

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
 Data File : BF136390.D
 Acq On : 04 Dec 2023 19:34
 Operator : CG\JU
 Sample : 05521-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3-COMP

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: BF136390.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	507	rBV	49503	55984	2.71%	0.303%
2	5.440	565	570	573	rBV	2203337	1894149	91.73%	10.263%
3	6.440	735	740	743	rBV	2123927	1859877	90.07%	10.077%
4	6.804	798	802	805	rBV	802756	676457	32.76%	3.665%
5	7.363	892	897	900	rBV	1331114	1146783	55.54%	6.214%
6	8.081	1015	1019	1022	rBV	1019426	852323	41.28%	4.618%
7	9.157	1198	1202	1205	rBV	2738609	2064853	100.00%	11.188%
8	9.275	1218	1222	1226	rVV	34598	30408	1.47%	0.165%
9	9.316	1226	1229	1232	rVB	43379	31409	1.52%	0.170%
10	9.834	1314	1317	1321	rVB	1064010	847150	41.03%	4.590%
11	10.628	1448	1452	1455	rBV	1258015	1111609	53.83%	6.023%
12	11.328	1567	1571	1573	rBV	984458	786125	38.07%	4.259%
13	11.351	1573	1575	1578	rVV	196655	153143	7.42%	0.830%
14	11.398	1580	1583	1587	rVB	50420	48819	2.36%	0.265%
15	11.833	1654	1657	1659	rBV	51140	49210	2.38%	0.267%
16	11.863	1659	1662	1666	rVV2	354607	320059	15.50%	1.734%
17	11.904	1667	1669	1672	rVV2	42851	43160	2.09%	0.234%
