

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
 Data File : BF136432.D
 Acq On : 06 Dec 2023 17:13
 Operator : CG\JU
 Sample : 05602-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROUTE-4-TP-4

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_F\Methods\8270-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	12	15	20	rVB2	20772	27876	1.80%	0.196%
2	5.028	497	500	505	rBV	32409	35208	2.27%	0.248%
3	5.428	564	568	571	rBV	1756231	1547695	100.00%	10.898%
4	6.428	734	738	741	rBV	1501189	1451401	93.78%	10.220%
5	6.799	797	801	806	rBV	635053	557159	36.00%	3.923%
6	6.922	818	822	827	rBV	35097	36006	2.33%	0.254%
7	7.069	844	847	849	rBV	31635	22724	1.47%	0.160%
8	7.134	855	858	861	rBV	22802	19829	1.28%	0.140%
9	7.357	891	896	899	rBV	994922	915295	59.14%	6.445%
10	8.075	1014	1018	1021	rBV	757705	631507	40.80%	4.447%
11	9.151	1197	1201	1204	rBV	1813235	1432503	92.56%	10.087%
12	9.828	1309	1316	1320	rBV	695787	563336	36.40%	3.967%
13	10.375	1406	1409	1416	rBV2	33643	33319	2.15%	0.235%
14	10.616	1447	1450	1463	rVB	834646	724817	46.83%	5.104%
15	10.928	1496	1503	1506	rBV3	20048	27839	1.80%	0.196%
16	11.322	1566	1570	1572	rBV	570966	535150	34.58%	3.768%
17	11.345	1572	1574	1577	rVV	308876	251060	16.22%	1.768%
18	11.392	1579	1582	1586	rVB	108831	96393	6.23%	0.679%
19	11.822	1649	1655	1658	rBV	67040	66067	4.27%	0.465%
20	11.851	1658	1660	1664	rVV	159637	155267	10.03%	1.093%
21	11.898	1665	1668	1671	rVV2	55077	56844	3.67%	0.400%
22	11.934	1671	1674	1677	rVV	111273	126872	8.20%	0.893%
23	11.957	1677	1678	1683	rVB	60957	40283	2.60%	0.284%
24	12.122	1697	1706	1709	rBV	40760	59396	3.84%	0.418%
25	12.375	1745	1749	1752	rBV	54655	60125	3.88%	0.423%
26	12.416	1752	1756	1761	rVB4	39139	59281	3.83%	0.417%
27	12.463	1761	1764	1769	rBV4	17906	30224	1.95%	0.213%
28	12.539	1773	1777	1780	rBV	440042	392226	25.34%	2.762%
29	12.645	1790	1795	1800	rBV7	13188	19578	1.26%	0.138%
30	12.769	1809	1816	1818	rBV	401705	424819	27.45%	2.991%
31	12.786	1818	1819	1822	rVV	40176	30810	1.99%	0.217%
32	12.816	1822	1824	1829	rVB2	26147	35554	2.30%	0.250%
33	12.886	1833	1836	1837	rVV	25657	22977	1.48%	0.162%
34	12.916	1837	1841	1844	rVV	1529050	1368029	88.39%	9.633%
35	12.986	1847	1853	1860	rBV4	35699	67575	4.37%	0.476%
36	13.075	1865	1868	1869	rBV2	25374	24142	1.56%	0.170%

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Filtering: 5

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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

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37	13.098	1869	1872	1876	rVB	90991	87430	5.65%	0.616%
38	13.163	1876	1883	1886	rBV	101003	109148	7.05%	0.769%
39	13.198	1886	1889	1893	rBV2	46102	50240	3.25%	0.354%
40	13.292	1902	1905	1908	rVB	34772	29966	1.94%	0.211%
41	13.322	1908	1910	1916	rBV	35932	45560	2.94%	0.321%
42	13.580	1951	1954	1957	rBV5	19809	26484	1.71%	0.186%
43	13.722	1973	1978	1980	rBV2	28933	43780	2.83%	0.308%
44	13.745	1980	1982	1984	rVV	25736	21014	1.36%	0.148%
45	13.969	2015	2020	2023	rBV2	666496	751041	48.53%	5.289%
46	13.998	2023	2025	2027	rVB	154097	116506	7.53%	0.820%
47	14.075	2033	2038	2041	rVB3	59059	62983	4.07%	0.443%
48	14.328	2078	2081	2083	rBV3	15410	19247	1.24%	0.136%
49	14.357	2084	2086	2090	rVV	44698	50610	3.27%	0.356%
50	14.392	2090	2092	2095	rVB	27094	24157	1.56%	0.170%
51	14.457	2099	2103	2105	rVV2	44952	48498	3.13%	0.342%
52	15.016	2195	2198	2201	rBV	92762	136295	8.81%	0.960%
53	15.322	2247	2250	2254	rVB	49078	57769	3.73%	0.407%
54	15.386	2257	2261	2267	rVB	90458	110411	7.13%	0.777%
55	15.451	2268	2272	2276	rBV	337262	402521	26.01%	2.834%
56	16.939	2522	2525	2532	rVB3	30454	58531	3.78%	0.412%

