

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
 Data File : BF097333.D
 Acq On : 3 Aug 2017 22:56
 Operator : SJ/JU
 Sample : I4541-05 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11936

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	4.557	451	454	475	rVB	386702	549970	35.53%	2.646%
2	5.034	532	535	554	rBV	1135746	1476312	95.39%	7.101%
3	6.110	715	718	733	rBV	1508967	1547712	100.00%	7.445%
4	6.216	733	736	743	rVB	1585918	1483881	95.88%	7.138%
5	6.445	771	775	783	rBV	751137	758631	49.02%	3.649%
6	6.598	797	801	813	rBV	1186712	1066215	68.89%	5.129%
7	7.010	868	871	880	rBV	893682	839667	54.25%	4.039%
8	7.728	989	993	1002	rBV	965539	957697	61.88%	4.607%
9	8.439	1109	1114	1118	rBV	19896	17727	1.15%	0.085%
10	8.533	1127	1130	1138	rVB3	16358	17677	1.14%	0.085%
11	8.798	1171	1175	1179	rBV	1678121	1375164	88.85%	6.615%
12	9.198	1241	1243	1247	rVB	188611	150426	9.72%	0.724%
13	9.327	1262	1265	1268	rBV	41349	36894	2.38%	0.177%
14	9.422	1277	1281	1284	rBV	30312	30736	1.99%	0.148%
15	9.463	1284	1288	1292	rVV2	1141760	1039568	67.17%	5.001%
16	9.498	1292	1294	1303	rVB	55238	51745	3.34%	0.249%
17	9.675	1318	1324	1327	rBV	33604	37887	2.45%	0.182%
