

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
 Data File : BF136385.D
 Acq On : 04 Dec 2023 16:55
 Operator : CG\JU
 Sample : 05434-13
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-7

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	497	502	509	rVB2	26936	35701	1.43%	0.165%
2	5.434	565	569	573	rBV	2084800	2049823	82.32%	9.489%
3	6.440	735	740	743	rBV	2146631	1962938	78.83%	9.087%
4	6.634	770	773	778	rBV2	33678	38886	1.56%	0.180%
5	6.798	798	801	805	rBV	765996	679843	27.30%	3.147%
6	7.363	892	897	900	rBV	1448522	1260967	50.64%	5.837%
7	8.081	1015	1019	1022	rBV	964481	874596	35.12%	4.049%
8	9.157	1198	1202	1205	rBV	3154868	2490119	100.00%	11.527%
9	9.275	1218	1222	1225	rVB	44577	36865	1.48%	0.171%
10	9.692	1290	1293	1297	rVB	63308	53548	2.15%	0.248%
11	9.834	1313	1317	1320	rBV	1183386	888885	35.70%	4.115%
12	10.622	1447	1451	1455	rBV	1290046	1225158	49.20%	5.672%
13	10.751	1470	1473	1480	rVB5	27985	39602	1.59%	0.183%
14	11.328	1567	1571	1573	rBV	950198	818184	32.86%	3.788%
15	11.351	1573	1575	1579	rVV	328217	264466	10.62%	1.224%
16	11.398	1579	1583	1586	rVB	70245	64904	2.61%	0.300%
17	11.557	1604	1610	1612	rBV2	28411	32131	1.29%	0.149%
18	11.728	1635	1639	1646	rVB3	16274	34275	1.38%	0.159%
19	11.828	1653	1656	1659	rBV	89556	87908	3.53%	0.407%
20	11.863	1659	1662	1667	rVV2	430780	391643	15.73%	1.813%
