

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
 Data File : BF097326.D
 Acq On : 3 Aug 2017 19:39
 Operator : SJ/JU
 Sample : I4541-13
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11944

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-BF072517.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	3.863	330	336	343	rBV3	11411	28613	1.00%	0.092%
2	4.575	452	457	478	rVB	675660	1131653	39.73%	3.645%
3	5.045	533	537	555	rBV	2320647	2656374	93.26%	8.557%
4	6.116	715	719	732	rBV	2541460	2848458	100.00%	9.175%
5	6.216	732	736	743	rVB	2434927	2579324	90.55%	8.309%
6	6.445	771	775	785	rVB	740832	701446	24.63%	2.260%
7	6.598	797	801	812	rBV	1970988	1810510	63.56%	5.832%
8	7.016	868	872	887	rBV	1793765	1742225	61.16%	5.612%
9	7.728	989	993	1001	rBV	982637	948115	33.29%	3.054%
10	8.798	1171	1175	1179	rBV	2443791	2449337	85.99%	7.890%
11	8.898	1185	1192	1195	rBV2	37112	39443	1.38%	0.127%
12	9.198	1240	1243	1248	rBV	371822	303868	10.67%	0.979%
13	9.422	1276	1281	1284	rBV	43203	44021	1.55%	0.142%
14	9.463	1284	1288	1292	rVV	1082265	957046	33.60%	3.083%
15	9.498	1292	1294	1298	rVB	47957	41188	1.45%	0.133%
16	9.922	1363	1366	1369	rVB	60062	51400	1.80%	0.166%
17	10.010	1378	1381	1384	rVB	33909	29140	1.02%	0.094%
18	10.139	1398	1403	1406	rBV3	24296	32211	1.13%	0.104%
19	10.251	1418	1422	1428	rBV	1424596	1388255	48.74%	4.472%
20	10.386	1442	1445	1455	rVB	84234	101243	3.55%	0.326%
21	10.704	1498	1499	1505	rVB5	26256	30937	1.09%	0.100%
22	10.833	1517	1521	1524	rVV	70694	61863	2.17%	0.199%
23	10.939	1535	1539	1541	rBV	903629	926720	32.53%	2.985%
24	10.957	1541	1542	1546	rVV	437184	351224	12.33%	1.131%
25	11.016	1546	1552	1556	rVB	118050	131010	4.60%	0.422%
26	11.180	1575	1580	1587	rBV2	50051	83522	2.93%	0.269%
27	11.257	1591	1593	1597	rVV2	31280	33855	1.19%	0.109%
