

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
 Data File : BF098660.D
 Acq On : 20 Sep 2017 15:17
 Operator : SJ/JU
 Sample : I5285-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CSTP-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.799	457	461	477	rBV	295588	466739	17.19%	1.764%
2	5.234	530	535	555	rBV	2354178	2624207	96.66%	9.920%
3	6.281	708	713	728	rBV	2453061	2664647	98.15%	10.073%
4	6.393	728	732	735	rBV	3091358	2714903	100.00%	10.263%
5	6.616	767	770	776	rBV	681787	608063	22.40%	2.299%
6	6.775	793	797	804	rBV	2209492	1878111	69.18%	7.099%
7	7.192	863	868	871	rBV	1855053	1665693	61.35%	6.296%
8	7.904	985	989	992	rBV	884411	799191	29.44%	3.021%
9	8.981	1167	1172	1175	rBV	2889421	2443483	90.00%	9.237%
10	9.375	1236	1239	1243	rBV	369787	335873	12.37%	1.270%
11	9.651	1282	1286	1290	rBV2	963419	821002	30.24%	3.103%
12	10.445	1416	1421	1433	rBV	1653643	1528683	56.31%	5.779%
13	10.563	1438	1441	1449	rVB5	22492	36502	1.34%	0.138%
14	11.133	1534	1538	1541	rBV	869642	787503	29.01%	2.977%
15	11.157	1541	1542	1546	rVV	214884	147354	5.43%	0.557%
16	11.216	1547	1552	1555	rVB	43321	47723	1.76%	0.180%
17	11.639	1621	1624	1626	rBV	49134	45081	1.66%	0.170%
18	11.669	1626	1629	1632	rVB	61894	58530	2.16%	0.221%
19	11.745	1639	1642	1645	rBV	62261	68450	2.52%	0.259%
20	11.769	1645	1646	1650	rVB	39575	29793	1.10%	0.113%