21	11.939	1672	1675	1678	rVV	143311	162548	6.53%	0.752%
22	11.963	1678	1679	1684	rVB	81997	52723	2.12%	0.244%
23	12.127	1704	1707	1709	rBV2	55577	46263	1.86%	0.214%
24	12.151	1709	1711	1714	rVB2	65586	57945	2.33%	0.268%
25	12.380	1747	1750	1753	rBV	96827	103382	4.15%	0.479%
26	12.416	1753	1756	1759	rVV4	66232	105388	4.23%	0.488%
27	12.469	1762	1765	1769	rBV5	57237	77575	3.12%	0.359%
28	12.545	1774	1778	1781	rBV	749889	618245	24.83%	2.862%
29	12.651	1791	1796	1799	rBV3	97598	115919	4.66%	0.537%
30	12.775	1811	1817	1820	rBV	676481	655208	26.31%	3.033%
31	12.827	1823	1826	1830	rVB3	50523	75554	3.03%	0.350%
32	12.892	1834	1837	1838	rBV3	40531	36770	1.48%	0.170%
33	12.922	1838	1842	1846	rVV	2498410	2145548	86.16%	9.932%
34	12.992	1850	1854	1858	rBV2	67309	95512	3.84%	0.442%
35	13.080	1866	1869	1871	rBV3	57942	73807	2.96%	0.342%
36	13.104	1871	1873	1877	rVB	125898	103689	4.16%	0.480%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.169	1880	1884	1887	rVB2	69724	78026	3.13%	0.361%
38	13.210	1887	1891	1893	rBV2	105071	101940	4.09%	0.472%
39	13.298	1904	1906	1909	rVB	63573	52976	2.13%	0.245%
40	13.333	1909	1912	1914	rBV	72214	67219	2.70%	0.311%
41	13.510	1939	1942	1944	rBV3	30494	30672	1.23%	0.142%
42	13.616	1957	1960	1964	rVB	72357	85747	3.44%	0.397%
43	13.727	1974	1979	1982	rBV3	78075	119104	4.78%	0.551%
