

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096576.D
 Acq On : 7 Jul 2017 23:12
 Operator : SJ/MA
 Sample : I4070-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-05-070517-C

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-BF070117.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	4.887	471	476	486	rVB	342127	461431	17.57%	1.894%
2	5.310	543	548	551	rBV	2522097	2619598	99.72%	10.751%
3	6.340	717	723	731	rBV	2407086	2626953	100.00%	10.782%
4	6.469	740	745	748	rBV	2587049	2557710	97.36%	10.497%
5	6.692	780	783	787	rBV	759316	673804	25.65%	2.765%
6	6.851	806	810	814	rBV	2078557	1923379	73.22%	7.894%
7	7.257	873	879	882	rBV	1708413	1603169	61.03%	6.580%
8	7.975	997	1001	1005	rBV	1025048	906578	34.51%	3.721%
9	9.057	1180	1185	1188	rBV	2667712	2425109	92.32%	9.953%
10	9.386	1238	1241	1244	rBV	30104	28516	1.09%	0.117%
11	9.445	1248	1251	1254	rBV	284168	211554	8.05%	0.868%
12	9.586	1272	1275	1278	rBV	48795	40760	1.55%	0.167%
13	9.622	1278	1281	1287	rVV4	16044	30808	1.17%	0.126%
14	9.728	1294	1299	1302	rBV	1036727	867860	33.04%	3.562%
15	10.139	1364	1369	1372	rBV3	29403	44569	1.70%	0.183%
16	10.175	1372	1375	1378	rVB2	62084	50957	1.94%	0.209%
17	10.269	1389	1391	1398	rVB2	36072	39540	1.51%	0.162%
18	10.392	1408	1412	1415	rBV3	24023	34552	1.32%	0.142%
19	10.510	1428	1432	1436	rBV	1321488	1232379	46.91%	5.058%
20	10.645	1451	1455	1462	rVB	76319	89879	3.42%	0.369%
21	11.092	1528	1531	1535	rBV2	40116	42281	1.61%	0.174%