28	11.439	1621	1624	1626	rBV	76659	66071	2.32%	0.213%
29	11.463	1626	1628	1631	rVV	96265	90577	3.18%	0.292%
30	11.498	1631	1634	1639	rVV2	177454	228718	8.03%	0.737%
31	11.545	1639	1642	1645	rVV	142573	161136	5.66%	0.519%
32	11.569	1645	1646	1652	rVB	64096	47847	1.68%	0.154%
33	11.733	1671	1674	1676	rBV	54958	48404	1.70%	0.156%
34	11.769	1677	1680	1684	rVB	43658	48579	1.71%	0.156%

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35	11.986	1714	1717	1719	rBV	64126	58992	2.07%	0.190%
36	12.021	1719	1723	1725	rVV3	38208	54642	1.92%	0.176%
37	12.074	1729	1732	1735	rVB3	58767	61212	2.15%	0.197%
38	12.139	1739	1743	1747	rBV	942704	830633	29.16%	2.676%
39	12.274	1763	1766	1773	rBV3	76693	134092	4.71%	0.432%
40	12.363	1776	1781	1784	rBV	822847	832211	29.22%	2.681%
41	12.421	1788	1791	1793	rBV	35489	34428	1.21%	0.111%
42	12.492	1800	1803	1804	rBV	36785	38312	1.35%	0.123%
43	12.521	1804	1808	1811	rVV	1617539	1662695	58.37%	5.356%
44	12.586	1817	1819	1823	rVB	36444	43956	1.54%	0.142%
45	12.698	1831	1838	1841	rVB2	129597	182170	6.40%	0.587%
46	12.763	1846	1849	1852	rVV2	89448	94008	3.30%	0.303%
47	12.798	1852	1855	1862	rVB2	97659	127238	4.47%	0.410%
48	12.886	1868	1870	1873	rBV	41150	37754	1.33%	0.122%
49	12.921	1873	1876	1878	rVV	44208	38098	1.34%	0.123%
50	13.210	1922	1925	1931	rVB	57556	61039	2.14%	0.197%
51	13.310	1939	1942	1944	rBV2	82804	86193	3.03%	0.278%
52	13.333	1944	1946	1948	rVB	57396	40788	1.43%	0.131%
53	13.357	1948	1950	1952	rBV	45689	36594	1.28%	0.118%
54	13.415	1957	1960	1962	rBV	61191	61090	2.14%	0.197%
55	13.439	1962	1964	1969	rVB2	109587	110088	3.86%	0.355%
56	13.557	1979	1984	1987	rBV2	790203	1092130	38.34%	3.518%
57	13.580	1987	1988	1992	rVB	360535	286638	10.06%	0.923%
58	13.663	1999	2002	2004	rVB	76997	66585	2.34%	0.214%
59	13.945	2048	2050	2053	rVB	62631	55215	1.94%	0.178%
