

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096414.D
 Acq On : 2 Jul 2017 14:21
 Operator : SJ/MA
 Sample : I3950-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B5-4-6

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	4.934	479	484	493	rBV	436690	590983	16.02%	1.892%
2	5.351	550	555	558	rVB	3147967	3285307	89.03%	10.517%
3	6.375	723	729	732	rBV	3289193	3690125	100.00%	11.813%
4	6.504	746	751	754	rBV	3422399	3393105	91.95%	10.863%
5	6.734	786	790	793	rBV	1332439	1062672	28.80%	3.402%
6	6.892	812	817	820	rVB	2765732	2448578	66.35%	7.839%
7	7.292	879	885	888	rBV	2180193	2196997	59.54%	7.033%
8	7.386	897	901	905	rVB2	40187	50586	1.37%	0.162%
9	8.016	1003	1008	1011	rBV	1508792	1298096	35.18%	4.156%
10	8.451	1078	1082	1086	rBV	38686	37606	1.02%	0.120%
11	8.622	1106	1111	1113	rBV	77084	63976	1.73%	0.205%
12	8.727	1123	1129	1131	rVB	50503	50259	1.36%	0.161%
13	9.092	1186	1191	1194	rBV	3087673	2732598	74.05%	8.748%
14	9.186	1201	1207	1210	rBV2	102734	110452	2.99%	0.354%
15	9.480	1254	1257	1260	rBV	592591	497677	13.49%	1.593%
