	3.47 ng	68133	Acenaphthene-d10	14.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclododecanone, 2-ethylidene	208	C14H24O	001138-01-8	49
2			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	35
3			Silane, chlorodiethyl(3-methylpe...	222	C10H23ClOSi	1000363-50-1	30
4			2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1000215-77-9	25
5			5-(4,5-Dihydro-3H-pyrrol-2-ylmet...	208	C11H16N2S	051430-88-7	18



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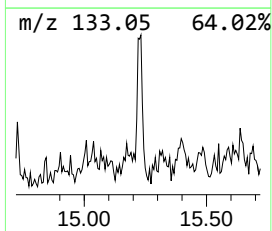
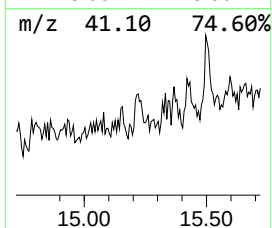
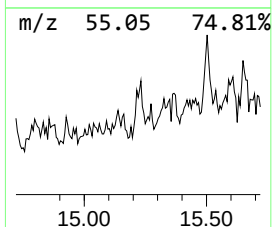
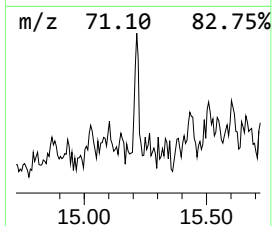
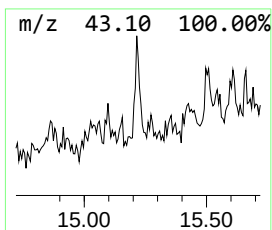
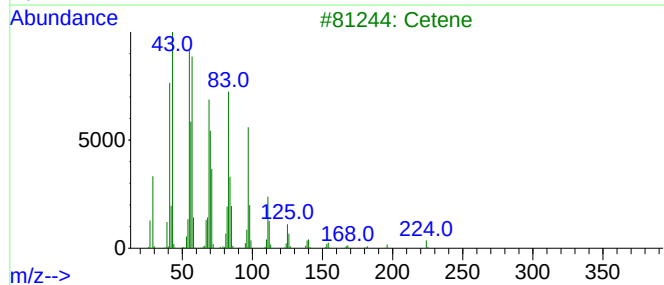
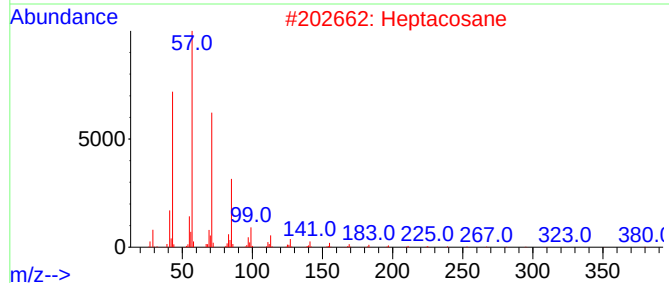
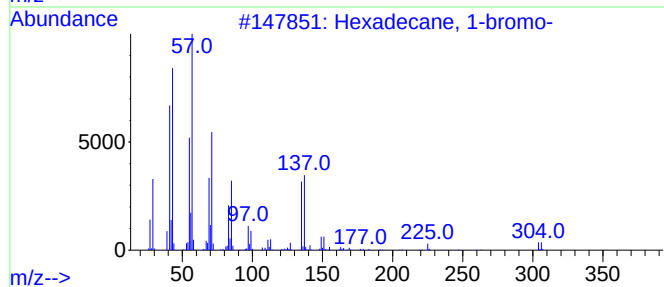
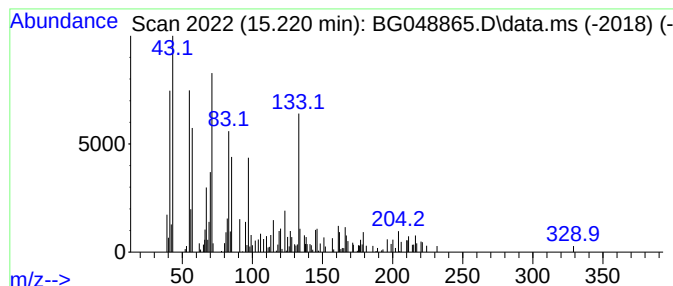
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.22 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.220	4.30 ng	84383	Acenaphthene-d10	14.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	38
2			Heptacosane	380	C27H56	000593-49-7	35
