

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
 Data File : BF135366.D
 Acq On : 20 Sep 2023 19:47
 Operator : CG\JU
 Sample : 04397-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B103-03

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135366.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	24	rVB	39993	58136	1.81%	0.204%
2	5.004	492	496	507	rVB	34971	50155	1.56%	0.176%
3	5.393	558	562	581	rBV	3013089	3208897	100.00%	11.287%
4	6.404	729	734	737	rBV	3098505	3062451	95.44%	10.772%
5	6.604	762	768	771	rBV5	20141	38786	1.21%	0.136%
6	6.757	790	794	801	rVB	989037	802277	25.00%	2.822%
7	7.322	885	890	893	rBV	2137755	1980237	61.71%	6.966%
8	8.034	1007	1011	1025	rBV	1152859	1028289	32.04%	3.617%
9	8.751	1128	1133	1139	rBV2	34763	32722	1.02%	0.115%
10	9.116	1190	1195	1198	rBV	3064412	2750294	85.71%	9.674%
11	9.234	1212	1215	1219	rVB	37652	35486	1.11%	0.125%
12	9.792	1306	1310	1313	rBV	1084577	917330	28.59%	3.227%
13	9.822	1313	1315	1321	rVB	171073	156887	4.89%	0.552%
14	9.998	1342	1345	1350	rBV	66581	61998	1.93%	0.218%
15	10.339	1400	1403	1408	rVB	117102	105796	3.30%	0.372%
16	10.586	1441	1445	1460	rBV	1474204	1468680	45.77%	5.166%
17	11.180	1543	1546	1553	rVB	54324	49589	1.55%	0.174%
18	11.286	1560	1564	1566	rBV	856582	852782	26.58%	3.000%
19	11.310	1566	1568	1571	rVV	876026	711478	22.17%	2.503%
20	11.357	1571	1576	1580	rVB	193799	202048	6.30%	0.711%
21	11.522	1598	1604	1612	rBV	100518	120686	3.76%	0.425%
22	11.786	1646	1649	1652	rBV	68293	68844	2.15%	0.242%
23	11.822	1652	1655	1660	rVV	311812	312665	9.74%	1.100%
24	11.863	1660	1662	1665	rVB	37156	34302	1.07%	0.121%
25	11.898	1665	1668	1671	rBV	140205	145225	4.53%	0.511%
26	12.086	1697	1700	1703	rBV	58871	50347	1.57%	0.177%
27	12.116	1703	1705	1709	rVB	52299	48078	1.50%	0.169%
28	12.339	1740	1743	1746	rBV2	30260	33968	1.06%	0.119%
29	12.504	1767	1771	1775	rBV	1222263	1060904	33.06%	3.732%
30	12.610	1786	1789	1793	rBV4	60799	76328	2.38%	0.268%
31	12.657	1793	1797	1800	rVV2	43200	62136	1.94%	0.219%
