

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
 Data File : BG048843.D
 Acq On : 22 Apr 2021 12:20
 Operator : CG/JU
 Sample : M2042-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FS-SB12A(7-8)

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: BG048843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.609	380	386	396	rVB	385198	595442	38.15%	5.585%
2	7.224	653	661	670	rBV	386515	670938	42.98%	6.293%
3	8.059	796	803	809	rBV	80616	135240	8.66%	1.268%
4	9.234	994	1003	1010	rBV	266275	453555	29.06%	4.254%
5	10.891	1276	1285	1291	rBV	103261	187309	12.00%	1.757%
6	13.341	1694	1702	1708	rBV	661982	987220	63.25%	9.259%
7	14.163	1837	1842	1849	rBV	36172	51508	3.30%	0.483%
8	14.722	1928	1937	1944	rBV	167960	260274	16.67%	2.441%
9	16.214	2185	2191	2204	rBV	530666	810730	51.94%	7.604%
10	17.477	2400	2406	2410	rBV	229487	338785	21.70%	3.178%
11	17.518	2410	2413	2421	rVB	82376	119381	7.65%	1.120%
12	17.612	2421	2429	2434	rBV	20097	37296	2.39%	0.350%
13	18.364	2551	2557	2561	rBV3	51021	79047	5.06%	0.741%
14	18.406	2561	2564	2572	rVB3	24829	39197	2.51%	0.368%
15	18.558	2584	2590	2593	rBV3	25439	51392	3.29%	0.482%
16	18.858	2634	2641	2645	rBV	13723	24732	1.58%	0.232%
17	19.275	2706	2712	2715	rBV4	17672	31138	1.99%	0.292%
18	19.416	2731	2736	2741	rBV5	14299	26907	1.72%	0.252%
19	19.534	2750	2756	2762	rBV	238806	355595	22.78%	3.335%
20	19.633	2768	2773	2777	rBV8	19281	29115	1.87%	0.273%
21	19.863	2806	2812	2814	rBV2	42422	63936	4.10%	0.600%
22	19.898	2814	2818	2824	rVV	239133	333635	21.37%	3.129%
23	19.968	2826	2830	2835	rVB4	20195	30954	1.98%	0.290%
24	20.092	2845	2851	2857	rBV	1206034	1560936	100.00%	14.640%
25	20.139	2857	2859	2863	rVB2	16767	20636	1.32%	0.194%
26	20.209	2866	2871	2874	rBV5	21497	38522	2.47%	0.361%
27	20.362	2891	2897	2898	rBV4	24181	38489	2.47%	0.361%
28	20.386	2898	2901	2906	rVB	35870	53774	3.44%	0.504%
29	20.491	2914	2919	2922	rBV3	14878	22315	1.43%	0.209%
30	20.550	2922	2929	2933	rBV4	30899	66873	4.28%	0.627%
31	20.691	2949	2953	2956	rVV2	16015	23200	1.49%	0.218%
32	20.732	2957	2960	2964	rVB	12993	15859	1.02%	0.149%
33	21.161	3028	3033	3038	rBV	41527	68240	4.37%	0.640%
34	21.343	3059	3064	3068	rBV4	29171	56263	3.60%	0.528%
35	21.390	3068	3072	3077	rVV2	89922	144427	9.25%	1.355%
36	21.443	3079	3081	3086	rVV3	32783	52901	3.39%	0.496%

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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 >

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37	21.496	3086	3090	3099	rVB2	34354	67845	4.35%	0.636%
38	21.778	3129	3138	3143	rBV2	256856	653068	41.84%	6.125%
39	21.825	3143	3146	3153	rVB	119877	186216	11.93%	1.747%
40	21.984	3169	3173	3179	rVB7	17081	30808	1.97%	0.289%
41	22.195	3206	3209	3216	rVB4	19801	38964	2.50%	0.365%
42	22.524	3258	3265	3273	rVB4	28383	62375	4.00%	0.585%
43	22.601	3273	3278	3285	rBV9	20677	41838	2.68%	0.392%
44	22.800	3310	3312	3317	rBV6	11127	16814	1.08%	0.158%
45	23.294	3395	3396	3402	rVB6	14873	15881	1.02%	0.149%
46	24.052	3516	3525	3532	rBV2	115603	373653	23.94%	3.505%
47	24.316	3564	3570	3576	rVB4	22873	52263	3.35%	0.490%
48	24.522	3602	3605	3607	rBV4	13045	16042	1.03%	0.150%
49	24.798	3644	3652	3663	rVB3	68922	212918	13.64%	1.997%
50	24.957	3670	3679	3689	rVB2	100733	283922	18.19%	2.663%
51	25.115	3694	3706	3715	rBV3	133009	408217	26.15%	3.829%
52	25.180	3715	3717	3727	rVB5	26806	64579	4.14%	0.606%
53	26.443	3924	3932	3933	rBV7	9758	22620	1.45%	0.212%
54	26.543	3946	3949	3958	rVB7	9016	21119	1.35%	0.198%
55	28.928	4343	4355	4367	rBV5	47505	216889	13.89%	2.034%