18	11.939	1672	1675	1678	rVV	86799	103230	5.00%	0.559%
19	11.963	1678	1679	1685	rVB	44927	38573	1.87%	0.209%
20	12.127	1702	1707	1709	rBV2	33576	43095	2.09%	0.234%
21	12.386	1747	1751	1753	rBV	48470	53992	2.61%	0.293%
22	12.422	1753	1757	1759	rVV2	38537	46221	2.24%	0.250%
23	12.469	1762	1765	1770	rVB3	35267	39604	1.92%	0.215%
24	12.545	1773	1778	1781	rBV	417563	350105	16.96%	1.897%
25	12.592	1784	1786	1792	rVB2	73417	66072	3.20%	0.358%
26	12.651	1793	1796	1802	rBV3	67079	79384	3.84%	0.430%
27	12.751	1809	1813	1815	rBV2	188096	204128	9.89%	1.106%
28	12.775	1815	1817	1820	rVV	469640	357524	17.31%	1.937%
29	12.827	1823	1826	1830	rVB2	56091	54944	2.66%	0.298%
30	12.922	1838	1842	1846	rVB	2298191	1996383	96.68%	10.817%
31	12.992	1850	1854	1862	rBV5	40930	69443	3.36%	0.376%
32	13.104	1871	1873	1876	rVB	66988	55049	2.67%	0.298%
33	13.174	1876	1885	1887	rBV2	48801	73925	3.58%	0.401%
34	13.210	1887	1891	1894	rVV2	64923	58699	2.84%	0.318%
35	13.304	1904	1907	1910	rBV2	40098	57441	2.78%	0.311%
36	13.333	1910	1912	1915	rVB	38613	35098	1.70%	0.190%

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37	13.463	1930	1934	1936	rBV	121322	121596	5.89%	0.659%
38	13.504	1939	1941	1944	rVV	32608	32696	1.58%	0.177%
39	13.616	1957	1960	1964	rBV	24690	28644	1.39%	0.155%