21	12.186	1713	1717	1720	rBV	60695	59634	2.20%	0.225%
22	12.222	1720	1723	1725	rVV2	39649	44230	1.63%	0.167%
23	12.280	1729	1733	1736	rBV2	29767	34384	1.27%	0.130%
24	12.345	1740	1744	1748	rBV	428332	375423	13.83%	1.419%
25	12.545	1776	1778	1779	rBV	72814	58203	2.14%	0.220%
26	12.575	1779	1783	1786	rVV	450294	422613	15.57%	1.598%
27	12.627	1789	1792	1796	rVB3	41004	57603	2.12%	0.218%
28	12.722	1800	1808	1811	rBV	1983392	1794982	66.12%	6.785%
29	12.792	1816	1820	1826	rVB4	49935	72838	2.68%	0.275%
30	12.880	1832	1835	1836	rBV3	36334	34824	1.28%	0.132%
31	12.904	1837	1839	1842	rVB2	43272	39195	1.44%	0.148%
32	12.951	1842	1847	1849	rBV4	21365	31946	1.18%	0.121%
33	13.010	1853	1857	1864	rBV2	73779	98117	3.61%	0.371%
34	13.098	1870	1872	1875	rBV	50457	44569	1.64%	0.168%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

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 Min Area: 3 % of largest Peak
 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.133	1875	1878	1881	rBV	41544	40241	1.48%	0.152%
36	13.251	1895	1898	1901	rBV	38705	32824	1.21%	0.124%
37	13.286	1901	1904	1908	rBV5	21872	40829	1.50%	0.154%
38	13.416	1924	1926	1930	rVB	42246	43846	1.62%	0.166%
39	13.527	1939	1945	1947	rBV2	50004	70493	2.60%	0.266%
40	13.621	1958	1961	1968	rVB3	120238	165464	6.09%	0.625%
41	13.774	1978	1987	1989	rBV2	687159	846798	31.19%	3.201%
