

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081023\
 Data File : BF134717.D
 Acq On : 10 Aug 2023 19:31
 Operator : CG\JU
 Sample : 03955-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-23

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.404	390	394	401	rBV	65310	74334	2.56%	0.273%
2	5.028	497	500	515	rVB	192430	218856	7.54%	0.803%
3	5.428	564	568	572	rBV	2503750	2428902	83.67%	8.909%
4	6.434	734	739	742	rBV	2732480	2505575	86.31%	9.191%
5	6.634	769	773	779	rBV	64947	66383	2.29%	0.243%
6	6.798	798	801	804	rBV	1507000	1122416	38.67%	4.117%
7	7.357	892	896	899	rBV	1844196	1606051	55.33%	5.891%
8	8.075	1014	1018	1021	rBV	1673329	1437910	49.53%	5.274%
9	9.151	1197	1201	1214	rBV	3171942	2902844	100.00%	10.648%
10	9.275	1219	1222	1232	rVB	53984	69794	2.40%	0.256%
11	9.834	1313	1317	1320	rBV	1750360	1443045	49.71%	5.293%
12	9.863	1320	1322	1327	rVB	84193	72953	2.51%	0.268%
13	10.039	1348	1352	1355	rBV2	40490	40588	1.40%	0.149%
14	10.381	1407	1410	1415	rVB	58149	56570	1.95%	0.208%
15	10.622	1447	1451	1462	rVB	1370958	1225531	42.22%	4.495%
16	10.745	1469	1472	1477	rVB4	24375	30340	1.05%	0.111%