18	9.780	1339	1342	1347	rBV6	10182	17995	1.16%	0.087%
19	9.922	1363	1366	1370	rVB	44018	38945	2.52%	0.187%
20	10.010	1378	1381	1388	rVB	40473	45069	2.91%	0.217%
21	10.251	1418	1422	1428	rBV	739465	721127	46.59%	3.469%
22	10.386	1442	1445	1450	rBV	53870	64030	4.14%	0.308%
23	10.757	1505	1508	1510	rBV2	21414	24036	1.55%	0.116%
24	10.833	1517	1521	1524	rBV	55782	49030	3.17%	0.236%
25	10.933	1535	1538	1541	rBV	826167	839704	54.25%	4.039%
26	10.957	1541	1542	1547	rVV	448601	353189	22.82%	1.699%
27	11.016	1547	1552	1556	rVB	115997	117297	7.58%	0.564%
28	11.057	1556	1559	1561	rBV3	16385	17019	1.10%	0.082%
29	11.180	1577	1580	1583	rBV	48305	43788	2.83%	0.211%
30	11.257	1591	1593	1596	rBV2	19431	21984	1.42%	0.106%
31	11.439	1621	1624	1626	rBV	62438	58443	3.78%	0.281%
32	11.469	1626	1629	1631	rVV	74223	74257	4.80%	0.357%
33	11.492	1631	1633	1635	rVV	63473	64474	4.17%	0.310%
34	11.516	1635	1637	1639	rVV	169364	136348	8.81%	0.656%

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Integrator: RTE

Smoothing : ON

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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35	11.545	1639	1642	1645	rVV	103581	118652	7.67%	0.571%