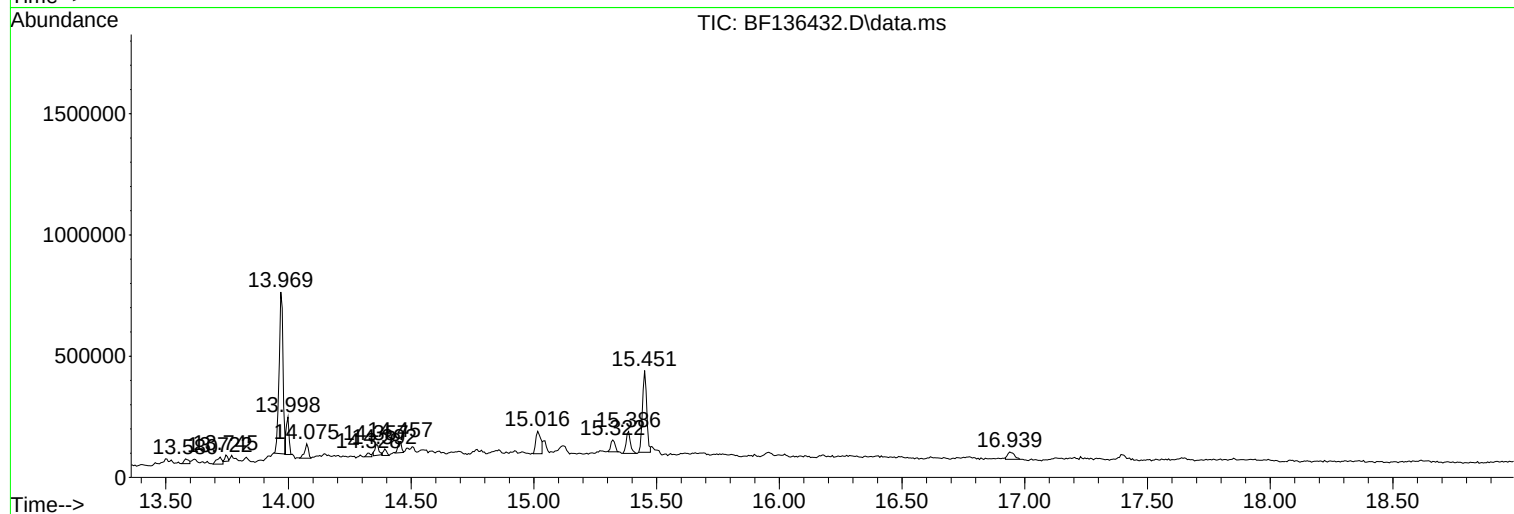
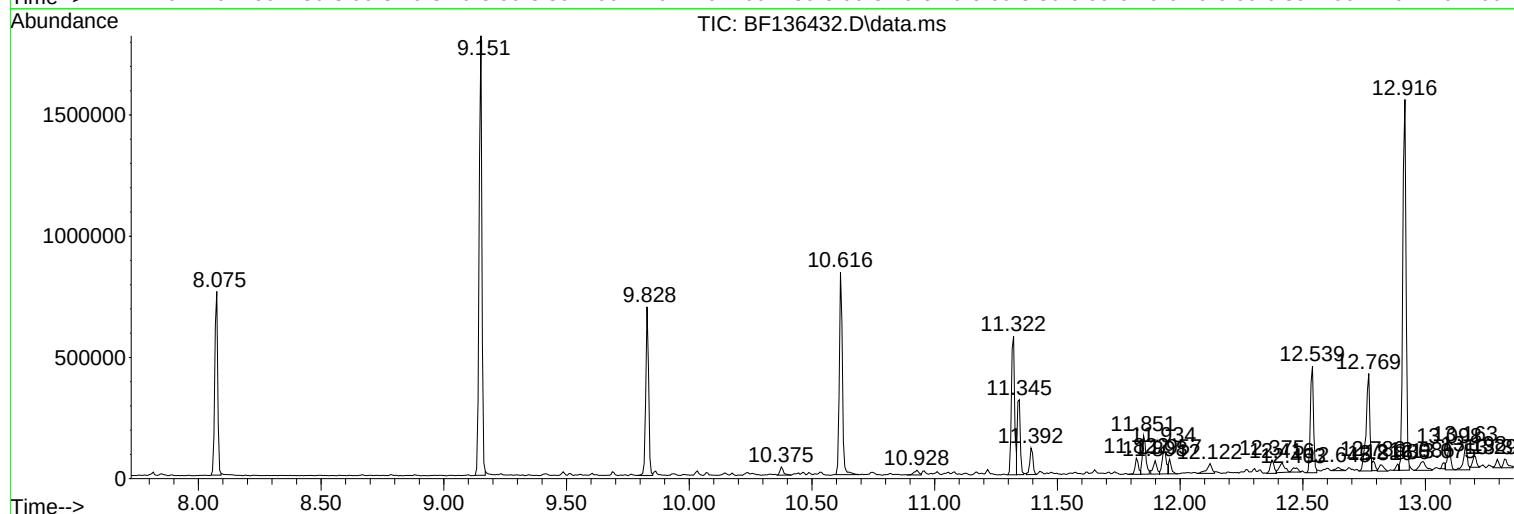
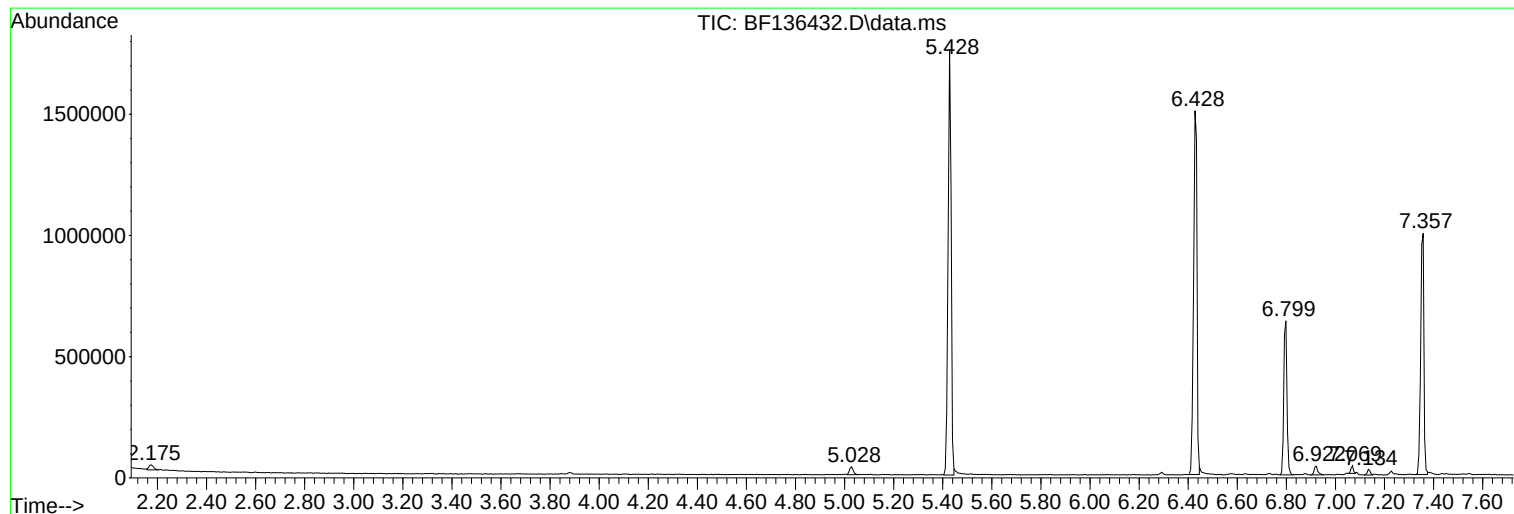
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

