

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
 Data File : BG055675.D
 Acq On : 17 Nov 2022 21:21
 Operator : CG/JU
 Sample : N5607-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-37

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.306	335	343	350	rBV	88215	138687	6.77%	0.911%
2	5.788	417	425	435	rBV	611895	998802	48.76%	6.559%
3	7.398	690	699	709	rBV	626612	1076541	52.55%	7.070%
4	8.250	836	844	851	rBV	171167	287604	14.04%	1.889%
5	9.425	1035	1044	1056	rBV	365039	664563	32.44%	4.364%
6	10.823	1276	1282	1295	rBV	72260	125497	6.13%	0.824%
7	11.082	1319	1326	1333	rBV	232250	419282	20.47%	2.753%
8	13.497	1729	1737	1745	rBV	992685	1568543	76.57%	10.300%
9	14.872	1964	1971	1979	rVB	379647	579720	28.30%	3.807%
10	15.253	2030	2036	2044	rBV3	10208	20660	1.01%	0.136%
11	16.352	2217	2223	2236	rBV	778147	1233143	60.20%	8.098%
12	17.474	2410	2414	2417	rBV5	12619	21066	1.03%	0.138%
13	17.615	2431	2438	2442	rBV	437221	686370	33.51%	4.507%
14	17.657	2442	2445	2452	rVB	90177	138965	6.78%	0.913%
15	17.745	2457	2460	2464	rVB	22995	29629	1.45%	0.195%
16	18.250	2543	2546	2552	rVB3	18394	24813	1.21%	0.163%
17	18.473	2579	2584	2590	rVV2	202961	316592	15.46%	2.079%
18	18.532	2590	2594	2600	rVB2	62662	97115	4.74%	0.638%
19	18.614	2604	2608	2613	rVV	20490	29153	1.42%	0.191%
20	18.673	2613	2618	2623	rVV2	66279	136096	6.64%	0.894%