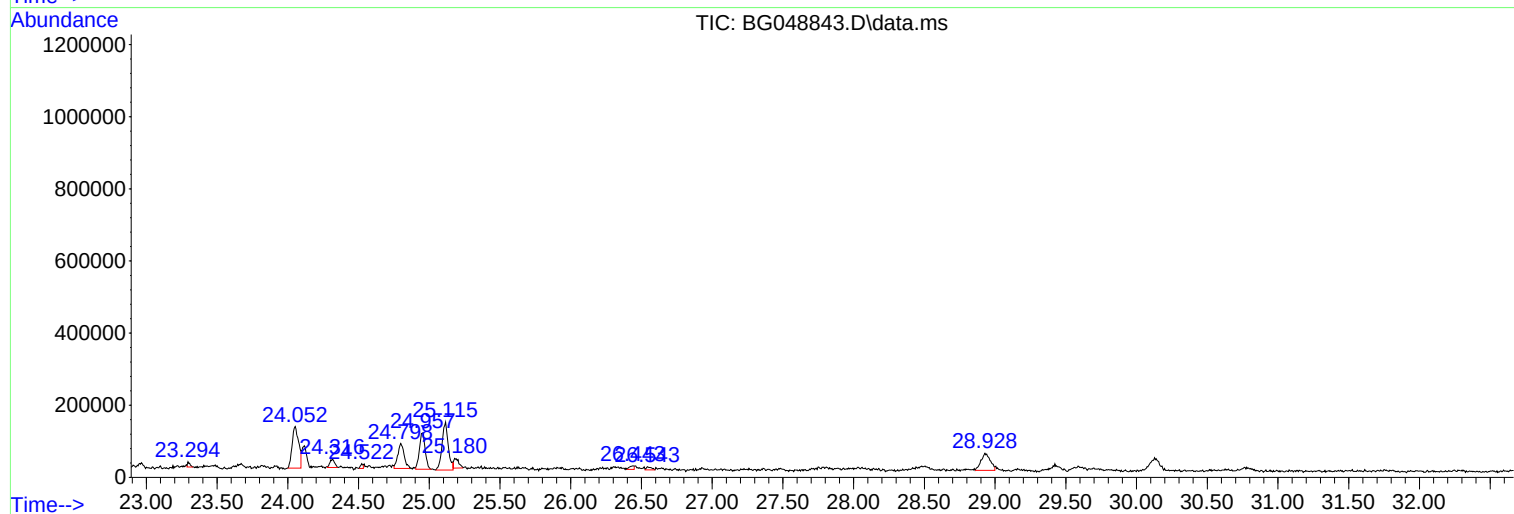
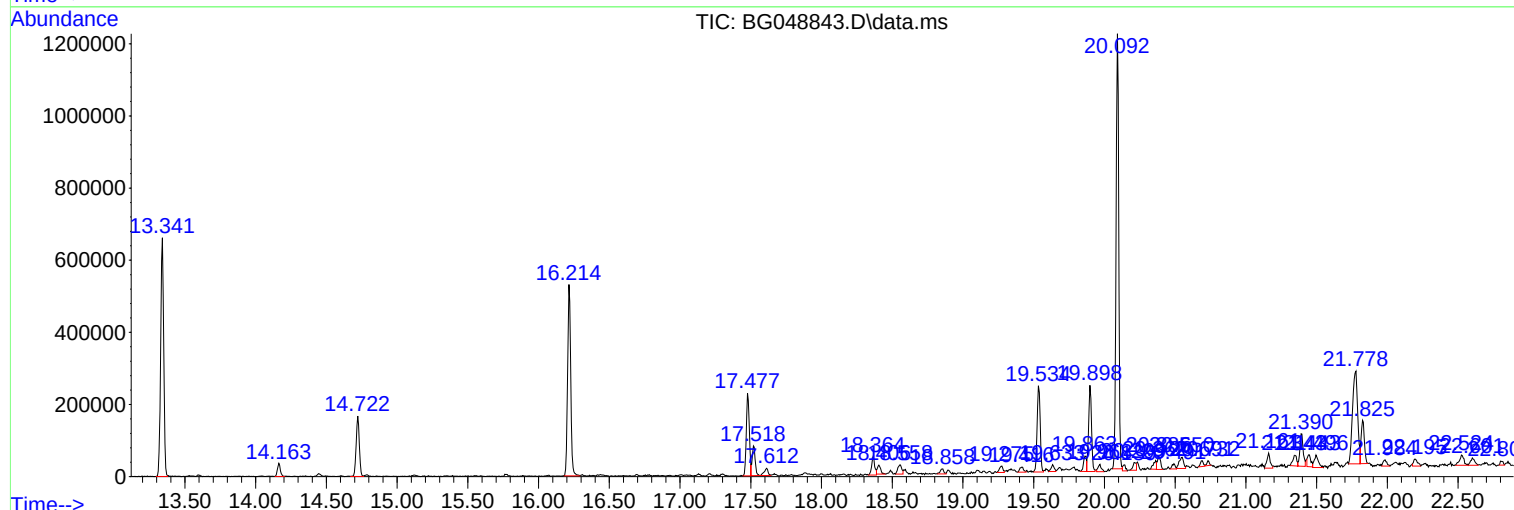
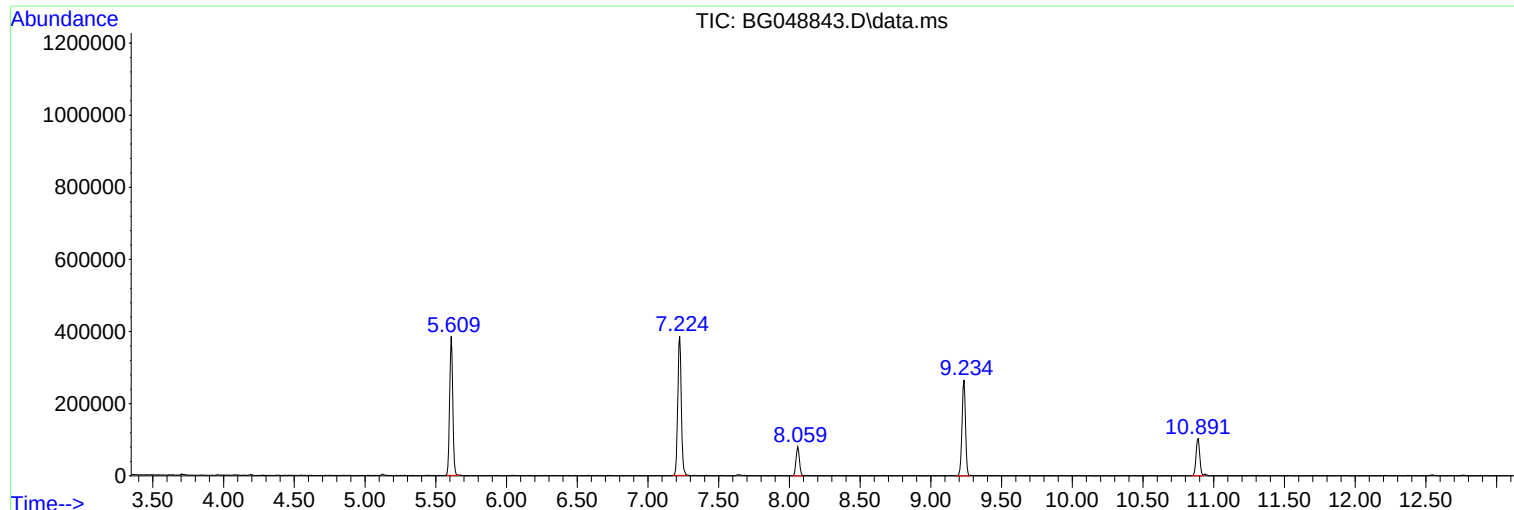
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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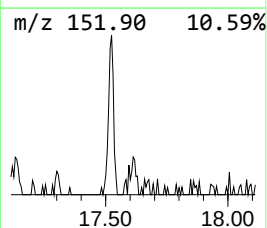
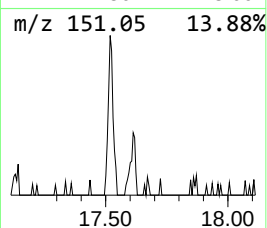
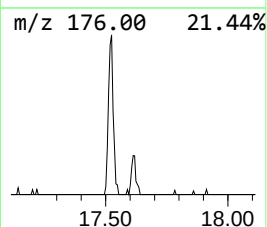
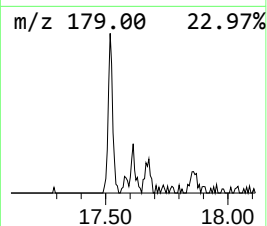
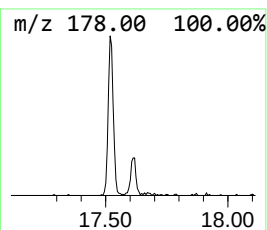
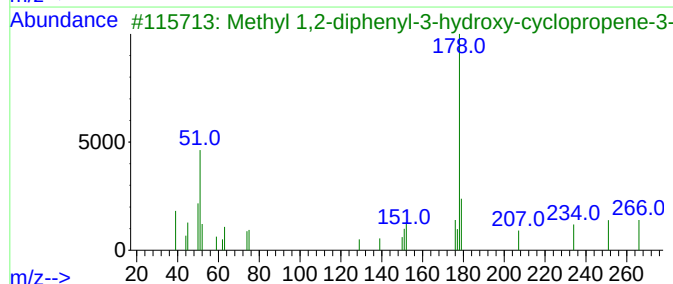
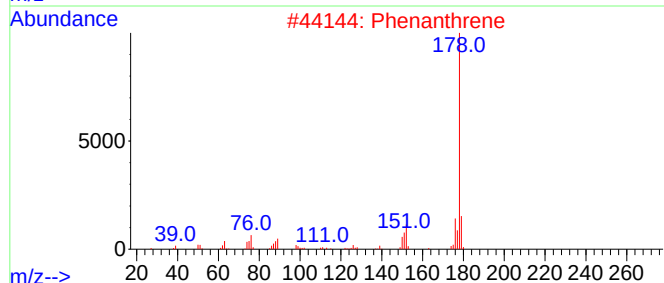
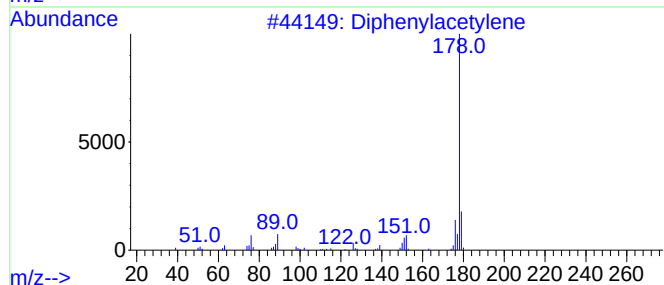
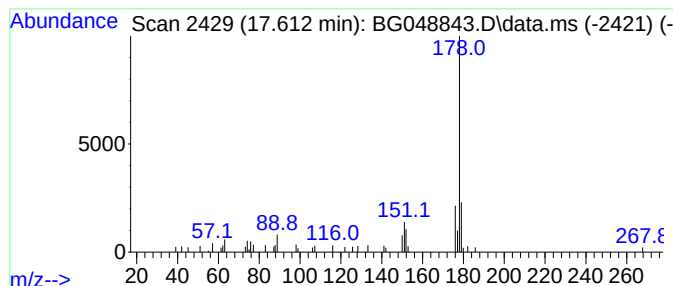
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Diphenylacetylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.612	2.20 ng	37296	Phenanthrene-d10	17.477