22	11.204	1546	1550	1552	rBV	782580	655490	24.95%	2.690%
23	11.227	1552	1554	1557	rVV	219683	158196	6.02%	0.649%
24	11.280	1559	1563	1566	rVB	35482	32622	1.24%	0.134%
25	11.704	1632	1635	1638	rBV	79397	69183	2.63%	0.284%
26	11.733	1638	1640	1645	rVB2	92760	93581	3.56%	0.384%
27	11.816	1650	1654	1656	rVV	89990	91984	3.50%	0.378%
28	11.839	1656	1658	1663	rVB	62970	49451	1.88%	0.203%
29	12.022	1687	1689	1696	rVB4	28297	32555	1.24%	0.134%
30	12.257	1725	1729	1732	rBV	68452	69417	2.64%	0.285%
31	12.292	1732	1735	1737	rVV2	35643	40634	1.55%	0.167%
32	12.339	1740	1743	1748	rBV4	30693	41929	1.60%	0.172%
33	12.410	1752	1755	1759	rVB	170286	159575	6.07%	0.655%
34	12.463	1759	1764	1765	rBV4	25108	27576	1.05%	0.113%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	12.639	1789	1794	1797	rBV	212864	213786	8.14%	0.877%
36	12.786	1815	1819	1823	rBV	1483708	1464381	55.74%	6.010%
37	12.857	1828	1831	1834	rBV3	36756	41890	1.59%	0.172%
38	12.969	1848	1850	1852	rVB	54493	41991	1.60%	0.172%
39	13.033	1859	1861	1864	rVB	36684	30332	1.15%	0.124%
40	13.069	1864	1867	1871	rBV2	49240	46100	1.75%	0.189%
41	13.163	1880	1883	1886	rVV	48436	43217	1.65%	0.177%
42	13.192	1886	1888	1892	rVB	45853	40563	1.54%	0.166%
43	13.474	1933	1936	1940	rVB3	30299	45415	1.73%	0.186%
44	13.580	1950	1954	1958	rBV3	36482	65889	2.51%	0.270%
45	13.692	1968	1973	1979	rVB2	116845	144335	5.49%	0.592%
46	13.833	1992	1997	1999	rBV	720956	735703	28.01%	3.020%
47	13.857	1999	2001	2003	rVB	100723	79148	3.01%	0.325%
