

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
 Data File : BF104284.D
 Acq On : 5 Apr 2018 21:53
 Operator : JU/SJ
 Sample : J2239-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-1-COMP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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	2.298	31	36	44	rVB	110668	160551	3.99%	0.451%
2	5.204	526	530	541	rBV	51168	110424	2.75%	0.310%
3	5.581	591	594	624	rBV	1490317	2980001	74.13%	8.369%
4	6.586	761	765	784	rBV	1569225	3244318	80.70%	9.111%
5	6.716	784	787	819	rVV	2243680	4020201	100.00%	11.290%
6	6.951	823	827	848	rVV	203723	733883	18.25%	2.061%
7	7.098	848	852	889	rVB	1868036	2843872	70.74%	7.986%
8	7.516	919	923	945	rBV	941701	2101296	52.27%	5.901%
9	7.657	945	947	964	rVB4	49444	130873	3.26%	0.368%
10	8.227	1040	1044	1085	rBV	427197	967989	24.08%	2.718%
11	9.298	1222	1226	1255	rBV	2742027	3882658	96.58%	10.904%
12	9.686	1287	1292	1306	rBV	172684	262333	6.53%	0.737%
13	9.886	1323	1326	1330	rBV	52115	45574	1.13%	0.128%
14	9.980	1338	1342	1361	rBV	829487	1098555	27.33%	3.085%
15	10.386	1409	1411	1415	rVB	78193	59663	1.48%	0.168%
16	10.780	1474	1478	1489	rBV	1598075	2408692	59.91%	6.764%
17	10.857	1489	1491	1506	rVB	114793	231498	5.76%	0.650%
18	11.310	1564	1568	1571	rBV	48556	48293	1.20%	0.136%
19	11.480	1593	1597	1609	rBV2	651293	1261309	31.37%	3.542%
20	11.980	1679	1682	1686	rBV3	69943	99295	2.47%	0.279%
21	12.015	1686	1688	1695	rVB3	30697	46165	1.15%	0.130%
22	12.527	1772	1775	1779	rBV	34778	41092	1.02%	0.115%
23	12.698	1800	1804	1813	rBV	301265	448045	11.14%	1.258%
24	12.857	1827	1831	1837	rBV6	32461	47204	1.17%	0.133%
25	12.927	1837	1843	1849	rBV	333350	506272	12.59%	1.422%