17	11.128	1534	1537	1541	rVB2	33624	31890	1.10%	0.117%
18	11.216	1550	1552	1557	rVB	43049	41287	1.42%	0.151%
19	11.322	1566	1570	1572	rBV	1605710	1318995	45.44%	4.838%
20	11.345	1572	1574	1578	rVV	780795	606425	20.89%	2.224%
21	11.392	1578	1582	1586	rVB	167550	172112	5.93%	0.631%
22	11.557	1604	1610	1616	rBV2	42990	66773	2.30%	0.245%
23	11.822	1651	1655	1658	rBV	87195	89606	3.09%	0.329%
24	11.851	1658	1660	1665	rVV	172301	166440	5.73%	0.611%
25	11.898	1665	1668	1671	rVV	56712	57839	1.99%	0.212%
26	11.933	1671	1674	1677	rVV	120910	146733	5.05%	0.538%
27	11.957	1677	1678	1683	rVB	76144	57336	1.98%	0.210%
28	12.122	1703	1706	1708	rBV	74271	61335	2.11%	0.225%
29	12.145	1708	1710	1714	rVB	42234	36761	1.27%	0.135%
30	12.275	1726	1732	1734	rBV	32175	44154	1.52%	0.162%
31	12.375	1746	1749	1752	rBV	66663	64402	2.22%	0.236%
32	12.416	1752	1756	1761	rVB3	37262	68754	2.37%	0.252%
33	12.457	1761	1763	1768	rBV	62946	69001	2.38%	0.253%
34	12.539	1773	1777	1780	rBV	899392	803256	27.67%	2.946%
35	12.769	1810	1816	1819	rBV	801152	854295	29.43%	3.134%
36	12.816	1822	1824	1829	rVB2	39270	52970	1.82%	0.194%