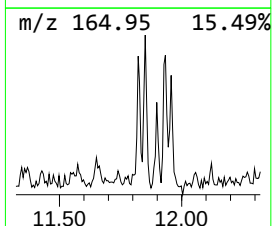
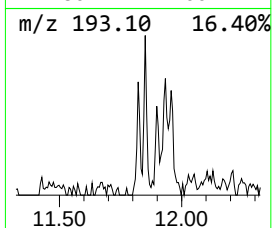
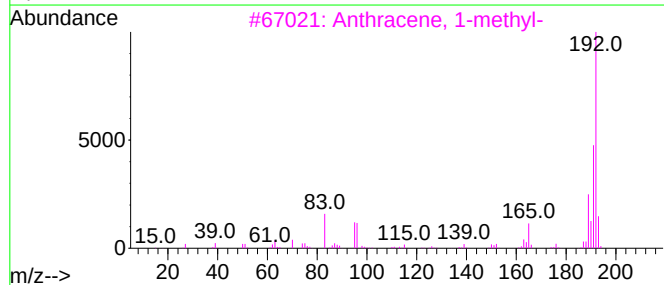
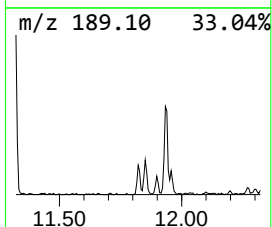
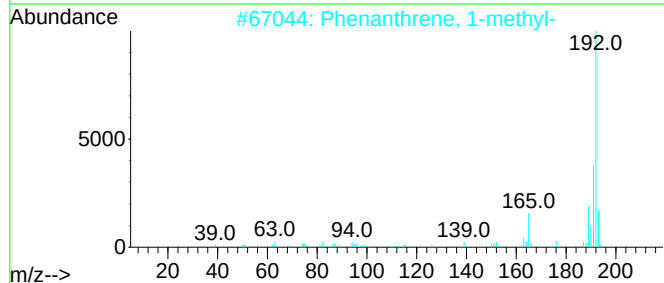
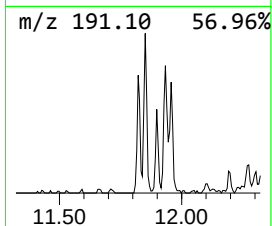
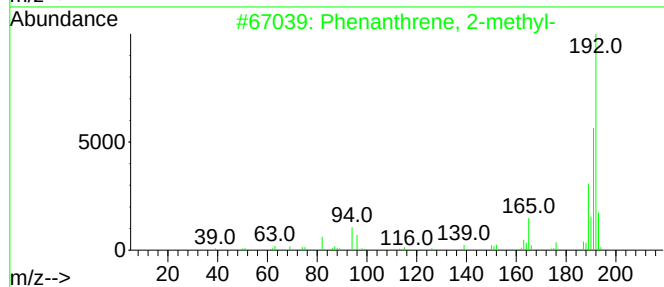
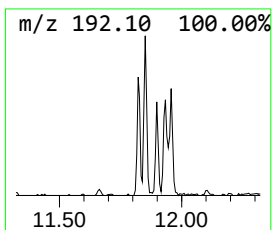
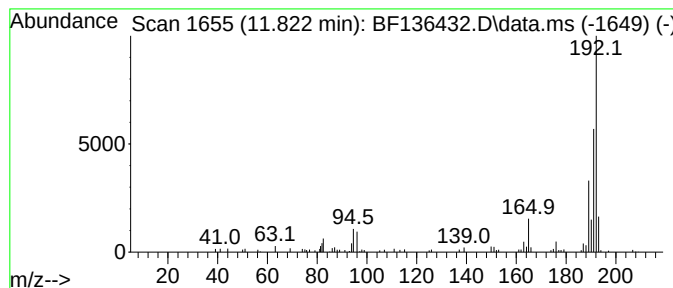
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.47 ng	66067	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	91
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	90



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

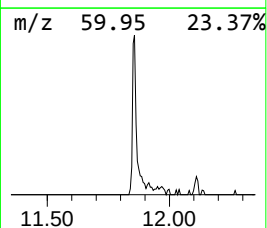
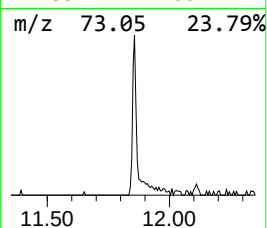
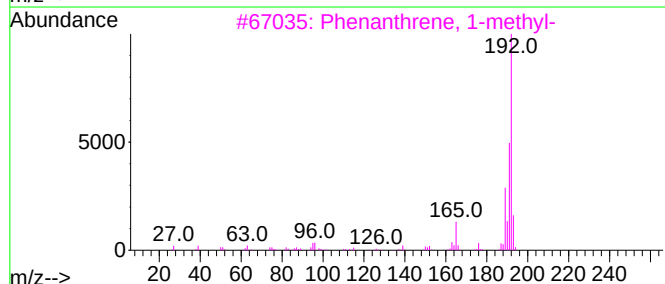
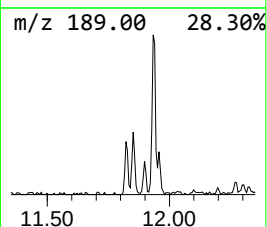
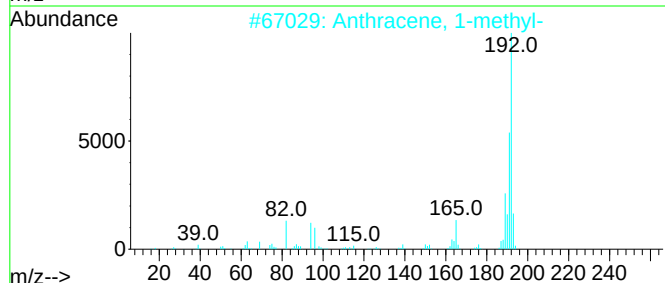
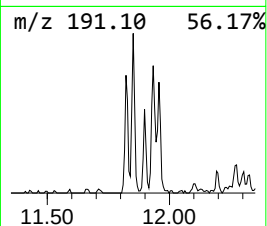
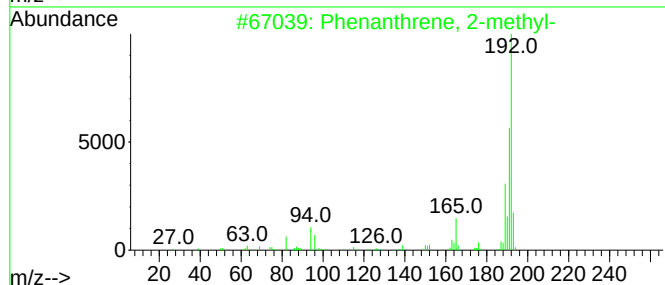
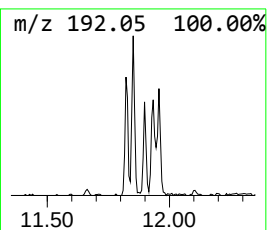
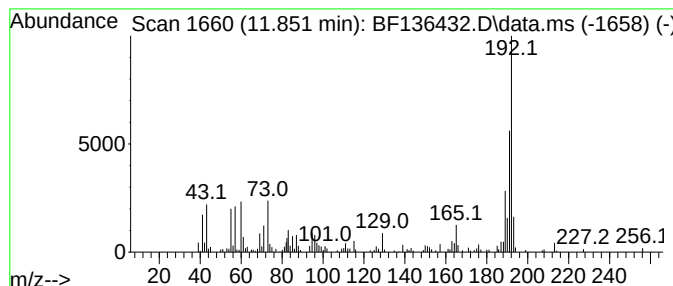
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	5.80 ng	155267	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
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Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

