

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
 Data File : BG051093.D
 Acq On : 17 Nov 2021 15:37
 Operator : CG/JU
 Sample : M4680-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-3

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-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051093.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.287	300	306	316	rVB	112846	175647	7.67%	0.988%
2	5.763	380	387	395	rBV	793778	1306900	57.10%	7.354%
3	7.379	651	662	678	rBV	828598	1481269	64.72%	8.336%
4	8.225	799	806	820	rBV	128708	220904	9.65%	1.243%
5	9.400	997	1006	1017	rBV	509232	937121	40.95%	5.274%
6	10.799	1235	1244	1255	rBV	24931	52922	2.31%	0.298%
7	11.051	1278	1287	1293	rBV	186955	349358	15.27%	1.966%
8	11.104	1293	1296	1302	rVB	26932	41641	1.82%	0.234%
9	12.690	1560	1566	1573	rVB2	14742	23541	1.03%	0.132%
10	13.472	1692	1699	1709	rBV	1216543	1926057	84.16%	10.839%
11	14.853	1923	1934	1940	rBV	313157	488880	21.36%	2.751%
12	14.917	1940	1945	1953	rVB	36481	57663	2.52%	0.324%
13	15.246	1995	2001	2008	rVB	28893	48818	2.13%	0.275%
14	15.893	2105	2111	2121	rVB2	46087	80606	3.52%	0.454%
15	16.339	2180	2187	2198	rBV	912553	1443033	63.05%	8.120%