21	18.714	2623	2625	2629	rVB	40540	44094	2.15%	0.290%
22	18.761	2630	2633	2641	rBV3	22559	42686	2.08%	0.280%
23	18.973	2665	2669	2673	rBV	29593	44575	2.18%	0.293%
24	19.266	2717	2719	2723	rVB	20480	21463	1.05%	0.141%
25	19.390	2735	2740	2745	rBV	86361	146955	7.17%	0.965%
26	19.531	2760	2764	2769	rBV5	34956	64743	3.16%	0.425%
27	19.654	2780	2785	2790	rVB	301384	439918	21.48%	2.889%
28	19.736	2795	2799	2806	rVB2	84901	140436	6.86%	0.922%
29	20.013	2842	2846	2853	rVB	360735	538092	26.27%	3.534%
30	20.201	2873	2878	2883	rBV	1621025	2048415	100.00%	13.452%
31	20.800	2977	2980	2984	rBV2	86198	131793	6.43%	0.865%
32	21.517	3098	3102	3107	rVB	141550	207458	10.13%	1.362%
33	21.910	3161	3169	3174	rBV2	466953	1135365	55.43%	7.456%
34	21.963	3175	3178	3191	rVB	198986	333027	16.26%	2.187%
35	23.838	3493	3497	3509	rVB2	140726	307851	15.03%	2.022%
36	24.237	3559	3565	3573	rBV	120050	383412	18.72%	2.518%

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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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.330	3744	3751	3760	rVB2	224704	604809	29.53%	3.972%
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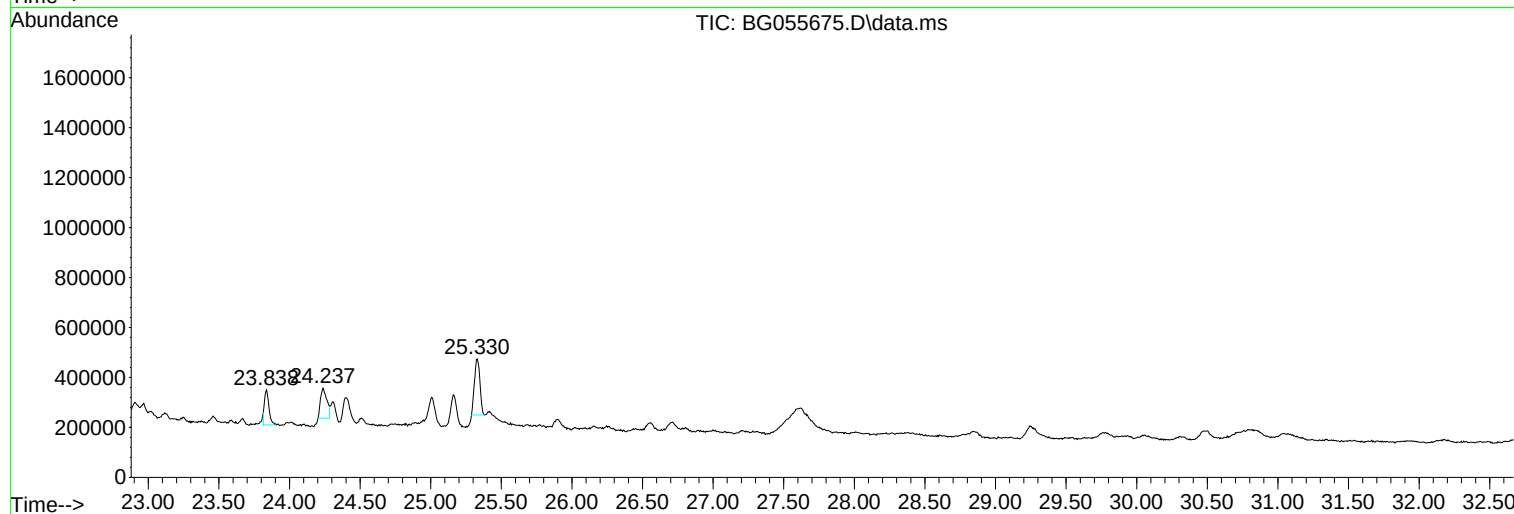
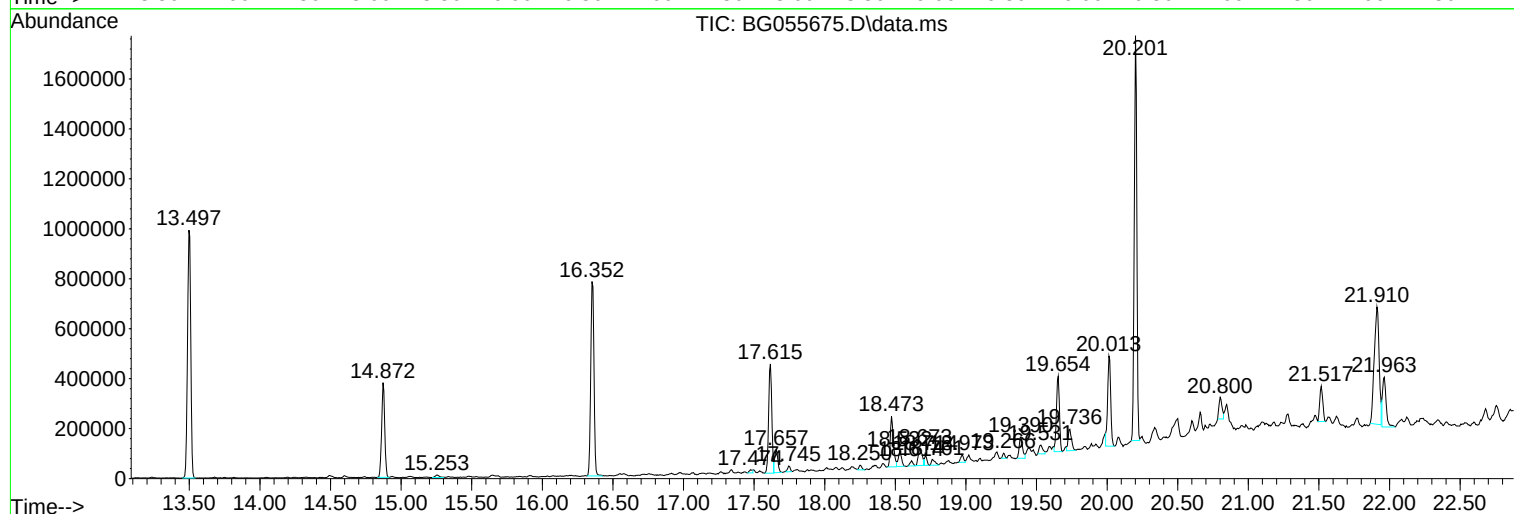
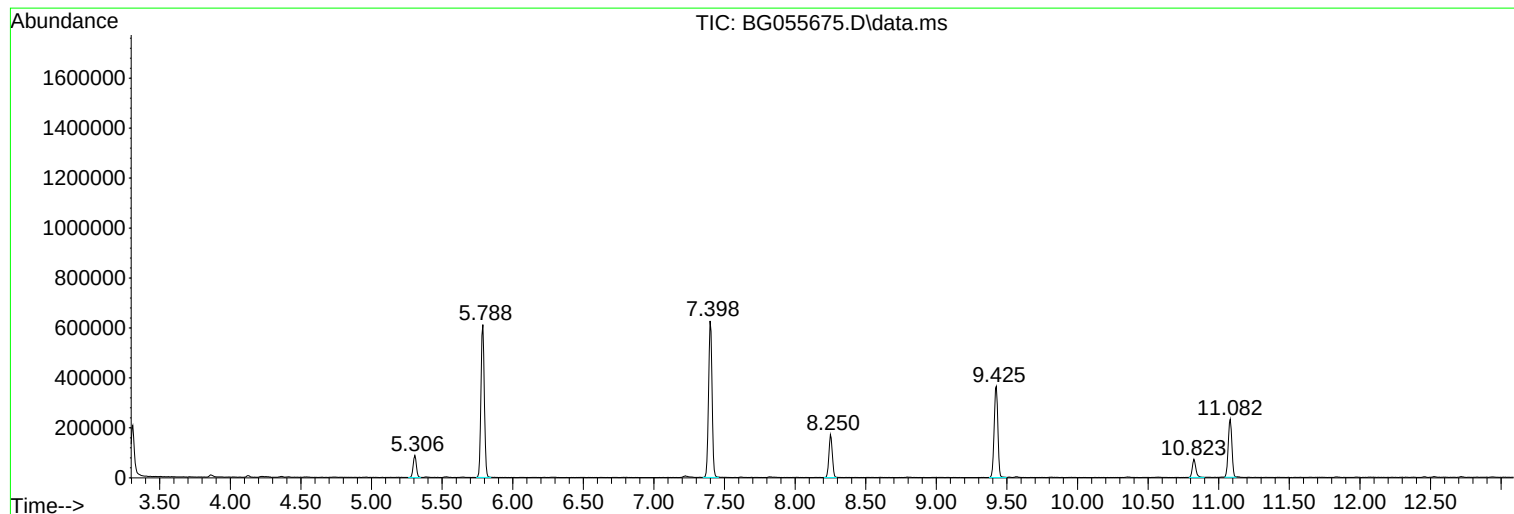