16	9.622	1278	1281	1285	rBV	46932	40412	1.10%	0.129%
17	9.710	1294	1296	1300	rVB	111877	93755	2.54%	0.300%
18	9.769	1300	1306	1309	rBV	1413830	1337154	36.24%	4.281%
19	9.969	1337	1340	1344	rVB2	53820	52449	1.42%	0.168%
20	10.210	1378	1381	1384	rVB	140616	110099	2.98%	0.352%
21	10.433	1415	1419	1421	rBV	40859	49001	1.33%	0.157%
22	10.551	1434	1439	1442	rBV	1760068	1629311	44.15%	5.216%
23	10.680	1458	1461	1468	rVB	152031	172440	4.67%	0.552%
24	11.127	1534	1537	1540	rBV3	64750	61568	1.67%	0.197%
25	11.245	1553	1557	1559	rBV	1104923	918286	24.88%	2.940%
26	11.269	1559	1561	1564	rVB	126680	96711	2.62%	0.310%
27	11.316	1564	1569	1572	rVB	79155	71970	1.95%	0.230%
28	11.780	1644	1648	1652	rBV2	101729	120244	3.26%	0.385%
29	11.857	1657	1661	1663	rBV3	35401	38500	1.04%	0.123%
30	12.292	1732	1735	1739	rBV4	44058	49666	1.35%	0.159%
31	12.451	1759	1762	1767	rBV	238173	200540	5.43%	0.642%
32	12.680	1795	1801	1804	rBV2	192666	217740	5.90%	0.697%
33	12.827	1822	1826	1830	rBV	1827522	1633151	44.26%	5.228%
34	12.904	1836	1839	1841	rBV	32361	38263	1.04%	0.122%