32	12.733	1803	1810	1816	rVV	1006777	1093690	34.08%	3.847%
33	12.780	1816	1818	1823	rVB2	45460	49754	1.55%	0.175%
34	12.880	1831	1835	1838	rBV	2030078	1750196	54.54%	6.156%
35	12.957	1843	1848	1851	rBV2	46596	79867	2.49%	0.281%
36	13.039	1859	1862	1864	rBV3	48064	61958	1.93%	0.218%

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 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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.069	1864	1867	1870	rVB	141890	142303	4.43%	0.501%
38	13.133	1874	1878	1881	rVV	131099	114424	3.57%	0.402%
39	13.169	1881	1884	1886	rVV2	74191	77195	2.41%	0.272%
40	13.192	1886	1888	1891	rVB	38321	35292	1.10%	0.124%
41	13.298	1903	1906	1909	rBV3	49122	62472	1.95%	0.220%
42	13.369	1913	1918	1924	rBV	335062	344588	10.74%	1.212%
43	13.457	1928	1933	1937	rBV5	26611	60249	1.88%	0.212%
44	13.580	1951	1954	1958	rVB	65638	61392	1.91%	0.216%
45	13.686	1969	1972	1975	rBV	103011	115211	3.59%	0.405%
46	13.716	1975	1977	1979	rVV	90043	79199	2.47%	0.279%