36	11.569	1645	1646	1650	rVB	46622	30380	1.96%	0.146%
37	11.663	1659	1662	1663	rBV2	20289	23324	1.51%	0.112%
38	11.733	1671	1674	1678	rBV	61674	66159	4.27%	0.318%
39	11.768	1678	1680	1685	rVB3	44002	46071	2.98%	0.222%
40	11.874	1697	1698	1703	rVB5	17098	16749	1.08%	0.081%
41	11.986	1714	1717	1719	rBV	35058	35478	2.29%	0.171%
42	12.021	1719	1723	1725	rVV5	21008	33561	2.17%	0.161%
43	12.074	1729	1732	1735	rVB2	44310	43301	2.80%	0.208%
44	12.139	1739	1743	1747	rBV	710851	611969	39.54%	2.944%
45	12.233	1757	1759	1762	rVB	37065	29651	1.92%	0.143%
46	12.286	1765	1768	1771	rVV2	42077	42346	2.74%	0.204%
47	12.363	1776	1781	1785	rVV	609158	623368	40.28%	2.999%
48	12.421	1788	1791	1796	rVB3	27970	40912	2.64%	0.197%
49	12.492	1800	1803	1804	rBV	31315	33019	2.13%	0.159%
50	12.515	1804	1807	1815	rVB	874054	794273	51.32%	3.821%
51	12.621	1823	1825	1828	rVB	26256	18461	1.19%	0.089%
52	12.674	1831	1834	1835	rBV3	32046	27269	1.76%	0.131%
53	12.692	1835	1837	1842	rVB	67083	79514	5.14%	0.382%
54	12.763	1846	1849	1852	rBV2	69378	79680	5.15%	0.383%
55	12.798	1852	1855	1860	rVV	68867	75805	4.90%	0.365%