42	13.798	1989	1991	1995	rVV	218097	194623	7.17%	0.736%
43	13.874	1999	2004	2011	rBV4	25706	40268	1.48%	0.152%
44	13.939	2011	2015	2020	rBV6	32119	54289	2.00%	0.205%
45	14.163	2048	2053	2056	rVB	65306	68726	2.53%	0.260%
46	14.239	2061	2066	2071	rBV7	39961	85051	3.13%	0.321%
47	14.286	2071	2074	2076	rBV	32052	31156	1.15%	0.118%
48	14.480	2105	2107	2110	rBV3	30422	40727	1.50%	0.154%
49	14.516	2111	2113	2119	rVB3	52906	75212	2.77%	0.284%
50	14.639	2131	2134	2138	rVB2	50751	64896	2.39%	0.245%
51	14.780	2155	2158	2165	rBV	211933	336386	12.39%	1.272%
52	14.880	2172	2175	2178	rVB	43266	45032	1.66%	0.170%
53	15.057	2201	2205	2208	rVB	146990	161456	5.95%	0.610%
54	15.110	2211	2214	2220	rVB	184345	230094	8.48%	0.870%
55	15.168	2220	2224	2228	rBV	489366	562817	20.73%	2.127%
56	15.568	2288	2292	2297	rBV5	23878	39387	1.45%	0.149%
57	16.498	2445	2450	2459	rVB3	55573	123368	4.54%	0.466%
58	16.898	2511	2518	2525	rBV3	42613	90998	3.35%	0.344%
59	17.139	2554	2559	2563	rVB8	17419	29488	1.09%	0.111%

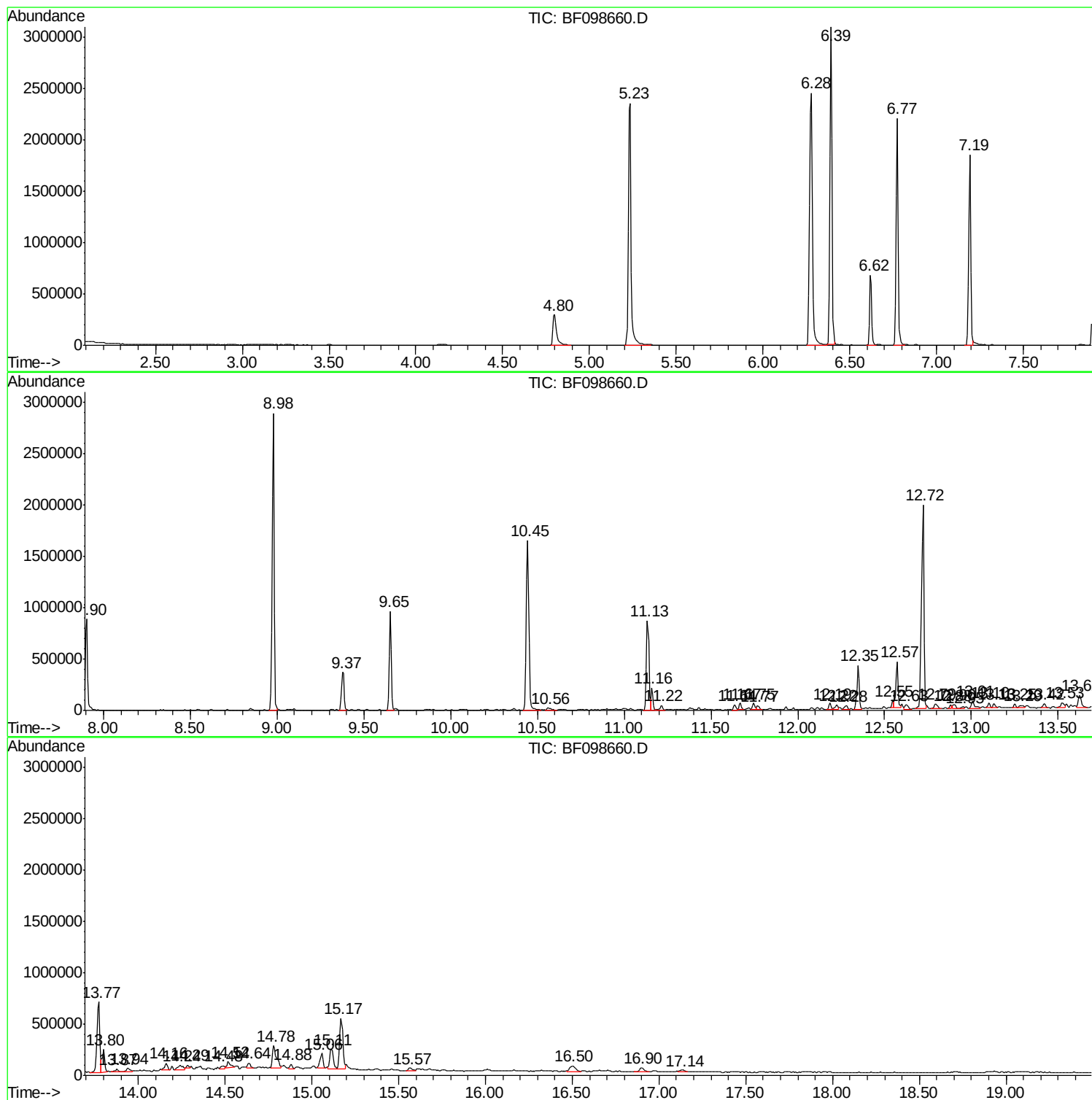
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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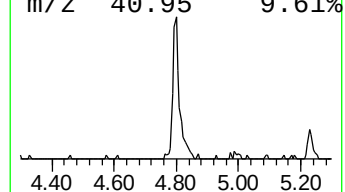
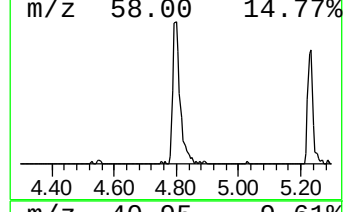
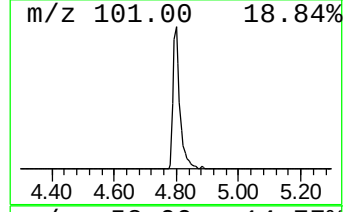
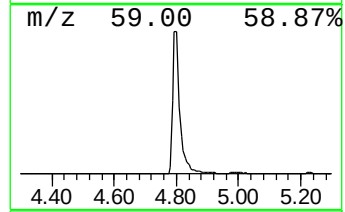
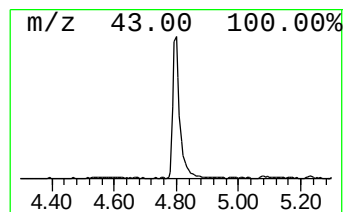