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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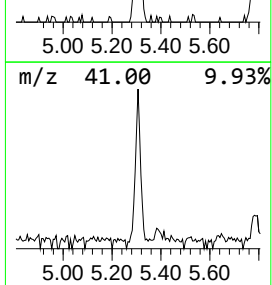
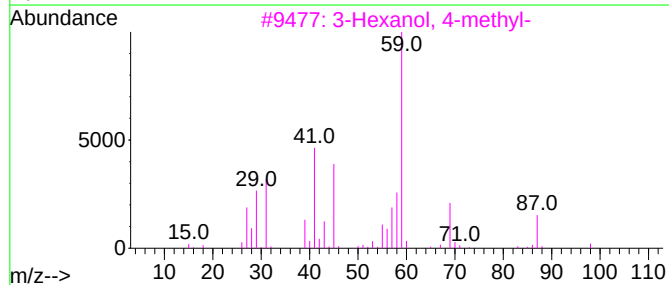
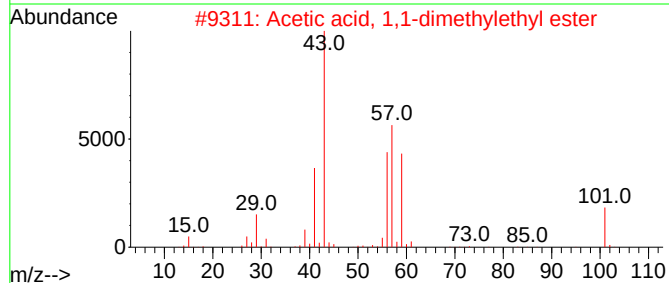
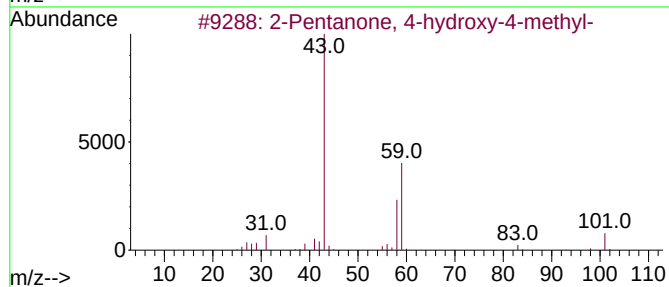
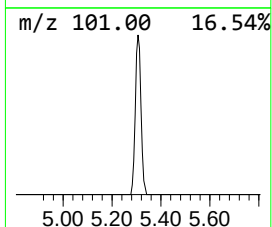
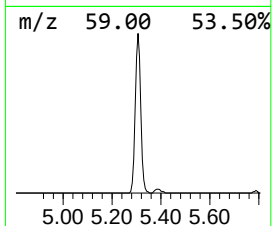
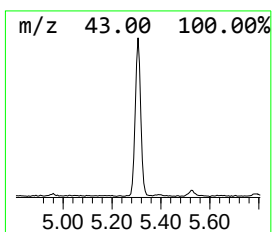
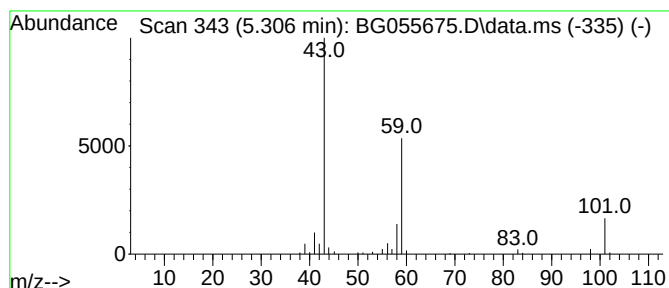
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.306	9.64 ng	138687	1,4-Dichlorobenzene-d4	8.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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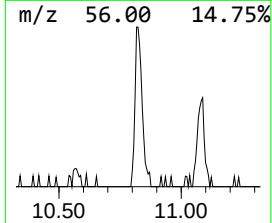
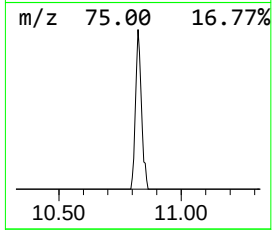
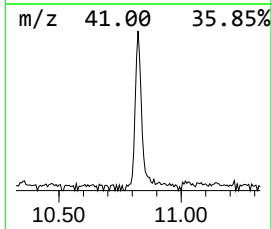
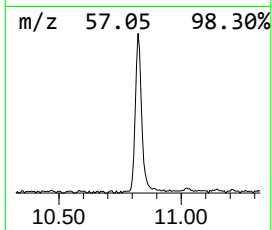
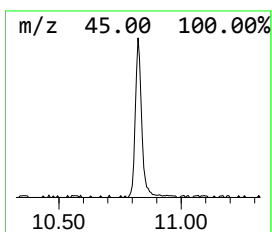
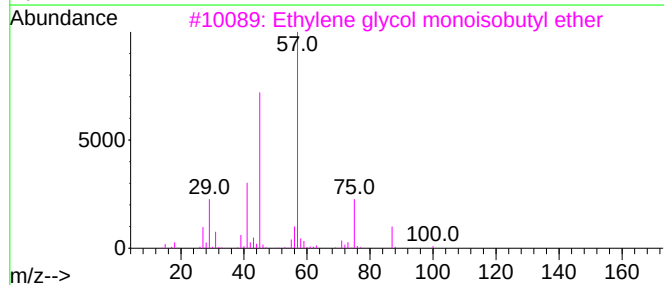
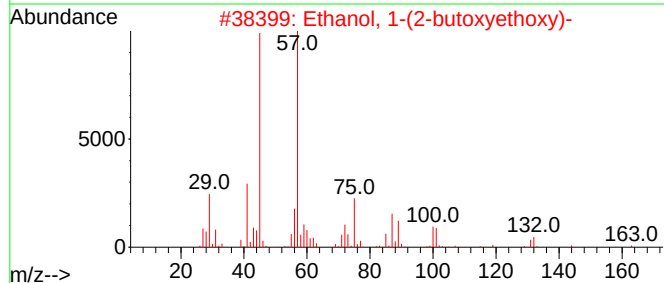
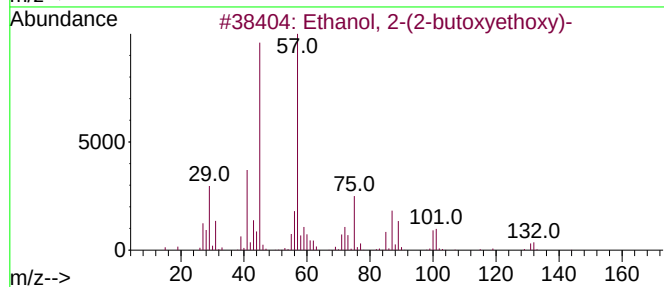
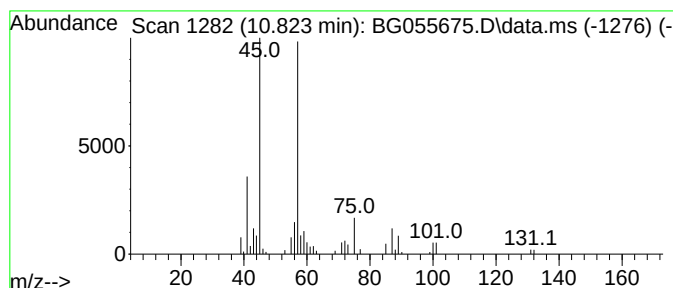
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.823	5.99 ng	125497	Naphthalene-d8	11.082	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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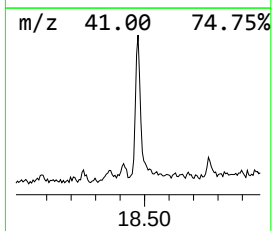
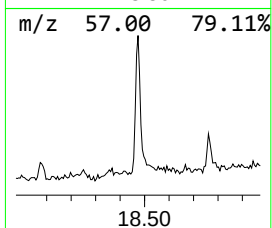
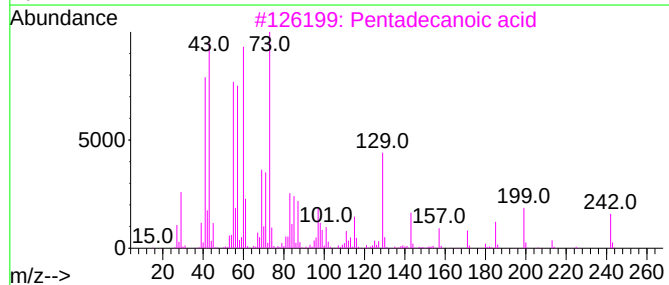
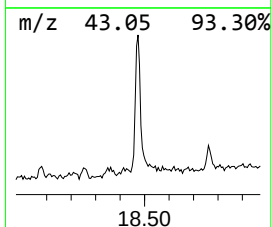