3			Cetene	224	C16H32	000629-73-2	30
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	27
5			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	27



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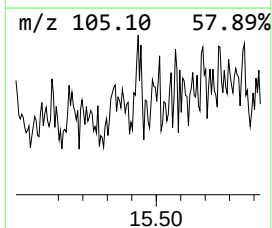
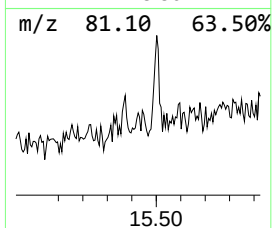
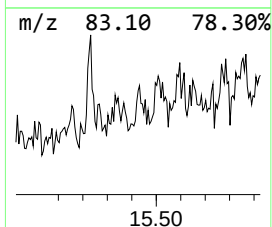
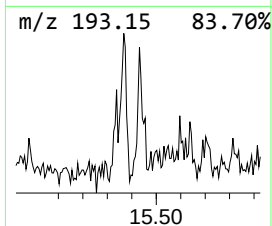
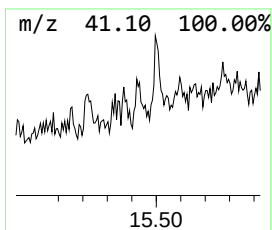
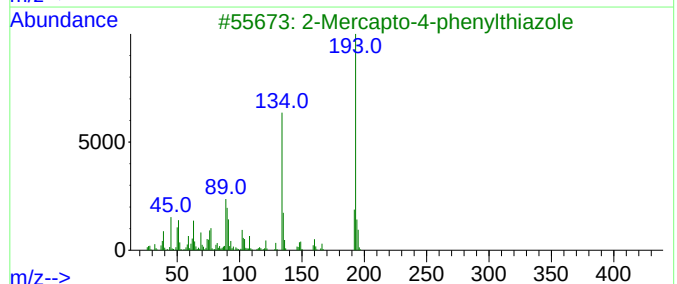
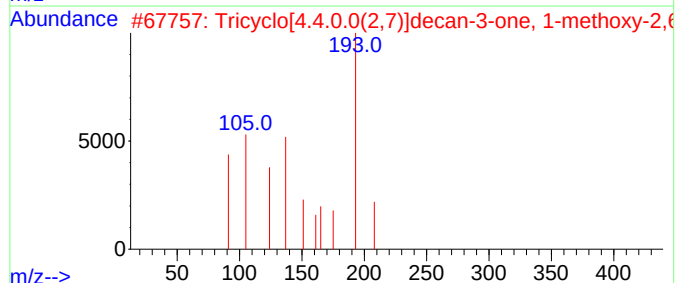
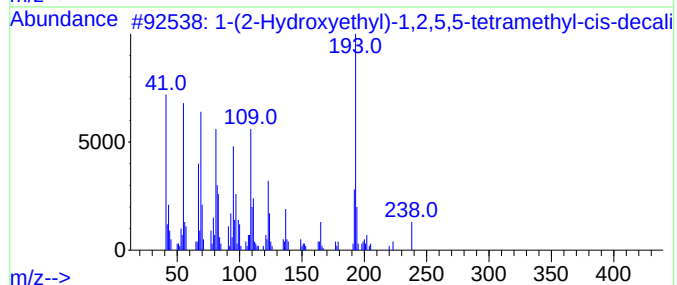
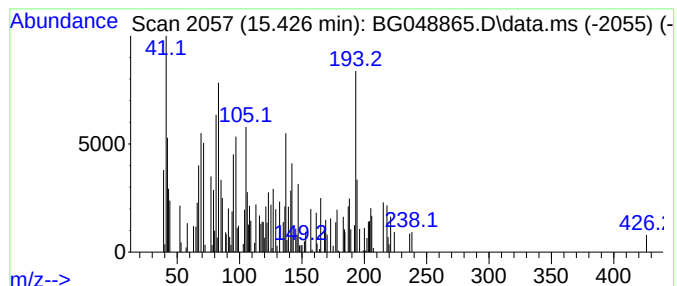
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.42 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	3.66 ng	71891	Acenaphthene-d10	14.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	25		
2	Tricyclo[4.4.0.0(2,7)]decan-3-on...	208	C13H20O2	062648-63-9	16		
3	2-Mercapto-4-phenylthiazole	193	C9H7NS2	002103-88-0	11		
4	Phosphonic acid, bicyclo[2.2.1]h...	202	C9H15O3P	027768-77-0	11		
5	1H-1,2,3-Triazole, 1,4-diphenyl-	221	C14H11N3	013148-78-2	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048865.D