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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

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37	12.886	1833	1836	1837	rBV2	45626	41723	1.44%	0.153%
38	12.916	1837	1841	1848	rVB	2762837	2303816	79.36%	8.450%
39	12.986	1848	1853	1857	rBV2	57261	98344	3.39%	0.361%
40	13.075	1865	1868	1869	rBV2	42534	44951	1.55%	0.165%
41	13.098	1869	1872	1875	rVB	71585	78578	2.71%	0.288%
42	13.163	1879	1883	1886	rVB3	50795	55547	1.91%	0.204%
43	13.198	1886	1889	1892	rBV	86664	93567	3.22%	0.343%
44	13.292	1902	1905	1908	rBV	57132	46977	1.62%	0.172%
45	13.322	1908	1910	1914	rBV	59279	53784	1.85%	0.197%
46	13.604	1955	1958	1962	rVB	73960	76078	2.62%	0.279%
47	13.716	1973	1977	1980	rBV2	64239	88986	3.07%	0.326%
48	13.745	1980	1982	1984	rVV	58304	44637	1.54%	0.164%
49	13.822	1991	1995	2001	rVB2	169060	222395	7.66%	0.816%
50	13.969	2013	2020	2023	rBV2	1228955	1497475	51.59%	5.493%
51	13.992	2023	2024	2030	rVB	350574	300891	10.37%	1.104%
52	14.074	2035	2038	2040	rVB	43881	37095	1.28%	0.136%
53	14.151	2048	2051	2055	rVB5	45224	43855	1.51%	0.161%