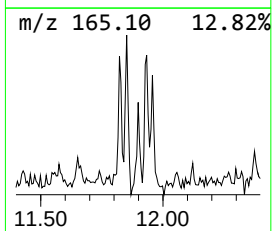
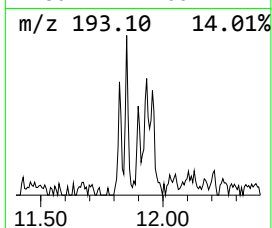
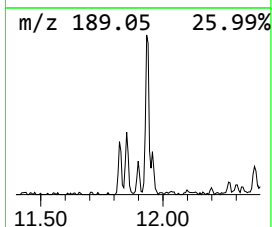
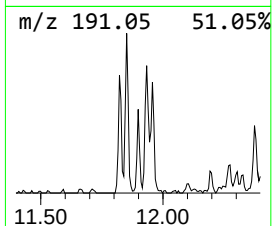
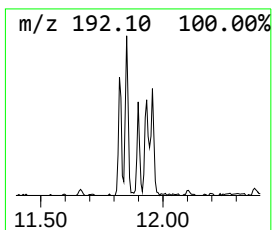
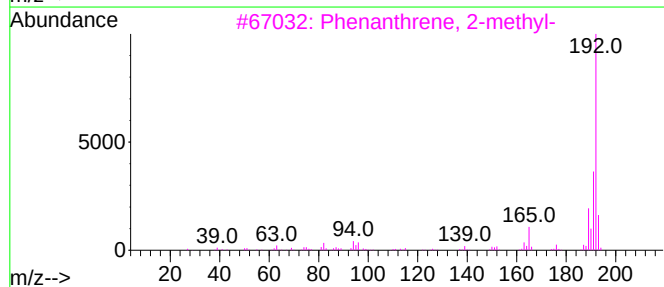
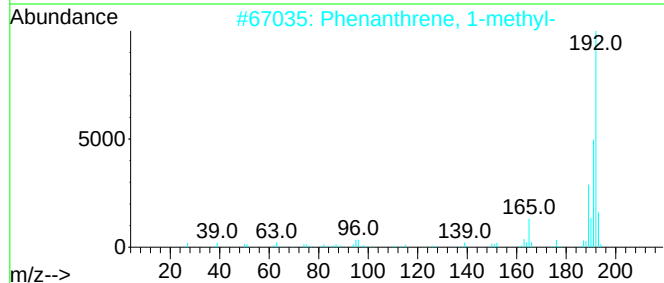
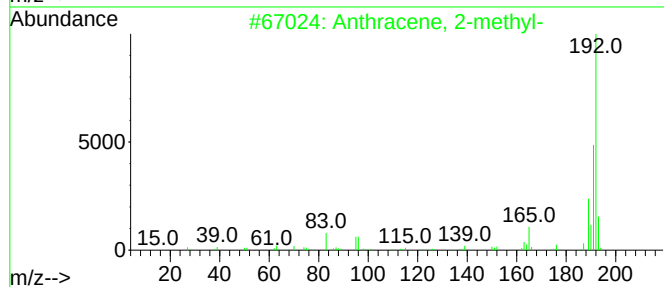
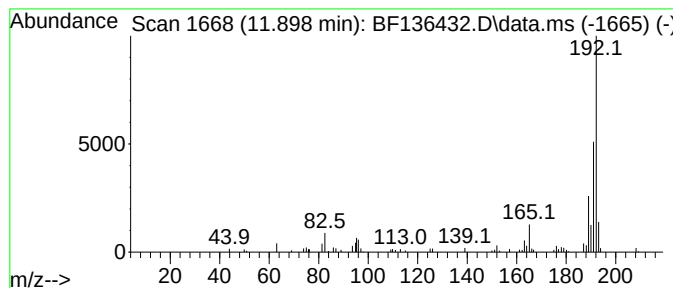
Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

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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 Anthracene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.898	2.12 ng	56844	Phenanthrene-d10		11.322	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-		192	C15H12	000613-12-7	96
2	Phenanthrene, 1-methyl-		192	C15H12	000832-69-9	95
3	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	93
4	Anthracene, 1-methyl-		192	C15H12	000610-48-0	93
5	Anthracene, 9-methyl-		192	C15H12	000779-02-2	93



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ALS Vial : 15 Sample Multiplier: 1

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ROUTE-4-TP-4

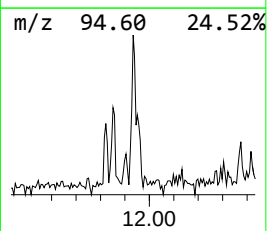
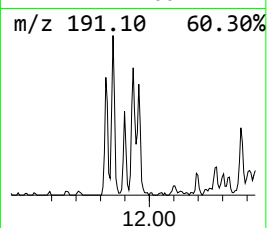
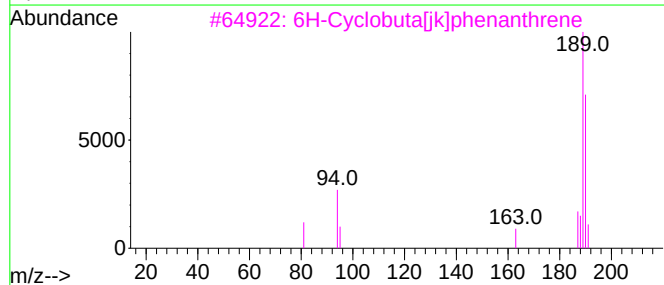
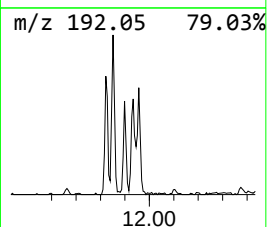
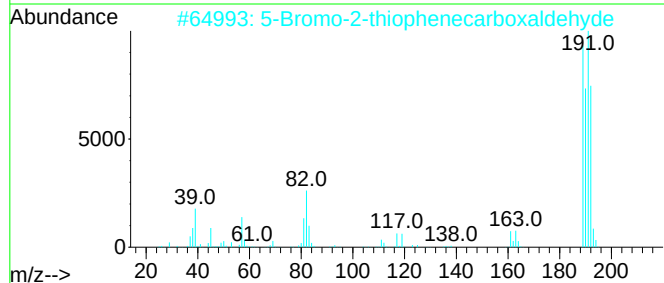
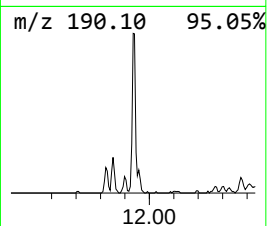
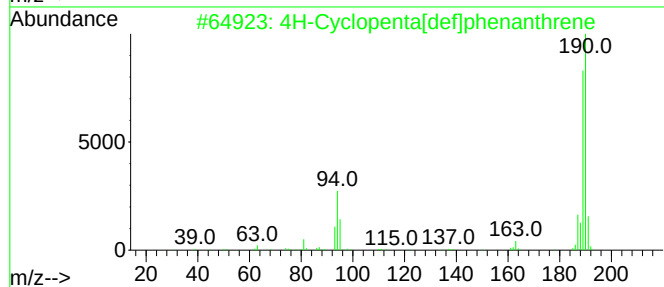
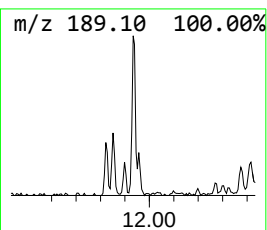
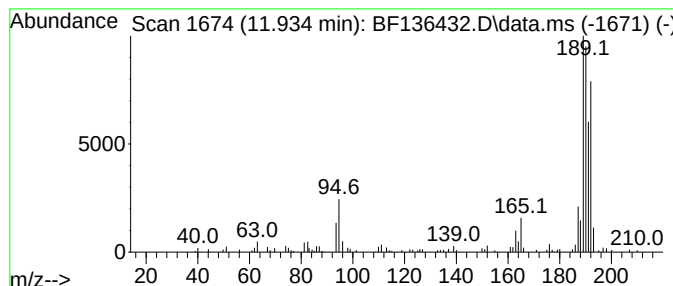
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	4.74 ng	126872	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2			5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
5			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	42



