

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
 Data File : BF133709.D
 Acq On : 12 Jun 2023 17:57
 Operator : CG\JU
 Sample : 03044-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-5.0-7.0-DUP

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	497	504	514	rVB	38977	54444	2.50%	0.265%
2	5.451	566	572	575	rBV	2109728	2017799	92.65%	9.817%
3	6.463	738	744	747	rBV	2144576	2071050	95.09%	10.077%
4	6.828	803	806	810	rBV	548800	473783	21.75%	2.305%
5	7.398	898	903	906	rBV	1448333	1354559	62.19%	6.591%
6	8.116	1021	1025	1028	rBV	691660	587936	26.99%	2.861%
7	9.192	1204	1208	1211	rBV	2697246	2177960	100.00%	10.597%
8	9.869	1317	1323	1326	rBV	768928	597776	27.45%	2.908%
9	9.898	1326	1328	1332	rVB	51203	43503	2.00%	0.212%
10	10.075	1354	1358	1362	rBV2	27492	26495	1.22%	0.129%
11	10.416	1412	1416	1421	rVB	42481	39043	1.79%	0.190%
12	10.580	1440	1444	1448	rVB2	150237	137899	6.33%	0.671%
13	10.657	1453	1457	1461	rBV	1476317	1273311	58.46%	6.195%
14	11.251	1556	1558	1564	rVB	32774	30873	1.42%	0.150%
15	11.357	1572	1576	1578	rBV	649287	526262	24.16%	2.560%
16	11.380	1578	1580	1584	rVV	554728	411873	18.91%	2.004%
17	11.433	1584	1589	1592	rVB	119382	104886	4.82%	0.510%
18	11.586	1609	1615	1617	rBV2	37751	36789	1.69%	0.179%
19	11.857	1656	1661	1663	rBV	64230	66286	3.04%	0.323%
20	11.886	1663	1666	1670	rVV2	192141	201310	9.24%	0.979%
21	11.933	1671	1674	1677	rVV2	43843	45429	2.09%	0.221%
22	11.968	1677	1680	1683	rVV2	109745	130293	5.98%	0.634%
23	11.992	1683	1684	1689	rVB	55928	37033	1.70%	0.180%
24	12.157	1709	1712	1714	rBV	51693	43799	2.01%	0.213%
25	12.180	1714	1716	1719	rVB2	33567	28238	1.30%	0.137%