60	14.410	2126	2129	2133	rBV2	130197	142544	5.00%	0.459%
61	14.551	2149	2153	2160	rBV	432653	665762	23.37%	2.145%
62	14.639	2165	2168	2171	rBV2	75839	81787	2.87%	0.263%
63	14.798	2192	2195	2200	rVB	233669	260904	9.16%	0.840%
64	14.851	2200	2204	2208	rBV	326466	363859	12.77%	1.172%
65	14.898	2208	2212	2215	rBV	490140	521316	18.30%	1.679%
66	16.098	2412	2416	2421	rVB	134821	235171	8.26%	0.758%
67	16.156	2423	2426	2434	rVB6	57524	80481	2.83%	0.259%
68	16.280	2445	2447	2452	rBV4	40889	52076	1.83%	0.168%
69	16.456	2472	2477	2484	rVB2	113009	218988	7.69%	0.705%
70	17.292	2616	2619	2624	rBV7	22082	40948	1.44%	0.132%
71	17.609	2670	2673	2674	rBV3	25884	29925	1.05%	0.096%

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72	18.050	2747	2748	2751	rBV3	25089	29404	1.03%	0.095%
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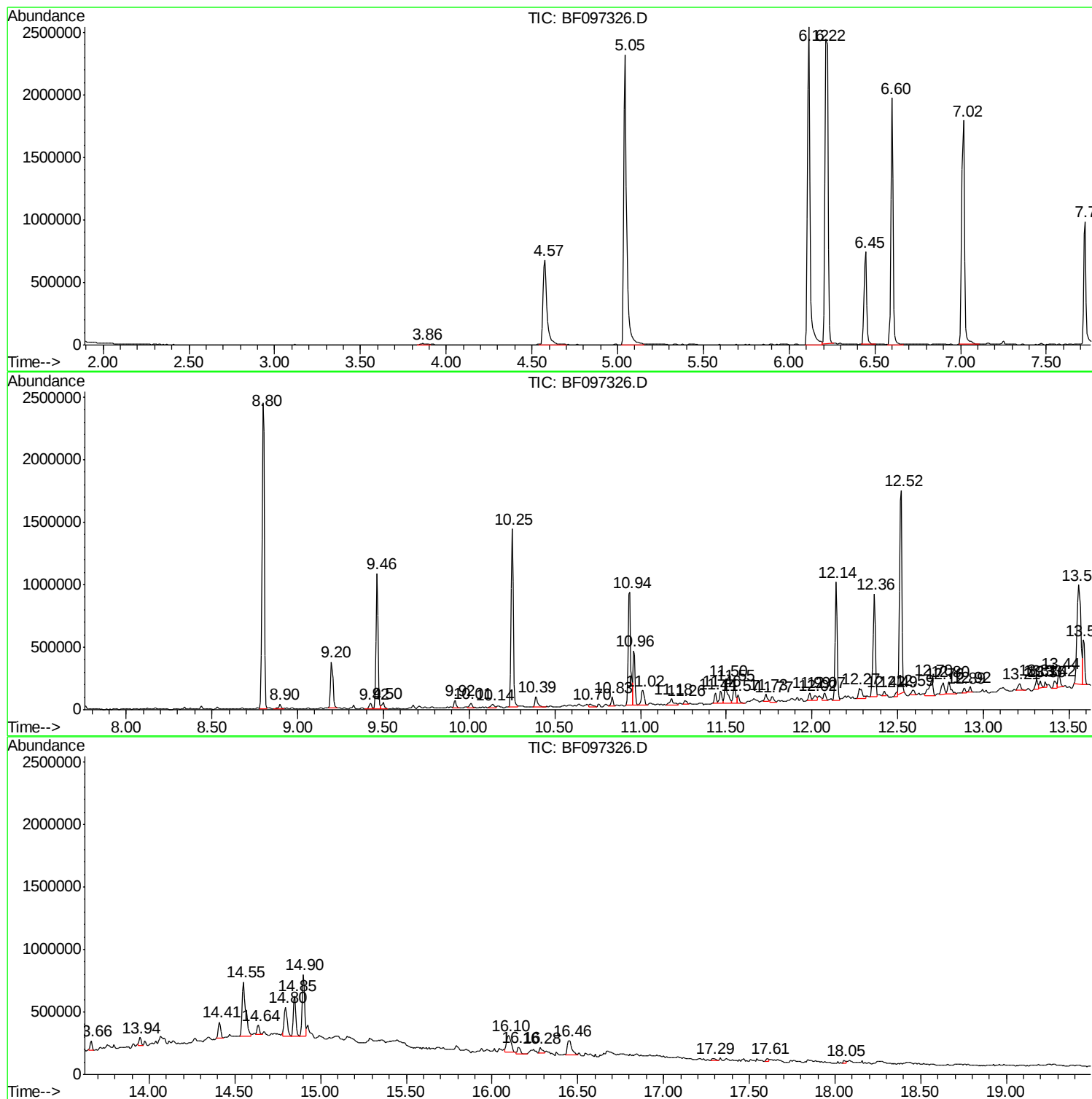
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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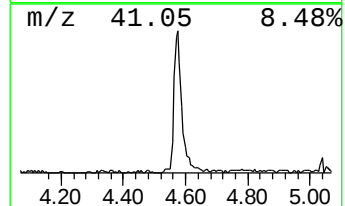
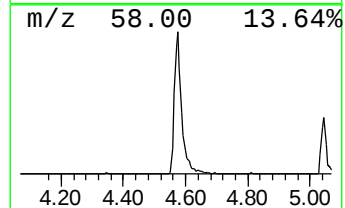
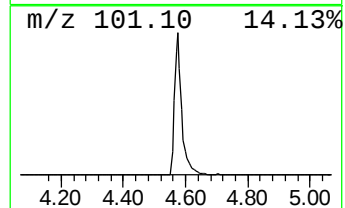
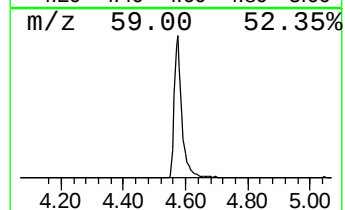
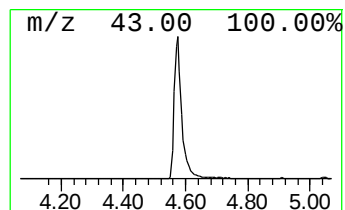
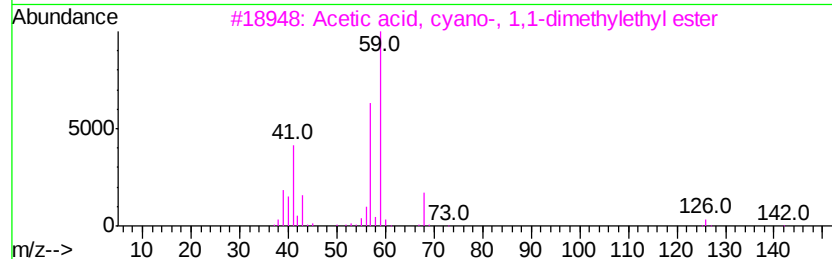
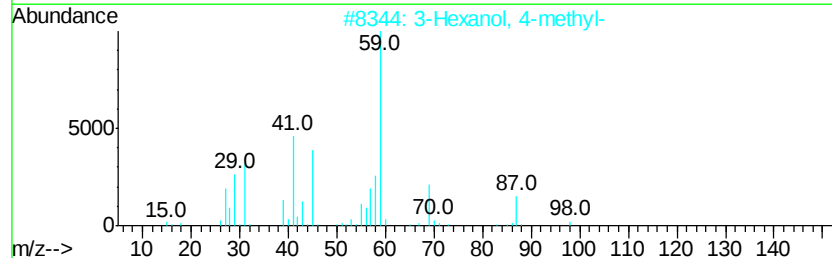
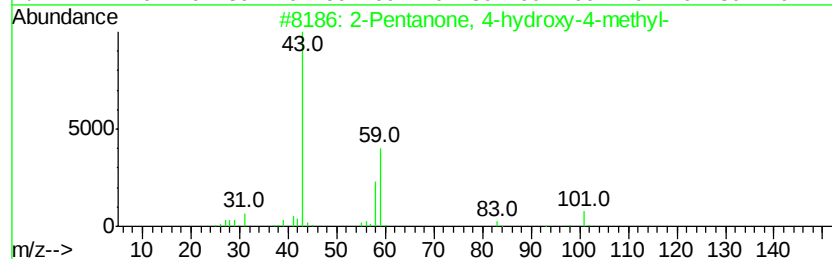
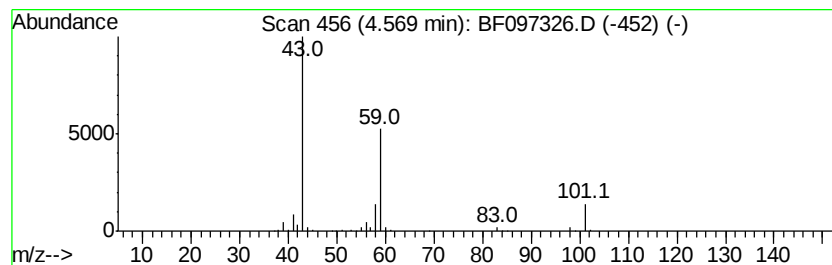
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	32.27 ng	1131650	1,4-Dichlorobenzene-d4	6.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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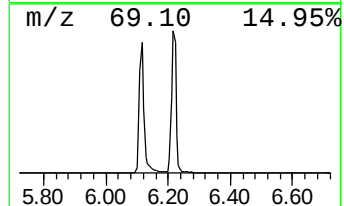
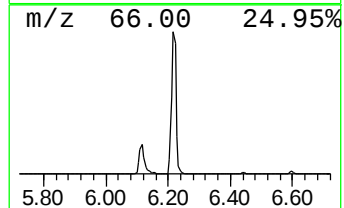
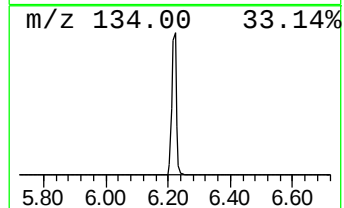
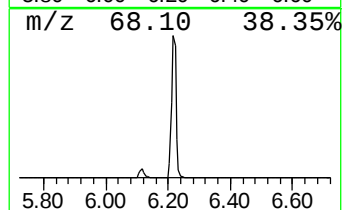
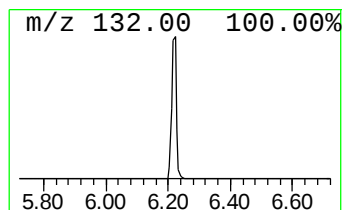
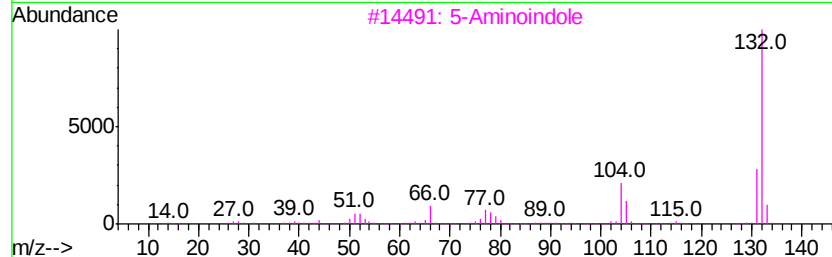