47	13.739	1979	1981	1983	rVV	81519	87372	2.72%	0.307%
48	13.792	1987	1990	1996	rVB	89691	86989	2.71%	0.306%
49	13.939	2008	2015	2018	rBV2	911581	1374502	42.83%	4.835%
50	13.969	2018	2020	2023	rVB	509582	387839	12.09%	1.364%
51	14.045	2030	2033	2036	rVB	119379	105138	3.28%	0.370%
52	14.139	2047	2049	2053	rBV2	38032	49881	1.55%	0.175%
53	14.174	2053	2055	2058	rVB	51198	45366	1.41%	0.160%
54	14.233	2063	2065	2068	rVV3	46885	33687	1.05%	0.118%
55	14.292	2073	2075	2077	rBV2	38579	33099	1.03%	0.116%
56	14.333	2080	2082	2084	rVB	67826	53094	1.65%	0.187%
57	14.457	2101	2103	2105	rBV2	36765	33588	1.05%	0.118%
58	14.474	2105	2106	2110	rVB2	62026	48385	1.51%	0.170%
59	14.651	2133	2136	2143	rBV5	35419	61843	1.93%	0.218%
60	14.827	2163	2166	2169	rBV2	37217	47573	1.48%	0.167%
61	14.980	2188	2192	2195	rBV	385973	554431	17.28%	1.950%
62	15.057	2203	2205	2208	rVB3	50695	43816	1.37%	0.154%
63	15.092	2208	2211	2214	rVB	61609	64523	2.01%	0.227%
64	15.280	2240	2243	2250	rVB	205949	253668	7.91%	0.892%
65	15.345	2250	2254	2260	rBV	298297	366294	11.41%	1.288%