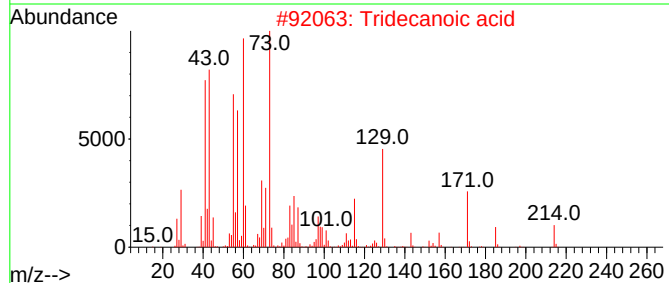
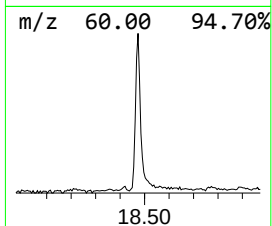
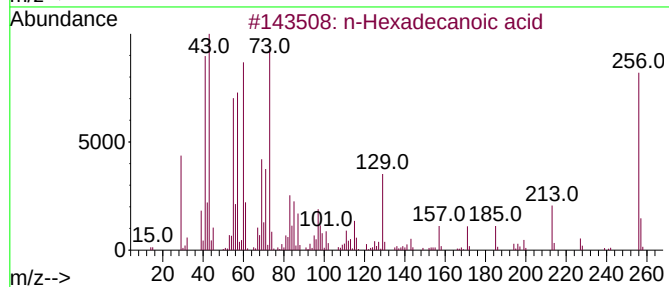
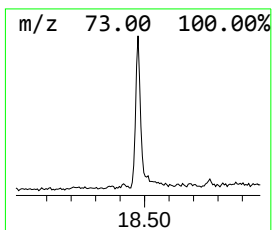
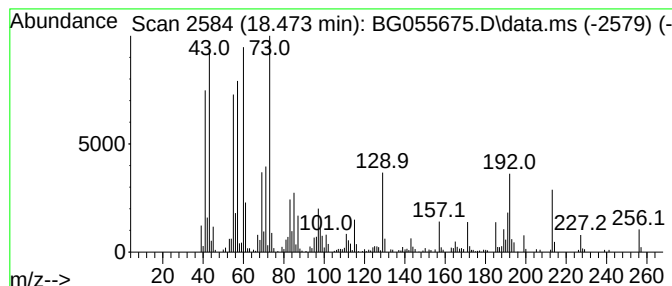
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.473	9.23 ng	316592	Phenanthrene-d10	17.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Undecanoic acid	186	C11H22O2	000112-37-8	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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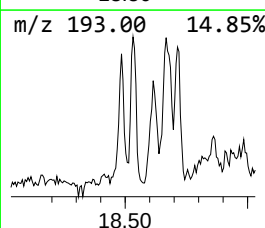
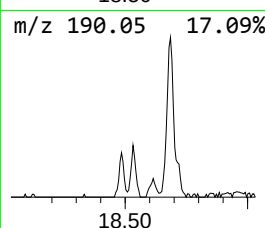
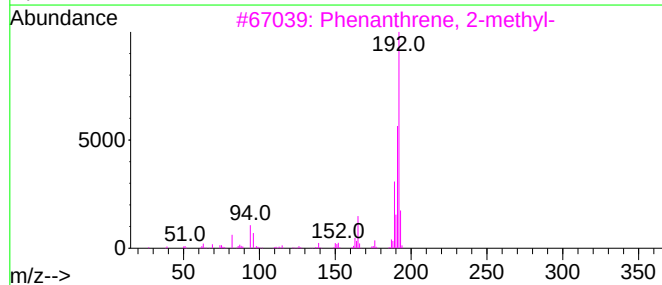
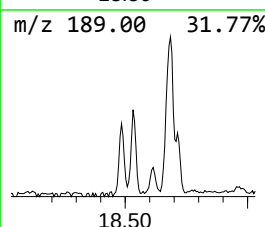
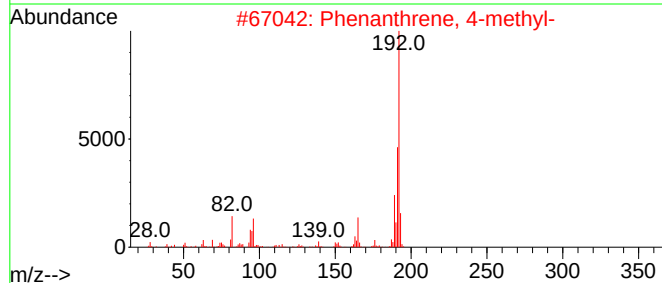
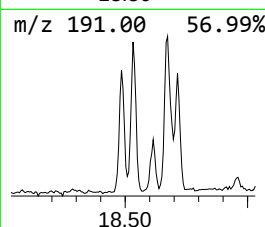
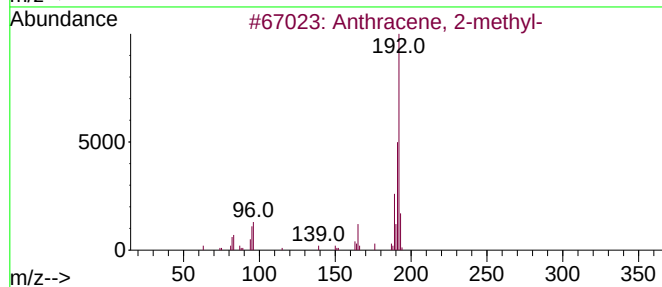
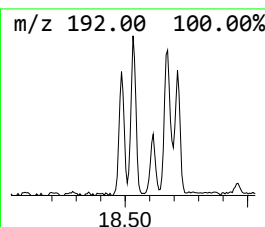
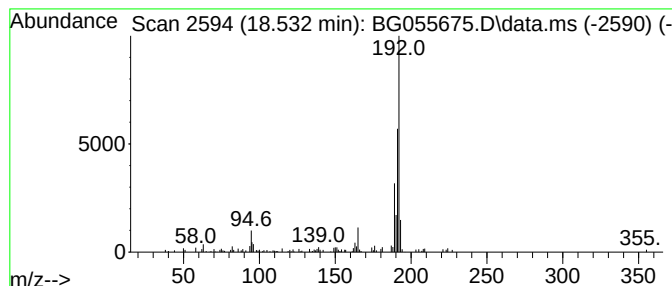
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.532	2.83 ng	97115	Phenanthrene-d10	17.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	90



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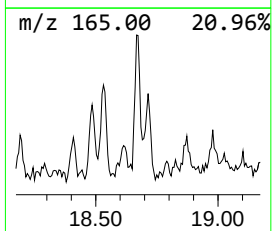
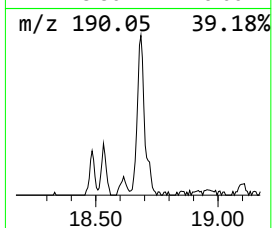
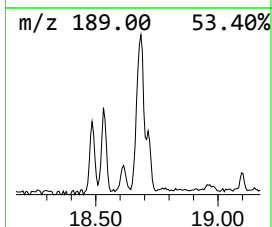
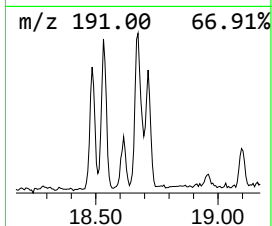
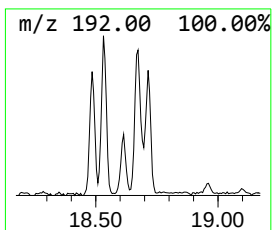
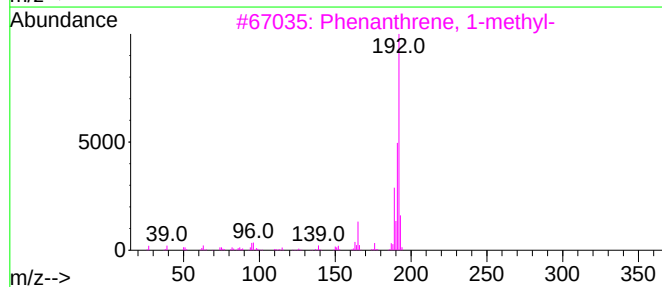
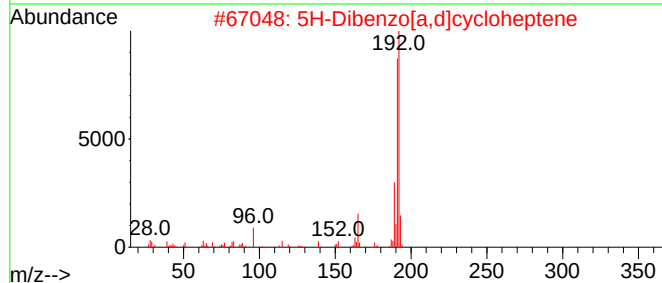
