

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
 Data File : BF136426.D
 Acq On : 06 Dec 2023 14:01
 Operator : CG\JU
 Sample : 05434-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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: BF136426.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	496	501	508	rBV	36168	46429	1.94%	0.209%
2	5.434	564	569	572	rBV	2166556	2102393	87.72%	9.442%
3	6.434	734	739	742	rBV	2109325	2020339	84.29%	9.073%
4	6.792	797	800	804	rBV	770595	654921	27.32%	2.941%
5	7.357	891	896	899	rBV	1451394	1320445	55.09%	5.930%
6	8.069	1014	1017	1021	rBV	892924	815781	34.04%	3.664%
7	9.151	1197	1201	1204	rBV	2980120	2396821	100.00%	10.764%
8	9.269	1216	1221	1226	rBV2	26693	30156	1.26%	0.135%
9	9.686	1289	1292	1296	rBV	68975	55137	2.30%	0.248%
10	9.828	1312	1316	1320	rBV	987234	778842	32.49%	3.498%
11	10.375	1406	1409	1415	rVB2	30648	33469	1.40%	0.150%
12	10.616	1446	1450	1465	rBV	1146439	1126796	47.01%	5.060%
13	11.316	1566	1569	1572	rBV	718386	689099	28.75%	3.095%
14	11.339	1572	1573	1577	rVV	362967	269215	11.23%	1.209%
15	11.392	1579	1582	1585	rVB	65396	55291	2.31%	0.248%
16	11.551	1602	1609	1612	rBV2	34599	41943	1.75%	0.188%
17	11.651	1623	1626	1630	rVB	38969	33911	1.41%	0.152%
18	11.710	1630	1636	1638	rBV7	26400	38946	1.62%	0.175%
19	11.822	1651	1655	1657	rBV	112363	92839	3.87%	0.417%
20	11.857	1657	1661	1665	rVV2	286162	296966	12.39%	1.334%
21	11.933	1670	1674	1676	rVV	140534	145090	6.05%	0.652%
22	11.957	1676	1678	1681	rVB	79252	61053	2.55%	0.274%