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B5-4-6

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	13.010	1854	1857	1860	rVB	53143	57814	1.57%	0.185%
36	13.074	1865	1868	1870	rBV2	48654	42029	1.14%	0.135%
37	13.110	1871	1874	1876	rBV	51069	48508	1.31%	0.155%
38	13.310	1904	1908	1914	rVB2	141678	169447	4.59%	0.542%
39	13.380	1917	1920	1923	rBV2	47553	63276	1.71%	0.203%
40	13.733	1977	1980	1984	rVB	160931	170581	4.62%	0.546%
41	13.874	1999	2004	2007	rBV2	911351	1010178	27.38%	3.234%
42	13.898	2007	2008	2011	rVB	188224	106326	2.88%	0.340%
43	14.886	2172	2176	2183	rVB	171311	306257	8.30%	0.980%
44	15.168	2221	2224	2229	rVB	125597	148152	4.01%	0.474%
45	15.221	2230	2233	2238	rBV	105759	134430	3.64%	0.430%
46	15.286	2240	2244	2248	rBV	461918	539474	14.62%	1.727%

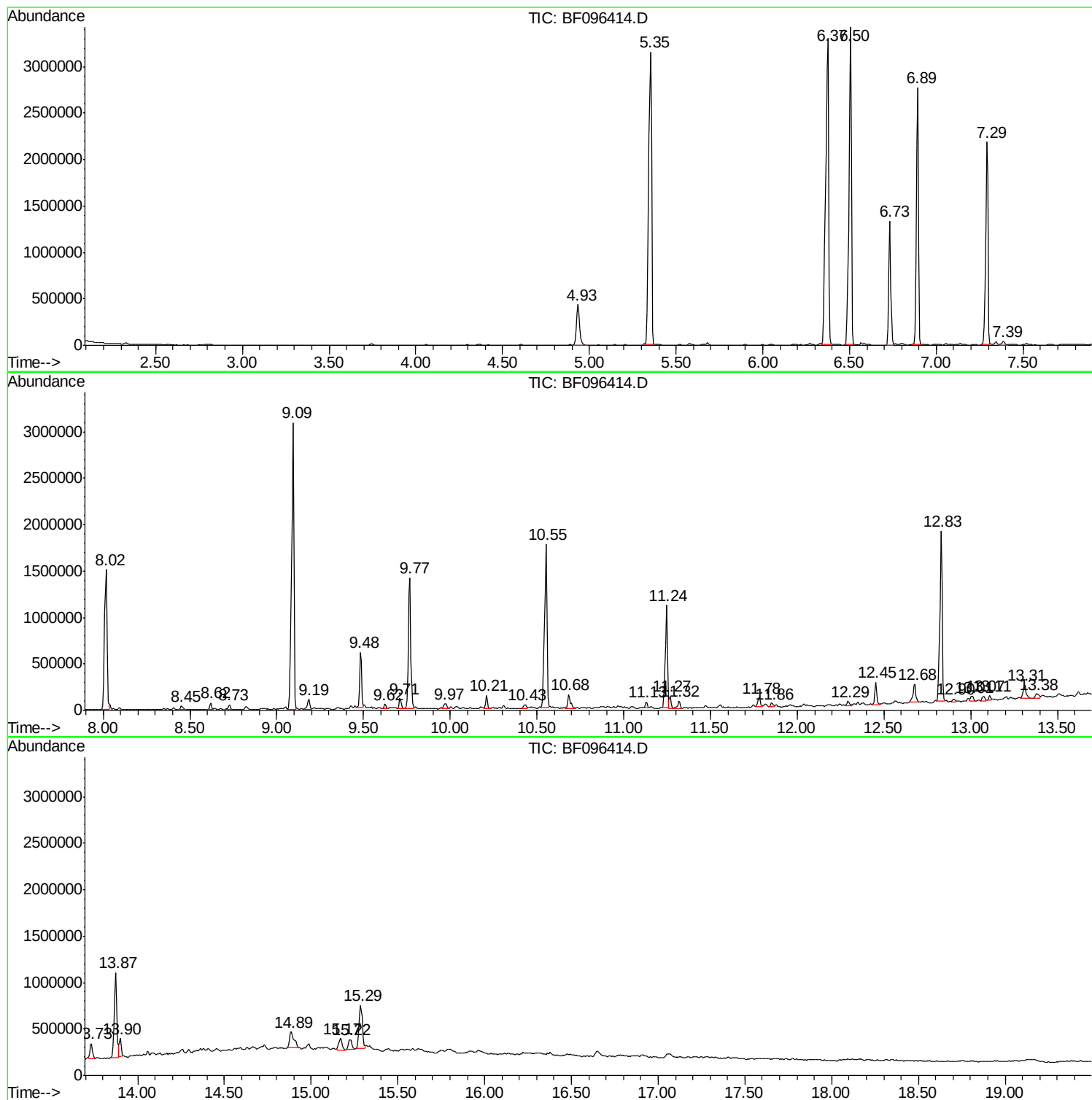
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Instrument :
BNA_F
ClientSampled :
B5-4-6

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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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B5-4-6

