

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
 Data File : BF136261.D
 Acq On : 28 Nov 2023 21:36
 Operator : CG\JU
 Sample : 05516-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11930

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: BF136261.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	498	502	508	rVB	36845	42995	1.93%	0.198%
2	5.434	565	569	572	rBV	2421784	2063759	92.51%	9.490%
3	6.434	734	739	742	rBV	2273003	1966523	88.15%	9.043%
4	6.804	798	802	805	rBV	986468	733892	32.90%	3.375%
5	7.363	892	897	900	rBV	1543820	1256386	56.32%	5.777%
6	8.081	1015	1019	1021	rBV	1199418	939401	42.11%	4.320%
7	8.098	1021	1022	1029	rVB	84927	59933	2.69%	0.276%
8	8.792	1135	1140	1143	rBV	99546	74318	3.33%	0.342%
9	8.892	1152	1157	1160	rBV	72099	58468	2.62%	0.269%
10	9.157	1198	1202	1205	rBV	3009531	2230916	100.00%	10.259%
11	9.275	1220	1222	1225	rVB	36664	30970	1.39%	0.142%
12	9.422	1239	1247	1252	rVB3	24846	36331	1.63%	0.167%
13	9.492	1256	1259	1262	rBV	38559	34319	1.54%	0.158%
14	9.833	1311	1317	1321	rBV	1050958	902331	40.45%	4.149%
15	9.869	1321	1323	1327	rVB	112616	85141	3.82%	0.392%