48	14.221	2058	2063	2065	rBV	49270	57271	2.18%	0.235%
49	14.251	2065	2068	2071	rVV	35506	30749	1.17%	0.126%
50	14.751	2150	2153	2156	rVB4	39935	45164	1.72%	0.185%
51	14.833	2164	2167	2171	rBV	74966	124175	4.73%	0.510%
52	14.933	2181	2184	2185	rBV	40242	37882	1.44%	0.155%
53	15.115	2212	2215	2219	rVB	63833	71301	2.71%	0.293%
54	15.168	2221	2224	2228	rBV	74414	86596	3.30%	0.355%
55	15.233	2230	2235	2242	rBV	539260	658781	25.08%	2.704%
56	15.462	2271	2274	2280	rVB8	21558	35761	1.36%	0.147%
57	15.680	2308	2311	2315	rBV2	27989	40120	1.53%	0.165%
58	15.727	2316	2319	2327	rVB7	39685	75278	2.87%	0.309%
59	16.574	2459	2463	2470	rVB3	27159	48232	1.84%	0.198%
60	16.974	2527	2531	2534	rVB2	17241	27383	1.04%	0.112%

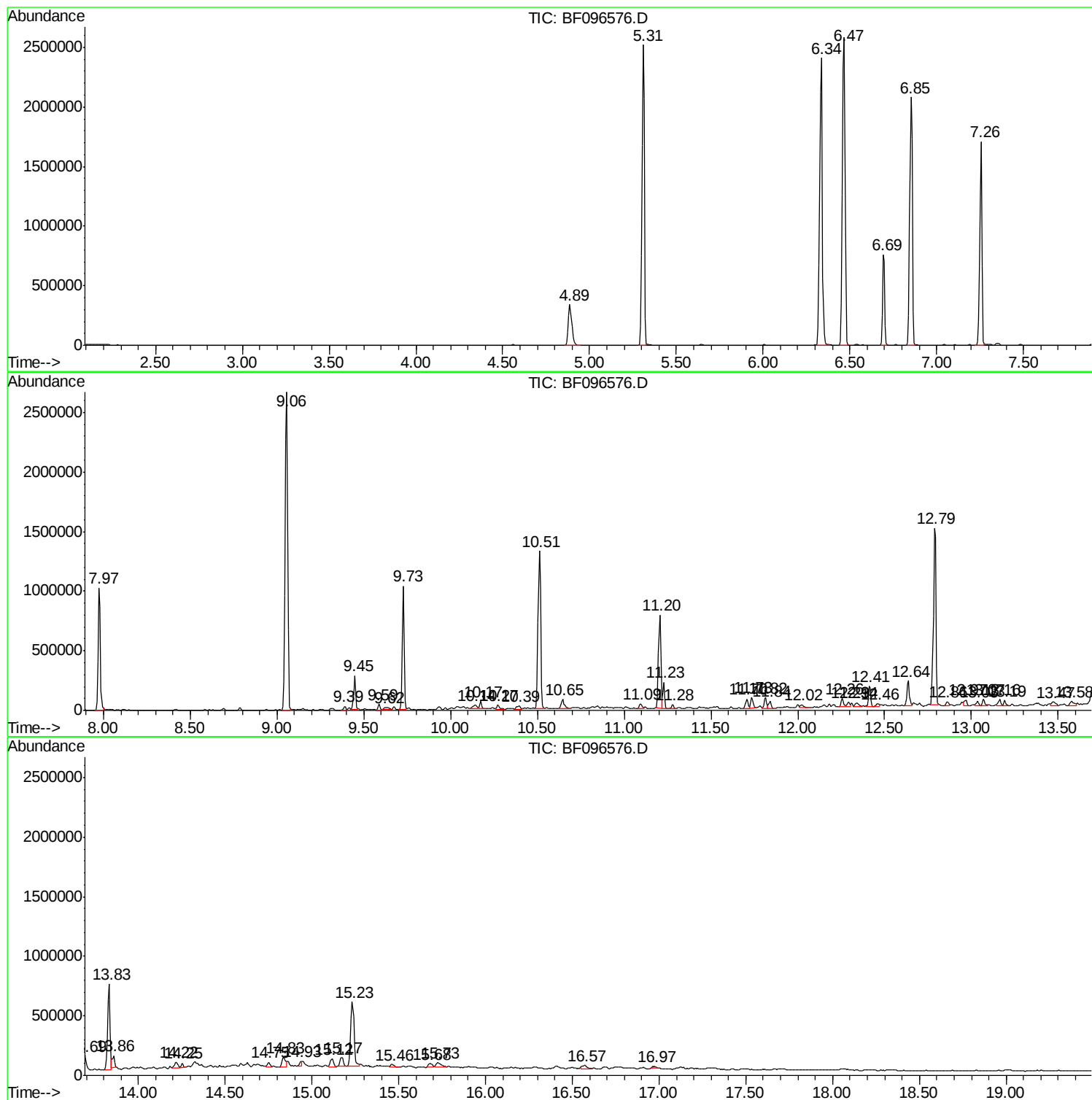
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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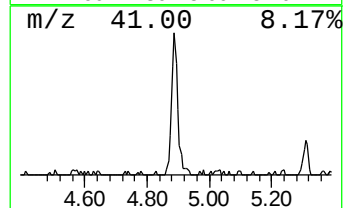
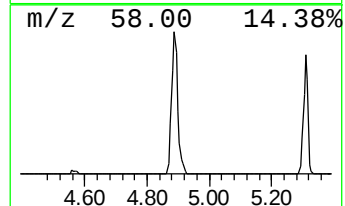
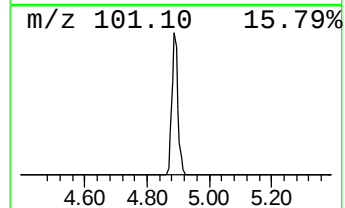
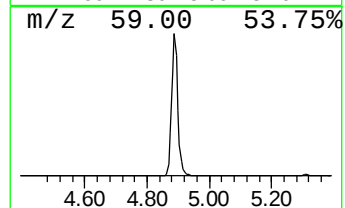
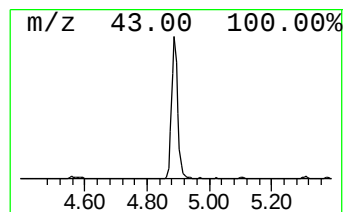
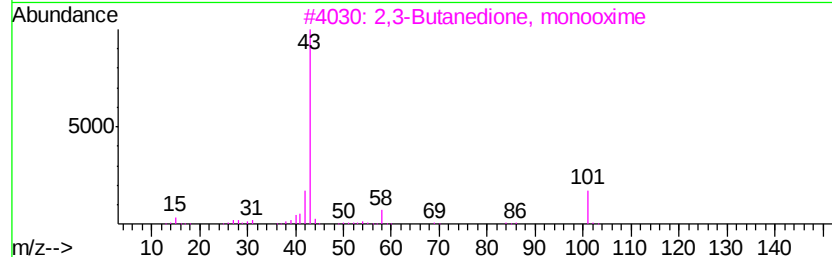
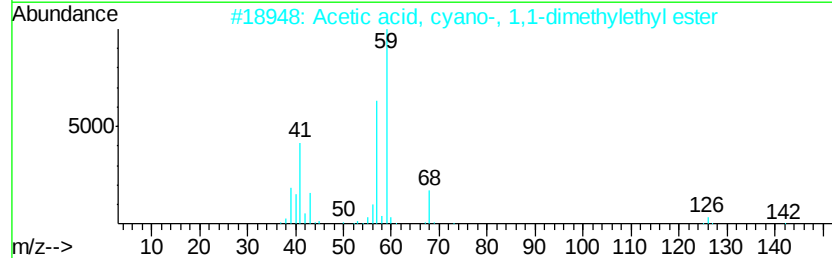
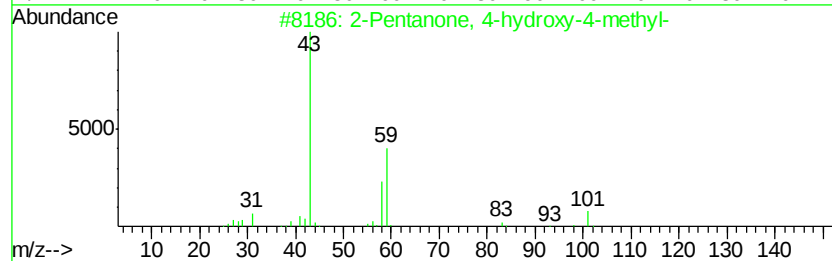
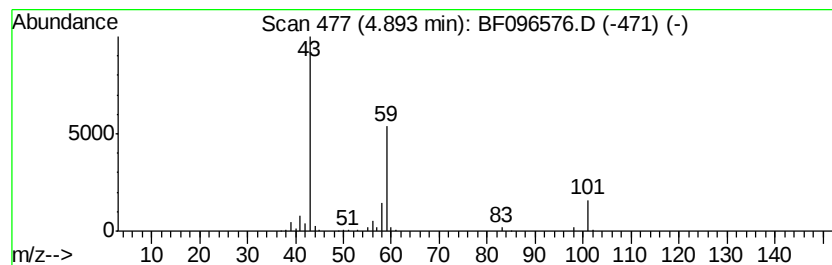
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	13.70 ng	461431	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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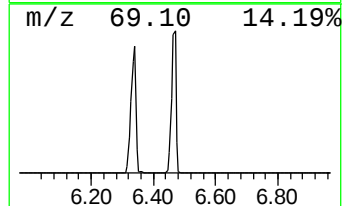
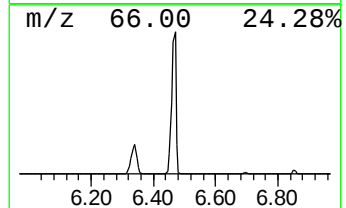