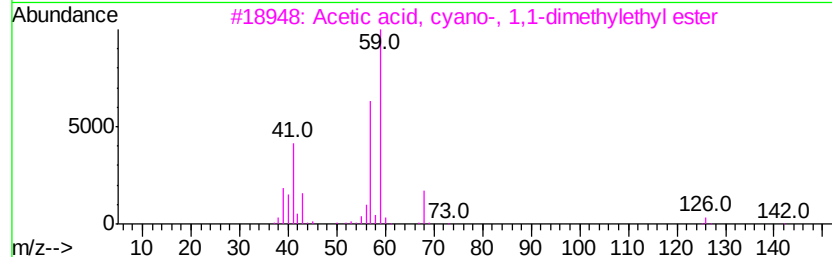
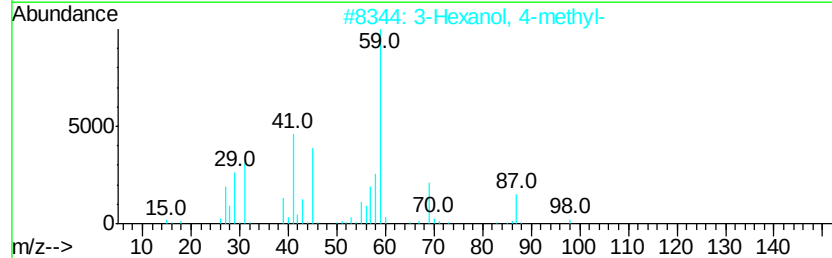
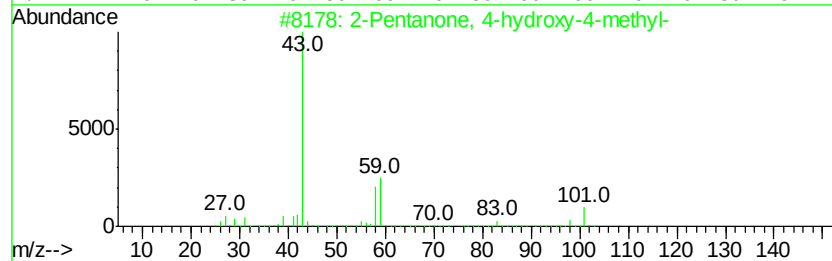
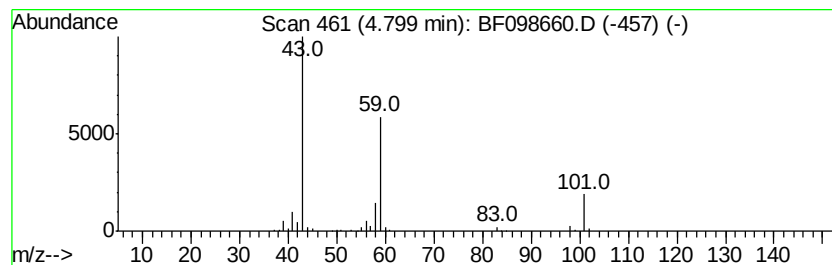
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	15.35 ng	466739	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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Instrument :
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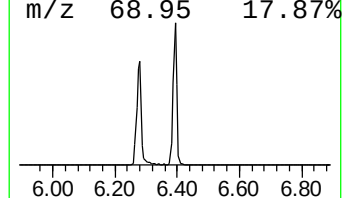
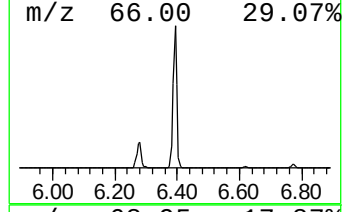
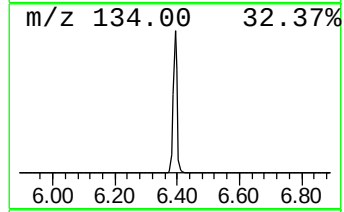
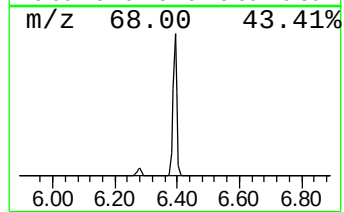
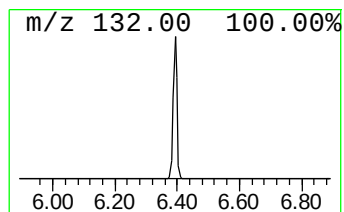
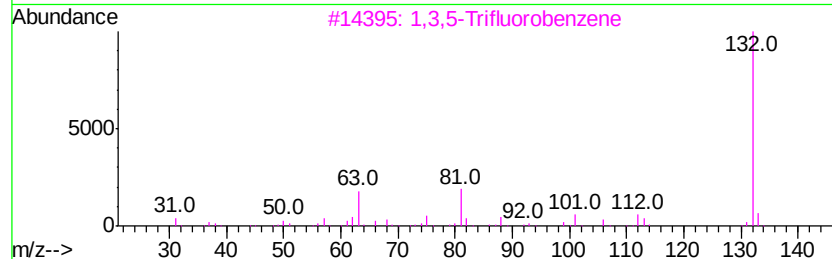
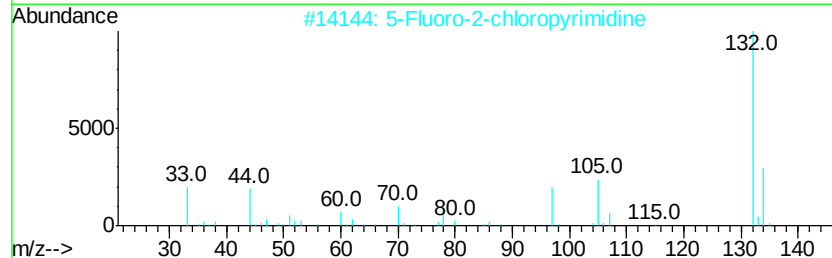
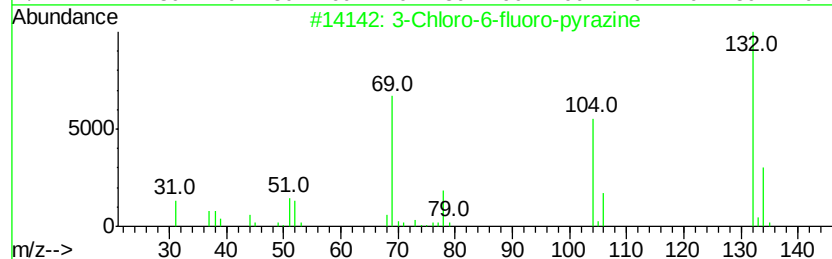
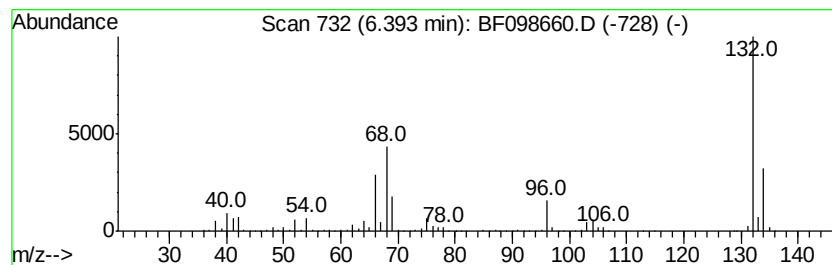
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	89.30 ng	2714900	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
4		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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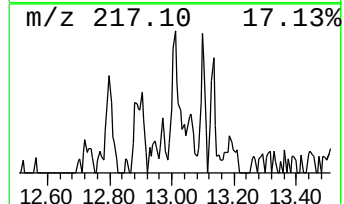
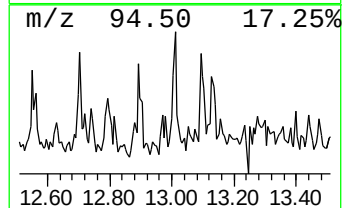
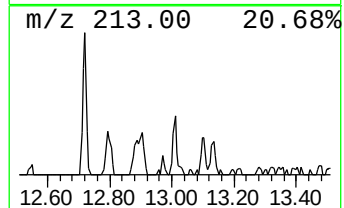
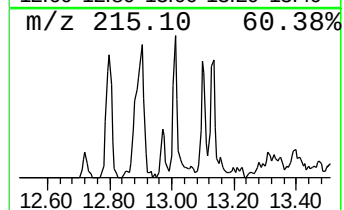
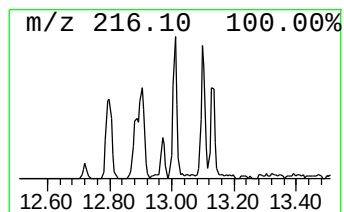
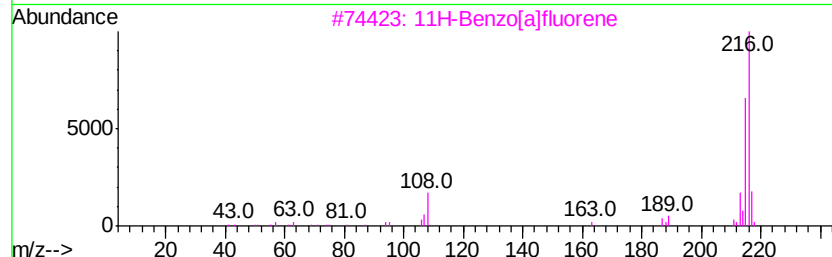
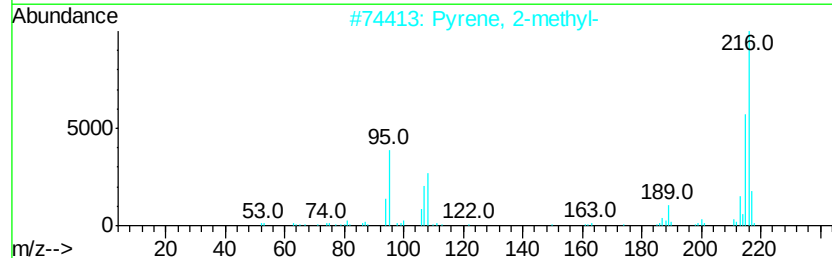
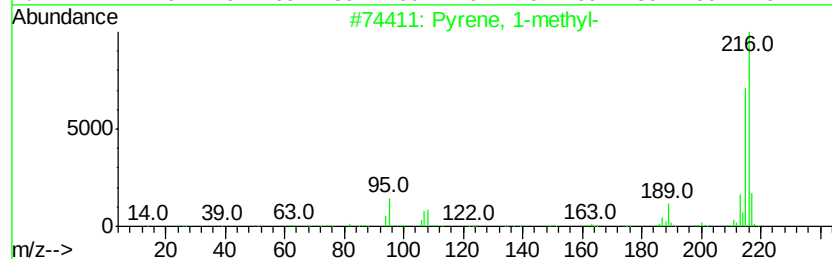