16	10.039	1348	1352	1356	rBV	82819	66318	2.97%	0.305%
17	10.381	1408	1410	1414	rVB	64659	59650	2.67%	0.274%
18	10.622	1448	1451	1459	rBV	1037922	937201	42.01%	4.310%
19	11.328	1567	1571	1573	rBV	874005	689949	30.93%	3.173%
20	11.351	1573	1575	1578	rVV	627987	447013	20.04%	2.056%
21	11.404	1578	1584	1587	rVB	64263	67706	3.03%	0.311%
22	11.557	1604	1610	1613	rBV2	51647	60416	2.71%	0.278%
23	11.833	1653	1657	1659	rBV	56133	55950	2.51%	0.257%
24	11.863	1659	1662	1667	rVV2	195552	195562	8.77%	0.899%
25	11.945	1672	1676	1678	rVV2	80481	92113	4.13%	0.424%
26	11.963	1678	1679	1685	rVB	37079	29428	1.32%	0.135%
27	12.127	1704	1707	1709	rBV	39867	38909	1.74%	0.179%
28	12.151	1709	1711	1715	rVB	85043	68779	3.08%	0.316%
29	12.380	1745	1750	1754	rBV2	28408	35562	1.59%	0.164%
30	12.469	1762	1765	1770	rVB	40216	44142	1.98%	0.203%
31	12.545	1774	1778	1782	rBV	939218	718407	32.20%	3.304%
32	12.598	1782	1787	1791	rVB5	26173	41110	1.84%	0.189%
33	12.657	1793	1797	1802	rBV3	74052	101261	4.54%	0.466%
34	12.774	1811	1817	1820	rBV	709568	718387	32.20%	3.303%
35	12.822	1823	1825	1830	rVB2	37496	43085	1.93%	0.198%
36	12.898	1834	1838	1839	rBV	38353	35486	1.59%	0.163%