Acq On : 23 Apr 2021 16:10
Operator : CG/JU
Sample : M2119-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

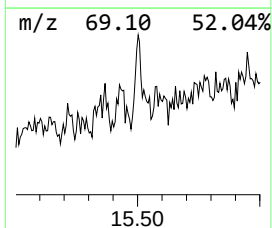
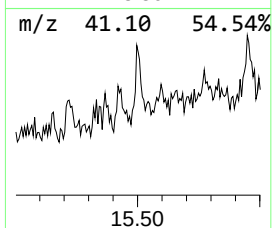
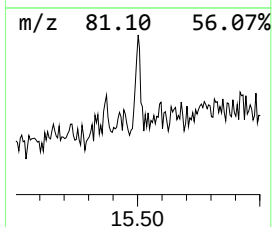
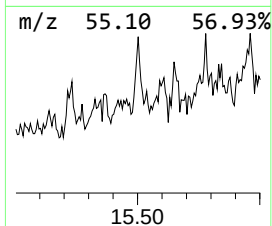
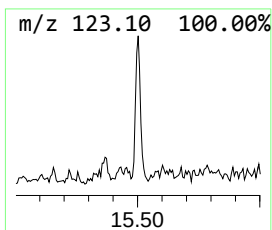
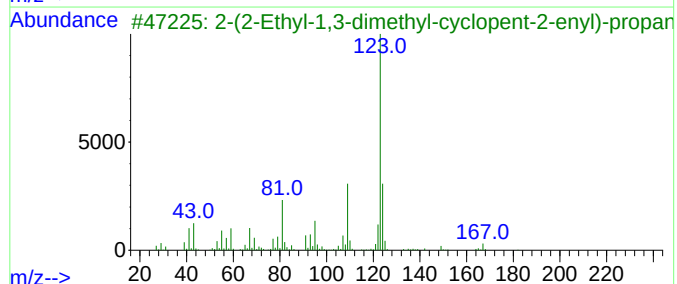
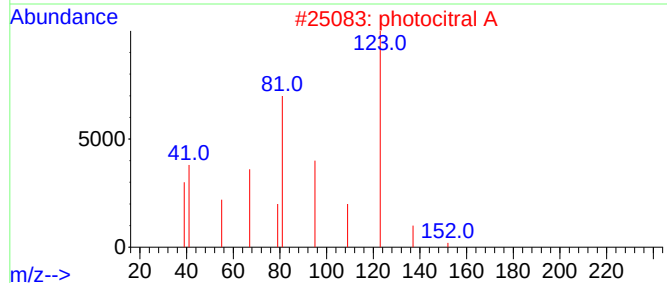
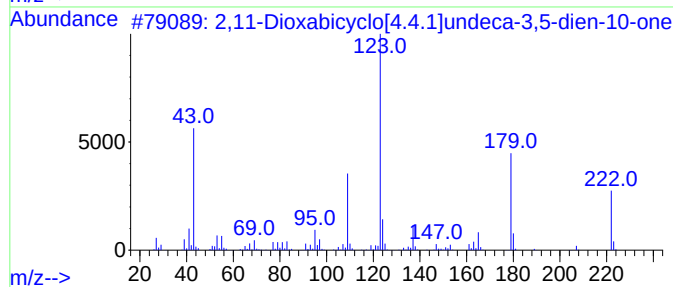
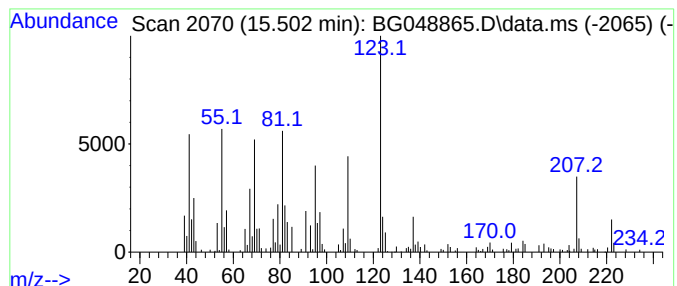
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.502	10.76 ng	211035	Acenaphthene-d10	14.715	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2	photocitral A	152	C10H16O	055253-28-6	47
3	2-(2-Ethyl-1,3-dimethyl-cyclopent...	182	C12H22O	1000186-82-4	47
4	4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	43
5	1-Butanone, 4-chloro-1-(4-fluoro...	200	C10H10ClFO	003874-54-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048865.D
Acq On : 23 Apr 2021 16:10
Operator : CG/JU
Sample : M2119-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
352

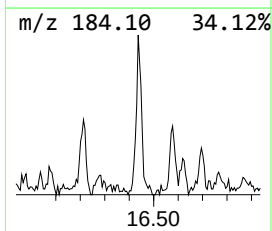