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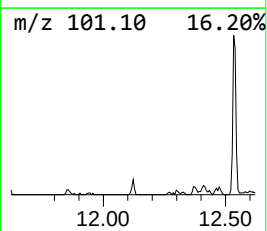
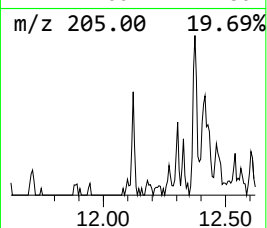
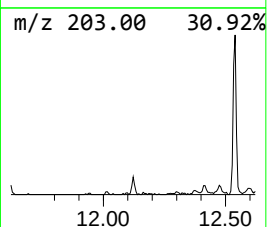
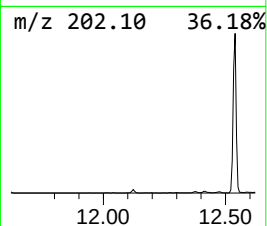
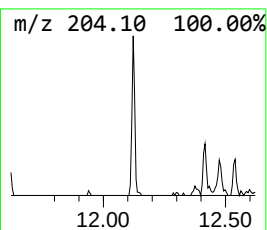
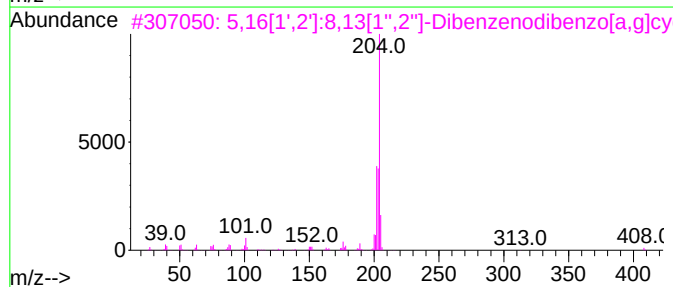
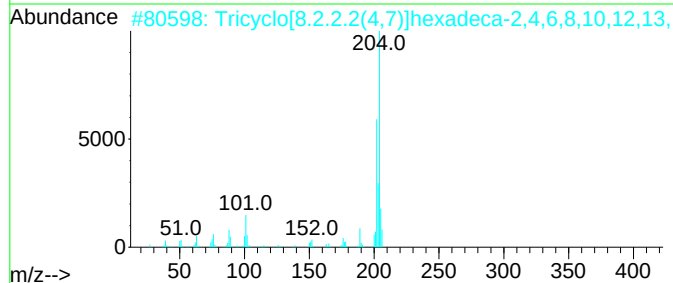
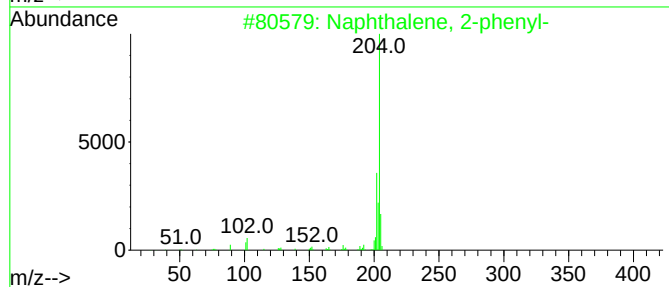
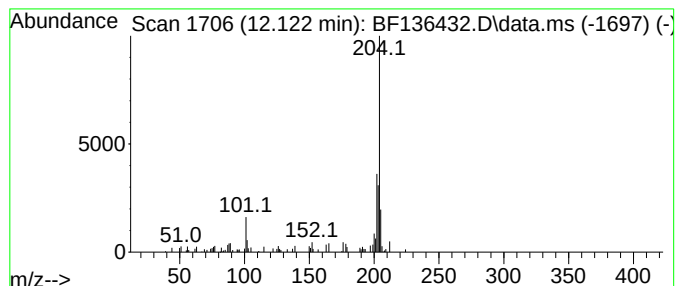
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Naphthalene, 2-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.122	2.22 ng	59396	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	81
2			Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	74
3			5,16[1',2'] :8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	72
4			Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	62
5			1,4-Ethenoanthracene, 1,4-dihydro-	204	C16H12	027765-96-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