54	14.357	2084	2086	2089	rVB	69127	59722	2.06%	0.219%
55	14.392	2090	2092	2096	rBV2	38527	31657	1.09%	0.116%
56	14.457	2100	2103	2105	rBV3	59342	61709	2.13%	0.226%
57	14.739	2149	2151	2154	rBV2	72735	89360	3.08%	0.328%
58	15.010	2193	2197	2200	rBV	273235	387262	13.34%	1.420%
59	15.316	2245	2249	2255	rVB	154161	193119	6.65%	0.708%
60	15.374	2255	2259	2265	rBV	215943	264844	9.12%	0.971%
61	15.439	2266	2270	2274	rBV	624373	823710	28.38%	3.021%
62	17.380	2596	2600	2606	rVB2	59296	110045	3.79%	0.404%

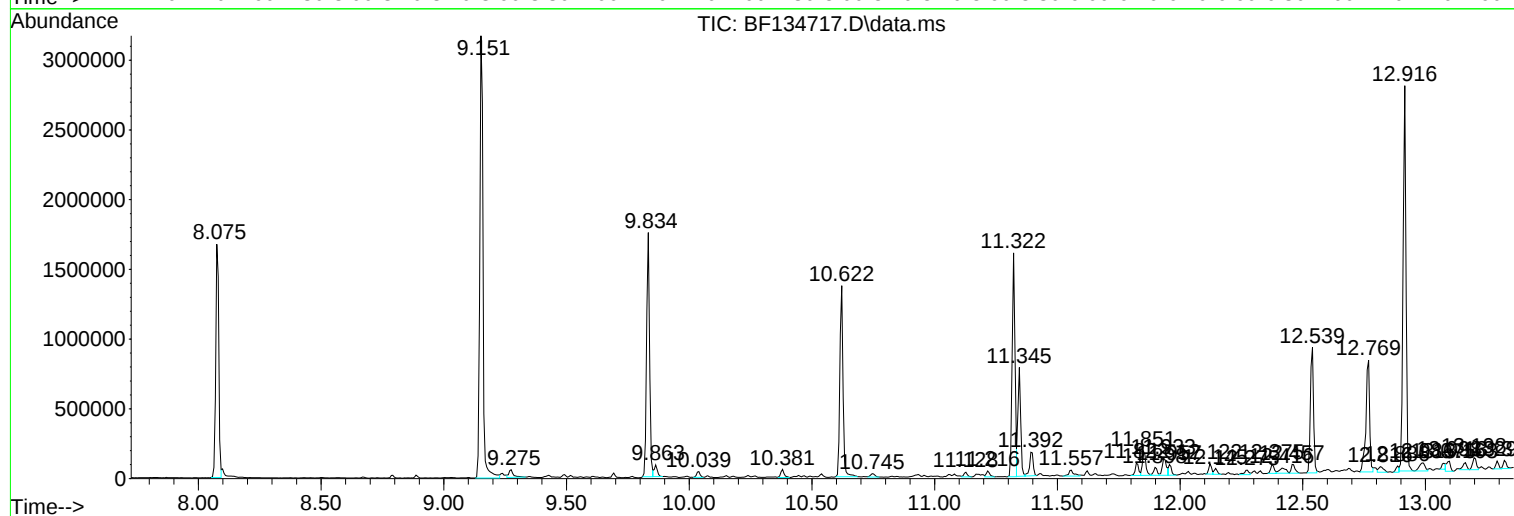
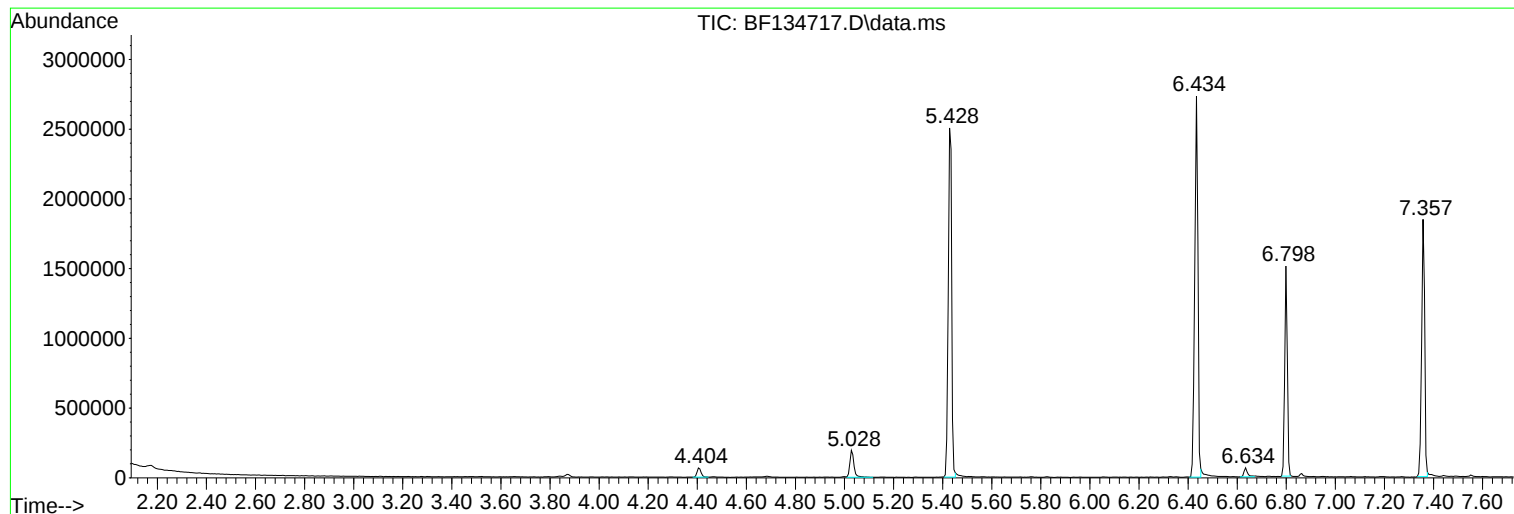
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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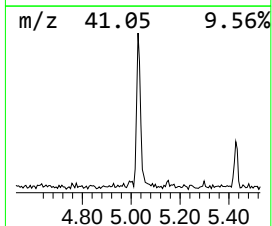
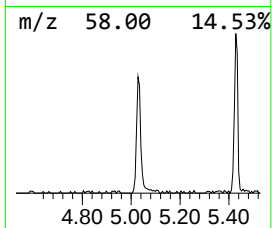
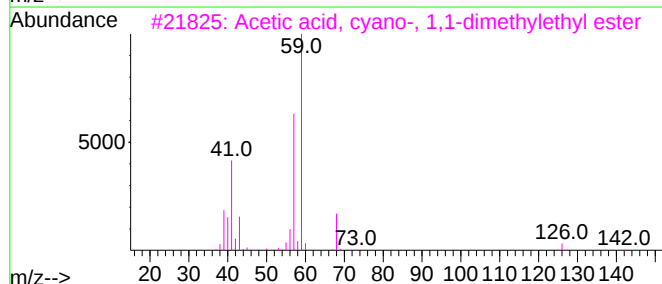
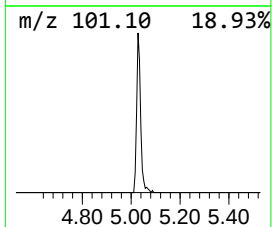
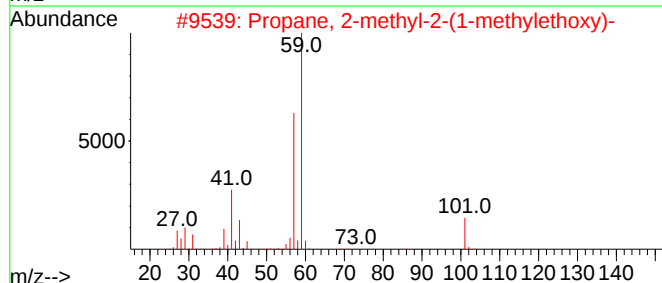
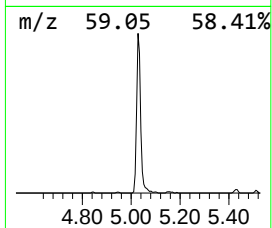
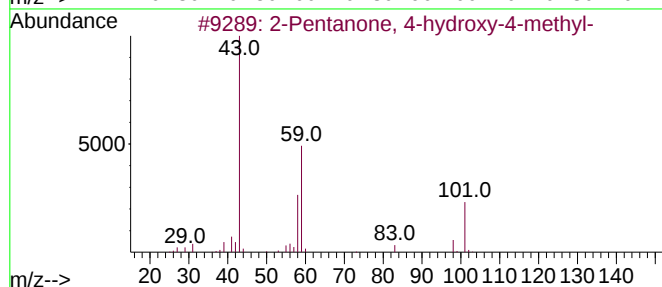
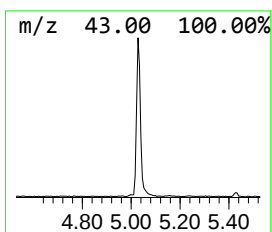
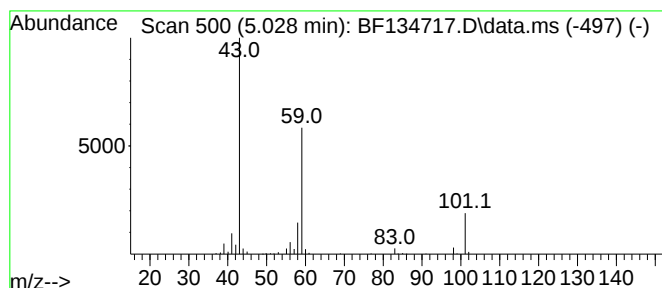