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37	12.922	1839	1842	1846	rVV	1724231	1538659	68.97%	7.075%
38	12.998	1849	1855	1858	rBV2	46264	75828	3.40%	0.349%
39	13.080	1865	1869	1871	rBV4	39790	51061	2.29%	0.235%
40	13.104	1871	1873	1877	rVB	82893	70175	3.15%	0.323%
41	13.169	1881	1884	1887	rBV2	49234	48411	2.17%	0.223%
42	13.210	1887	1891	1893	rBV2	77179	77899	3.49%	0.358%
43	13.233	1893	1895	1899	rVB	29192	29527	1.32%	0.136%
44	13.333	1909	1912	1914	rBV	30577	30419	1.36%	0.140%
45	13.616	1956	1960	1965	rVB	81070	84279	3.78%	0.388%
46	13.727	1974	1979	1982	rBV2	75454	99647	4.47%	0.458%
47	13.757	1982	1984	1986	rVV	62254	50663	2.27%	0.233%
48	13.780	1986	1988	1992	rVB2	37535	47049	2.11%	0.216%
49	13.821	1992	1995	2000	rBV2	76424	66366	2.97%	0.305%
50	13.869	2000	2003	2007	rBV2	40607	70781	3.17%	0.325%
51	13.980	2014	2022	2025	rBV2	1001426	1245960	55.85%	5.729%
52	14.004	2025	2026	2033	rVB	391176	306653	13.75%	1.410%
53	14.086	2037	2040	2042	rVB	47581	37975	1.70%	0.175%
54	14.368	2085	2088	2090	rVB	59304	48641	2.18%	0.224%
55	14.404	2091	2094	2098	rVB2	51377	56200	2.52%	0.258%
56	14.463	2101	2104	2107	rBV2	41662	50484	2.26%	0.232%