23	12.122	1703	1706	1707	rBV2	48491	41723	1.74%	0.187%
24	12.145	1707	1710	1714	rVB2	70827	73662	3.07%	0.331%
25	12.298	1734	1736	1739	rBV	36583	28598	1.19%	0.128%
26	12.374	1745	1749	1752	rBV	109148	110875	4.63%	0.498%
27	12.410	1752	1755	1757	rVV2	56551	70258	2.93%	0.316%
28	12.457	1761	1763	1768	rBV2	64097	75444	3.15%	0.339%
29	12.533	1773	1776	1780	rVV	648702	582471	24.30%	2.616%
30	12.586	1780	1785	1786	rVV4	32663	43338	1.81%	0.195%
31	12.645	1790	1795	1797	rVV3	90067	113256	4.73%	0.509%
32	12.686	1800	1802	1806	rVV3	42288	48485	2.02%	0.218%
33	12.763	1810	1815	1818	rVV	636692	662987	27.66%	2.977%
34	12.821	1822	1825	1829	rVB3	52403	64014	2.67%	0.287%
35	12.886	1832	1836	1837	rBV2	34147	32799	1.37%	0.147%
36	12.916	1837	1841	1844	rVV	2524741	2081840	86.86%	9.349%

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37	12.986	1848	1853	1856	rBV2	74213	107797	4.50%	0.484%
38	13.074	1864	1868	1869	rBV3	55946	64094	2.67%	0.288%
39	13.092	1869	1871	1875	rVB	102852	104794	4.37%	0.471%
40	13.163	1876	1883	1886	rBV2	87138	105426	4.40%	0.473%
41	13.198	1886	1889	1893	rBV	110073	109549	4.57%	0.492%
42	13.292	1902	1905	1908	rVB	89287	69161	2.89%	0.311%
43	13.321	1908	1910	1914	rBV	77489	63940	2.67%	0.287%
44	13.604	1955	1958	1963	rVB	72294	80579	3.36%	0.362%
45	13.716	1972	1977	1980	rBV3	83509	118227	4.93%	0.531%
46	13.745	1980	1982	1984	rVV	61208	51293	2.14%	0.230%
47	13.768	1984	1986	1991	rVV3	57079	82713	3.45%	0.371%
48	13.816	1991	1994	1998	rVB2	63548	88160	3.68%	0.396%