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	3.90 ng	218856	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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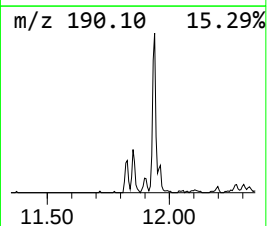
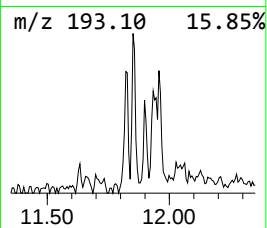
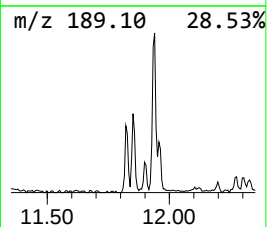
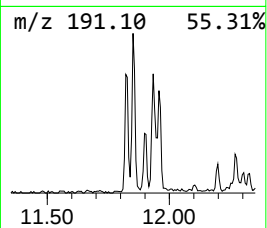
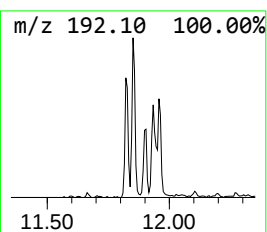
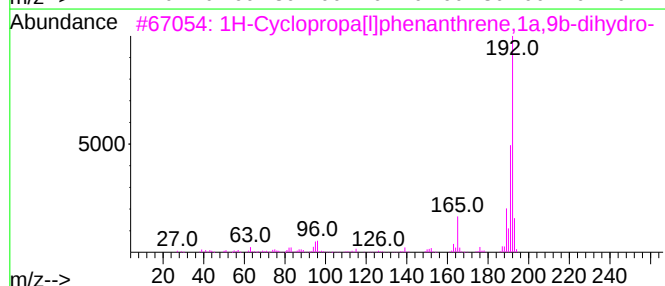
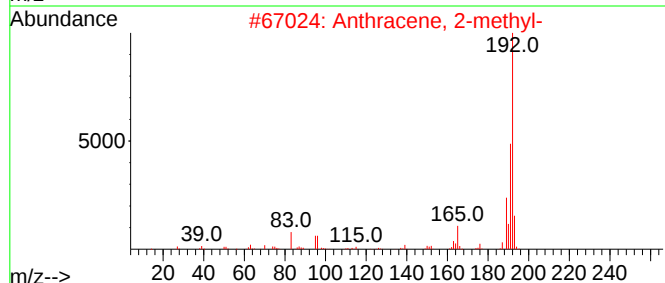
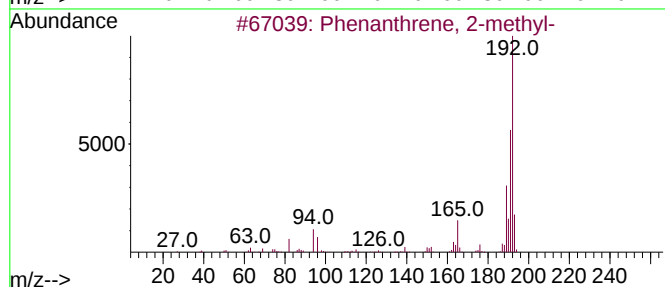
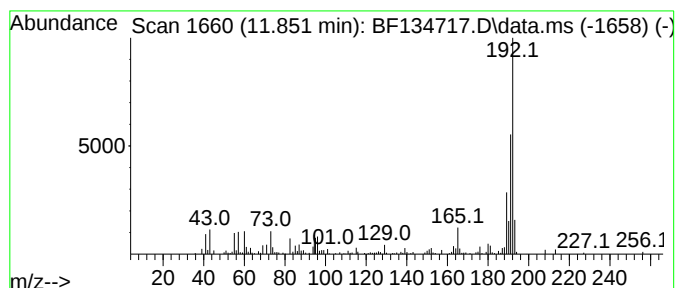
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.52 ng	166440	Phenanthrene-d10	11.322

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
3		1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
5		Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	94



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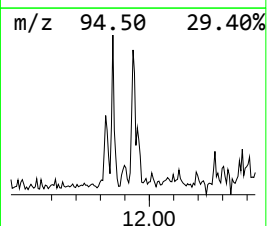
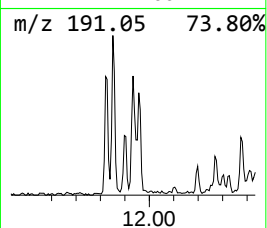
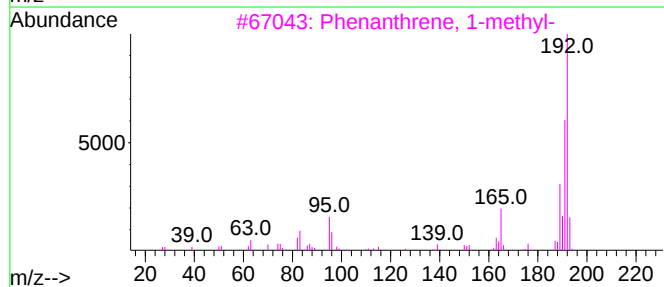
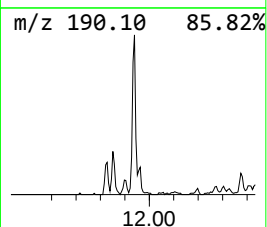
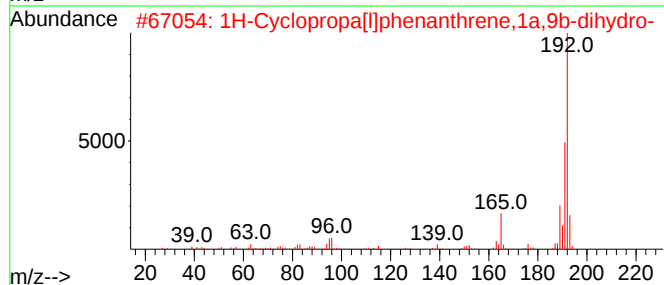
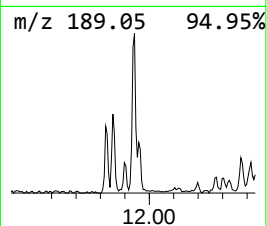
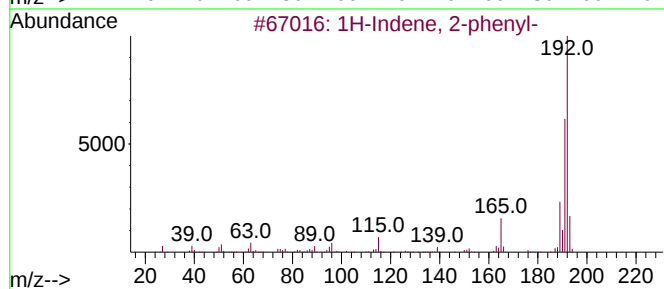