57	14.627	2128	2132	2137	rBV	645469	570920	25.59%	2.625%
58	14.674	2137	2140	2143	rVV2	46665	49474	2.22%	0.228%
59	14.763	2152	2155	2157	rBV4	29487	31443	1.41%	0.145%
60	14.933	2181	2184	2187	rVB3	70949	67604	3.03%	0.311%
61	15.027	2195	2200	2203	rBV	304352	455414	20.41%	2.094%
62	15.133	2215	2218	2223	rVB2	89477	105446	4.73%	0.485%
63	15.333	2248	2252	2258	rVB	151515	193681	8.68%	0.891%
64	15.398	2259	2263	2269	rBV	184992	216735	9.72%	0.997%
65	15.463	2269	2274	2278	rBV	494571	590451	26.47%	2.715%
66	15.980	2358	2362	2368	rBV2	45635	68033	3.05%	0.313%
67	16.957	2522	2528	2539	rVB2	60331	136549	6.12%	0.628%
68	17.145	2555	2560	2567	rBV7	14916	33184	1.49%	0.153%
69	17.404	2600	2604	2611	rVB	40903	78847	3.53%	0.363%

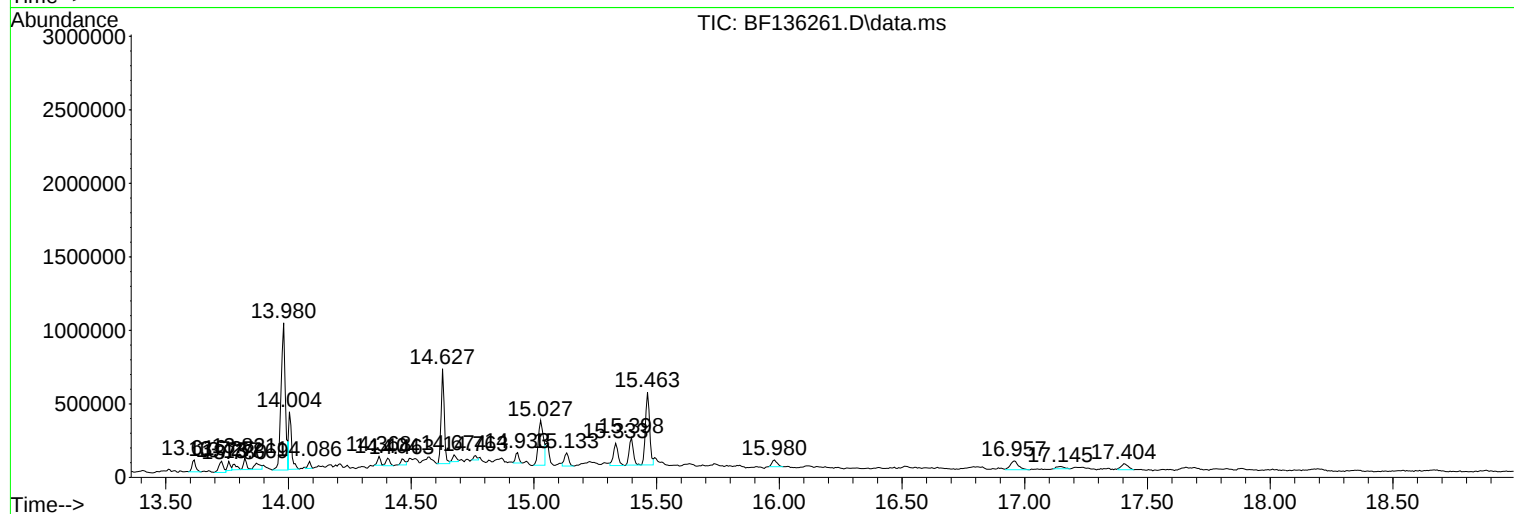
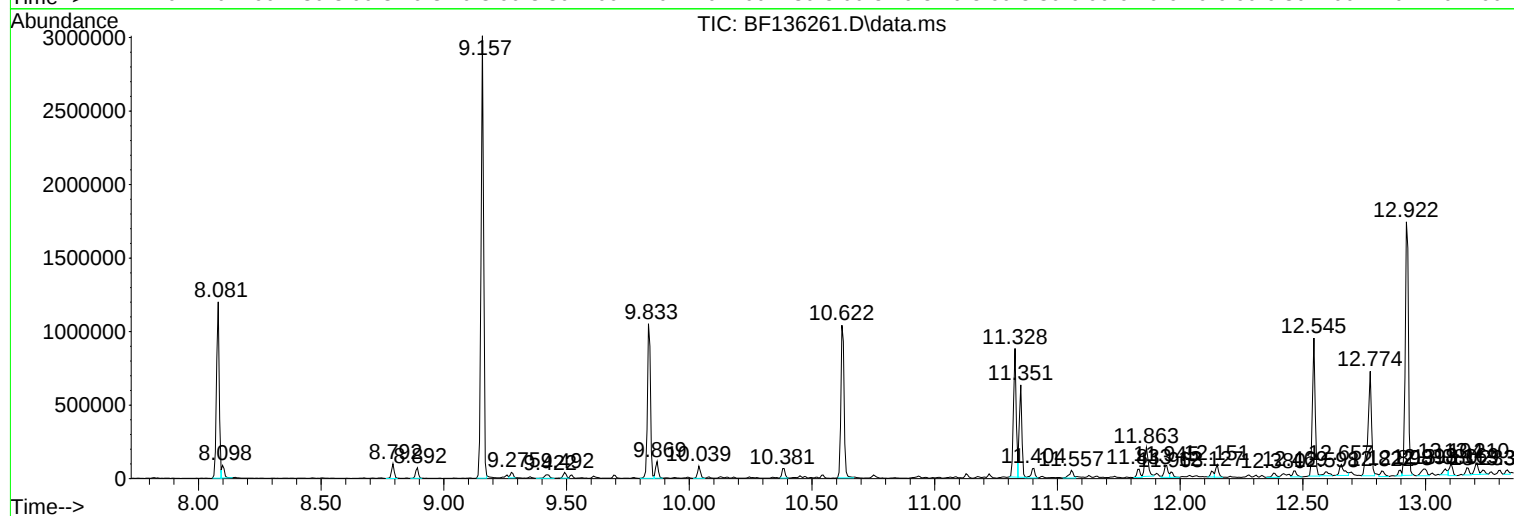
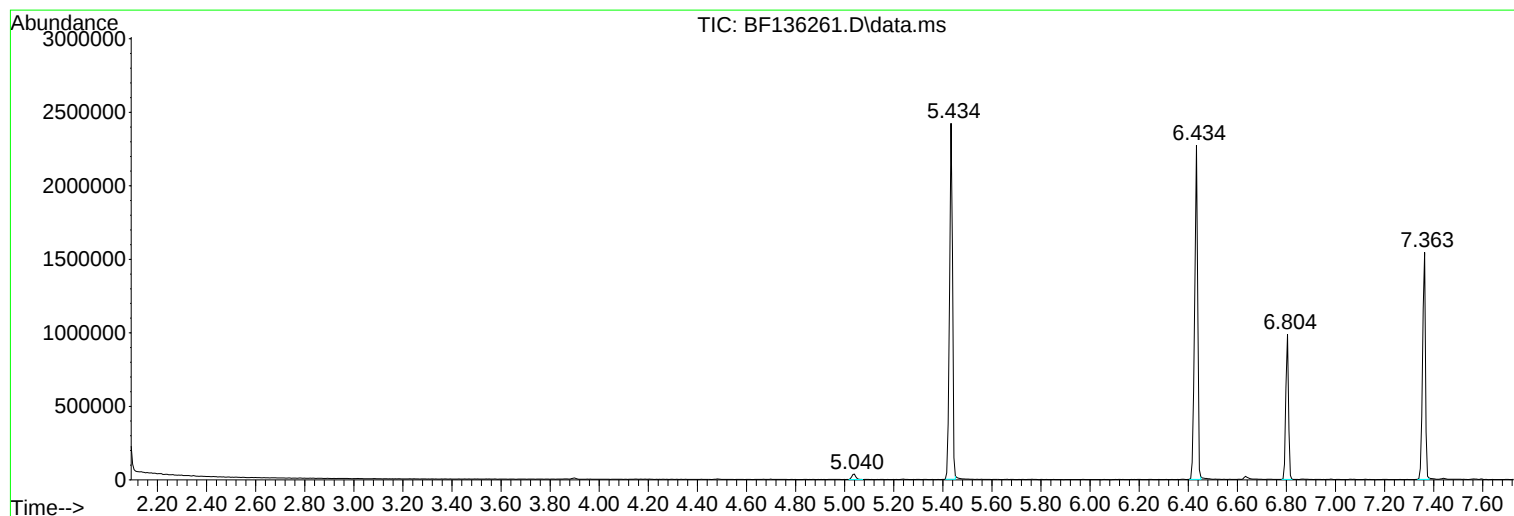
Sum of corrected areas: 21746575

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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



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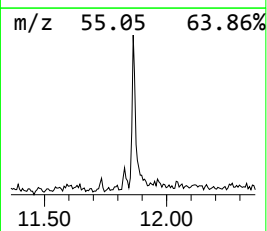
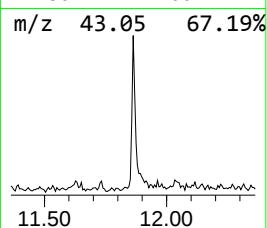