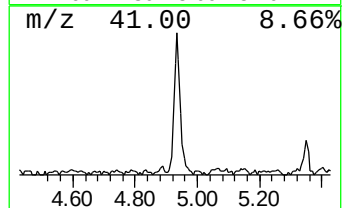
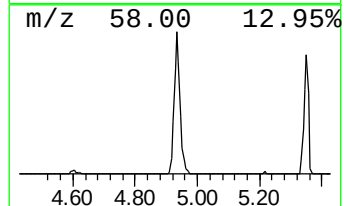
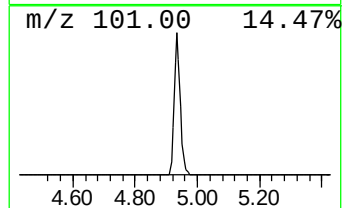
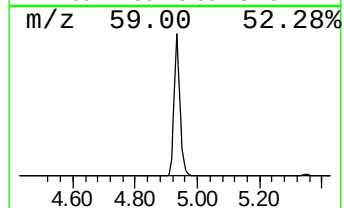
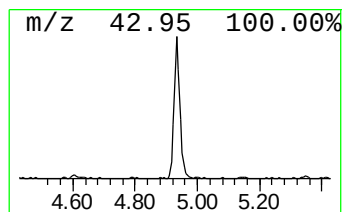
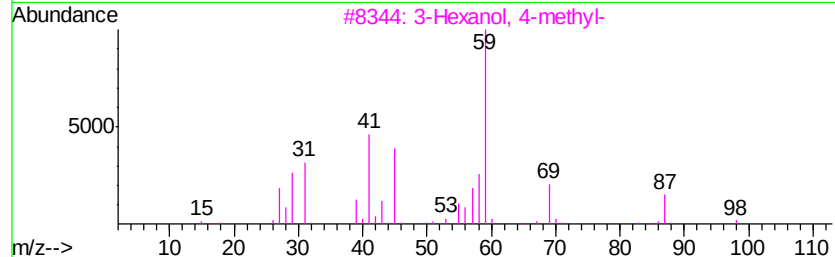
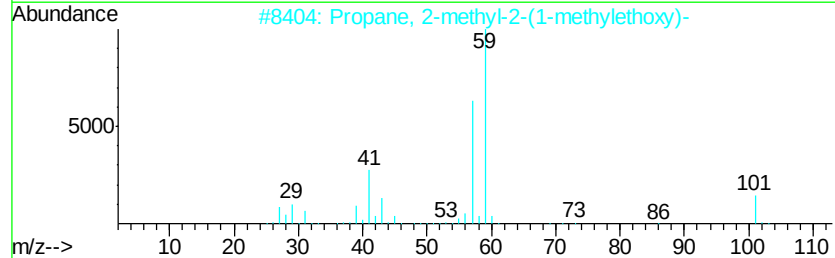
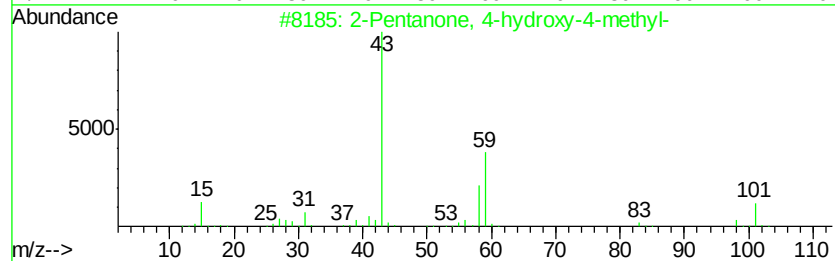
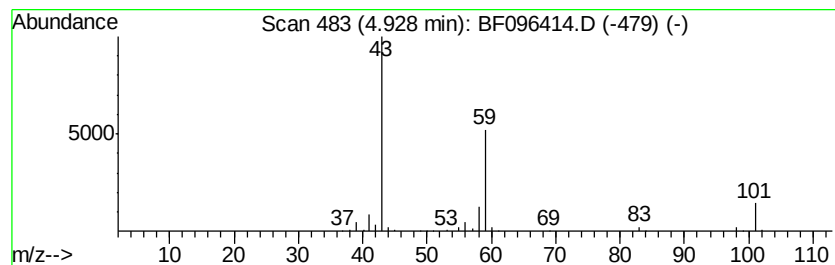
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.93	11.12 ng	590983	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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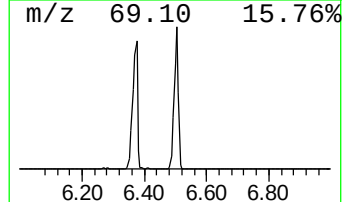
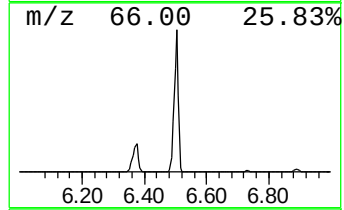
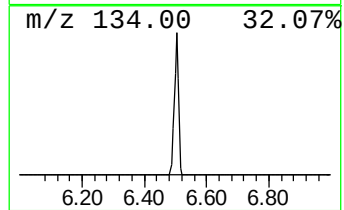
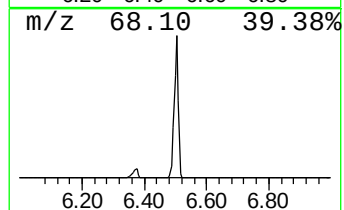
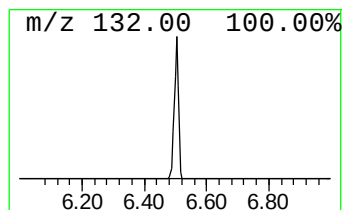
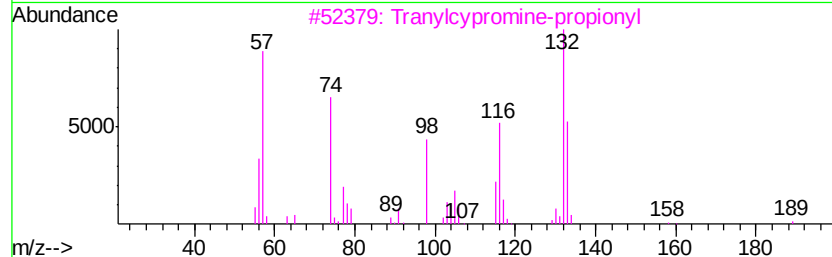
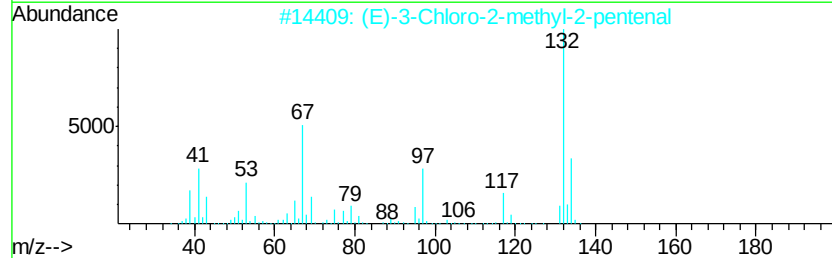
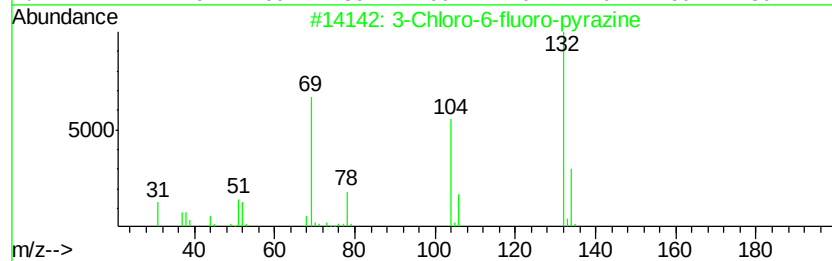
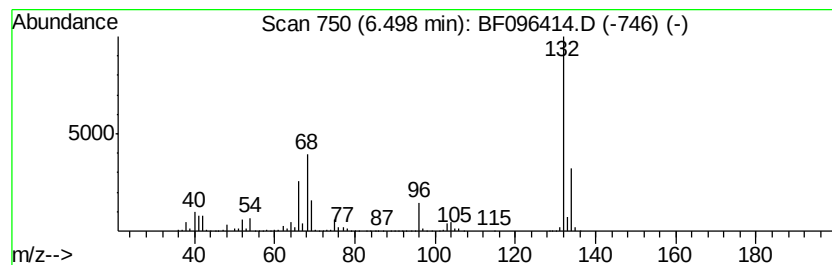