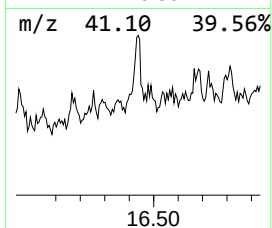
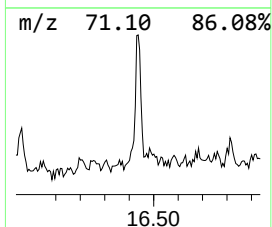
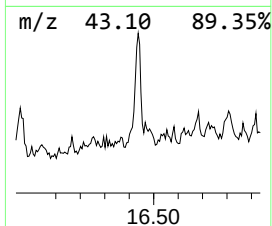
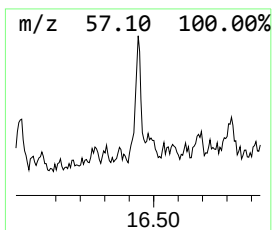
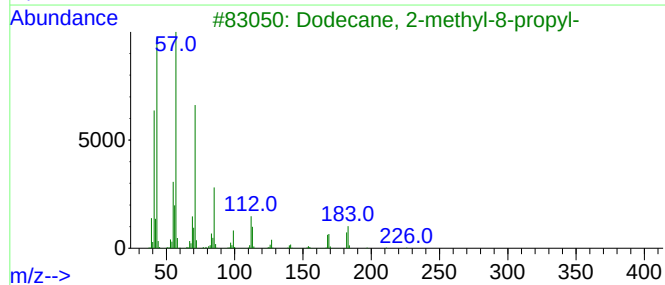
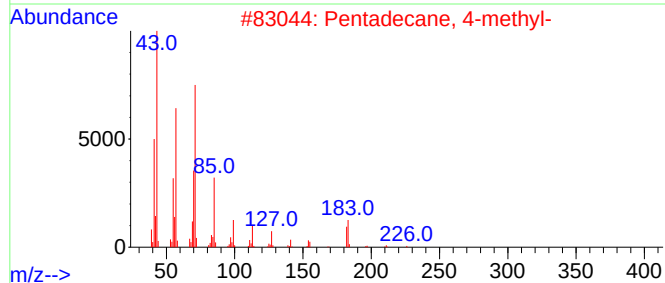
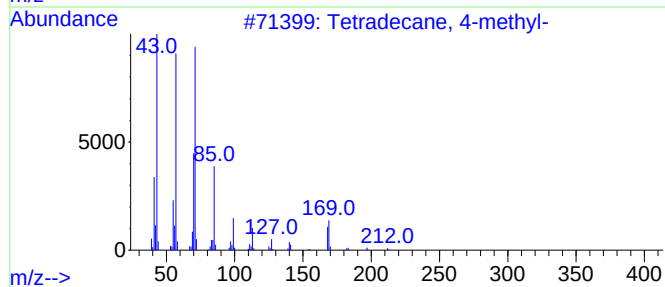
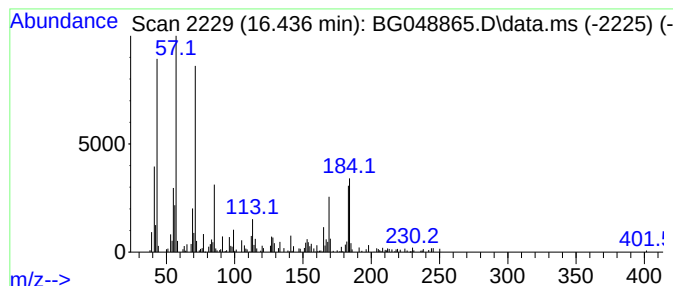
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.436	12.62 ng	258656	Phenanthrene-d10	17.471

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	64
2			Pentadecane, 4-methyl-	226	C16H34	002801-87-8	58
3			Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	58
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	53
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048865.D
Acq On : 23 Apr 2021 16:10
Operator : CG/JU
Sample : M2119-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
352

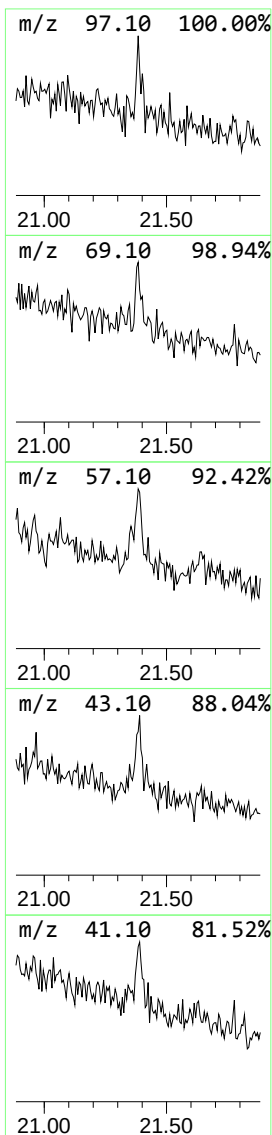
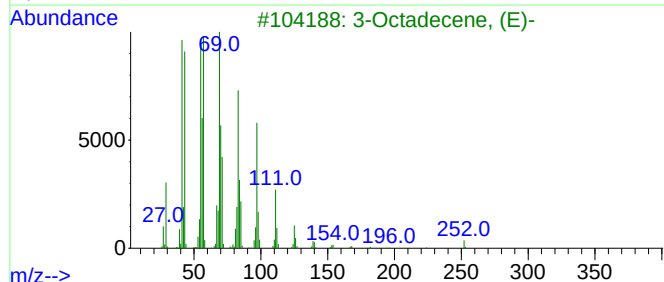
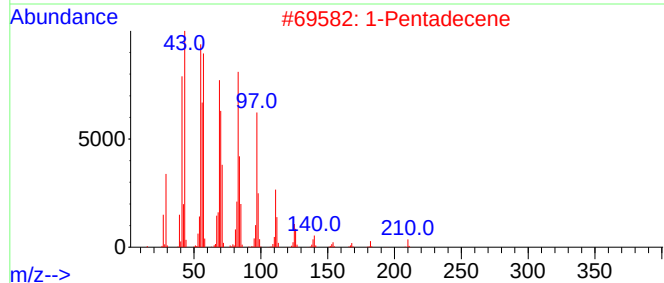
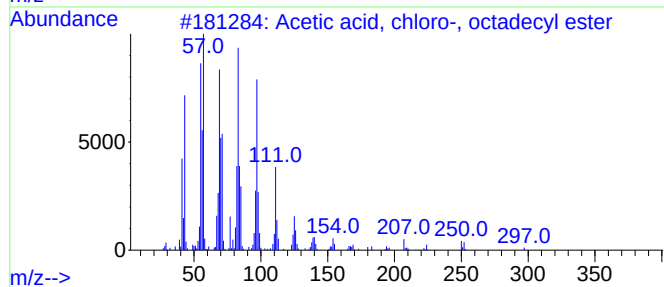
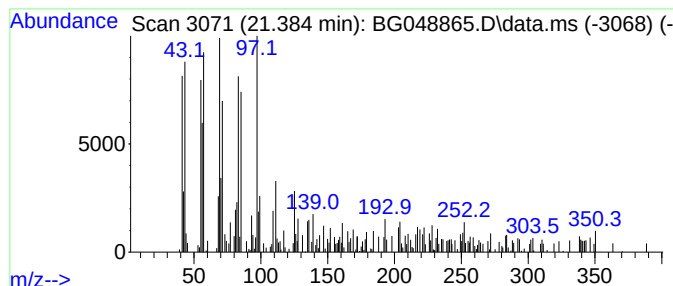
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Acetic acid, chloro-, octad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.384	5.40 ng	90677	Chrysene-d12	21.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	58
2			1-Pentadecene	210	C15H30	013360-61-7	58
3			3-Octadecene, (E)-	252	C18H36	007206-19-1	49
4			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	49
5			7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048865.D
Acq On : 23 Apr 2021 16:10
Operator : CG/JU
Sample : M2119-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
352

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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
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unknown14.45	14.451	5.0	ng	98050	3	14.715	392400	20.0
unknown14.54	14.545	10.4	ng	203938	3	14.715	392400	20.0
unknown14.62	14.621	3.5	ng	68133	3	14.715	392400	20.0
unknown15.22	15.220	4.3	ng	84383	3	14.715	392400	20.0
unknown15.42	15.426	3.7	ng	71891	3	14.715	392400	20.0
2,11-Dioxabicyc...	15.502	10.8	ng	211035	3	14.715	392400	20.0
Tetradecane, 4-...	16.436	12.6	ng	258656	4	17.471	409806	20.0
Acetic acid, ch...	21.384	5.4	ng	90677	5	21.771	336010	20.0