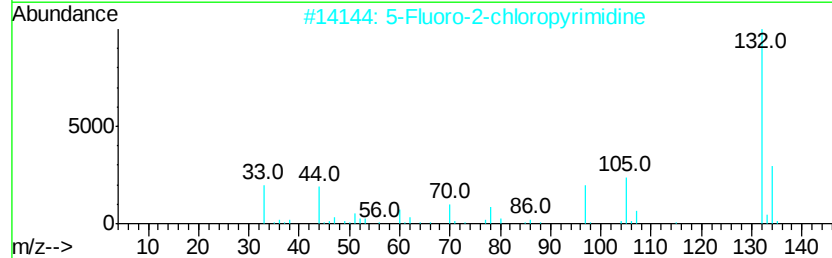
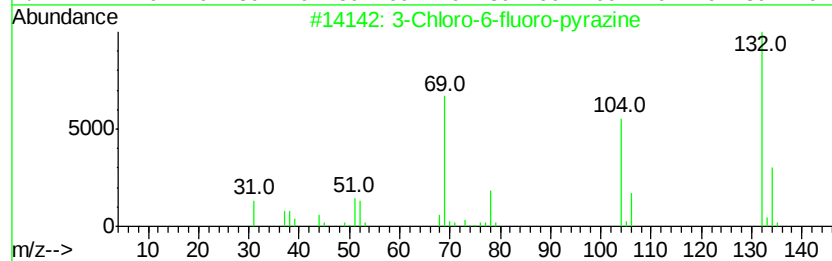
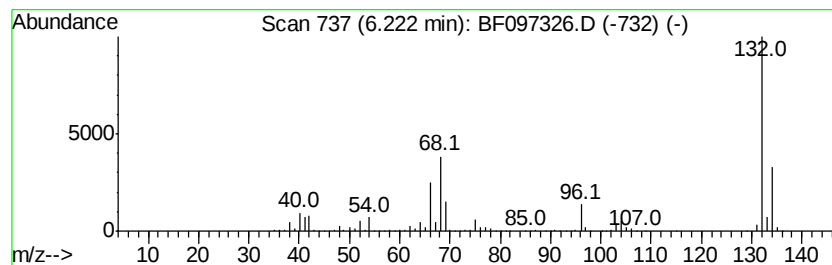
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	73.54 ng	2579320	1,4-Dichlorobenzene-d4	6.45

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-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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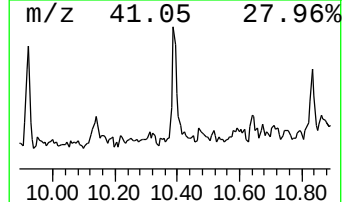
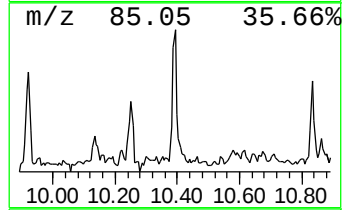
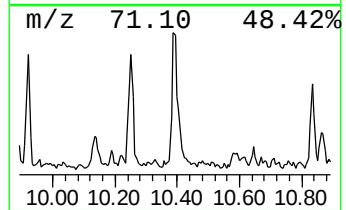
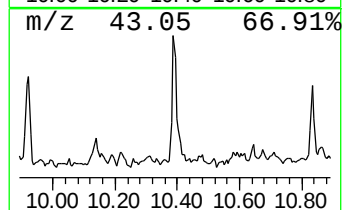
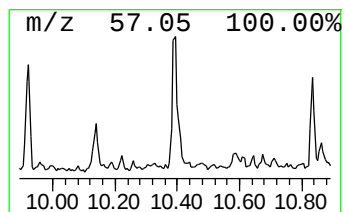
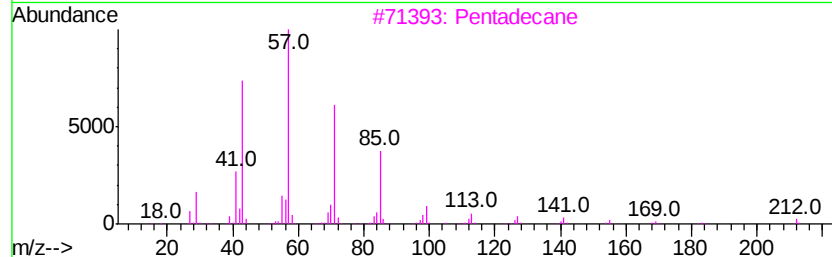
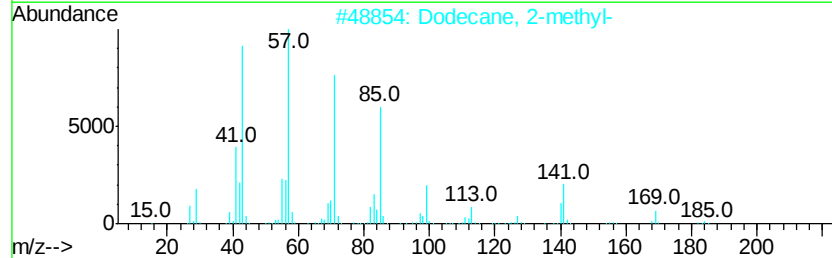
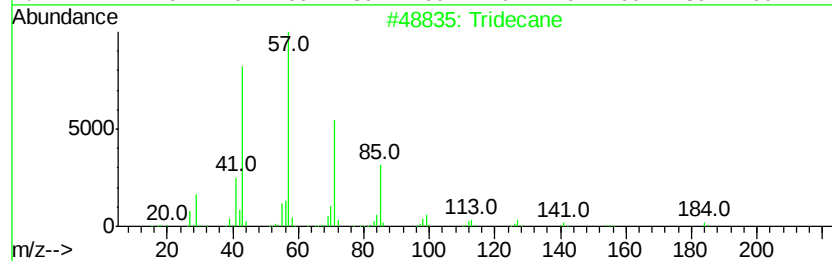
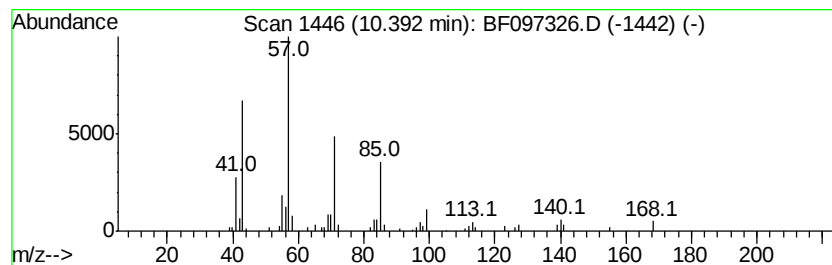
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.39	2.18 ng	101243	Phenanthrene-d10		10.94	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	94
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
3		Pentadecane	212	C15H32	000629-62-9	64
4		Hexadecane	226	C16H34	000544-76-3	64
5		Heptacosane	380	C27H56	000593-49-7	64



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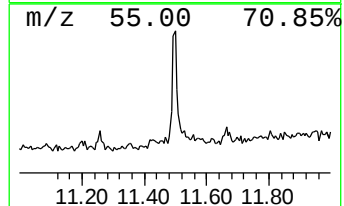
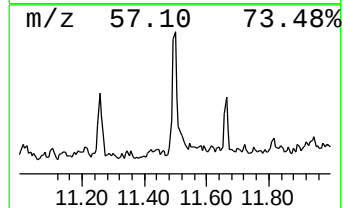
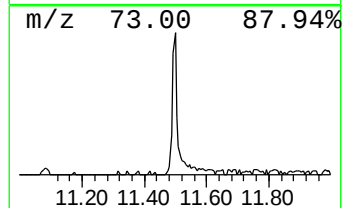
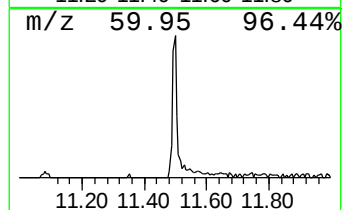
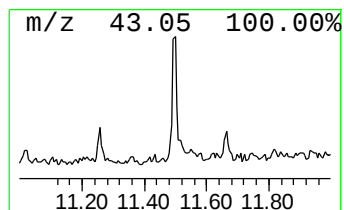
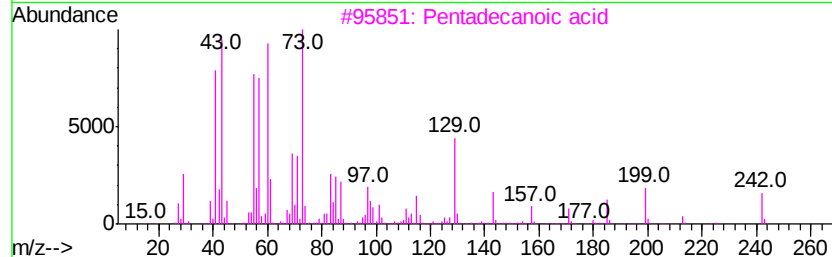
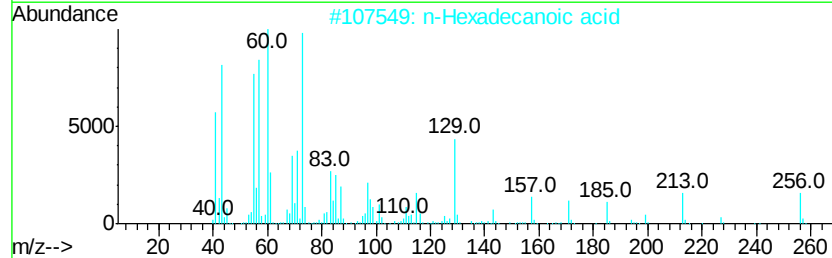
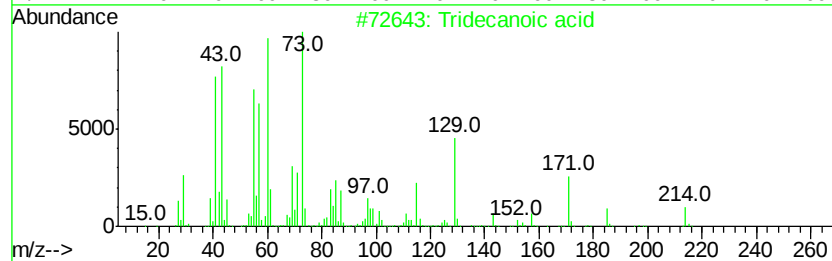
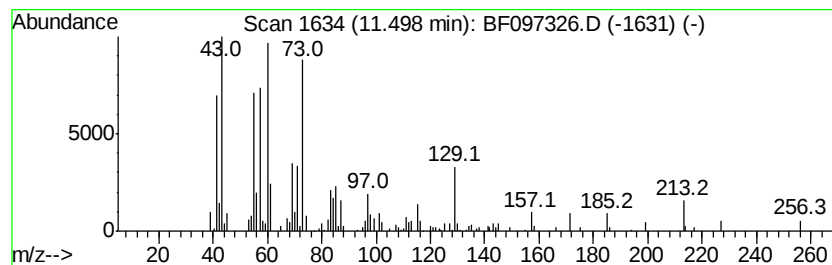
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	4.94 ng	228718	Phenanthrene-d10	10.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
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Operator : SJ/JU
Sample : I4541-13
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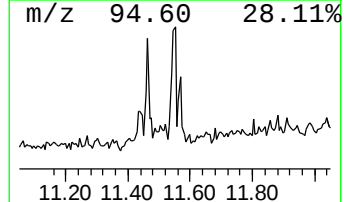