16	17.320	2349	2354	2359	rBV6	17559	35576	1.55%	0.200%
17	17.420	2366	2371	2377	rVB	22729	38439	1.68%	0.216%
18	17.602	2395	2402	2405	rBV	347243	559070	24.43%	3.146%
19	17.643	2405	2409	2415	rVV	368858	554971	24.25%	3.123%
20	17.732	2415	2424	2430	rVV	89373	169990	7.43%	0.957%
21	18.002	2463	2470	2476	rBV	46977	81476	3.56%	0.458%
22	18.472	2542	2550	2554	rBV2	55779	121514	5.31%	0.684%
23	18.519	2554	2558	2564	rVB	69052	108878	4.76%	0.613%
24	18.601	2567	2572	2576	rVB	30176	46785	2.04%	0.263%
25	18.672	2577	2584	2587	rBV2	66668	135635	5.93%	0.763%
26	18.701	2587	2589	2594	rVB2	31187	36799	1.61%	0.207%
27	18.960	2629	2633	2637	rBV	35462	48870	2.14%	0.275%
28	19.012	2637	2642	2647	rBV	26290	37225	1.63%	0.209%
29	19.371	2698	2703	2709	rBV	31807	66148	2.89%	0.372%
30	19.524	2724	2729	2734	rBV4	23353	42378	1.85%	0.238%
31	19.641	2743	2749	2755	rBV	505086	743277	32.48%	4.183%
32	19.970	2800	2805	2807	rBV2	81588	135095	5.90%	0.760%
33	20.005	2807	2811	2818	rVV	409125	605749	26.47%	3.409%
34	20.064	2818	2821	2828	rVB2	31087	52973	2.31%	0.298%
35	20.188	2836	2842	2848	rBV	1725815	2288610	100.00%	12.879%
36	20.329	2860	2866	2871	rVB3	32754	70052	3.06%	0.394%