66	15.410	2260	2265	2268	rBV	529742	653847	20.38%	2.300%
67	16.886	2511	2516	2524	rVB2	96784	198314	6.18%	0.698%
68	17.333	2588	2592	2601	rVB2	61158	130294	4.06%	0.458%

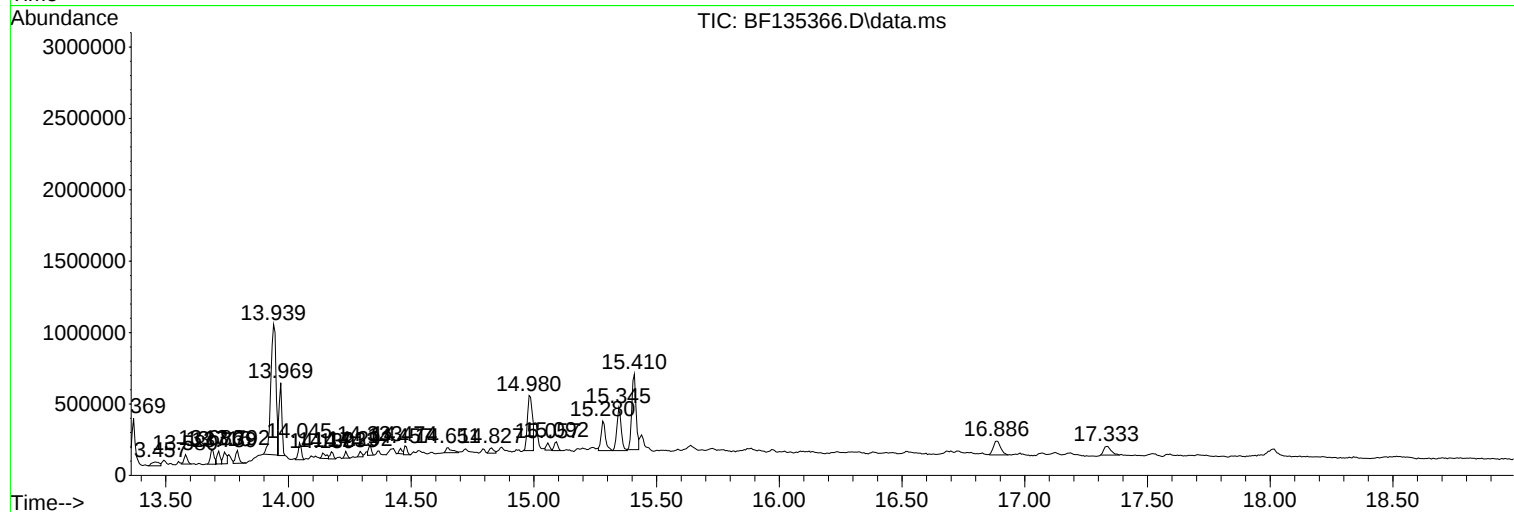
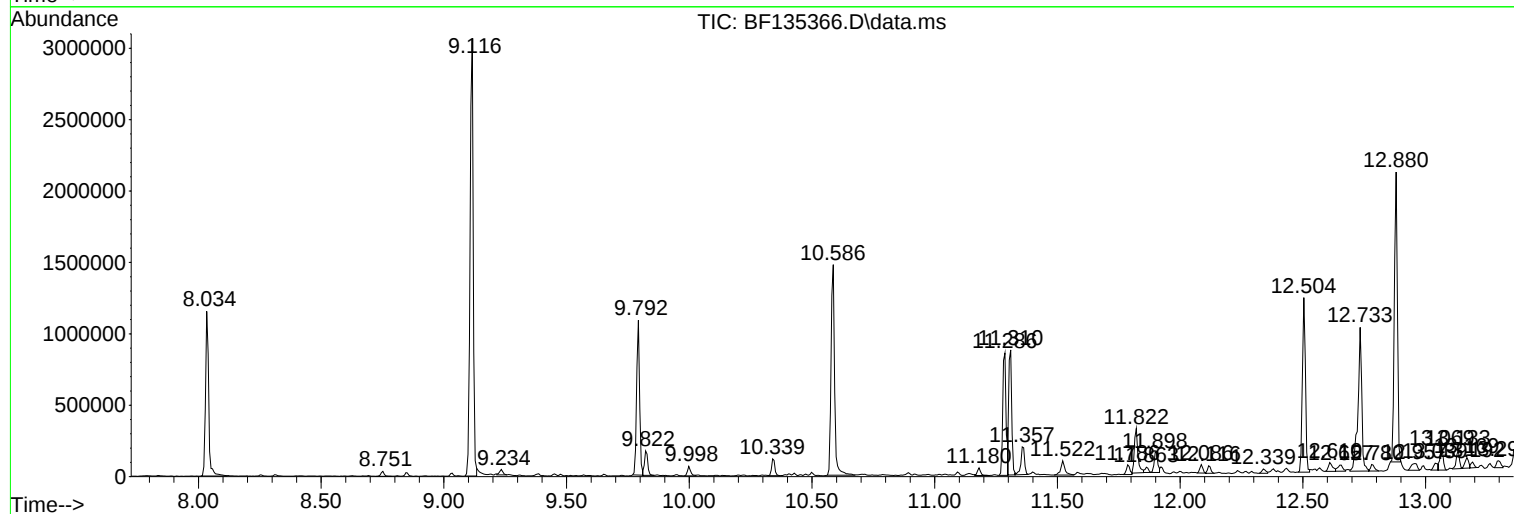
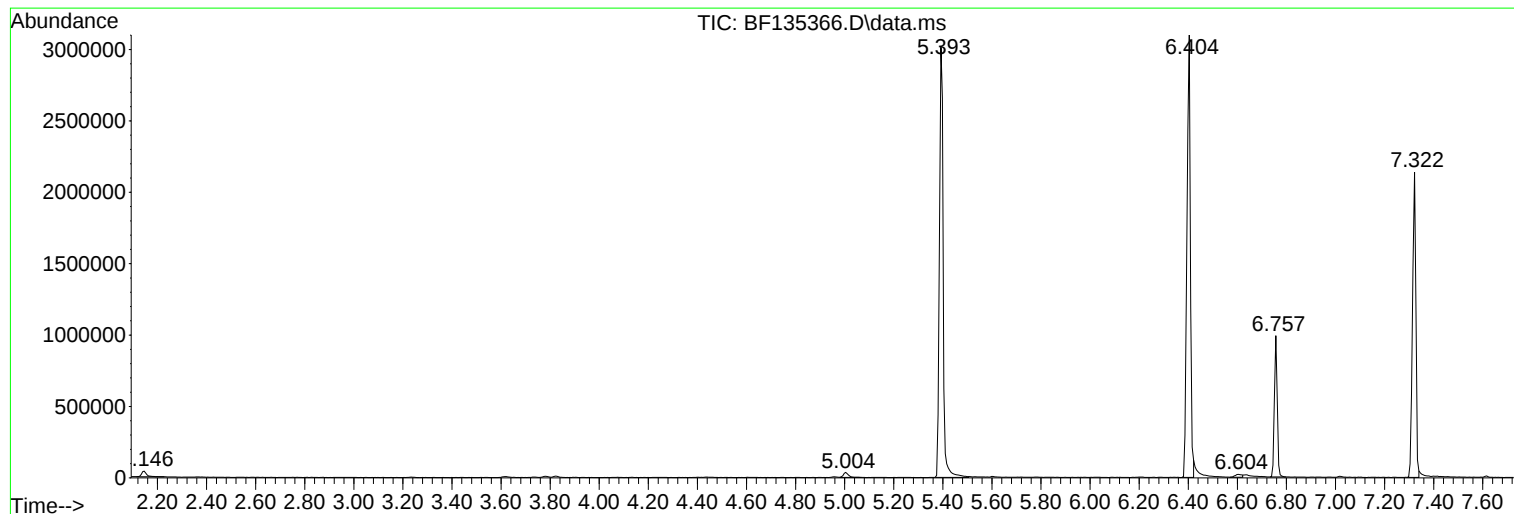
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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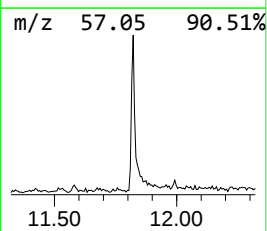
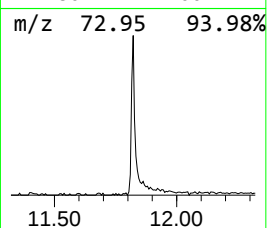
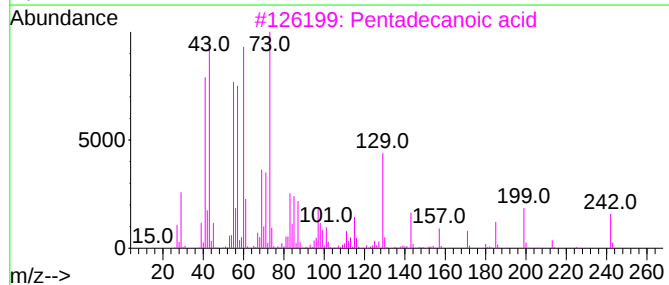
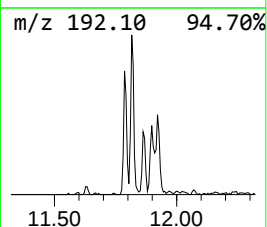
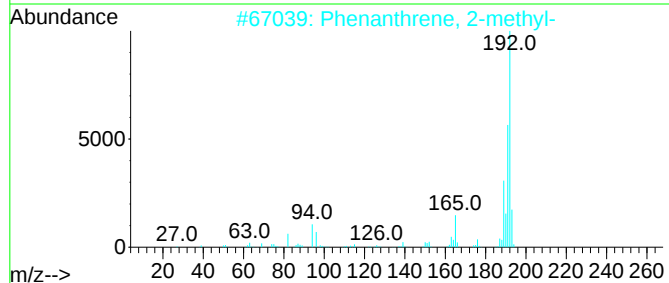
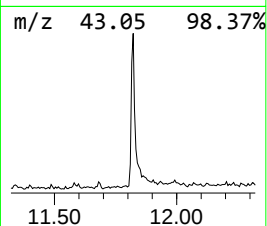
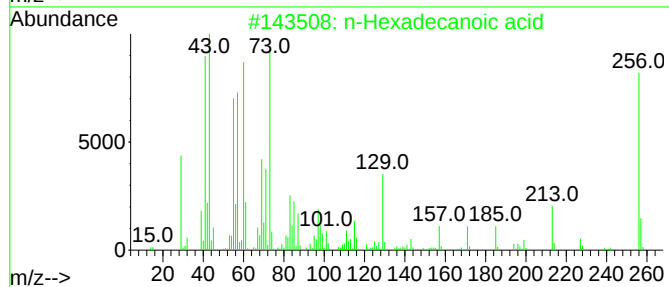
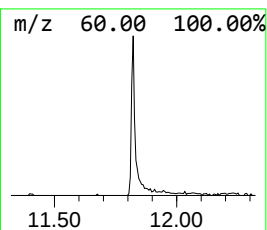
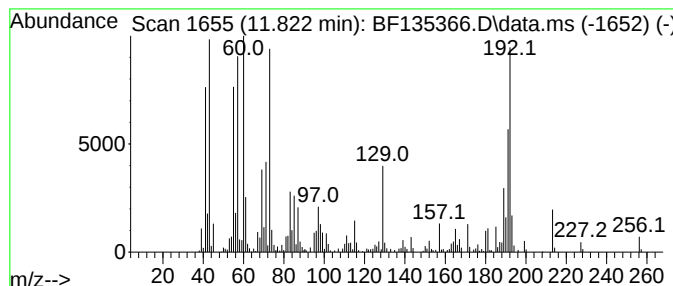
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	7.33 ng	312665	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60



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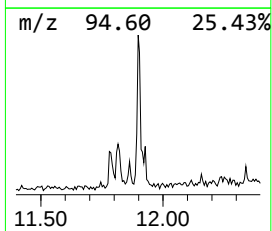
