

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136741.D
 Acq On : 27 Dec 2023 02:43
 Operator : CG\JU
 Sample : 05602-07
 Misc :
 ALS Vial : 18 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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136741.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	7	12	19	rBV	14831	21120	1.90%	0.208%
2	5.016	495	498	503	rBV	27270	28437	2.56%	0.281%
3	5.428	564	568	582	rVB	1125445	1109868	100.00%	10.954%
4	6.428	734	738	741	rBV	1220674	1034876	93.24%	10.214%
5	6.781	795	798	804	rVB	479854	395055	35.59%	3.899%
6	6.904	814	819	823	rBV	31361	30245	2.73%	0.299%
7	7.051	842	844	852	rVB	31360	29913	2.70%	0.295%
8	7.122	852	856	858	rBV	16580	14373	1.30%	0.142%
9	7.210	868	871	881	rVB	11611	13983	1.26%	0.138%
10	7.345	889	894	897	rBV	730261	657450	59.24%	6.489%
11	8.057	1012	1015	1019	rBV	536651	433923	39.10%	4.283%
12	9.133	1195	1198	1202	rBV	1195120	1009561	90.96%	9.964%
13	9.816	1310	1314	1317	rBV	499806	383996	34.60%	3.790%
14	10.022	1343	1349	1353	rBV3	12780	16434	1.48%	0.162%
15	10.363	1404	1407	1413	rVB3	23273	25582	2.30%	0.252%
16	10.610	1445	1449	1460	rVB	591384	517489	46.63%	5.108%
17	10.733	1466	1470	1475	rVB6	12859	14694	1.32%	0.145%
18	10.916	1495	1501	1504	rBV2	16671	21992	1.98%	0.217%
19	11.204	1547	1550	1555	rVB	15388	14086	1.27%	0.139%
20	11.310	1564	1568	1570	rBV	417896	390660	35.20%	3.856%
21	11.333	1570	1572	1575	rVV	228721	176985	15.95%	1.747%
22	11.380	1577	1580	1584	rVB	80907	68422	6.16%	0.675%
23	11.810	1650	1653	1656	rBV	47309	45091	4.06%	0.445%
24	11.839	1656	1658	1663	rVV	160950	154542	13.92%	1.525%
25	11.886	1663	1666	1669	rVV	37451	40599	3.66%	0.401%