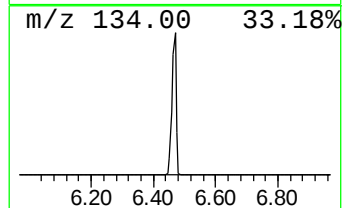
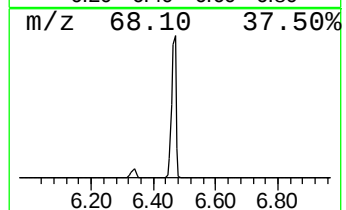
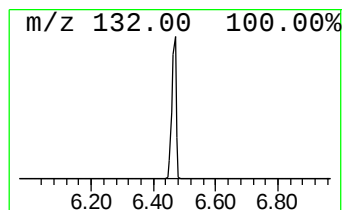
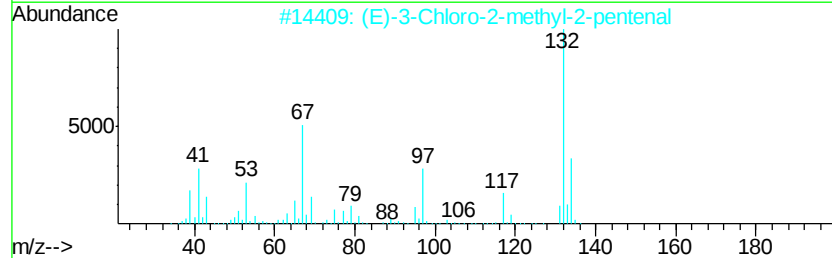
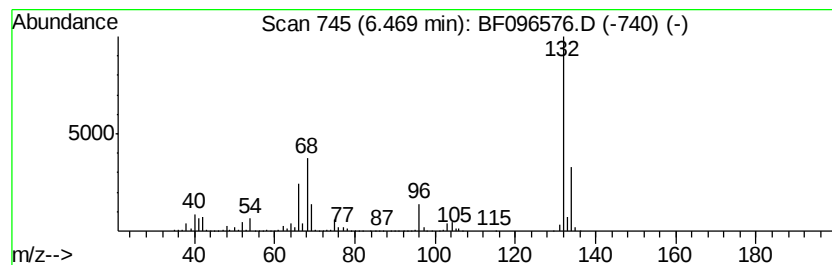
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	75.92 ng	2557710	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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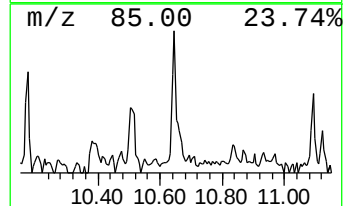
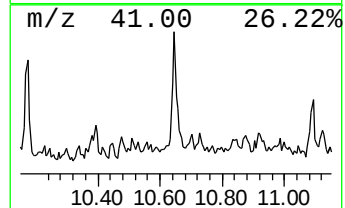
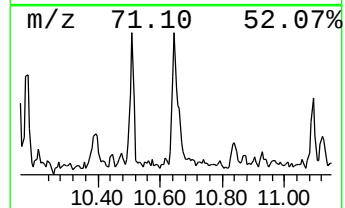
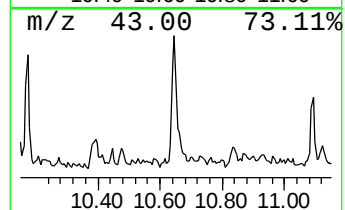
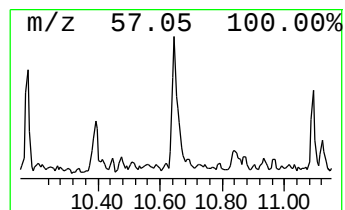
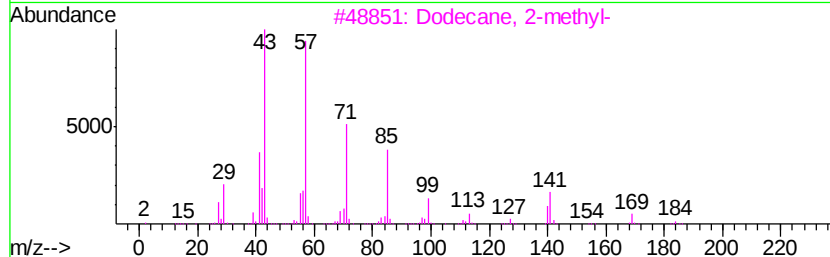
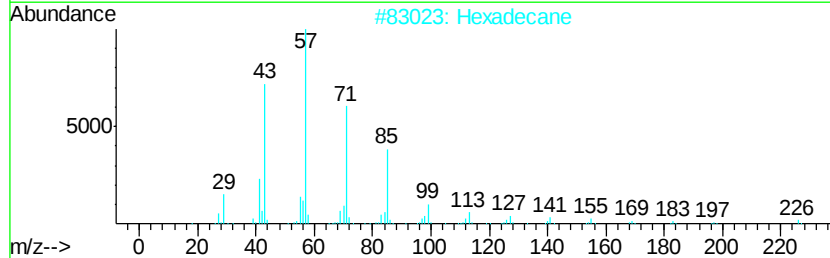
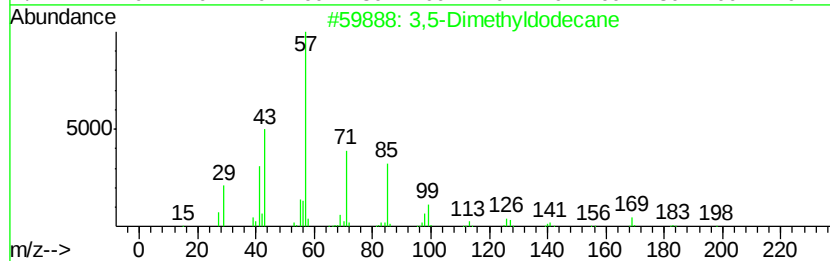
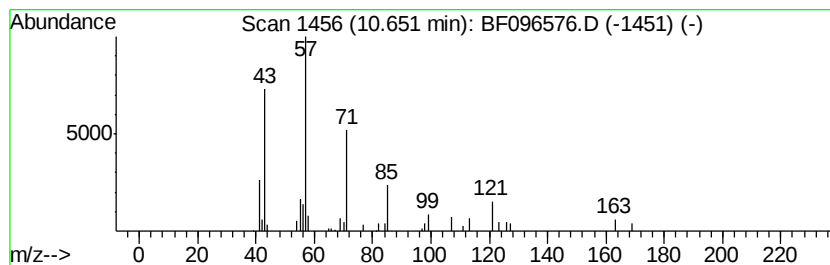
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3,5-Dimethyldodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.65	2.74 ng	89879	Phenanthrene-d10		11.20	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyldodecane		198	C14H30	107770-99-0	90
2	Hexadecane		226	C16H34	000544-76-3	86
3	Dodecane, 2-methyl-		184	C13H28	001560-97-0	83
4	Tridecane		184	C13H28	000629-50-5	80
5	Pentadecane		212	C15H32	000629-62-9	78



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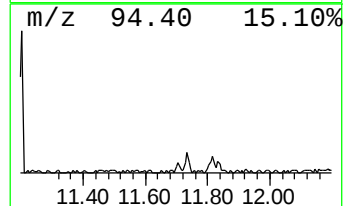
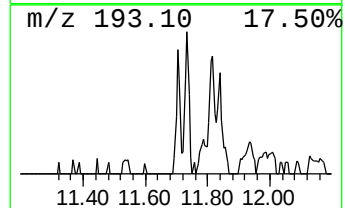
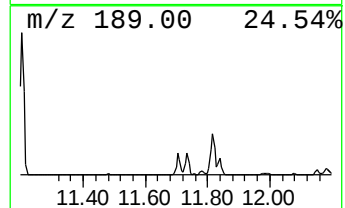
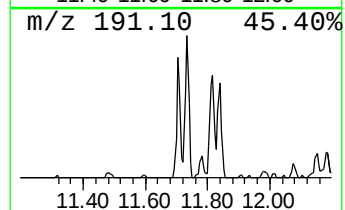
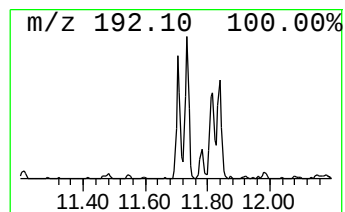
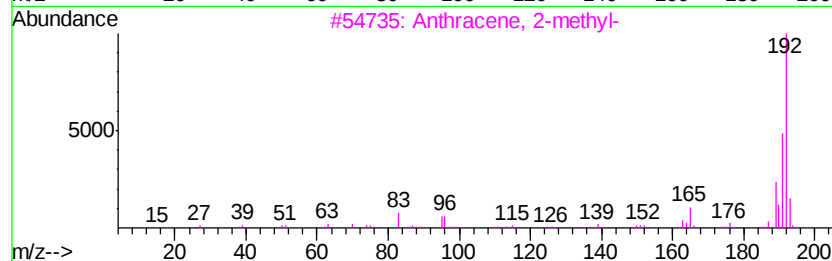