44	13.821	1993	1995	1998	rBV	59619	76473	3.07%	0.354%
45	13.857	1998	2001	2007	rVV3	96234	154220	6.19%	0.714%
46	13.980	2017	2022	2024	rBV2	931958	1091111	43.82%	5.051%
47	14.004	2024	2026	2029	rVB	320698	244171	9.81%	1.130%
48	14.369	2086	2088	2091	rVB	88215	71345	2.87%	0.330%
49	14.404	2091	2094	2097	rBV2	65422	66550	2.67%	0.308%
50	14.463	2101	2104	2106	rVV2	83253	74424	2.99%	0.345%
51	15.027	2196	2200	2203	rBV	260161	409276	16.44%	1.895%
52	15.333	2249	2252	2259	rVB	142506	175443	7.05%	0.812%
53	15.398	2260	2263	2270	rVB	207515	241833	9.71%	1.120%
54	15.463	2270	2274	2278	rBV	482697	604547	24.28%	2.799%

Sum of corrected areas: 21601595

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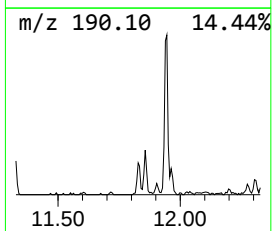
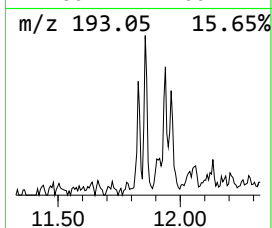
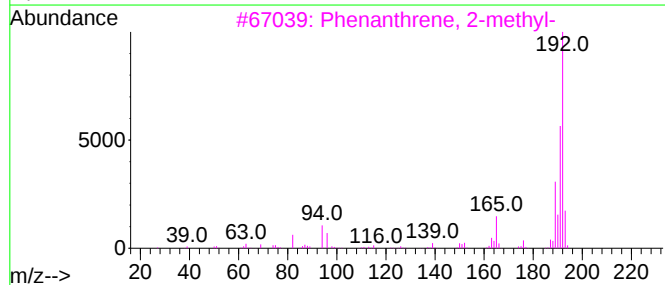
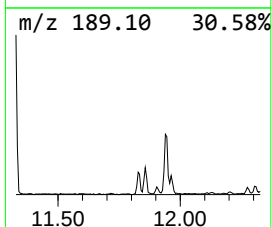
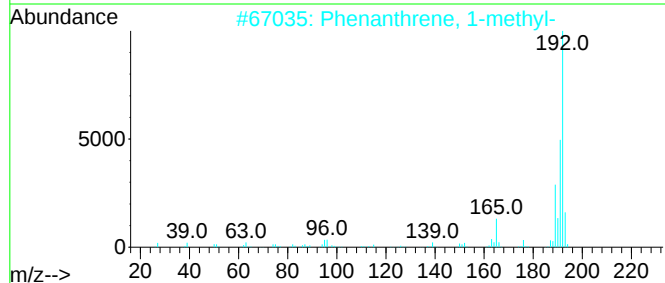
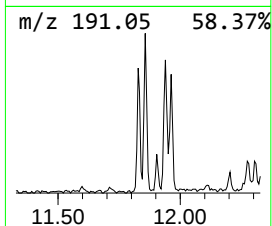
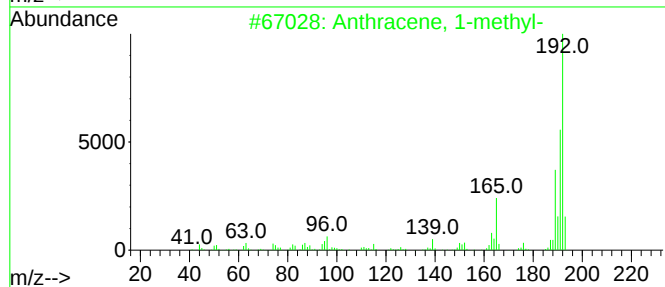
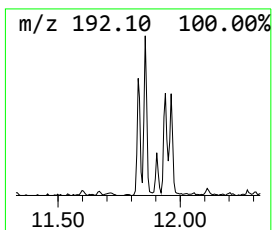
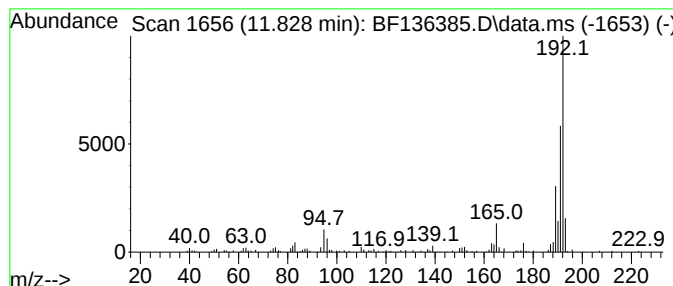
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Anthracene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.828	2.15 ng	87908	Phenanthrene-d10	11.328

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	93



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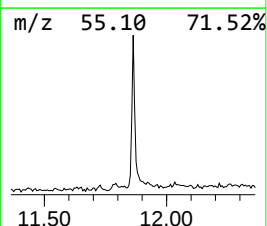