40	13.727	1977	1979	1982	rVB2	29555	26129	1.27%	0.142%
41	13.833	1993	1997	1999	rBV2	34284	47932	2.32%	0.260%
42	13.857	1999	2001	2009	rVB6	61327	110355	5.34%	0.598%
43	13.980	2017	2022	2025	rBV2	958171	989071	47.90%	5.359%
44	14.004	2025	2026	2032	rVB	177407	125921	6.10%	0.682%
45	14.157	2050	2052	2055	rVB2	45577	35888	1.74%	0.194%
46	14.369	2086	2088	2091	rVB	42864	32777	1.59%	0.178%
47	14.463	2101	2104	2107	rVB3	66011	58403	2.83%	0.316%
48	14.774	2155	2157	2160	rVB	43724	39433	1.91%	0.214%
49	14.851	2167	2170	2176	rVB2	54906	69365	3.36%	0.376%
50	15.027	2196	2200	2203	rBV	101163	152997	7.41%	0.829%
51	15.121	2213	2216	2223	rVB3	58408	81975	3.97%	0.444%
52	15.333	2249	2252	2258	rVB	58982	76216	3.69%	0.413%
53	15.398	2259	2263	2269	rVB	76832	99590	4.82%	0.540%
54	15.463	2270	2274	2279	rBV	444703	572516	27.73%	3.102%

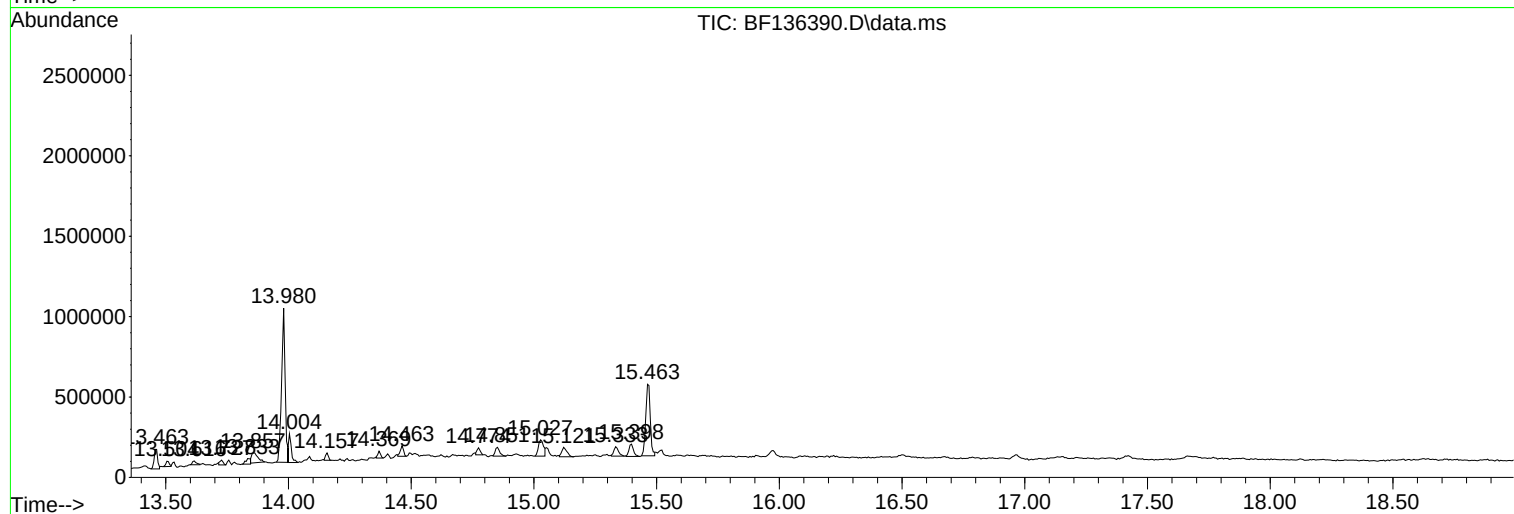
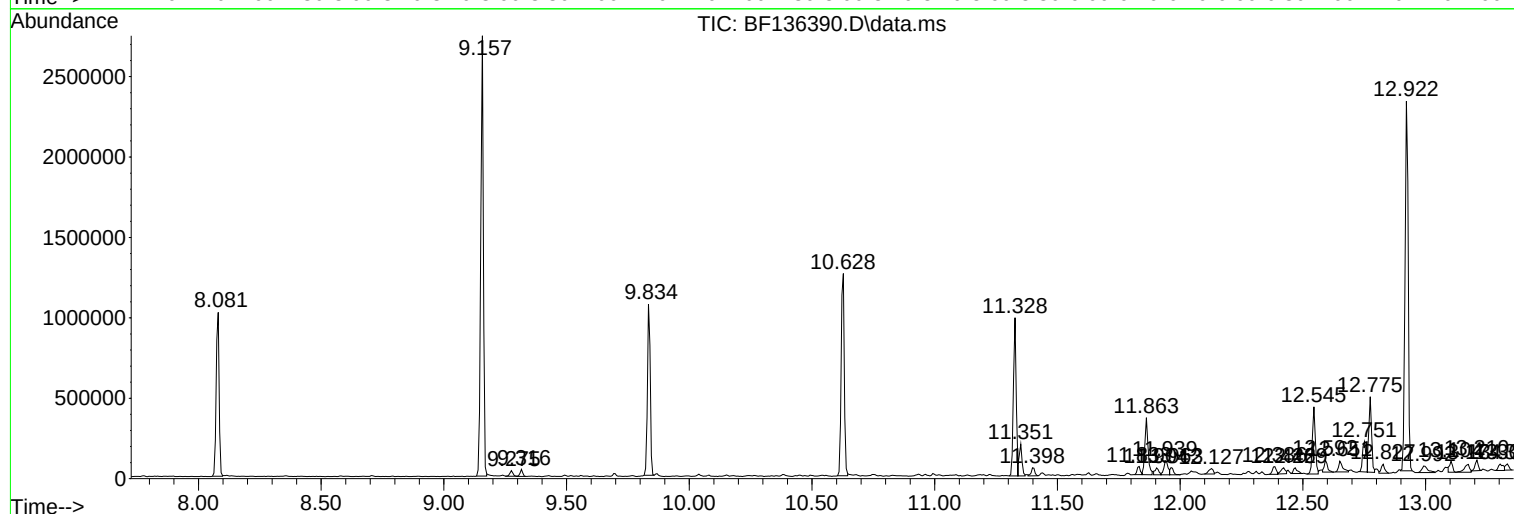
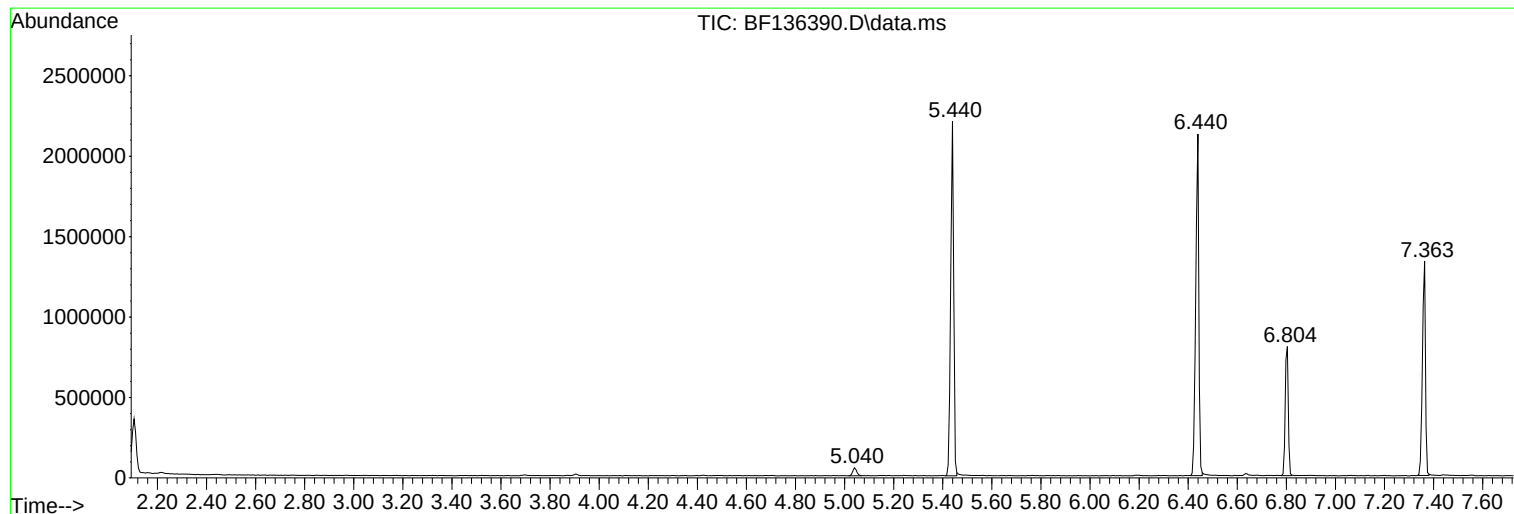
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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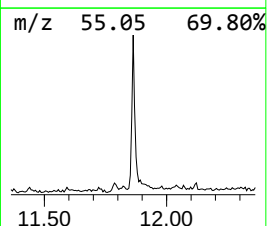
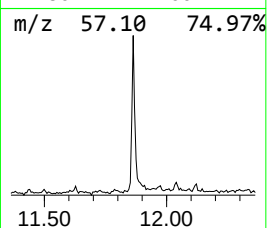
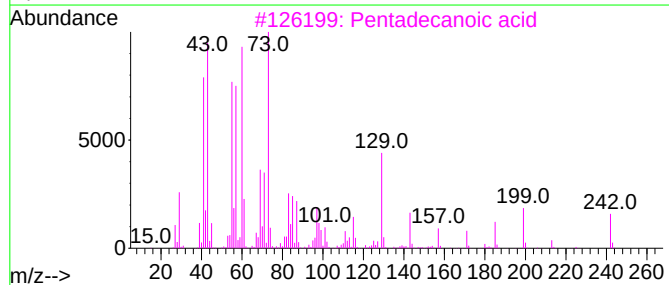
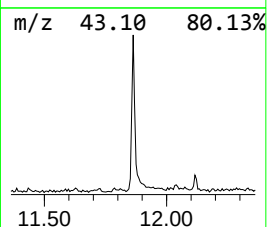