26	11.922	1669	1672	1675	rVV	78258	90040	8.11%	0.889%
27	11.945	1675	1676	1683	rVB	41823	30799	2.78%	0.304%
28	12.110	1697	1704	1708	rBV	30598	43855	3.95%	0.433%
29	12.257	1724	1729	1732	rBV4	14488	17368	1.56%	0.171%
30	12.292	1732	1735	1737	rBV	12569	12213	1.10%	0.121%
31	12.363	1742	1747	1750	rBV	45614	50069	4.51%	0.494%
32	12.404	1750	1754	1759	rVB4	27103	40961	3.69%	0.404%
33	12.451	1759	1762	1770	rVB4	15139	28832	2.60%	0.285%
34	12.527	1771	1775	1778	rBV	338070	272375	24.54%	2.688%
35	12.627	1789	1792	1798	rBV6	16357	27483	2.48%	0.271%
36	12.757	1807	1814	1816	rBV	288114	298007	26.85%	2.941%

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.774	1816	1817	1820	rVV	36044	27962	2.52%	0.276%
38	12.810	1820	1823	1827	rVB2	17305	24145	2.18%	0.238%
39	12.874	1832	1834	1835	rBV2	16821	14726	1.33%	0.145%
40	12.904	1835	1839	1842	rVB	1109504	930333	83.82%	9.182%
41	12.980	1847	1852	1855	rBV4	25138	38302	3.45%	0.378%
42	13.086	1867	1870	1873	rVB	69669	62443	5.63%	0.616%
43	13.151	1876	1881	1884	rBV2	63503	73351	6.61%	0.724%
44	13.192	1884	1888	1891	rVV2	36989	37198	3.35%	0.367%
45	13.286	1901	1904	1906	rVB	20014	16352	1.47%	0.161%
46	13.316	1906	1909	1913	rBV2	25809	22037	1.99%	0.218%
47	13.492	1935	1939	1941	rBV5	13825	19365	1.74%	0.191%
48	13.692	1971	1973	1975	rBV3	10829	13595	1.22%	0.134%
49	13.739	1979	1981	1983	rVV	20863	16770	1.51%	0.166%
50	13.810	1991	1993	1996	rVB2	18383	16779	1.51%	0.166%
51	13.863	1996	2002	2004	rBV6	33440	71182	6.41%	0.703%
52	13.963	2014	2019	2022	rBV2	507427	549509	49.51%	5.424%
53	13.986	2022	2023	2030	rVB	120174	98725	8.90%	0.974%
54	14.068	2034	2037	2040	rVB	39233	30317	2.73%	0.299%