26	13.062	1862	1866	1877	rBV	2592434	3230149	80.35%	9.071%
27	13.262	1892	1900	1905	rVB	40959	81540	2.03%	0.229%
28	13.362	1914	1917	1924	rVB3	53065	89536	2.23%	0.251%
29	13.457	1929	1933	1936	rBV	38623	52160	1.30%	0.146%
30	13.486	1936	1938	1944	rVB3	28663	40647	1.01%	0.114%
31	13.821	1992	1995	1999	rVB	43005	42648	1.06%	0.120%
32	13.862	1999	2002	2003	rBV	47521	45985	1.14%	0.129%
33	13.886	2003	2006	2011	rVV2	62947	108981	2.71%	0.306%
34	13.933	2011	2014	2019	rVV5	138267	206728	5.14%	0.581%

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35	13.974	2019	2021	2030	rVB7	42779	99257	2.47%	0.279%
36	14.133	2042	2048	2051	rBV2	686081	1027244	25.55%	2.885%
37	14.209	2058	2061	2064	rVB2	45738	54023	1.34%	0.152%
38	14.504	2105	2111	2112	rBV2	59675	74551	1.85%	0.209%
39	14.521	2112	2114	2118	rVV	82150	101075	2.51%	0.284%
40	14.562	2118	2121	2125	rVV2	61814	76908	1.91%	0.216%
41	14.868	2168	2173	2180	rBV3	66773	143388	3.57%	0.403%
42	14.927	2180	2183	2185	rVV	35273	45784	1.14%	0.129%
43	14.956	2185	2188	2193	rVB2	97387	130233	3.24%	0.366%
44	15.039	2198	2202	2210	rBV10	44688	88191	2.19%	0.248%
45	15.215	2227	2232	2247	rBV	169278	563219	14.01%	1.582%
46	15.533	2282	2286	2294	rBV	113122	218296	5.43%	0.613%
47	15.603	2294	2298	2305	rVV	134638	278728	6.93%	0.783%
48	15.668	2305	2309	2324	rVB	332169	701755	17.46%	1.971%
49	16.074	2375	2378	2384	rVB2	42963	68466	1.70%	0.192%
50	17.256	2571	2579	2590	rBV5	47252	159395	3.96%	0.448%
51	17.733	2654	2660	2663	rBV3	46555	100259	2.49%	0.282%

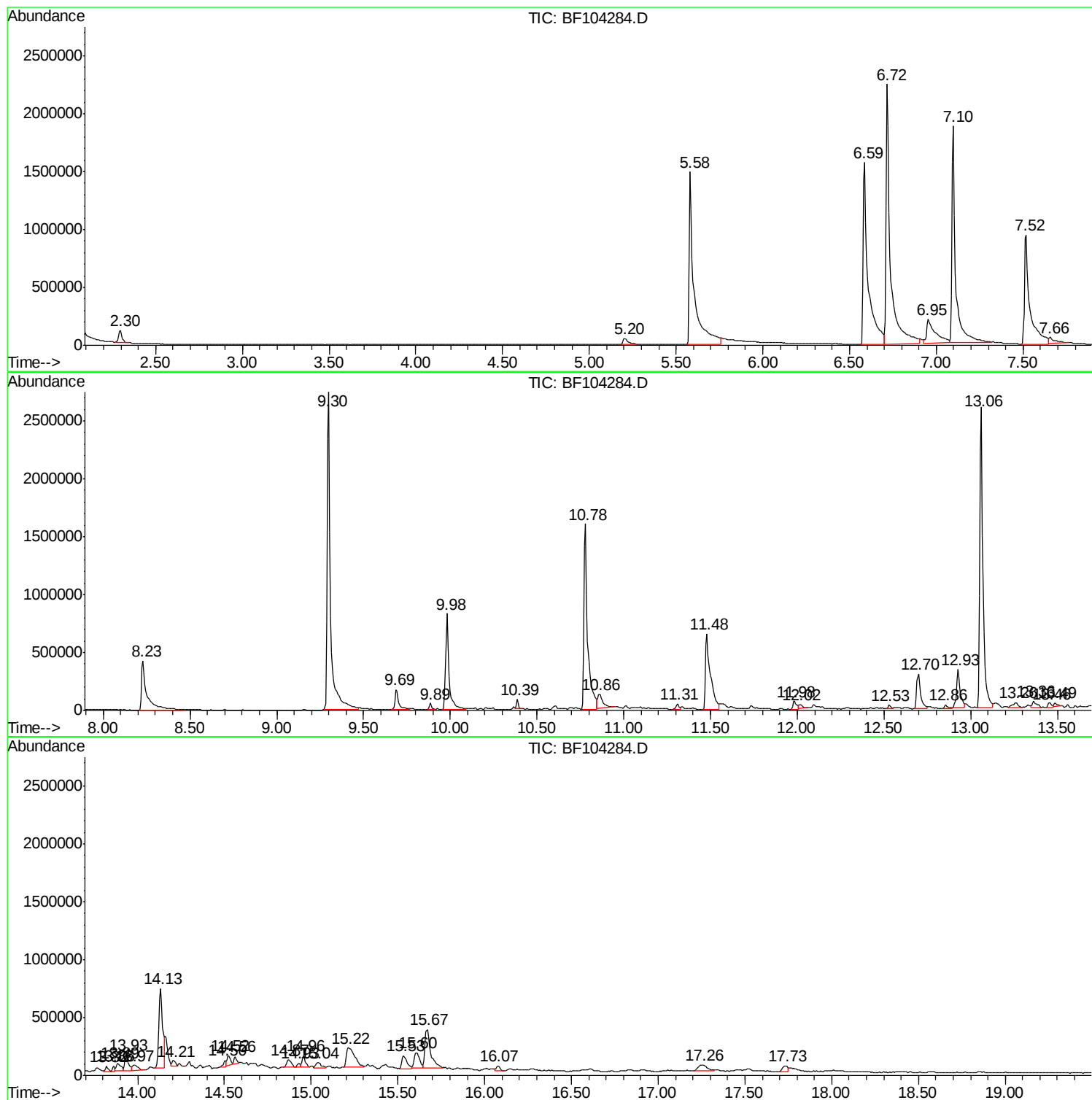
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ClientSampled :