56	12.886	1868	1870	1873	rBV	37891	33189	2.14%	0.160%
57	12.921	1873	1876	1880	rBV2	39878	44668	2.89%	0.215%
58	13.210	1922	1925	1928	rBV	57799	59762	3.86%	0.287%
59	13.310	1940	1942	1944	rBV2	40356	30752	1.99%	0.148%
60	13.357	1948	1950	1952	rBV	30132	24667	1.59%	0.119%
61	13.415	1958	1960	1962	rBV	49493	39023	2.52%	0.188%
62	13.439	1962	1964	1969	rVB3	45416	44150	2.85%	0.212%
63	13.557	1974	1984	1987	rBV2	838217	1256974	81.21%	6.046%
64	13.580	1987	1988	1997	rVB	301625	280331	18.11%	1.348%
65	13.945	2048	2050	2054	rVB	62113	54960	3.55%	0.264%
66	14.551	2149	2153	2161	rBV	342239	545959	35.28%	2.626%
67	14.639	2165	2168	2170	rBV2	72781	66813	4.32%	0.321%
68	14.798	2192	2195	2200	rVB	198258	207549	13.41%	0.998%
69	14.851	2200	2204	2208	rBV	261926	289778	18.72%	1.394%
70	14.898	2209	2212	2215	rBV	391361	426898	27.58%	2.054%
71	16.098	2412	2416	2421	rVB	123788	187169	12.09%	0.900%

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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

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72	16.456	2473	2477	2487	rVB	97923	201524	13.02%	0.969%
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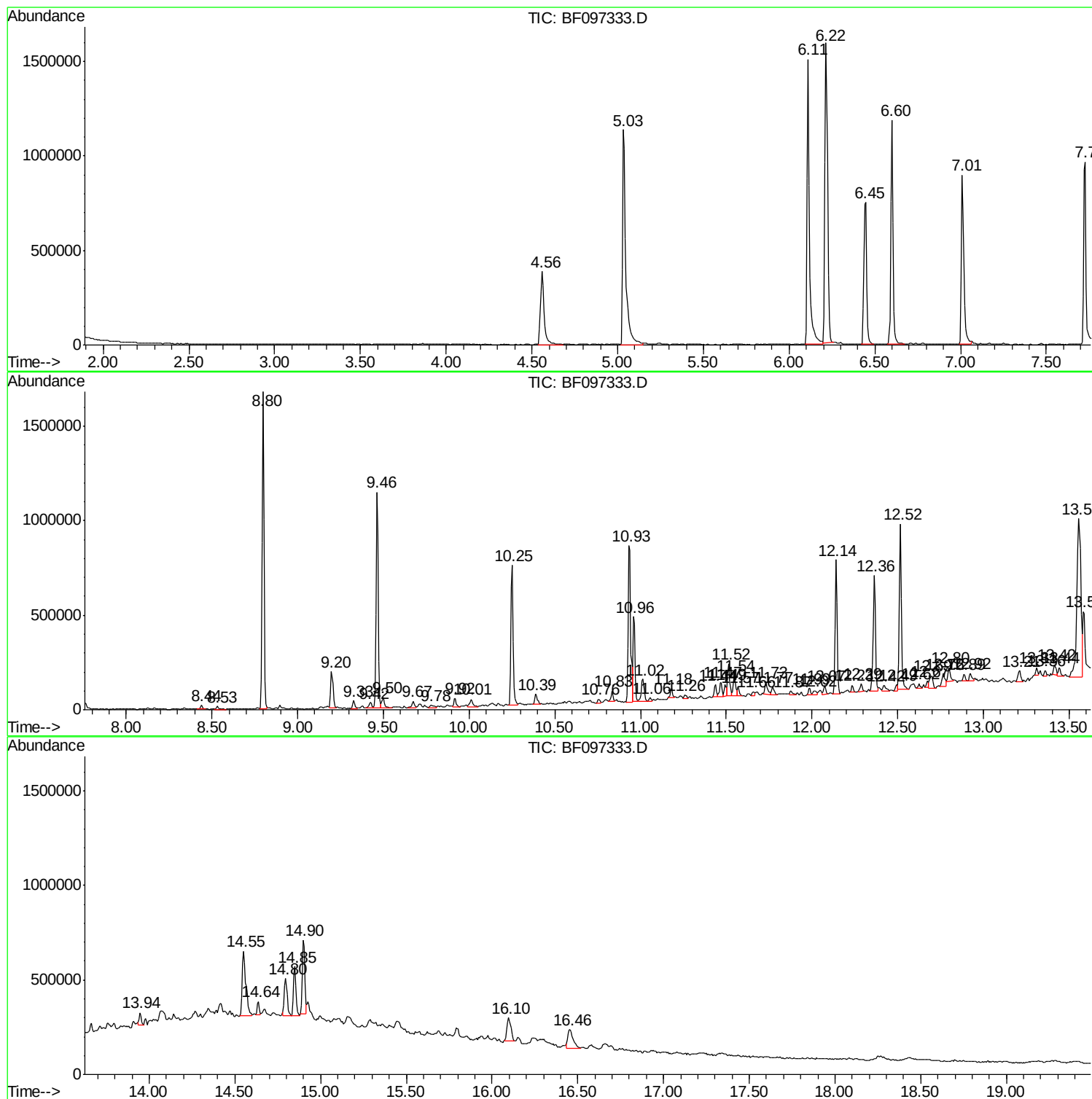