55	14.351	2083	2085	2088	rVB	32274	26300	2.37%	0.260%
56	14.498	2108	2110	2114	rVB4	19408	19622	1.77%	0.194%
57	15.010	2193	2197	2200	rBV	59346	91509	8.25%	0.903%
58	15.315	2246	2249	2256	rVB	35970	51291	4.62%	0.506%
59	15.380	2256	2260	2265	rVB	53547	74047	6.67%	0.731%
60	15.445	2266	2271	2274	rBV	196090	244646	22.04%	2.415%

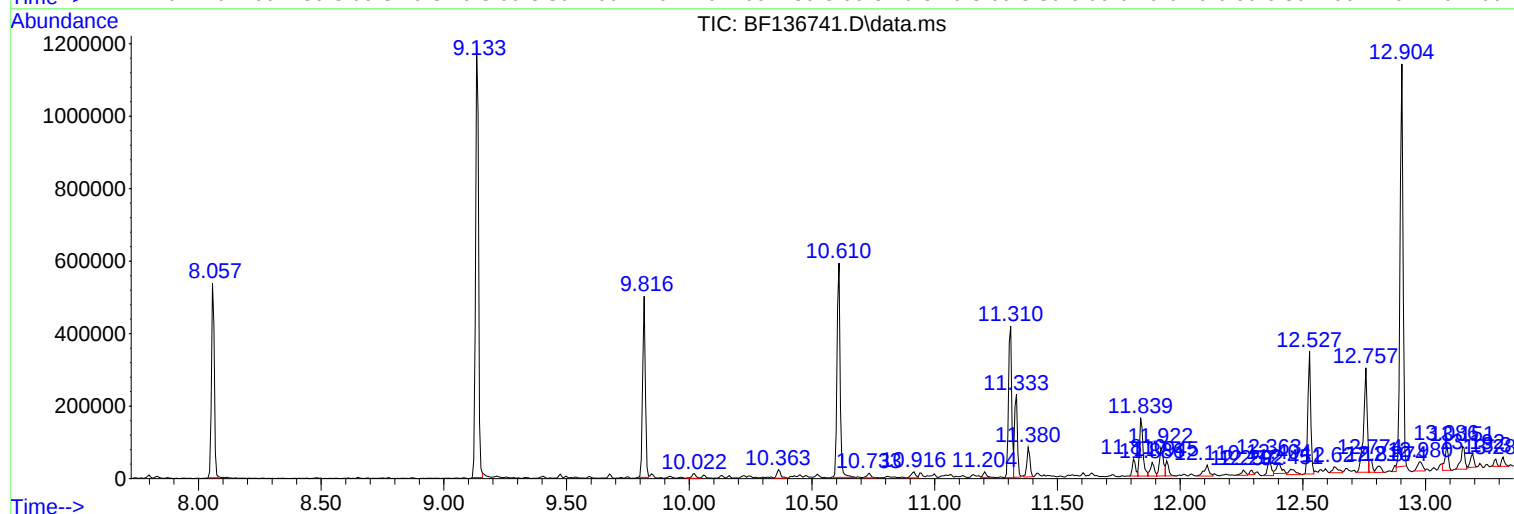
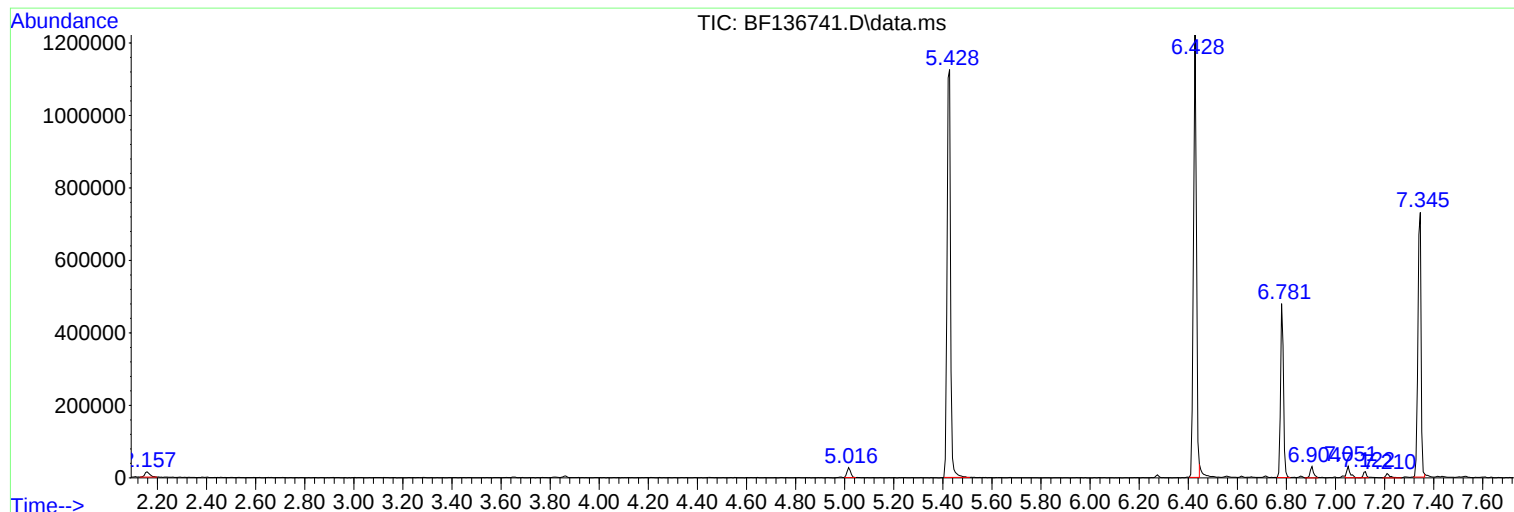
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ROUTE-4-TP-4

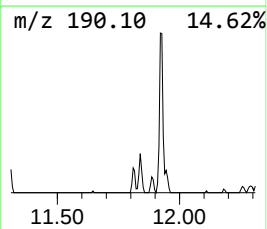
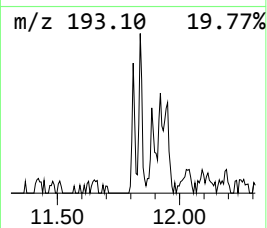
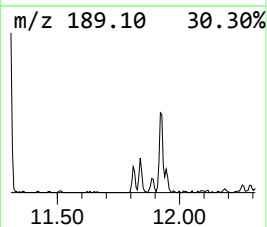
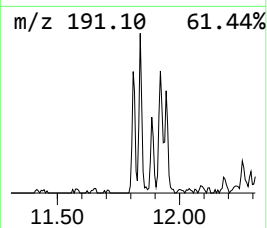
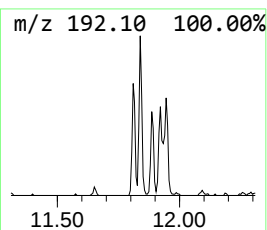
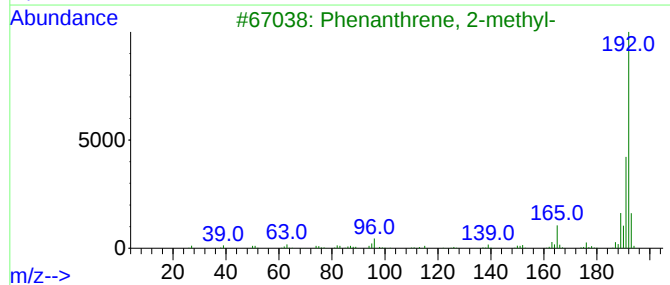
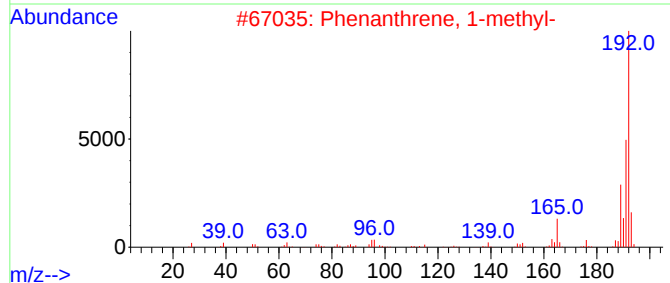
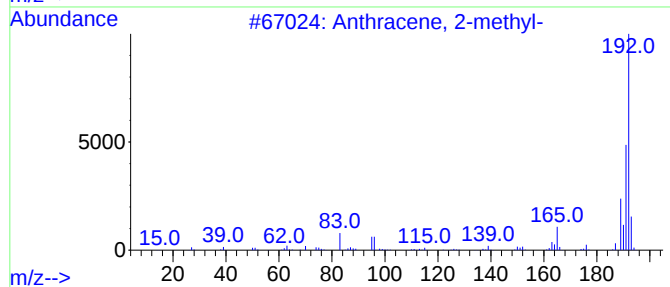
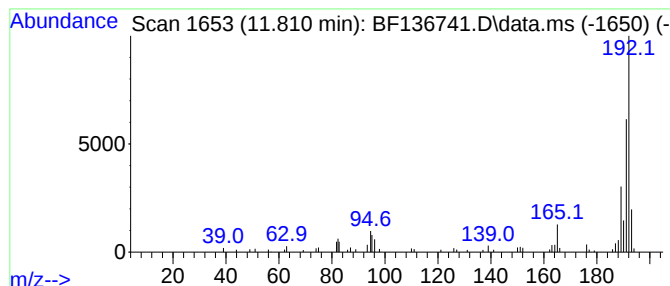
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.31 ng	45091	Phenanthrene-d10	11.310

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	96
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
5			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	94



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Misc :
ALS Vial : 18 Sample Multiplier: 1

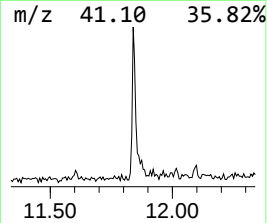
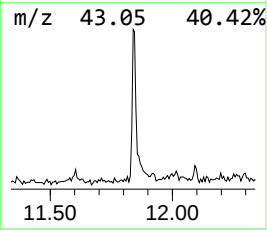
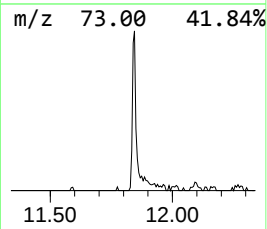
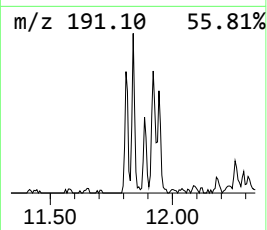
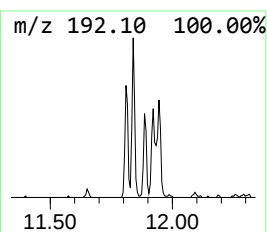
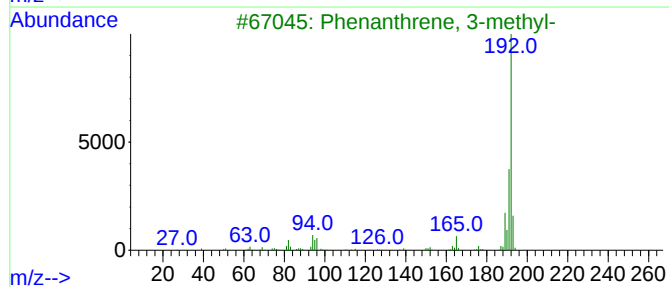
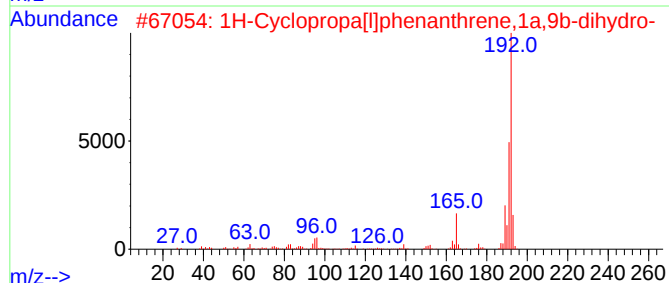
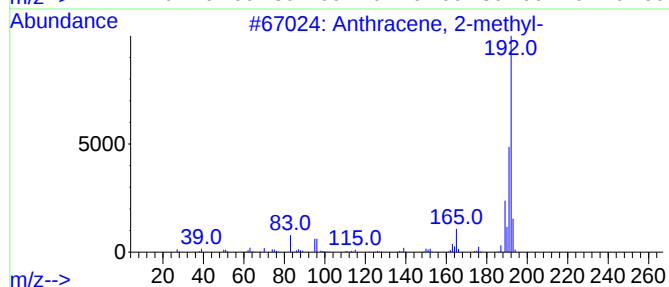
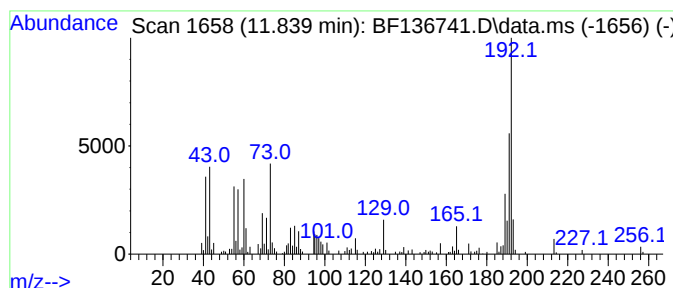
Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1H-Cyclopropa[l]phenanthren... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.839	7.91 ng	154542	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-		192	C15H12	000613-12-7	96
2	1H-Cyclopropa[1]phenanthrene,1a,...		192	C15H12	000949-41-7	94
3	Phenanthrene, 3-methyl-		192	C15H12	000832-71-3	94
4	Anthracene, 9-methyl-		192	C15H12	000779-02-2	93
5	1H-Indene, 2-phenyl-		192	C15H12	004505-48-0	93



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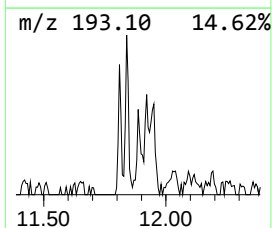
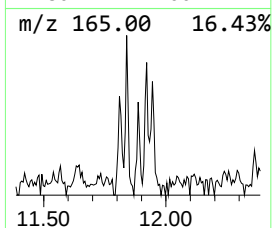
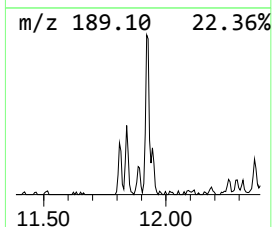
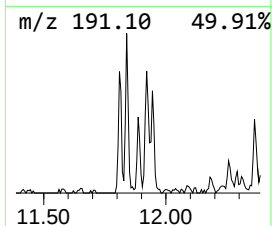
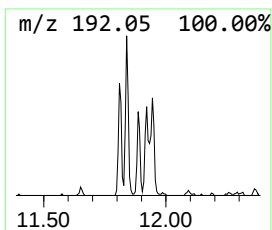
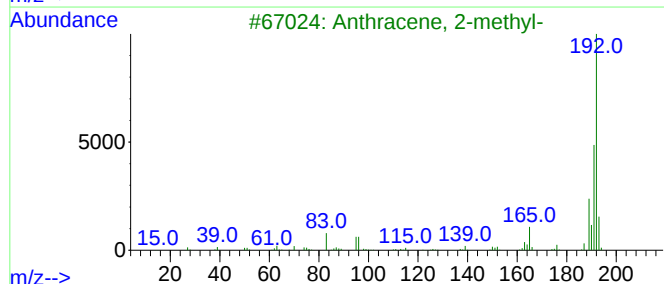
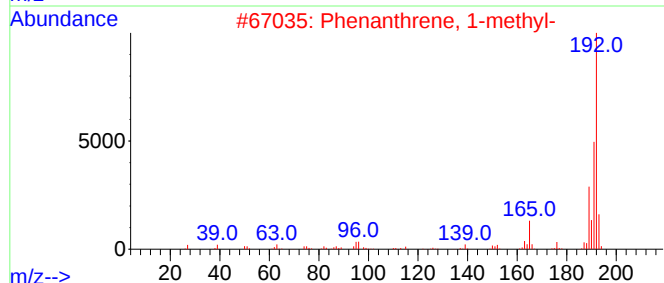
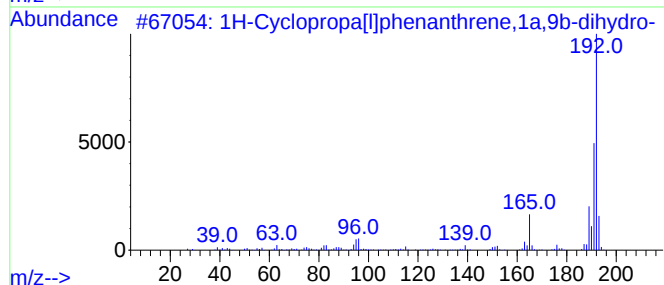
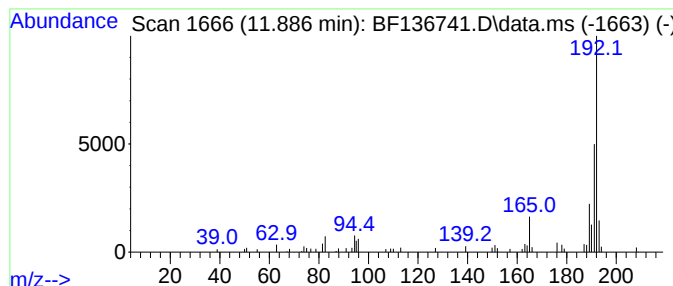
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.08 ng	40599	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	97
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94



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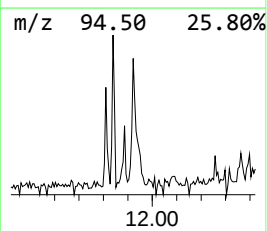
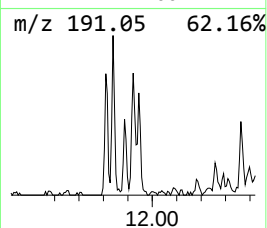
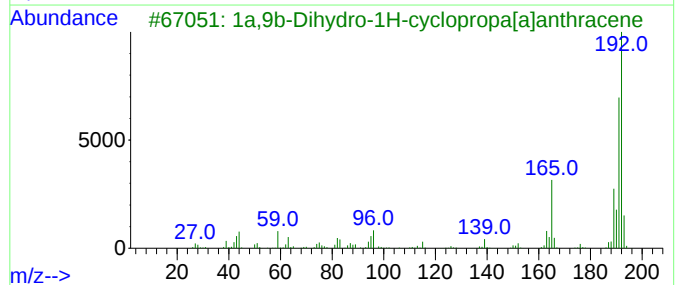
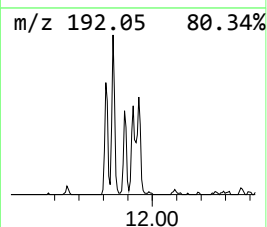
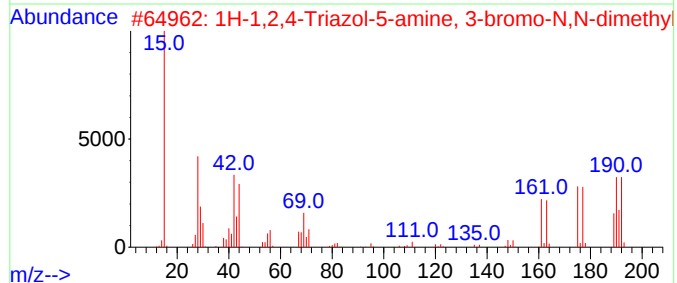
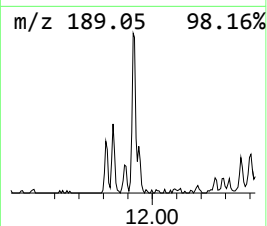
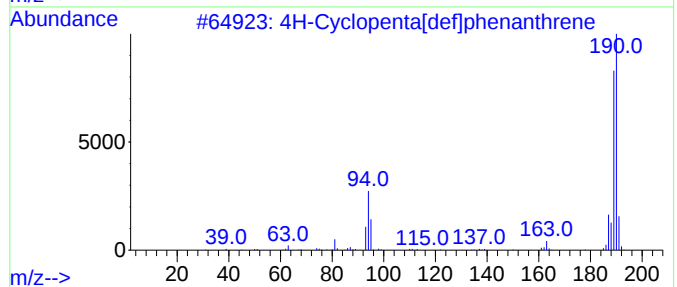
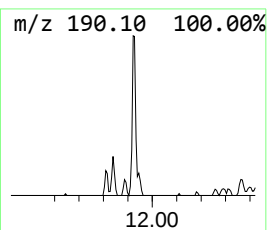
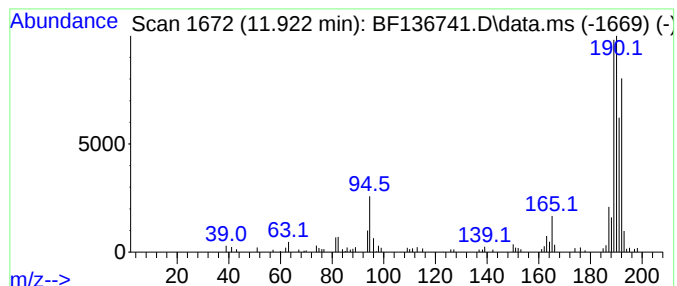
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.61 ng	90040	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2			1H-1,2,4-Triazol-5-amine, 3-brom...	190	C4H7BrN4	1000460-85-7	53
3			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	42