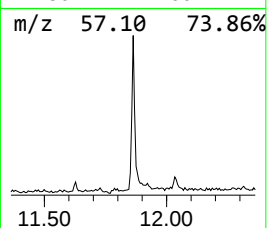
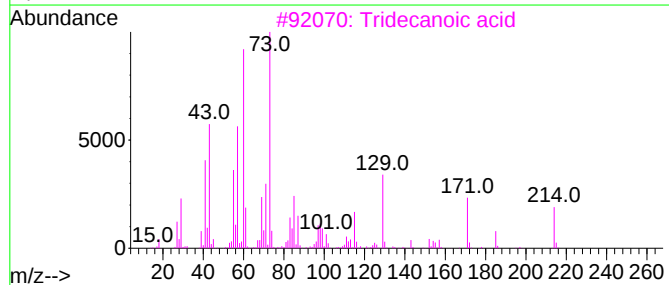
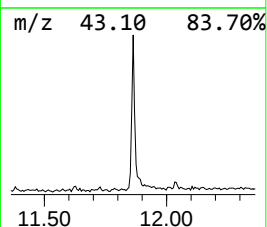
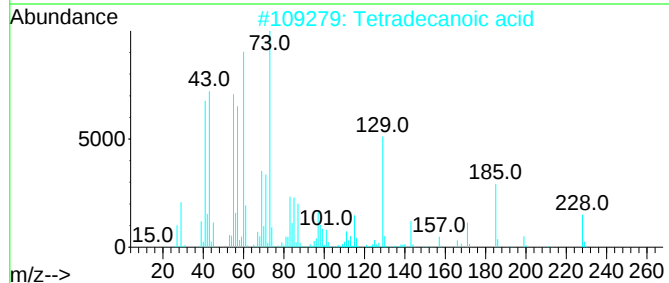
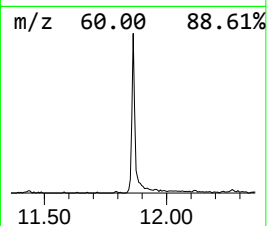
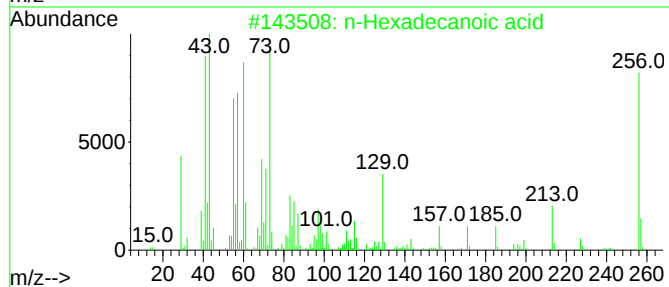
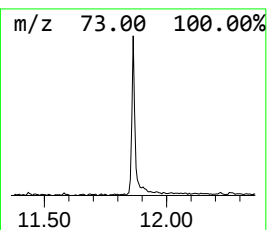
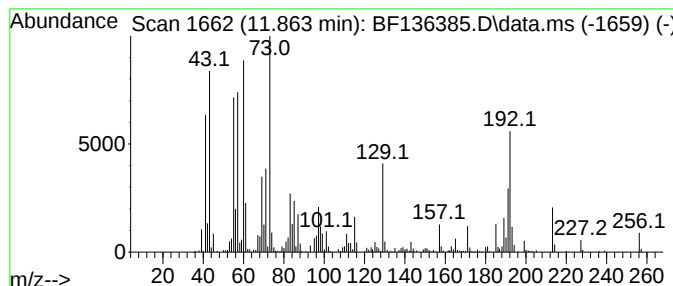
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.863	9.57 ng	391643	Phenanthrene-d10	11.328

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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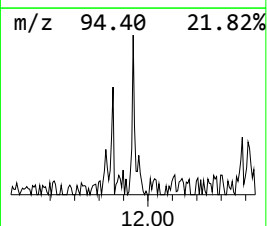
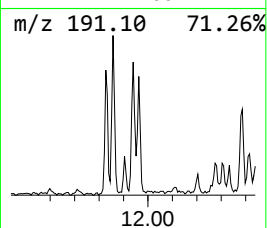
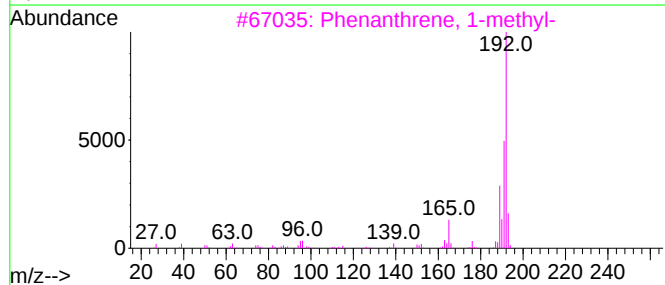
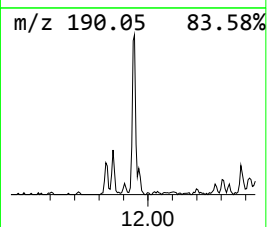
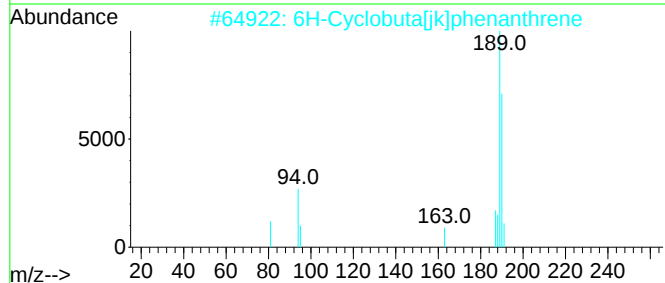
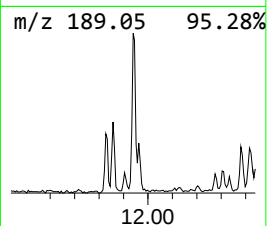
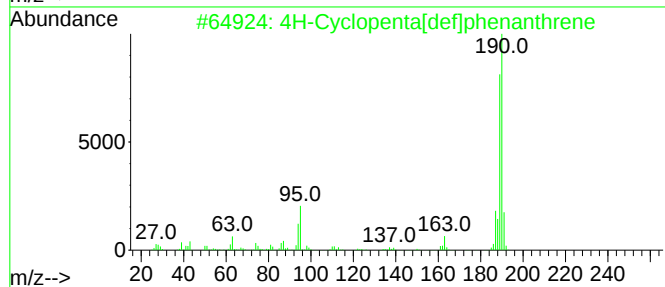
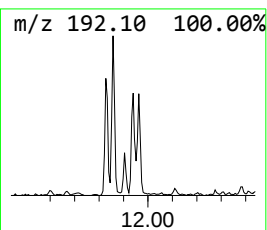
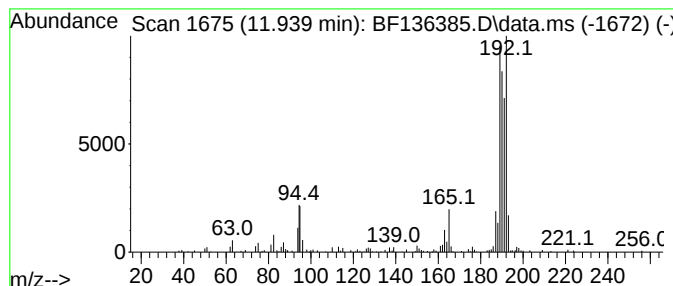
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.97 ng	162548	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	43
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42



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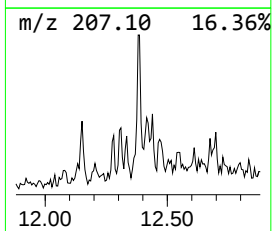
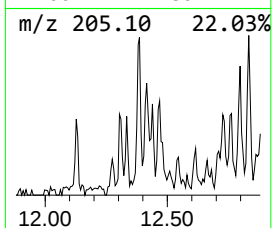
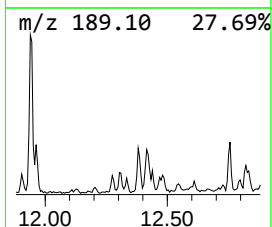
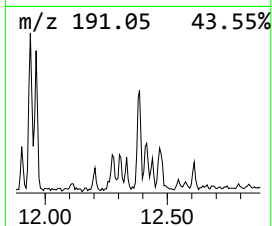