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Instrument :
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ClientSampled :
72-11936

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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Operator : SJ/JU
Sample : I4541-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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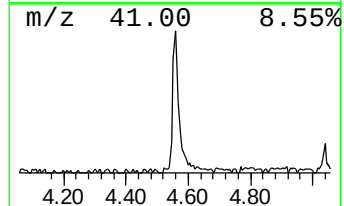
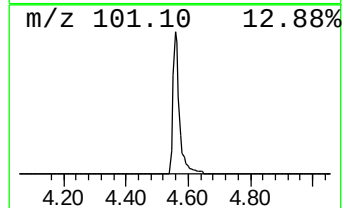
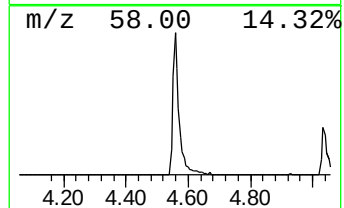
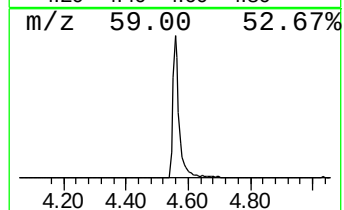
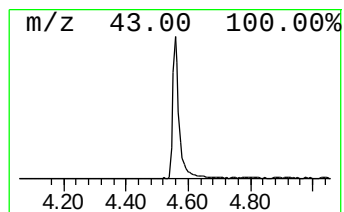
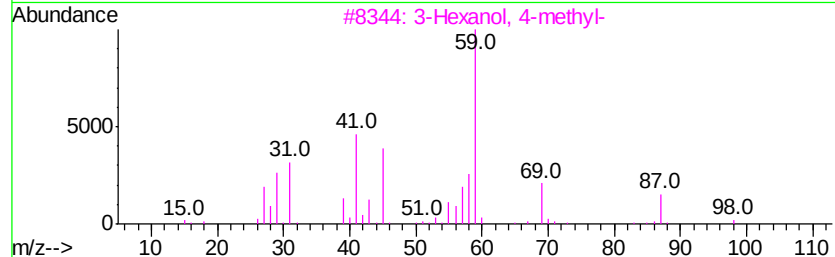
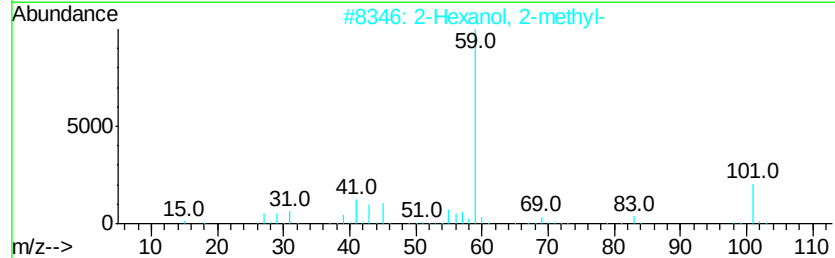
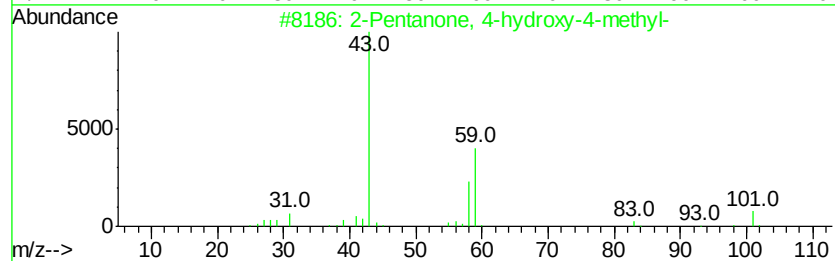
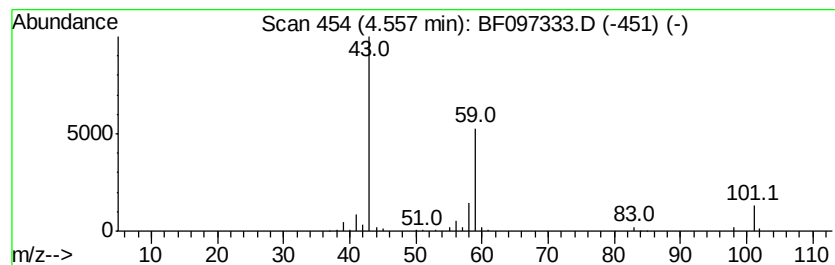
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	14.50 ng	549970	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		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		3-Octanol	130	C8H18O	000589-98-0	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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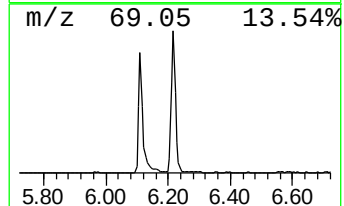