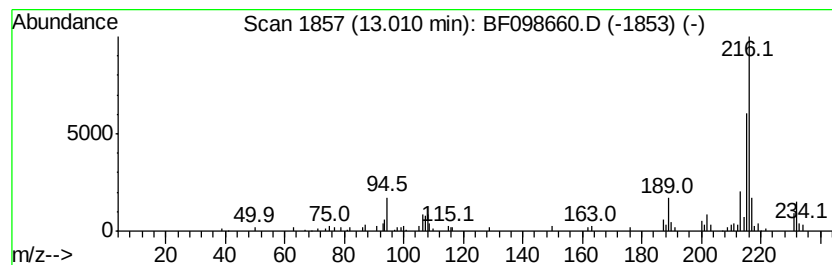
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	2.32 ng	98117	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	58



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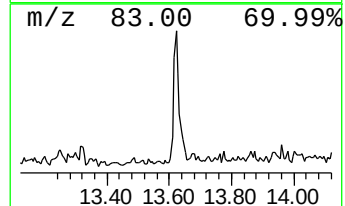
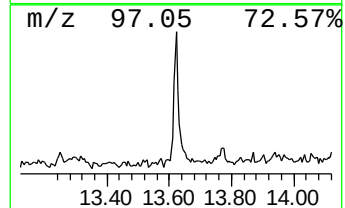
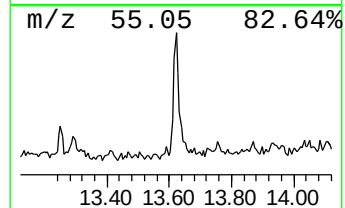
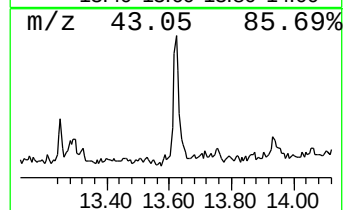
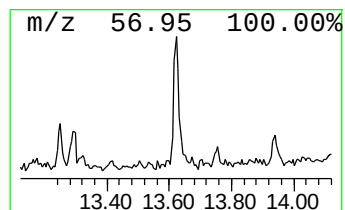
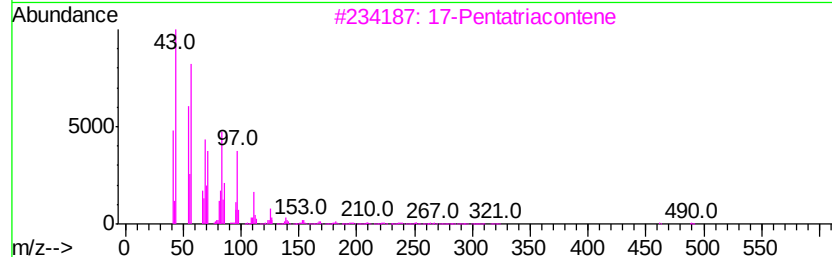
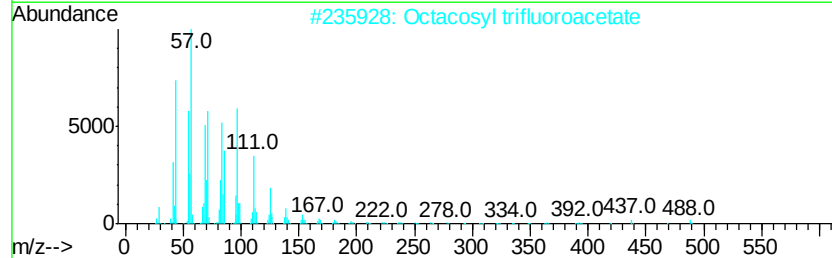
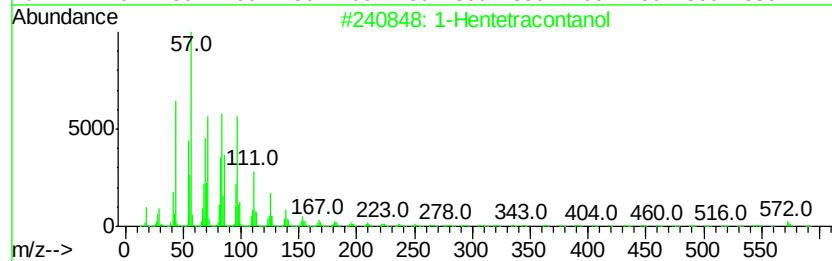
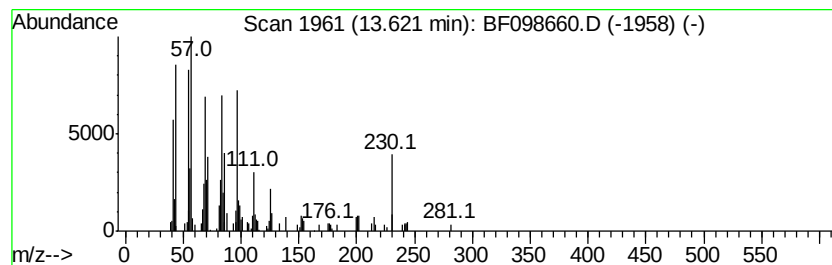
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hentetracontanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	3.91 ng	165464	Chrysene-d12	13.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hentetracontanol	593	C41H84O	040710-42-7	74
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	74
3		17-Pentatriacontene	491	C35H70	006971-40-0	68
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	64
5		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	62



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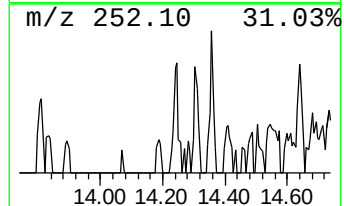
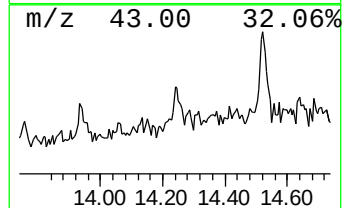
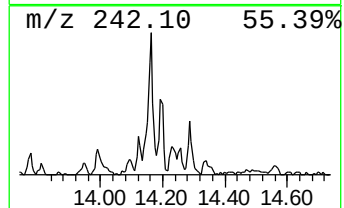
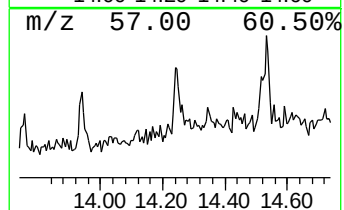
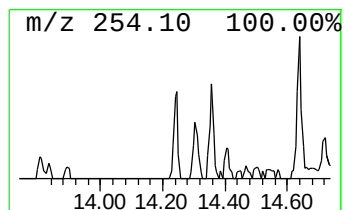
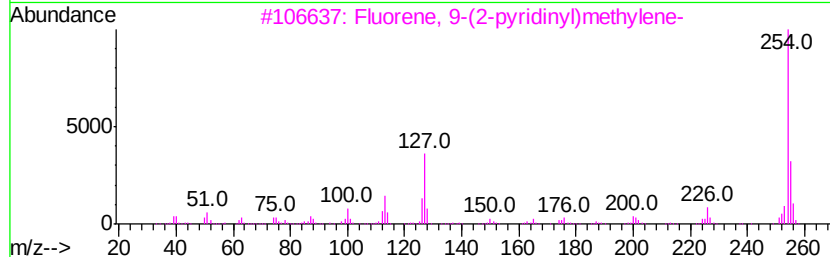