26	12.410	1752	1755	1758	rBV	51437	55447	2.55%	0.270%
27	12.451	1758	1762	1763	rVV2	36965	43806	2.01%	0.213%
28	12.492	1767	1769	1774	rVB3	37817	42686	1.96%	0.208%
29	12.574	1779	1783	1786	rVB	800358	677950	31.13%	3.299%
30	12.668	1796	1799	1801	rBV2	39457	32840	1.51%	0.160%
31	12.804	1816	1822	1827	rBV	722565	748861	34.38%	3.644%
32	12.851	1827	1830	1835	rVB3	38696	54451	2.50%	0.265%
33	12.921	1839	1842	1843	rBV	35700	32194	1.48%	0.157%
34	12.945	1843	1846	1850	rVV	1744976	1656363	76.05%	8.059%
35	13.015	1853	1858	1862	rBV2	46116	83385	3.83%	0.406%
36	13.104	1866	1873	1874	rBV4	44959	53633	2.46%	0.261%

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37	13.127	1875	1877	1880	rVB	93859	87113	4.00%	0.424%
38	13.174	1880	1885	1887	rBV4	36663	47874	2.20%	0.233%
39	13.198	1887	1889	1891	rVB	75809	54924	2.52%	0.267%
40	13.233	1891	1895	1898	rBV2	80997	81723	3.75%	0.398%
41	13.327	1908	1911	1914	rBV	41908	35557	1.63%	0.173%
42	13.357	1914	1916	1920	rBV	45879	39239	1.80%	0.191%
43	13.521	1939	1944	1946	rBV3	53501	73363	3.37%	0.357%
44	13.639	1961	1964	1969	rVB	49528	57814	2.65%	0.281%
45	13.751	1978	1983	1986	rBV3	65521	96964	4.45%	0.472%
46	13.780	1986	1988	1990	rVV	75209	64776	2.97%	0.315%
47	13.804	1990	1992	1996	rVV2	54840	81804	3.76%	0.398%
48	13.845	1996	1999	2006	rVB2	169044	195999	9.00%	0.954%
49	14.004	2018	2026	2028	rBV2	670664	952319	43.73%	4.633%
50	14.027	2028	2030	2036	rVB	368254	333765	15.32%	1.624%
51	14.110	2041	2044	2046	rVB	67454	57688	2.65%	0.281%
52	14.168	2051	2054	2056	rBV2	52074	46087	2.12%	0.224%
53	14.386	2089	2091	2095	rVB	69803	64082	2.94%	0.312%
54	14.421	2095	2097	2101	rVB	41453	36202	1.66%	0.176%