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	63.86 ng	3393110	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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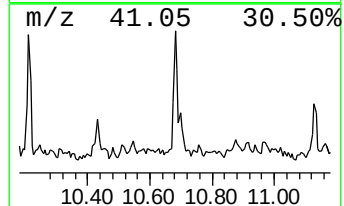
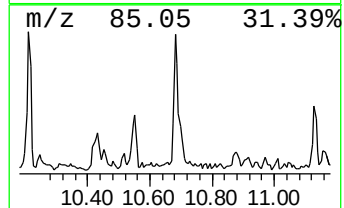
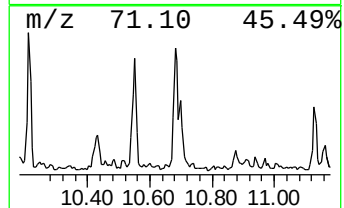
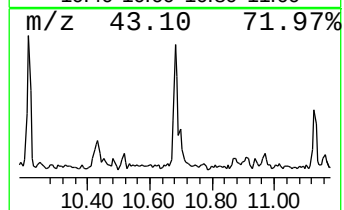
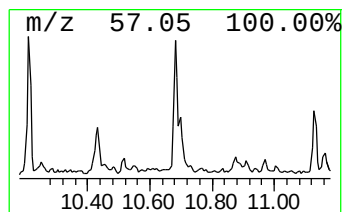
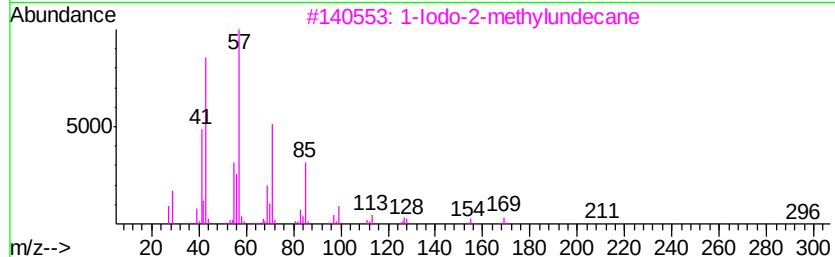
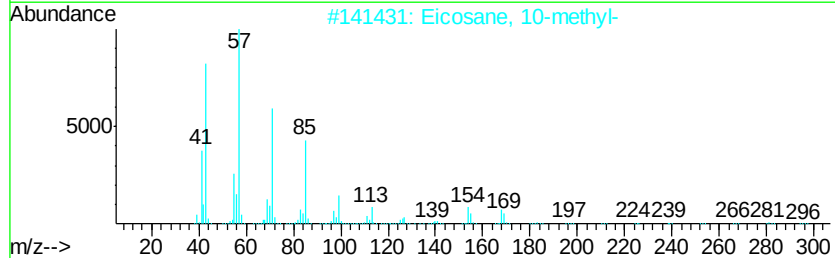
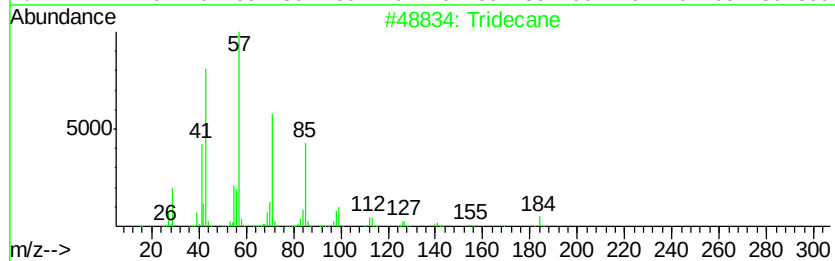
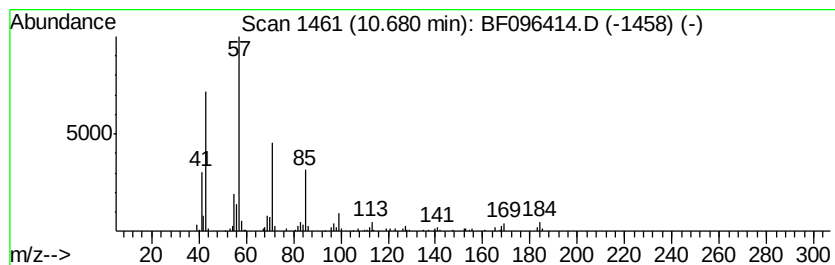
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.68	3.76 ng	172440	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	86
4	Hexadecane	226	C16H34	000544-76-3	83
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	80



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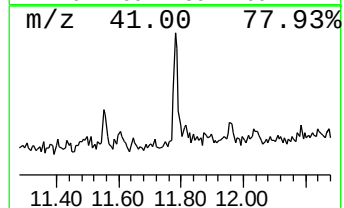
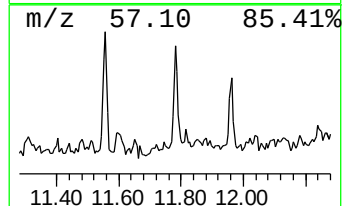
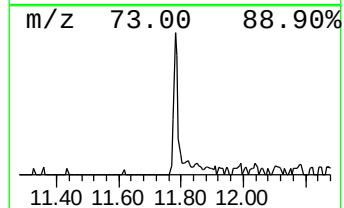
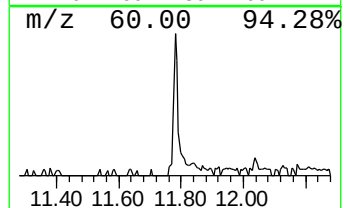
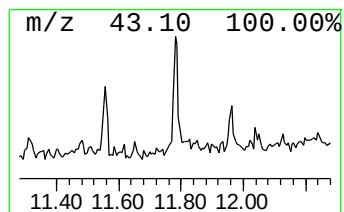
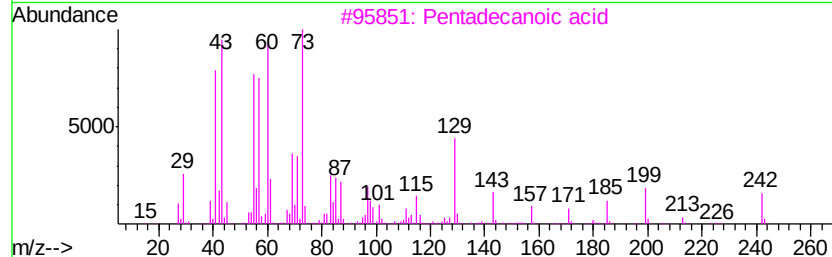
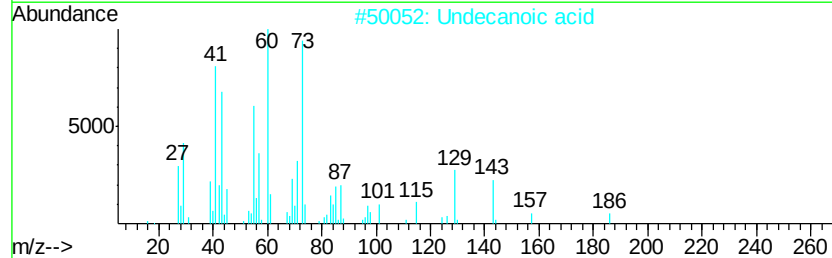
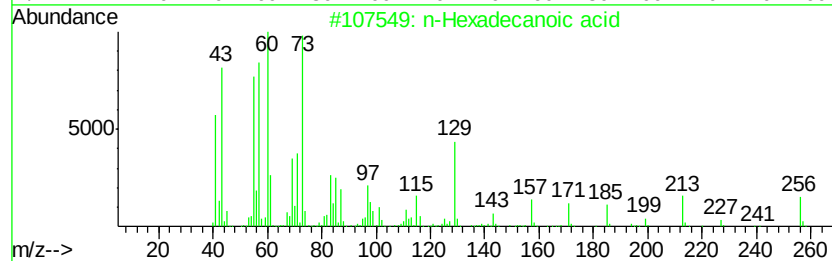