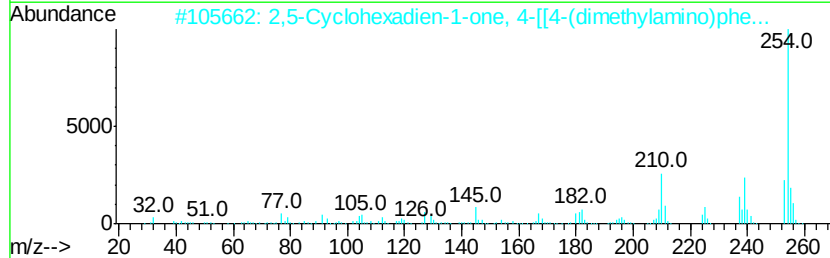
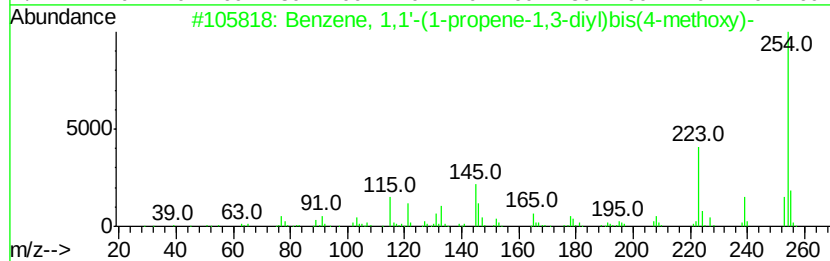
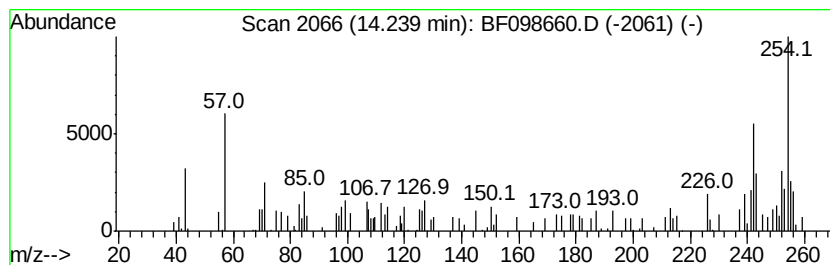
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.24 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.01 ng	85051	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,1'-(1-propene-1,3-div...	254	C17H18O2	1000362-20-9	38
2		2,5-Cyclohexadien-1-one, 4-[[4-(...	254	C16H18N2O	1000319-40-8	38
3		Fluorene, 9-(2-pyridinyl)methylene-	255	C19H13N	002871-27-4	35
4		Benzenamine, 4-(2-benzothiazolyl...	254	C15H14N2S	010205-56-8	30
5		6,6'-Biazulene,	254	C20H14	073393-11-0	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098660.D
Acq On : 20 Sep 2017 15:17
Operator : SJ/JU
Sample : I5285-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSTP-1

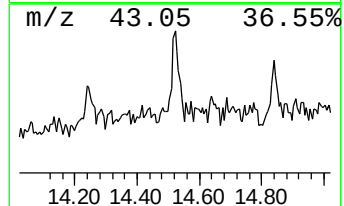
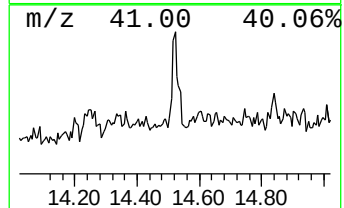
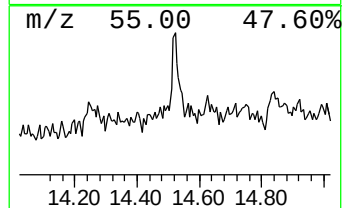
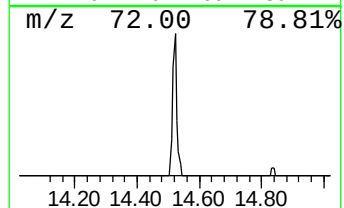
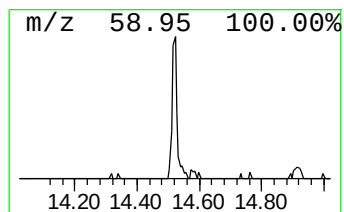
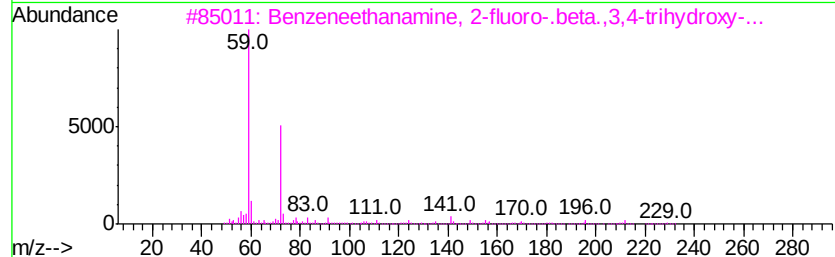
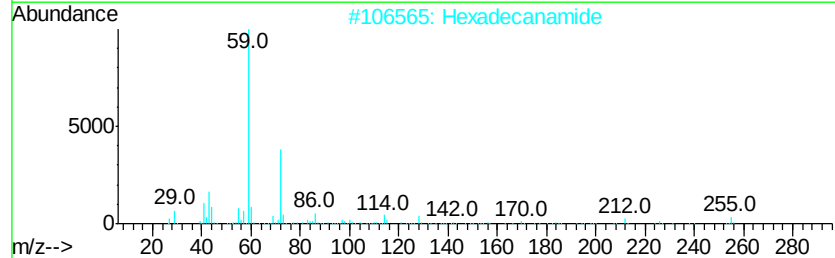
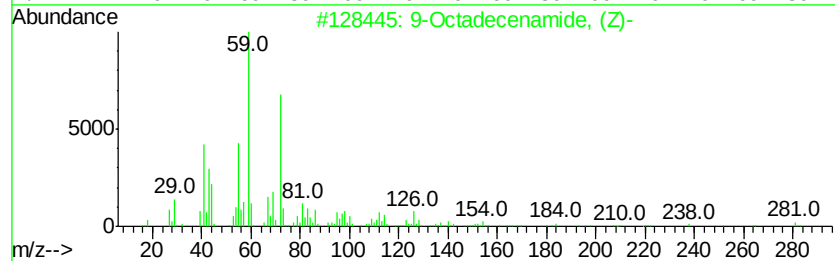
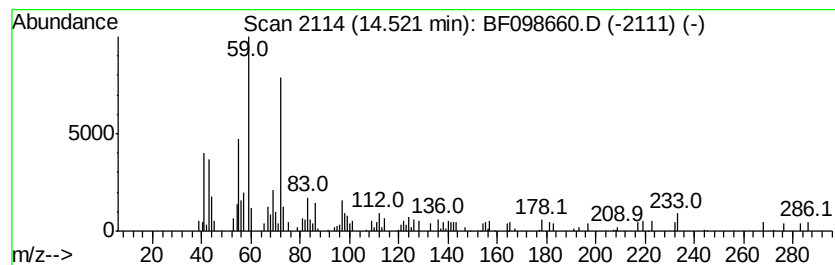
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.67 ng	75212	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Hexadecanamide	255	C16H33NO	000629-54-9	53