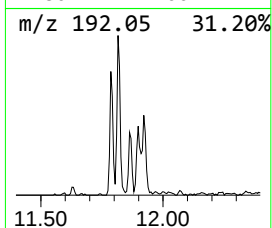
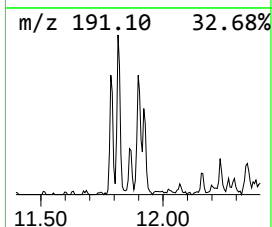
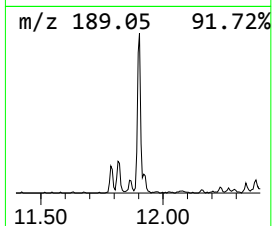
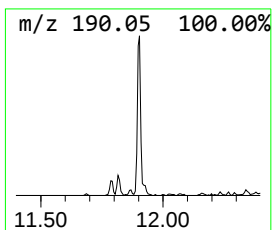
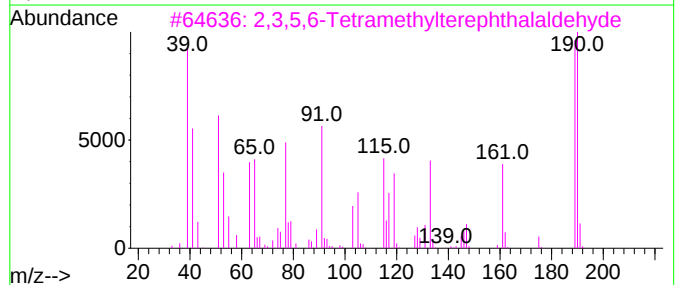
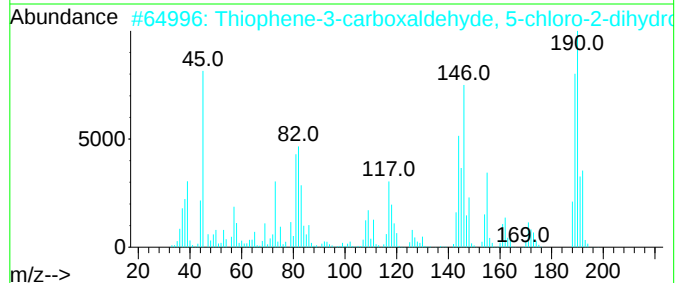
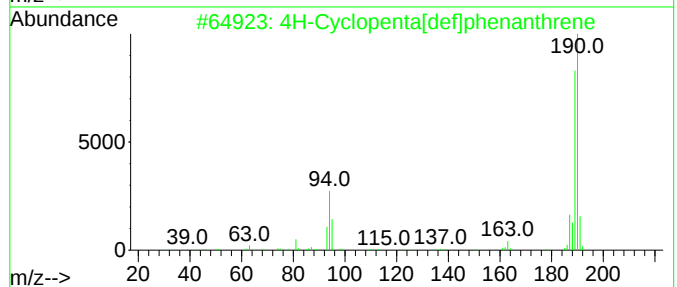
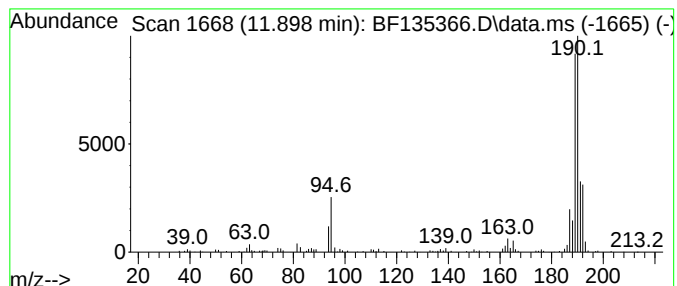
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.41 ng	145225	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45



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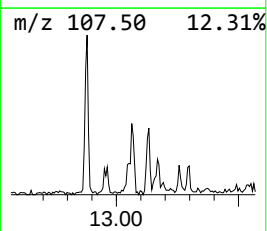
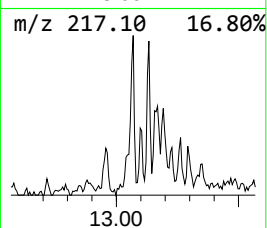
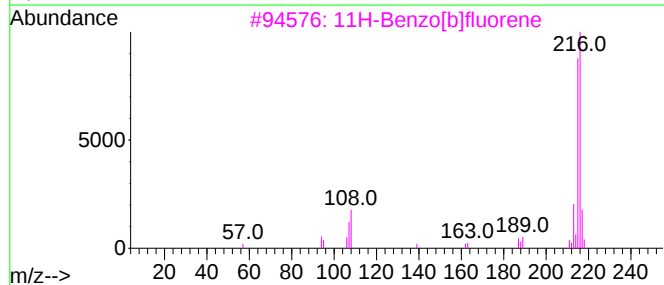
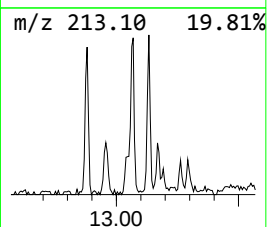
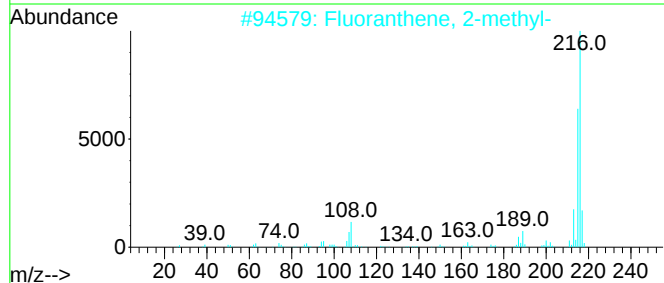
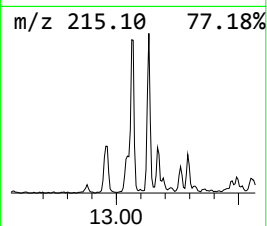
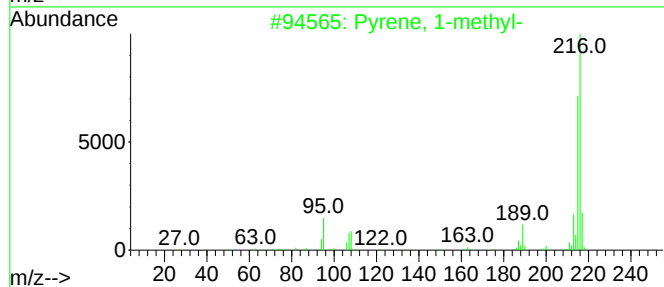
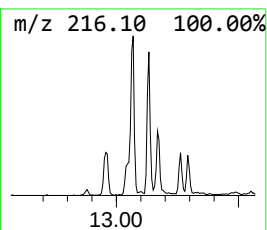
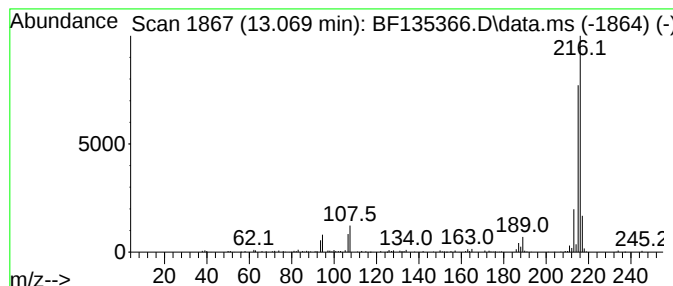
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pyrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	2.07 ng	142303	Chrysene-d12	13.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87