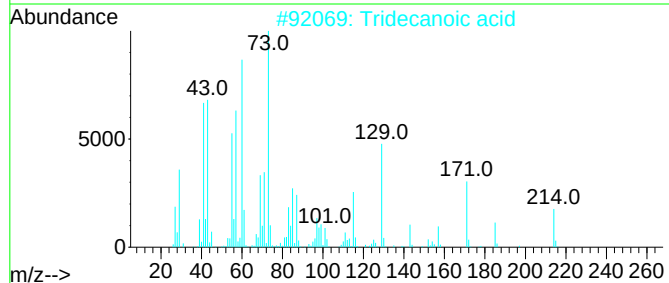
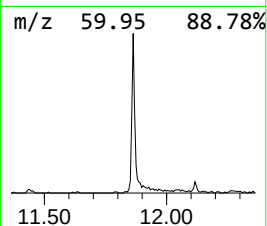
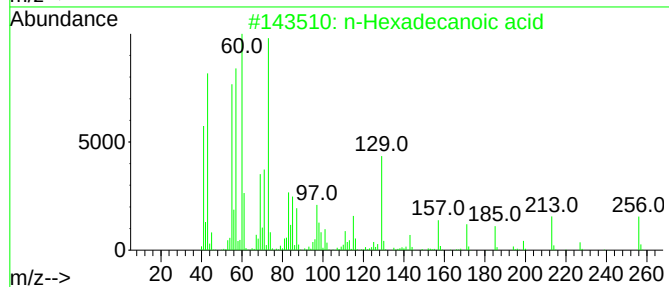
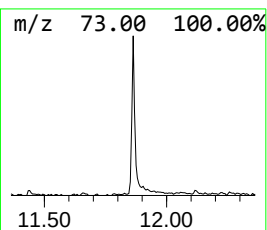
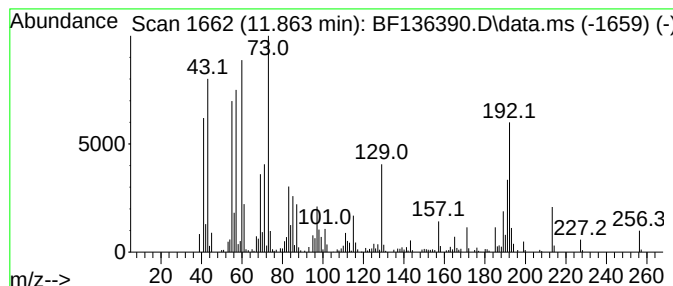
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	8.14 ng	320059	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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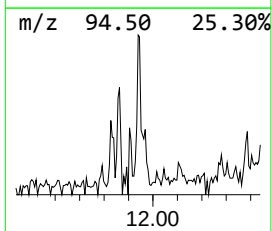
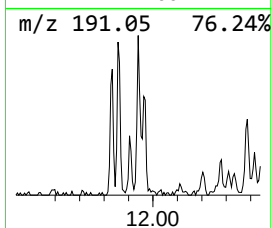
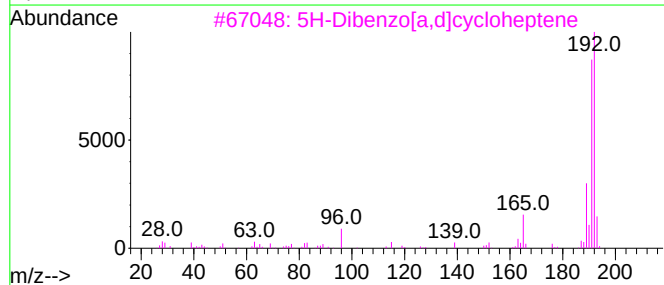
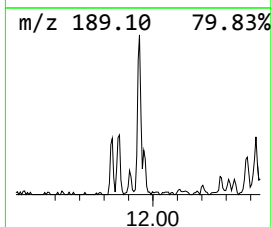
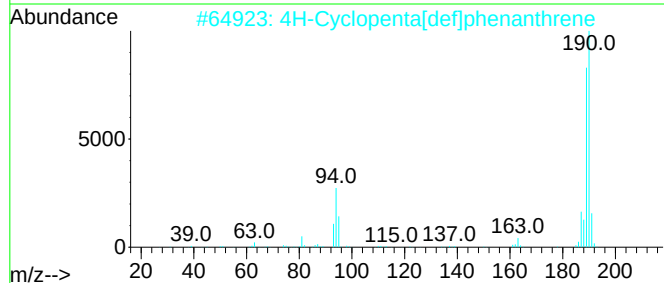
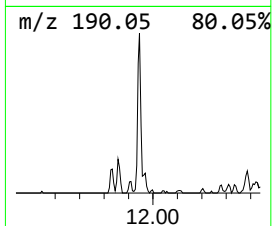
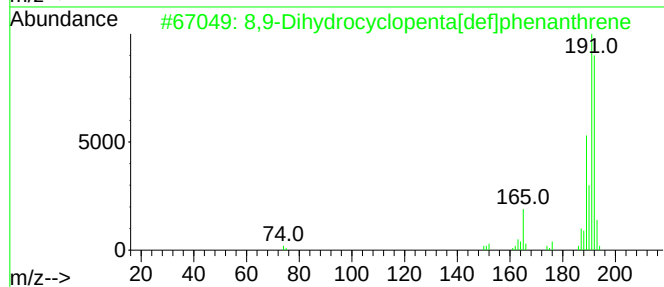
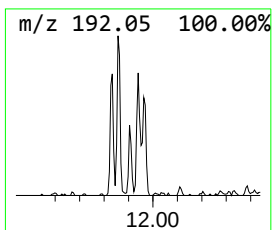
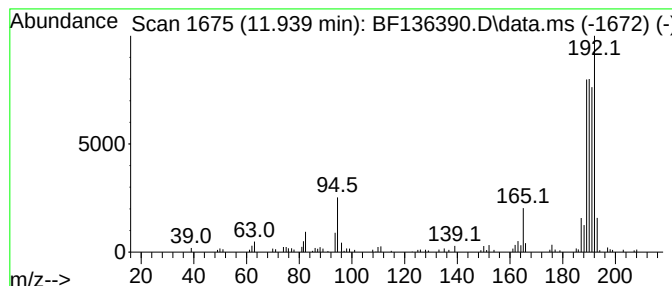
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 8,9-Dihydrocyclopenta[def]p... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.63 ng	103230	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	64
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
3			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	50
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	50



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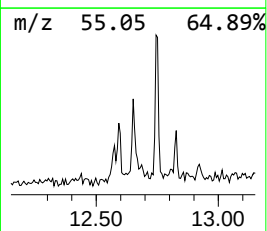