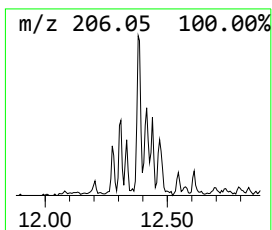
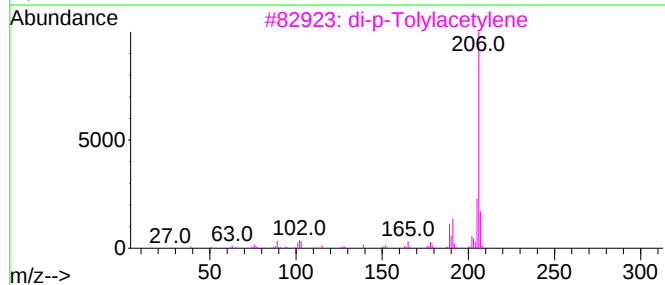
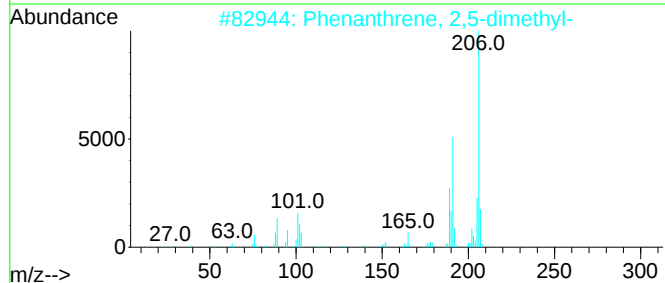
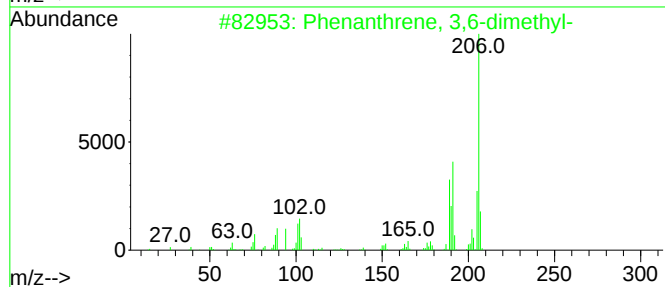
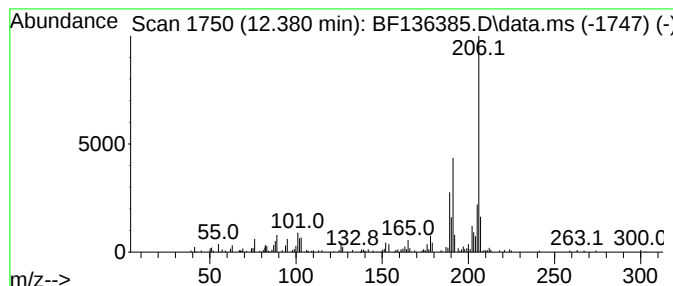
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 3,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	2.53 ng	103382	Phenanthrene-d10	11.328

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	95
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	94
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	94
5			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	94



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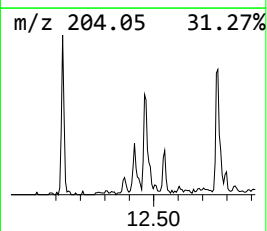
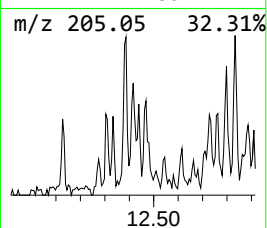
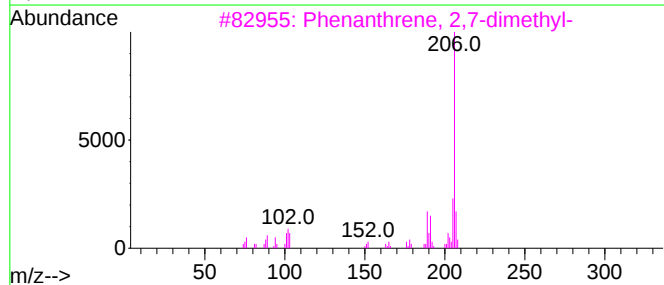
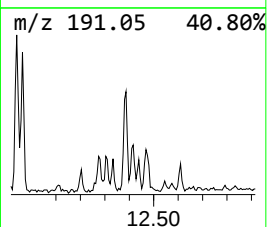
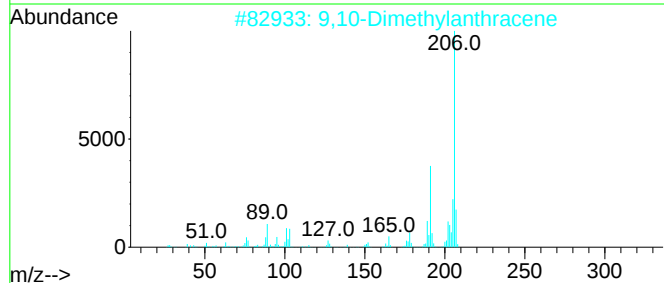
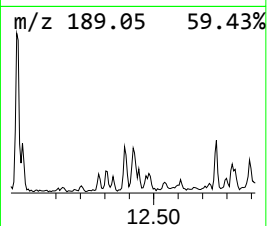
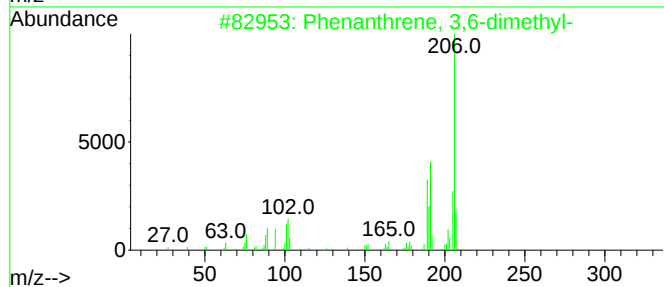
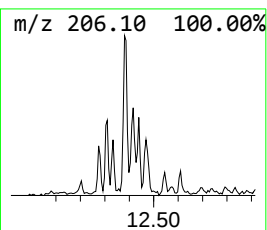
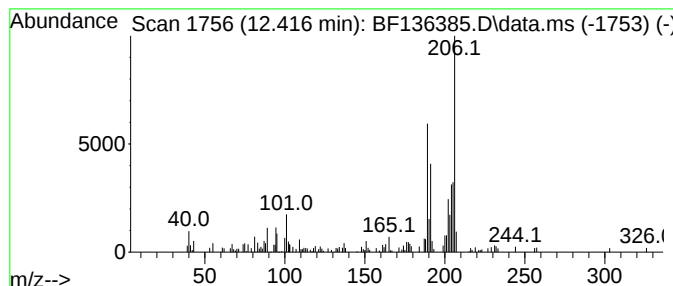
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,10-Dimethylantracene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	2.58 ng	105388	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	62
2			9,10-Dimethylantracene	206	C16H14	000781-43-1	58
3			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	58