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
5			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38



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ROUTE-4-TP-4

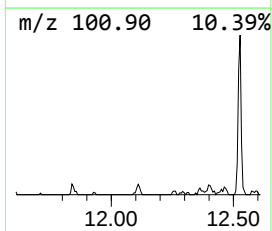
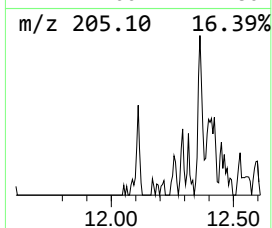
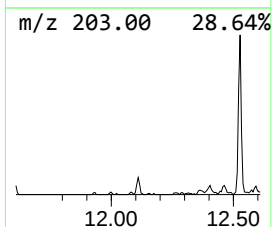
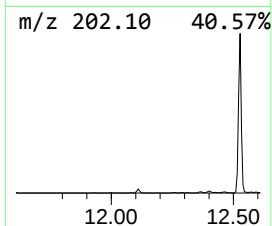
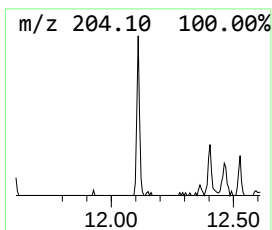
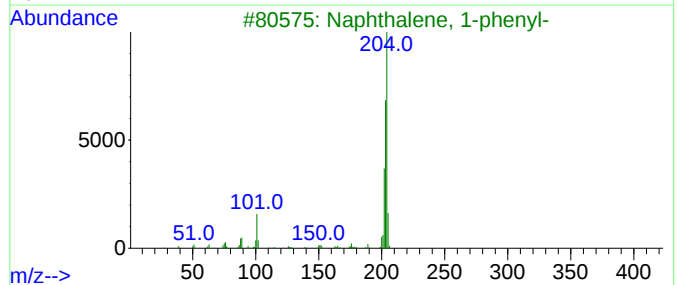
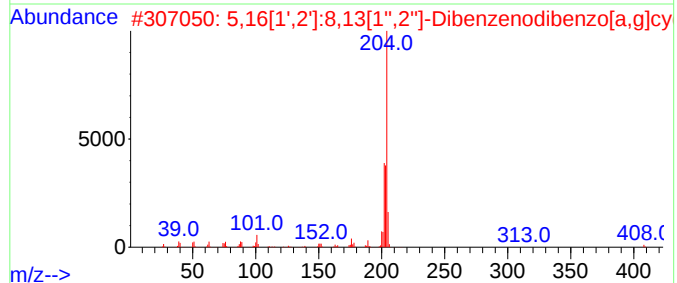
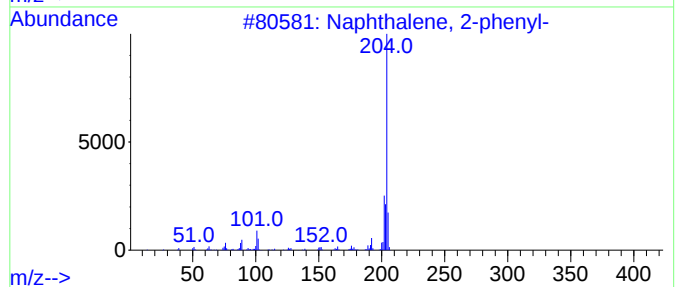
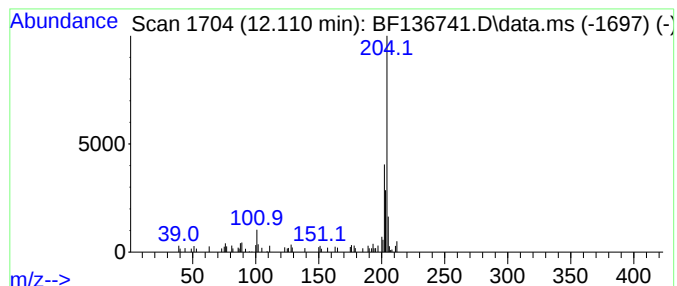
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.25 ng	43855	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	86
2			5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	86
3			Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	70
4			Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	70
5			Benzene, 1,1'-(1-buten-3-yne-1,4...	204	C16H12	013141-45-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136741.D
Acq On : 27 Dec 2023 02:43
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

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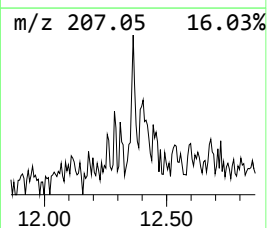
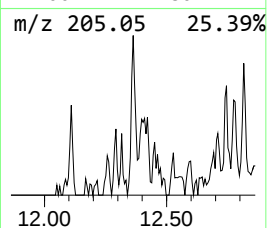
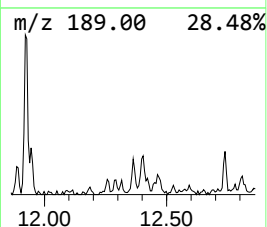
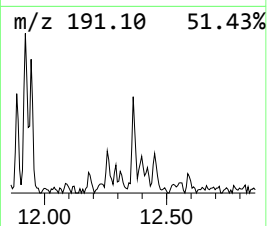
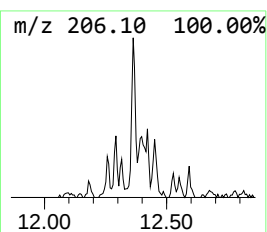
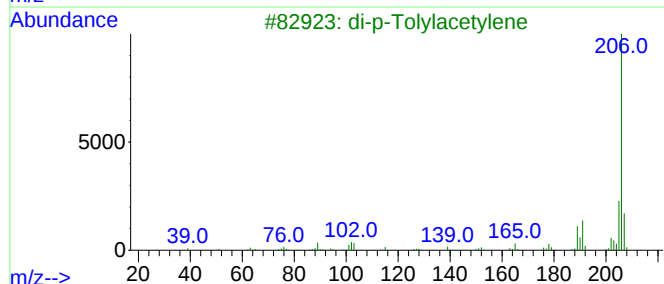
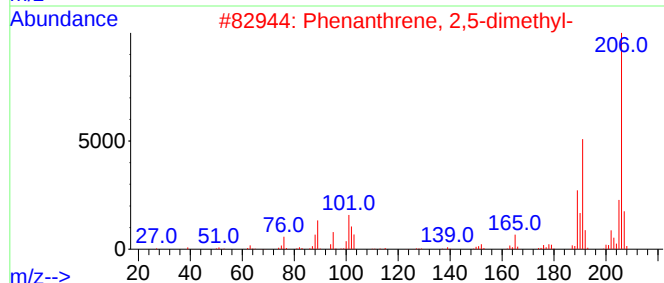
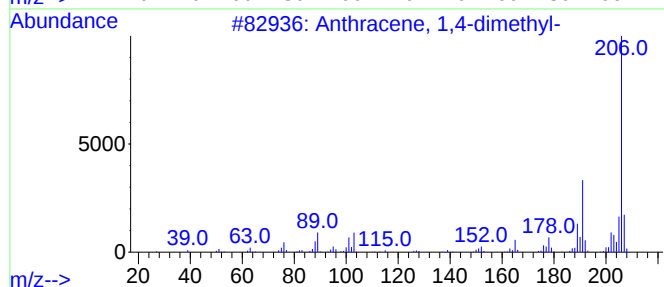
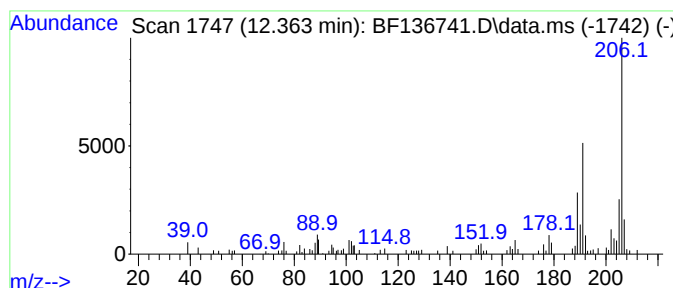
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Anthracene, 1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	2.56 ng	50069	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	93