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenylacetylene	178	C14H10	000501-65-5	87
2			Phenanthrene	178	C14H10	000085-01-8	76
3			Methyl 1,2-diphenyl-3-hydroxy-cy...	266	C17H14O3	043123-04-2	72
4			1,4-Dihydro-1,4-ethanoanthracene	206	C16H14	055431-80-6	72
5			Anthracene	178	C14H10	000120-12-7	68



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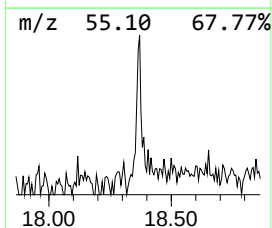
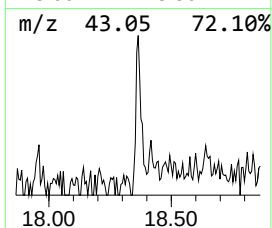
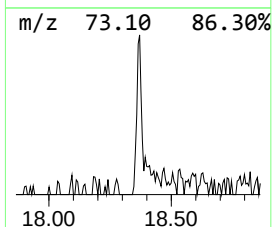
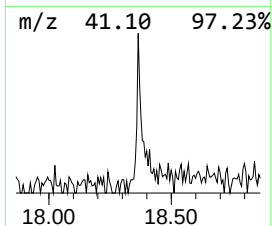
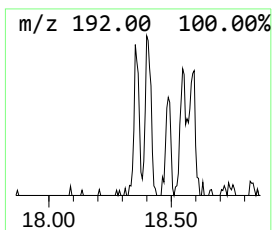
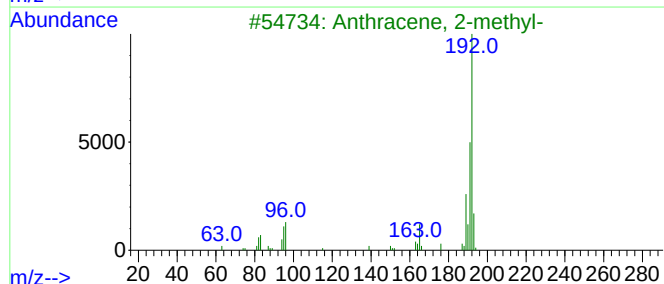
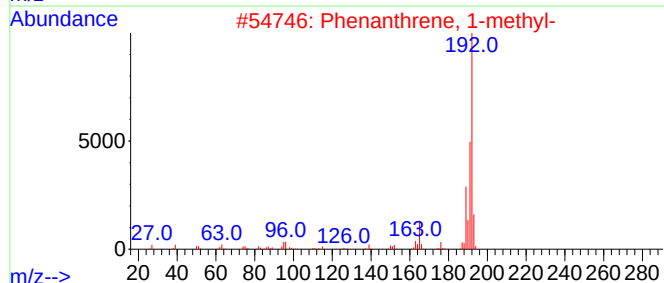
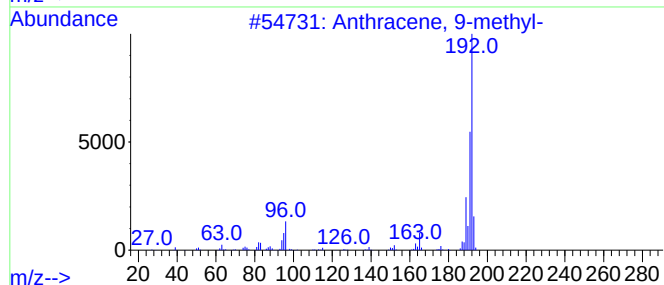
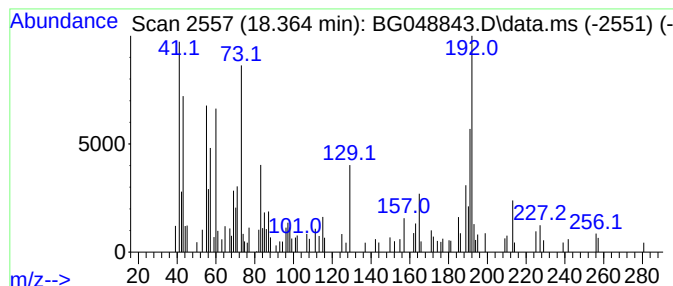
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown18.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.364	4.67 ng	79047	Phenanthrene-d10	17.477

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	46
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	43
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	38