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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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.458	2882	2888	2890	rBV6	33303	67606	2.95%	0.380%
38	20.487	2890	2893	2899	rVB	69429	102511	4.48%	0.577%
39	20.587	2906	2910	2914	rBV	53472	80177	3.50%	0.451%
40	21.269	3023	3026	3032	rVB	37370	57094	2.49%	0.321%
41	21.498	3061	3065	3071	rVB4	69356	140495	6.14%	0.791%
42	21.891	3125	3132	3138	rBV3	341587	886639	38.74%	4.989%
43	21.950	3138	3142	3148	rVB	176653	297655	13.01%	1.675%
44	24.224	3522	3529	3548	rVB2	121409	584264	25.53%	3.288%
45	24.994	3656	3660	3676	rVB2	69651	202938	8.87%	1.142%
46	25.152	3680	3687	3699	rVB2	106780	323128	14.12%	1.818%
47	25.317	3707	3715	3724	rVB3	143018	413984	18.09%	2.330%

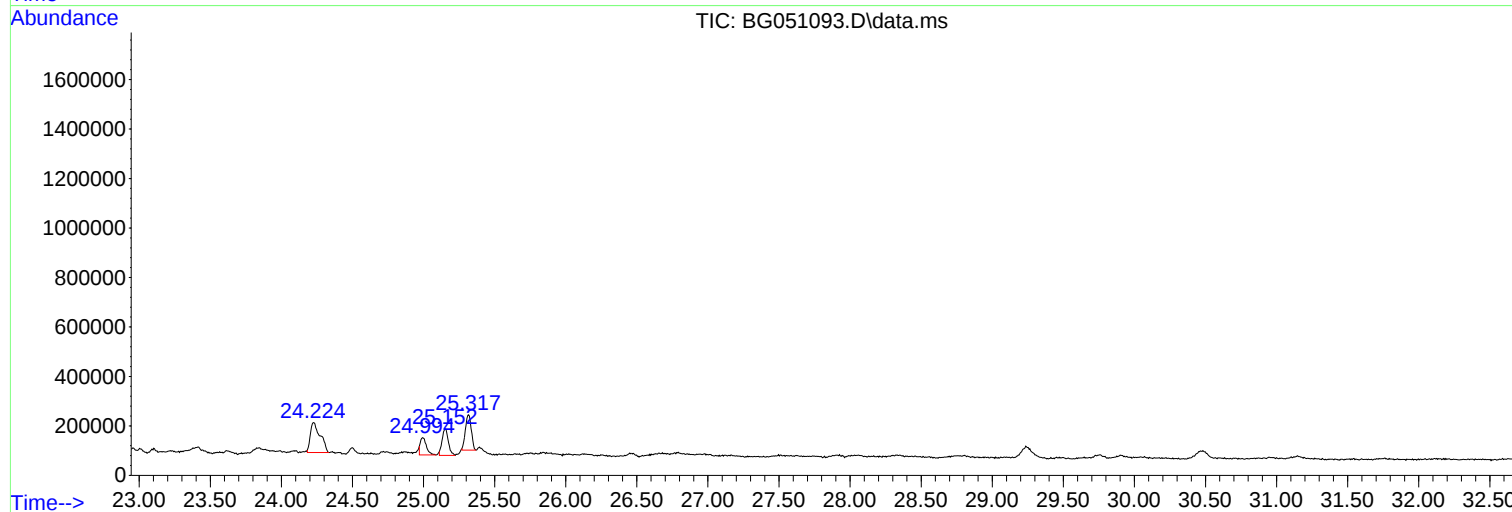
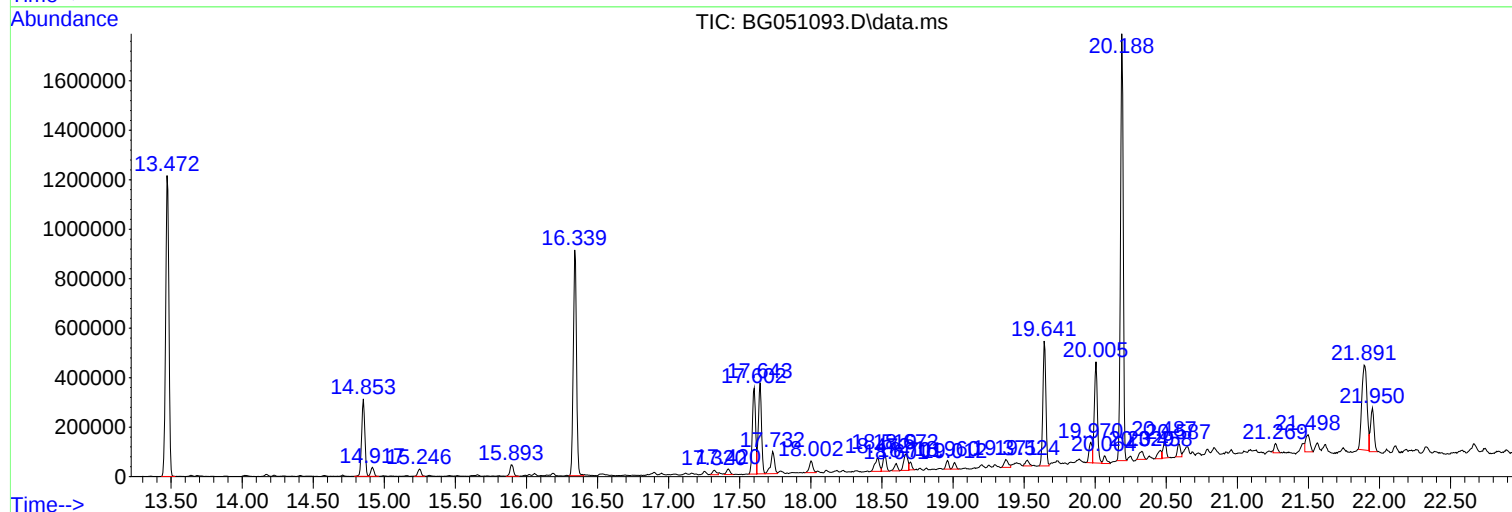
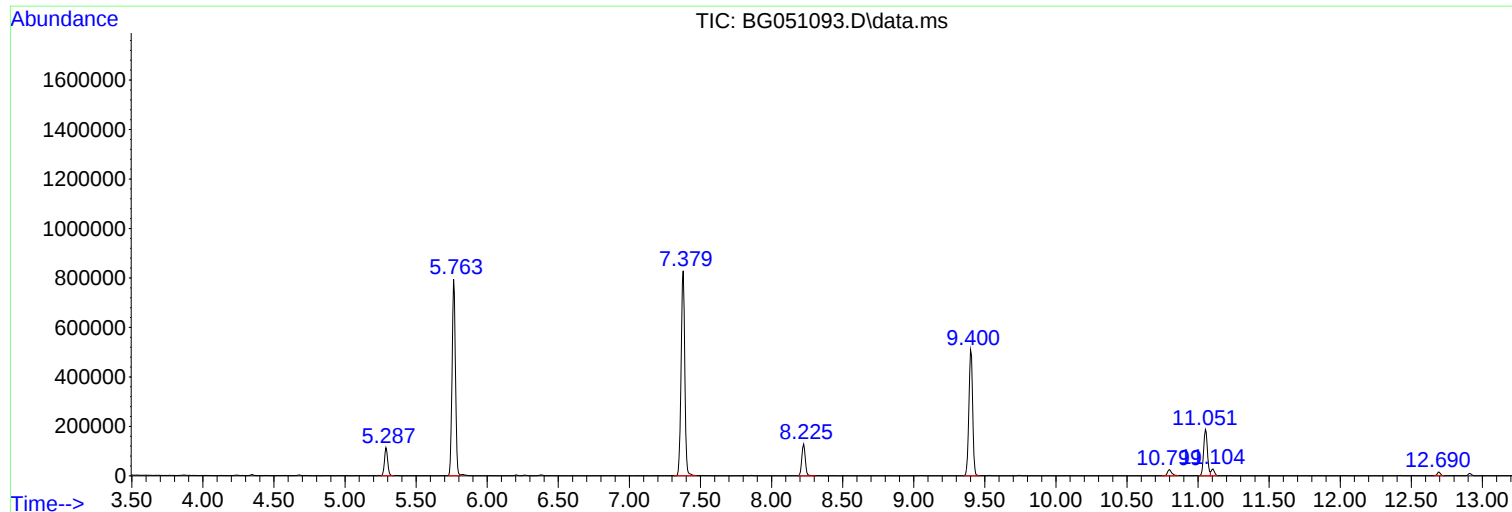
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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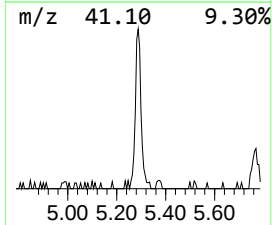
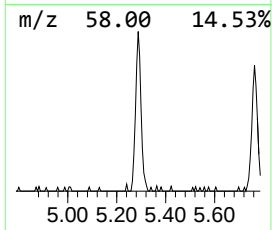
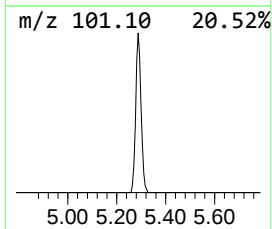