49	13.968	2009	2020	2023	rBV2	932348	1263648	52.72%	5.675%
50	13.998	2023	2025	2031	rVB	350033	309383	12.91%	1.389%
51	14.145	2048	2050	2055	rVB4	56298	62230	2.60%	0.279%
52	14.357	2082	2086	2090	rVB	94991	107580	4.49%	0.483%
53	14.392	2090	2092	2095	rBV2	71364	63010	2.63%	0.283%
54	14.451	2100	2102	2105	rVB2	92414	81960	3.42%	0.368%
55	14.486	2105	2108	2110	rBV	53951	58598	2.44%	0.263%
56	14.915	2178	2181	2185	rVB5	46939	62042	2.59%	0.279%
57	15.015	2194	2198	2201	rBV	281139	404958	16.90%	1.819%
58	15.110	2211	2214	2221	rVB2	87950	148040	6.18%	0.665%
59	15.321	2246	2250	2257	rVB	184374	239407	9.99%	1.075%
60	15.386	2257	2261	2267	rVB	201155	249311	10.40%	1.120%
61	15.451	2267	2272	2276	rBV	508426	628034	26.20%	2.820%
62	15.957	2353	2358	2362	rBV	79188	131059	5.47%	0.589%
63	16.939	2521	2525	2536	rVB2	77530	168437	7.03%	0.756%
64	17.392	2598	2602	2609	rVB	55580	107835	4.50%	0.484%

Sum of corrected areas: 22266897

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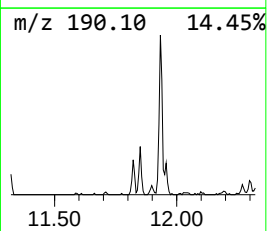
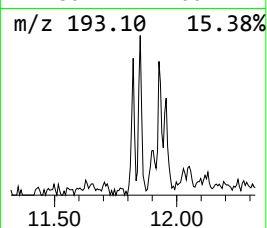
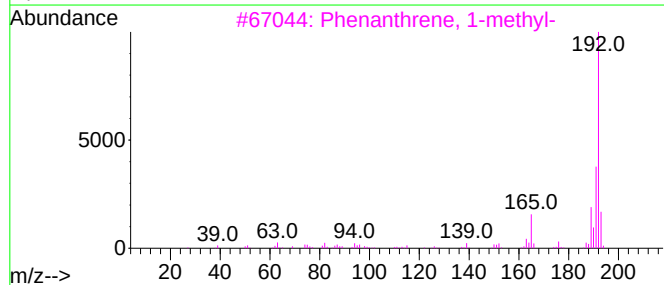
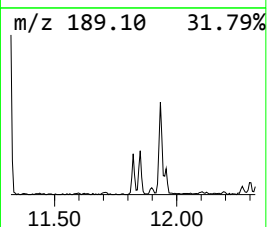
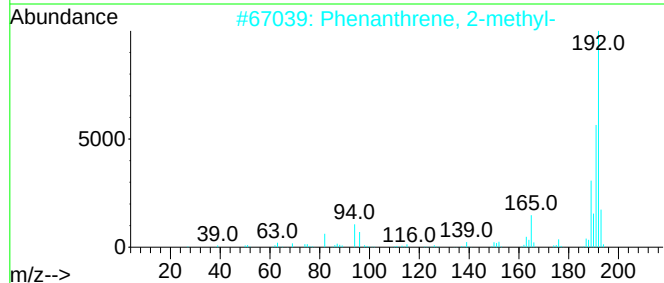
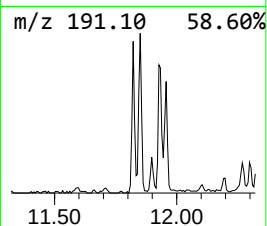
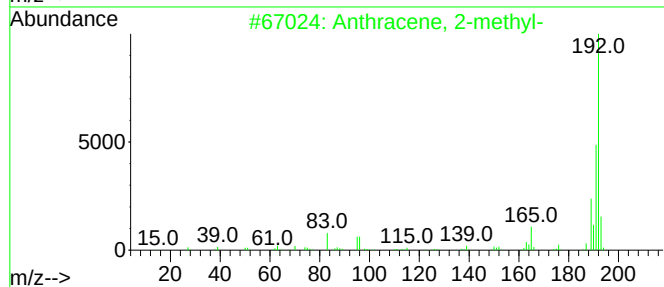
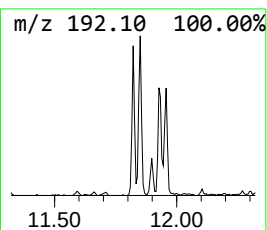
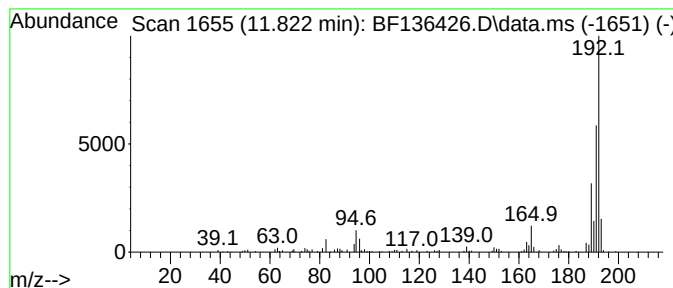
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.69 ng	92839	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
4			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91