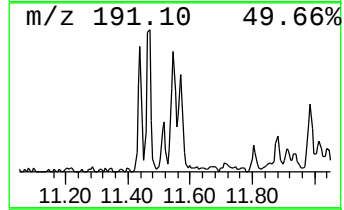
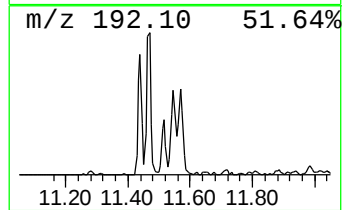
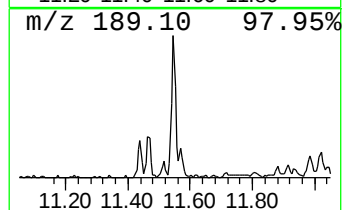
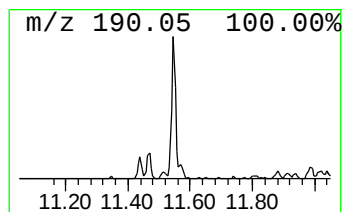
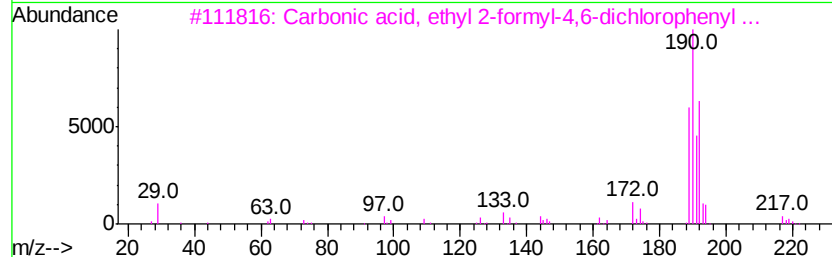
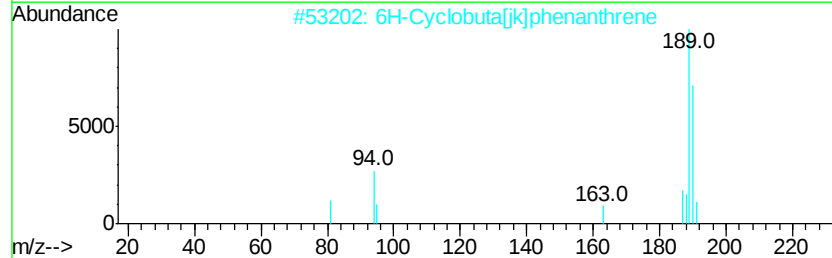
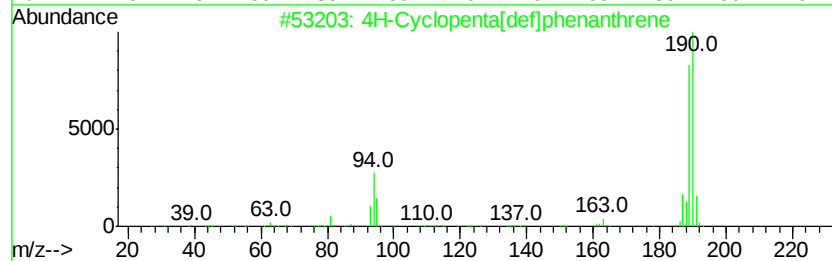
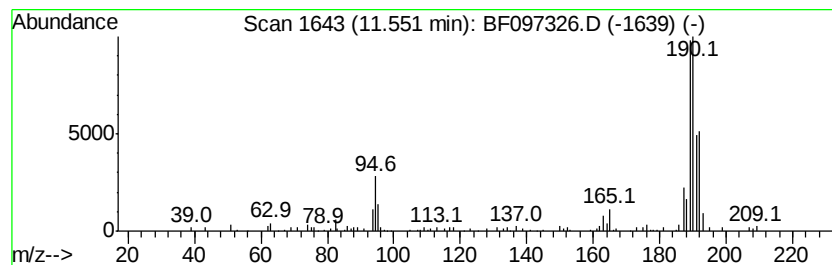
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.55	3.48 ng	161136	Phenanthrene-d10	10.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[ikl]phenanthrene	190	C15H10	083469-43-6	53
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	35
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18



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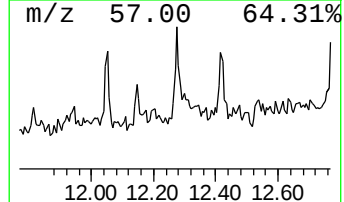
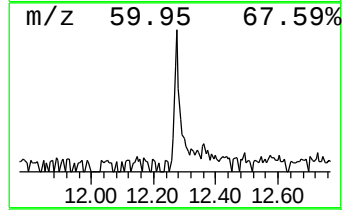
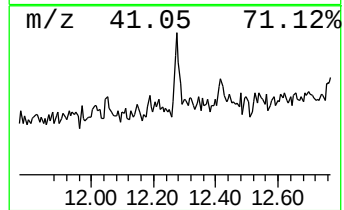
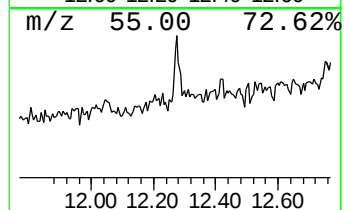
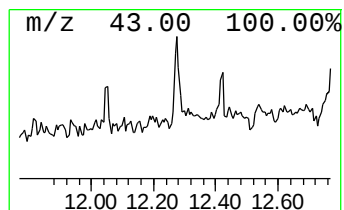
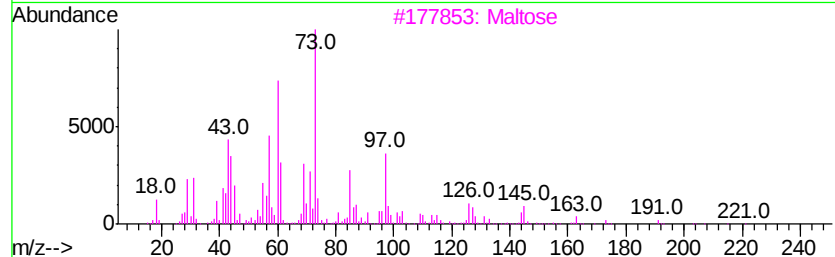
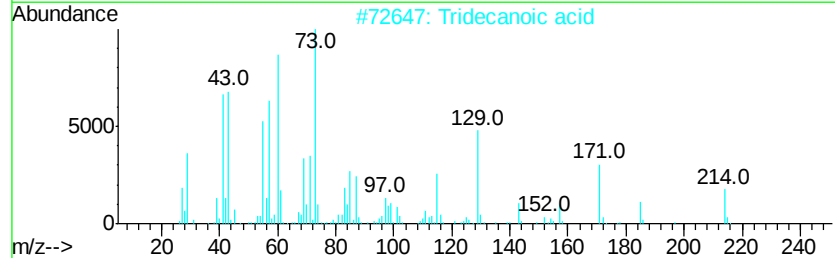
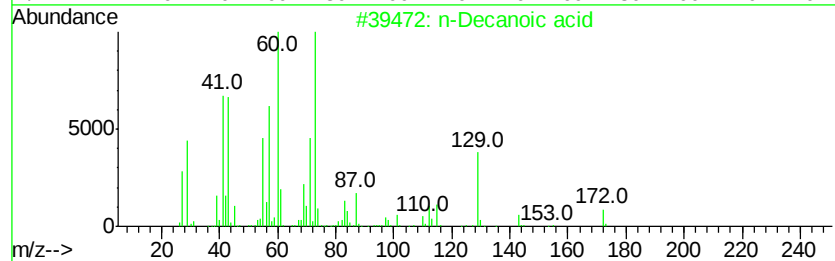
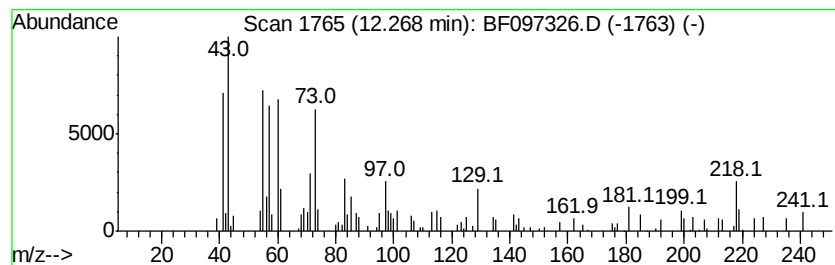
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Decanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	2.46 ng	134092	Chrysene-d12	13.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Decanoic acid	172 C10H20O2	000334-48-5	55
2	Tridecanoic acid	214 C13H26O2	000638-53-9	52
3	Maltose	342 C12H22O11	000069-79-4	50
4	Dodecanoic acid	200 C12H24O2	000143-07-7	50
5	Tetradecanoic acid	228 C14H28O2	000544-63-8	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
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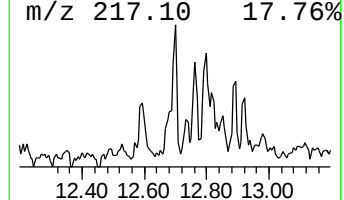
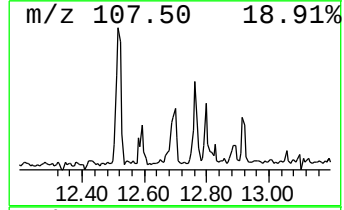
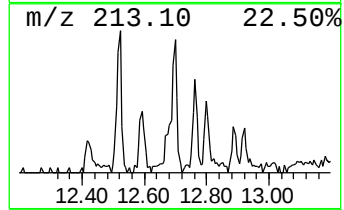
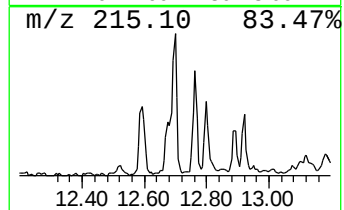