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
5			9,10-Dimethylanthracene	206	C16H14	000781-43-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136741.D
Acq On : 27 Dec 2023 02:43
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

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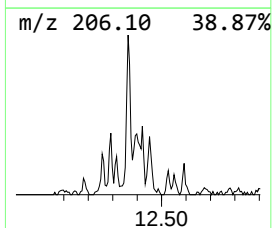
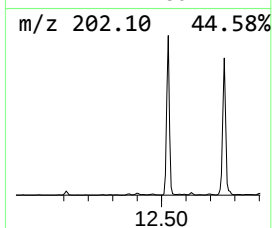
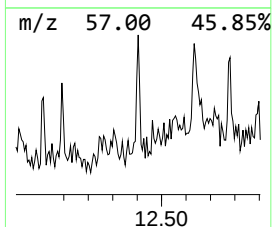
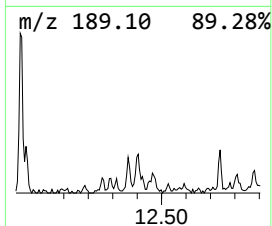
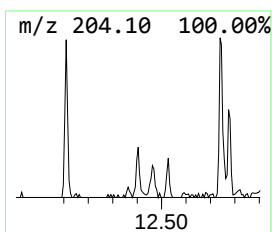
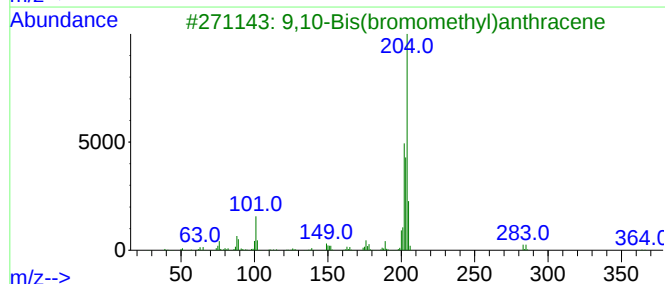
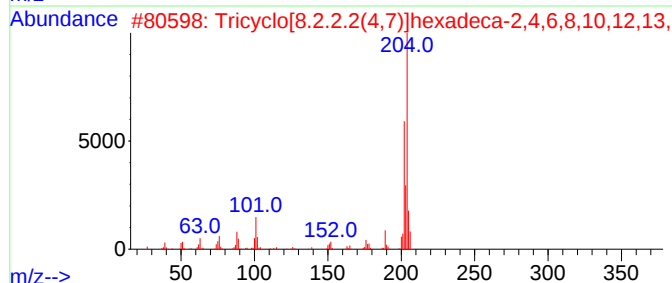
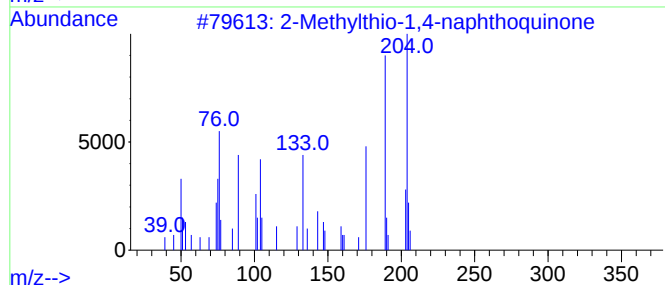
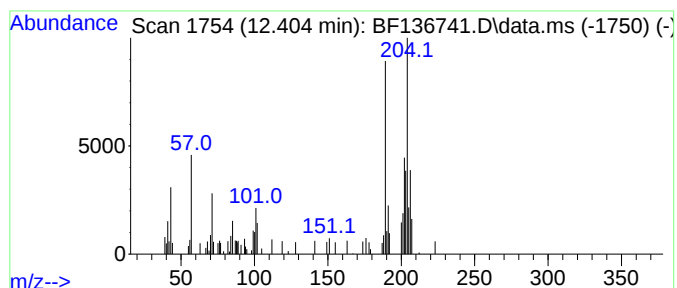
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.404 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	2.10 ng	40961	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylthio-1,4-naphthoquinone	204	C11H8O2S	026037-60-5	47
2			Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	46
3			9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	43
4			[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	43
5			1-(5-Nitro-1H-indol-3-yl)ethan-1...	204	C10H8N2O3	004771-10-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
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ClientSampleId :
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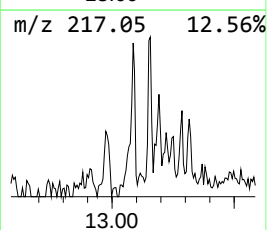
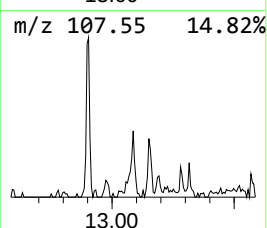
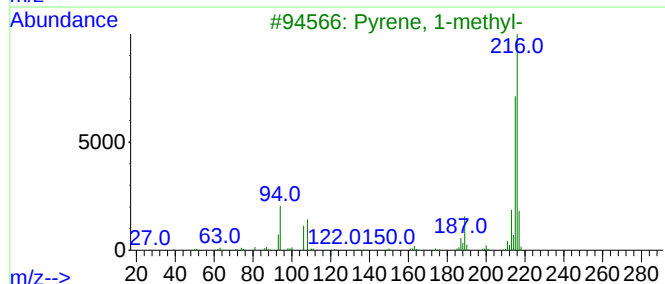
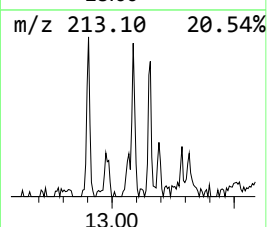
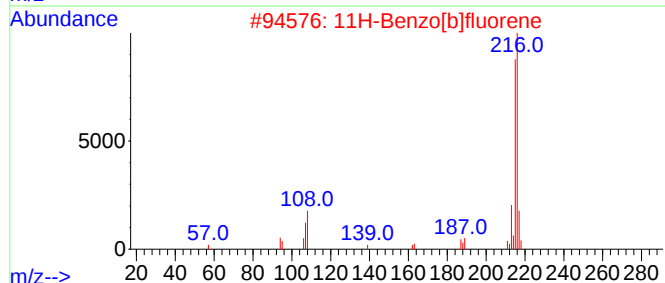
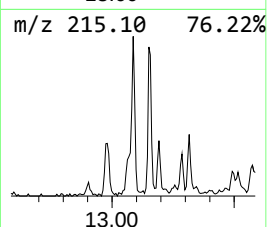
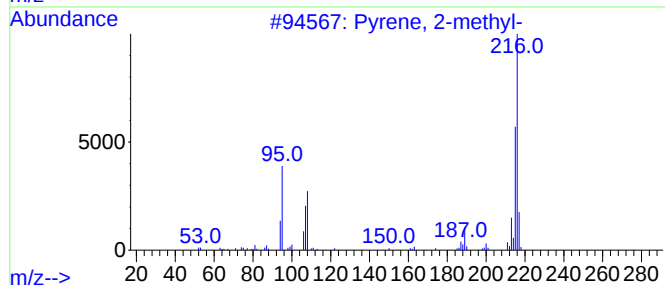