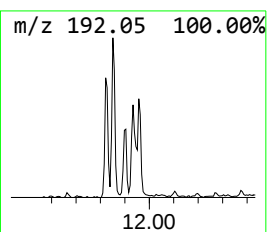
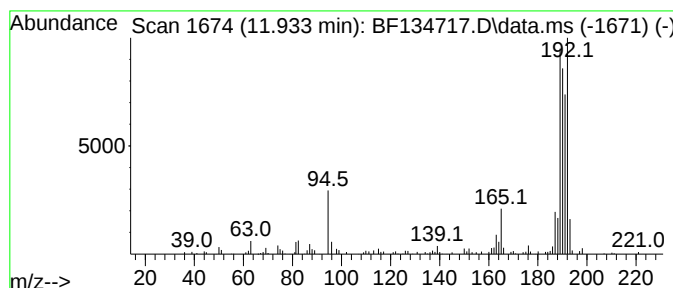
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1H-Indene, 2-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.22 ng	146733	Phenanthrene-d10	11.322

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	50
2		1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	50
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
4		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	50
5		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	46



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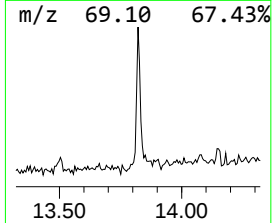
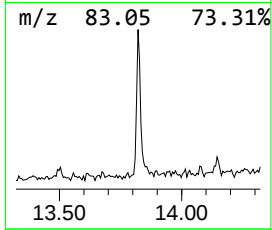
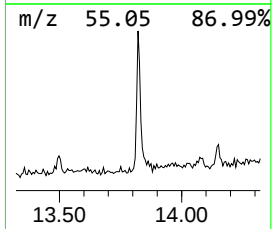
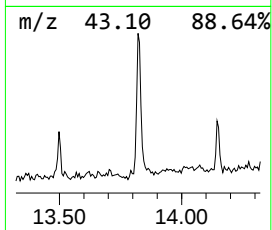
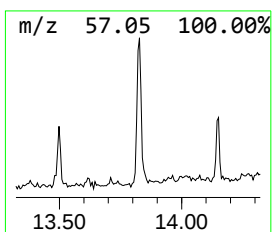
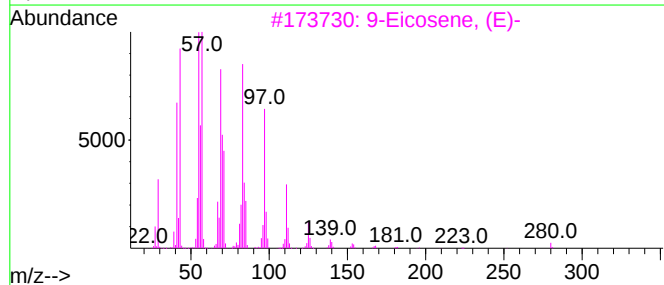
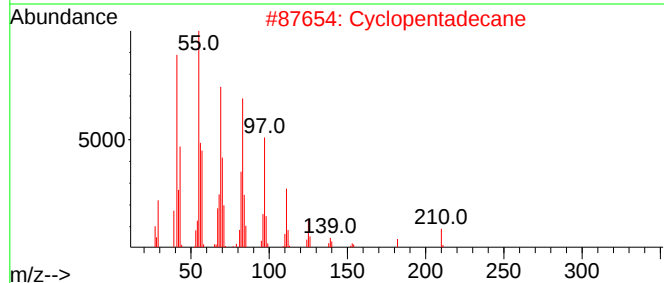
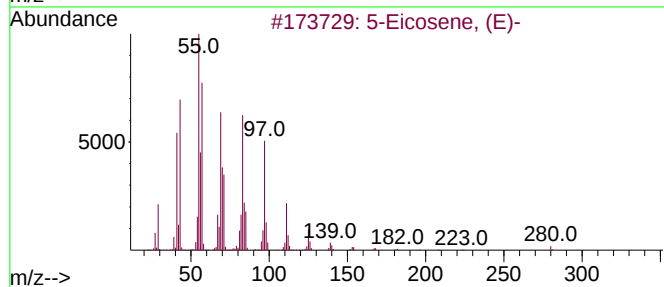
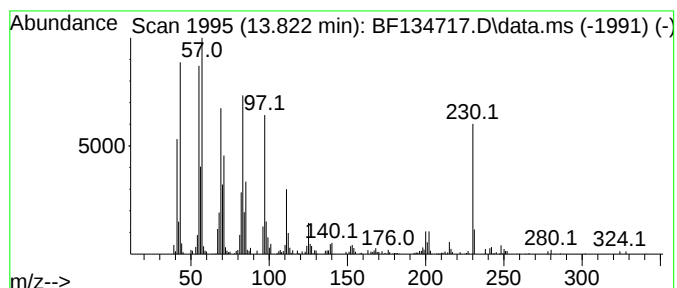
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.822	2.97 ng	222395	Chrysene-d12	13.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	92