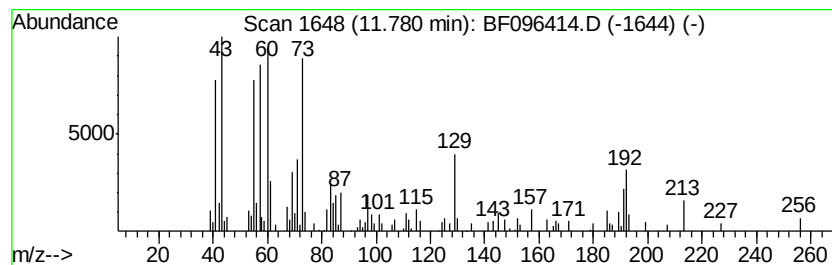
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	2.62 ng	120244	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	60
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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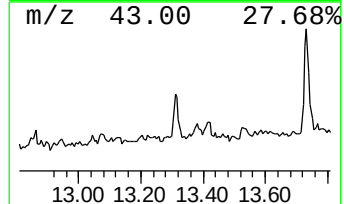
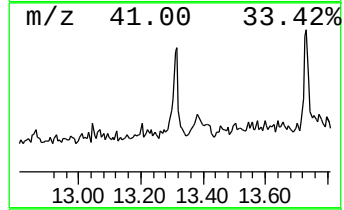
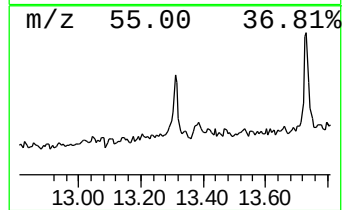
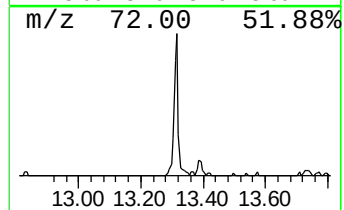
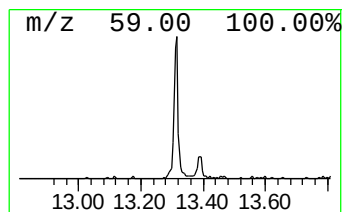
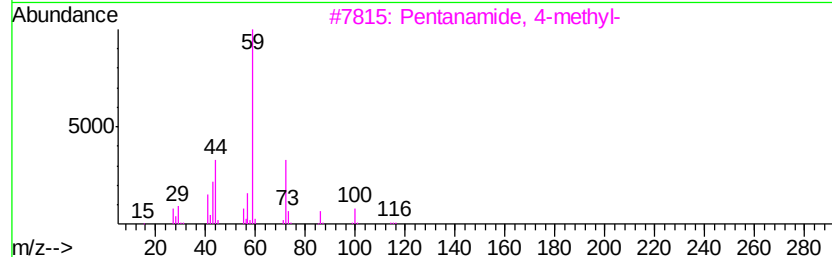
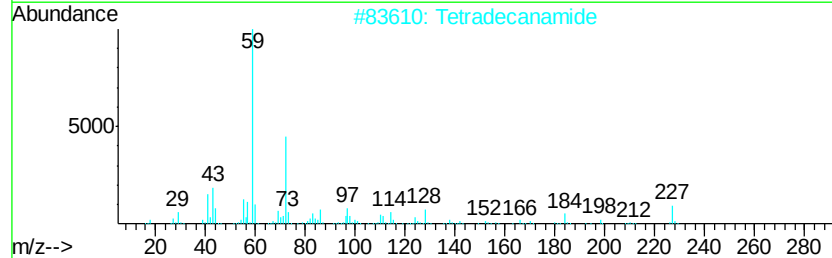
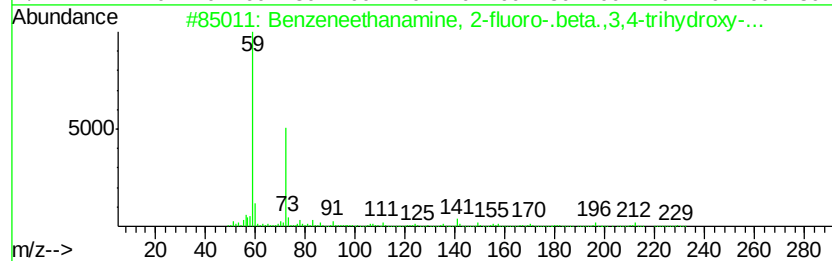
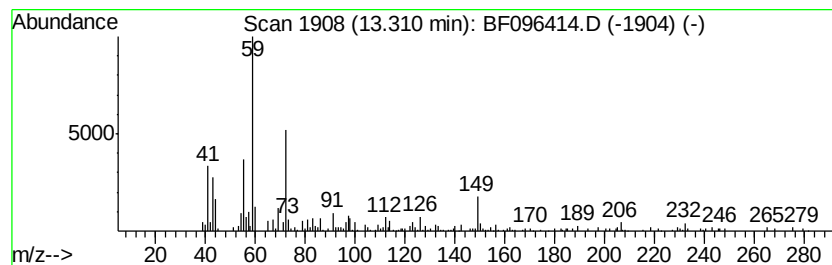
Instrument :
BNA_F
ClientSampleId :
B5-4-6

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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 Benzeneethanamine, 2-fluoro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.31	3.35 ng	169447	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096414.D
Acq On : 2 Jul 2017 14:21
Operator : SJ/MA