55	14.474	2103	2106	2110	rBV2	70270	89850	4.13%	0.437%
56	14.515	2110	2113	2115	rVV	43631	46203	2.12%	0.225%
57	14.533	2115	2116	2120	rVB3	45411	36733	1.69%	0.179%
58	14.780	2155	2158	2161	rBV2	47326	48395	2.22%	0.235%
59	15.039	2198	2202	2205	rBV	270175	413594	18.99%	2.012%
60	15.115	2213	2215	2217	rBV	43540	39665	1.82%	0.193%
61	15.145	2218	2220	2226	rVB	65740	71932	3.30%	0.350%
62	15.339	2250	2253	2259	rVB	170050	223985	10.28%	1.090%
63	15.404	2259	2264	2270	rBV	251008	318019	14.60%	1.547%
64	15.468	2270	2275	2278	rVV	337432	450763	20.70%	2.193%
65	15.498	2278	2280	2286	rVB2	103642	119108	5.47%	0.580%
66	16.921	2517	2522	2529	rVB2	95713	192165	8.82%	0.935%
67	17.356	2593	2596	2601	rVB2	58447	95238	4.37%	0.463%

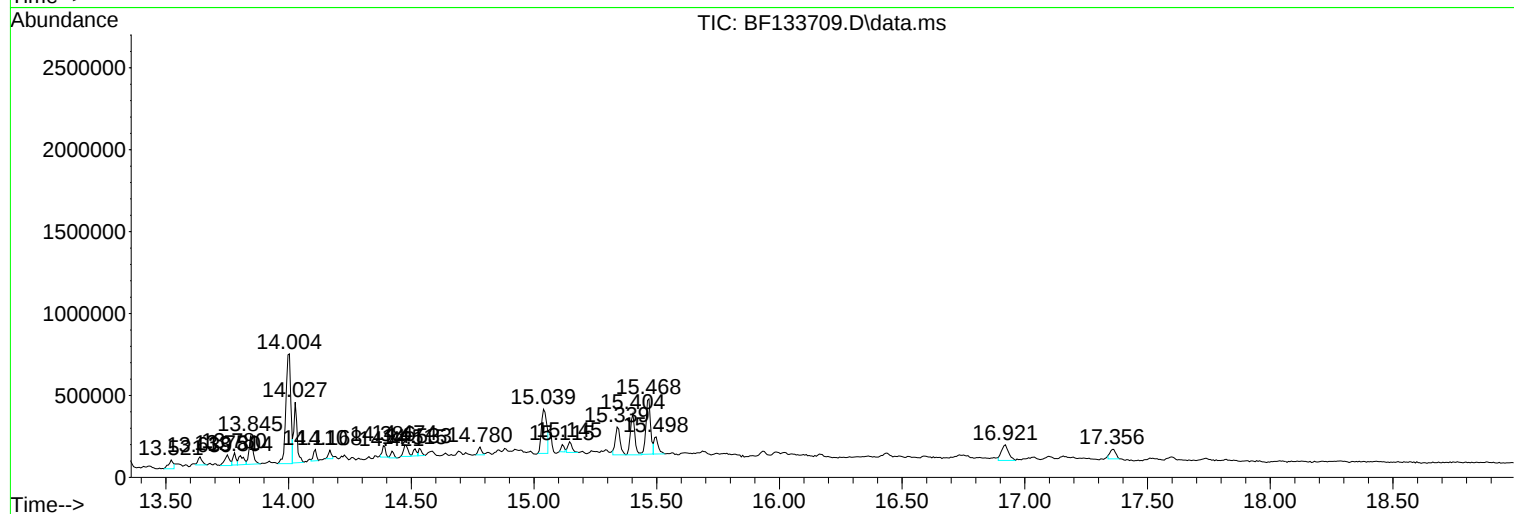
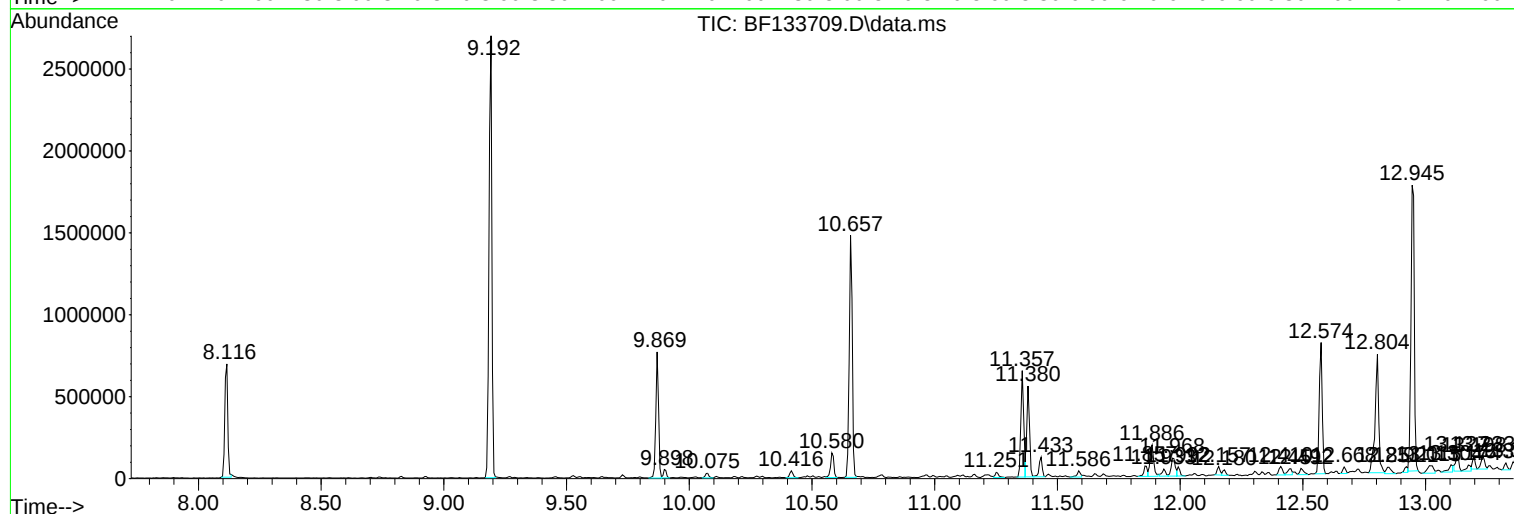
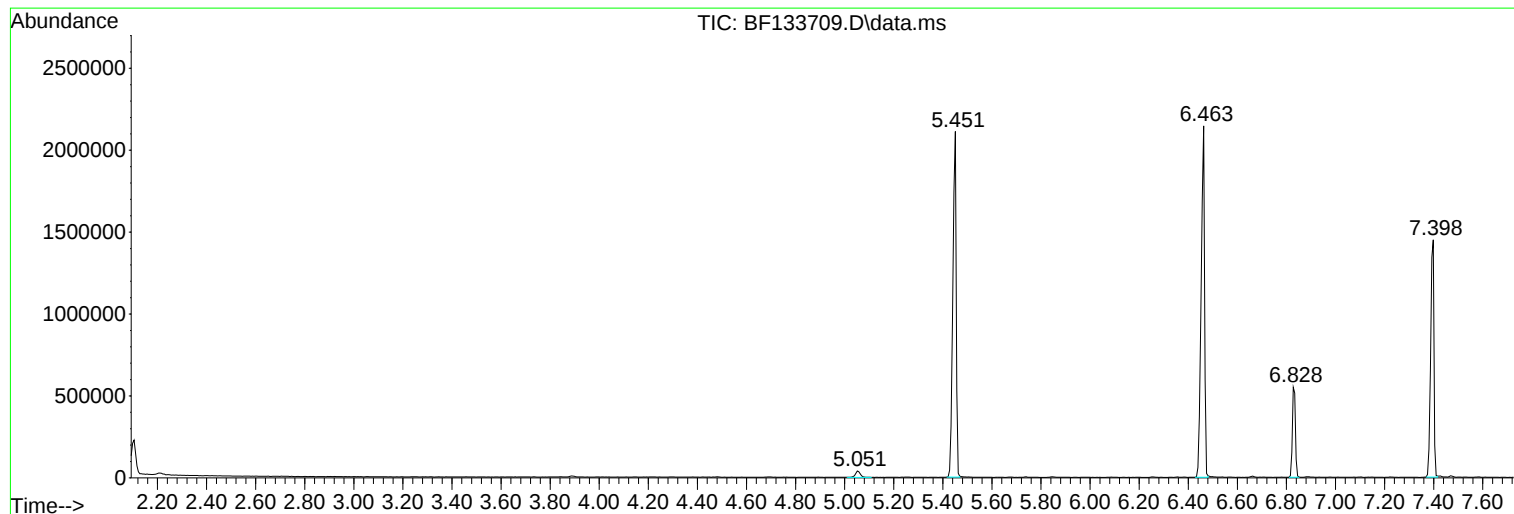
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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SB-02-5.0-7.0-DUP

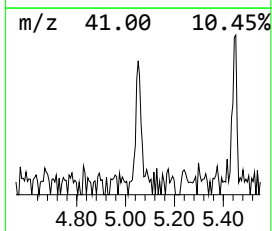
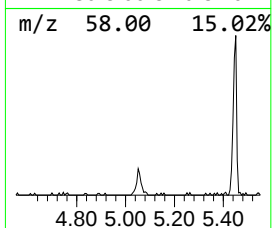
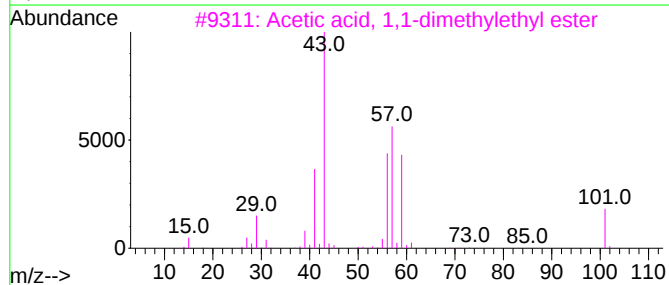
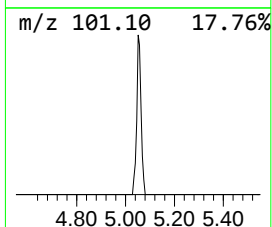
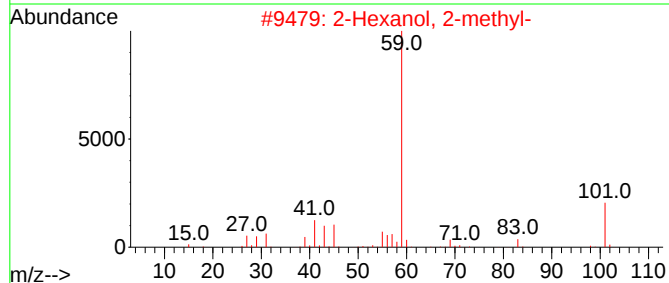
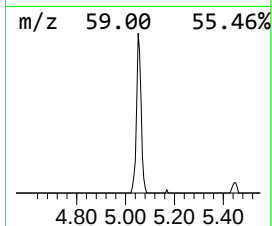
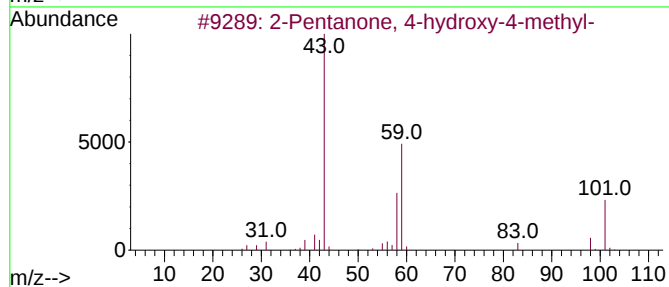
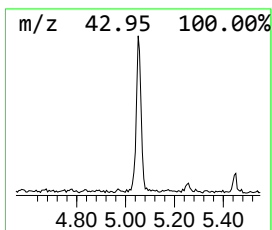
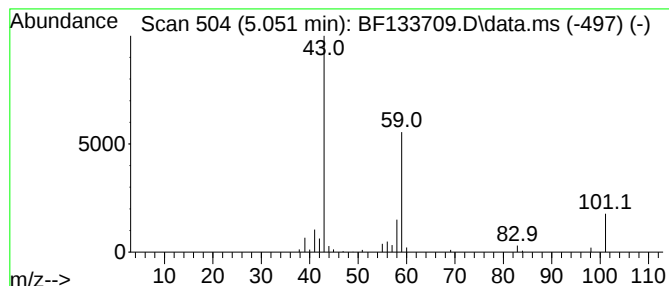
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.30 ng	54444	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33		
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	25		



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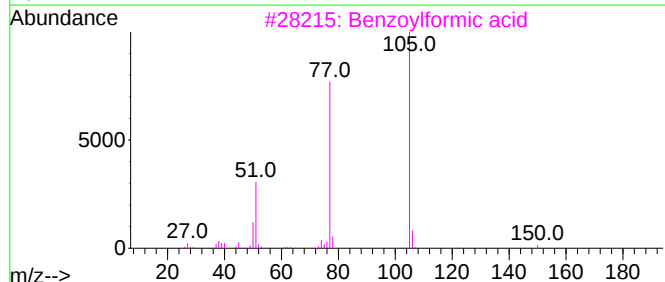
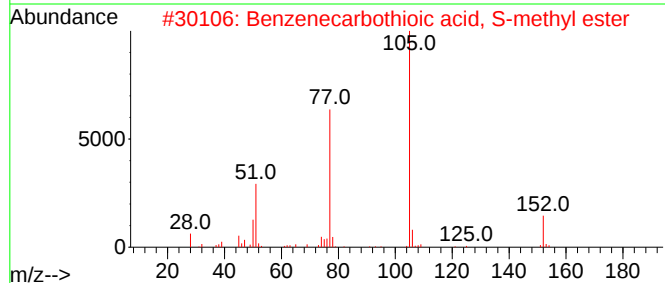