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



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ALS Vial : 18 Sample Multiplier: 1

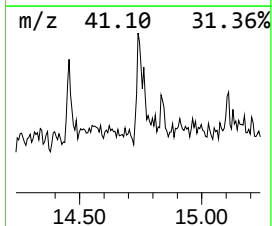
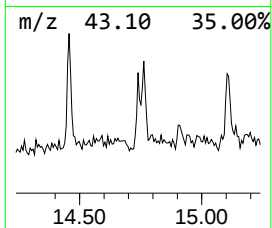
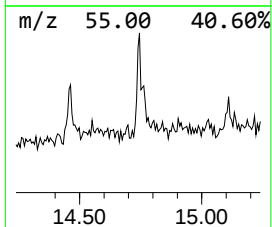
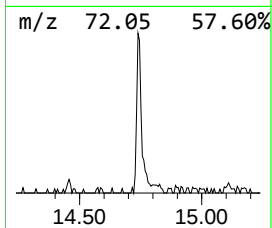
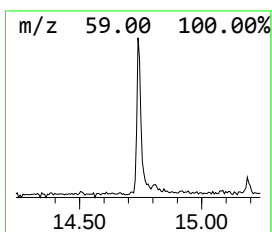
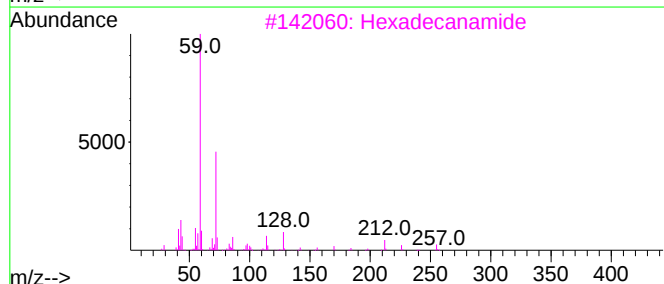
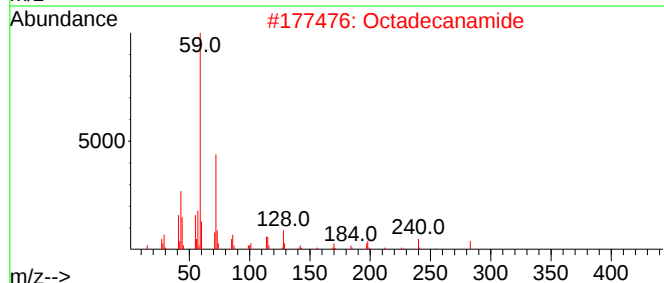
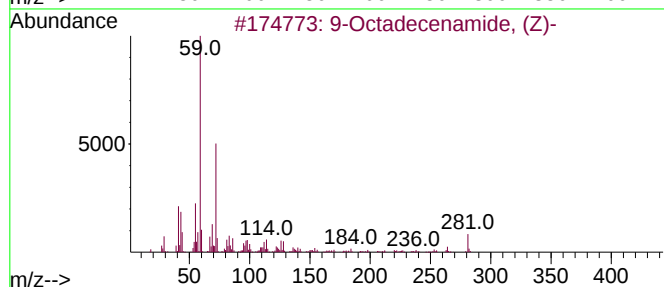
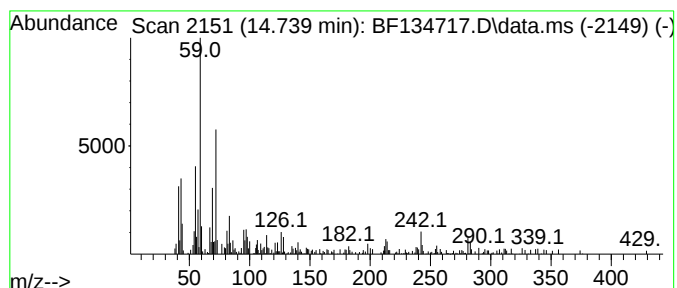
Instrument :
BNA_F
ClientSampleId :
WC-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.739	2.17 ng	89360	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Octadecanamide	283	C18H37NO	000124-26-5	89
3	Hexadecanamide	255	C16H33NO	000629-54-9	76
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
5	Behenic amide	339	C22H45NO	003061-75-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081023\
Data File : BF134717.D
Acq On : 10 Aug 2023 19:31
Operator : CG\JU
Sample : 03955-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-23

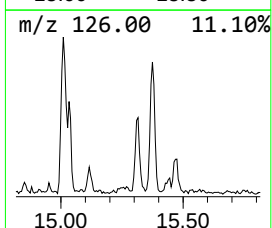