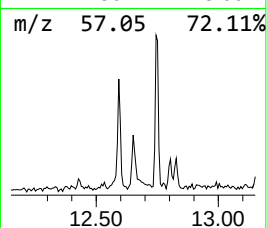
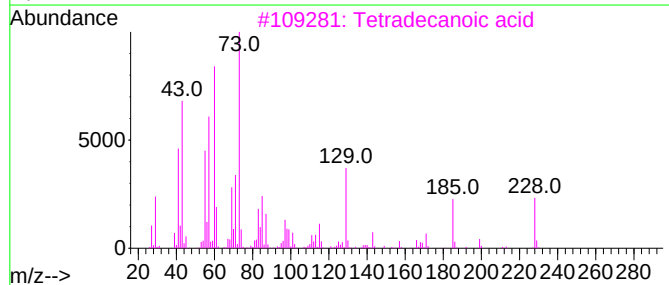
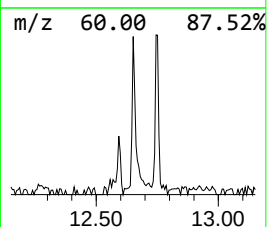
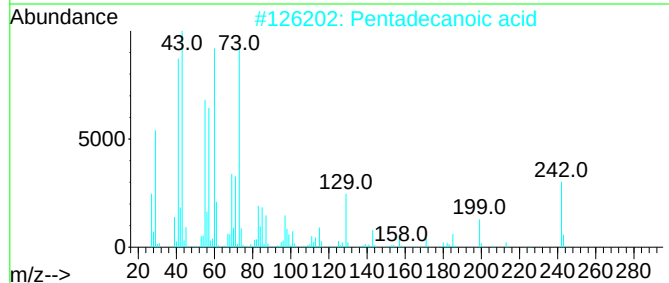
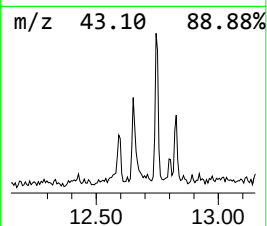
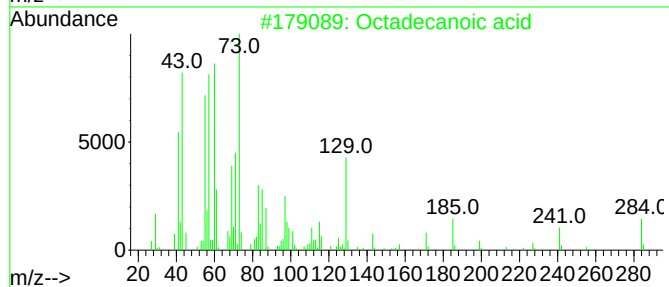
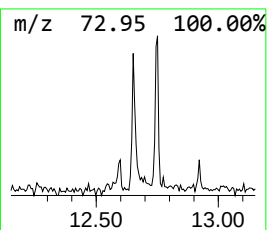
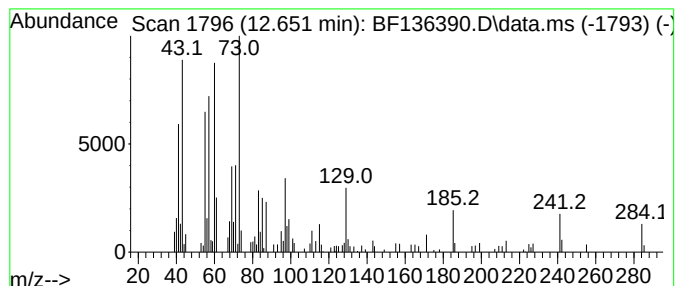
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.02 ng	79384	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Hexadecane	226	C16H34	000544-76-3	25



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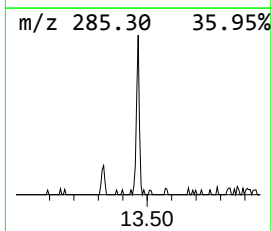
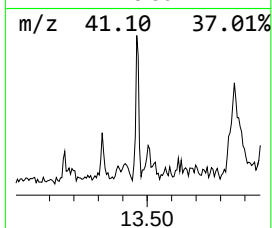
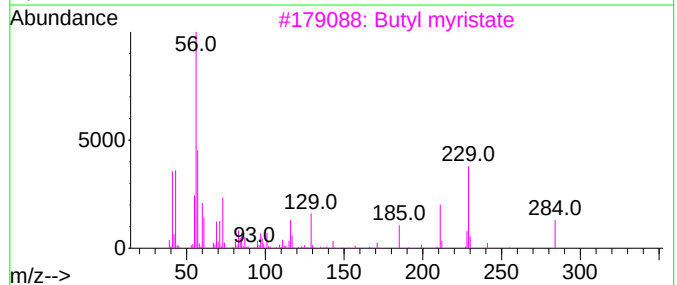
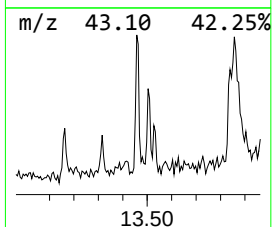
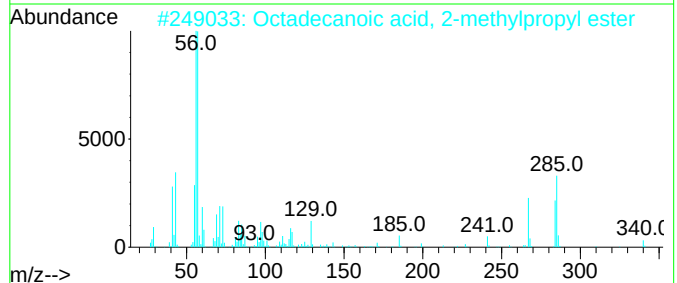
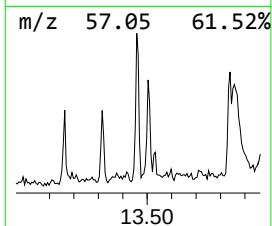
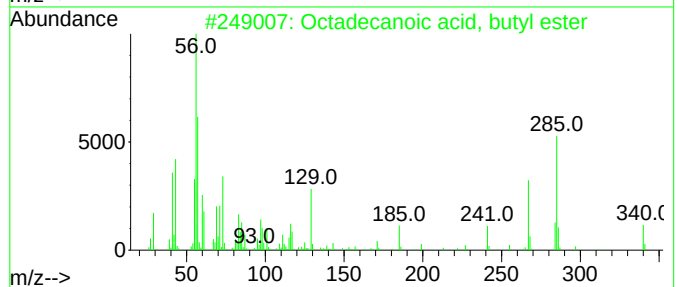
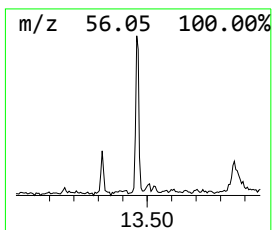
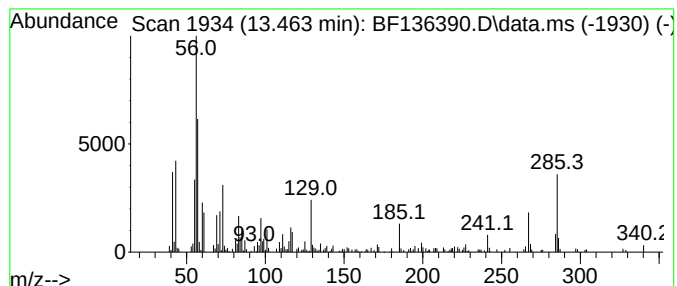
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.463	2.46 ng	121596	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	55
3	Butyl myristate	284	C18H36O2	000110-36-1	53
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30



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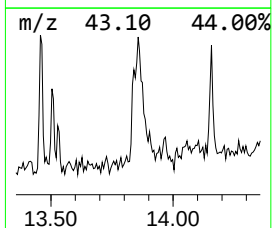
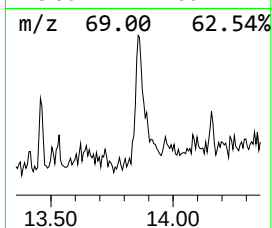