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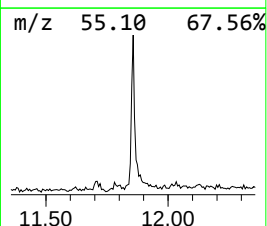
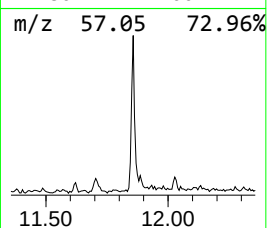
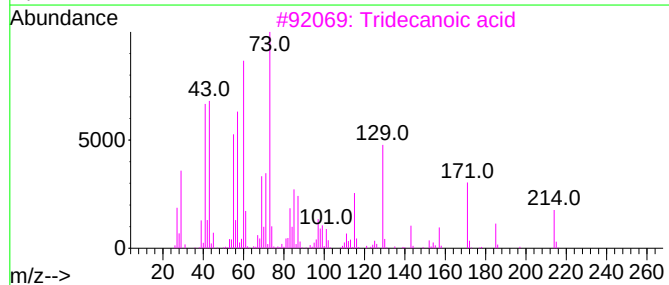
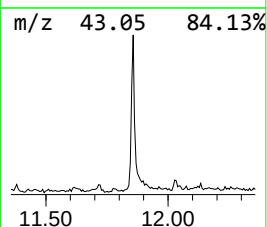
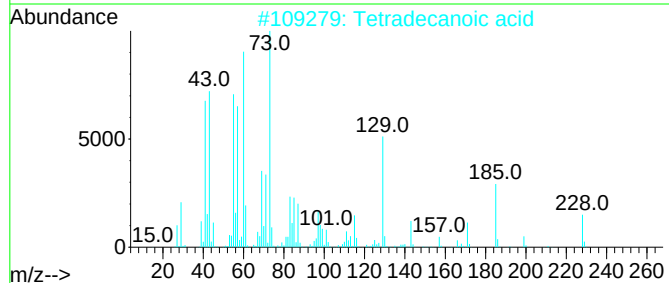
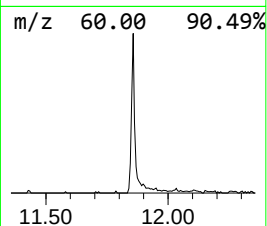
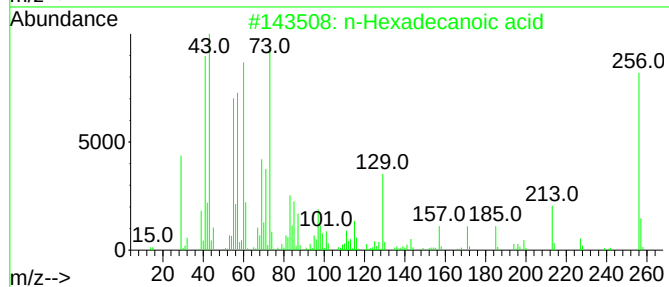
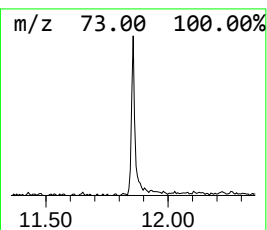
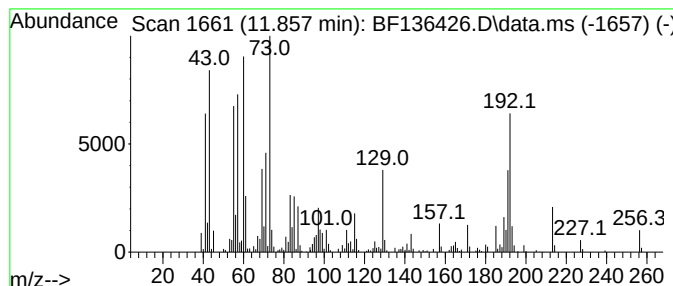
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.62 ng	296966	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	98
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Undecanoic acid	186	C11H22O2	000112-37-8	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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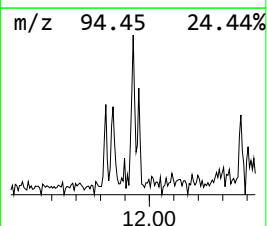
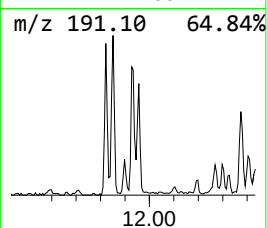
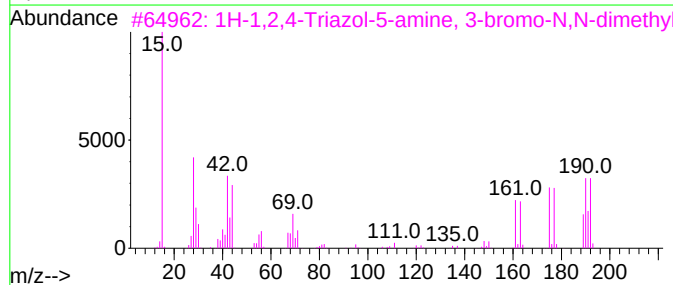
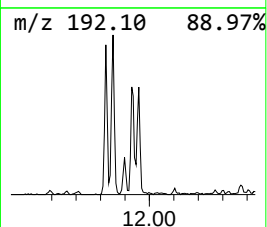
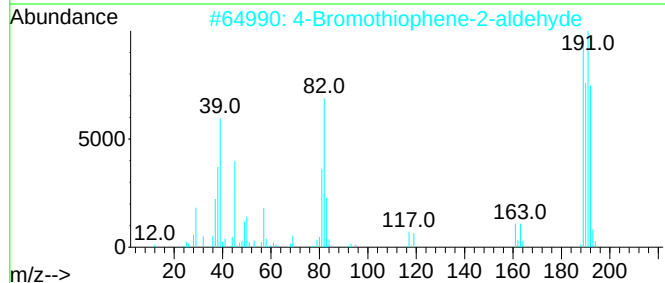
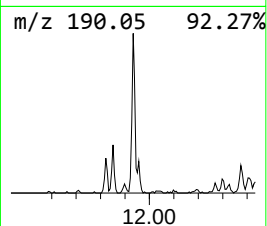
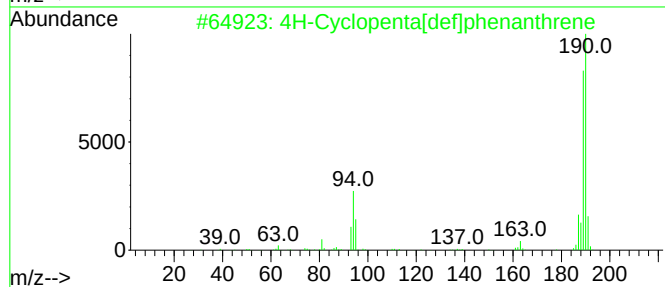
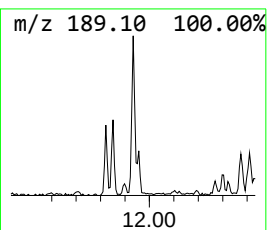
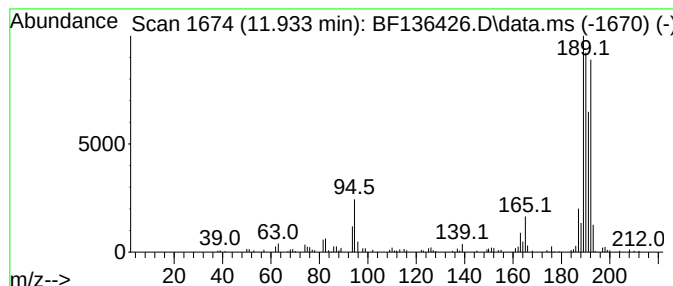
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.21 ng	145090	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
3			1H-1,2,4-Triazol-5-amine, 3-brom...	190	C4H7BrN4	1000460-85-7	53
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
5			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42



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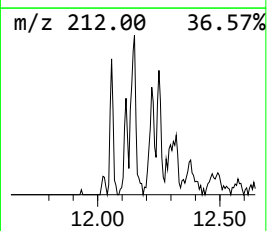