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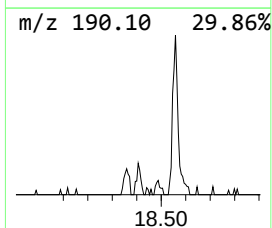
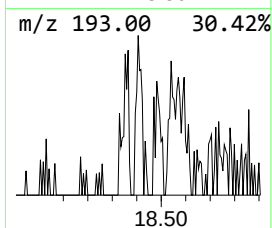
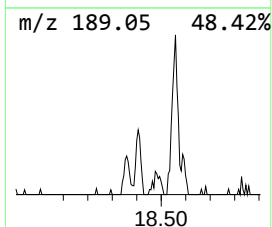
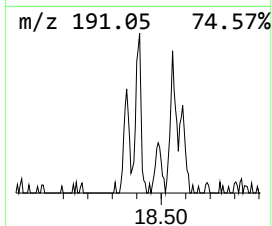
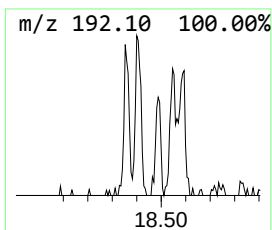
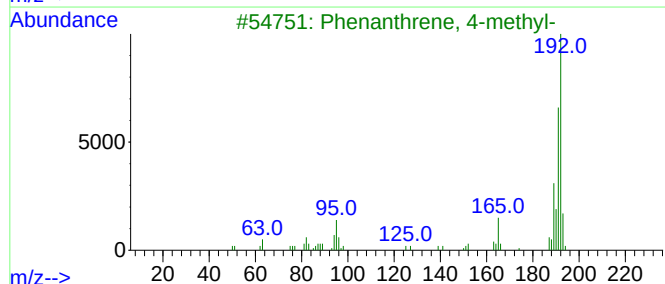
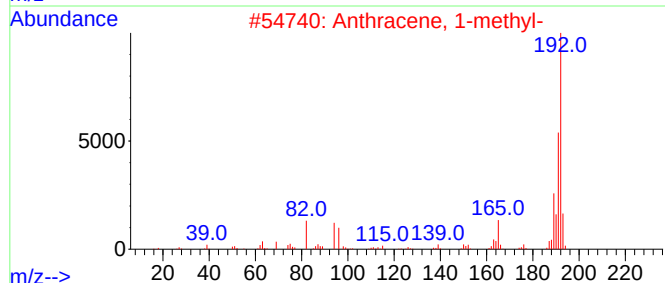
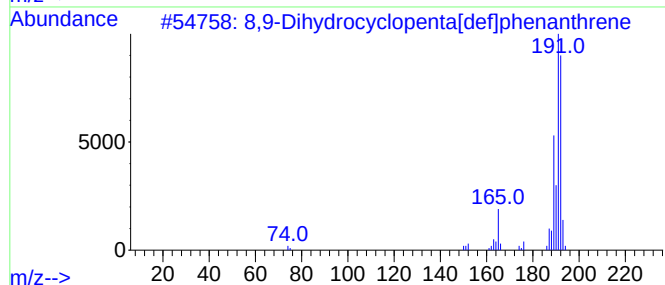
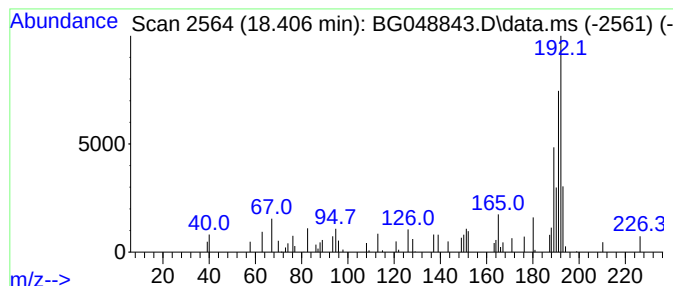
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 8,9-Dihydrocyclopenta[def]p... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.406	2.31 ng	39197	Phenanthrene-d10	17.477

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	58
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	52
3		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	52
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	52
5		Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	52



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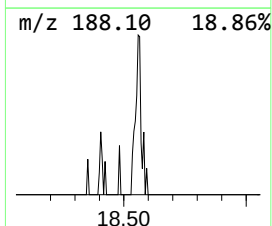
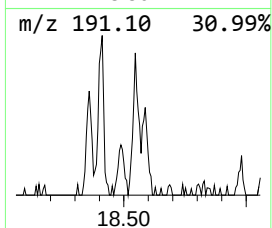
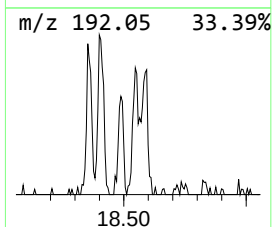
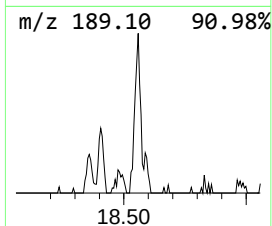
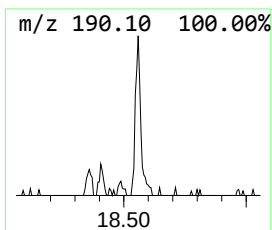
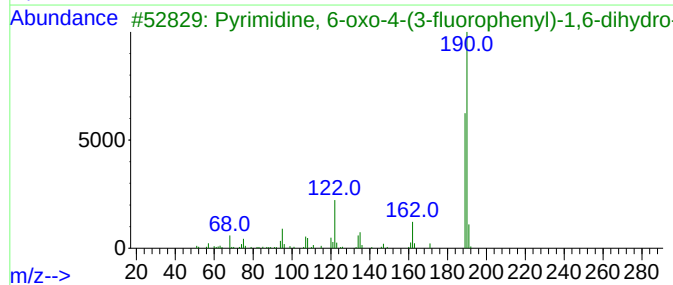
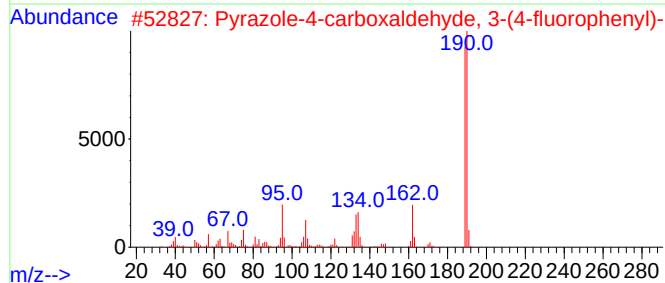
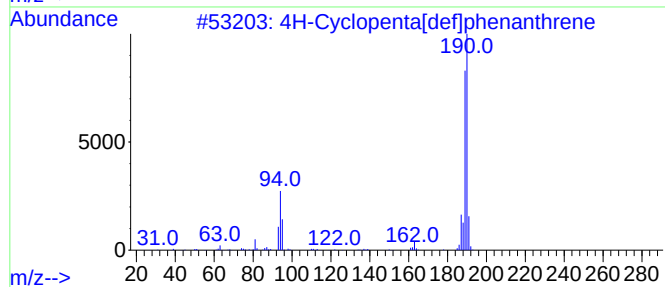
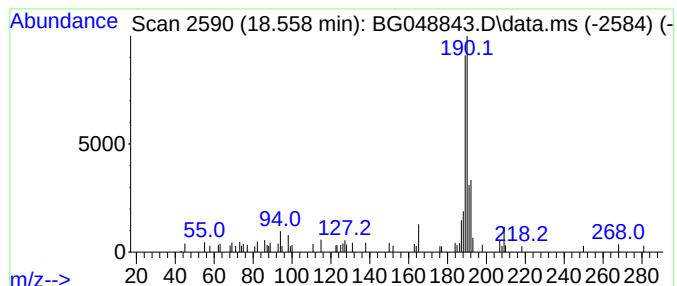
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.558	3.03 ng	51392	Phenanthrene-d10	17.477

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
3			Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	42
4			Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	36
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33