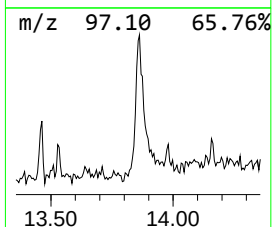
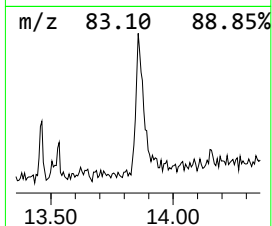
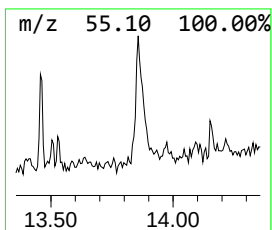
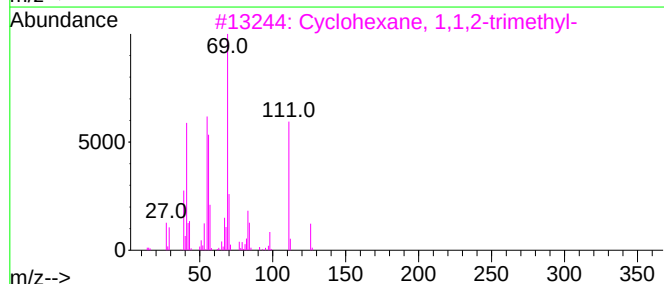
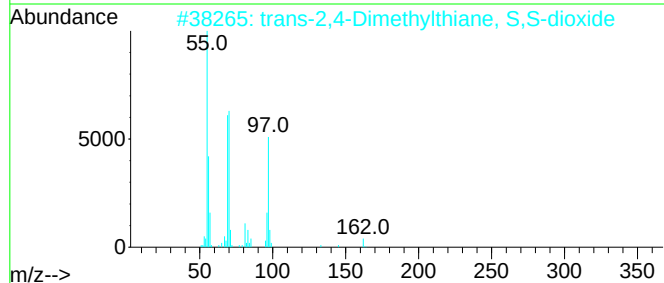
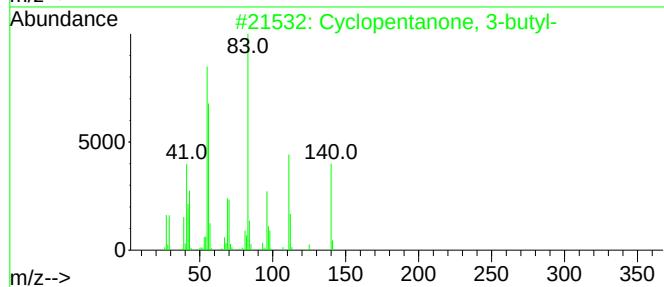
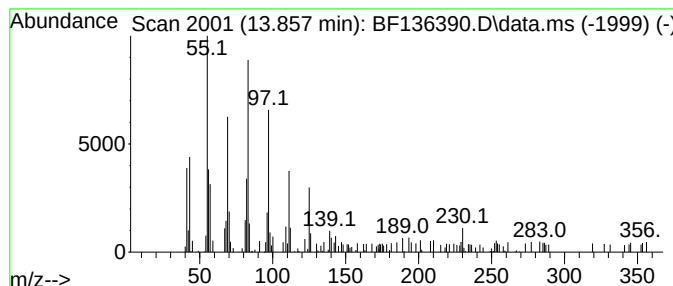
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.857 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.23 ng	110355	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 3-butyl-	140	C9H16O	057283-81-5	49
2			trans-2,4-Dimethylthiane, S,S-di...	162	C7H14O2S	1000215-67-6	38
3			Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	35
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	30
5			1,4-Cyclooctanedione	140	C8H12O2	055794-45-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136390.D
Acq On : 04 Dec 2023 19:34
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

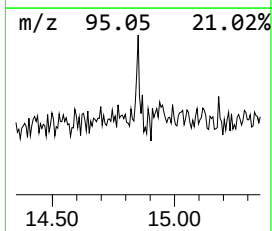
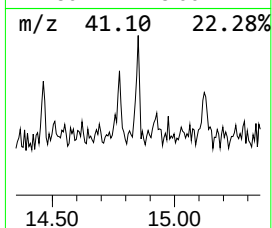
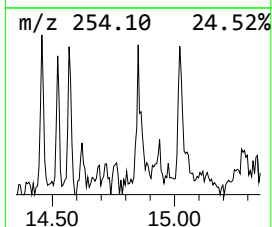
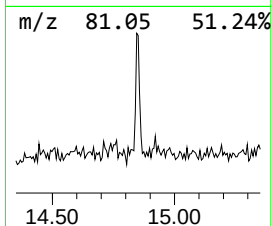
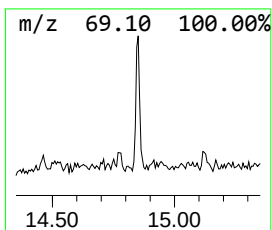
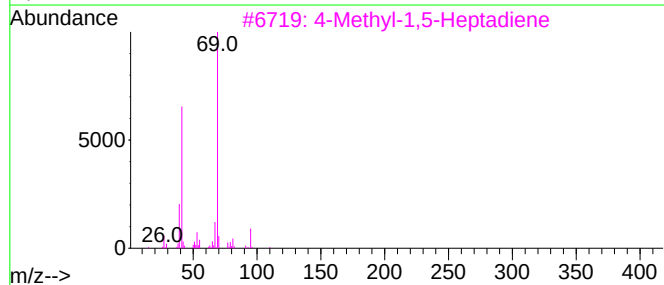
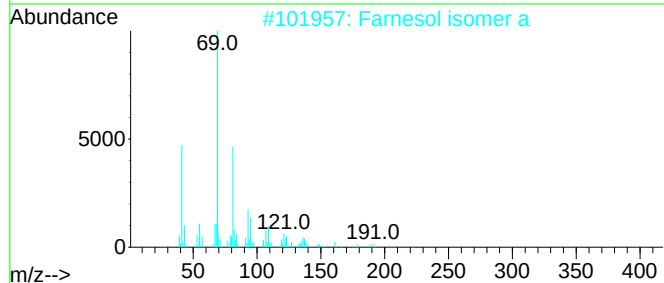
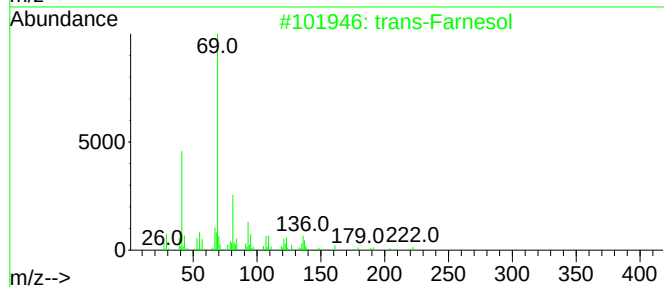