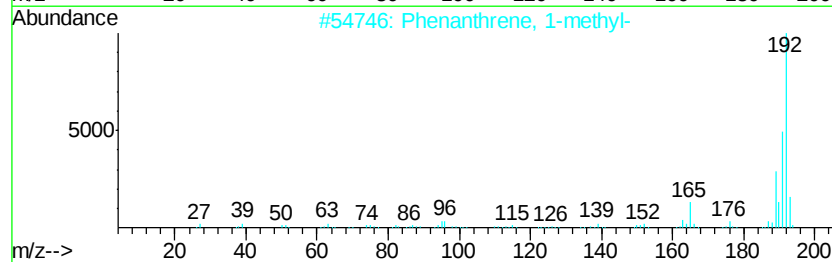
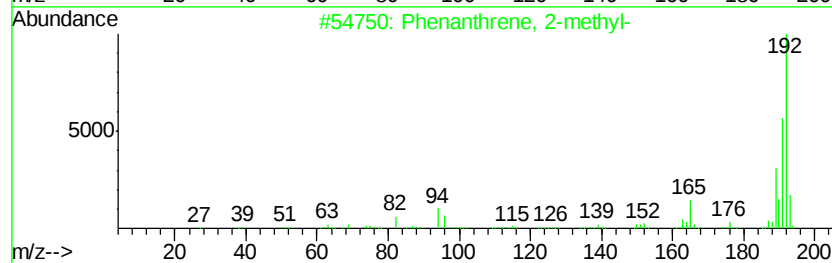
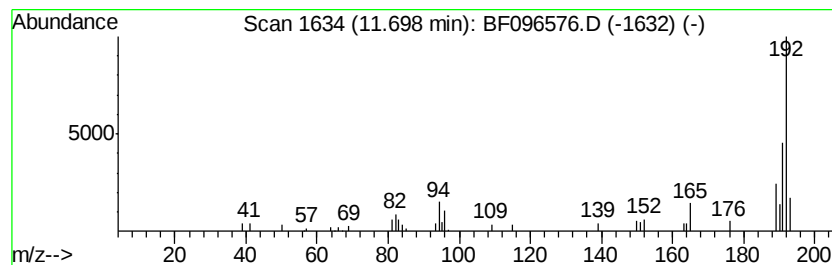
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.70	2.11 ng	69183	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
5	1H-Cyclopropa[1]phenanthrene, 1a, ...	192	C15H12	000949-41-7	94



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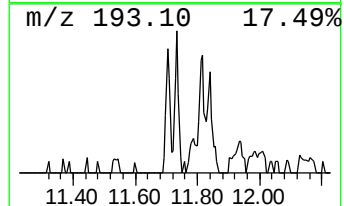
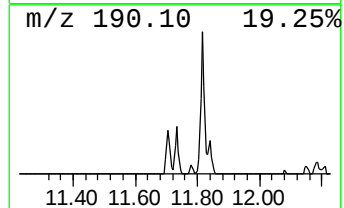
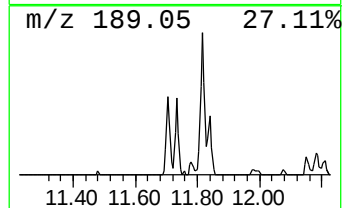
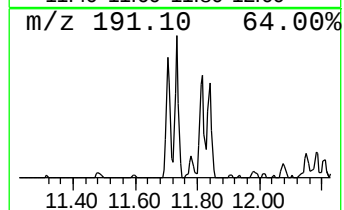
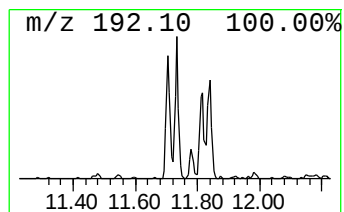
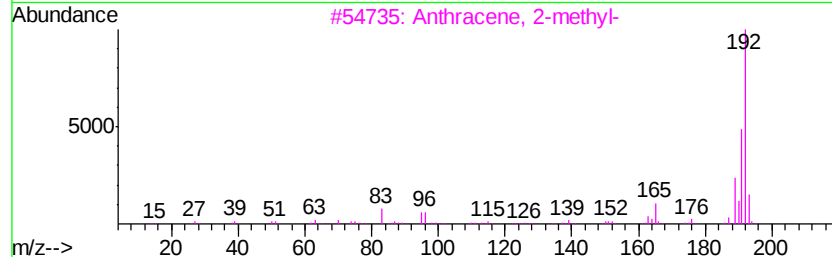
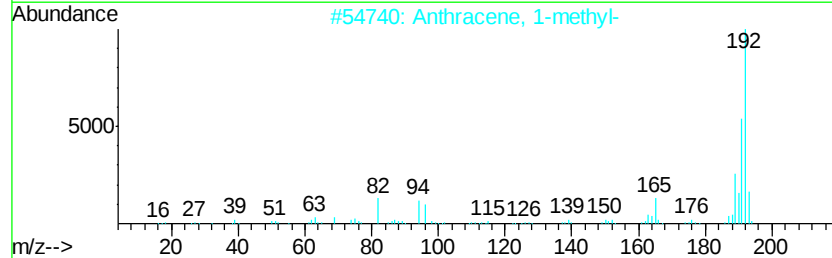
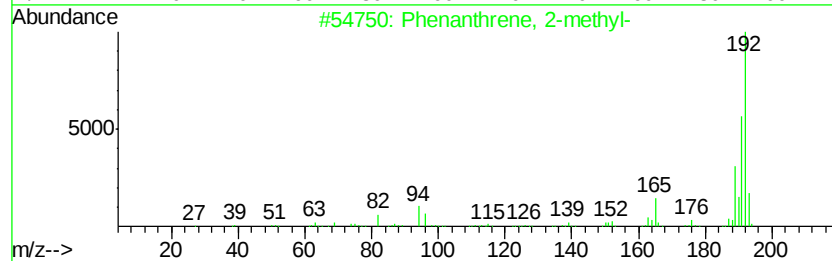
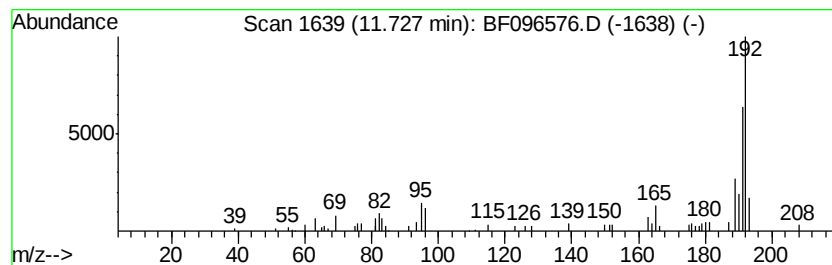
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.86 ng	93581	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096576.D
Acq On : 7 Jul 2017 23:12
Operator : SJ/MA
Sample : I4070-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-070517-C

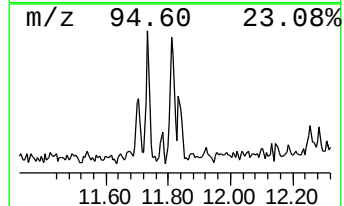
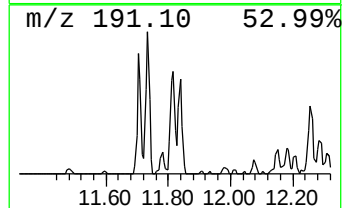
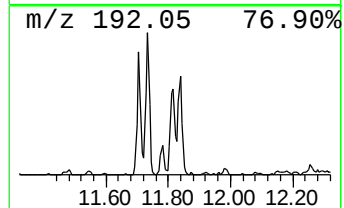
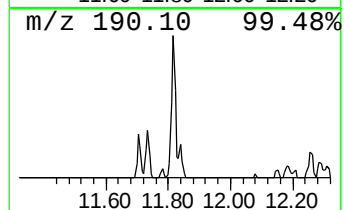
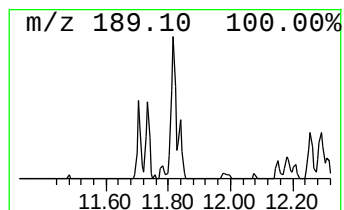
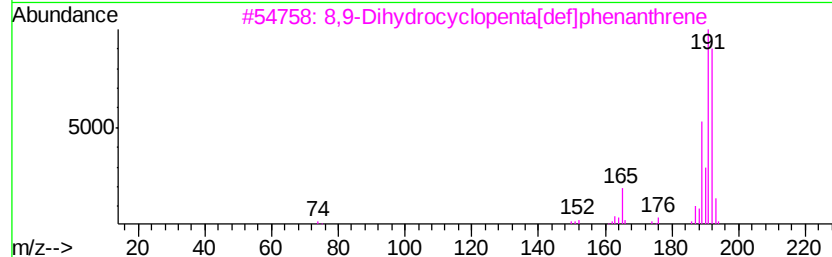
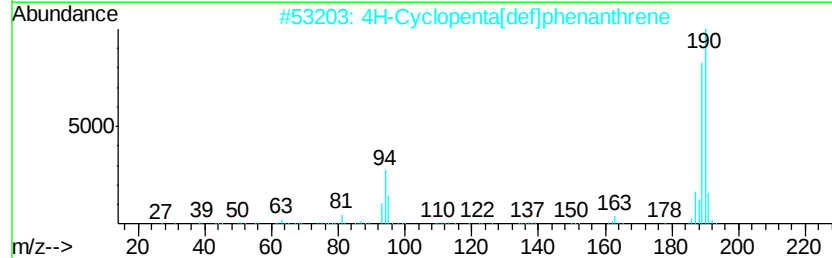
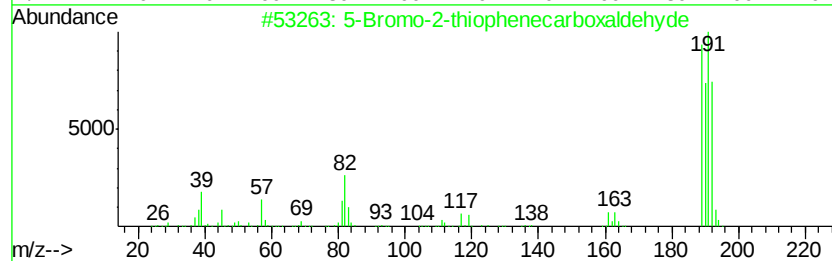
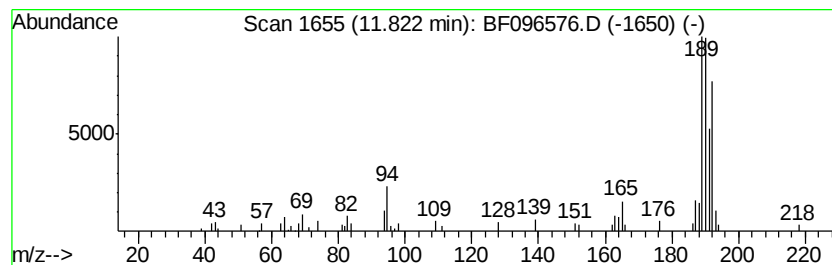
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Bromo-2-thiophenecarboxal... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.81 ng	91984	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	52