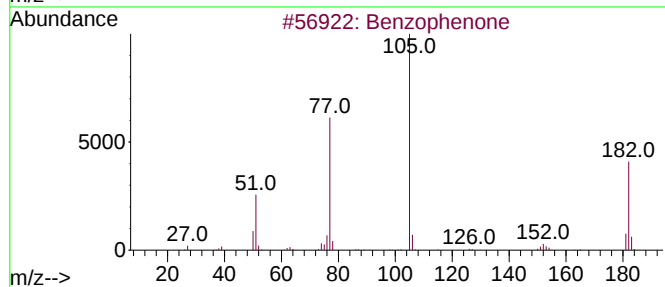
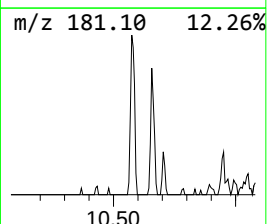
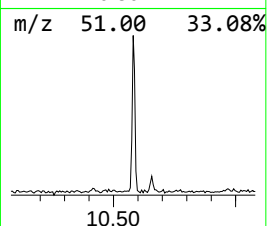
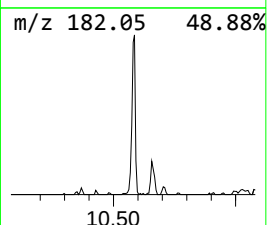
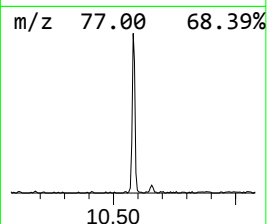
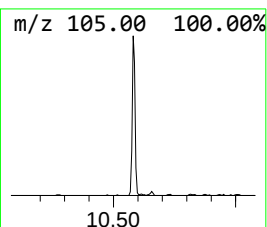
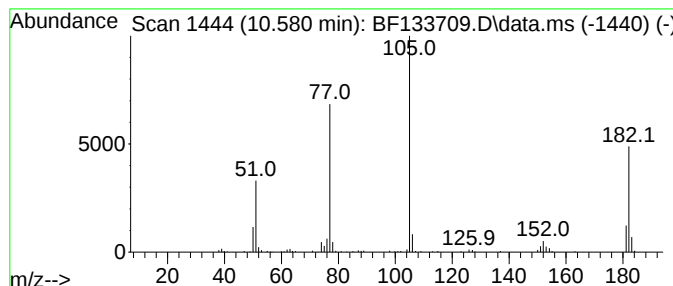
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	4.61 ng	137899	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			Benzoyl chloride	140	C7H5ClO	000098-88-4	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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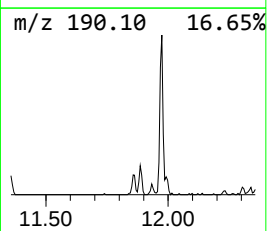
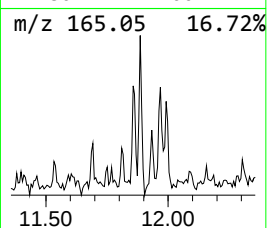
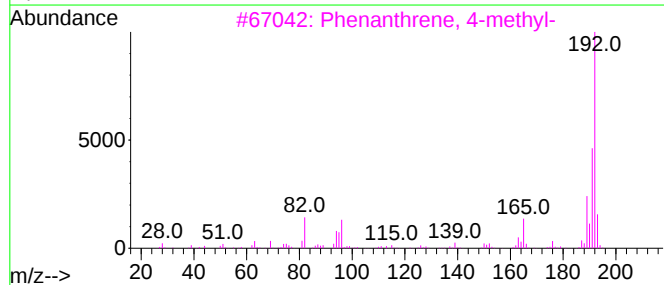
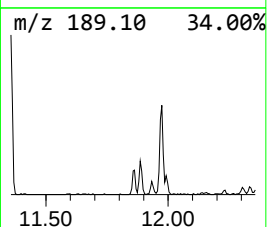
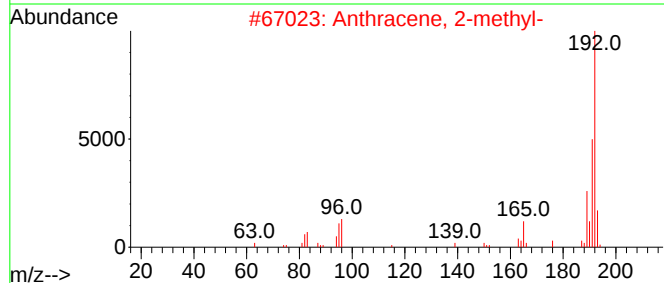
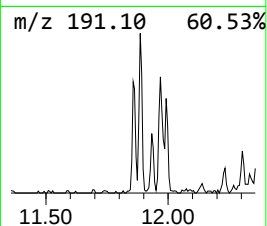
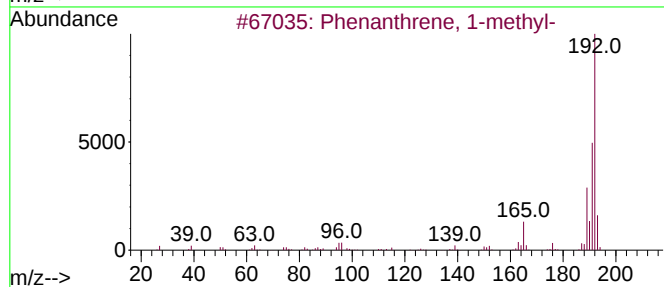
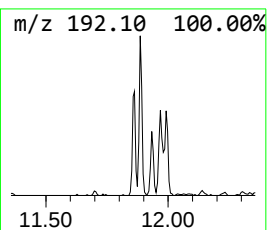
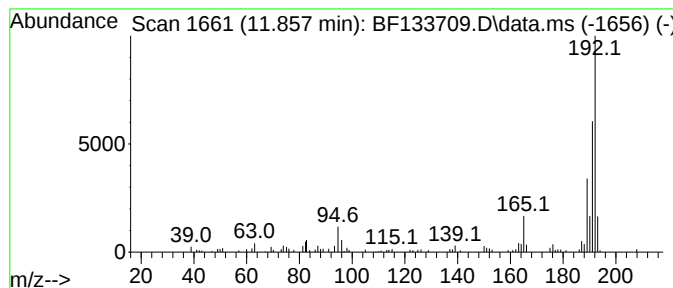
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Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.52 ng	66286	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90



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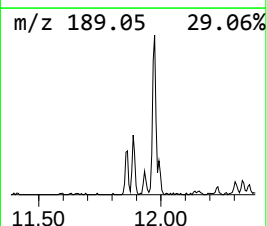
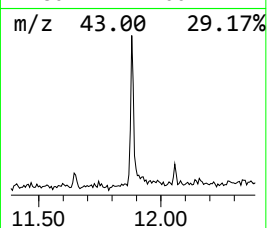
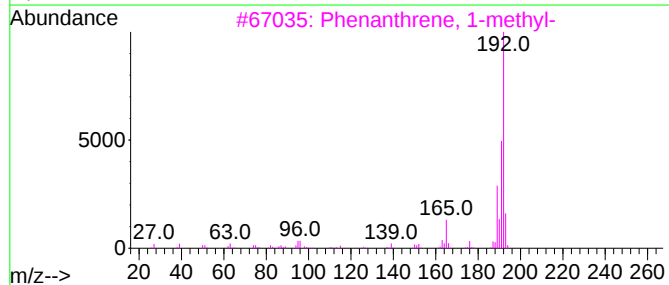
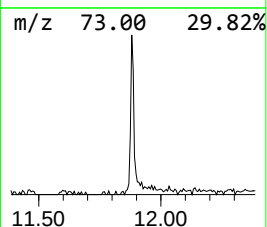
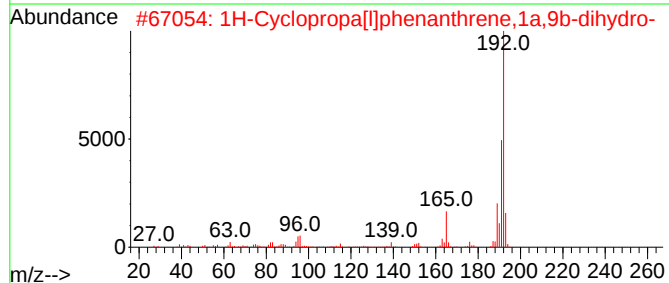
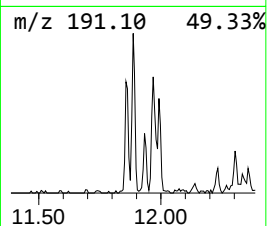
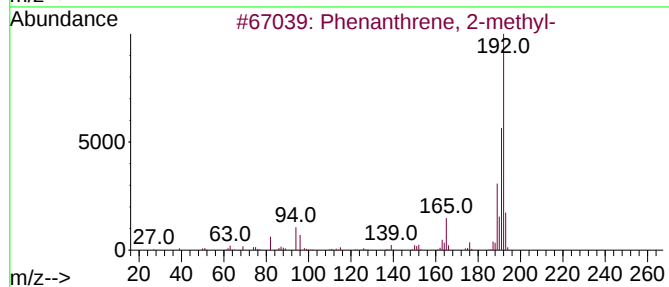
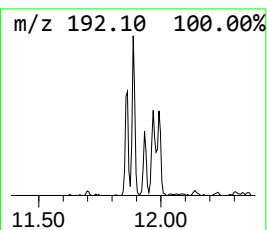
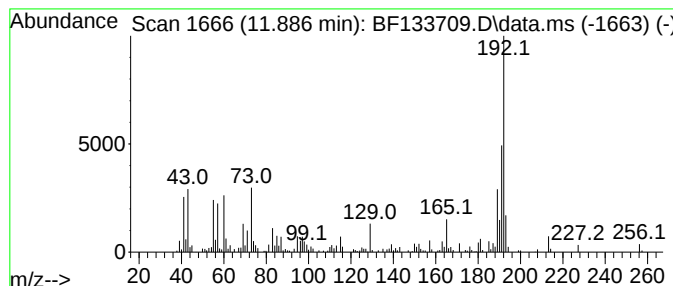
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	7.65 ng	201310	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133709.D