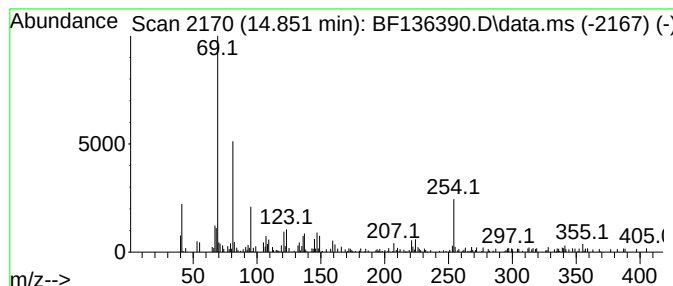
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 trans-Farnesol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	2.42 ng	69365	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Farnesol	222	C15H26O	000106-28-5	53
2			Farnesol isomer a	222	C15H26O	1000108-92-4	47
3			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	43
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	42
5			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136390.D
Acq On : 04 Dec 2023 19:34
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

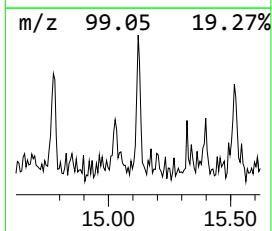
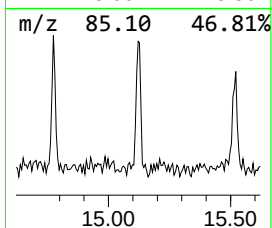
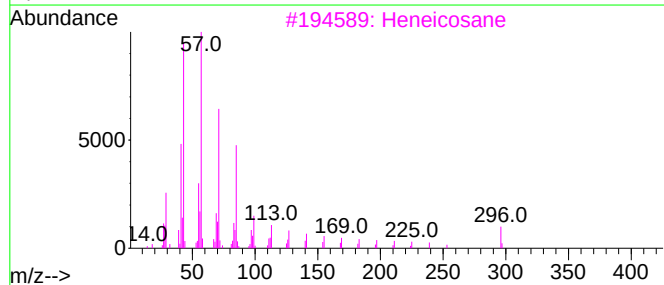
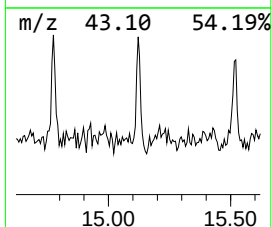
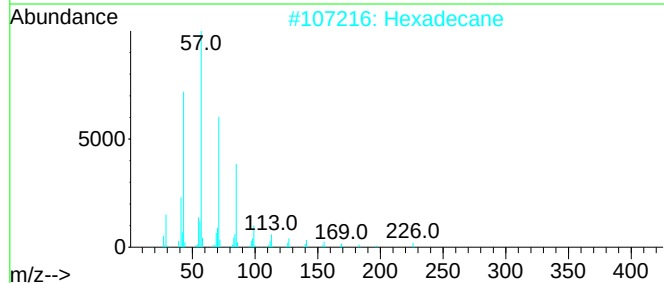
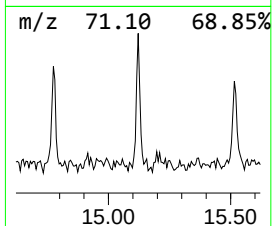
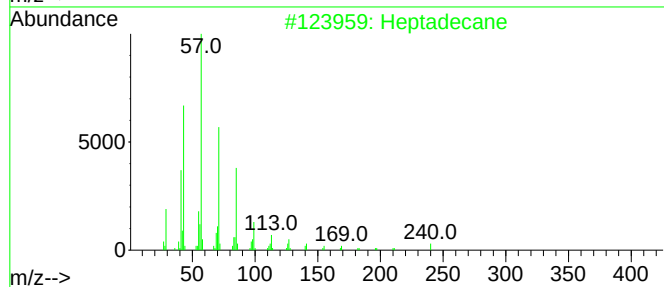
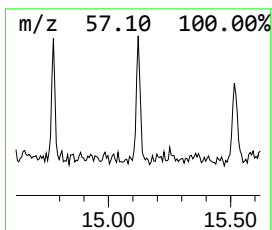
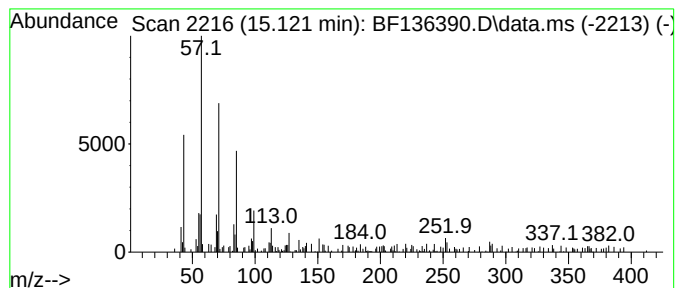
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	2.86 ng	81975	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	96
2			Hexadecane	226	C16H34	000544-76-3	93
3			Heneicosane	296	C21H44	000629-94-7	93
4			Tetracosane	338	C24H50	000646-31-1	93
5			Docosane	310	C22H46	000629-97-0	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136390.D