4			3,5-Dichloro-4-hydroxybenzoic acid	206	C7H4Cl2O3	003336-41-2	58
5			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136385.D
Acq On : 04 Dec 2023 16:55
Operator : CG\JU
Sample : 05434-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

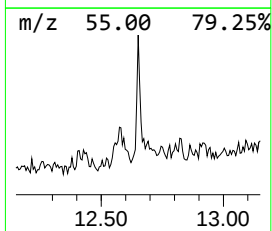
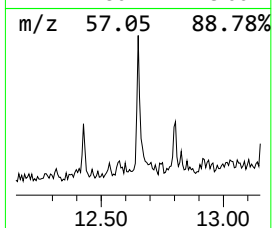
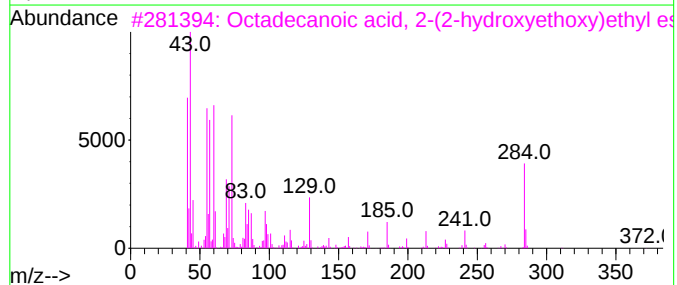
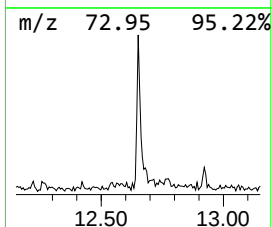
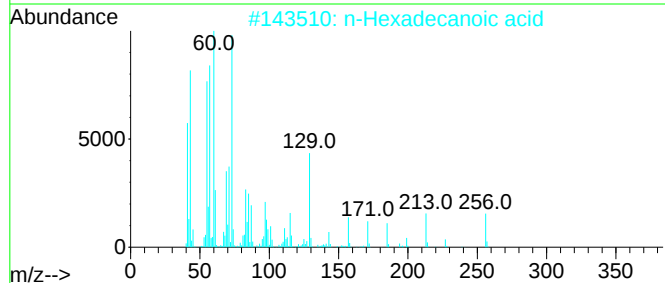
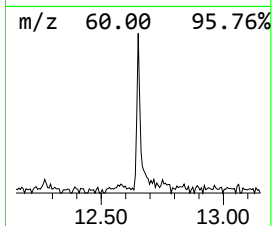
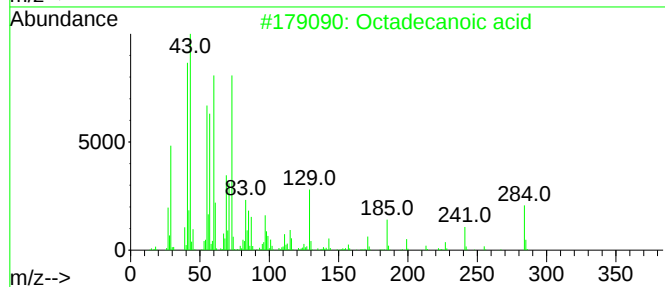
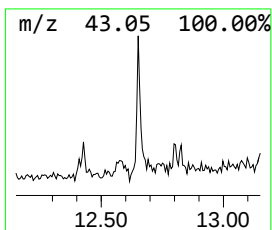
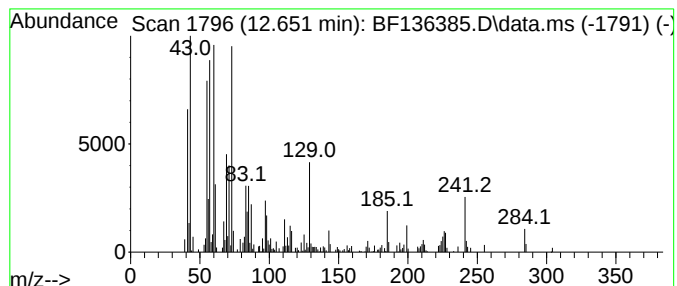
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.83 ng	115919	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136385.D
Acq On : 04 Dec 2023 16:55
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Sample : 05434-13
Misc :
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Instrument :
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ClientSampleId :
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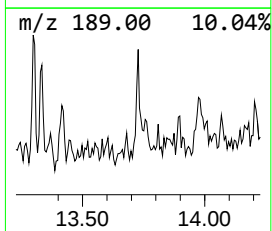
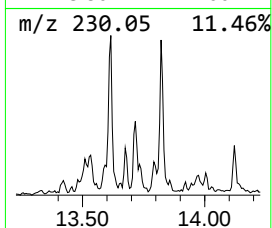
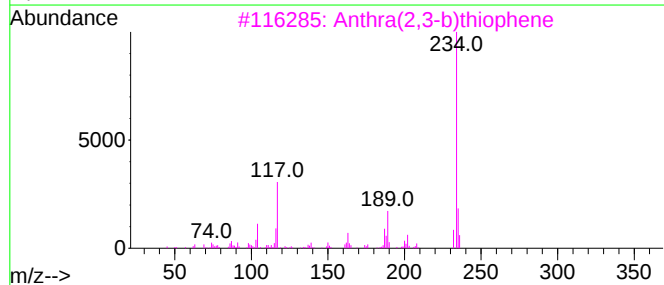
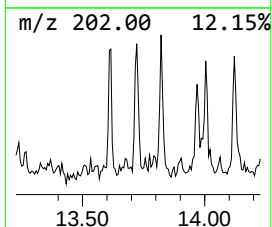
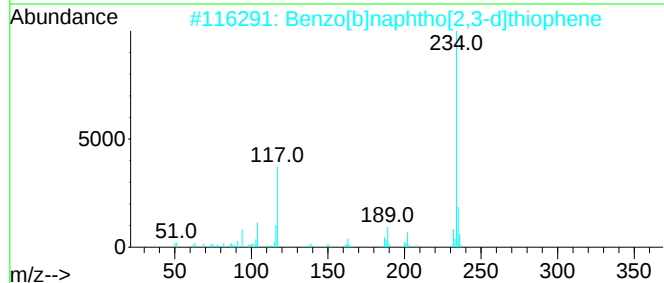
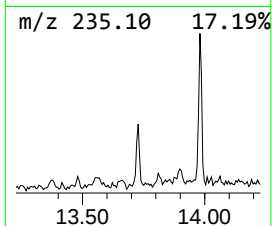
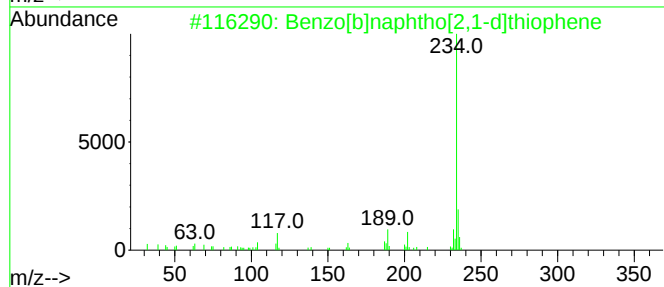