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	50
5			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096576.D
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ClientSampleId :
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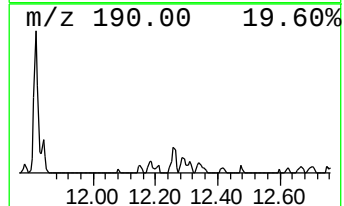
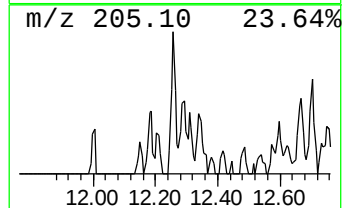
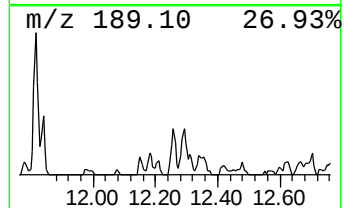
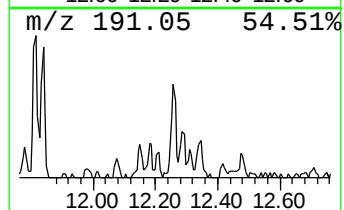
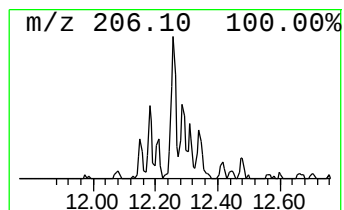
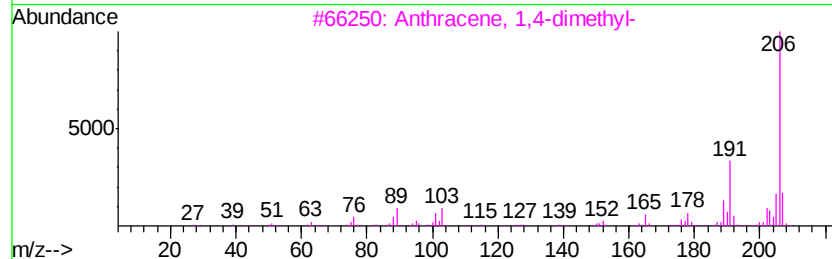
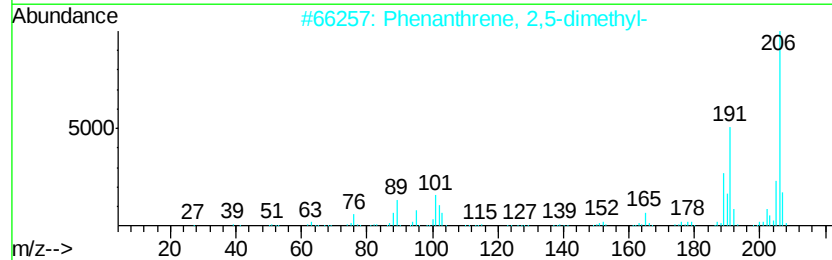
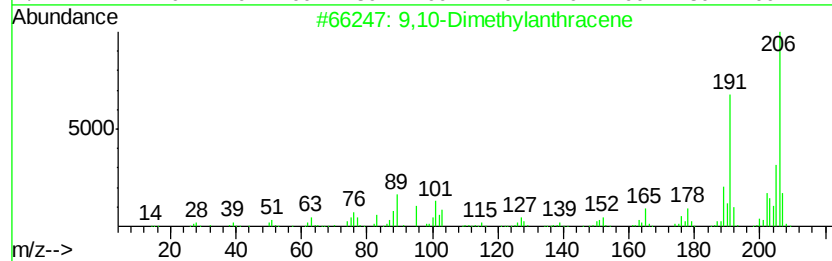
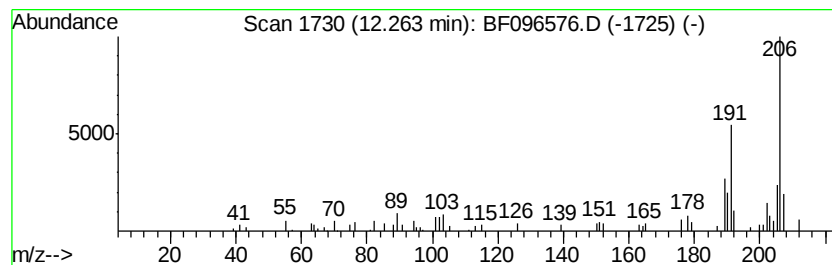
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,10-Dimethylantracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	2.12 ng	69417	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,10-Dimethylantracene	206	C16H14	000781-43-1	94
2		Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
3		Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	91
4		di-p-Tolylacetylene	206	C16H14	002789-88-0	91
5		Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90



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Data File : BF096576.D
Acq On : 7 Jul 2017 23:12
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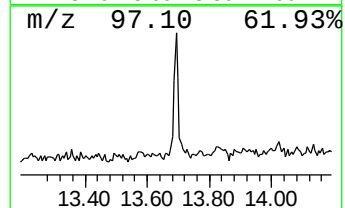
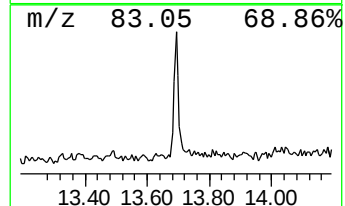
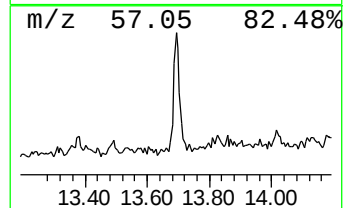