Acq On : 04 Dec 2023 19:34
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

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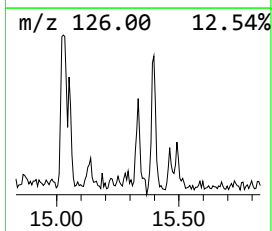
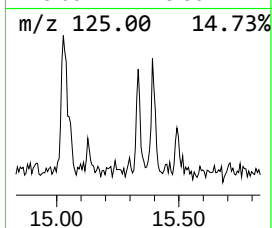
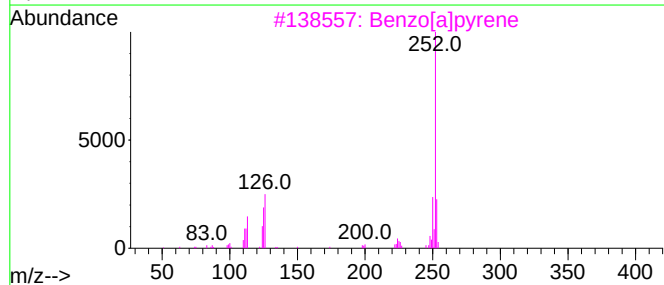
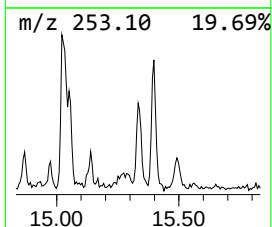
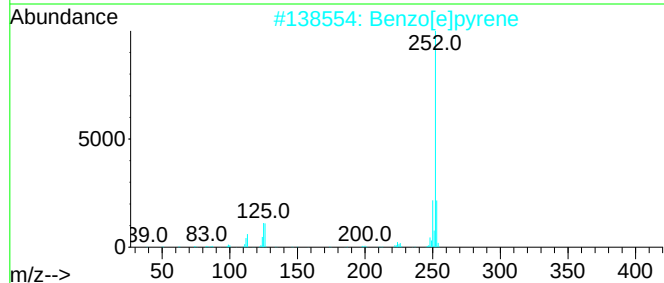
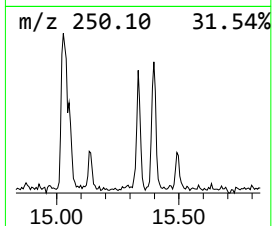
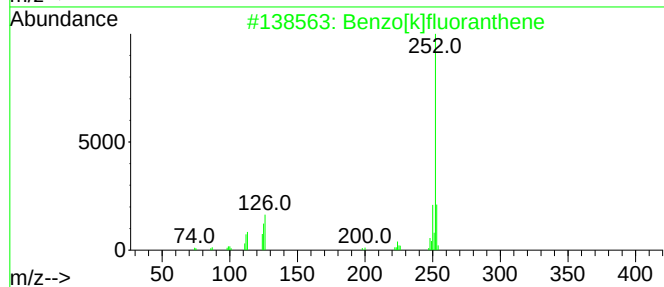
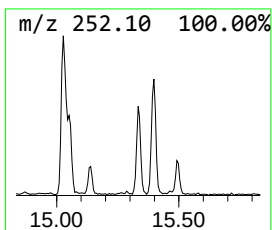
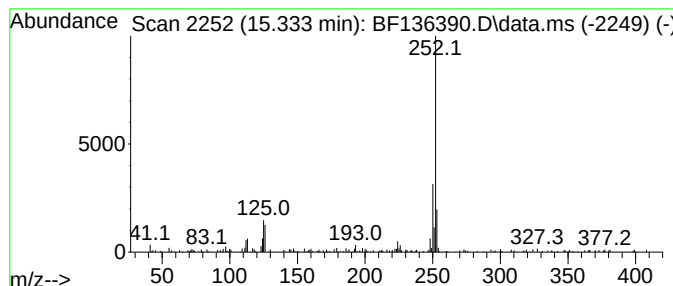
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	2.66 ng	76216	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136390.D
Acq On : 04 Dec 2023 19:34
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

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	8.1	ng	320059	4	11.328	786125	20.0
8,9-Dihydrocycl...	11.939	2.6	ng	103230	4	11.328	786125	20.0
Octadecanoic acid	12.651	2.0	ng	79384	4	11.328	786125	20.0
Octadecanoic ac...	13.463	2.5	ng	121596	5	13.980	989071	20.0
unknown13.857	13.857	2.2	ng	110355	5	13.980	989071	20.0
trans-Farnesol	14.851	2.4	ng	69365	6	15.469	572516	20.0
Heptadecane	15.121	2.9	ng	81975	6	15.469	572516	20.0
Benzo[e]pyrene	15.333	2.7	ng	76216	6	15.469	572516	20.0