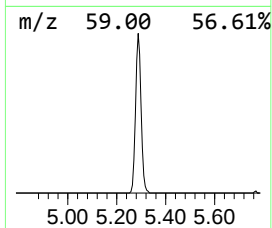
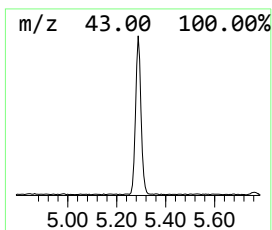
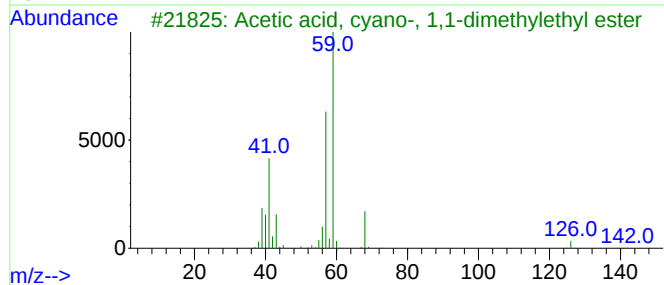
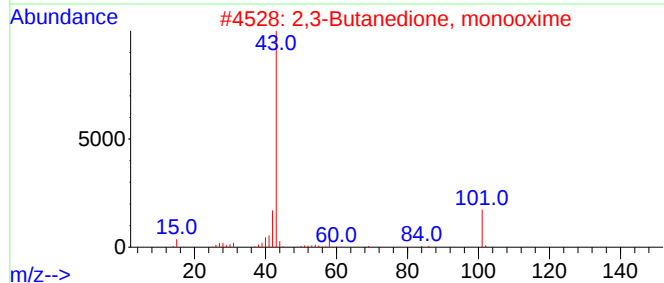
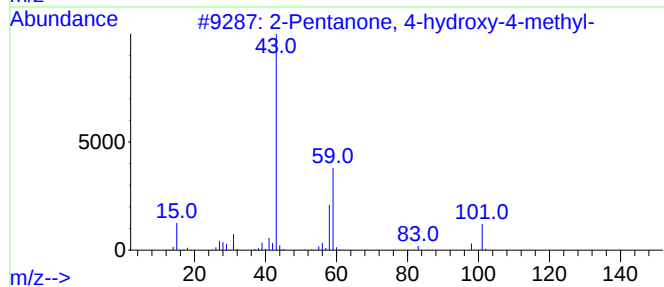
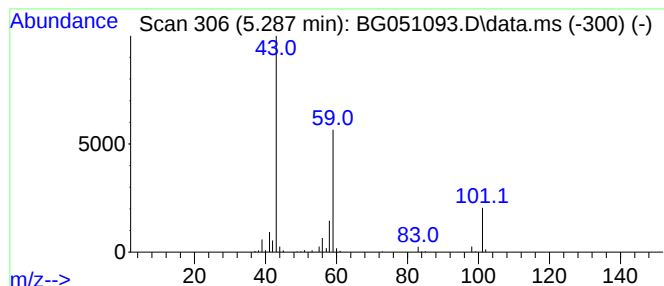
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.287	15.90 ng	175647	1,4-Dichlorobenzene-d4	8.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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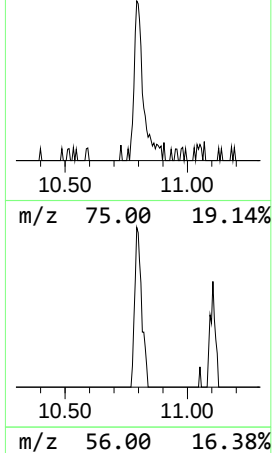
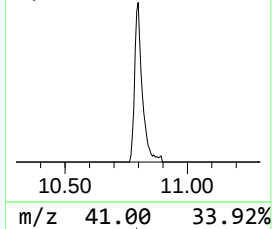
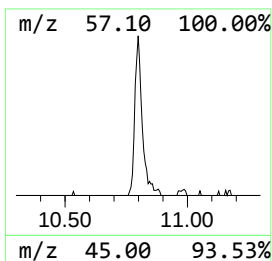
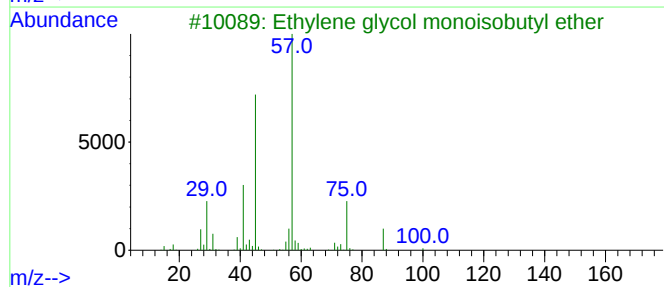
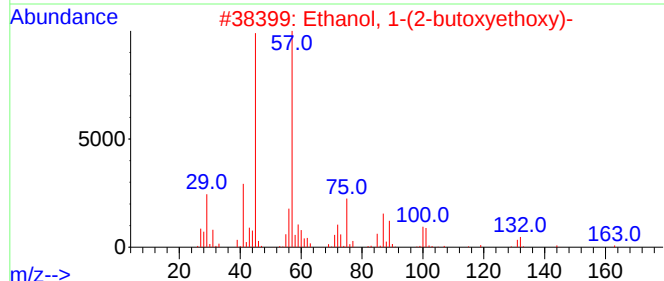
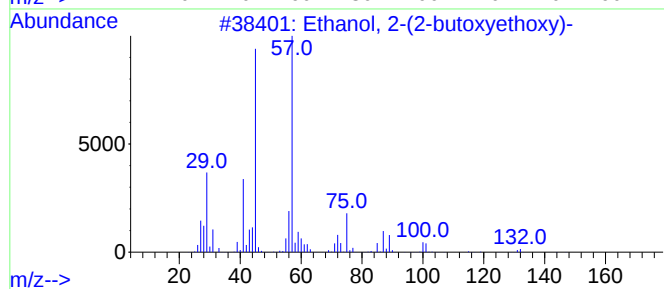
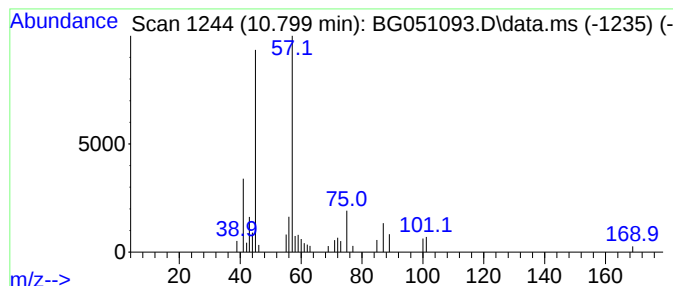
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.799	3.03 ng	52922	Naphthalene-d8	11.051

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	86
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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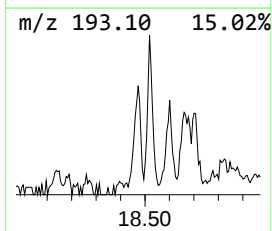
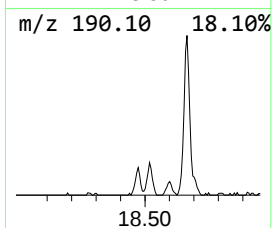
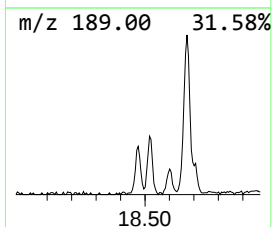
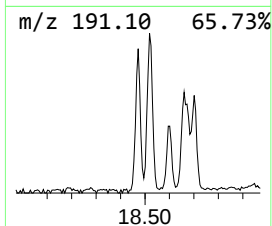
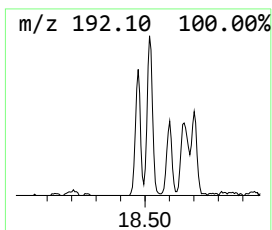