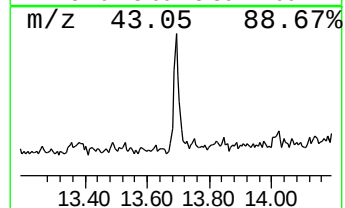
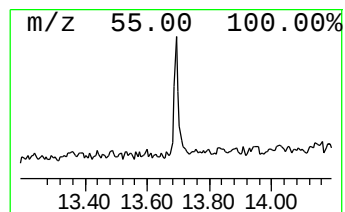
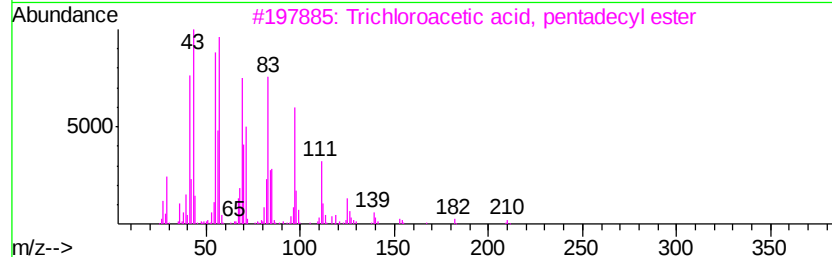
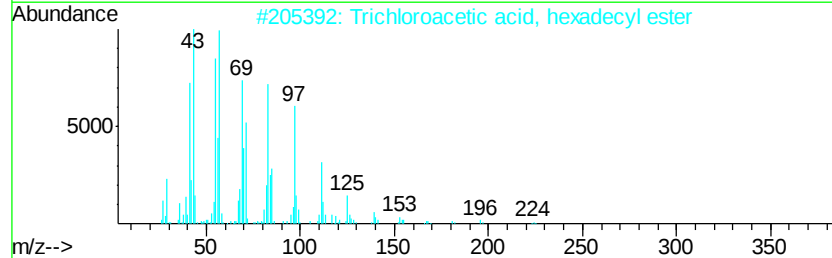
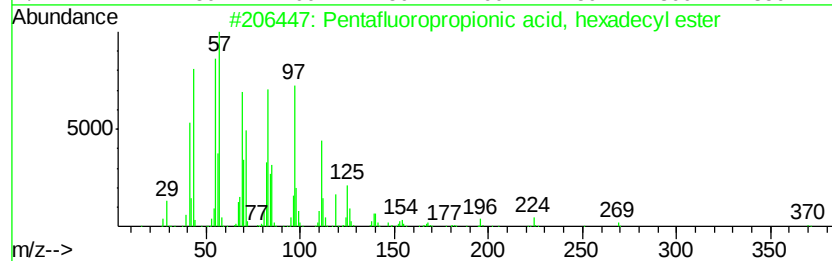
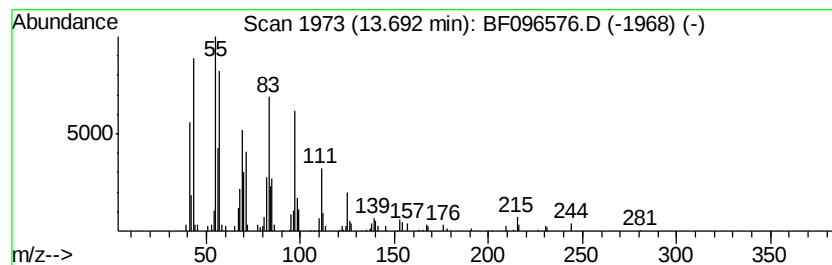
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.92 ng	144335	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hexadecyl...	388	C19H33F5O2	006222-07-7	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1000314-61-3	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
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Misc :
ALS Vial : 14 Sample Multiplier: 1

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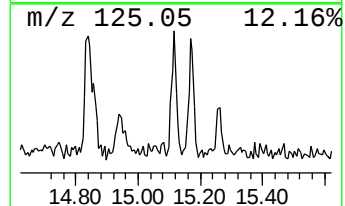
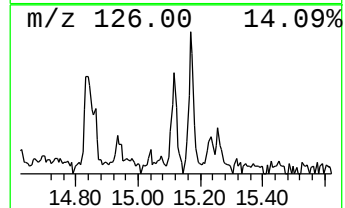
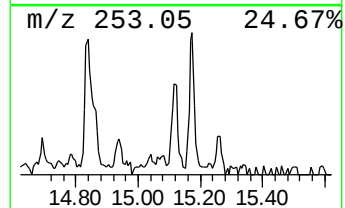
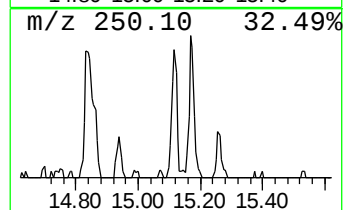
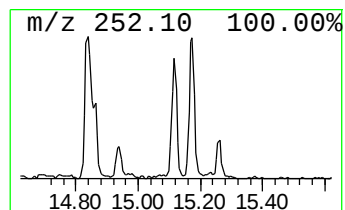
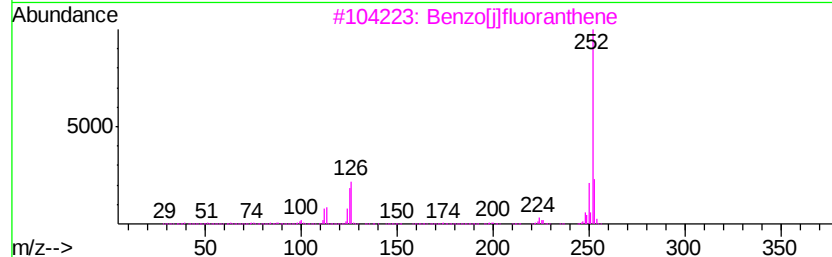
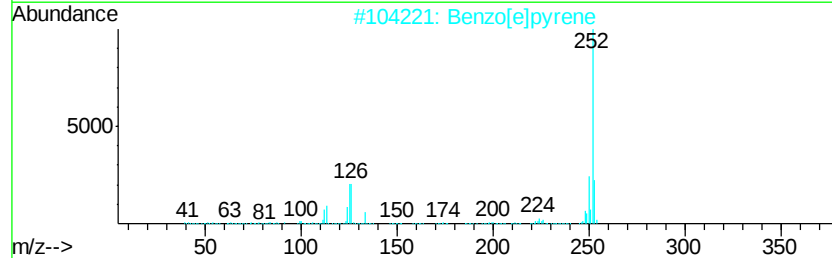
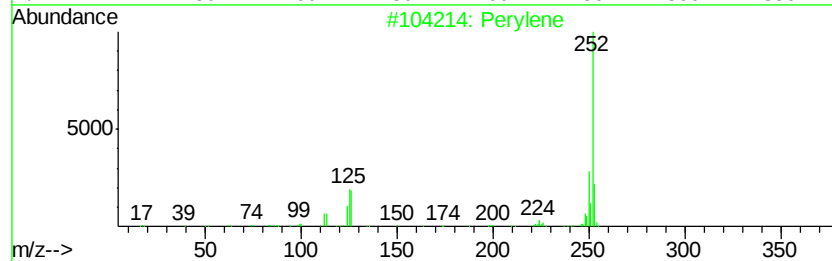
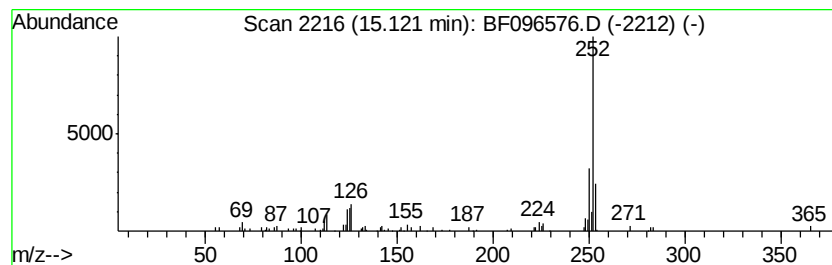
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	2.16 ng	71301	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	93
2	Benzo[e]pyrene		252	C20H12	000192-97-2	91
3	Benzo[j]fluoranthene		252	C20H12	000205-82-3	91
4	Benzo[k]fluoranthene		252	C20H12	000207-08-9	90
5	Benz[e]acephenanthrylene		252	C20H12	000205-99-2	89



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
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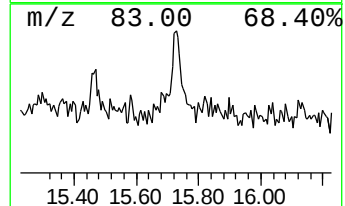