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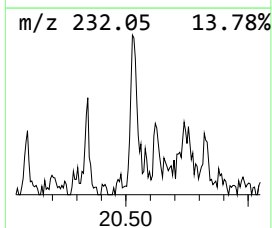
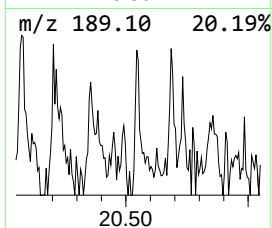
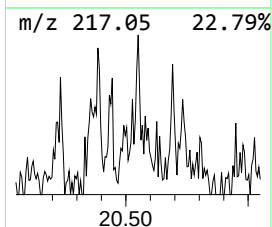
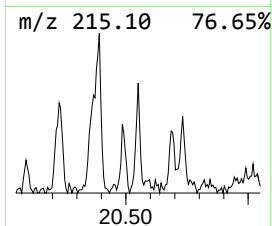
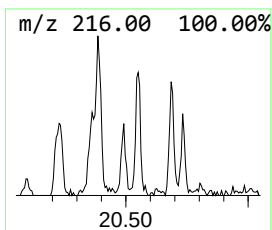
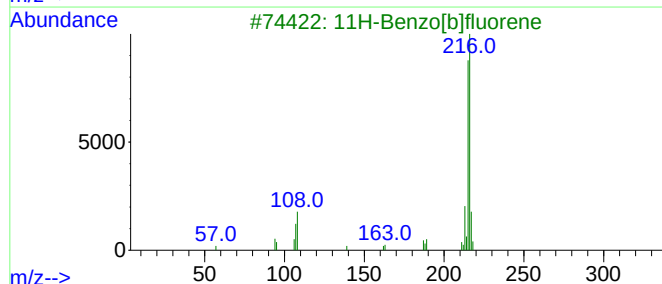
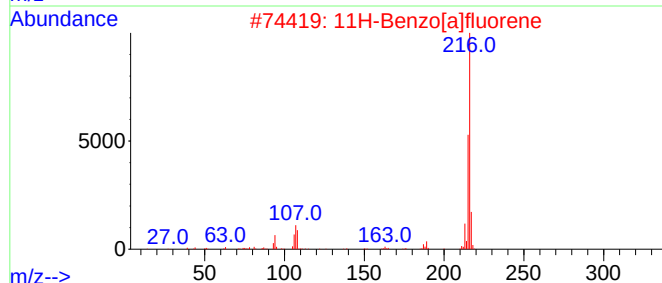
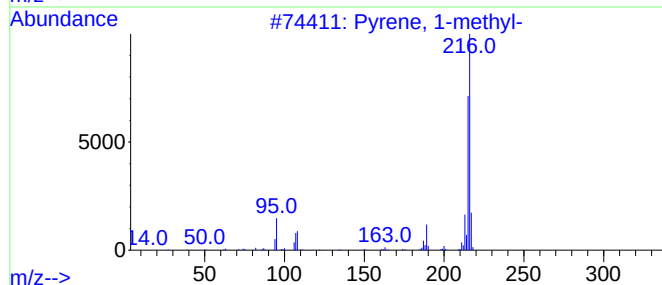
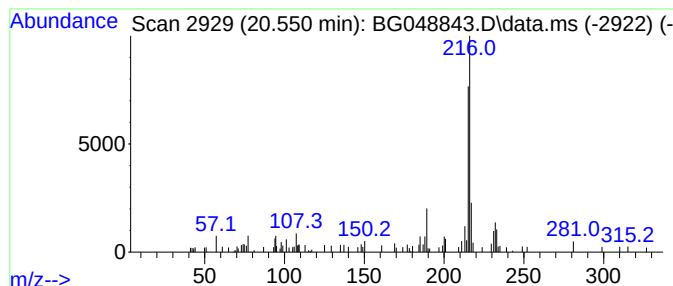
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.550	2.05 ng	66873	Chrysene-d12	21.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	68
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5			3-Pyridinamine, 6-chloro-N-(phen...	216	C12H9ClN2	005325-71-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FS-SB12A(7-8)

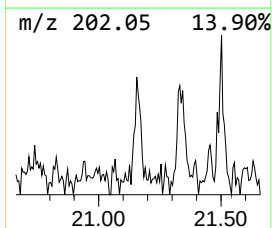
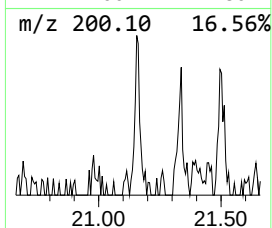
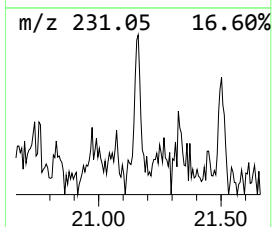
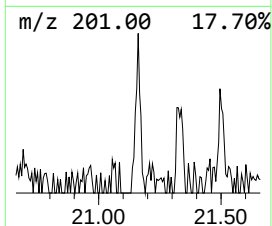
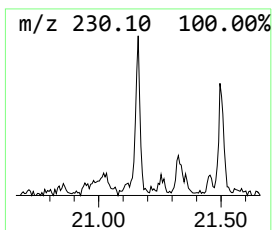
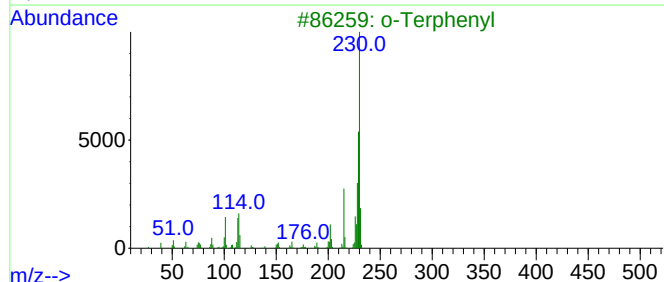
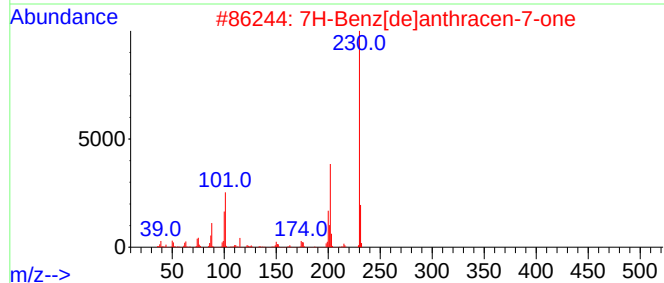
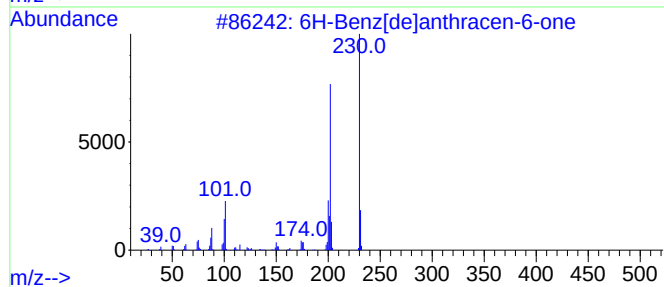
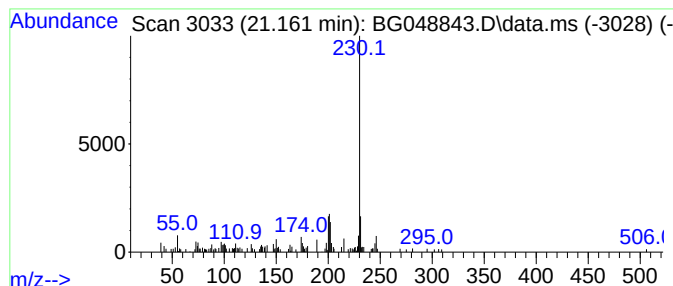
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 6H-Benz[de]anthracen-6-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.161	2.09 ng	68240	Chrysene-d12	21.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	68
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	64
3			o-Terphenyl	230	C18H14	000084-15-1	64
4			4,4'-Stilbenedicarbonitrile	230	C16H10N2	006292-62-2	59
5			Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB12A(7-8)