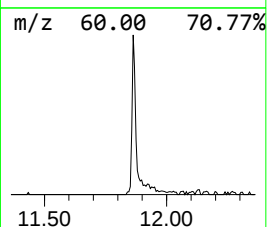
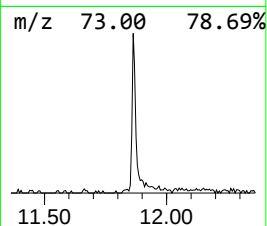
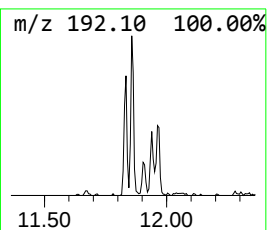
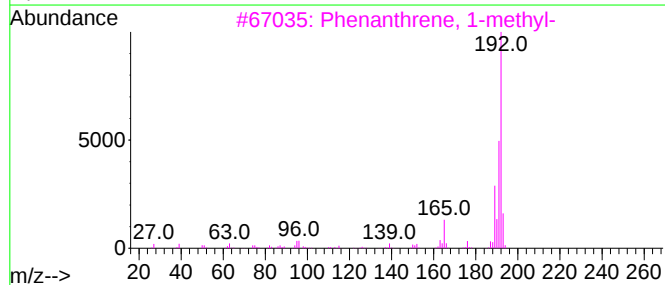
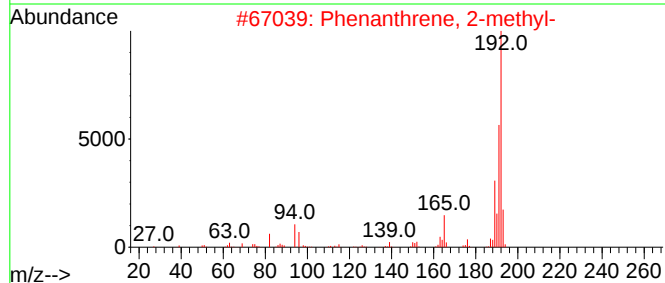
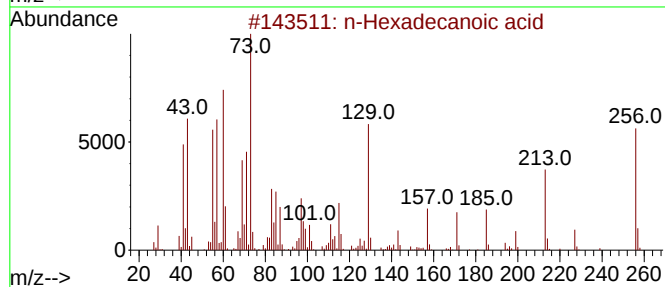
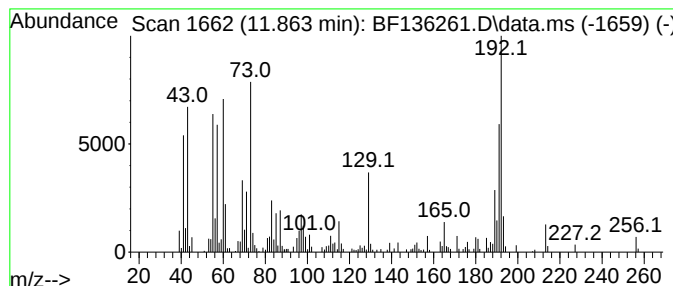
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	5.67 ng	195562	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	89
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
5			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	87



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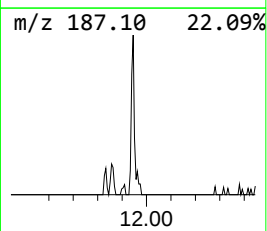
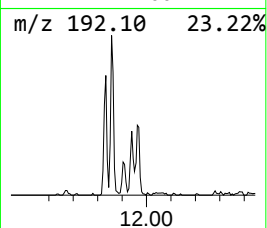
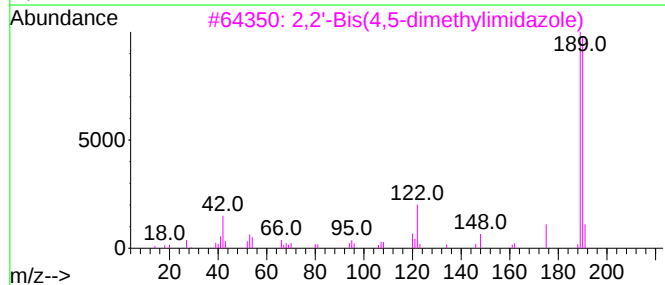
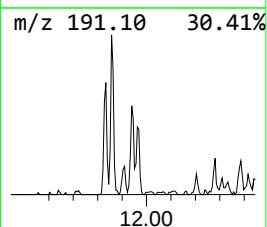
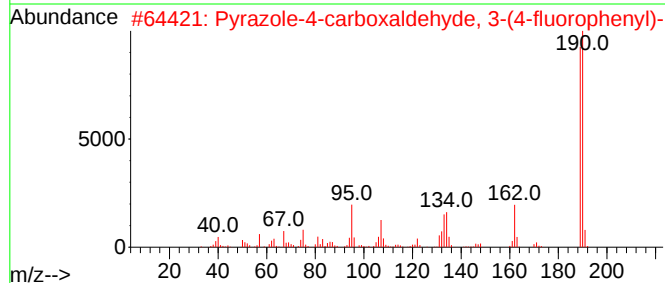
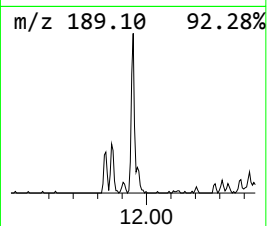
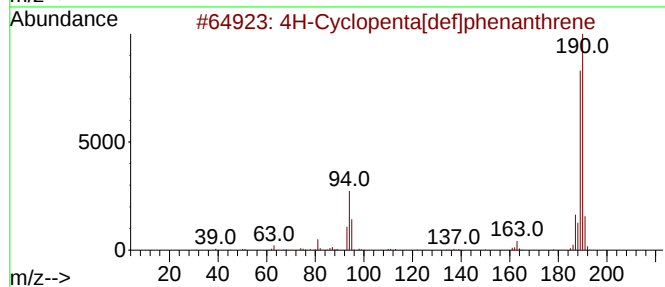
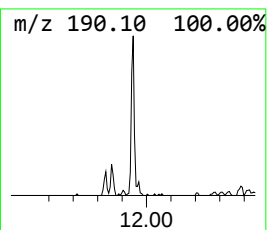
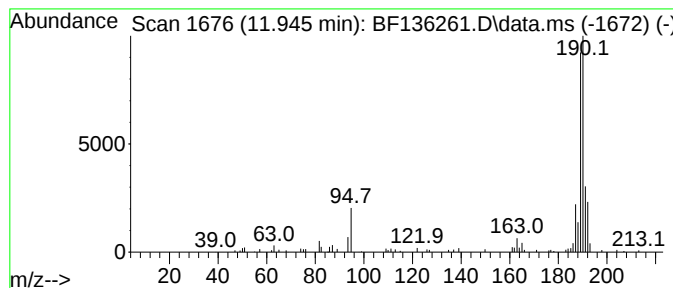
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.67 ng	92113	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22
5			1-Aminocyclopentanecarboxylic ac...	291	C13H22ClNO4	1000392-54-9	16