Acq On : 12 Jun 2023 17:57
Operator : CG\JU
Sample : 03044-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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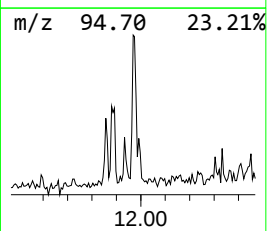
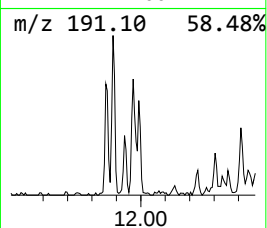
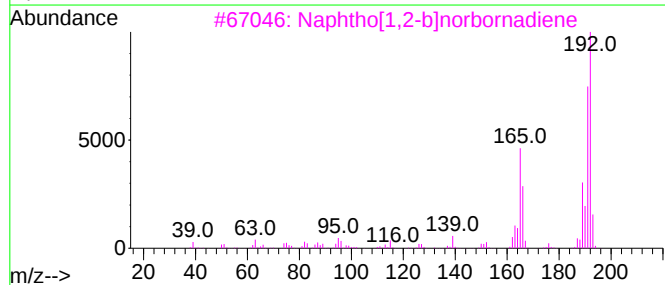
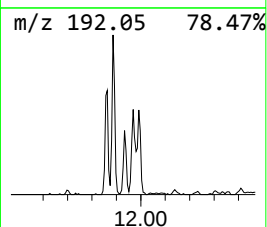
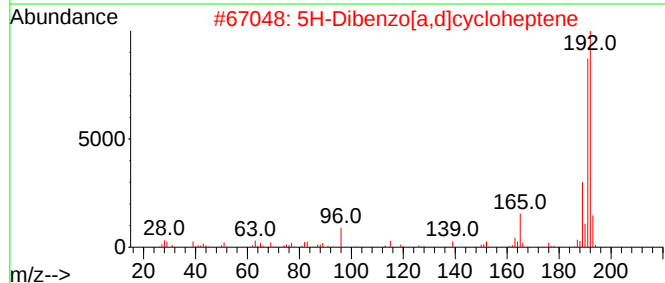
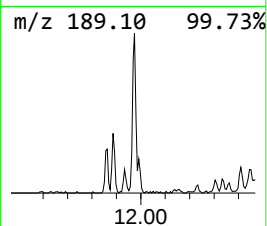
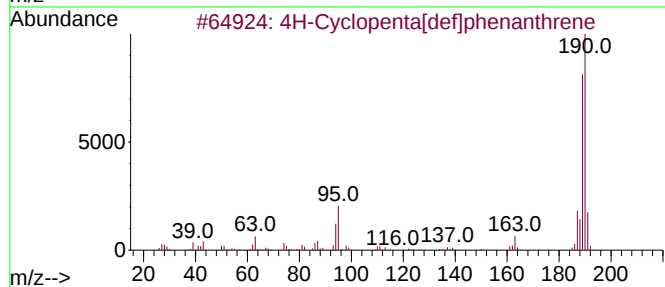
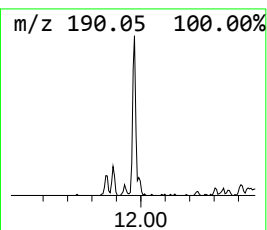
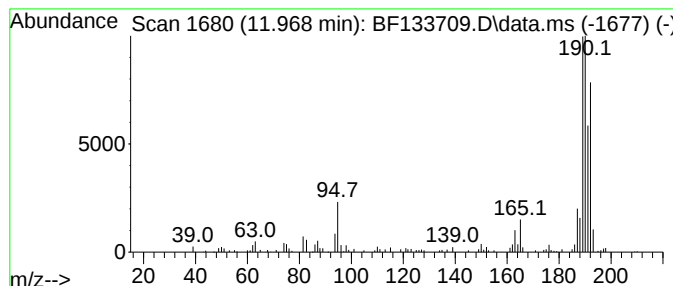
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	4.95 ng	130293	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
3			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	41
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	38



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Data File : BF133709.D
Acq On : 12 Jun 2023 17:57
Operator : CG\JU
Sample : 03044-03
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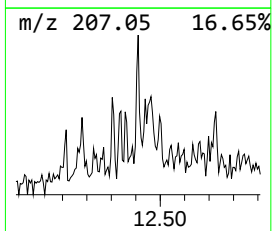
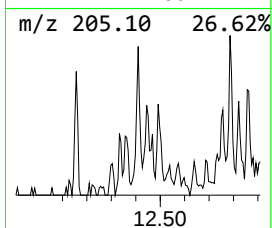
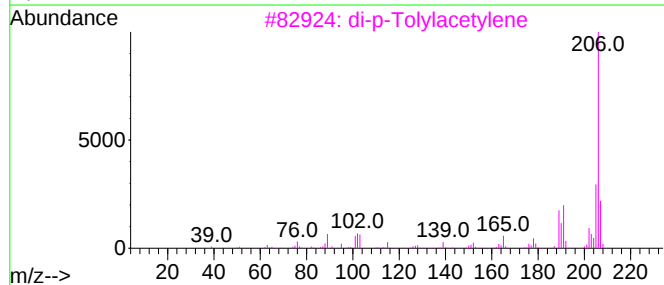
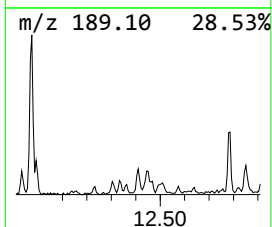
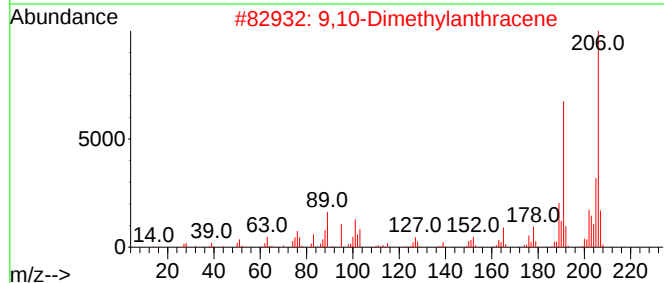
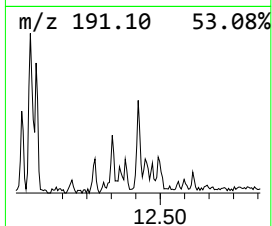
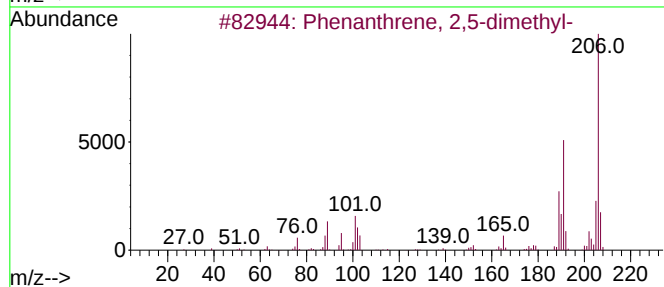
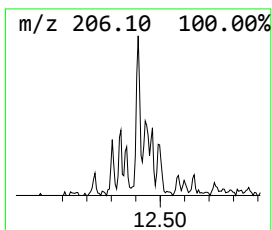
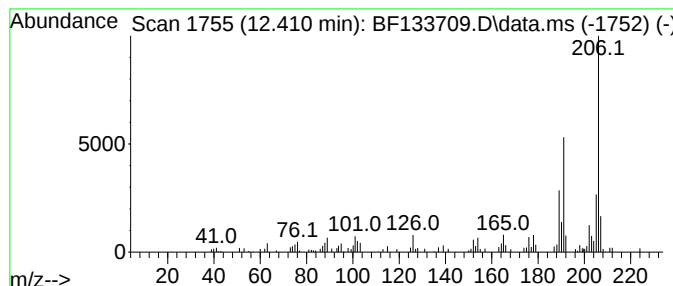
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.11 ng	55447	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2			9,10-Dimethylantracene	206	C16H14	000781-43-1	93
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	92
4			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	91