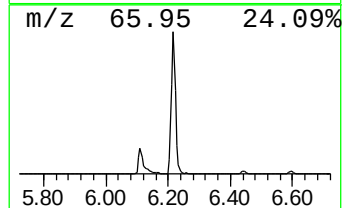
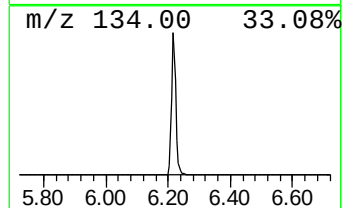
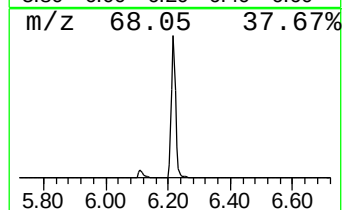
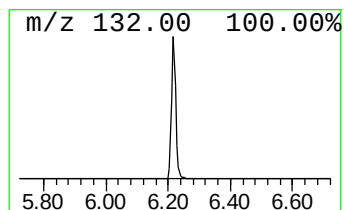
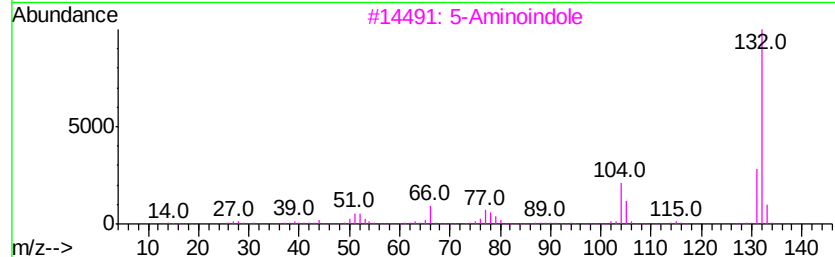
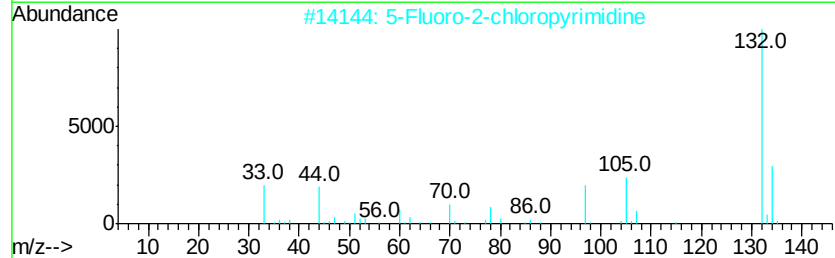
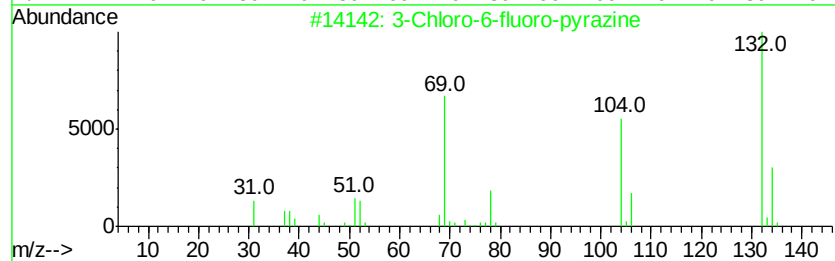
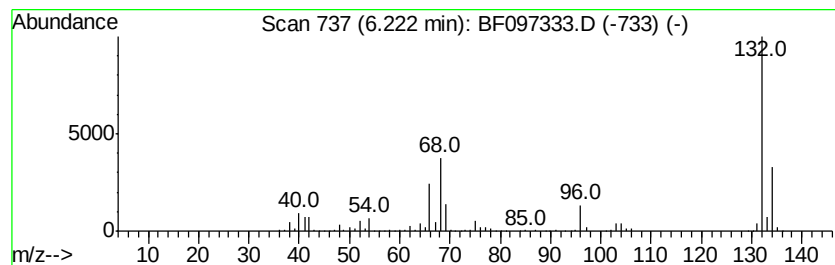
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	39.12 ng	1483880	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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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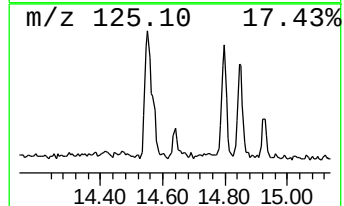
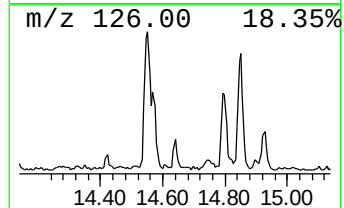
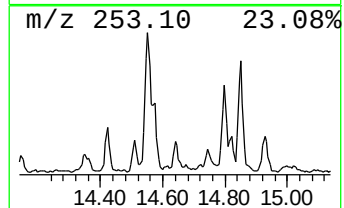
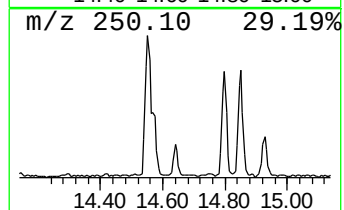
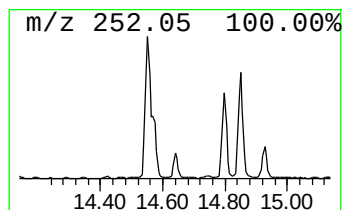
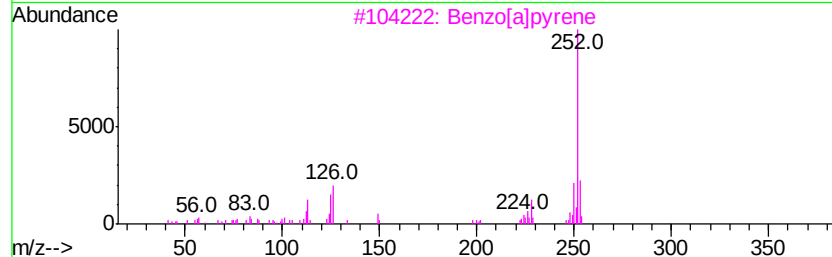
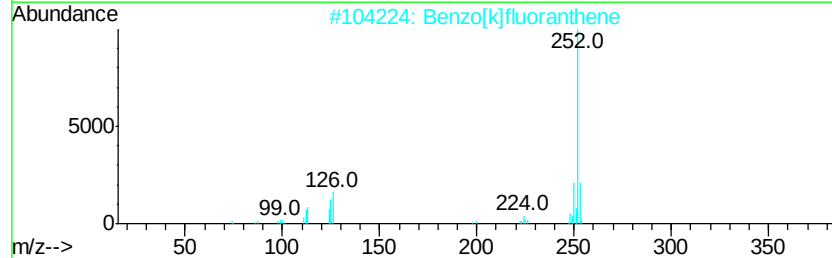
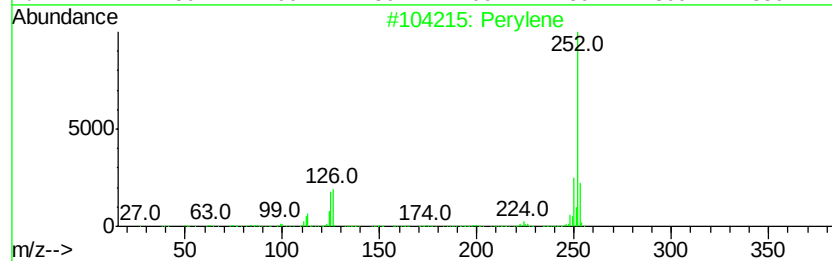
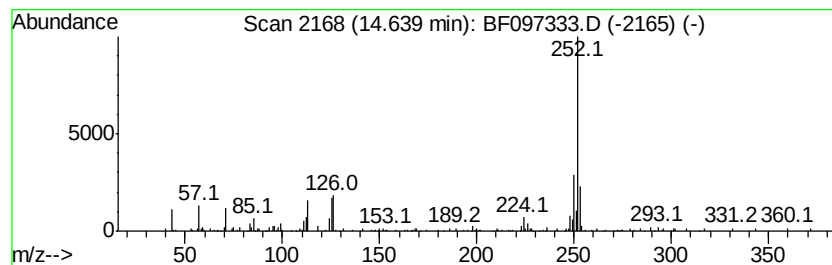
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.13 ng	66813	Perylene-d12	14.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	94
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
3		Benzo[a]pyrene	252	C20H12	000050-32-8	91