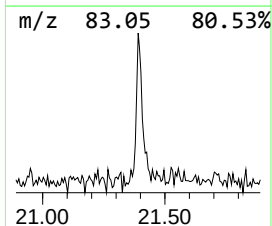
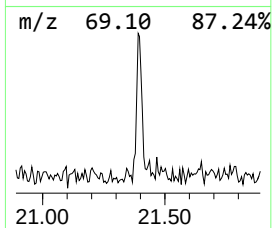
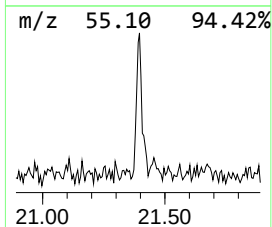
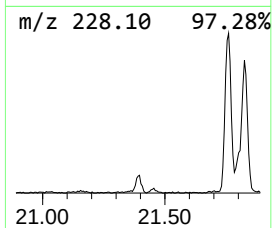
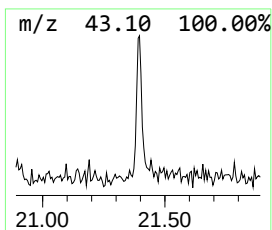
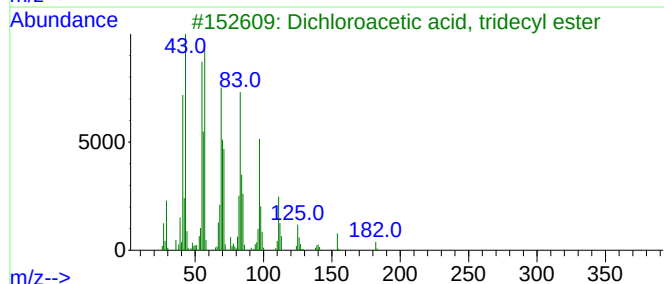
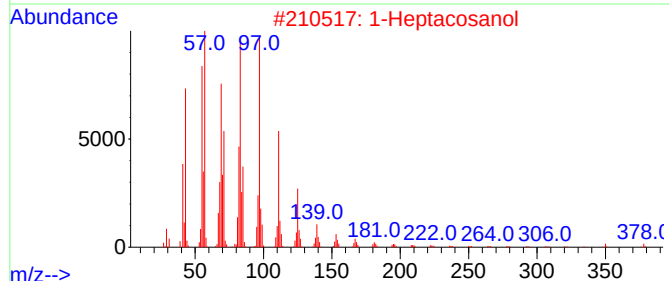
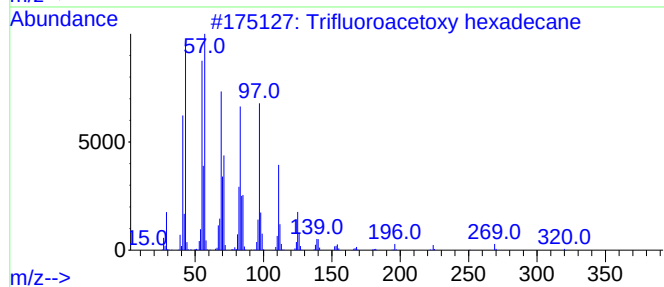
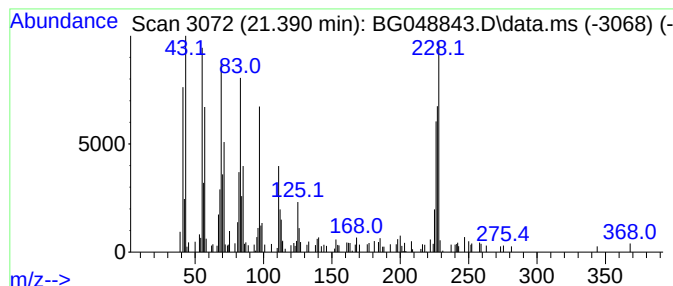
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.390	4.42 ng	144427	Chrysene-d12	21.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	55
2			1-Heptacosanol	396	C27H56O	002004-39-9	53
3			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	53
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	49
5			Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB12A(7-8)

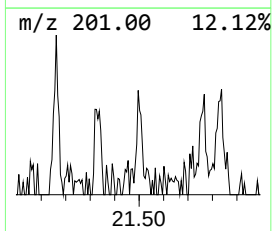
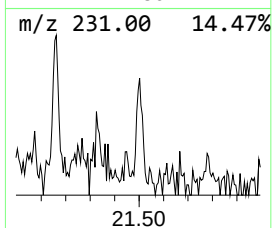
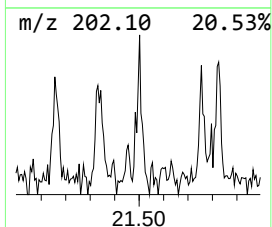
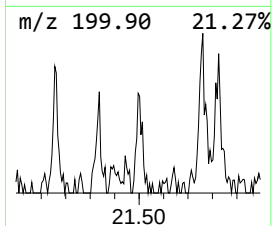
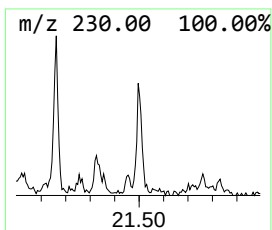
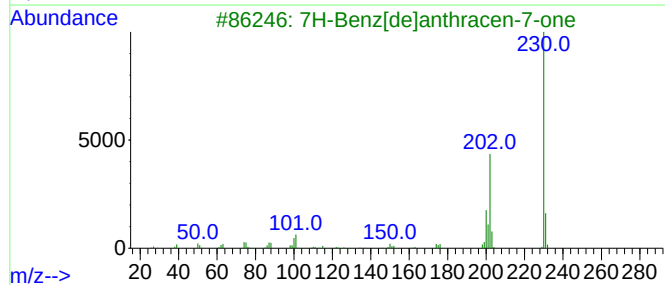
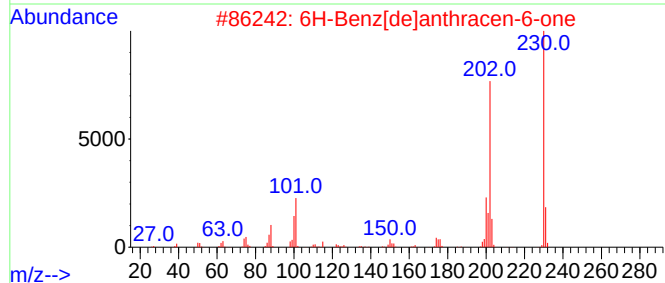
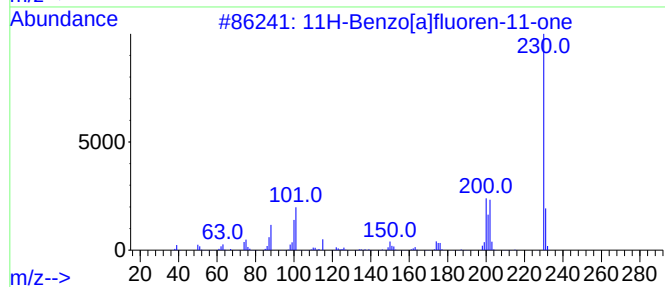
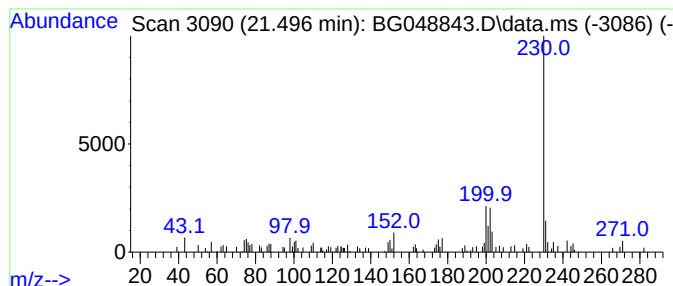
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.496	2.08 ng	67845	Chrysene-d12	21.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	81
2			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	76
3			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	76
4			Benzene, 1-phenyl-4-(2,2-dicyano...	230	C16H10N2	026089-09-8	62
5			p-Terphenyl	230	C18H14	000092-94-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB12A(7-8)