5			3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133709.D
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Sample : 03044-03
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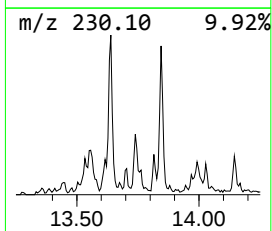
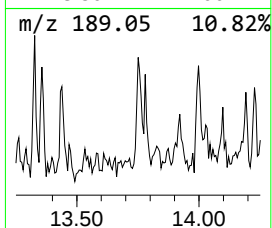
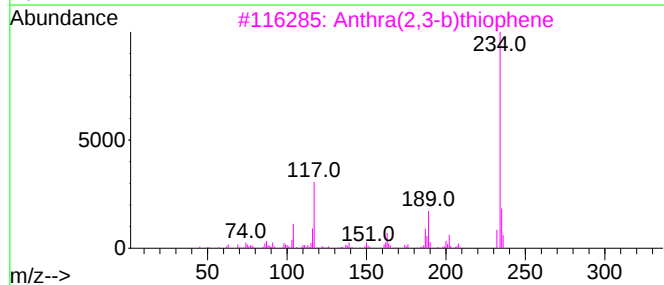
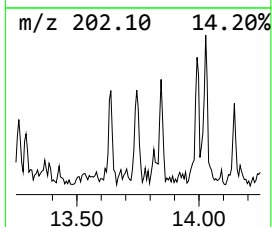
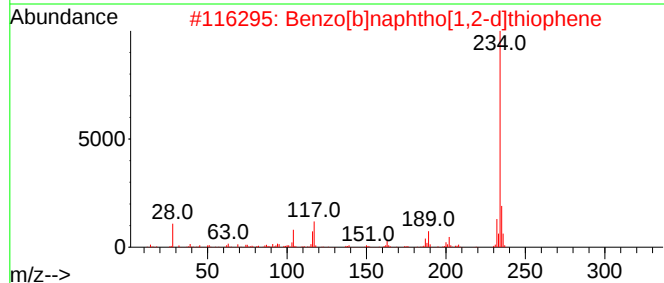
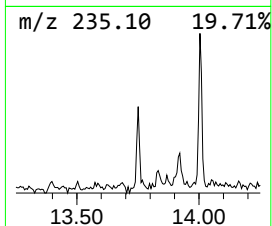
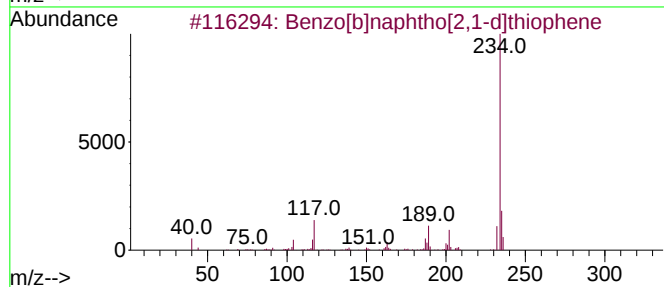
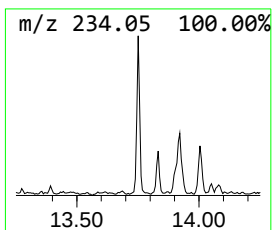
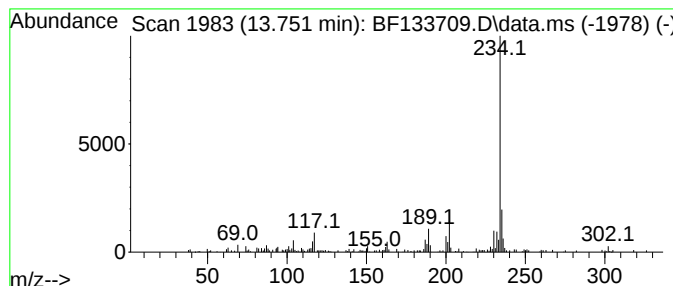
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.751	2.04 ng	96964	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	95
2	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	94
3	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	94
4	Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	93
5	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
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Acq On : 12 Jun 2023 17:57
Operator : CG\JU
Sample : 03044-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

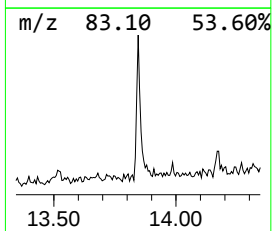
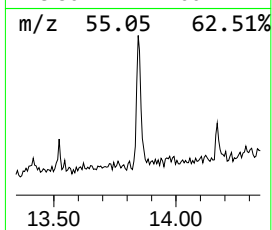
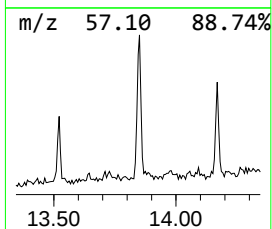
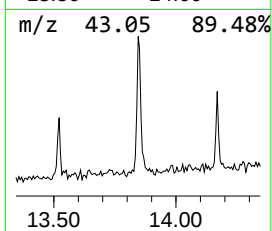
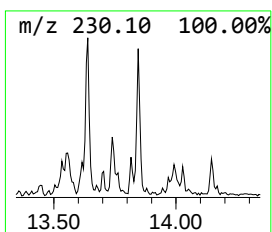
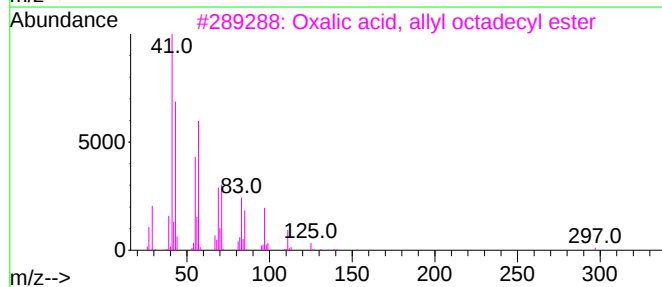
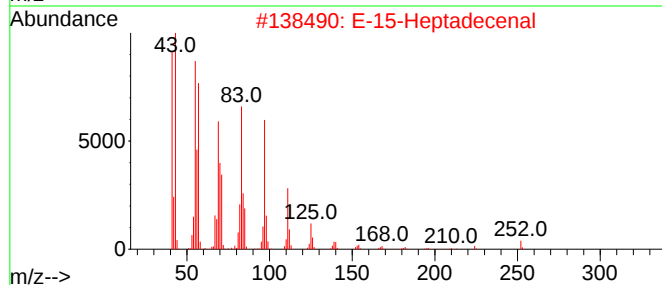
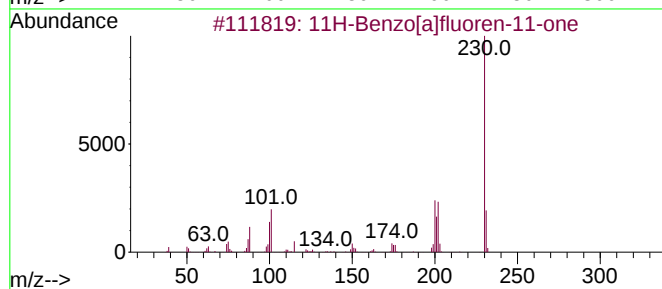
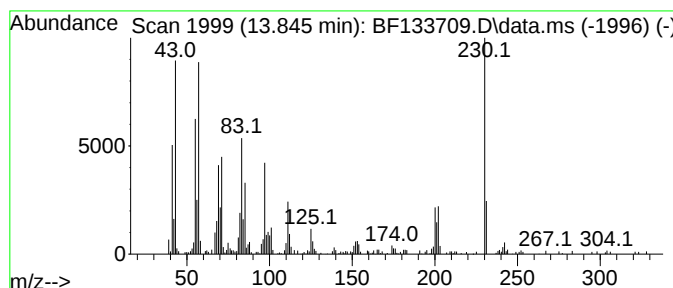
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.845	4.12 ng	195999	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	89
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	64