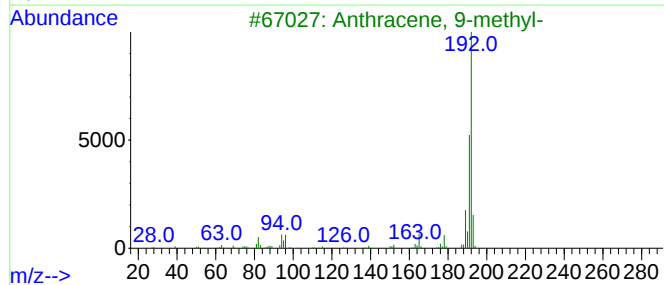
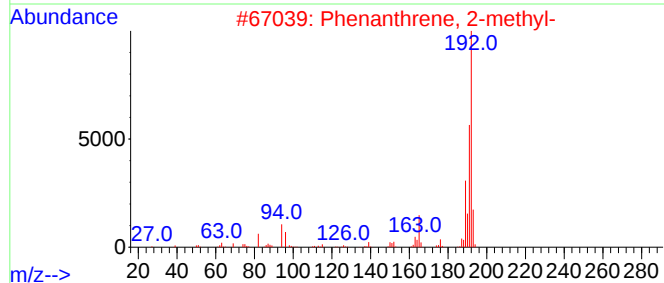
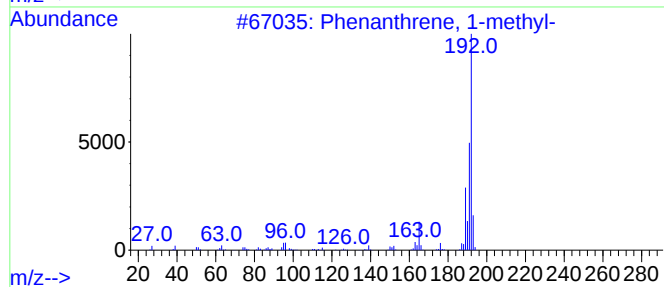
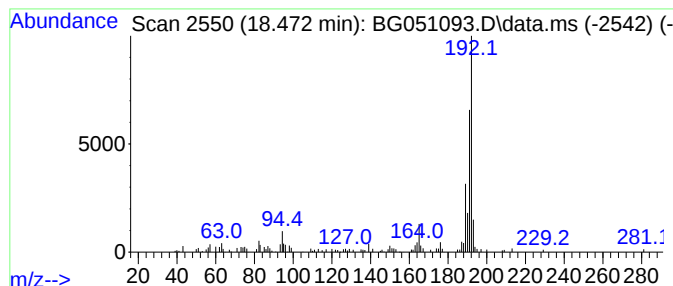
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.472	4.35 ng	121514	Phenanthrene-d10	17.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87
5			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	81



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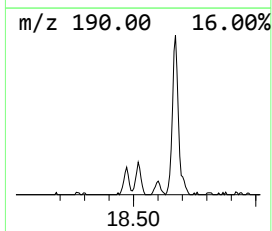
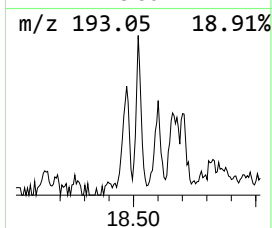
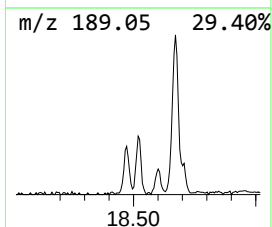
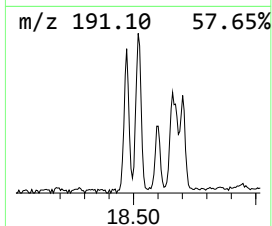
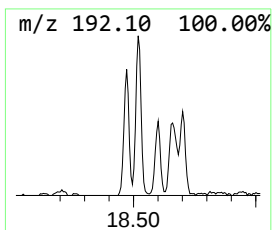
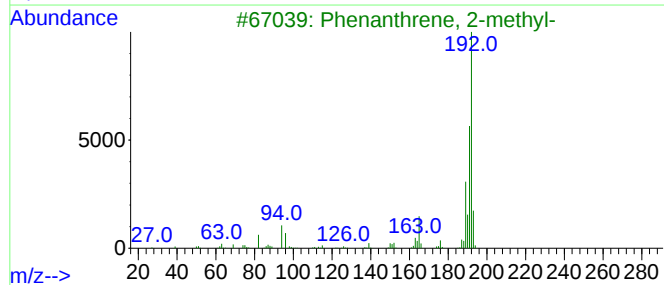
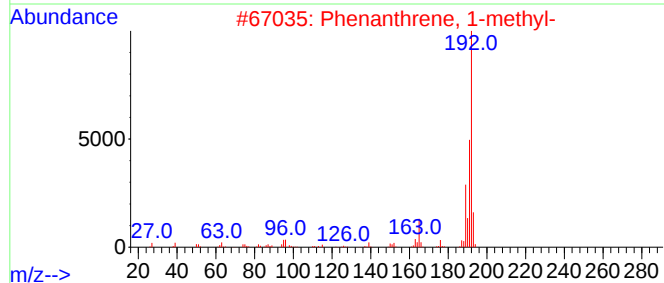
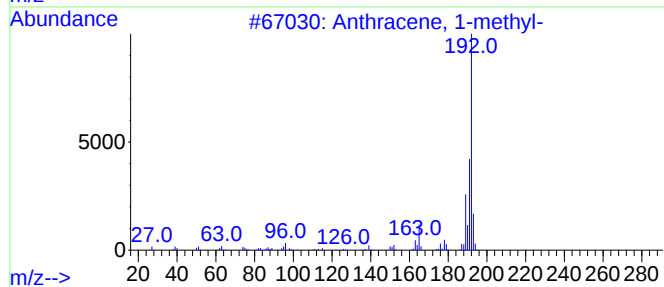
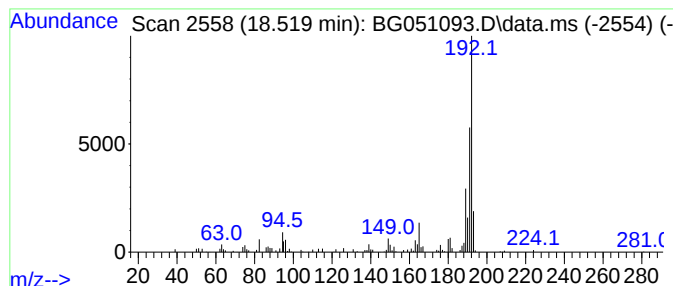
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.519	3.89 ng	108878	Phenanthrene-d10	17.602

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	90



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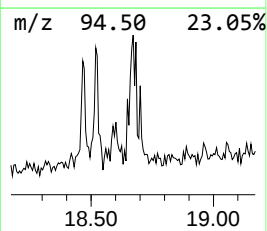
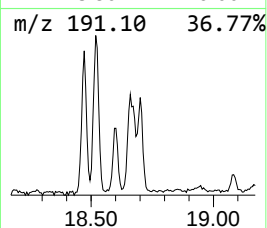
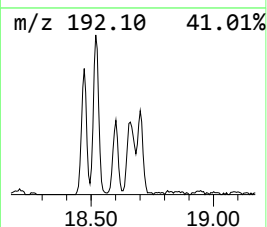