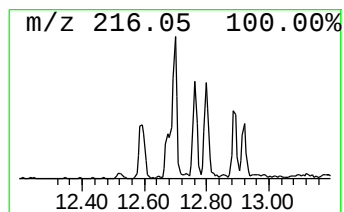
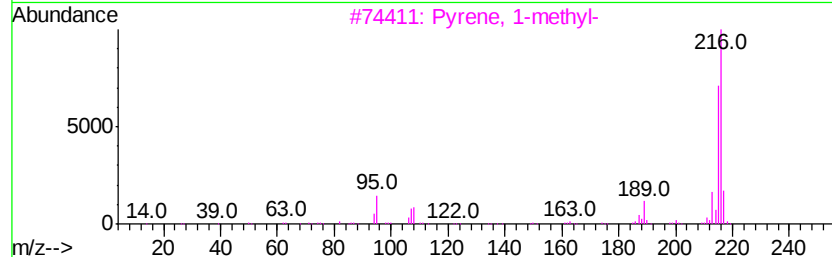
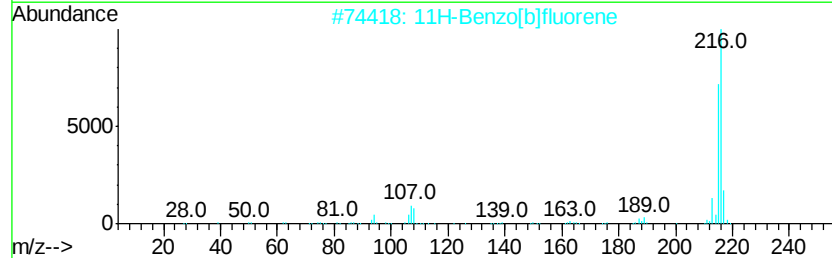
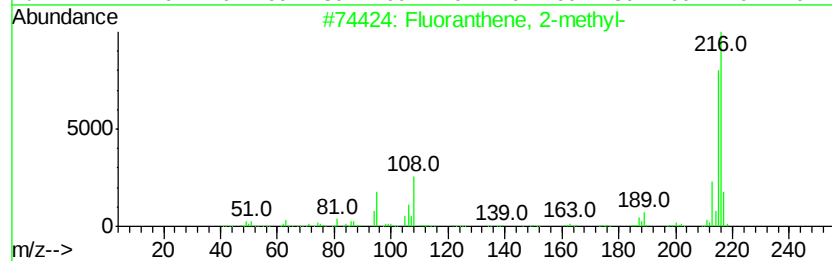
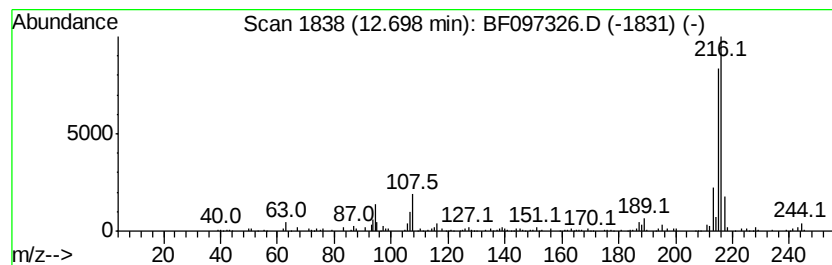
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Fluoranthene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.70	3.34 ng	182170	Chrysene-d12	13.56	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
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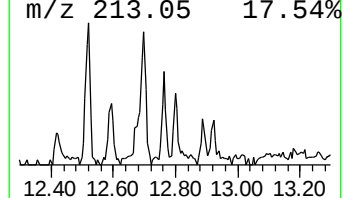
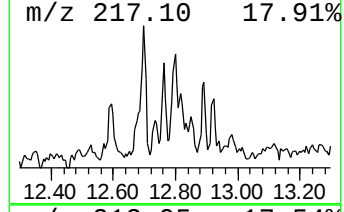
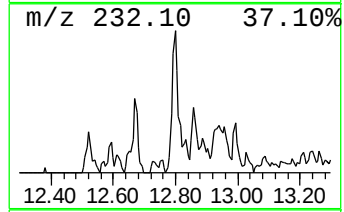
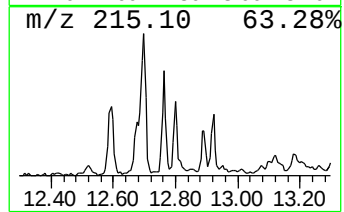
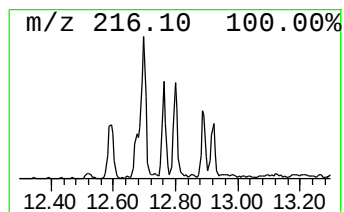
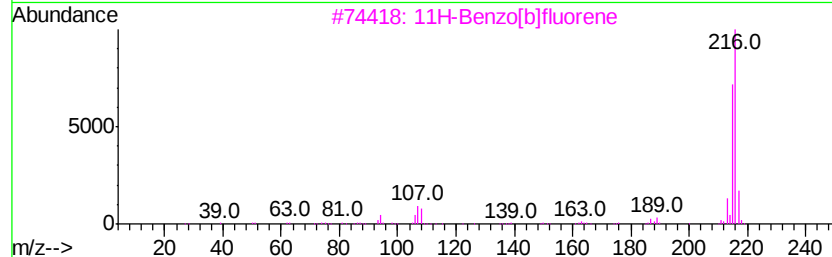
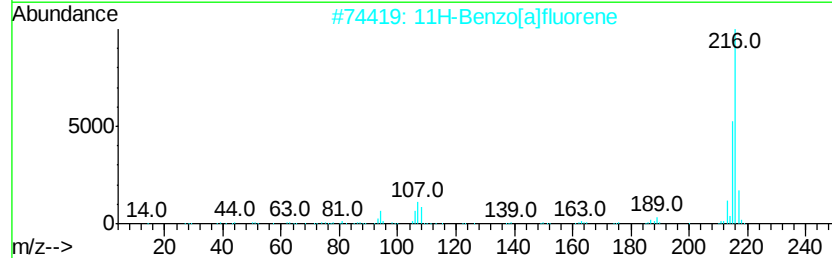
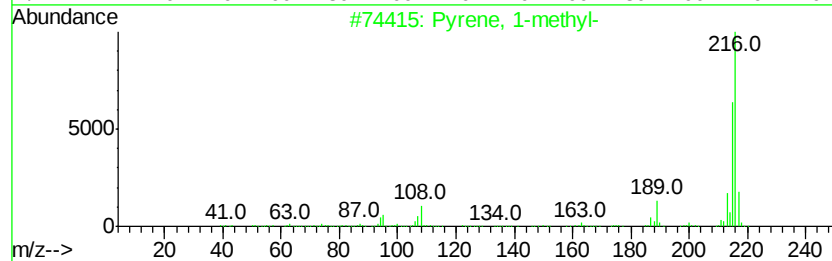
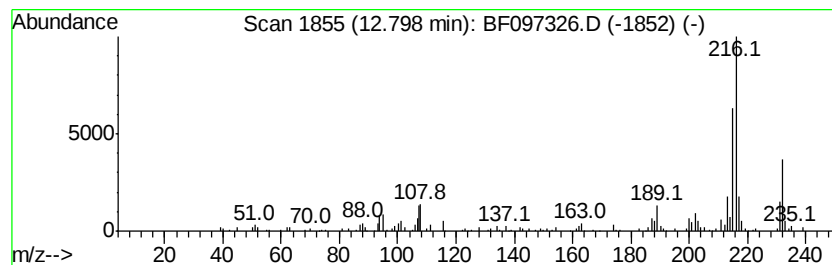
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.33 ng	127238	Chrysene-d12	13.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 96
2		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 89
3		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 89
4		Pyrene, 2-methyl-	216 C17H12	003442-78-2 89
5		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 64



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Sample : I4541-13
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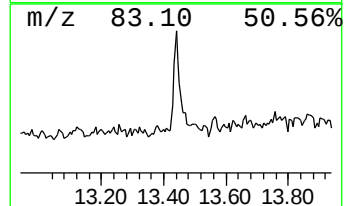
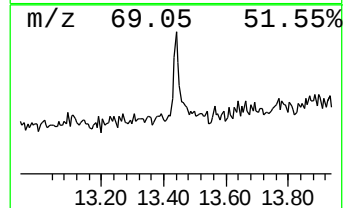
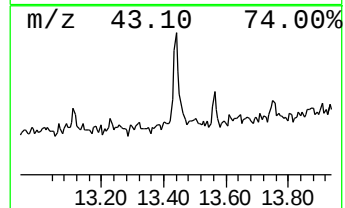
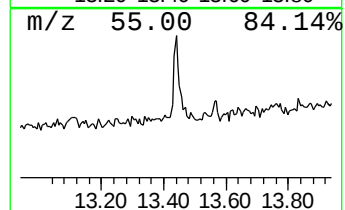
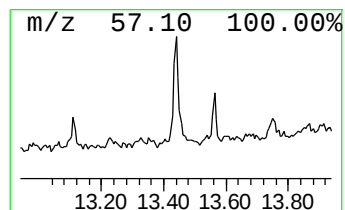
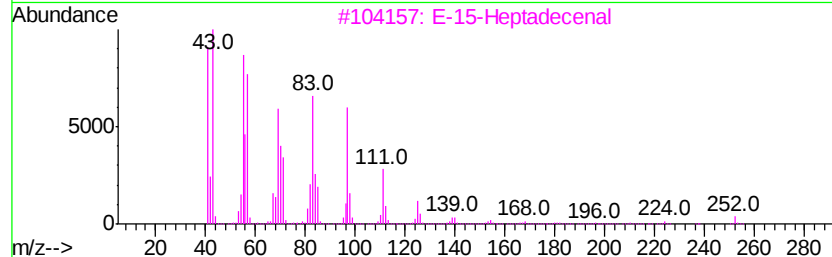
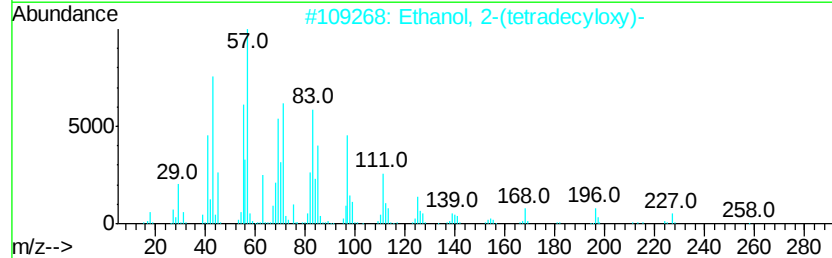
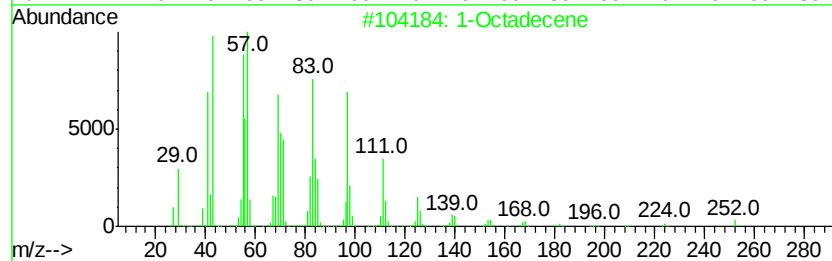
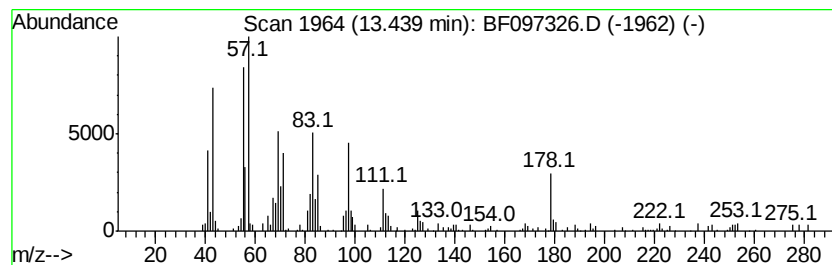