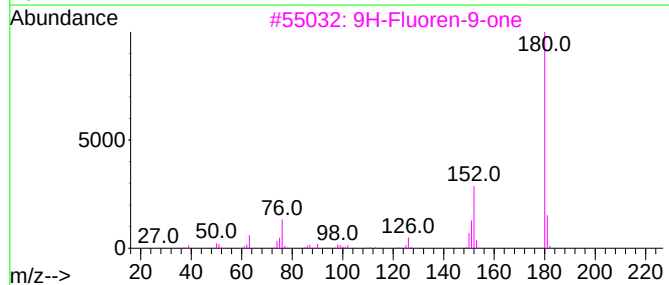
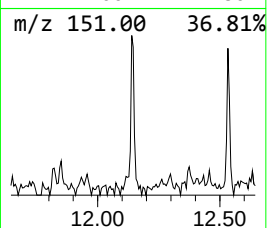
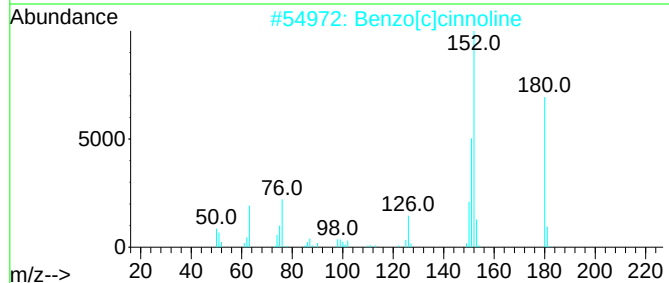
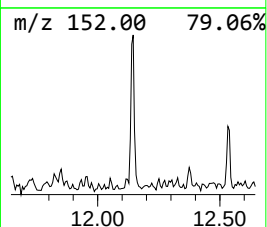
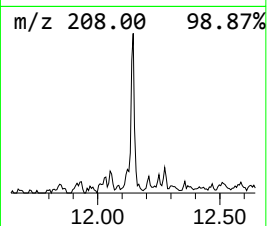
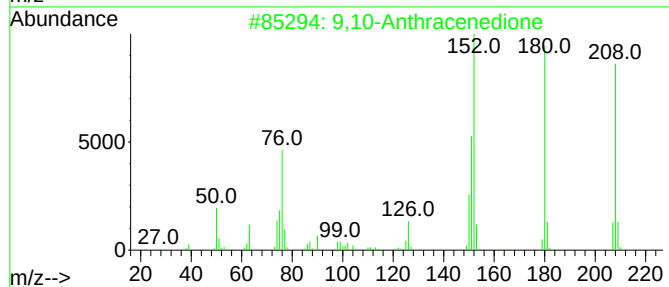
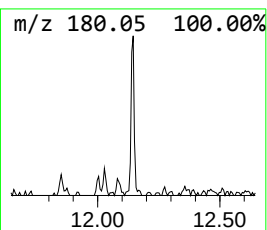
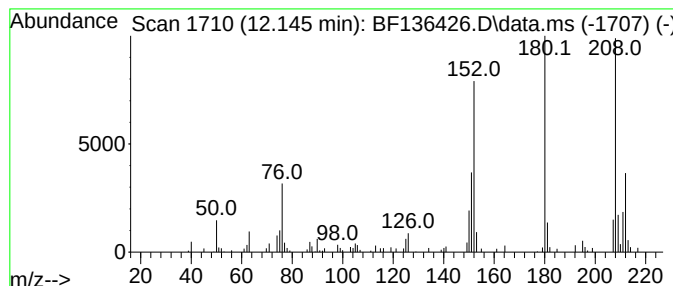
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9,10-Anthracenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.145	2.14 ng	73662	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione			208	C14H8O2	000084-65-1	93
2	Benzo[c]cinnoline			180	C12H8N2	000230-17-1	60
3	9H-Fluoren-9-one			180	C13H8O	000486-25-9	60
4	1H-Phenalen-1-one			180	C13H8O	000548-39-0	55
5	Benzo[h]cinnoline			180	C12H8N2	000230-31-9	53



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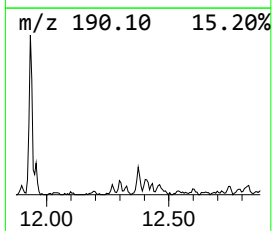
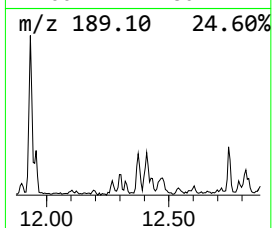
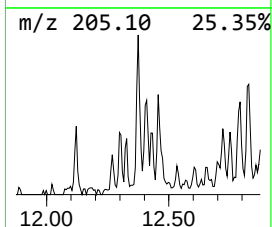
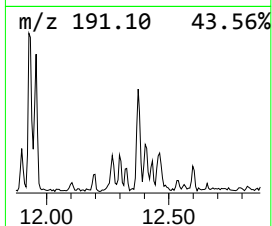
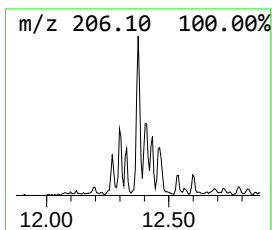
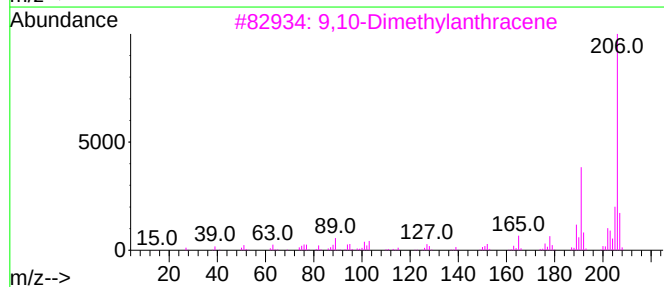
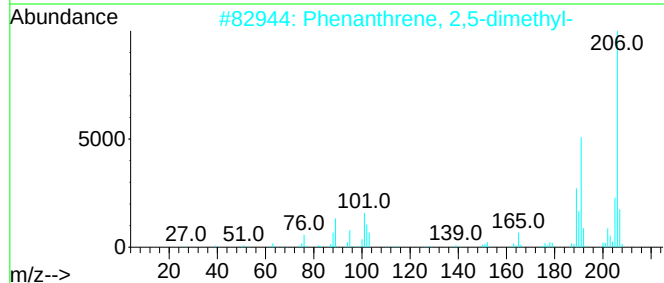
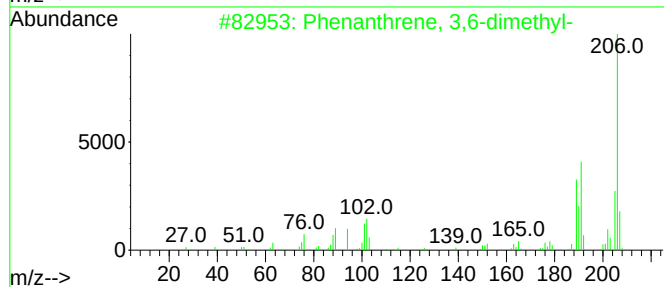
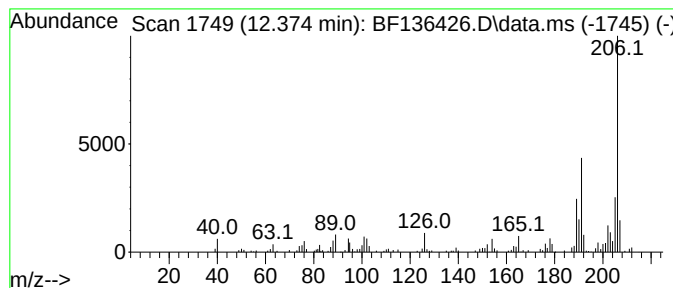
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	3.22 ng	110875	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
3			9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
4			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87
5			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