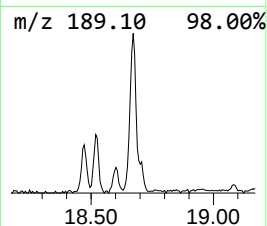
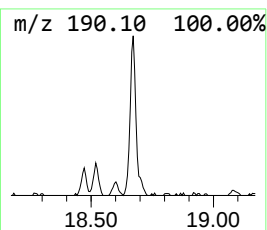
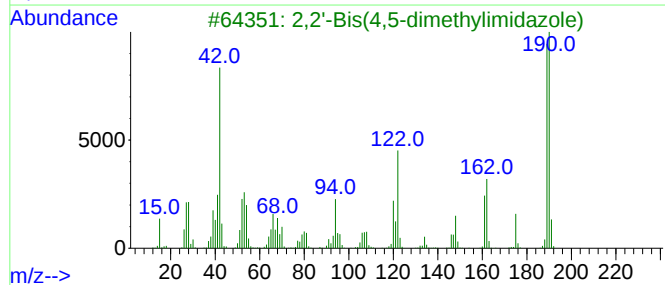
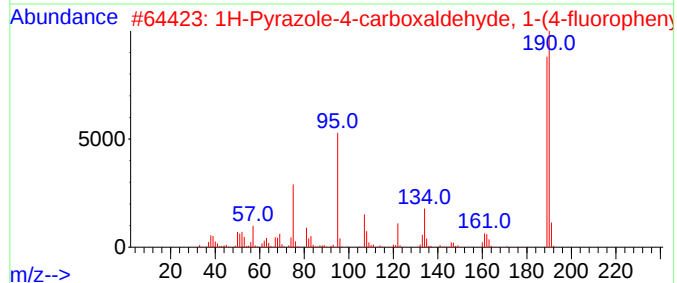
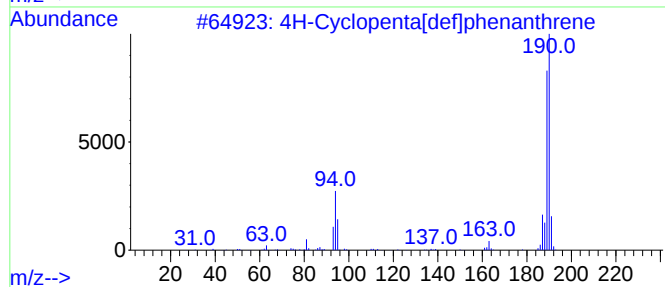
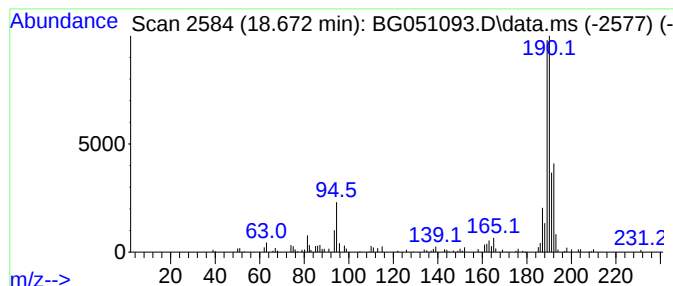
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.672	4.85 ng	135635	Phenanthrene-d10	17.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2			1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	49
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25
5			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051093.D
Acq On : 17 Nov 2021 15:37
Operator : CG/JU
Sample : M4680-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

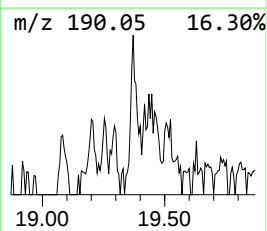
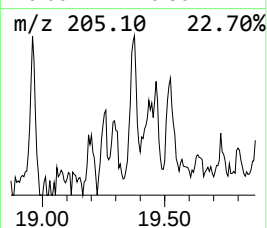
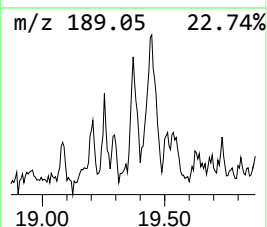
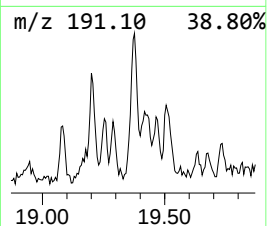
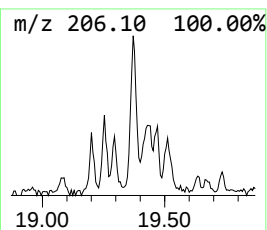
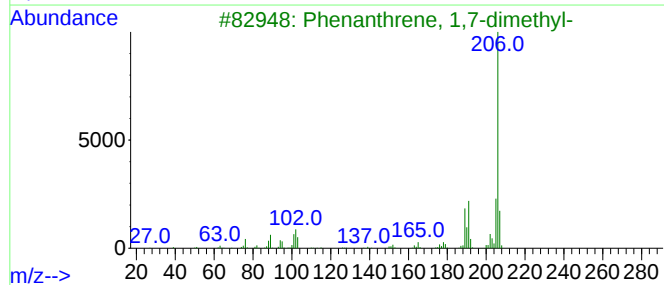
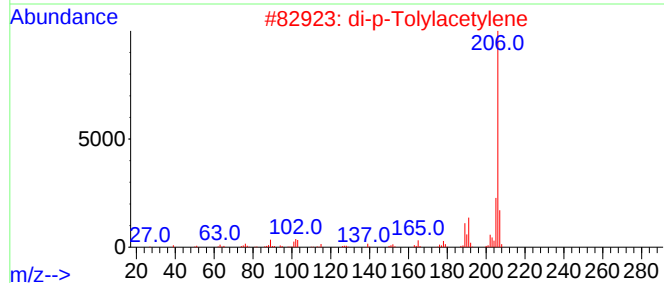
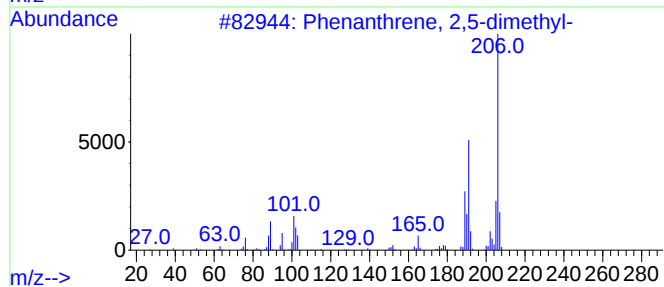
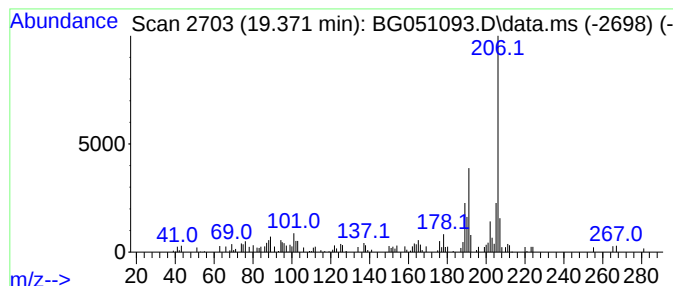
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ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.371	2.37 ng	66148	Phenanthrene-d10		17.602	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	97