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Octadecene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.02 ng	110088	Chrysene-d12	13.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecene	252 C18H36	000112-88-9	96
2	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	93
3	E-15-Heptadecenal	252 C17H32O	1000130-97-9	83
4	Pentafluoropropionic acid, hepta...	402 C20H35F5O2	959218-78-1	81
5	Heneicosyl heptafluorobutyrate	508 C25H43F7O2	1000351-83-8	81



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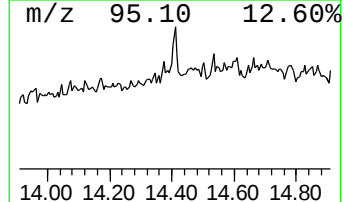
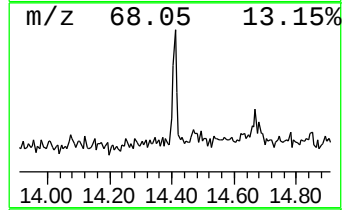
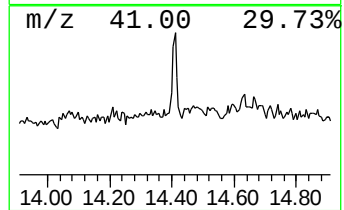
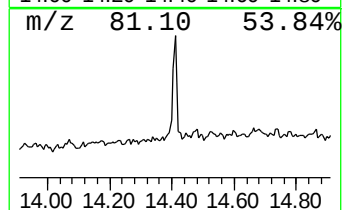
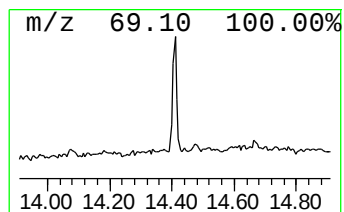
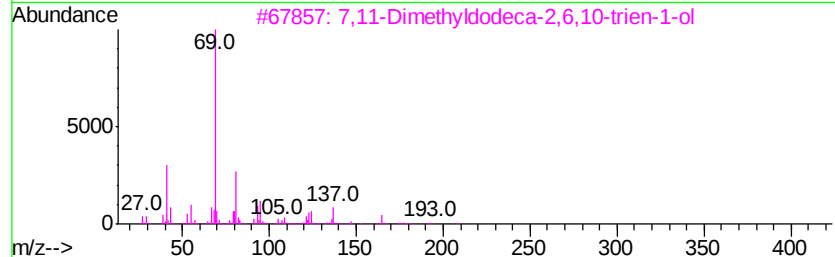
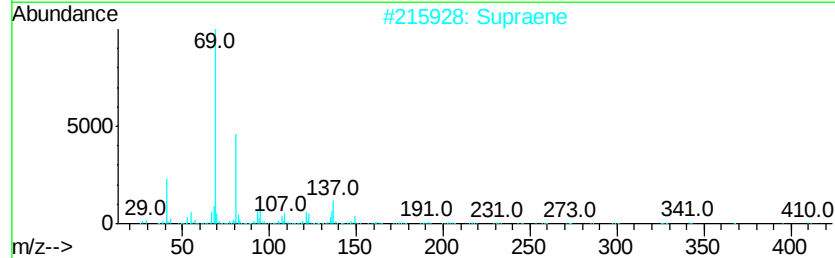
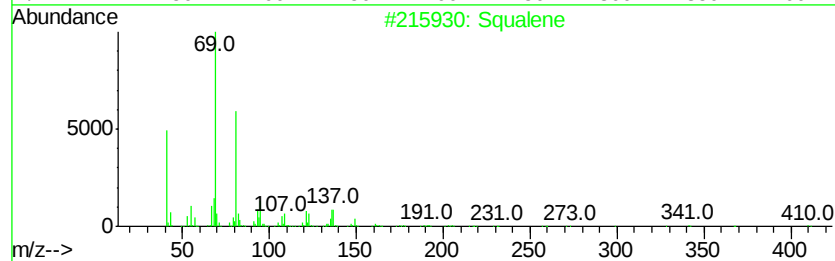
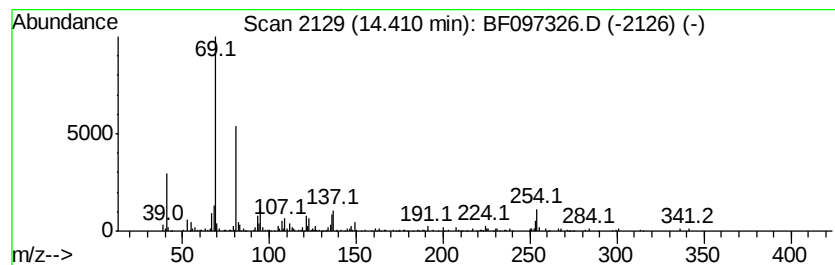
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	5.47 ng	142544	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	81
2		Supraene	410	C30H50	007683-64-9	74
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4		Farnesol isomer a	222	C15H26O	1000108-92-4	62
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53



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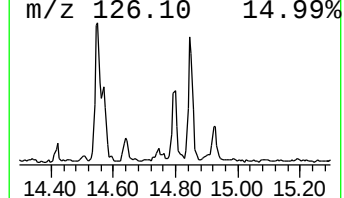
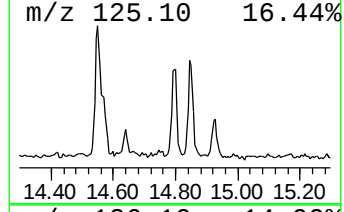
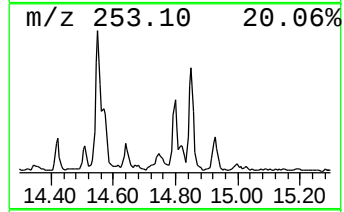
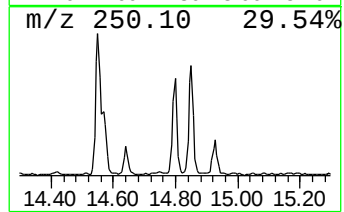
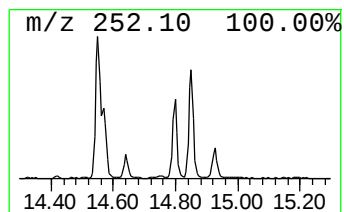
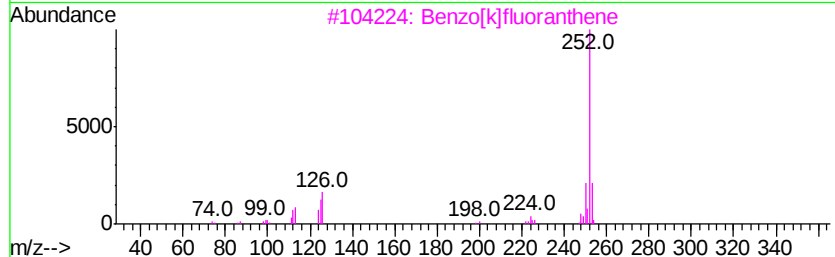
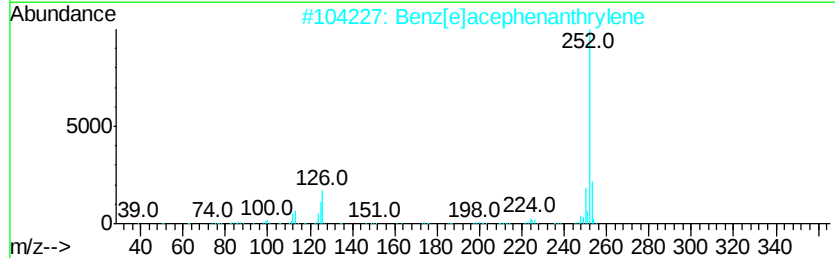
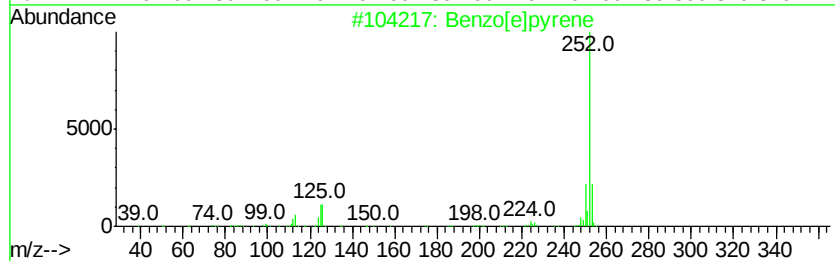
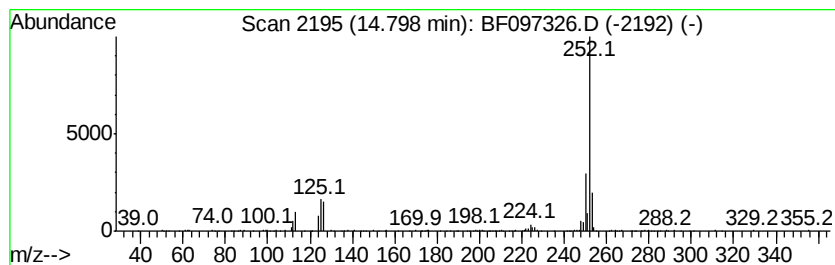
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	10.01 ng	260904	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4		Perylene	252	C20H12	000198-55-0	94
5		Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097326.D
Acq On : 3 Aug 2017 19:39
Operator : SJ/JU