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
4		Tetradecanamide	227	C14H29NO	000638-58-4	53
5		Octanamide	143	C8H17NO	000629-01-6	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
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Acq On : 20 Sep 2017 15:17
Operator : SJ/JU
Sample : I5285-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

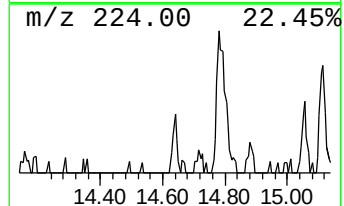
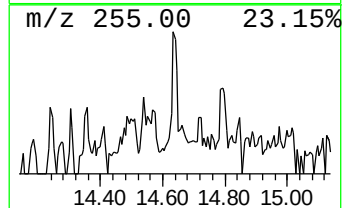
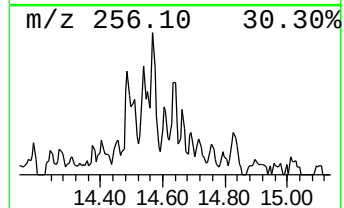
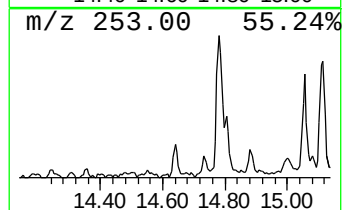
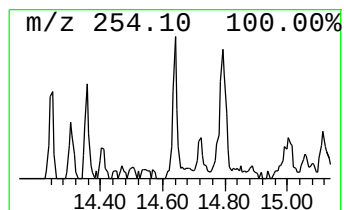
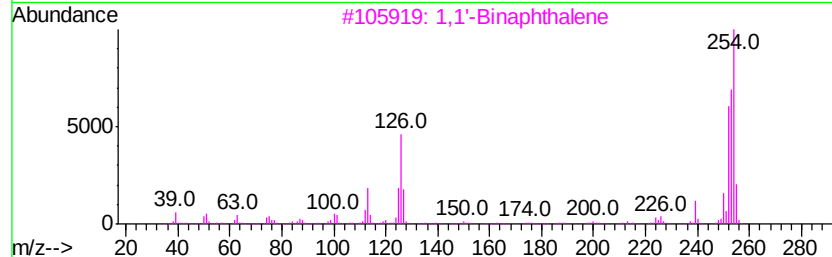
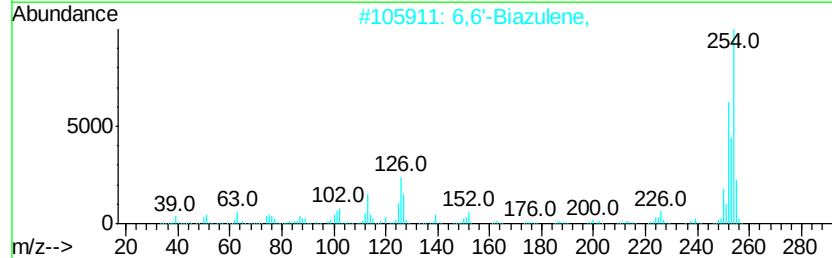
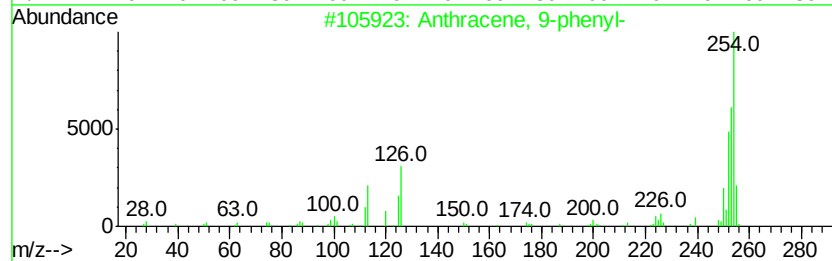
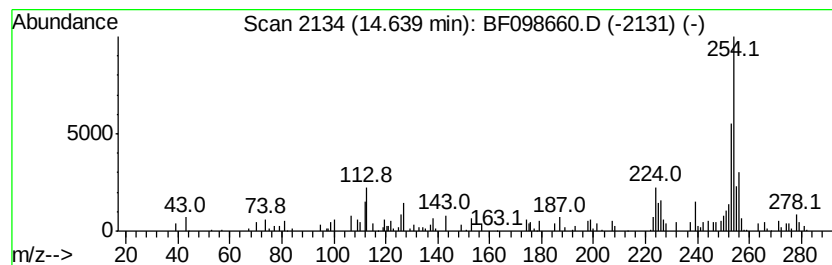
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Anthracene, 9-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.31 ng	64896	Perylene-d12	15.17
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Anthracene, 9-phenyl-	254 C20H14	000602-55-1 76
2		6,6'-Biazulene,	254 C20H14	073393-11-0 58
3		1,1'-Binaphthalene	254 C20H14	000604-53-5 58
4		Benzo(e)pyrene, 9,10-dihydro-	254 C20H14	066788-01-0 53
5		1,2'-Binaphthalene	254 C20H14	004325-74-0 53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092017\
Data File : BF098660.D
Acq On : 20 Sep 2017 15:17
Operator : SJ/JU
Sample : I5285-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSTP-1