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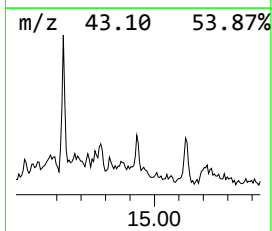
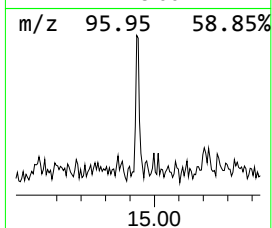
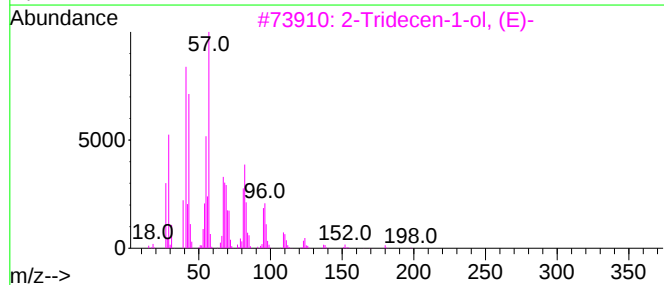
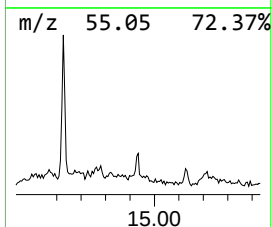
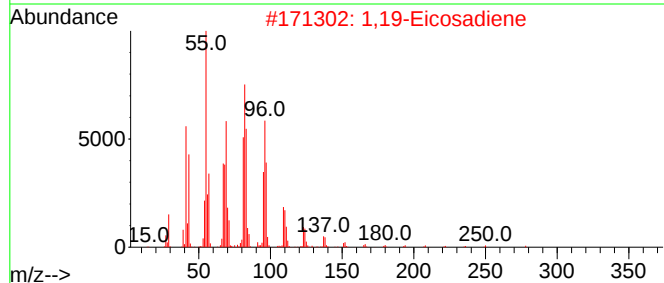
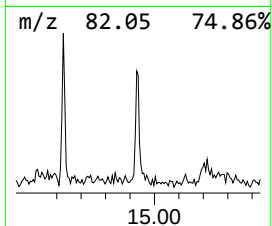
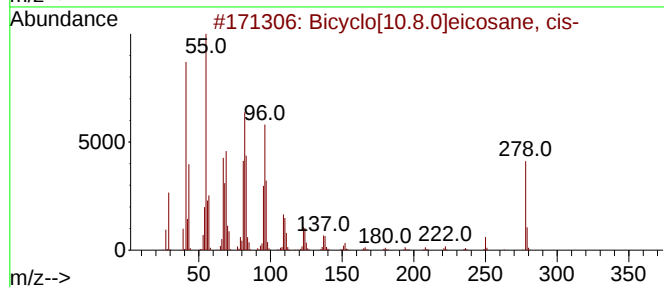
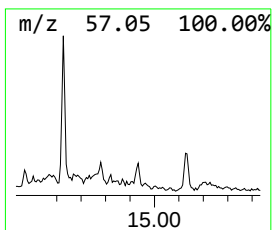
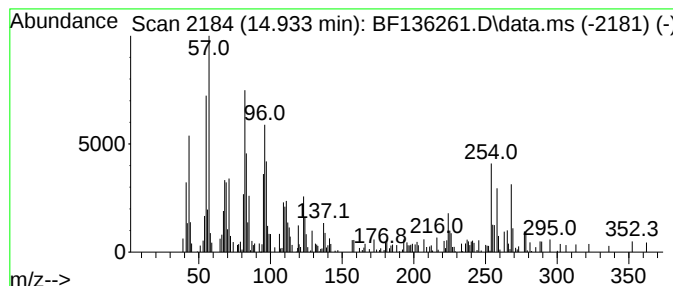
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Peak Number 3 Bicyclo[10.8.0]eicosane, cis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.29 ng	67604	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	90
2			1,19-Eicosadiene	278	C20H38	014811-95-1	78
3			2-Tridecen-1-ol, (E)-	198	C13H26O	074962-98-4	64
4			1-Methoxy-9-octadecene	282	C19H38O	1000430-37-3	56
5			17-Octadecenal	266	C18H34O	056554-86-0	49



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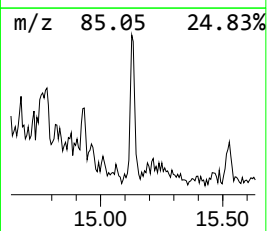
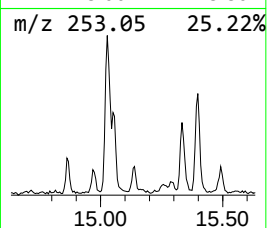
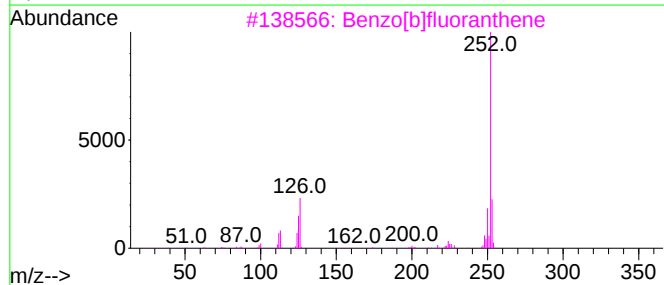
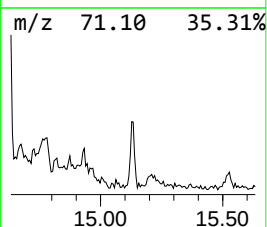
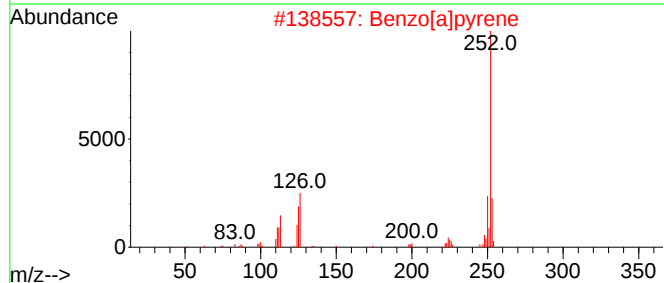
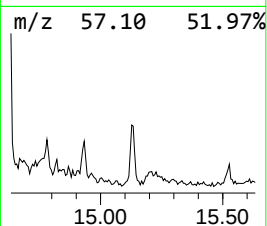