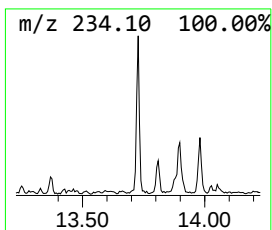
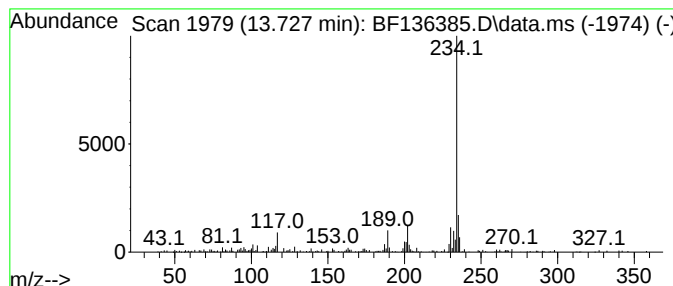
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	2.18 ng	119104	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	93
2			Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	87
3			Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	83
4			Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	76
5			Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136385.D
Acq On : 04 Dec 2023 16:55
Operator : CG\JU
Sample : 05434-13
Misc :
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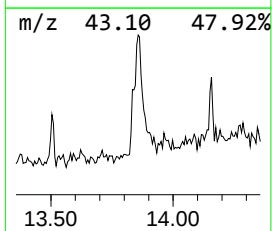
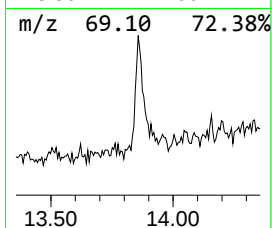
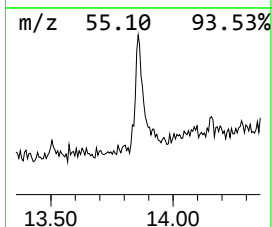
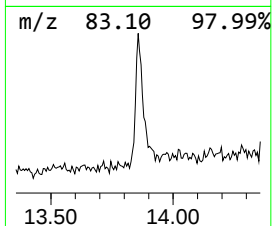
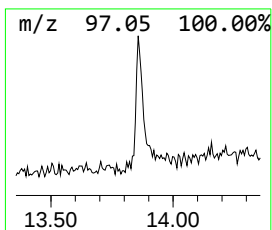
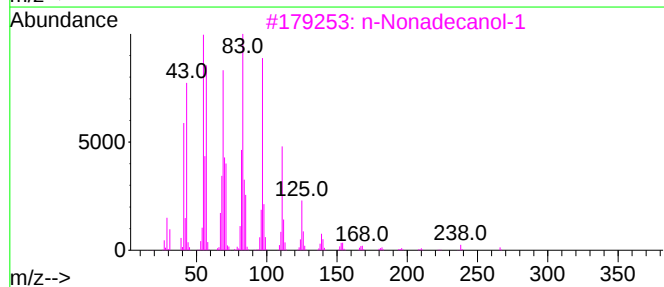
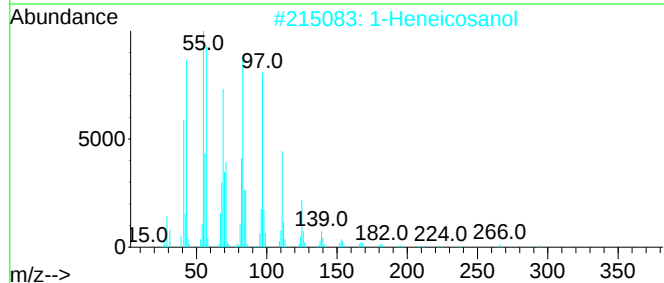
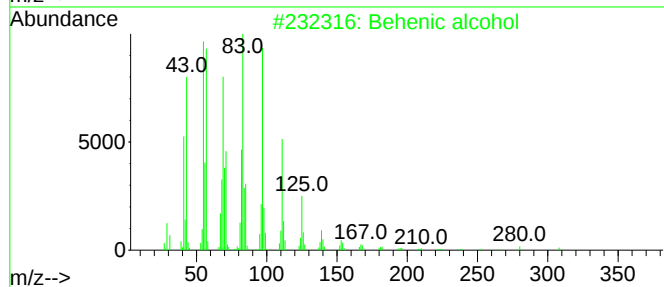
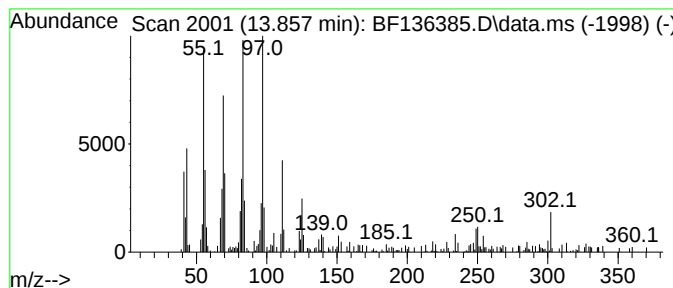
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	2.83 ng	154220	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	76
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	76
4	1-Tetracosene	336	C24H48	010192-32-2	70
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136385.D
Acq On : 04 Dec 2023 16:55
Operator : CG\JU
Sample : 05434-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