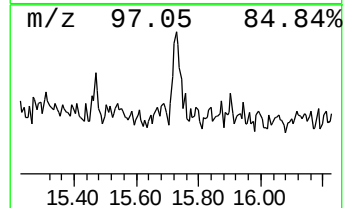
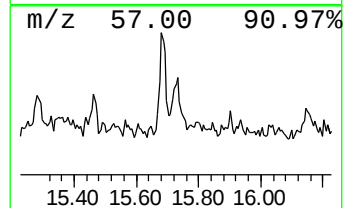
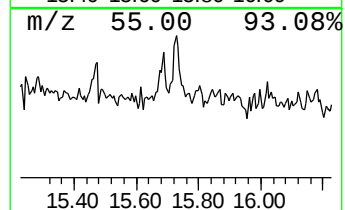
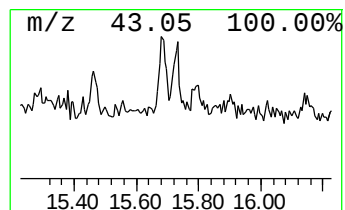
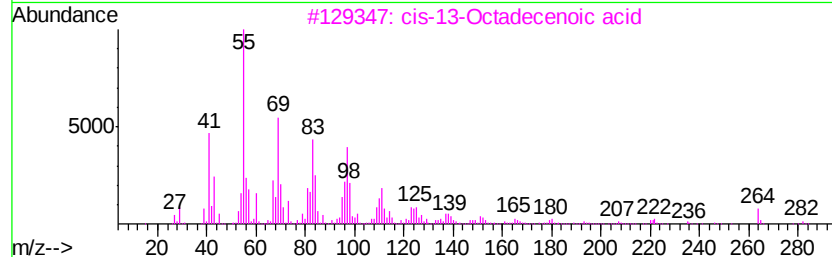
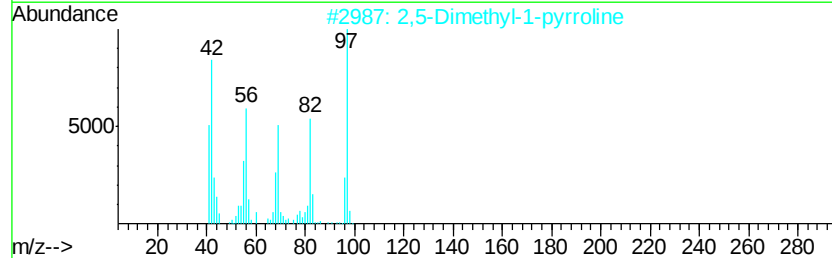
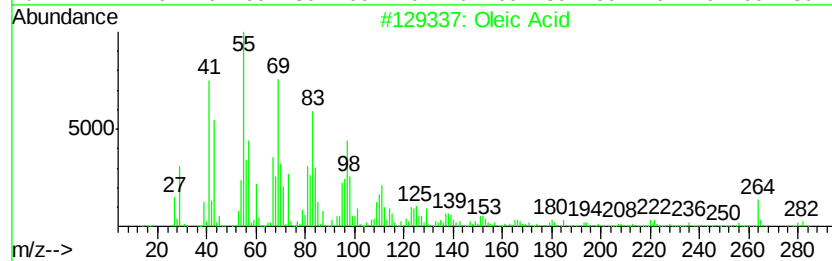
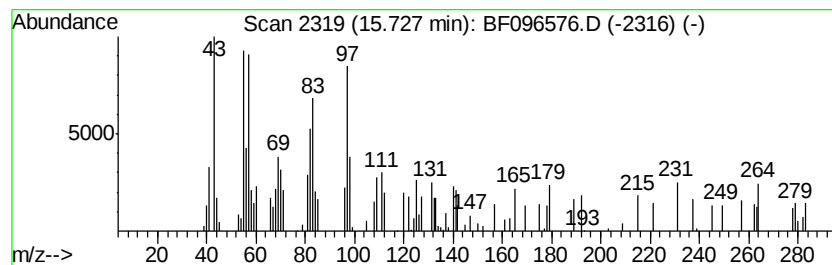
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.73 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.29 ng	75278	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oleic Acid	282	C18H34O2	000112-80-1	43
2		2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	38
3		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	38
4		Heptacosyl acetate	438	C29H58O2	1000351-78-2	30
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	30



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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
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unknown6.47	6.47	75.9	ng	2557710	1	6.69	673804	20.0
3,5-Dimethyldodecane	10.65	2.7	ng	89879	4	11.20	655490	20.0
Phenanthrene, 2-m...	11.70	2.1	ng	69183	4	11.20	655490	20.0
Anthracene, 1-met...	11.73	2.9	ng	93581	4	11.20	655490	20.0
5-Bromo-2-thiophe...	11.82	2.8	ng	91984	4	11.20	655490	20.0
9,10-Dimethylanth...	12.26	2.1	ng	69417	4	11.20	655490	20.0
Pentafluoropropio...	13.69	3.9	ng	144335	5	13.83	735703	20.0
Perylene	15.12	2.2	ng	71301	6	15.23	658781	20.0
unknown15.73	15.73	2.3	ng	75278	6	15.23	658781	20.0