2	di-p-Tolylacetylene		206	C16H14	002789-88-0	94
3	Phenanthrene, 1,7-dimethyl-		206	C16H14	000483-87-4	93
4	Phenanthrene, 2,3-dimethyl-		206	C16H14	003674-65-5	91
5	3,4-Dimethylphenanthrene		206	C16H14	1000452-24-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051093.D
Acq On : 17 Nov 2021 15:37
Operator : CG/JU
Sample : M4680-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

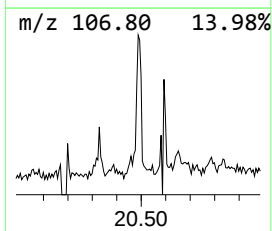
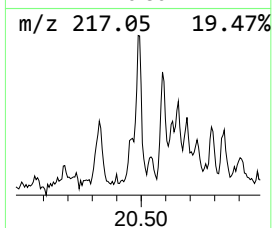
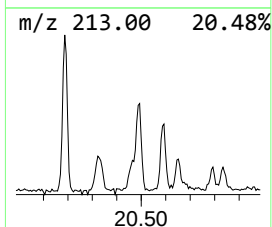
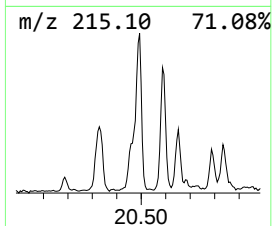
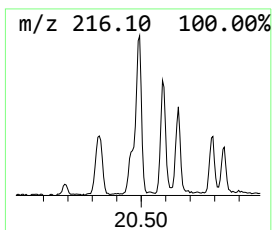
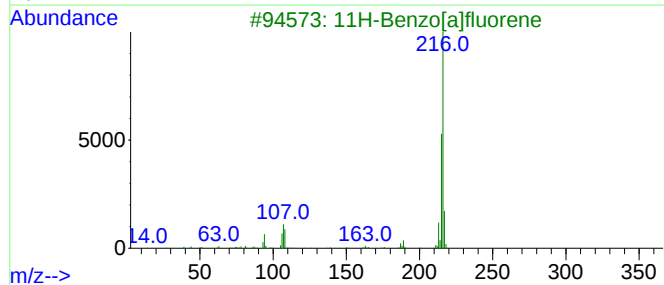
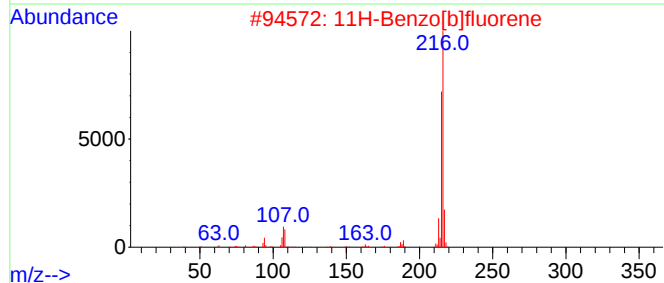
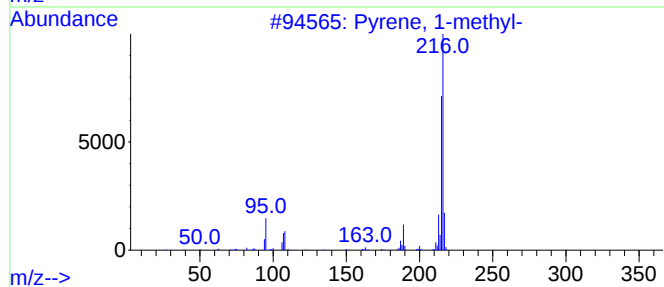
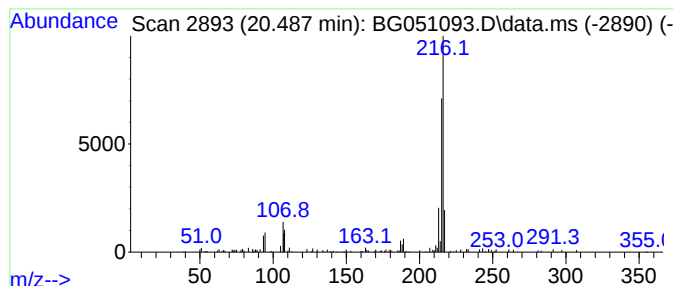
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.487	2.31 ng	102511	Chrysene-d12	21.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051093.D
Acq On : 17 Nov 2021 15:37
Operator : CG/JU
Sample : M4680-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

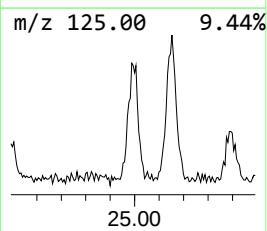