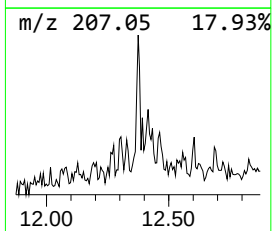
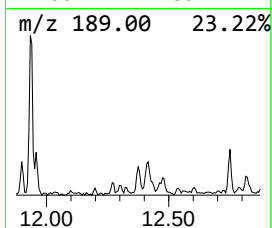
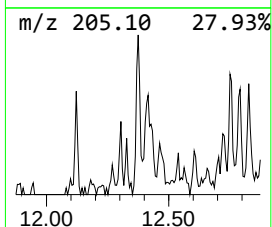
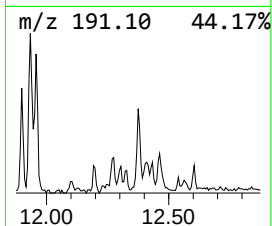
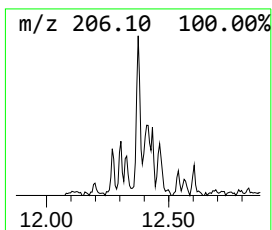
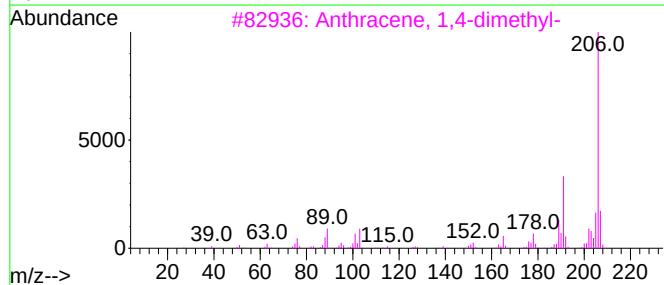
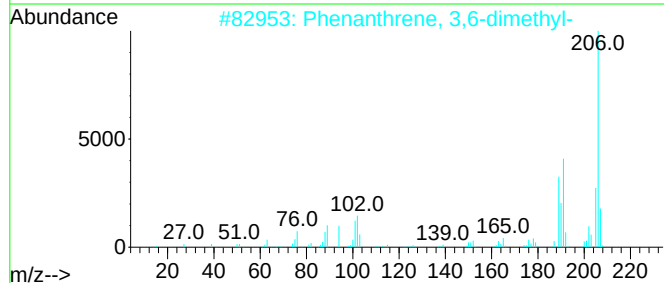
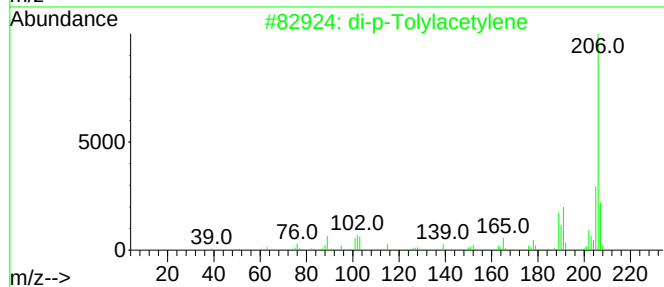
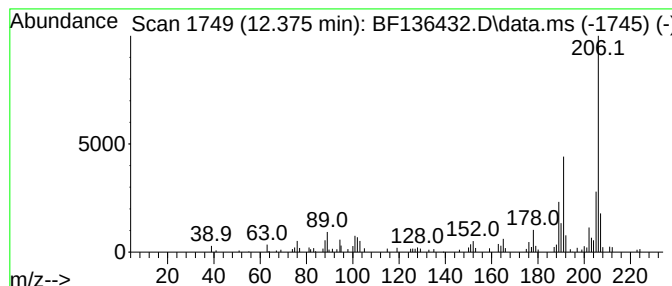
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 di-p-Tolylacetylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.375	2.25 ng	60125	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-p-Tolylacetylene	206	C16H14	002789-88-0	96
2			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	94
3			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
5			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
Sample : 05602-07
Misc :
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Instrument :
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ClientSampleId :
ROUTE-4-TP-4

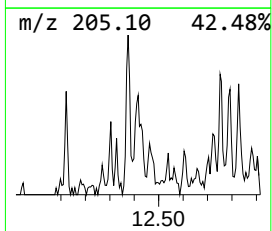
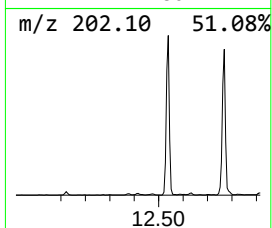
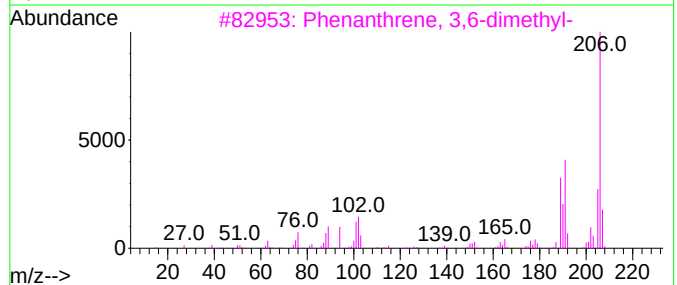
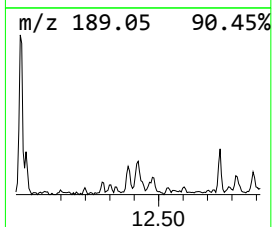
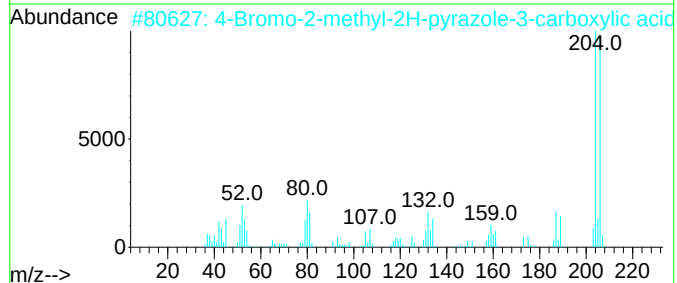
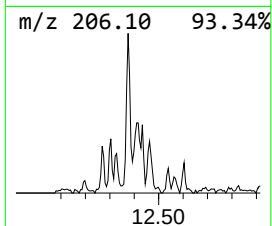
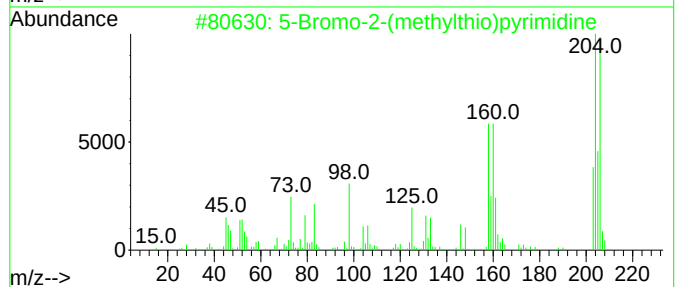
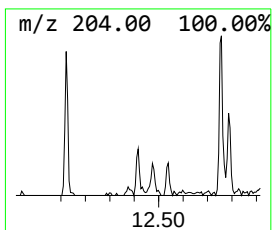
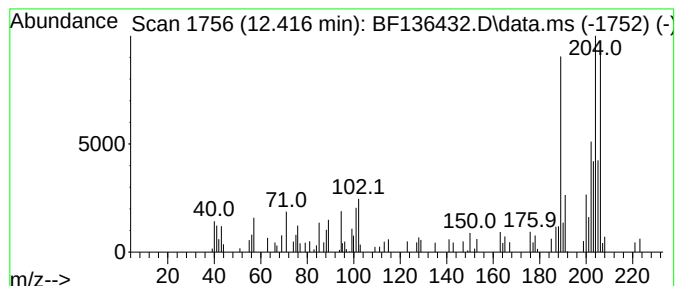
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.416 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	2.22 ng	59281	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-2-(methylthio)pyrimidine	204	C5H5BrN2S	014001-67-3	46
2			4-Bromo-2-methyl-2H-pyrazole-3-c...	204	C5H5BrN2O2	1000300-50-8	27
3			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	25
4			[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	25
5			Isoquinoline, 1-phenyl-	205	C15H11N	003297-72-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