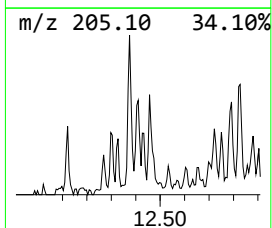
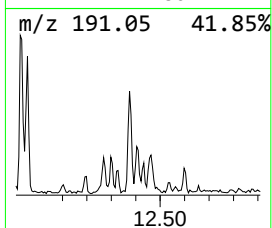
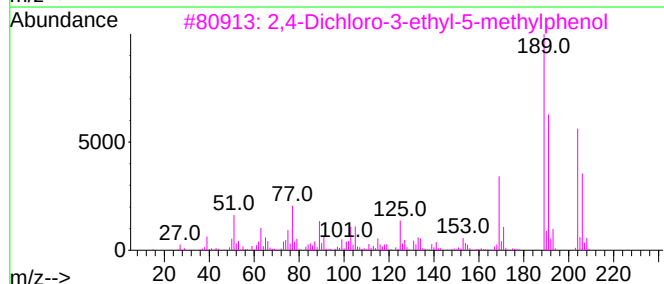
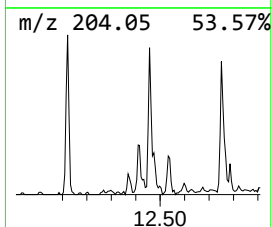
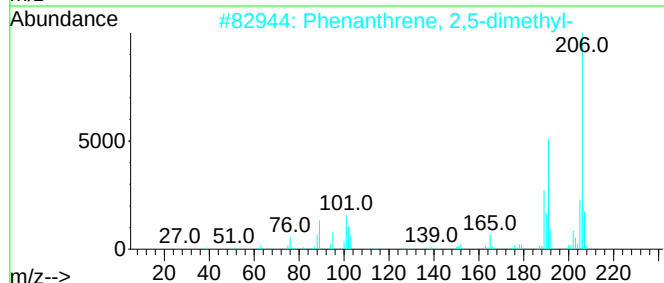
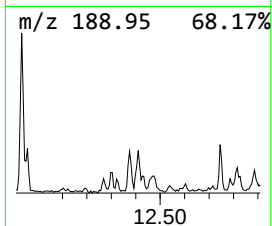
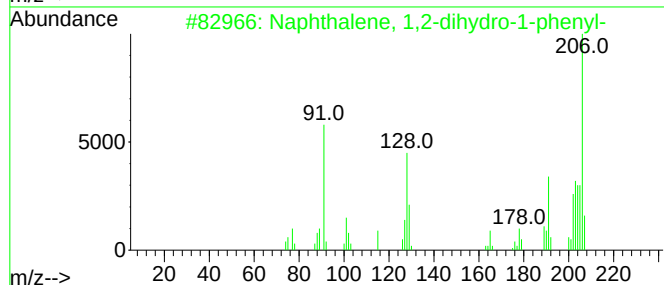
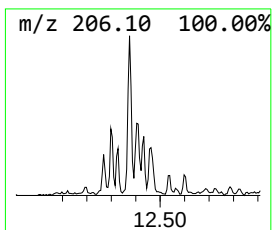
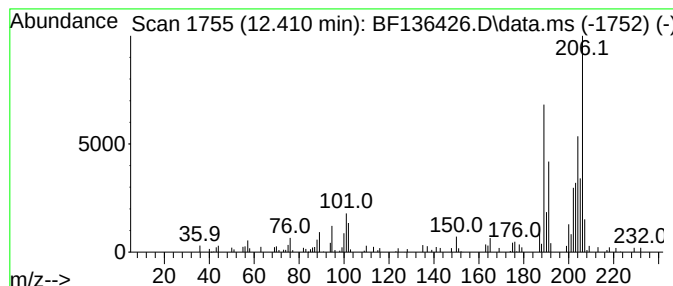
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.410 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.04 ng	70258	Phenanthrene-d10	11.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2-dihydro-1-phenyl-	206	C16H14	016606-46-5	49
2		Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	49
3		2,4-Dichloro-3-ethyl-5-methylphenol	204	C9H10Cl2O	001127-60-2	46
4		Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	46
5		Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

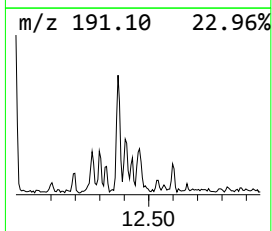
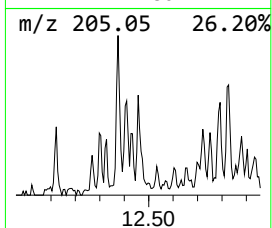
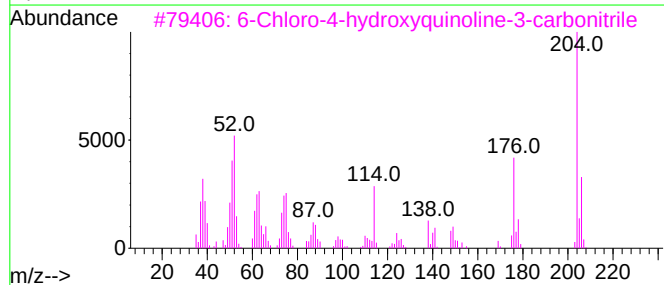
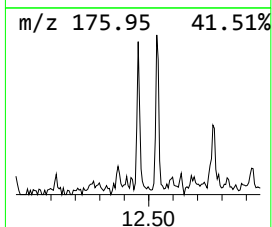
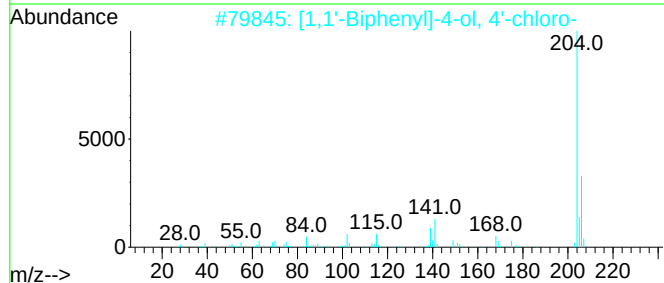
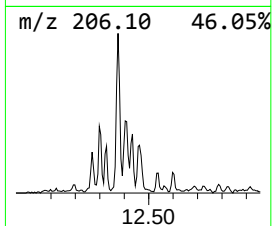
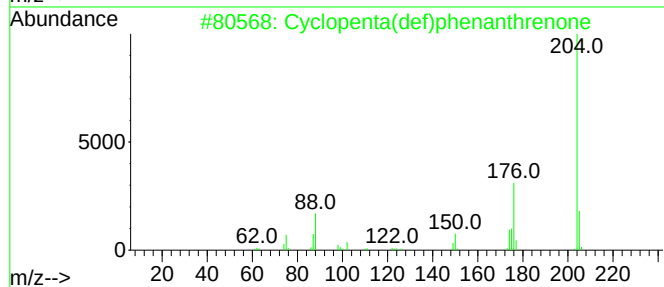
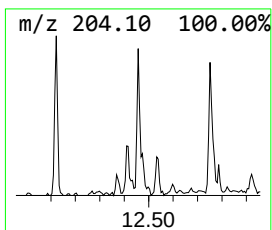
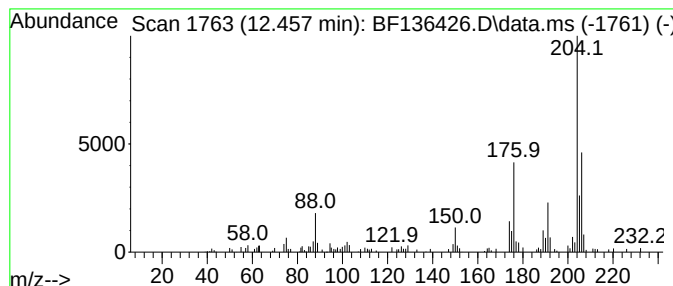
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopenta(def)phenanthrenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.457	2.19 ng	75444	Phenanthrene-d10			11.316
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone		204	C15H8O	005737-13-3	55