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	87
5		Benzo[e]pyrene	252	C20H12	000192-97-2	87



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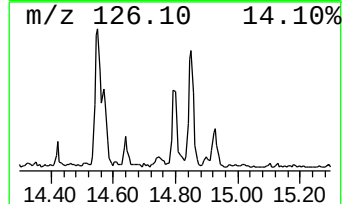
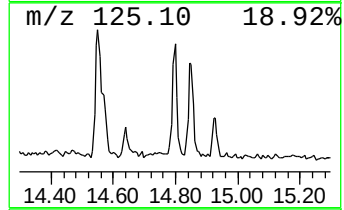
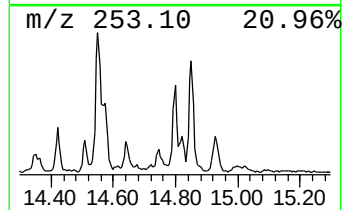
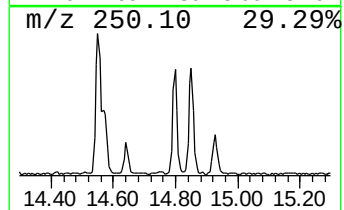
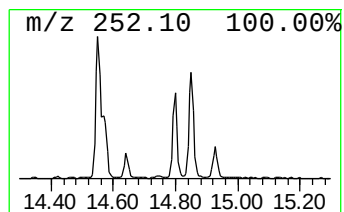
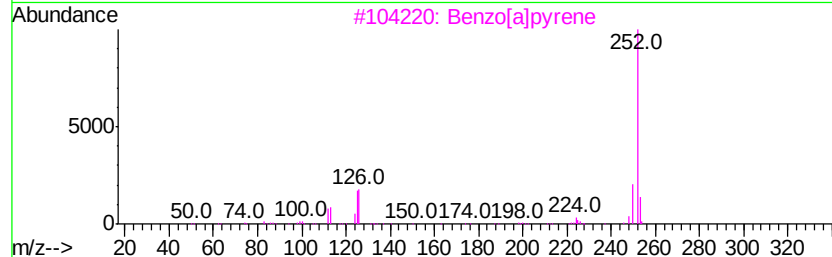
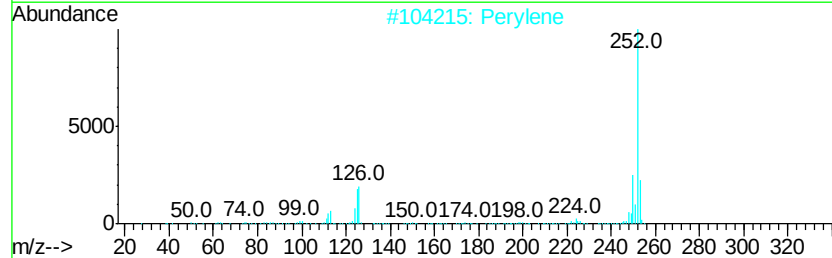
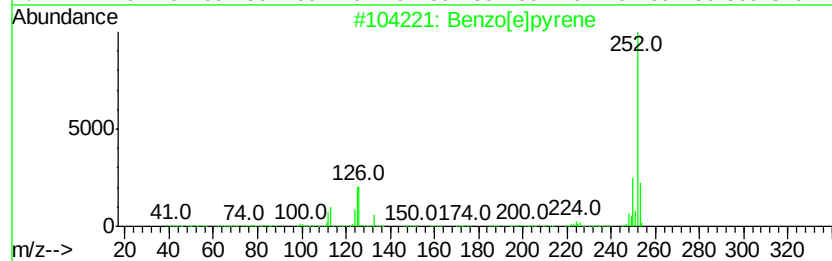
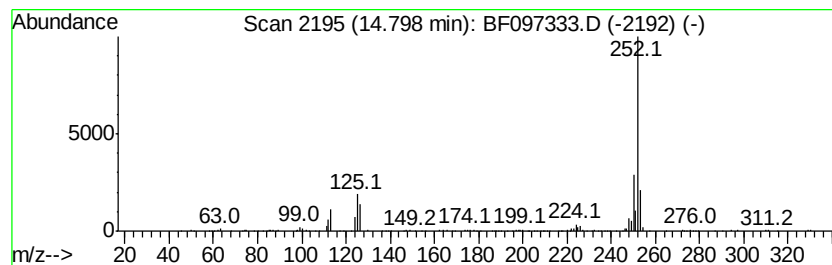
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	9.72 ng	207549	Perylene-d12	14.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Perylene	252	C20H12	000198-55-0	98
3		Benzo[a]pyrene	252	C20H12	000050-32-8	93
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097333.D
Acq On : 3 Aug 2017 22:56
Operator : SJ/JU
Sample : I4541-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11936

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...	4.56	14.5	ng	549970	1	6.45	758631	20.0
unknown6.22	6.22	39.1	ng	1483880	1	6.45	758631	20.0
Perylene	14.64	3.1	ng	66813	6	14.90	426898	20.0
Benzo[e]pyrene	14.80	9.7	ng	207549	6	14.90	426898	20.0