3	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	50
4	Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	49
5	Propionic acid, 3-iodo-, heptade...	438	C20H39IO2	1000406-24-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
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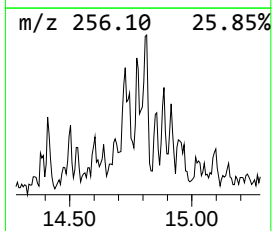
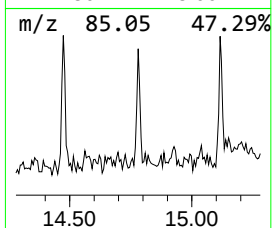
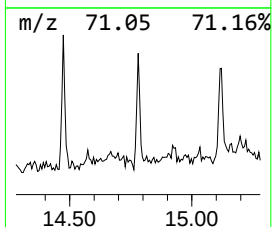
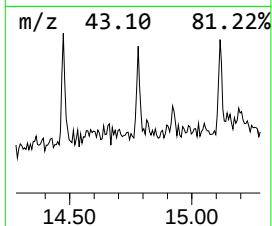
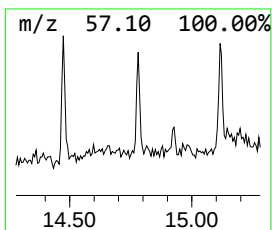
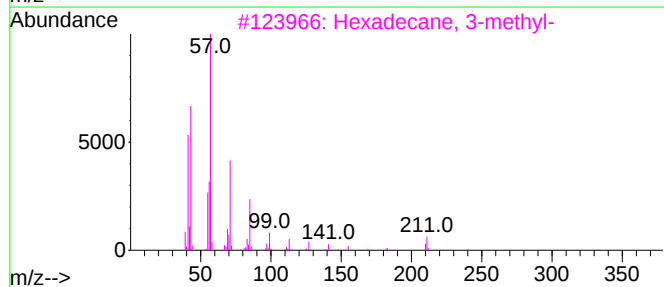
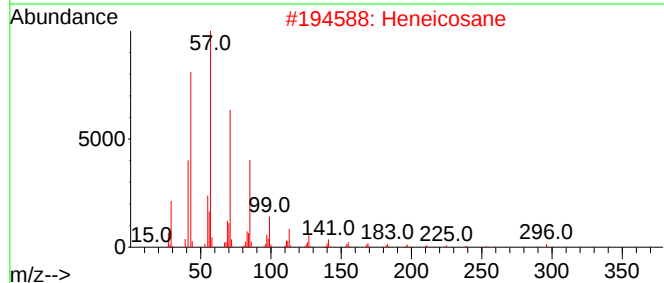
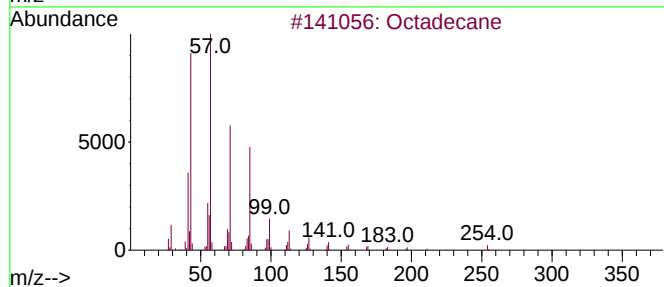
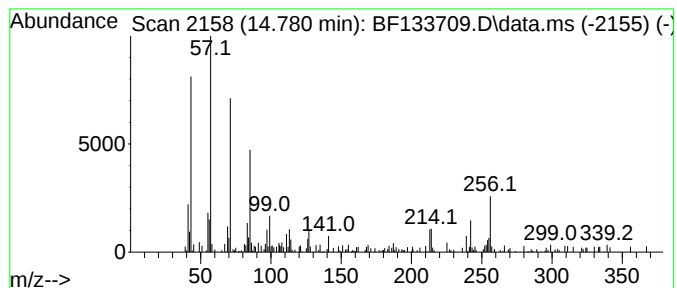
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	2.15 ng	48395	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	90
2		Heneicosane	296	C21H44	000629-94-7	89
3		Hexadecane, 3-methyl-	240	C17H36	006418-43-5	55
4		Tricosane	324	C23H48	000638-67-5	55
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
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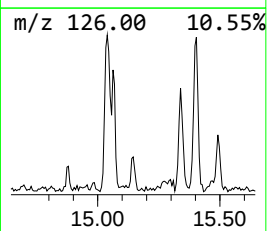
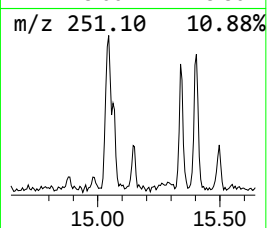
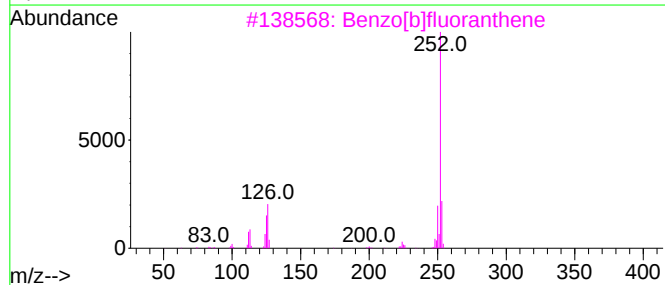
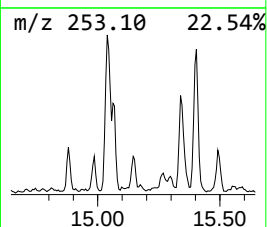
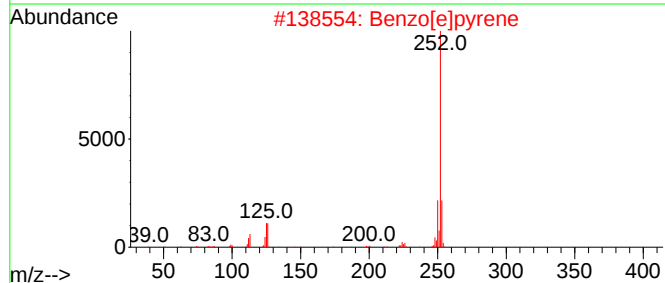
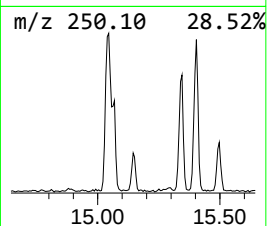
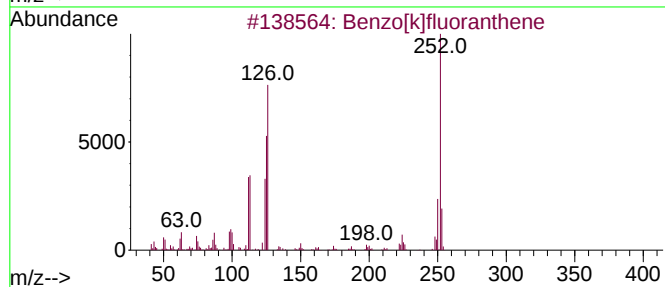
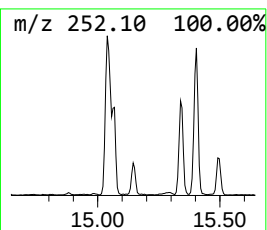
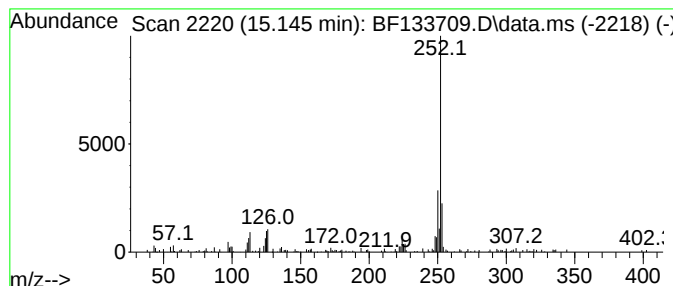
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.19 ng	71932	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2		Benzo[e]pyrene	252	C20H12	000192-97-2	93
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	87
4		Perylene	252	C20H12	000198-55-0	86