S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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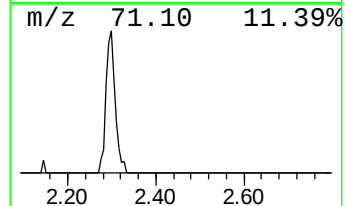
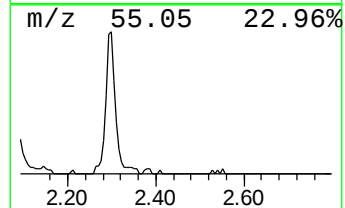
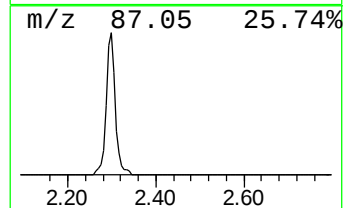
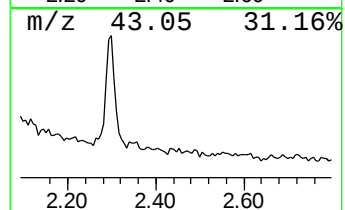
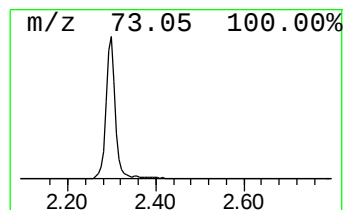
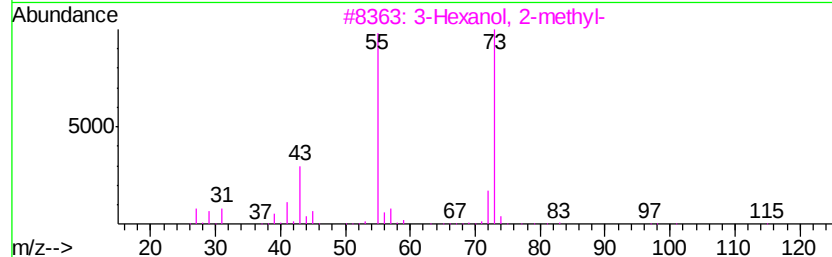
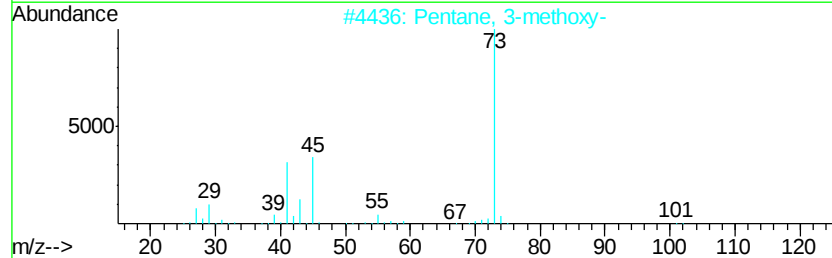
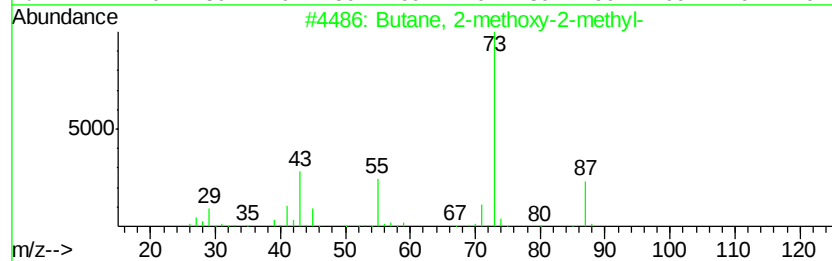
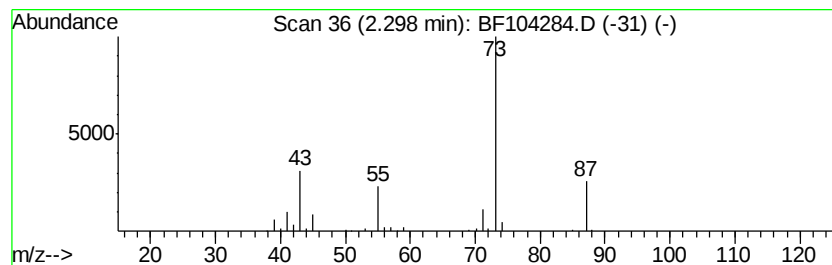
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	4.38 ng	160551	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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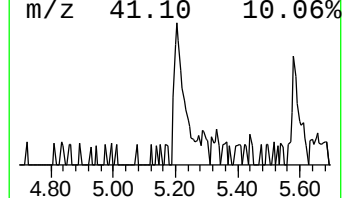
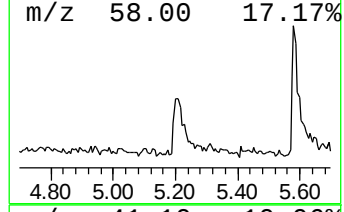
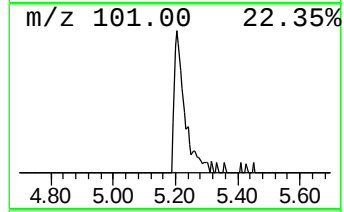
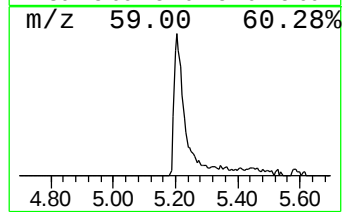
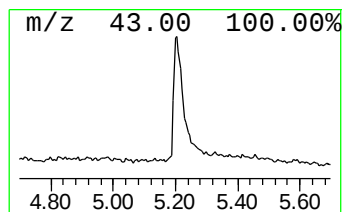
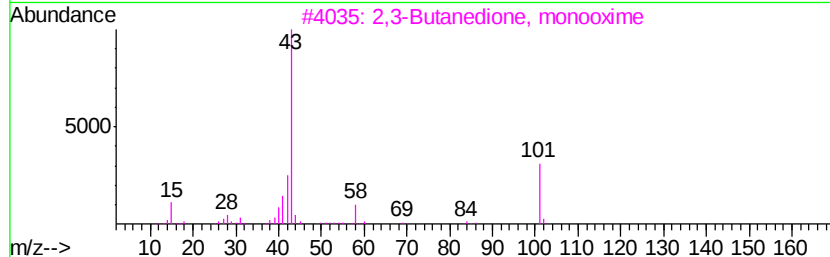
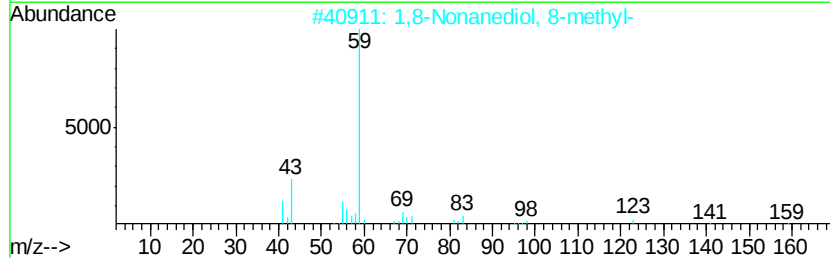
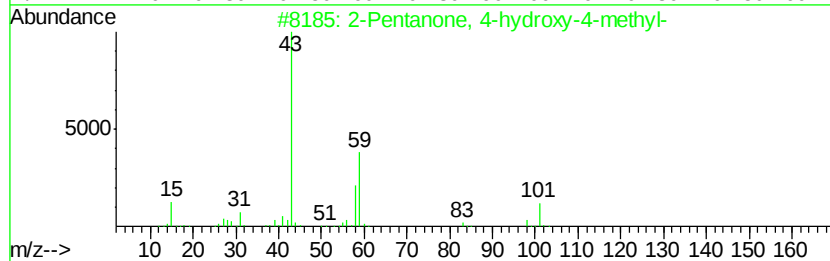
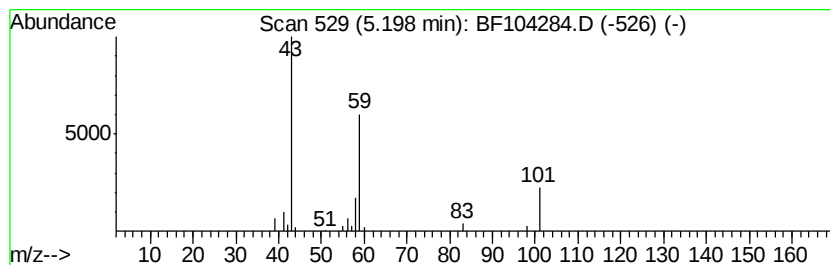
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.01 ng	110424	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	17
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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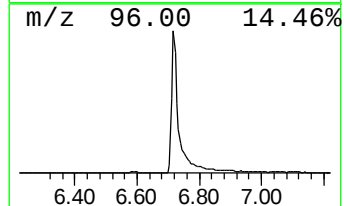
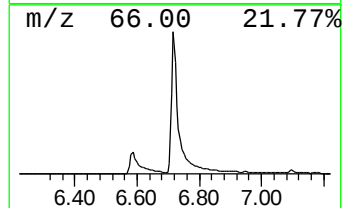
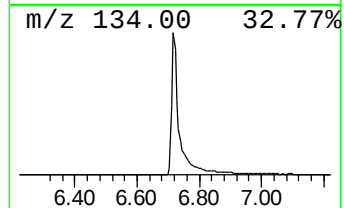
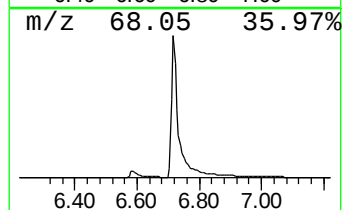
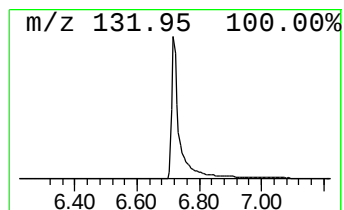
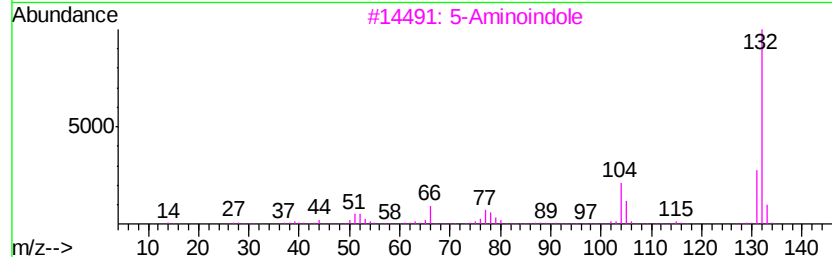
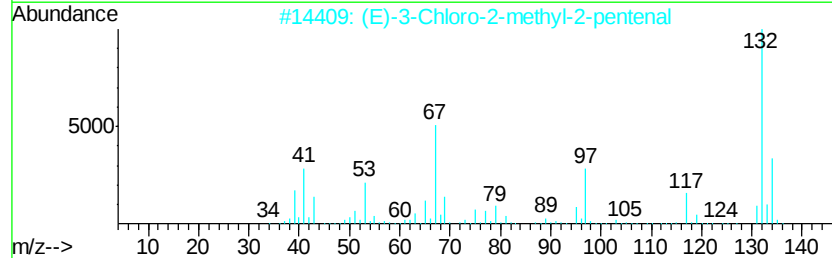
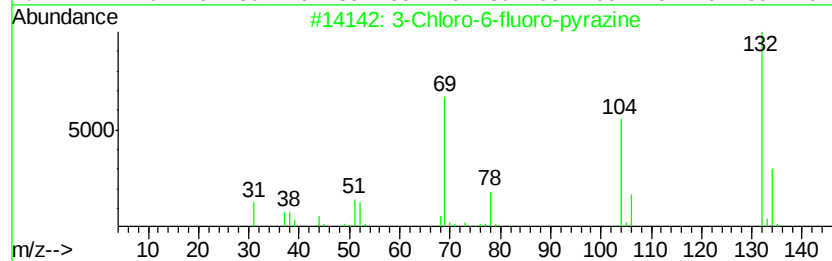
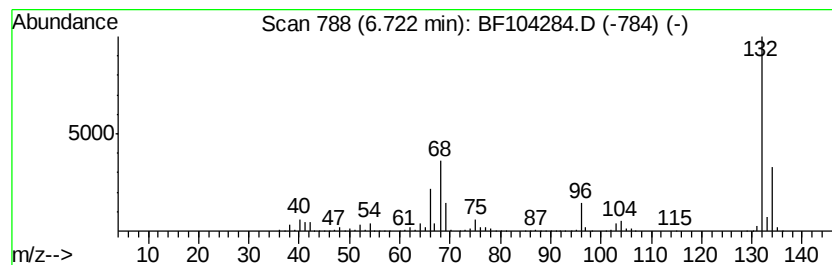
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	109.56 ng	4020200	1,4-Dichlorobenzene-d4	6.95