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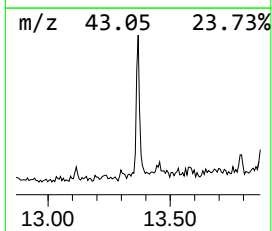
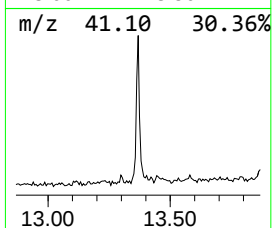
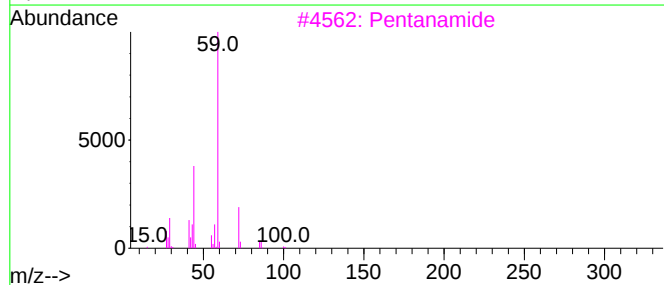
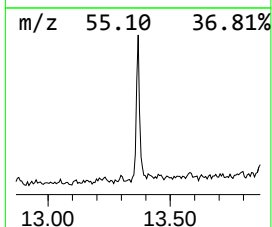
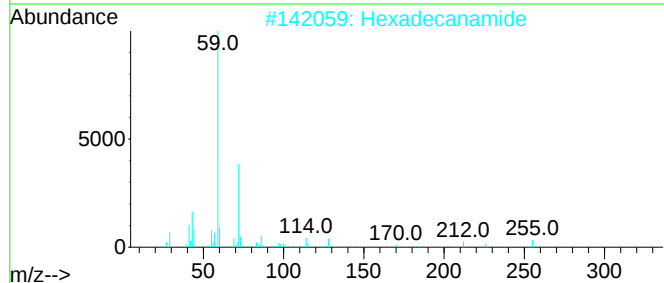
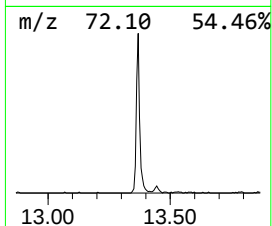
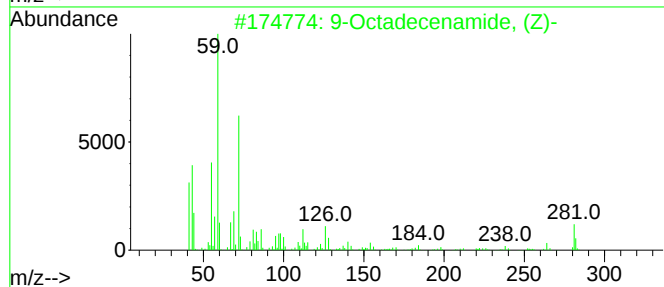
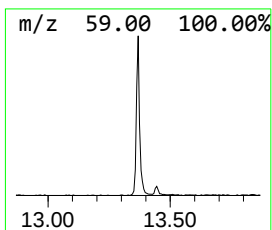
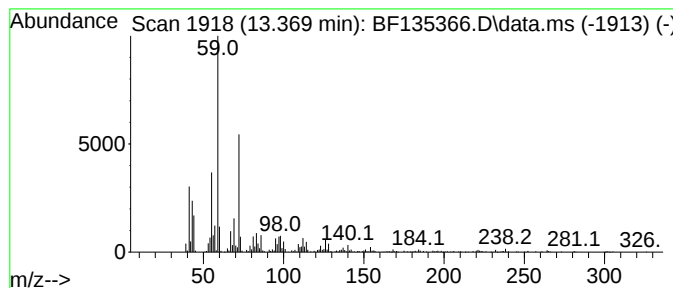
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	5.01 ng	344588	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Pentanamide	101	C5H11NO	000626-97-1	59
4			Methyl 2-[(2-methoxypropanoyl)(m...	231	C11H21NO4	1000495-86-8	47
5			Methyl 2-[(2-methoxypropanoyl)(m...	231	C11H21NO4	1000495-86-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135366.D
Acq On : 20 Sep 2023 19:47
Operator : CG\JU
Sample : 04397-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B103-03

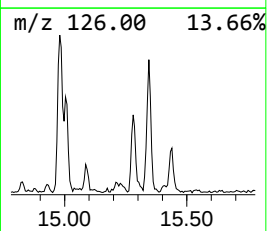