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
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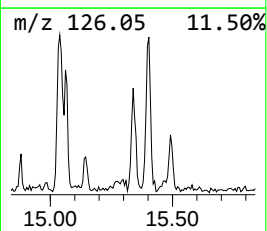
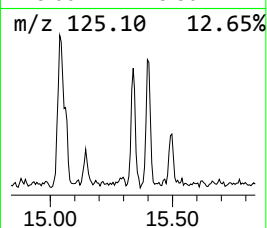
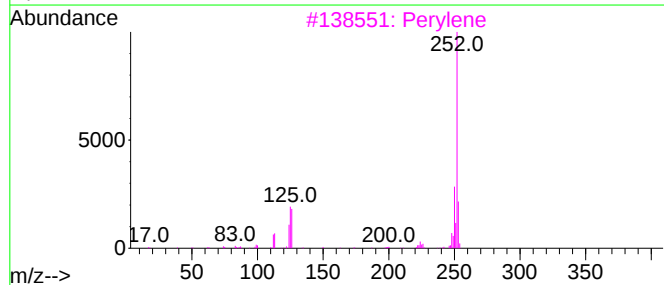
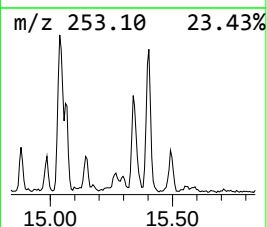
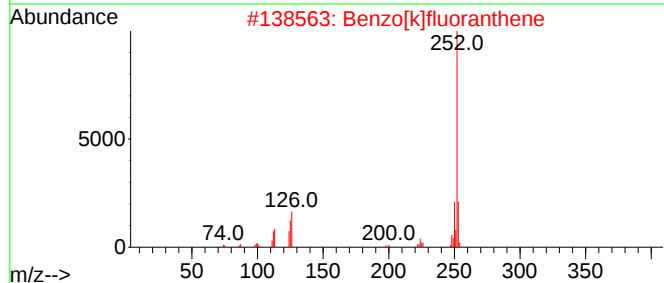
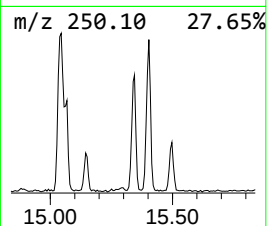
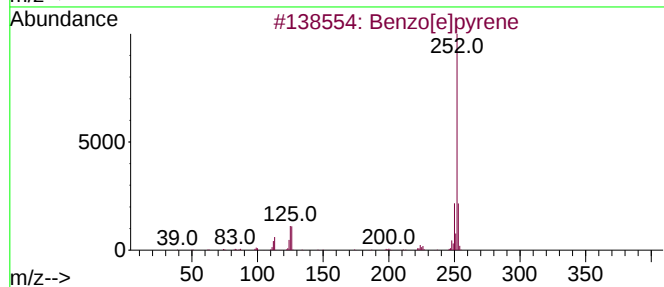
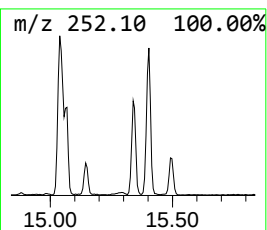
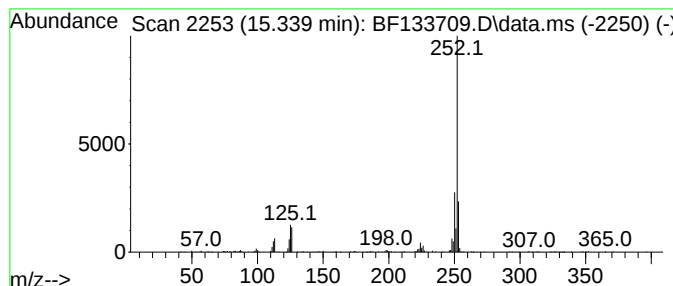
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	9.94 ng	223985	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3		Perylene	252	C20H12	000198-55-0	95
4		Benzo[a]pyrene	252	C20H12	000050-32-8	93
5		Benzo[b]fluoranthene	252	C20H12	000205-99-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133709.D
Acq On : 12 Jun 2023 17:57
Operator : CG\JU
Sample : 03044-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-5.0-7.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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-...	5.051	2.3	ng	54444	1	6.834	473783	20.0
Benzophenone	10.580	4.6	ng	137899	3	9.869	597776	20.0
Phenanthrene, 1...	11.857	2.5	ng	66286	4	11.357	526262	20.0
Phenanthrene, 2...	11.886	7.7	ng	201310	4	11.357	526262	20.0
4H-Cyclopenta[d...	11.969	5.0	ng	130293	4	11.357	526262	20.0
Phenanthrene, 2...	12.410	2.1	ng	55447	4	11.357	526262	20.0
Benzo[b]naphtho...	13.751	2.0	ng	96964	5	14.004	952319	20.0
11H-Benzo[a]flu...	13.845	4.1	ng	195999	5	14.004	952319	20.0
Octadecane	14.780	2.1	ng	48395	6	15.468	450763	20.0
Benzo[e]pyrene	15.145	3.2	ng	71932	6	15.468	450763	20.0
Perylene	15.339	9.9	ng	223985	6	15.468	450763	20.0