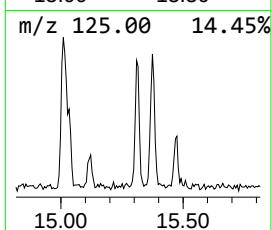
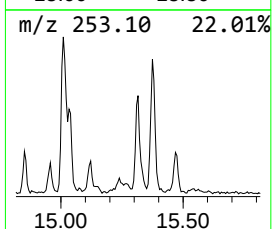
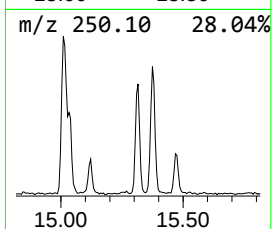
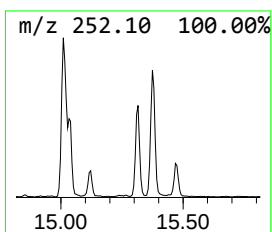
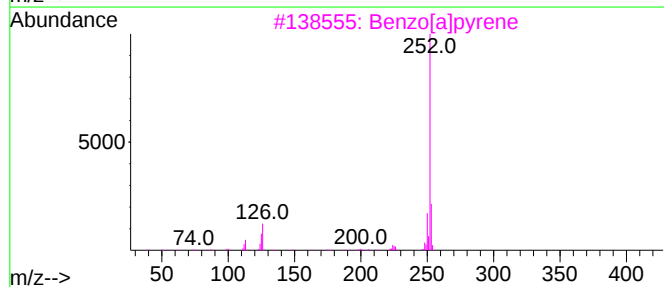
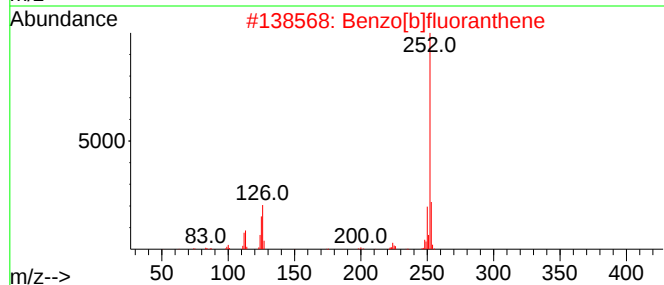
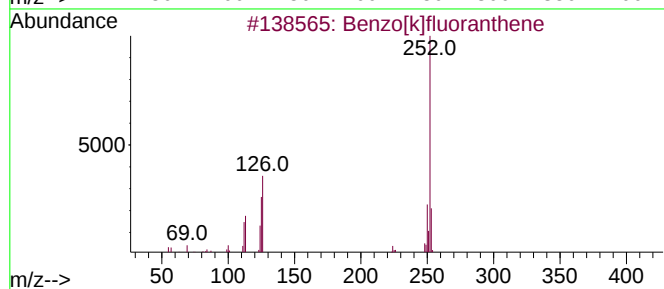
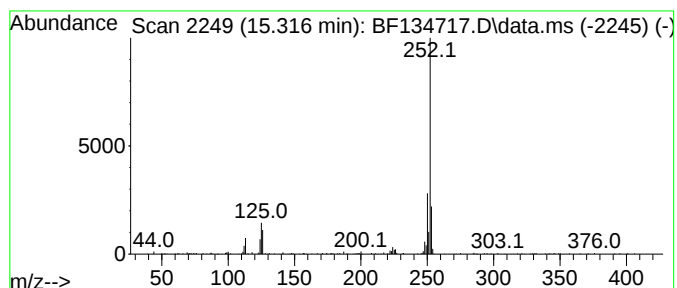
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.316	4.69 ng	193119	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Benzo[e]pyrene	252	C20H12	000192-97-2	95
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081023\
Data File : BF134717.D
Acq On : 10 Aug 2023 19:31
Operator : CG\JU
Sample : 03955-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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-...	5.028	3.9	ng	218856	1	6.798	1122420	20.0
Phenanthrene, 2...	11.851	2.5	ng	166440	4	11.322	1319000	20.0
1H-Indene, 2-ph...	11.933	2.2	ng	146733	4	11.322	1319000	20.0
5-Eicosene, (E)-	13.822	3.0	ng	222395	5	13.969	1497480	20.0
9-Octadecenamid...	14.739	2.2	ng	89360	6	15.439	823710	20.0
Benzo[e]pyrene	15.316	4.7	ng	193119	6	15.439	823710	20.0