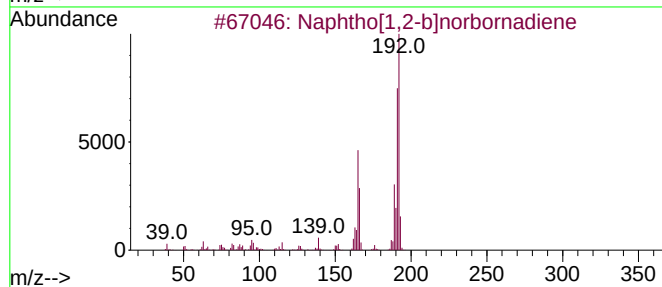
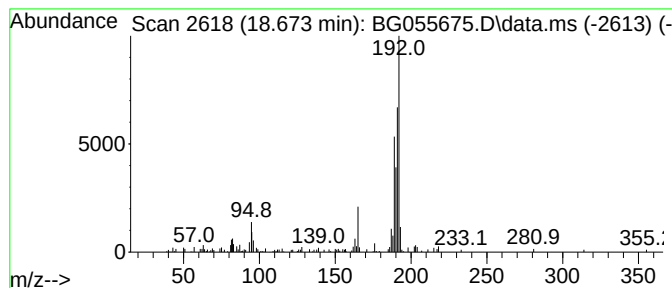
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Naphtho[1,2-b]norbornadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.673	3.97 ng	136096	Phenanthrene-d10	17.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	60
2			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	53
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
4			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	49
5			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055675.D
Acq On : 17 Nov 2022 21:21
Operator : CG/JU
Sample : N5607-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

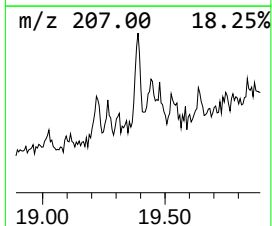
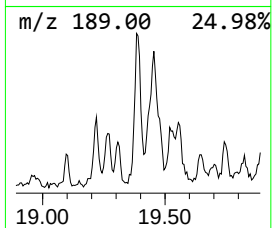
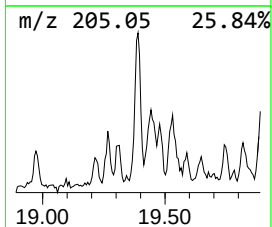
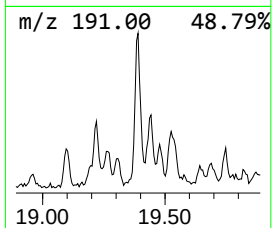
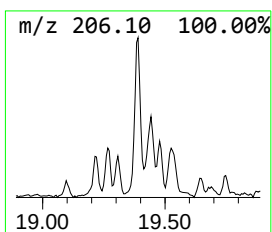
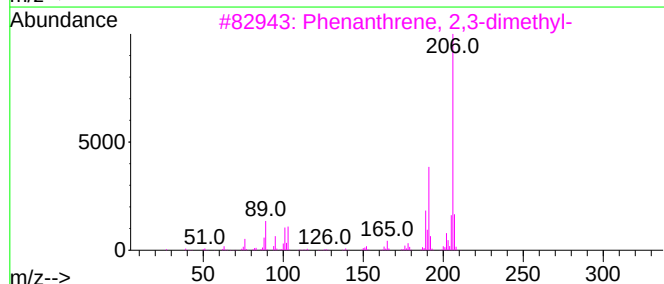
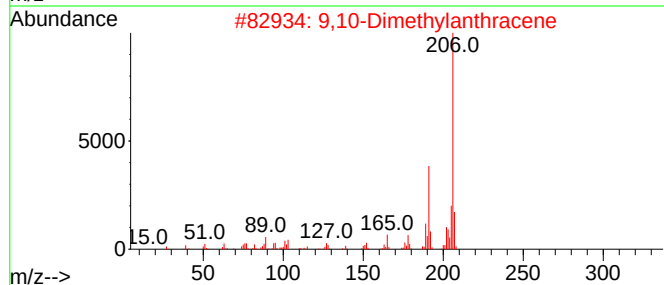
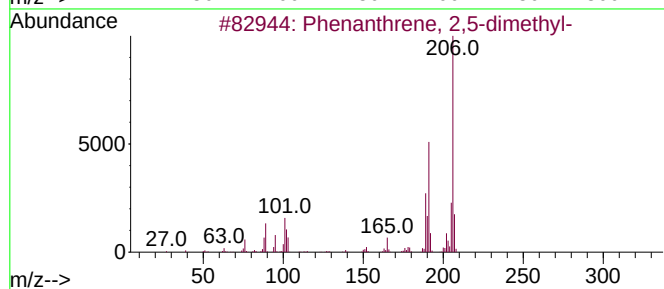
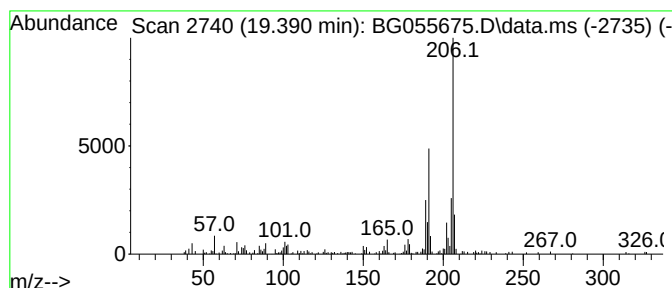
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.390	4.28 ng	146955	Phenanthrene-d10		17.615	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	93
2	9,10-Dimethylanthracene		206	C16H14	000781-43-1	91
3	Phenanthrene, 2,3-dimethyl-		206	C16H14	003674-65-5	87
4	di-p-Tolylacetylene		206	C16H14	002789-88-0	83