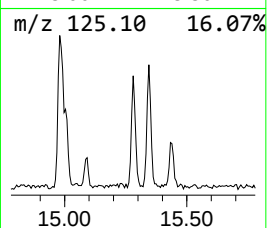
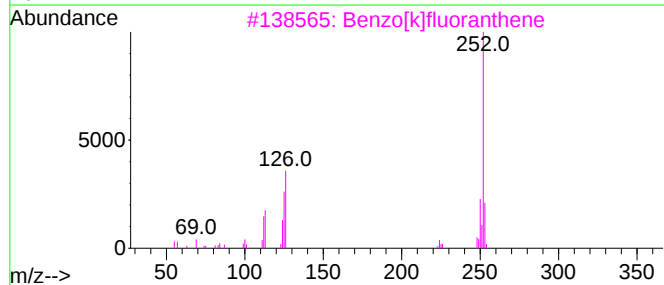
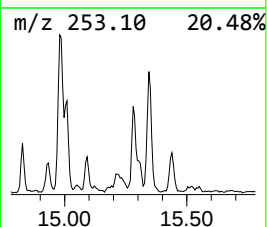
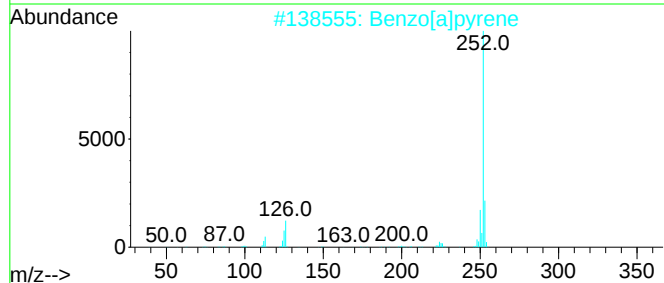
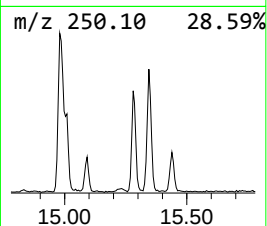
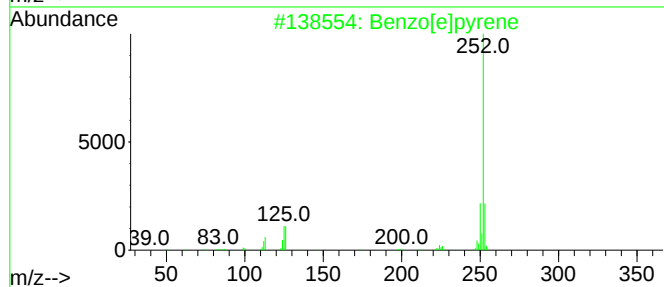
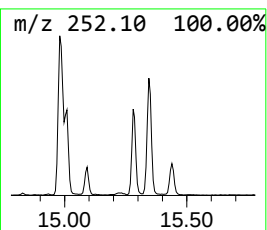
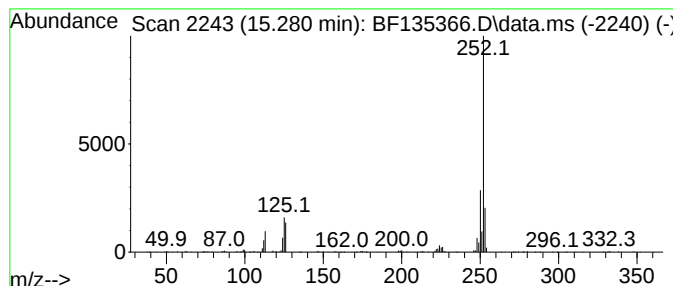
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	7.76 ng	253668	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Perylene	252	C20H12	000198-55-0	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135366.D
Acq On : 20 Sep 2023 19:47
Operator : CG\JU
Sample : 04397-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B103-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.822	7.3	ng	312665	4	11.286	852782	20.0
4H-Cyclopenta[d]...	11.898	3.4	ng	145225	4	11.286	852782	20.0
Pyrene, 1-methyl-	13.069	2.1	ng	142303	5	13.945	1374500	20.0
9-Octadecenamid...	13.368	5.0	ng	344588	5	13.945	1374500	20.0
Benzo[e]pyrene	15.280	7.8	ng	253668	6	15.410	653847	20.0