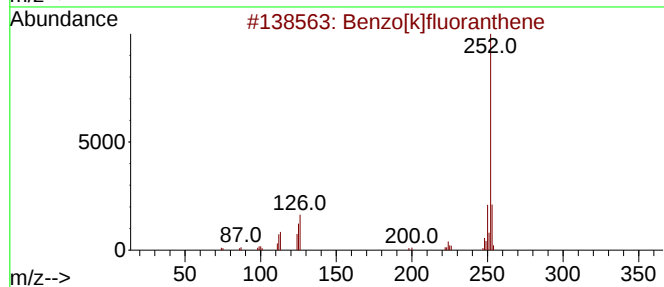
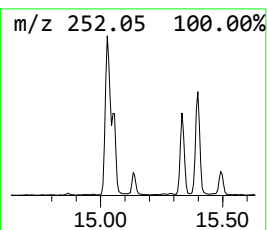
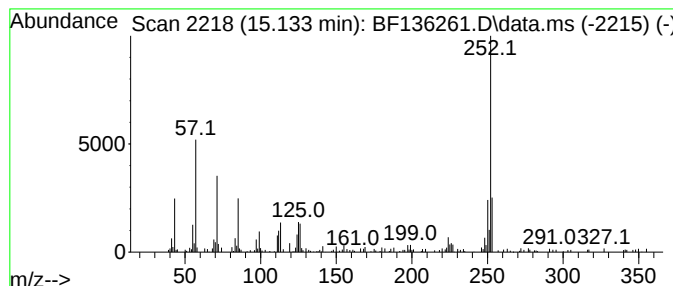
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.57 ng	105446	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	86
4			Benzo[e]pyrene	252	C20H12	000192-97-2	76
5			Perylene	252	C20H12	000198-55-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136261.D
Acq On : 28 Nov 2023 21:36
Operator : CG\JU
Sample : 05516-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

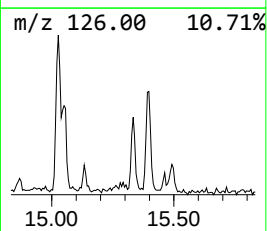
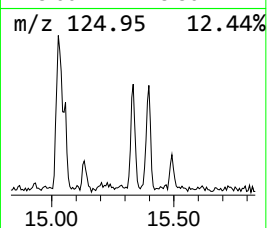
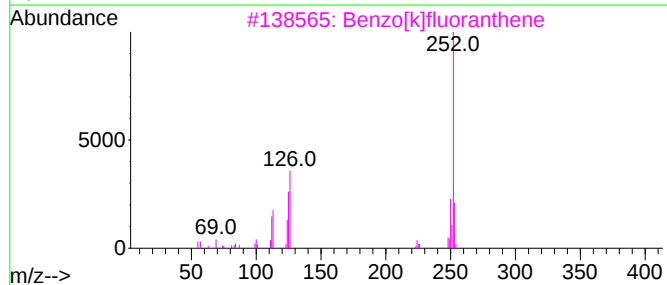
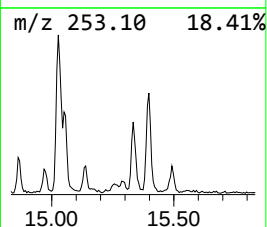
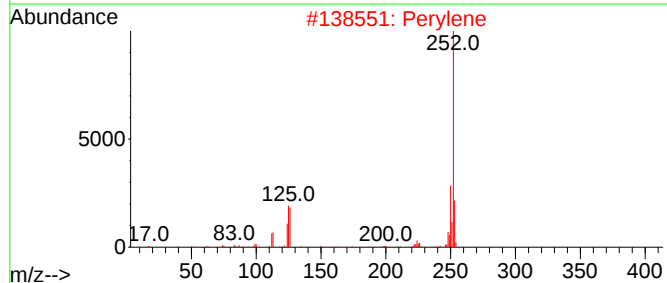
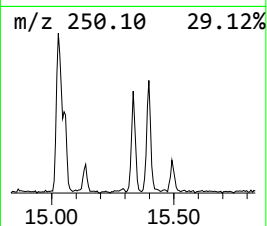
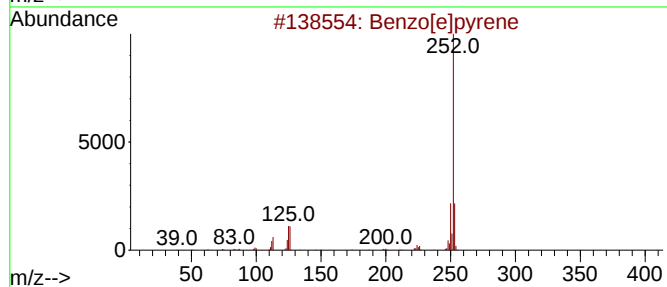
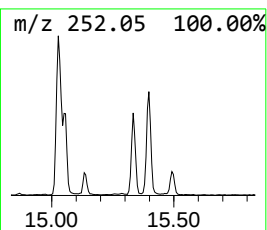
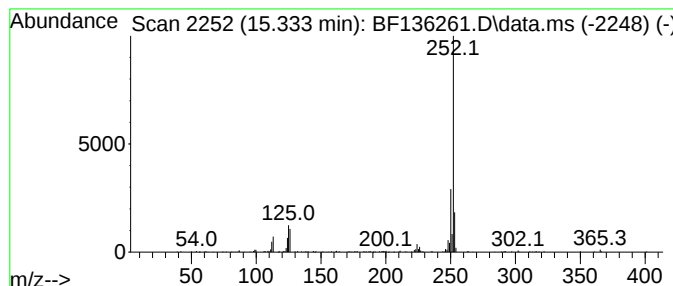
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	6.56 ng	193681	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	95
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136261.D
Acq On : 28 Nov 2023 21:36
Operator : CG\JU
Sample : 05516-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