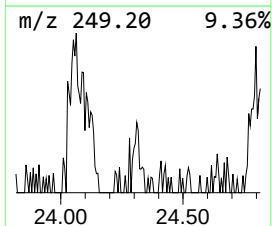
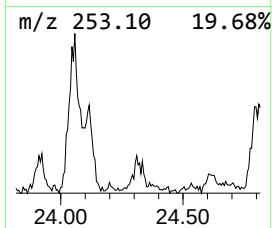
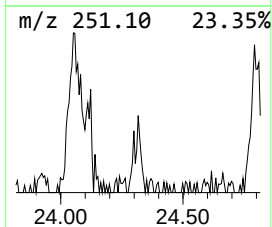
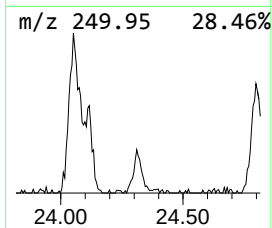
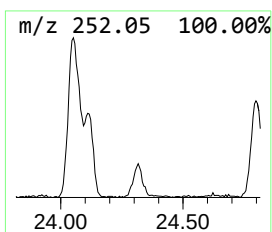
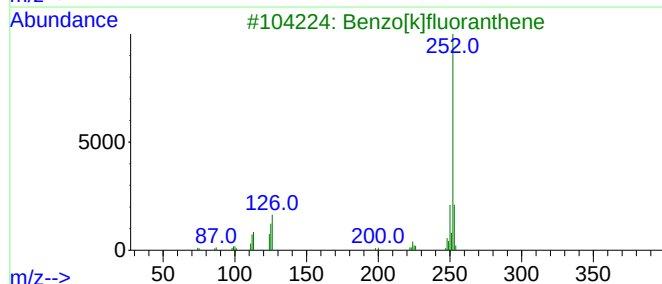
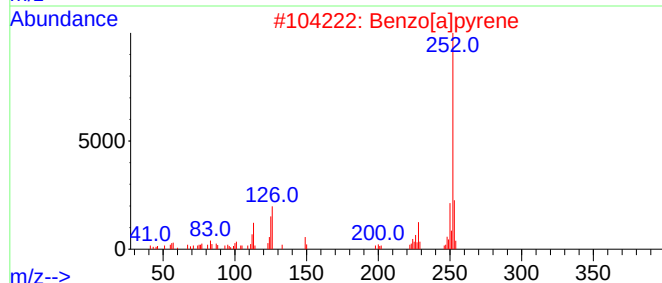
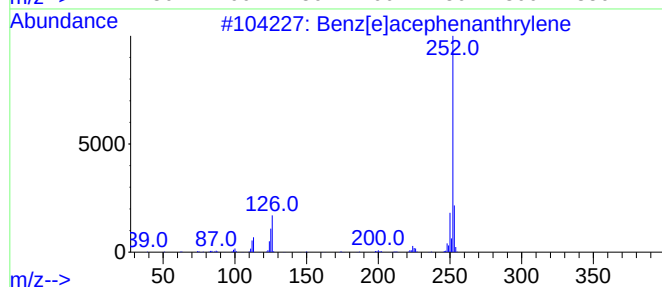
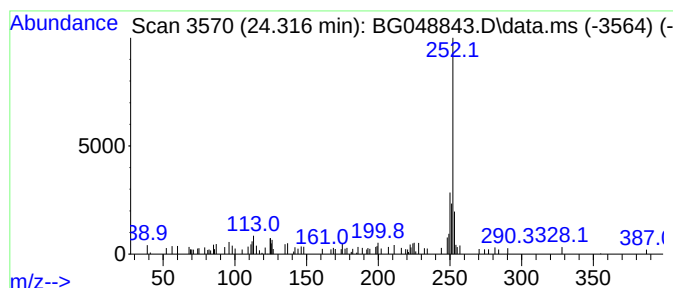
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 (1-Cyclopentenyl)ferrocene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.316	2.56 ng	52263	Perylene-d12	25.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
2			Benzo[a]pyrene	252	C20H12	000050-32-8	70
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	62
4			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	59
5			1H-Pyrrolo[2,3-g]quinoline, 1,2,...	252	C17H20N2	1000338-03-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB12A(7-8)