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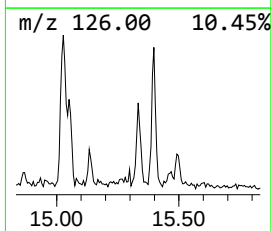
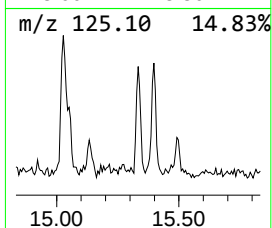
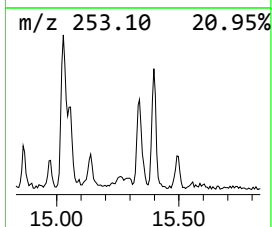
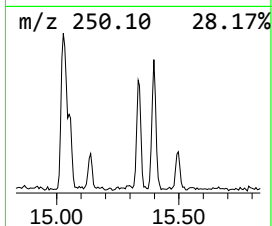
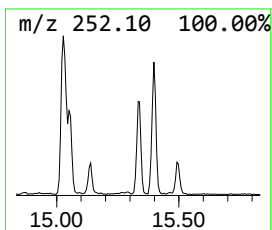
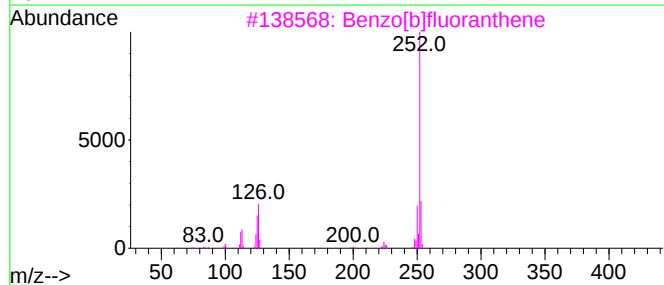
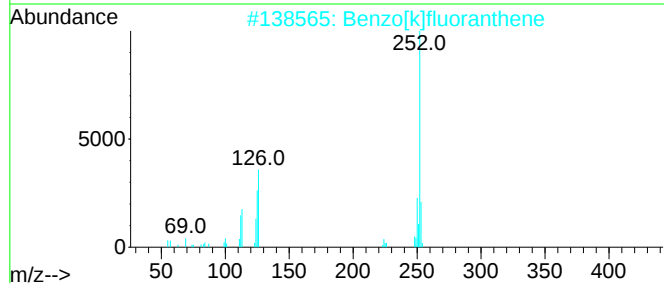
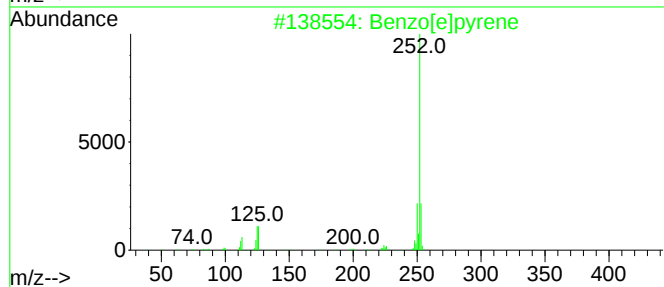
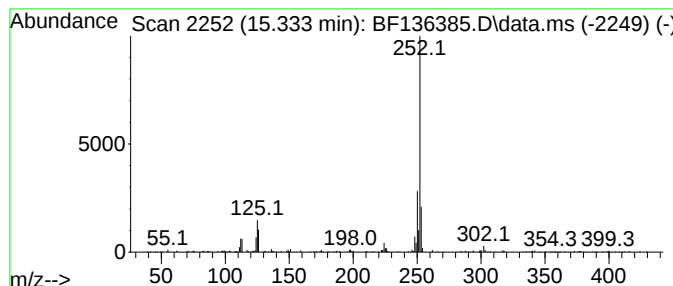
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	5.80 ng	175443	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5			Perylene	252	C20H12	000198-55-0	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136385.D
Acq On : 04 Dec 2023 16:55
Operator : CG\JU
Sample : 05434-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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, 1-m...	11.828	2.1	ng	87908	4	11.328	818184	20.0
n-Hexadecanoic ...	11.863	9.6	ng	391643	4	11.328	818184	20.0
4H-Cyclopenta[d...	11.939	4.0	ng	162548	4	11.328	818184	20.0
Phenanthrene, 3...	12.380	2.5	ng	103382	4	11.328	818184	20.0
9,10-Dimethylan...	12.416	2.6	ng	105388	4	11.328	818184	20.0
Octadecanoic acid	12.651	2.8	ng	115919	4	11.328	818184	20.0
Benzo[b]naphtho...	13.727	2.2	ng	119104	5	13.980	1091110	20.0
Behenic alcohol	13.857	2.8	ng	154220	5	13.980	1091110	20.0
Benzo[e]pyrene	15.333	5.8	ng	175443	6	15.463	604547	20.0