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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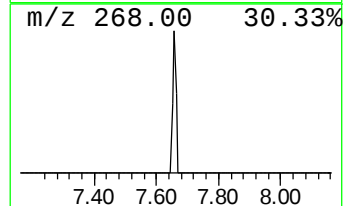
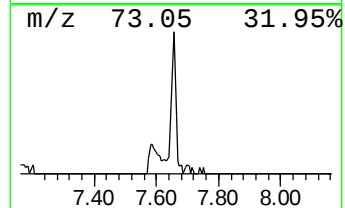
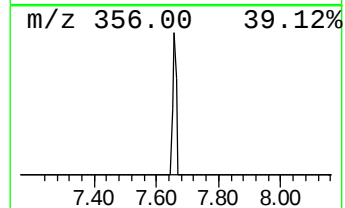
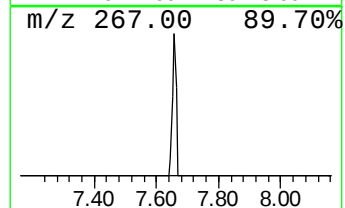
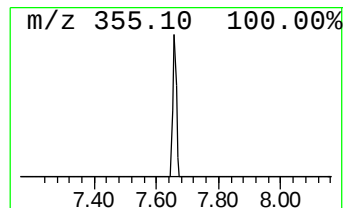
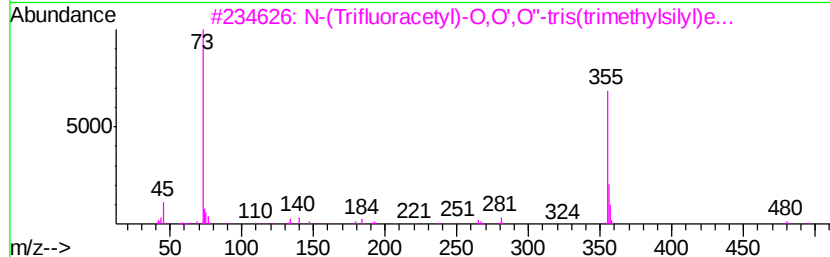
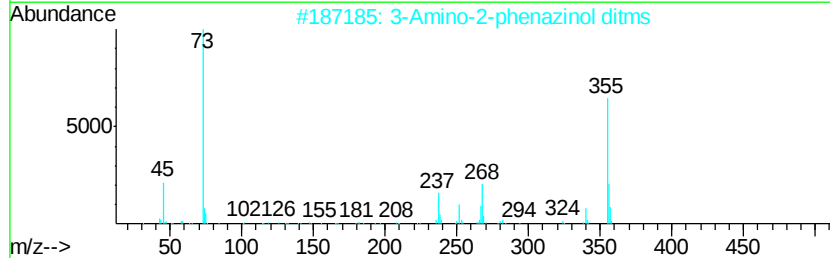
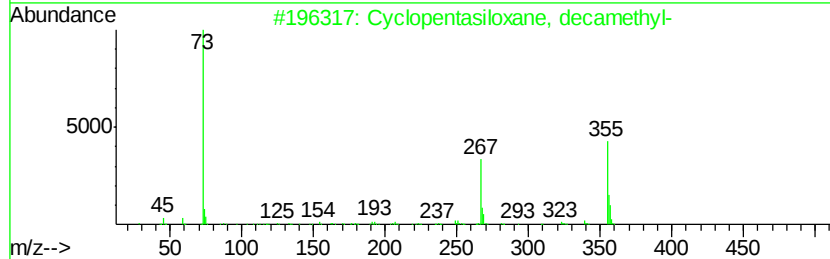
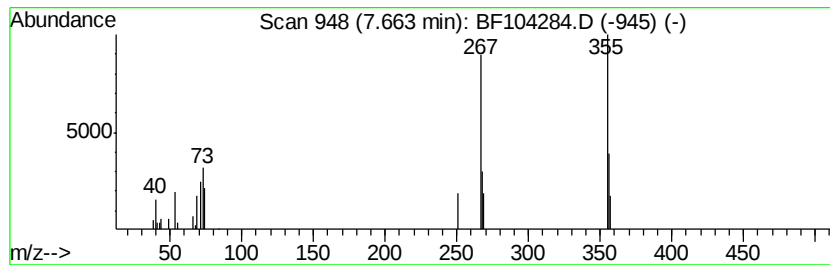
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentasiloxane, decamet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	2.70 ng	130873	Naphthalene-d8	8.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	83
2		3-Amino-2-phenazinol ditms	355	C18H25N3OSi2	1000332-15-5	50
3		N-(Trifluoroacetyl)-O,O',O''-tris...	495	C20H36F3N04Si3	054135-51-2	43
4		N-(Trifluoroacetyl)-N,O,O',O''-t...	553	C22H42F3N04Si4	1000072-26-7	43
5		N-(Trifluoroacetyl)-O,O',O''-tri...	481	C19H34F3N04Si3	1000072-26-3	43



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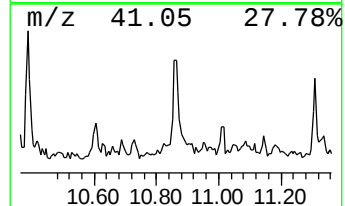
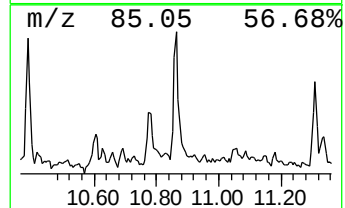
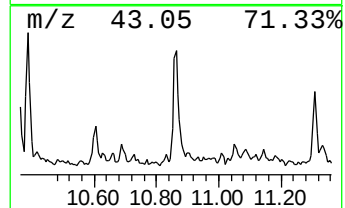
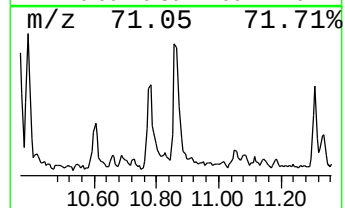
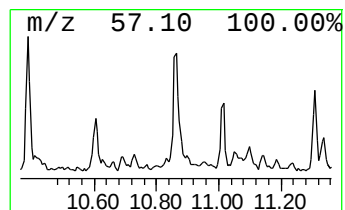
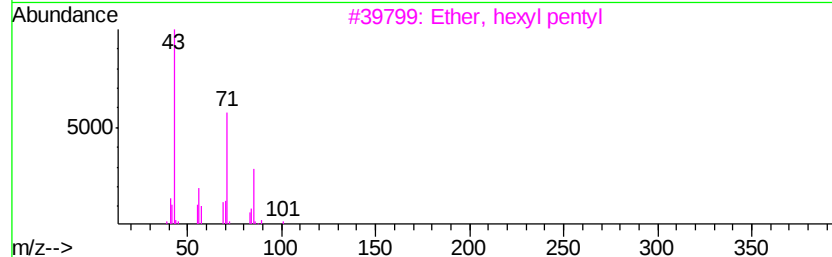
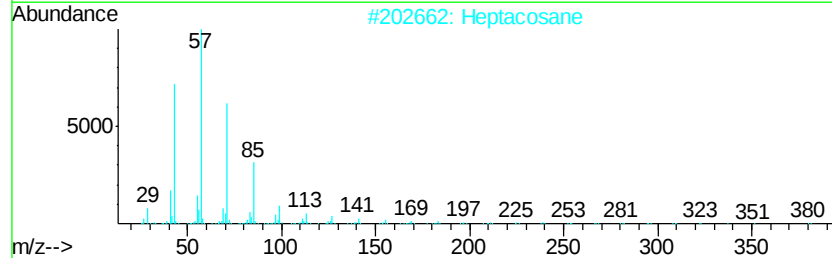
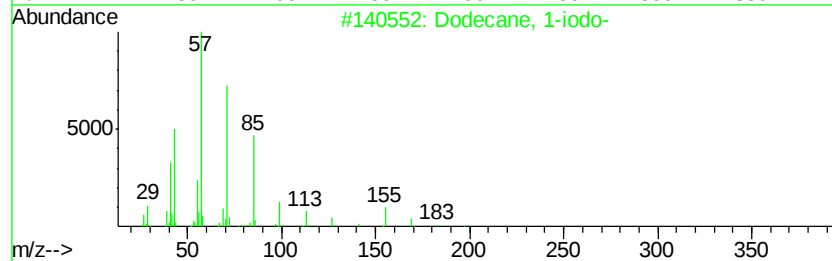
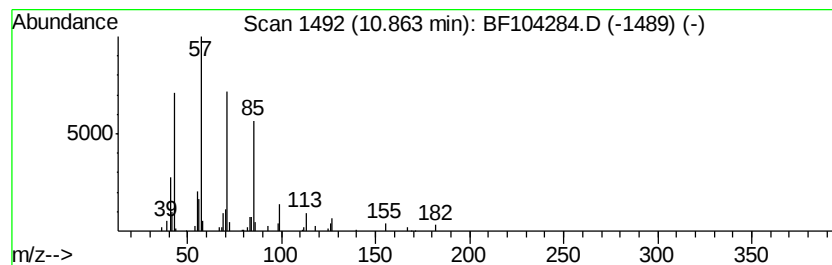
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	3.67 ng	231498	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86	
2	Heptacosane	380	C27H56	000593-49-7	83	
3	Ether, hexyl pentyl	172	C11H24O	032357-83-8	64	
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64	