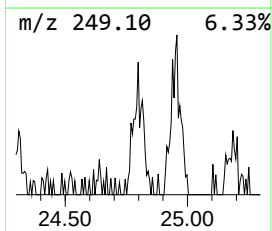
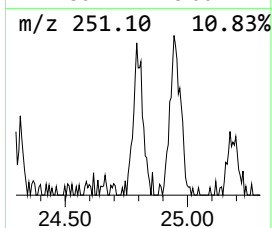
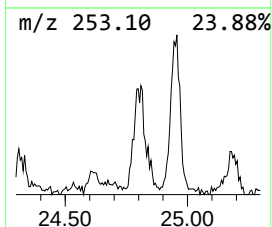
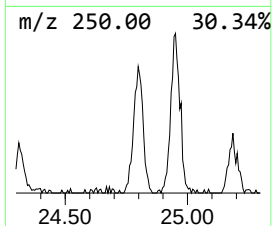
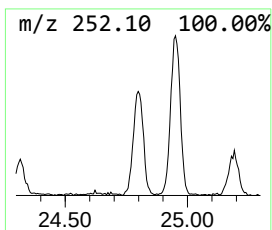
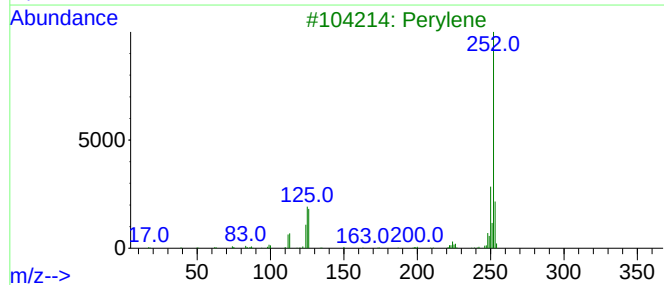
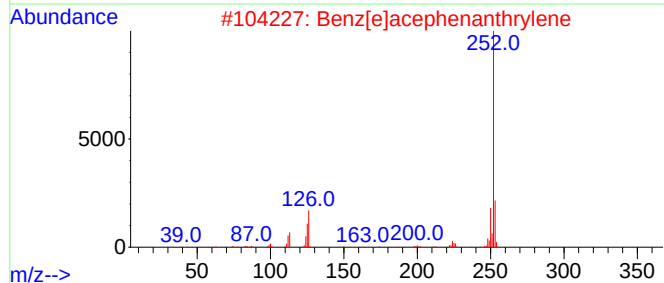
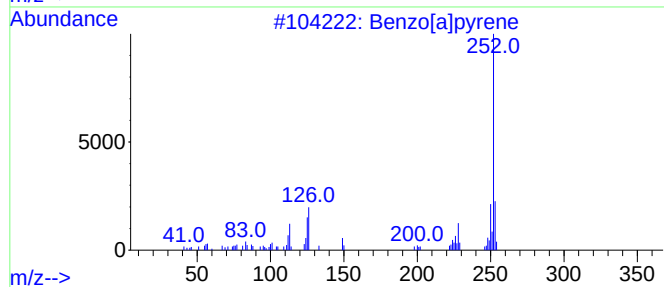
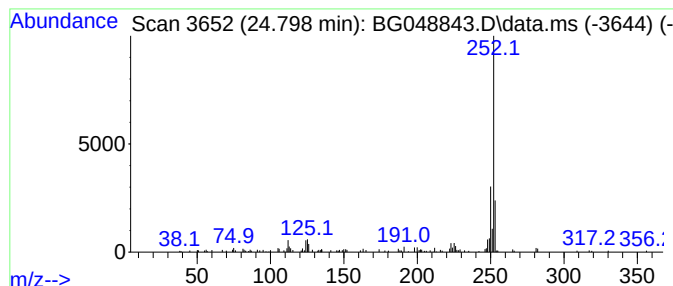
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.798	10.43 ng	212918	Perylene-d12	25.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	89
2			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3			Perylene	252	C20H12	000198-55-0	76
4			Benzo[e]pyrene	252	C20H12	000192-97-2	68
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB12A(7-8)

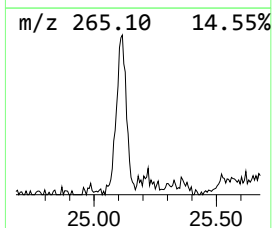
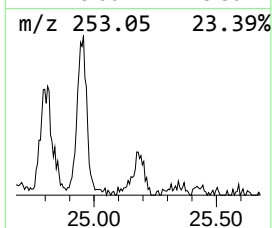
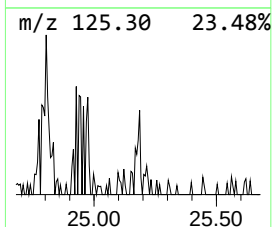
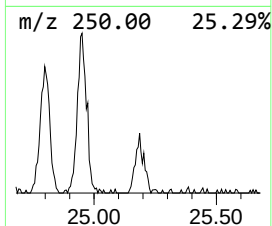
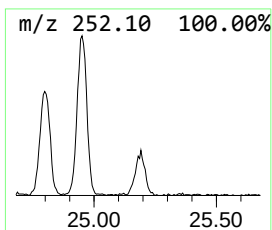
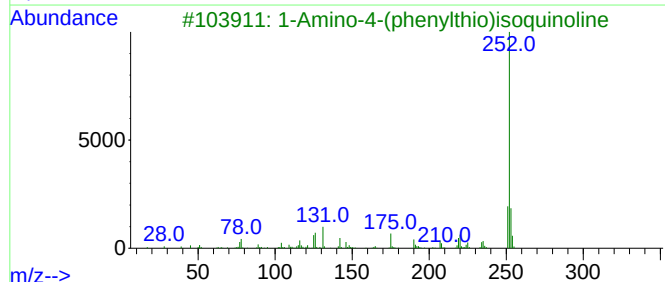
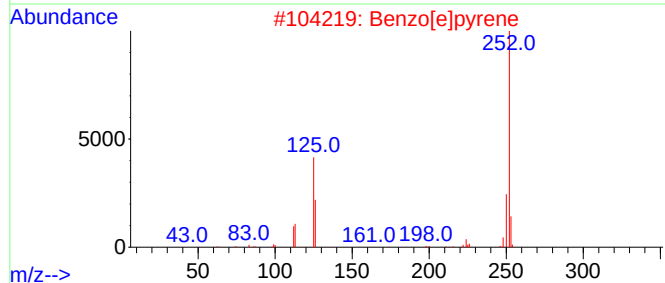
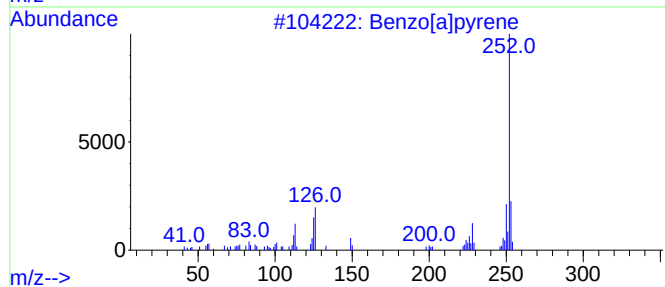
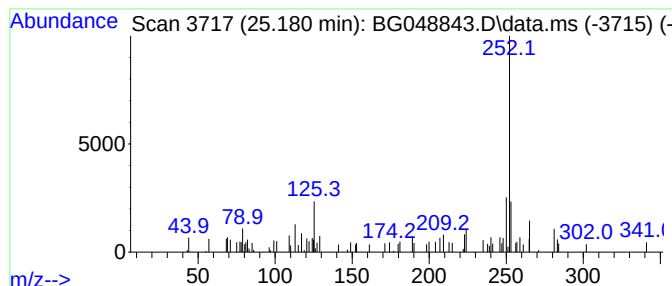
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.180	3.16 ng	64579	Perylene-d12	25.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	46
2			Benzo[e]pyrene	252	C20H12	000192-97-2	43
3			1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	43
4			12-H-Benzimidazo(2,1-b)-1,3-benz...	252	C14H8N2OS	063586-54-9	43
5			Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-06-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048843.D
Acq On : 22 Apr 2021 12:20
Operator : CG/JU
Sample : M2042-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FS-SB12A(7-8)

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
Diphenylacetylene	17.612	2.2	ng	37296	4	17.477	338785	20.0
unknown18.36	18.364	4.7	ng	79047	4	17.477	338785	20.0
8,9-Dihydrocyclo...	18.406	2.3	ng	39197	4	17.477	338785	20.0
4H-Cyclopenta[d]...	18.558	3.0	ng	51392	4	17.477	338785	20.0
Pyrene, 1-methyl-	20.550	2.0	ng	66873	5	21.778	653068	20.0
6H-Benz[de]anth...	21.161	2.1	ng	68240	5	21.778	653068	20.0
Trifluoroacetox...	21.390	4.4	ng	144427	5	21.778	653068	20.0
11H-Benzo[a]flu...	21.496	2.1	ng	67845	5	21.778	653068	20.0
(1-Cyclopentenyl...	24.316	2.6	ng	52263	6	25.115	408217	20.0
Perylene	24.798	10.4	ng	212918	6	25.115	408217	20.0
Benzo[e]pyrene	25.180	3.2	ng	64579	6	25.115	408217	20.0