5	Phenanthrene, 3,6-dimethyl-		206	C16H14	001576-67-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055675.D
Acq On : 17 Nov 2022 21:21
Operator : CG/JU
Sample : N5607-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

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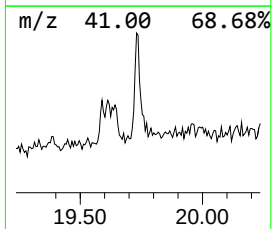
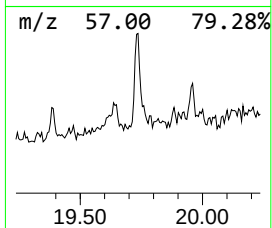
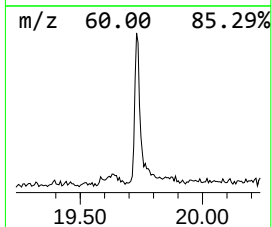
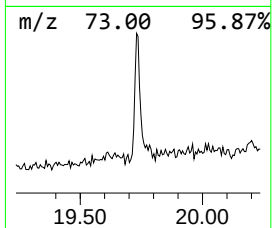
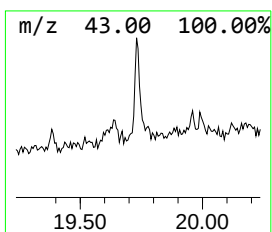
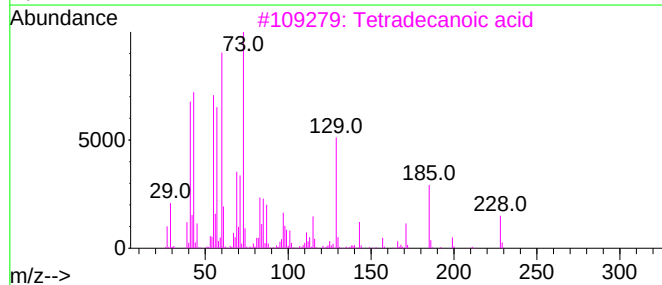
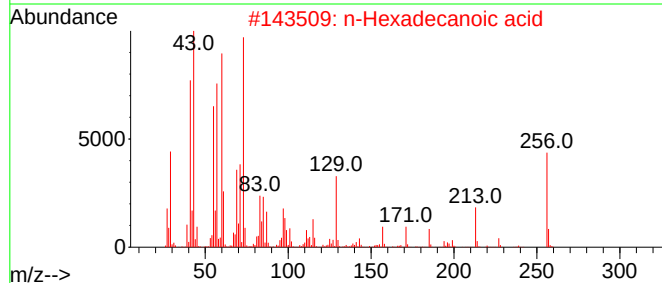
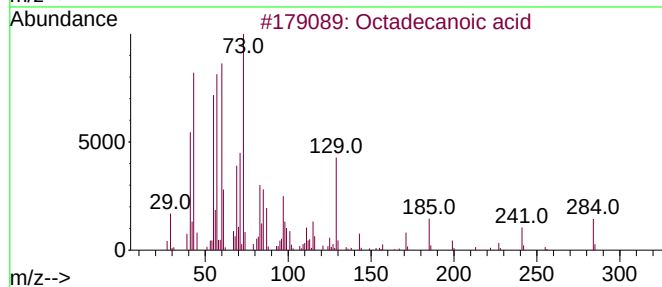
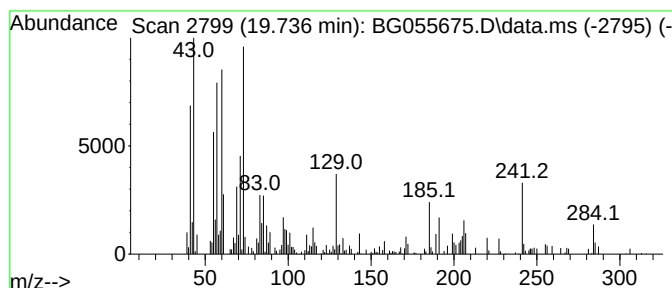
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.736	4.09 ng	140436	Phenanthrene-d10	17.615

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055675.D
Acq On : 17 Nov 2022 21:21
Operator : CG/JU
Sample : N5607-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-37

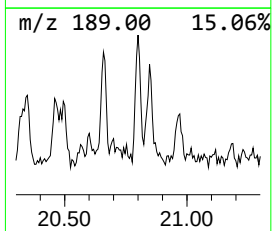
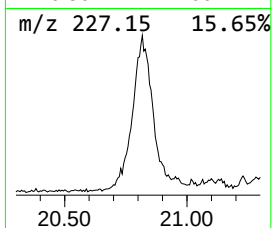
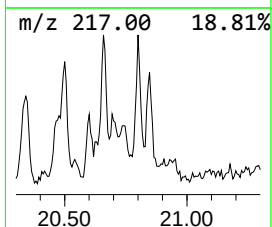
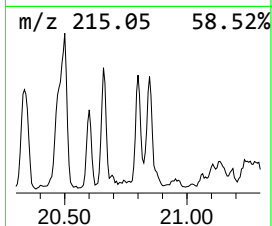
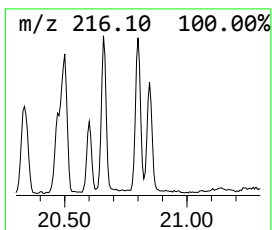
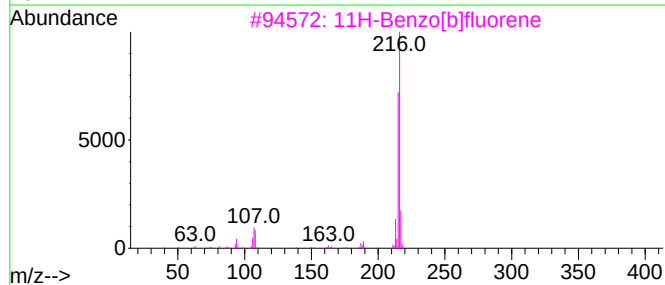
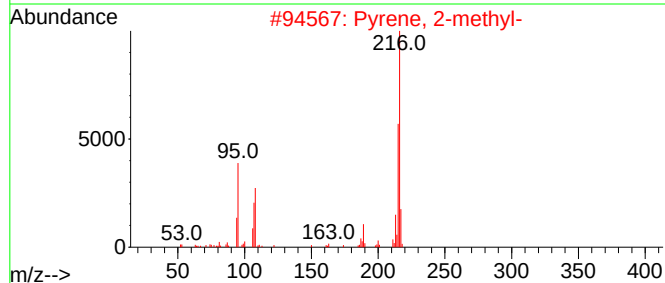
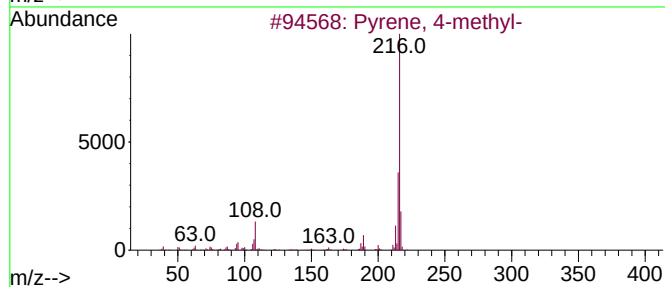
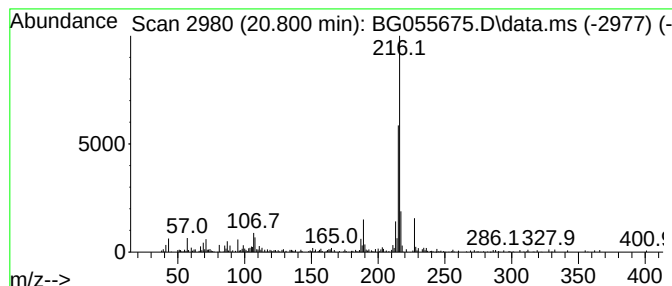