Sample : I3950-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

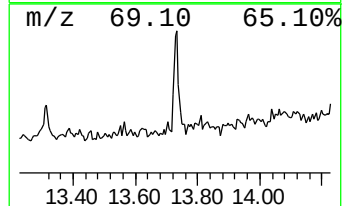
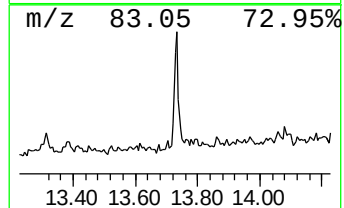
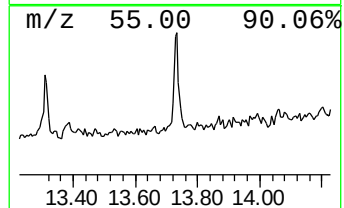
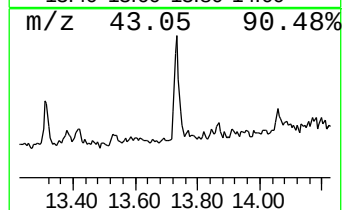
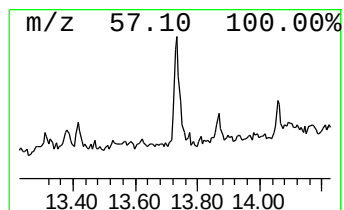
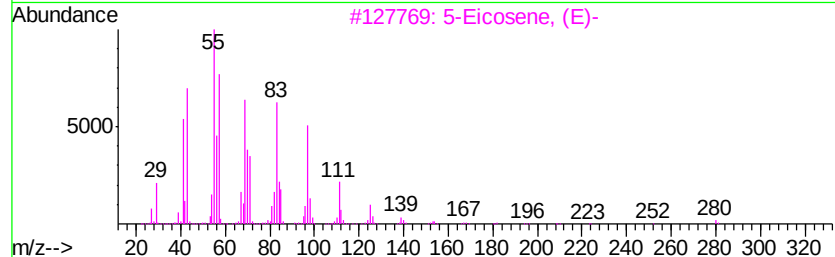
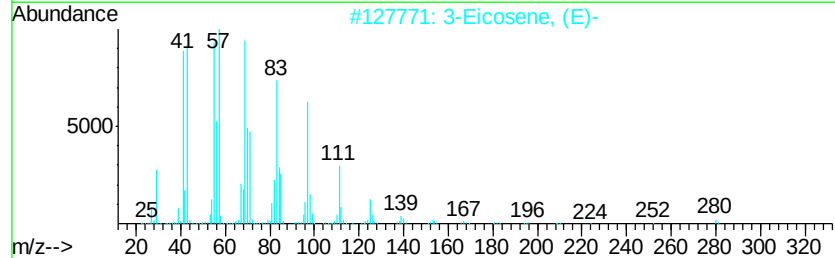
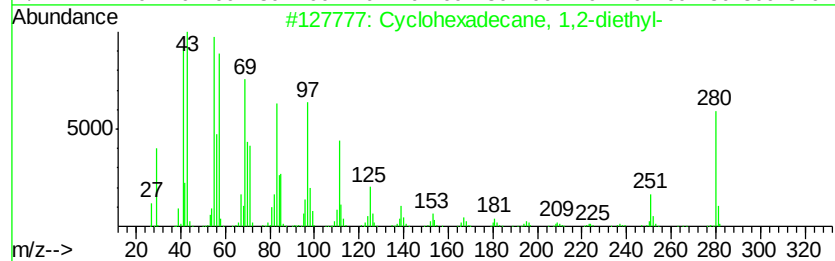
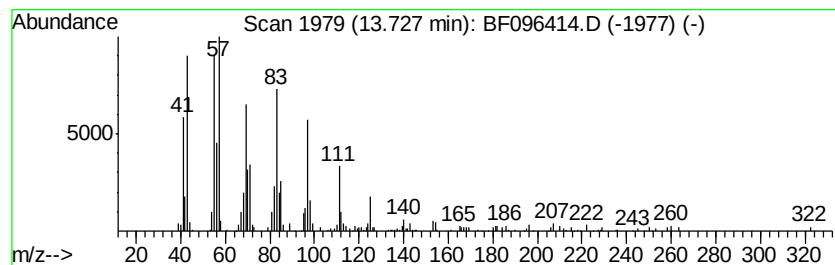
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.38 ng	170581	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane, 1,2-diethyl-	280 C20H40	1000155-85-3 94
2		3-Eicosene, (E)-	280 C20H40	074685-33-9 93
3		5-Eicosene, (E)-	280 C20H40	074685-30-6 92
4		Heptafluorobutyric acid, hexadec...	438 C20H33F7O2	006385-15-5 91
5		n-Tetracosanol-1	354 C24H50O	000506-51-4 90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
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Operator : SJ/MA
Sample : I3950-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

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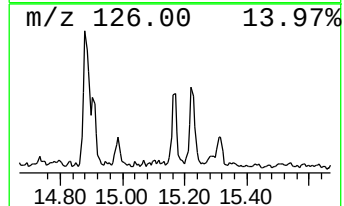