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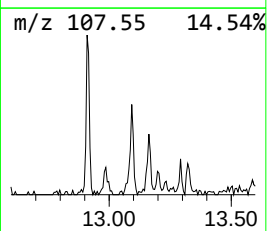
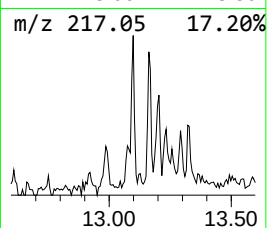
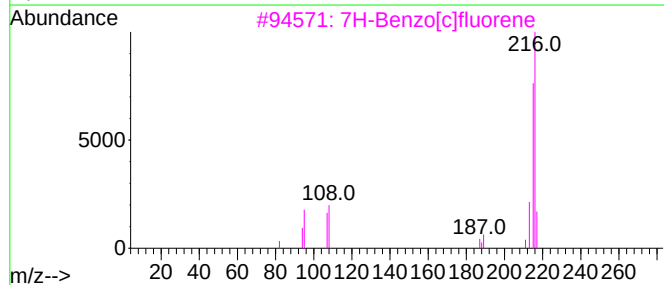
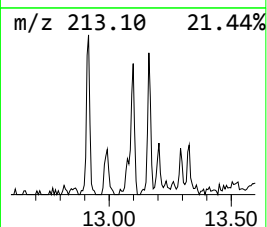
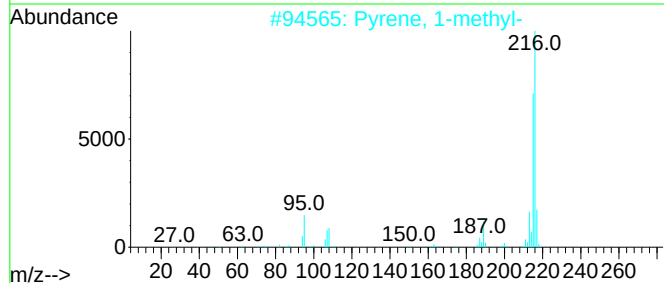
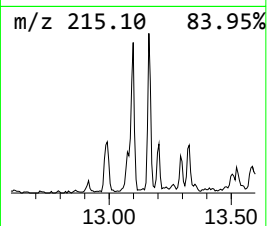
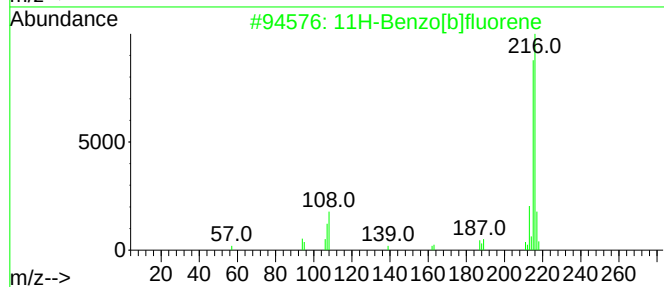
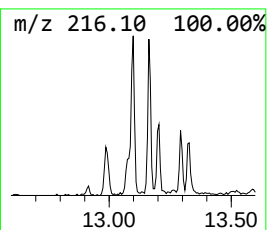
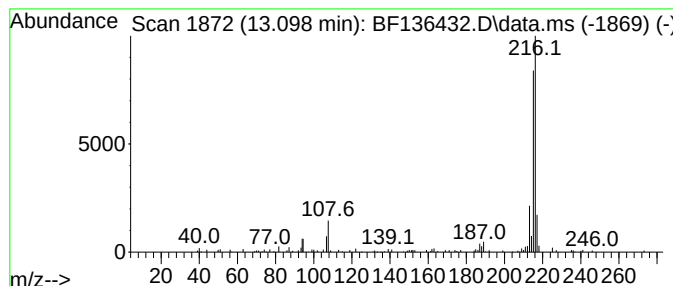
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	2.33 ng	87430	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	80
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ROUTE-4-TP-4

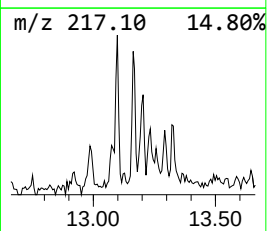
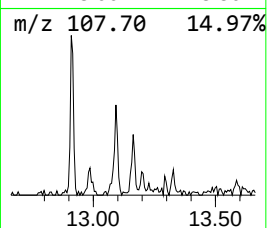
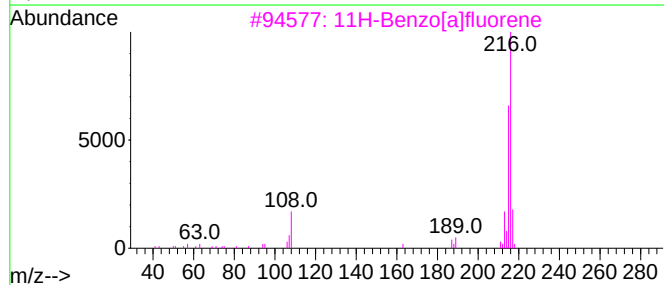
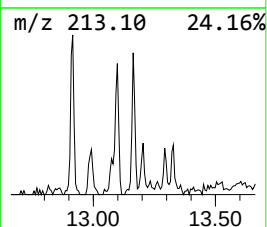
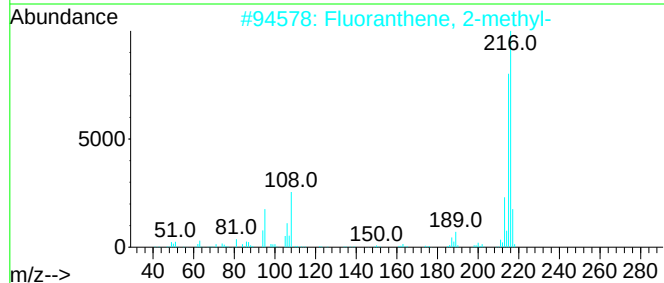
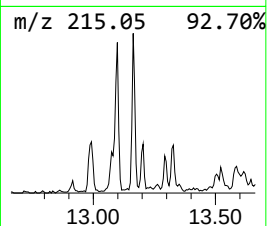
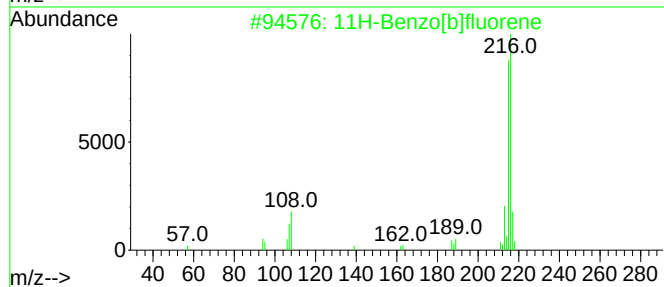
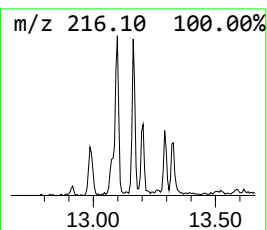
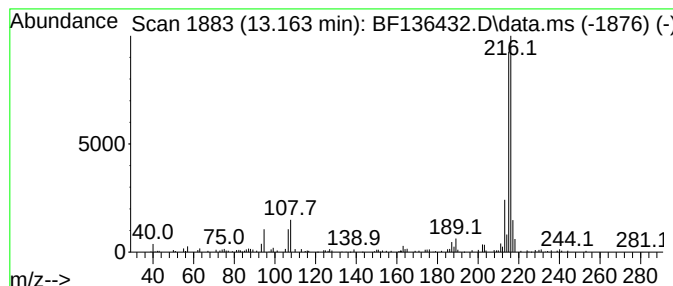
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.91 ng	109148	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	70
5			7H-Benzanthrene	216	C17H12	000199-94-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ROUTE-4-TP-4