2	[1,1'-Biphenyl]-4-ol, 4'-chloro-		204	C12H9ClO	028034-99-3	46
3	6-Chloro-4-hydroxyquinoline-3-ca...		204	C10H5ClN2O	1000435-79-8	42
4	2,4-Dichloro-3-ethyl-5-methylphe...		290	C13H16Cl2O3	1000487-42-9	38
5	2-Chloro-4-phenylphenol		204	C12H9ClO	000092-04-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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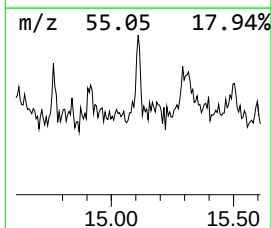
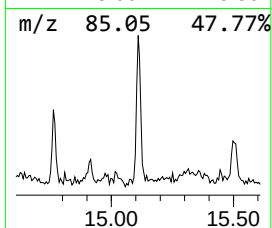
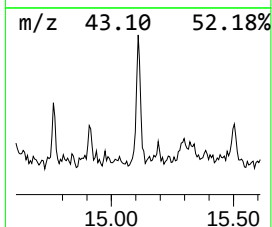
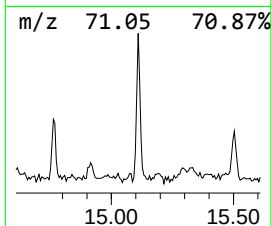
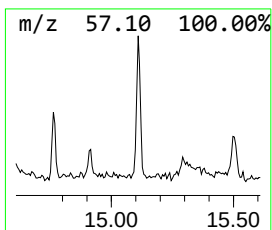
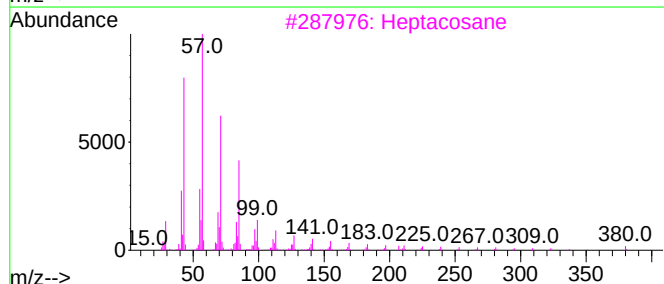
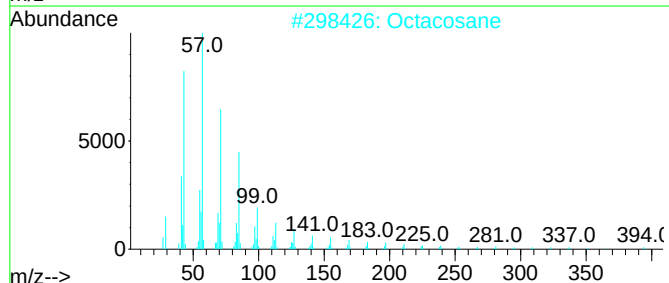
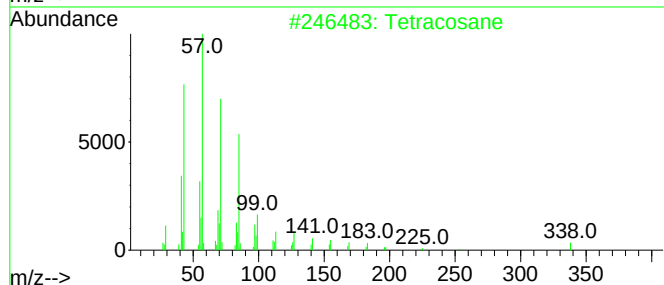
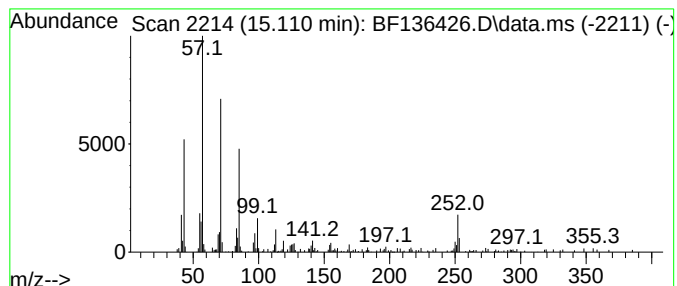
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	4.71 ng	148040	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	83
2		Octacosane	394	C28H58	000630-02-4	83
3		Heptacosane	380	C27H56	000593-49-7	83
4		Heptadecane	240	C17H36	000629-78-7	83
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

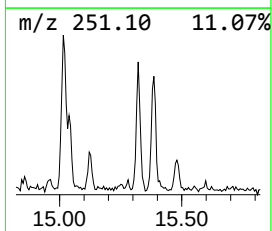
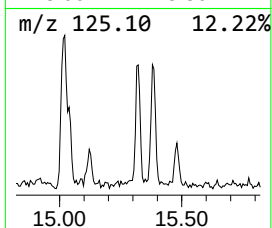
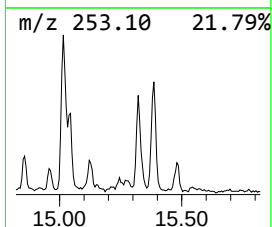
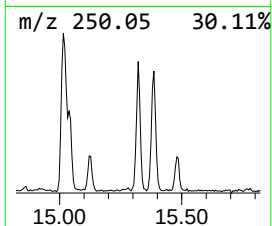
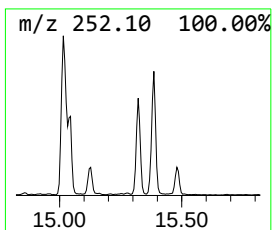
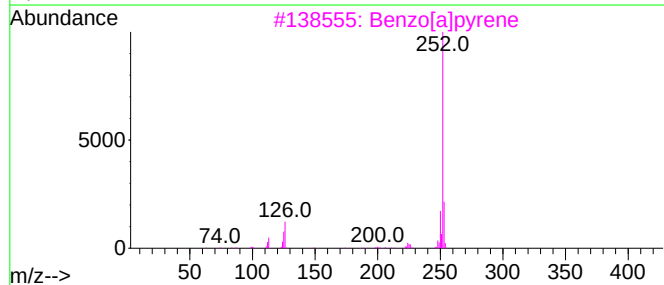
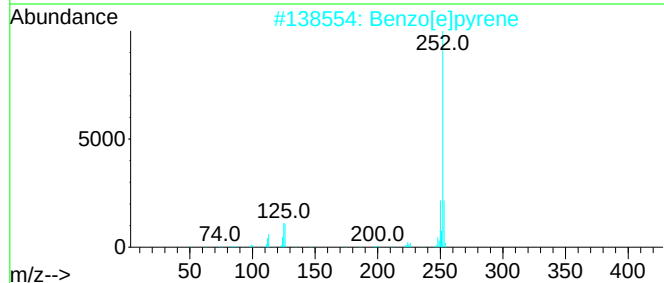
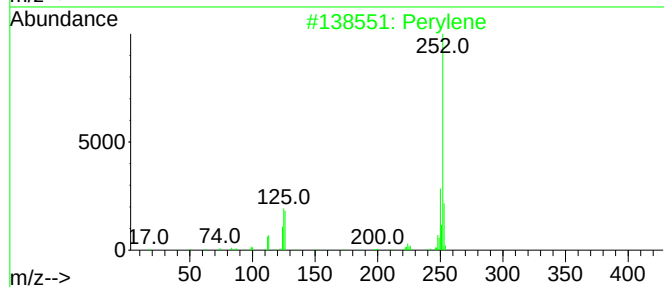
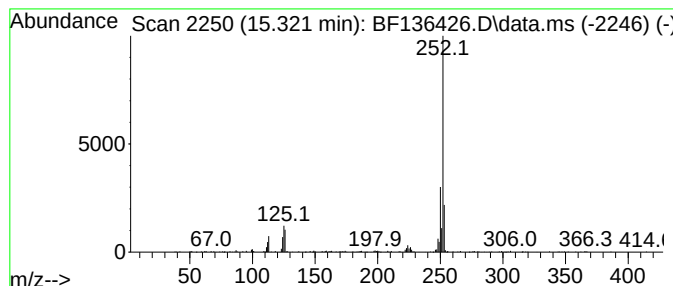
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	7.62 ng	239407	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	94