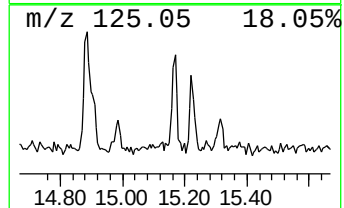
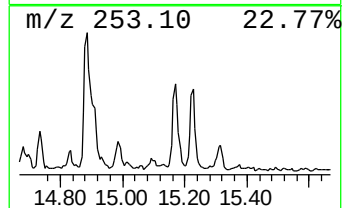
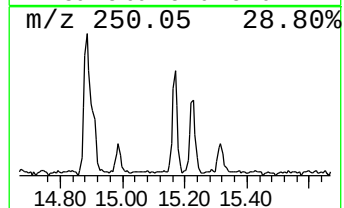
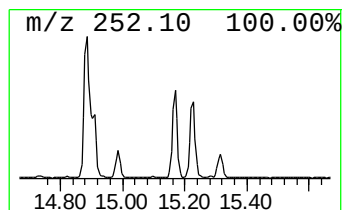
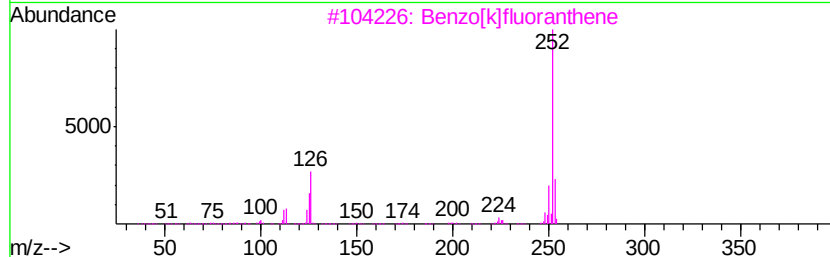
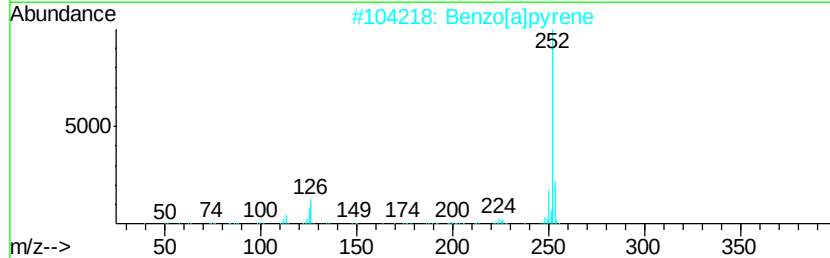
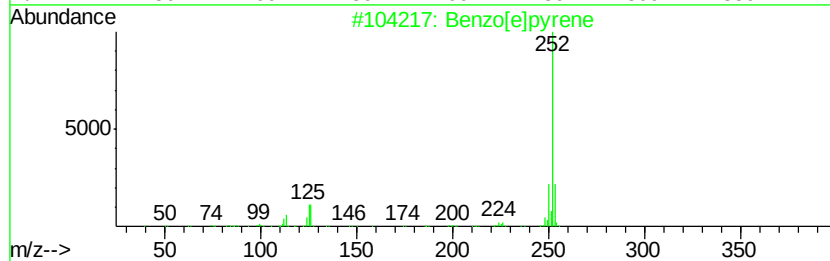
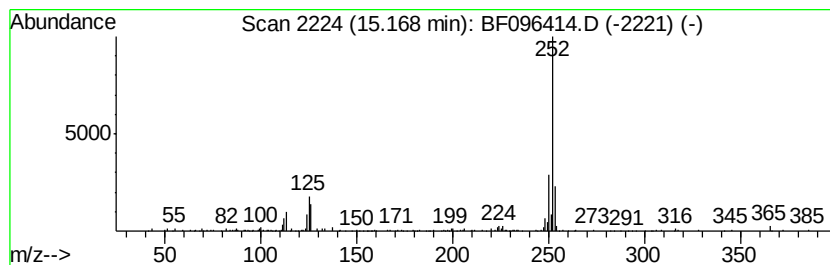
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	5.49 ng	148152	Perylene-d12	15.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



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Sample : I3950-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B5-4-6

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	11.1 ng		590983	1	6.73	1062670	20.0
unknown6.50	6.50	63.9 ng		3393110	1	6.73	1062670	20.0
Tridecane	10.68	3.8 ng		172440	4	11.24	918286	20.0
n-Hexadecanoic acid	11.78	2.6 ng		120244	4	11.24	918286	20.0
Benzeneethanamine...	13.31	3.4 ng		169447	5	13.87	1010180	20.0
Cyclohexadecane, ...	13.73	3.4 ng		170581	5	13.87	1010180	20.0
Benzo[e]pyrene	15.17	5.5 ng		148152	6	15.29	539474	20.0