5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
Data File : BF104284.D
Acq On : 5 Apr 2018 21:53
Operator : JU/SJ
Sample : J2239-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1-COMP

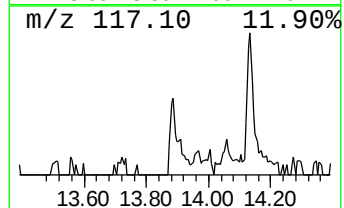
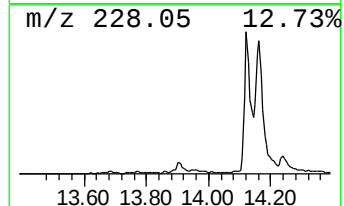
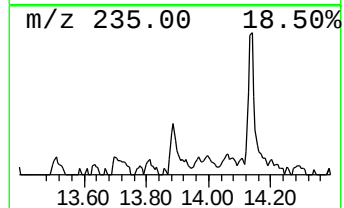
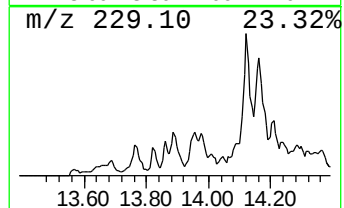
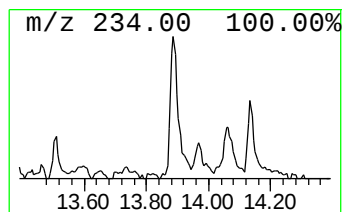
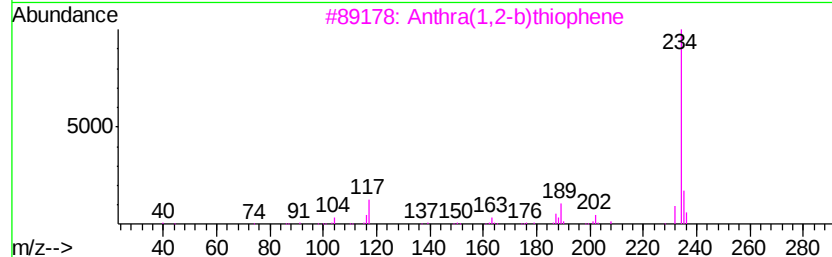
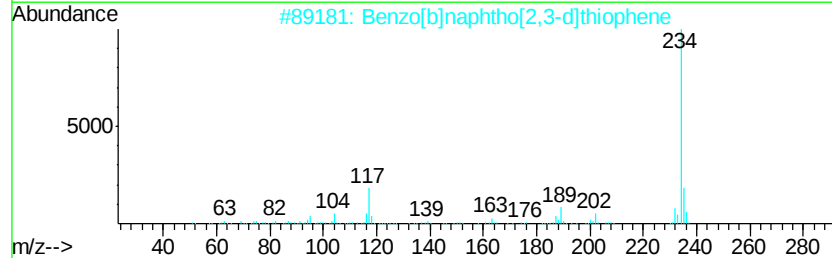
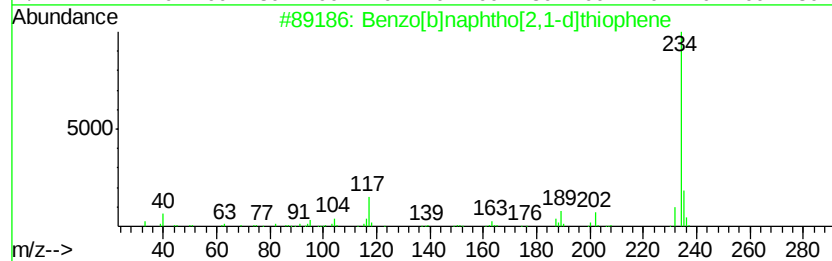
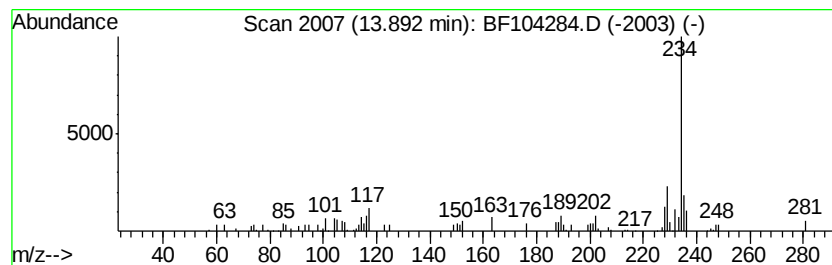
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.12 ng	108981	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	93
2		Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	86
3		Anthra(1,2-b)thiophene	234	C16H10S	000227-86-1	64
4		Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	50
5		Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
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Sample : J2239-01
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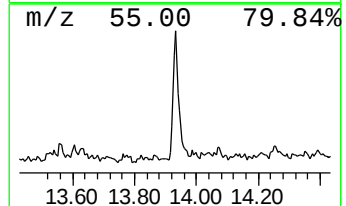
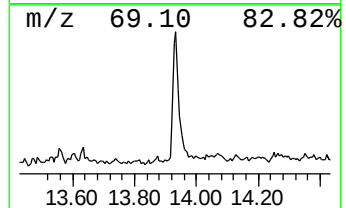
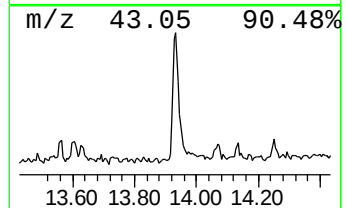
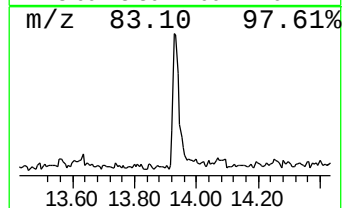
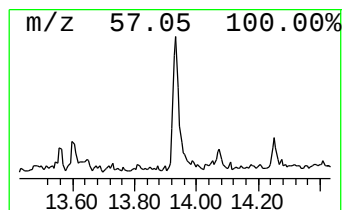
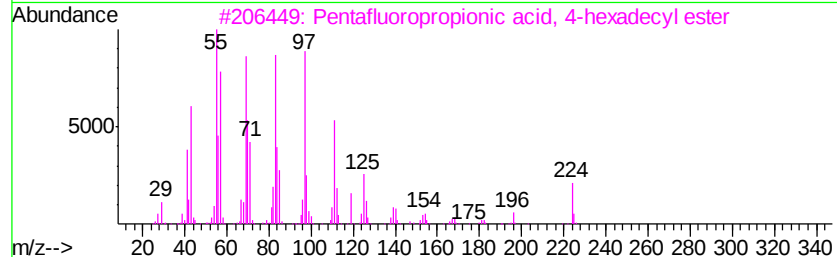
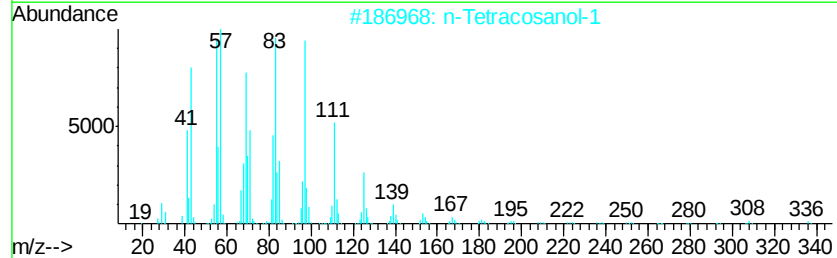
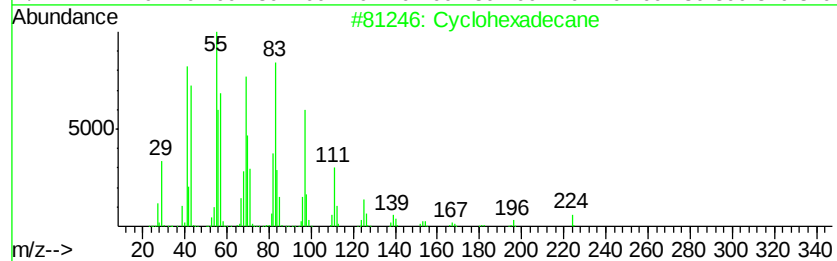
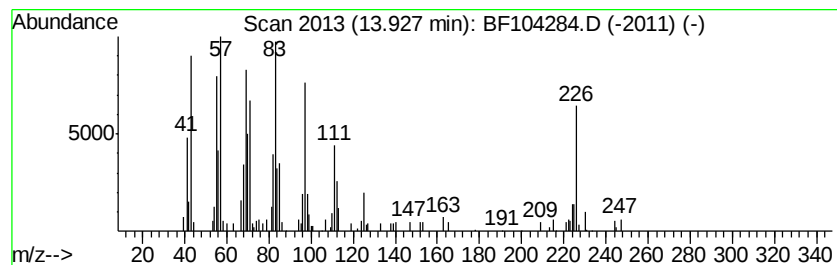
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.93	4.02 ng	206728	Chrysene-d12	14.13	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclohexadecane	224	C16H32	000295-65-8	98
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