Sample : I4541-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11944

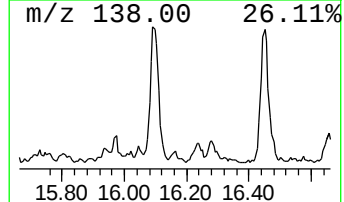
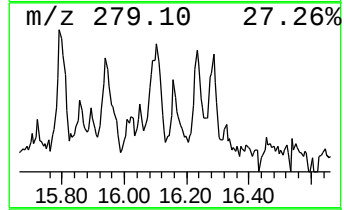
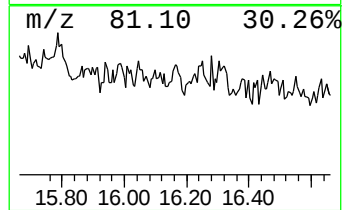
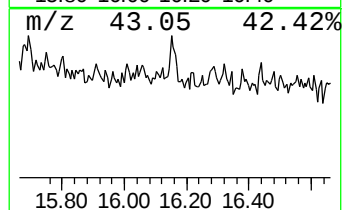
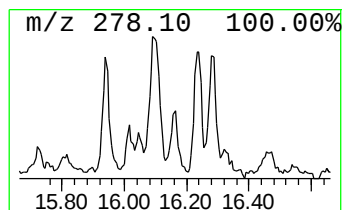
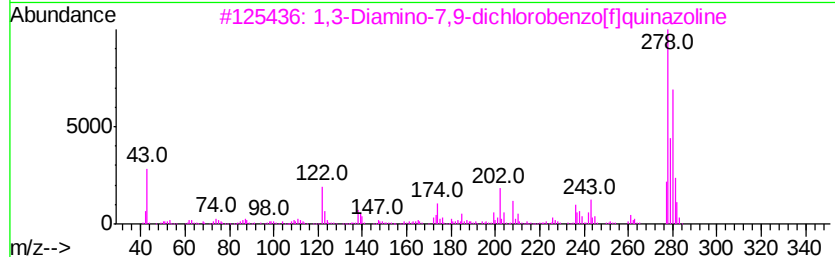
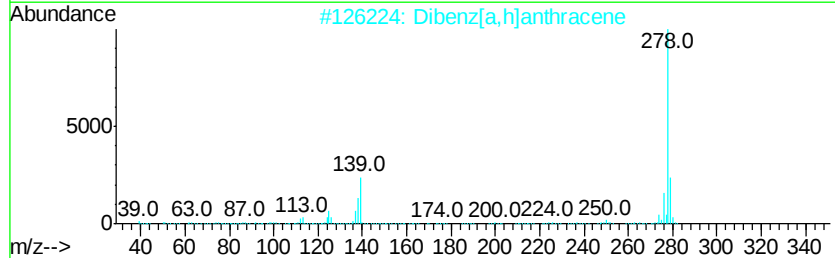
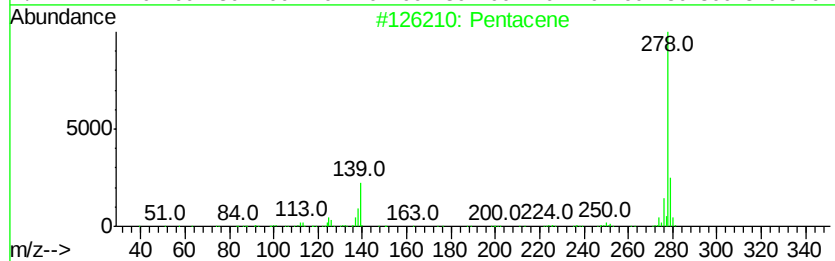
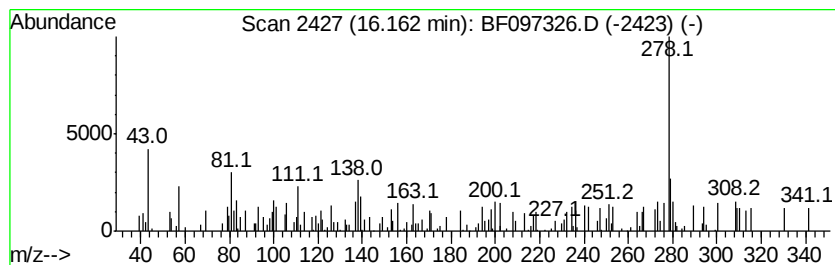
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.16 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	3.09 ng	80481	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacene	278	C22H14	000135-48-8	38
2		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	38
3		1,3-Diamino-7,9-dichlorobenzo[f]...	278	C12H8Cl2N4	037521-58-7	35
4		Benzo[b]triphenylene	278	C22H14	000215-58-7	32
5		Pyrimidine, 5-ethyl-2-(4'-fluoro...	278	C18H15FN2	095495-16-2	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097326.D
Acq On : 3 Aug 2017 19:39
Operator : SJ/JU
Sample : I4541-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11944

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
2-Pentanone, 4-hy...	4.57	32.3	ng	1131650	1	6.45	701446	20.0
unknown6.22	6.22	73.5	ng	2579320	1	6.45	701446	20.0
Tridecane	10.39	2.2	ng	101243	4	10.94	926720	20.0
Tridecanoic acid	11.50	4.9	ng	228718	4	10.94	926720	20.0
4H-Cyclopenta[def...	11.55	3.5	ng	161136	4	10.94	926720	20.0
n-Decanoic acid	12.27	2.5	ng	134092	5	13.56	1092130	20.0
Fluoranthene, 2-m...	12.70	3.3	ng	182170	5	13.56	1092130	20.0
Pyrene, 1-methyl-	12.80	2.3	ng	127238	5	13.56	1092130	20.0
1-Octadecene	13.44	2.0	ng	110088	5	13.56	1092130	20.0
Squalene	14.41	5.5	ng	142544	6	14.90	521316	20.0
Benzo[e]pyrene	14.80	10.0	ng	260904	6	14.90	521316	20.0
unknown16.16	16.16	3.1	ng	80481	6	14.90	521316	20.0