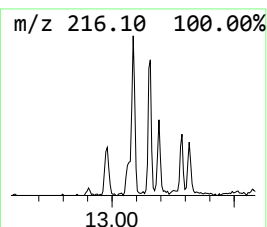
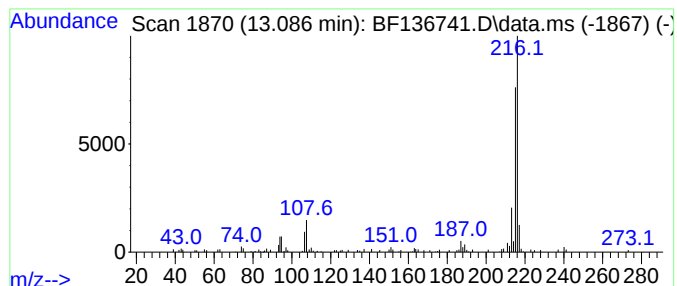
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	2.27 ng	62443	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 2-methyl-	216	C17H12	003442-78-2	89
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136741.D
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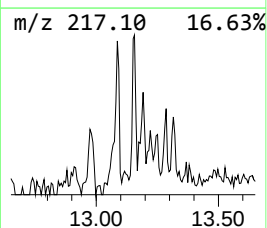
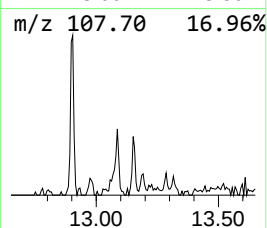
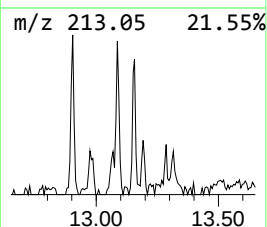
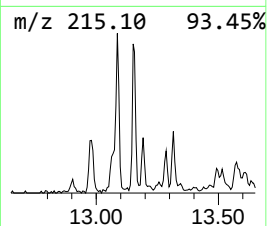
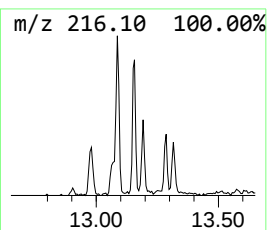
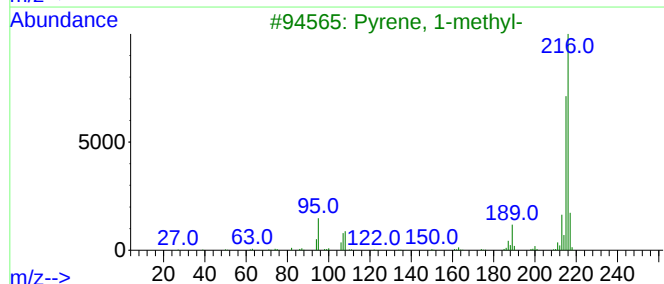
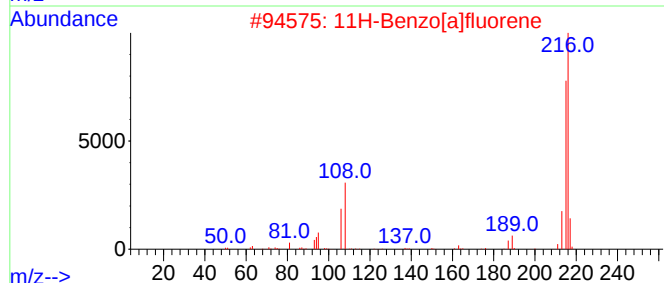
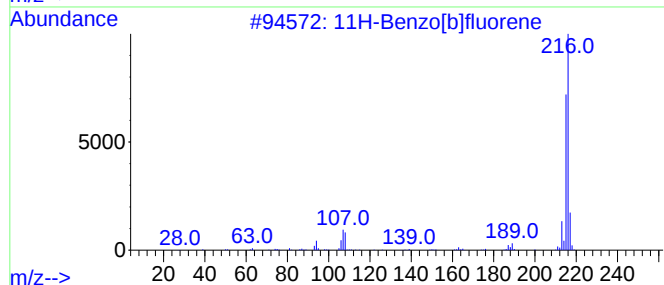
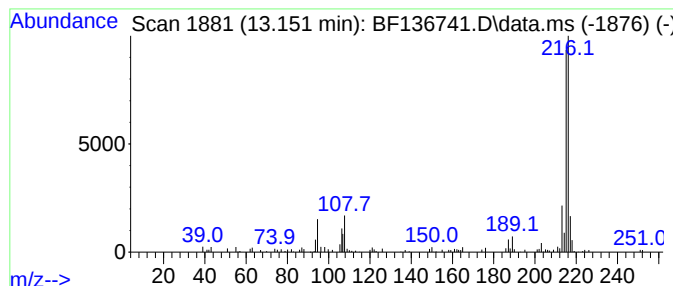
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.151	2.67 ng	73351	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5			Pyrene, 4-methyl-	216	C17H12	003353-12-6	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136741.D
Acq On : 27 Dec 2023 02:43
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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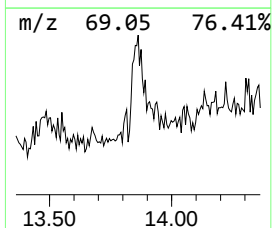
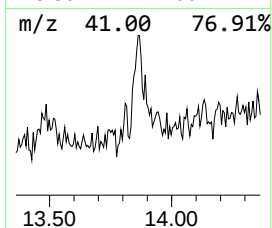
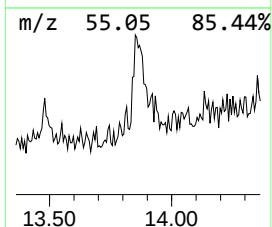
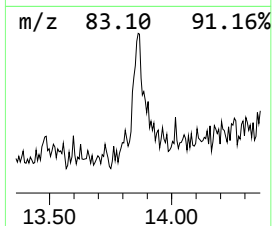
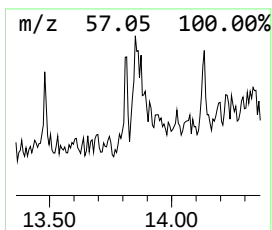
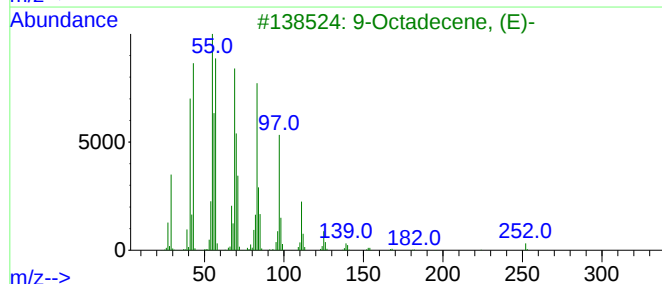
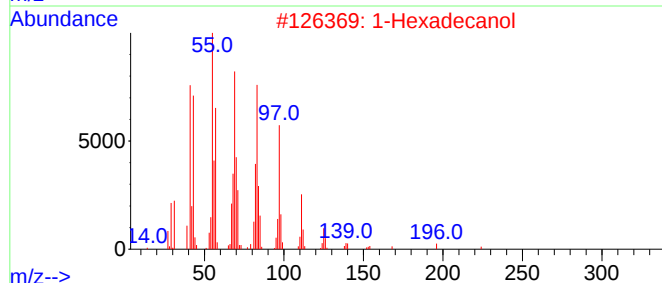
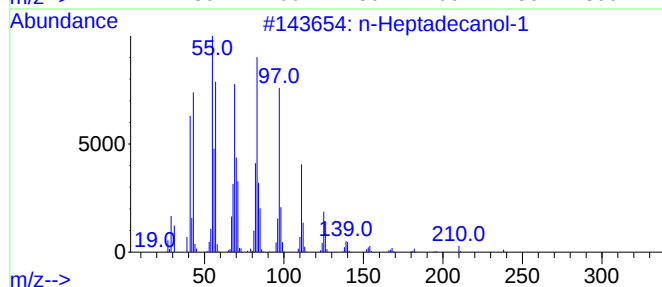
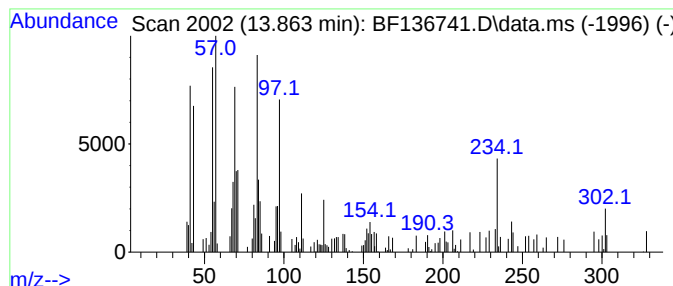
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Heptadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	2.59 ng	71182	Chrysene-d12	13.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	52