3	Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	70
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	64
5	Cetene	224	C16H32	000629-73-2	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
Data File : BF104284.D
Acq On : 5 Apr 2018 21:53
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Sample : J2239-01
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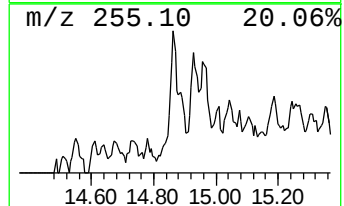
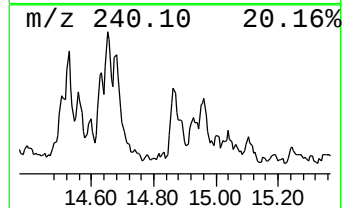
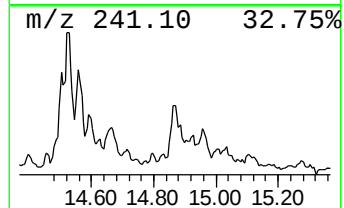
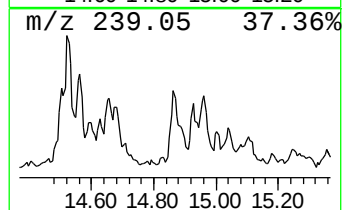
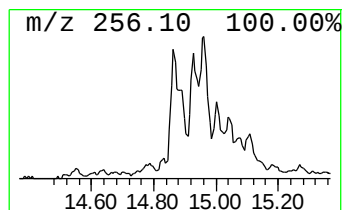
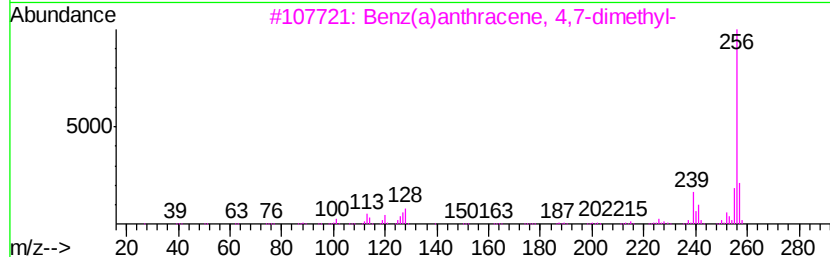
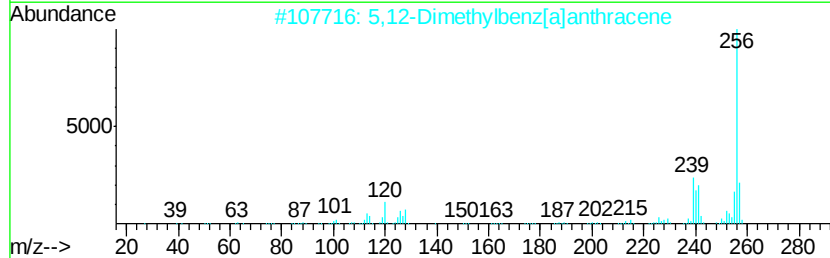
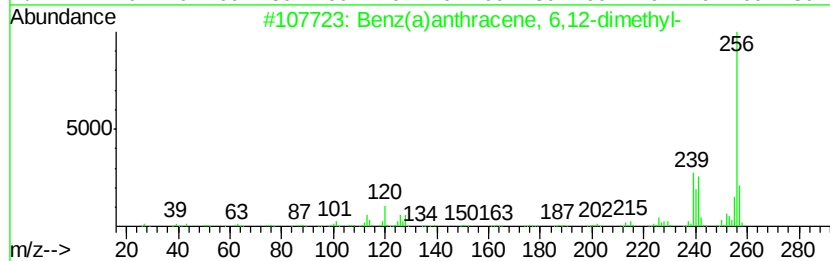
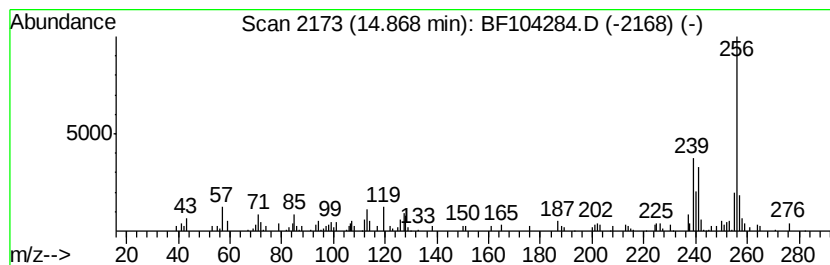
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benz(a)anthracene, 6,12-dim... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.79 ng	143388	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz(a)anthracene, 6,12-dimethyl-	256	C20H16	000568-81-0	91
2		5,12-Dimethylbenz[a]anthracene	256	C20H16	021297-22-3	91
3		Benz(a)anthracene, 4,7-dimethyl-	256	C20H16	035187-18-9	90
4		Benz[a]anthracene, 7,12-dimethyl-	256	C20H16	000057-97-6	90
5		4,12-Dimethylbenz[a]anthracene	256	C20H16	035187-19-0	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
Data File : BF104284.D
Acq On : 5 Apr 2018 21:53
Operator : JU/SJ
Sample : J2239-01
Misc :
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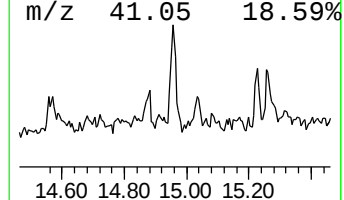
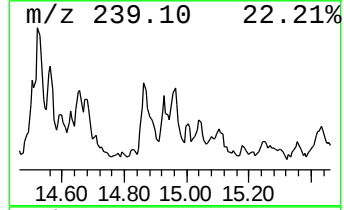
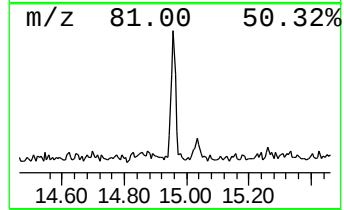
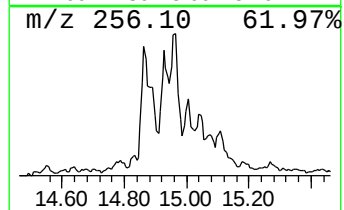
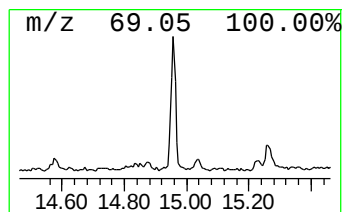
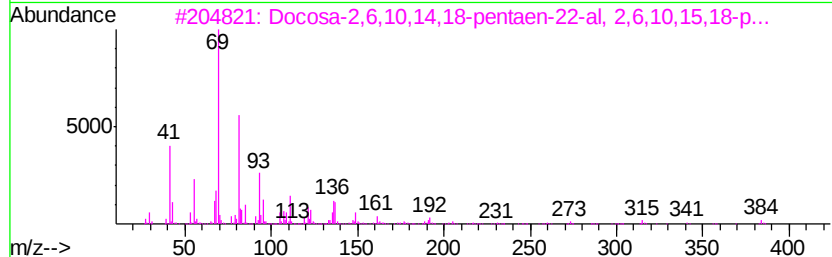