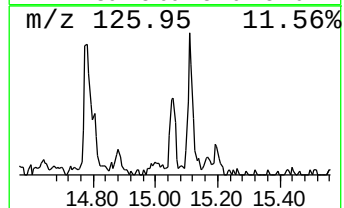
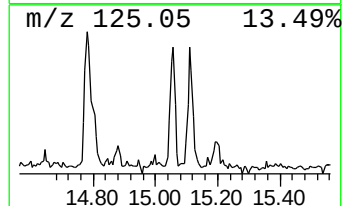
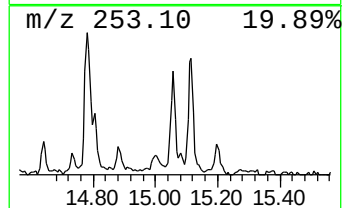
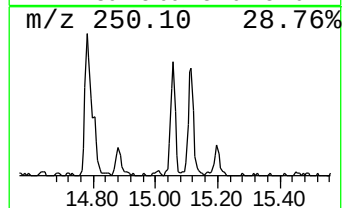
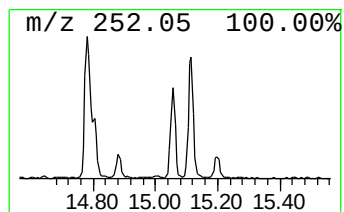
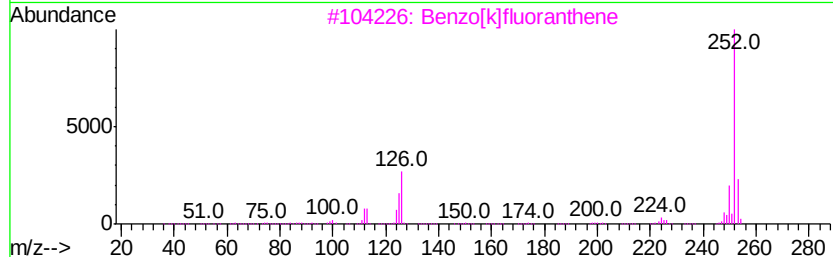
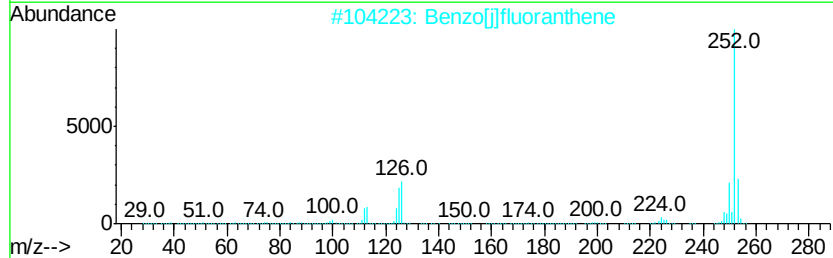
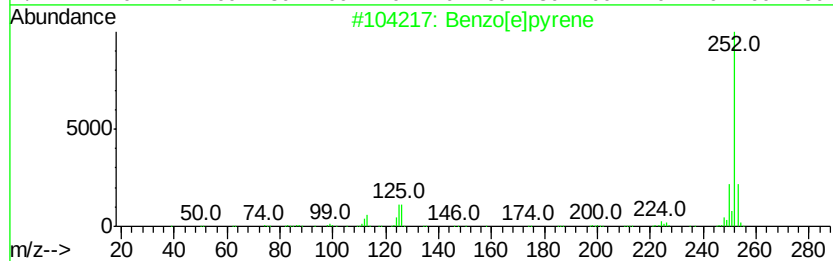
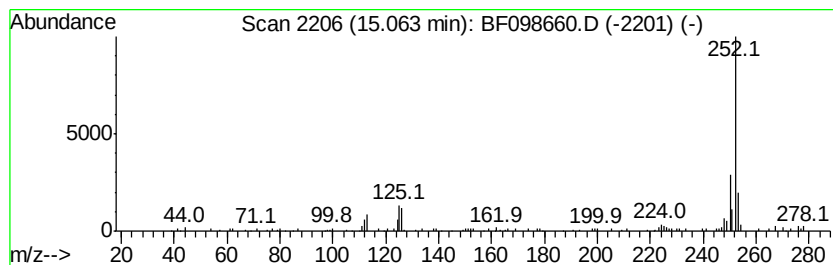
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.74 ng	161456	Perylene-d12	15.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[i]fluoranthene	252	C20H12	000205-82-3	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Perylene	252	C20H12	000198-55-0	93
5			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092017\
Data File : BF098660.D
Acq On : 20 Sep 2017 15:17
Operator : SJ/JU
Sample : I5285-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSTP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.80	4.80	15.4	ng	466739	1	6.62	608063	20.0
unknown6.39	6.39	89.3	ng	2714900	1	6.62	608063	20.0
Pyrene, 1-methyl-	13.01	2.3	ng	98117	5	13.77	846798	20.0
1-Hentetracontanol	13.62	3.9	ng	165464	5	13.77	846798	20.0
unknown14.24	14.24	2.0	ng	85051	5	13.77	846798	20.0
9-Octadecenamide, ...	14.52	2.7	ng	75212	6	15.17	562817	20.0
Anthracene, 9-phe...	14.64	2.3	ng	64896	6	15.17	562817	20.0
Benzo[e]pyrene	15.06	5.7	ng	161456	6	15.17	562817	20.0