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.800	2.32 ng	131793	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 4-methyl-	216	C17H12	003353-12-6	94
2			Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055675.D
Acq On : 17 Nov 2022 21:21
Operator : CG/JU
Sample : N5607-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

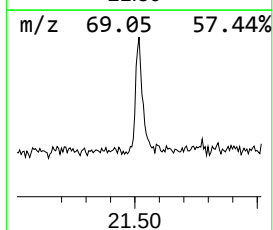
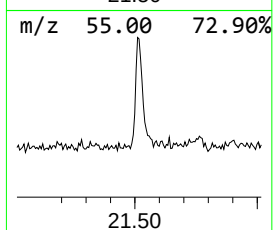
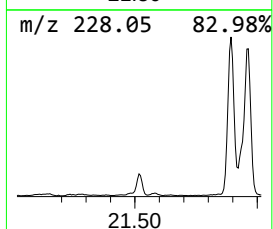
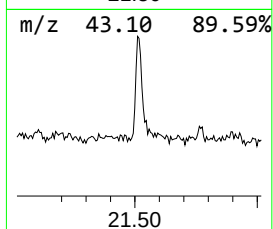
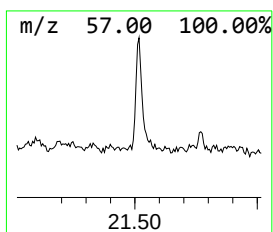
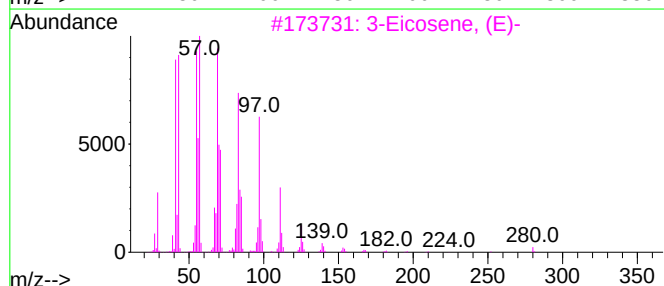
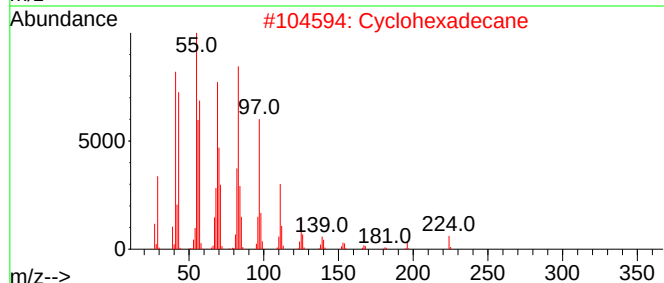
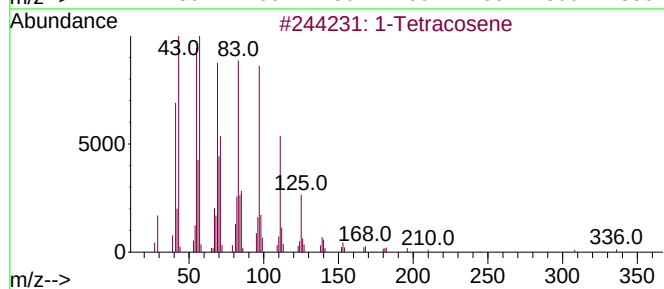
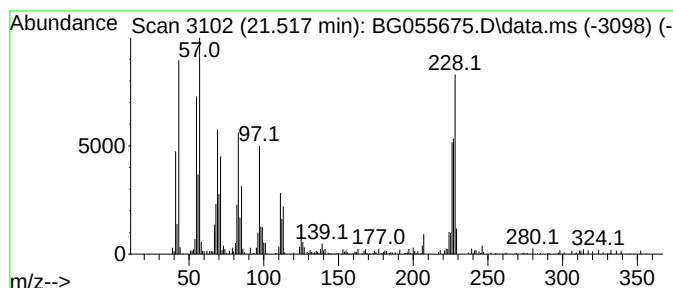
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetracosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.517	3.65 ng	207458	Chrysene-d12	21.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	Cyclohexadecane	224	C16H32	000295-65-8	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055675.D
Acq On : 17 Nov 2022 21:21
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Sample : N5607-05
Misc :
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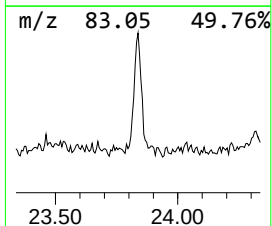
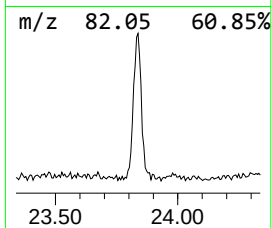
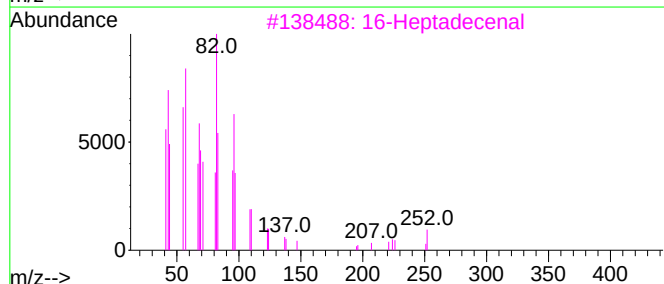
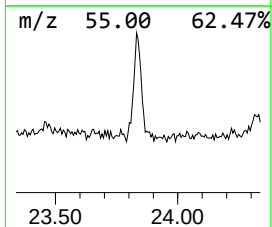
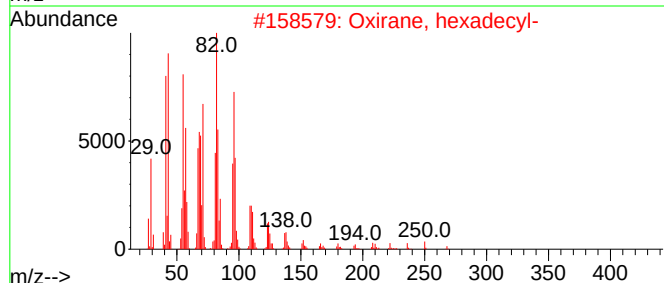