3			Benzo[a]pyrene	252	C20H12	000050-32-8	91
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

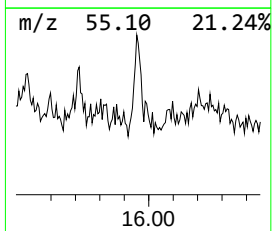
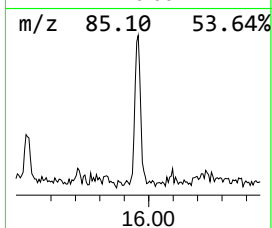
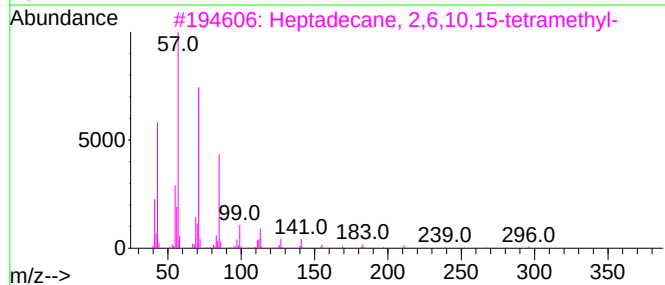
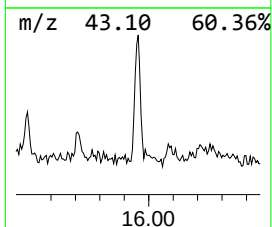
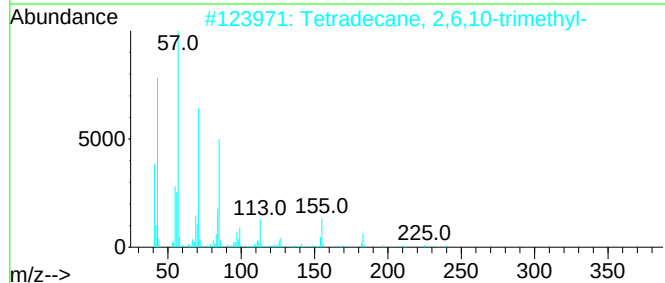
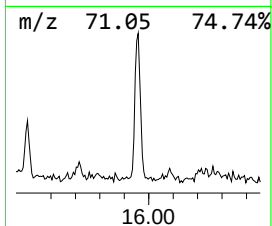
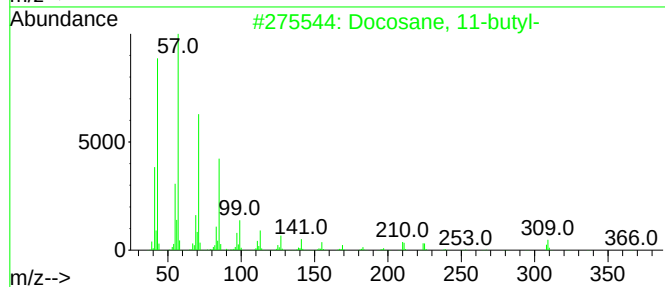
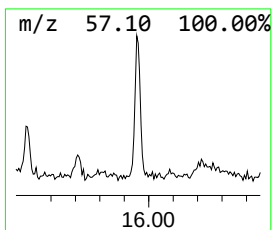
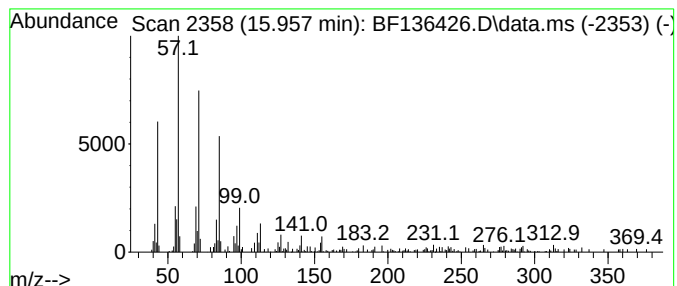
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 11-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	4.17 ng	131059	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
2		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	91
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136426.D
Acq On : 06 Dec 2023 14:01
Operator : CG\JU
Sample : 05434-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-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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n-Hexadecanoic ...	11.857	8.6	ng	296966	4	11.316	689099	20.0
4H-Cyclopenta[d...	11.933	4.2	ng	145090	4	11.316	689099	20.0
9,10-Anthracene...	12.145	2.1	ng	73662	4	11.316	689099	20.0
Phenanthrene, 3...	12.374	3.2	ng	110875	4	11.316	689099	20.0
unknown12.410	12.410	2.0	ng	70258	4	11.316	689099	20.0
Cyclopenta(def)...	12.457	2.2	ng	75444	4	11.316	689099	20.0
Tetracosane	15.110	4.7	ng	148040	6	15.451	628034	20.0
Perylene	15.321	7.6	ng	239407	6	15.451	628034	20.0
Docosane, 11-bu...	15.957	4.2	ng	131059	6	15.451	628034	20.0