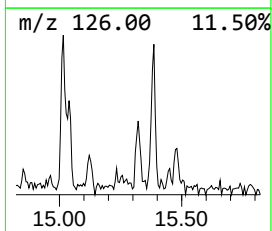
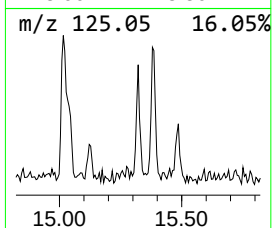
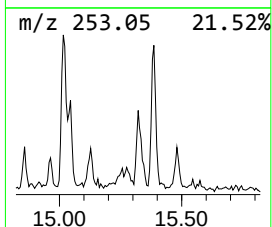
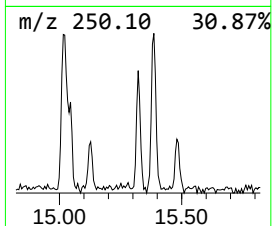
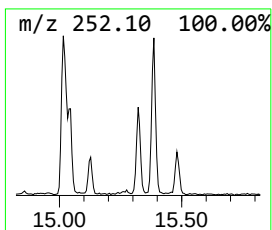
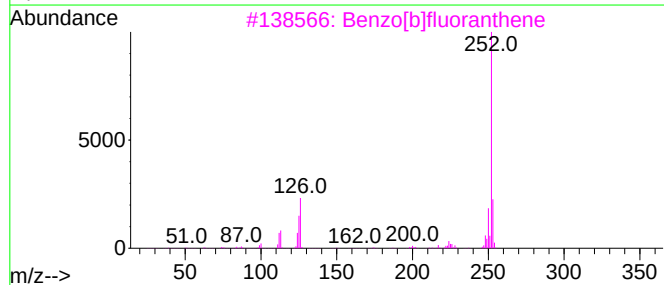
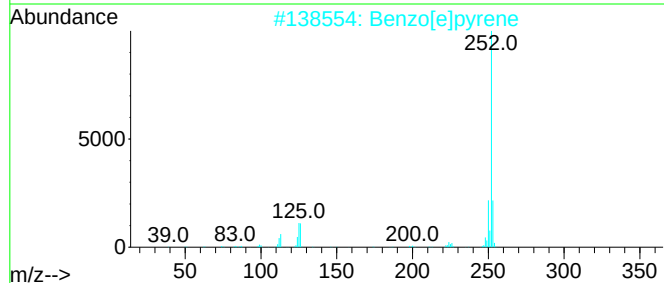
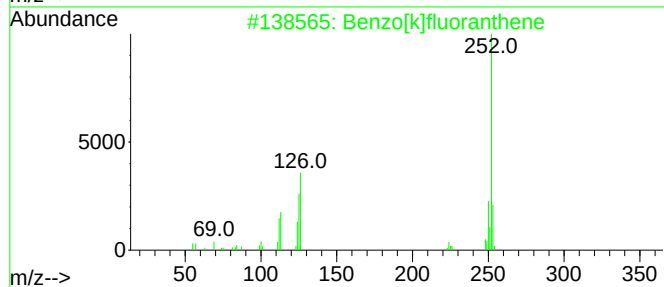
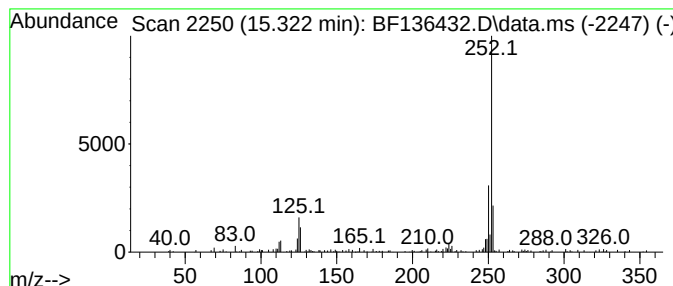
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.322	2.87 ng	57769	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
2		Benzo[e]pyrene	252	C20H12	000192-97-2	91
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4		Perylene	252	C20H12	000198-55-0	90
5		Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136432.D
Acq On : 06 Dec 2023 17:13
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
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Anthracene, 1-m...	11.851	5.8	ng	155267	4	11.322	535150	20.0
Anthracene, 2-m...	11.898	2.1	ng	56844	4	11.322	535150	20.0
4H-Cyclopenta[d...	11.934	4.7	ng	126872	4	11.322	535150	20.0
Naphthalene, 2-...	12.122	2.2	ng	59396	4	11.322	535150	20.0
di-p-Tolylacety...	12.375	2.3	ng	60125	4	11.322	535150	20.0
unknown12.416	12.416	2.2	ng	59281	4	11.322	535150	20.0
11H-Benzo[b]flu...	13.098	2.3	ng	87430	5	13.969	751041	20.0
Fluoranthene, 2...	13.163	2.9	ng	109148	5	13.969	751041	20.0
Benzo[e]pyrene	15.322	2.9	ng	57769	6	15.451	402521	20.0