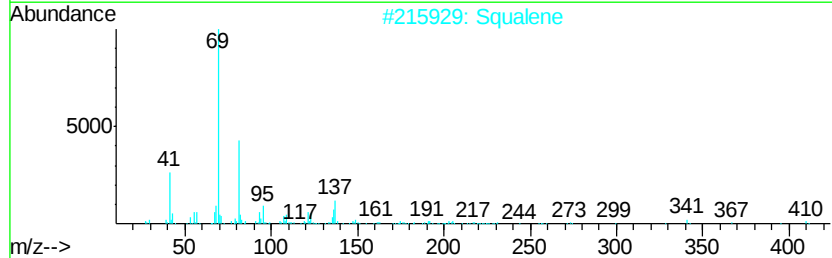
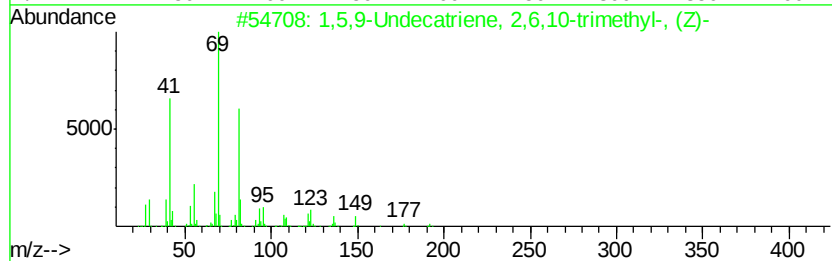
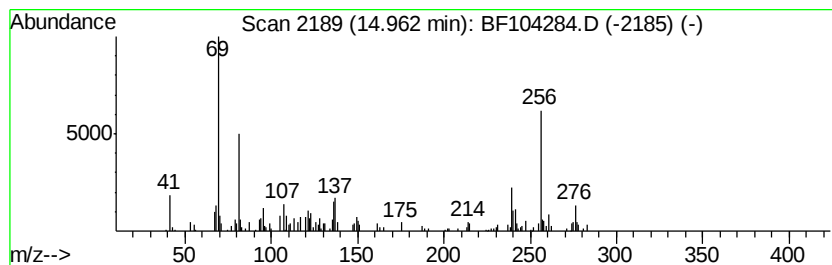
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.71 ng	130233	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	46
2			Squalene	410	C30H50	000111-02-4	45
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	43
4			Supraene	410	C30H50	007683-64-9	43
5			2,6-Dimethyl-2-trans-6-octadiene	138	C10H18	002609-23-6	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
Data File : BF104284.D
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Operator : JU/SJ
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Misc :
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ClientSampleId :
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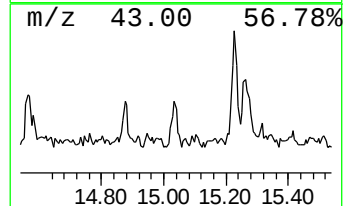
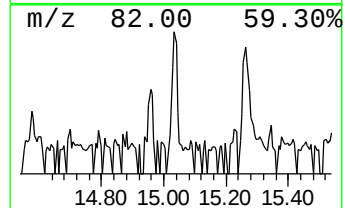
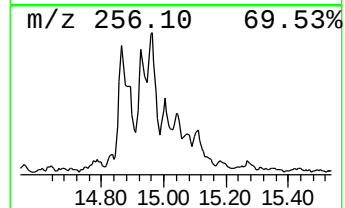
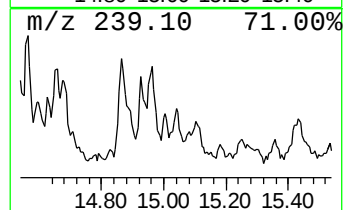
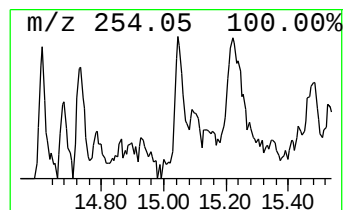
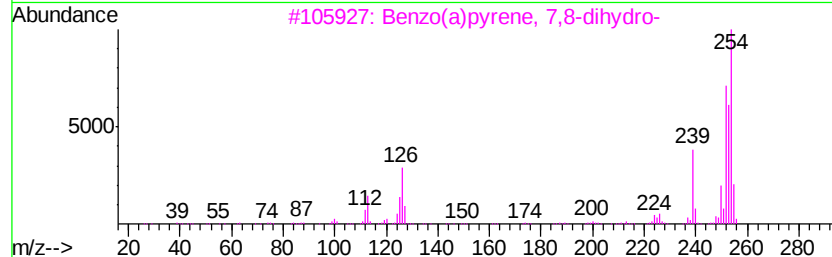
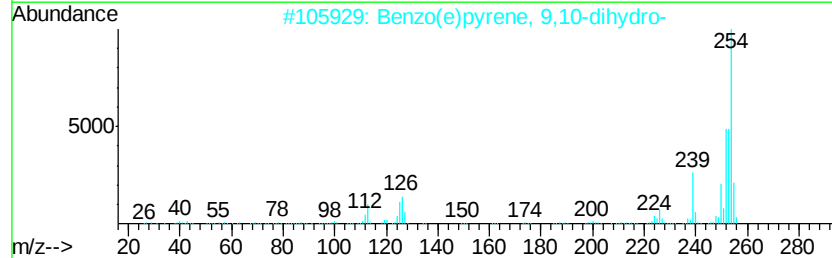
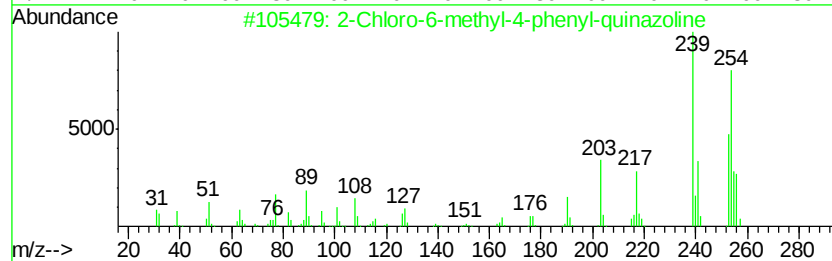
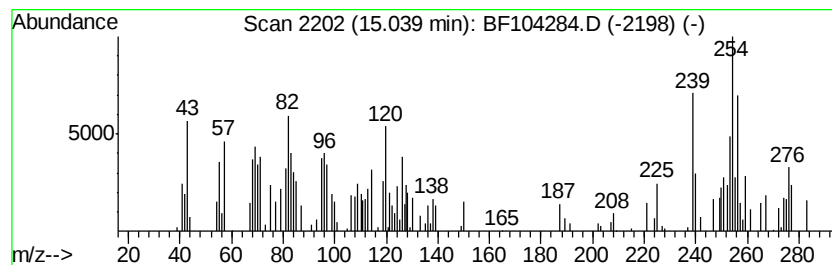
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.04 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	2.51 ng	88191	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-6-methyl-4-phenyl-quinazoline...	254	C15H11ClN2	1000317-62-9	47
2			Benzo(e)pyrene, 9,10-dihydro-	254	C20H14	066788-01-0	43
3			Benzo(a)pyrene, 7,8-dihydro-	254	C20H14	017573-23-8	43
4			6,6'-Biazulene,	254	C20H14	073393-11-0	38
5			4-Bromo-7-methylbenzo(b)thiophen...	254	C10H7BrOS	010476-16-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