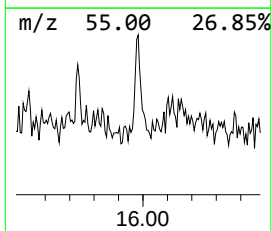
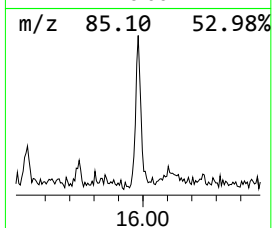
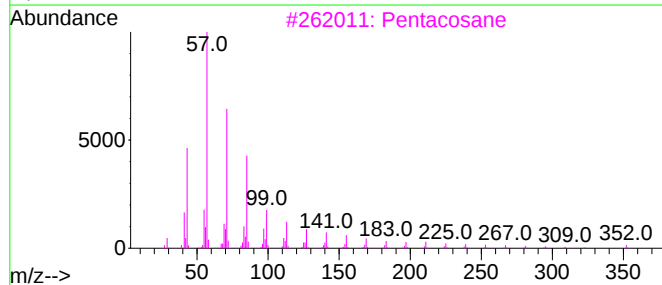
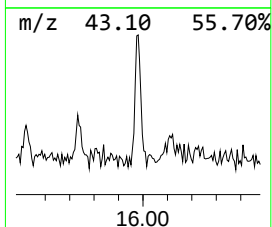
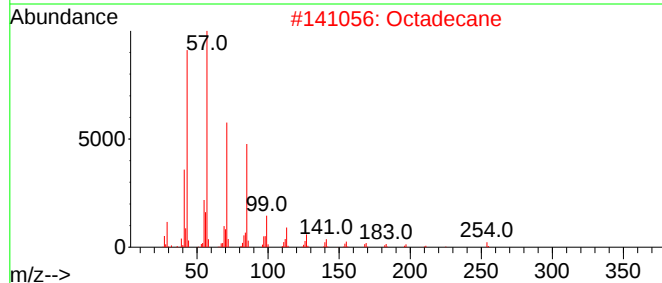
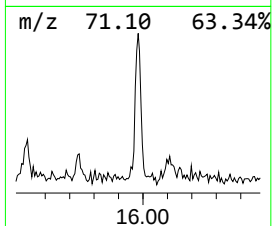
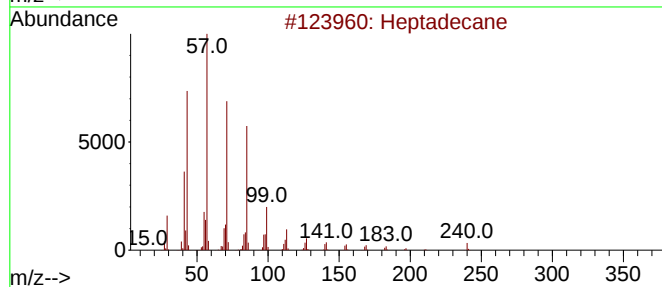
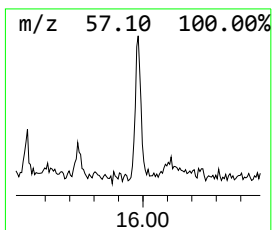
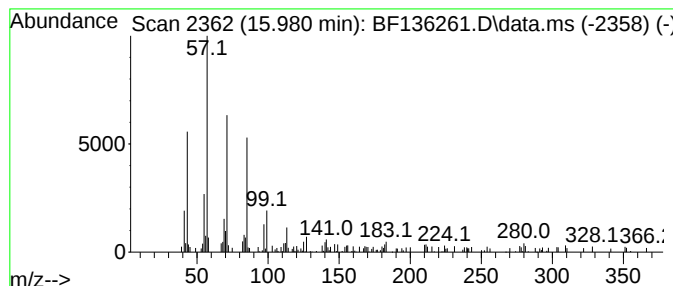
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	2.30 ng	68033	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	93
2		Octadecane	254	C18H38	000593-45-3	91
3		Pentacosane	352	C25H52	000629-99-2	89
4		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	87
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136261.D
Acq On : 28 Nov 2023 21:36
Operator : CG\JU
Sample : 05516-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.863	5.7	ng	195562	4	11.328	689949	20.0
4H-Cyclopenta[d...]	11.945	2.7	ng	92113	4	11.328	689949	20.0
Bicyclo[10.8.0]...	14.933	2.3	ng	67604	6	15.463	590451	20.0
Benzo[e]pyrene	15.133	3.6	ng	105446	6	15.463	590451	20.0
Perylene	15.333	6.6	ng	193681	6	15.463	590451	20.0
Heptadecane	15.980	2.3	ng	68033	6	15.463	590451	20.0