2		1-Hexadecanol	242	C16H34O	036653-82-4	52
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	52
4		7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	52
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
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ALS Vial : 18 Sample Multiplier: 1

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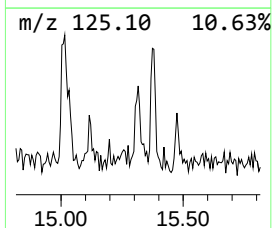
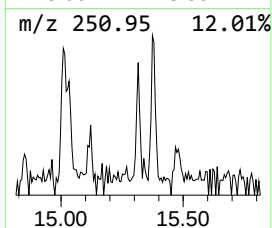
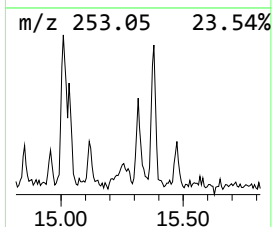
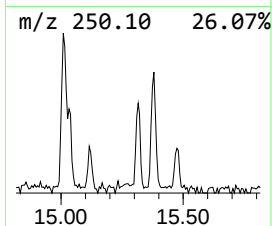
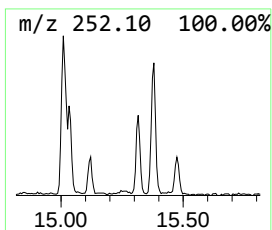
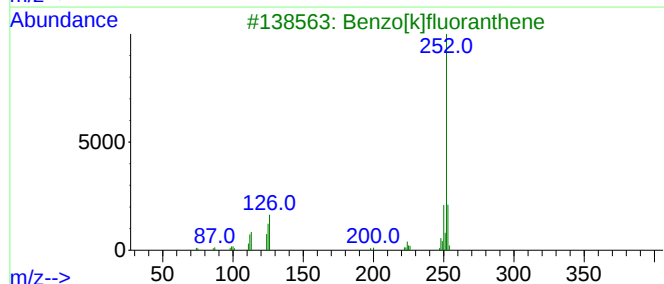
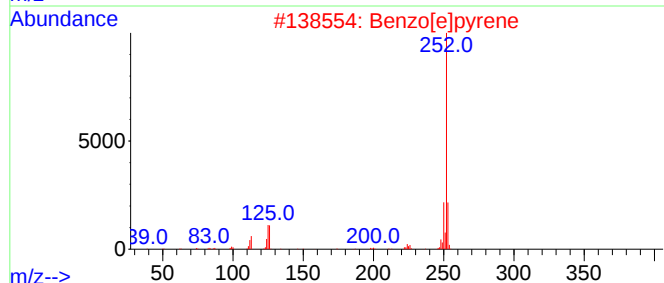
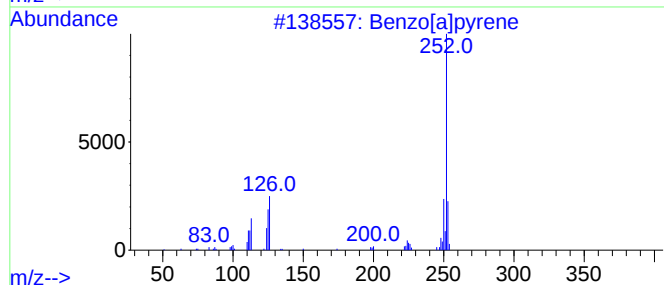
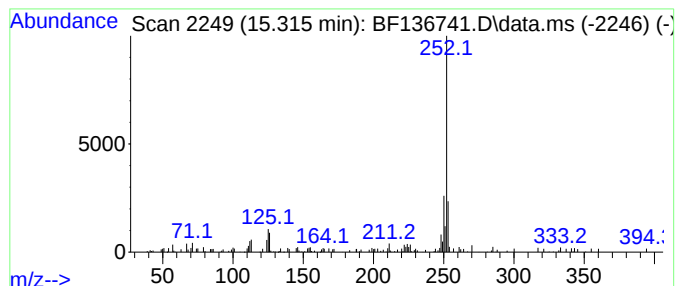
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	4.19 ng	51291	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136741.D
Acq On : 27 Dec 2023 02:43
Operator : CG\JU
Sample : 05602-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
Anthracene, 2-m...	11.810	2.3	ng	45091	4	11.310	390660	20.0
1H-Cyclopropa[1...	11.839	7.9	ng	154542	4	11.310	390660	20.0
Phenanthrene, 1...	11.886	2.1	ng	40599	4	11.310	390660	20.0
4H-Cyclopenta[d...	11.922	4.6	ng	90040	4	11.310	390660	20.0
Naphthalene, 2-...	12.110	2.3	ng	43855	4	11.310	390660	20.0
Anthracene, 1,4...	12.363	2.6	ng	50069	4	11.310	390660	20.0
unknown12.404	12.404	2.1	ng	40961	4	11.310	390660	20.0
Pyrene, 2-methyl-	13.086	2.3	ng	62443	5	13.963	549509	20.0
11H-Benzo[b]flu...	13.151	2.7	ng	73351	5	13.963	549509	20.0
n-Heptadecanol-1	13.863	2.6	ng	71182	5	13.963	549509	20.0
Benzo[e]pyrene	15.315	4.2	ng	51291	6	15.445	244646	20.0