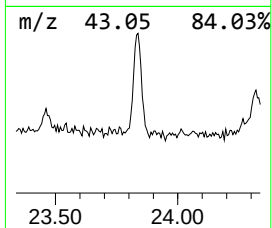
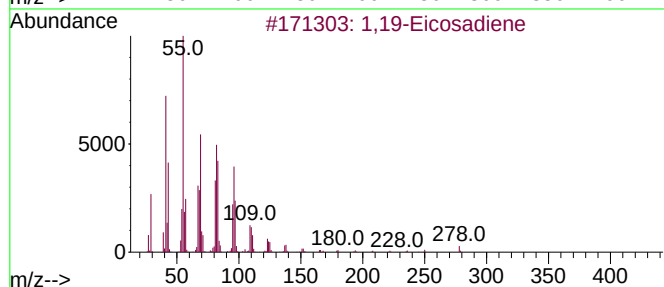
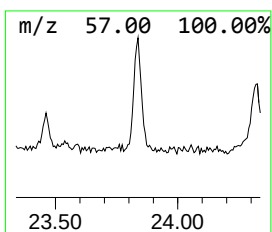
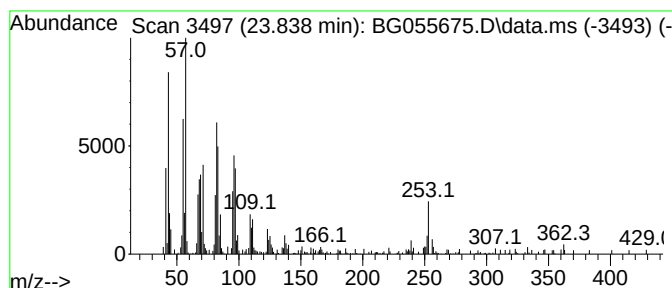
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,19-Eicosadiene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.837	10.18 ng	307851	Perylene-d12	25.330	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
3	16-Heptadecenal	252	C17H32O	1010144-57-9	78
4	Tetracosanal	352	C24H48O	057866-08-7	68
5	Octadecanal	268	C18H36O	000638-66-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
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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-BG111622.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
2-Pentanone, 4-...	5.306	9.6	ng	138687	1	8.250	287604	20.0
Ethanol, 2-(2-b...	10.823	6.0	ng	125497	2	11.082	419282	20.0
n-Hexadecanoic ...	18.473	9.2	ng	316592	4	17.615	686370	20.0
Anthracene, 2-m...	18.532	2.8	ng	97115	4	17.615	686370	20.0
Naphtho[1,2-b]n...	18.673	4.0	ng	136096	4	17.615	686370	20.0
Phenanthrene, 2...	19.390	4.3	ng	146955	4	17.615	686370	20.0
Octadecanoic acid	19.736	4.1	ng	140436	4	17.615	686370	20.0
Pyrene, 4-methyl-	20.800	2.3	ng	131793	5	21.916	1135370	20.0
1-Tetracosene	21.517	3.6	ng	207458	5	21.916	1135370	20.0
1,19-Eicosadiene	23.837	10.2	ng	307851	6	25.330	604809	20.0