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Acq On : 5 Apr 2018 21:53
Operator : JU/SJ
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ALS Vial : 14 Sample Multiplier: 1

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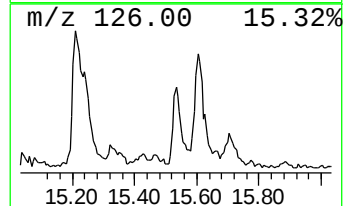
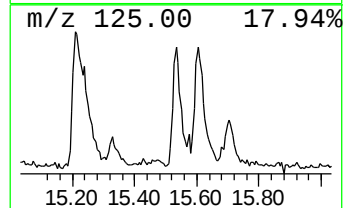
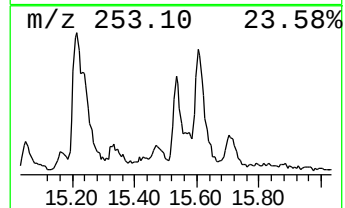
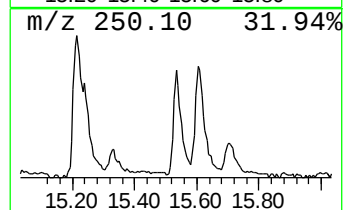
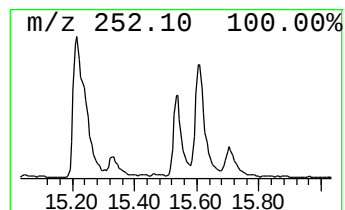
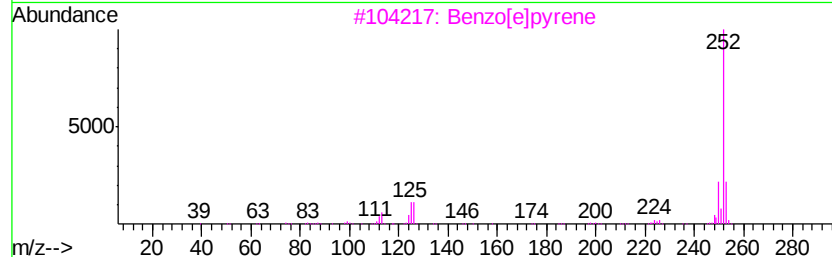
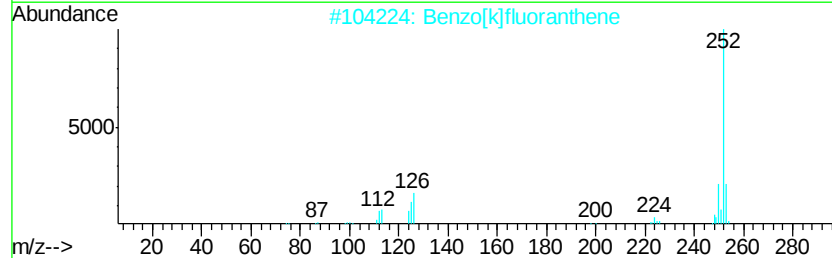
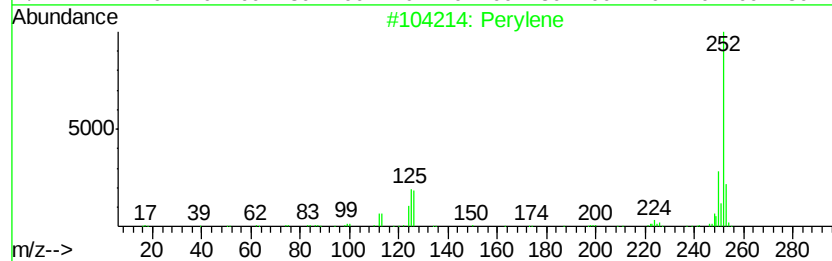
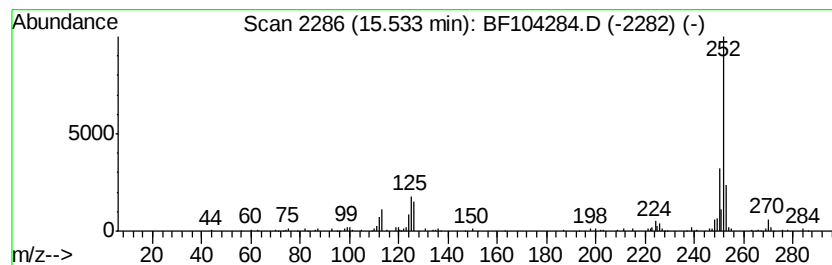
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	6.22 ng	218296	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3		Benzo[e]pyrene	252	C20H12	000192-97-2	97
4		Benzo[i]fluoranthene	252	C20H12	000205-82-3	94
5		Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
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 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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
Butane, 2-methoxy...	2.30	4.4	ng	160551	1	6.95	733883	20.0
2-Pentanone, 4-hy...	5.20	3.0	ng	110424	1	6.95	733883	20.0
unknown6.72	6.72	109.6	ng	4020200	1	6.95	733883	20.0
Cyclopentasiloxan...	7.66	2.7	ng	130873	2	8.23	967989	20.0
Dodecane, 1-iodo-	10.86	3.7	ng	231498	4	11.48	1261310	20.0
Benzo[b]naphtho[2...	13.89	2.1	ng	108981	5	14.13	1027240	20.0
Cyclohexadecane	13.93	4.0	ng	206728	5	14.13	1027240	20.0
Benz(a)anthracene...	14.87	2.8	ng	143388	5	14.13	1027240	20.0
unknown14.96	14.96	3.7	ng	130233	6	15.67	701755	20.0
unknown15.04	15.04	2.5	ng	88191	6	15.67	701755	20.0
Perylene	15.53	6.2	ng	218296	6	15.67	701755	20.0