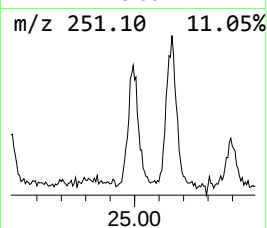
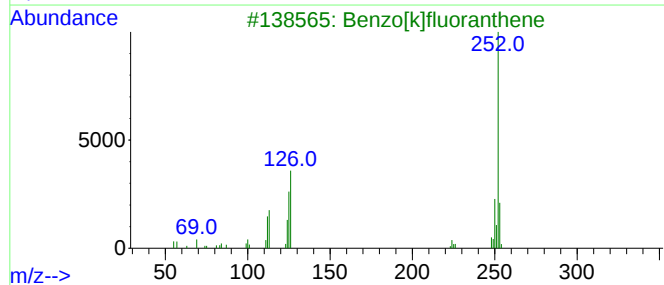
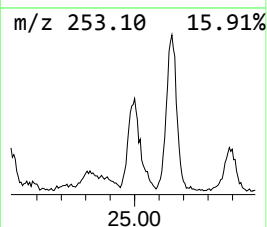
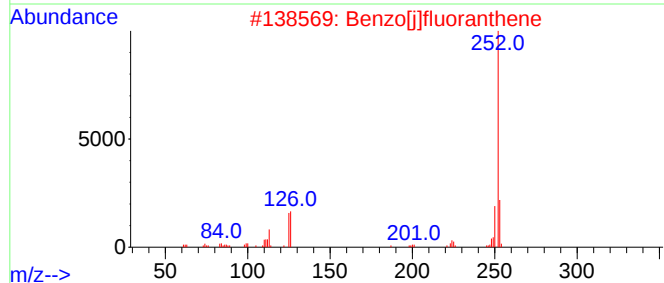
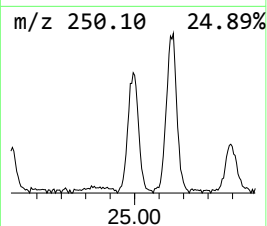
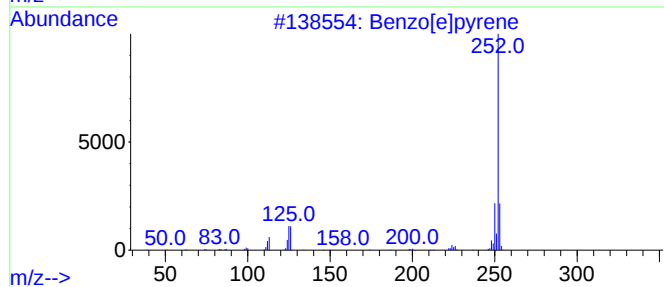
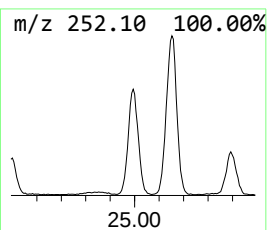
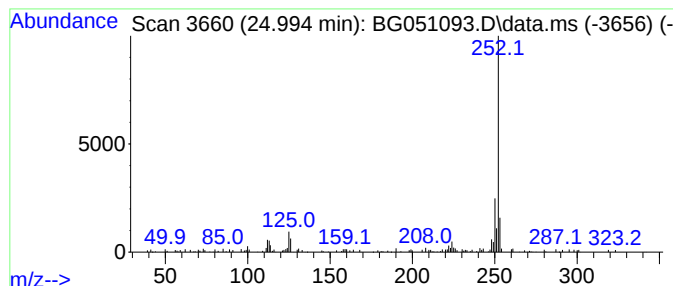
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.994	9.80 ng	202938	Perylene-d12	25.317

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	90
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
5			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051093.D
Acq On : 17 Nov 2021 15:37
Operator : CG/JU
Sample : M4680-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.287	15.9	ng	175647	1	8.225	220904	20.0
Ethanol, 2-(2-b...	10.799	3.0	ng	52922	2	11.051	349358	20.0
Phenanthrene, 1...	18.472	4.3	ng	121514	4	17.602	559070	20.0
Anthracene, 1-m...	18.519	3.9	ng	108878	4	17.602	559070	20.0
4H-Cyclopenta[d...	18.672	4.8	ng	135635	4	17.602	559070	20.0
Phenanthrene, 2...	19.371	2.4	ng	66148	4	17.602	559070	20.0
Pyrene, 1-methyl-	20.487	2.3	ng	102511	5	21.903	886639	20.0
Benzo[e]pyrene	24.994	9.8	ng	202938	6	25.317	413984	20.0