

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
 Data File : BF091356.D
 Acq On : 30 Nov 2016 16:05
 Operator : UM/SJ
 Sample : H5749-07
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-MM4-4

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-BF112916.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	5.064	240	243	252	rVB	1779007	2891760	34.68%	3.697%
2	5.476	275	279	281	rBV	6001613	7153989	85.81%	9.146%
3	6.504	365	369	371	rBV	5901375	8337218	100.00%	10.659%
4	6.630	377	380	383	rBV	4997255	7602070	91.18%	9.719%
5	6.859	398	400	402	rBV	1210998	1459800	17.51%	1.866%
6	7.019	411	414	417	rVB	4224951	5279531	63.32%	6.750%
7	7.430	446	450	452	rBV	4211605	4644615	55.71%	5.938%
8	8.150	510	513	515	rBV	2146277	2023842	24.27%	2.588%
9	9.225	604	607	610	rBV	5046537	6973248	83.64%	8.915%
10	9.556	634	636	640	rBV	75379	159266	1.91%	0.204%
11	9.613	640	641	644	rVV	464751	550792	6.61%	0.704%
12	9.899	664	666	668	rVV	2061074	1901395	22.81%	2.431%
13	10.105	681	684	685	rVV	131527	112599	1.35%	0.144%
14	10.139	685	687	692	rBV3	71011	88269	1.06%	0.113%
15	10.310	699	702	703	rBV	86294	129129	1.55%	0.165%
16	10.345	703	705	706	rVB	156750	154012	1.85%	0.197%
17	10.448	712	714	715	rVV2	96017	92755	1.11%	0.119%
18	10.688	732	735	737	rBV	4056877	4047824	48.55%	5.175%
19	10.813	744	746	750	rVB	295337	328747	3.94%	0.420%
20	11.122	770	773	777	rBV4	45513	120207	1.44%	0.154%
21	11.259	784	785	786	rVV	219300	191585	2.30%	0.245%
22	11.293	786	788	791	rVB2	80619	122976	1.48%	0.157%
23	11.385	793	796	800	rBV2	1801354	2691693	32.29%	3.441%
24	11.453	800	802	804	rVB	342512	293733	3.52%	0.376%
25	11.682	820	822	826	rVV2	128795	191741	2.30%	0.245%
26	11.888	837	840	841	rBV	142544	246748	2.96%	0.315%
27	11.911	841	842	844	rVV	574884	633236	7.60%	0.810%
28	11.956	844	846	847	rVV2	147594	143486	1.72%	0.183%
29	11.991	847	849	854	rVB2	353287	541593	6.50%	0.692%
30	12.093	854	858	861	rBV3	86806	163912	1.97%	0.210%
31	12.173	863	865	871	rVB3	128674	245611	2.95%	0.314%
32	12.322	875	878	880	rBV4	62442	100267	1.20%	0.128%
33	12.356	880	881	885	rVB	94131	129467	1.55%	0.166%
34	12.436	885	888	889	rBV	135513	200075	2.40%	0.256%

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Integration Parameters: rteint.p
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 Sampling : 1
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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 >
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35	12.471	889	891	893	rBV2	74568	138809	1.66%	0.177%
36	12.516	893	895	897	rVB3	73090	94397	1.13%	0.121%
37	12.596	899	902	904	rBV	1052785	1395702	16.74%	1.784%
38	12.699	909	911	914	rBV3	207998	290509	3.48%	0.371%
39	12.813	918	921	924	rBV2	1022812	1713741	20.56%	2.191%
40	12.871	924	926	929	rVB2	116559	174723	2.10%	0.223%
41	12.973	932	935	937	rVB	4651961	5088495	61.03%	6.506%
42	13.042	937	941	944	rVB3	112270	186471	2.24%	0.238%
43	13.145	947	950	952	rVB	291679	373690	4.48%	0.478%
44	13.214	954	956	957	rVB	271192	221749	2.66%	0.284%
45	13.248	957	959	961	rBV	230672	238938	2.87%	0.305%
46	13.339	965	967	968	rBV	114873	92771	1.11%	0.119%
47	13.374	968	970	972	rBV2	106663	91223	1.09%	0.117%
48	13.499	979	981	984	rBV3	156841	240824	2.89%	0.308%
49	13.545	984	985	988	rVB2	61026	94012	1.13%	0.120%
50	13.648	992	994	997	rVB	85516	114730	1.38%	0.147%
51	13.762	1001	1004	1005	rBV2	139146	204436	2.45%	0.261%
52	13.876	1013	1014	1018	rVB2	217957	220213	2.64%	0.282%
53	14.014	1023	1026	1031	rVB2	1750772	2830429	33.95%	3.619%
54	14.402	1058	1060	1061	rVB	118789	143860	1.73%	0.184%
55	14.436	1061	1063	1064	rBV	74371	93621	1.12%	0.120%
56	14.494	1066	1068	1069	rBV2	94683	91857	1.10%	0.117%
57	15.031	1113	1115	1120	rBV	425232	945949	11.35%	1.209%
58	15.134	1122	1124	1126	rVB	155823	183546	2.20%	0.235%
59	15.328	1139	1141	1144	rVB	286373	359427	4.31%	0.460%
60	15.385	1144	1146	1148	rBV	357216	460733	5.53%	0.589%
61	15.442	1149	1151	1153	rBV	692647	1033873	12.40%	1.322%
62	15.602	1163	1165	1168	rBV2	109090	168625	2.02%	0.216%
63	16.140	1210	1212	1217	rVB3	140130	292513	3.51%	0.374%
64	16.562	1247	1249	1255	rVB2	119958	240517	2.88%	0.308%
65	16.848	1271	1274	1278	rVB2	127452	276773	3.32%	0.354%
66	17.260	1308	1310	1317	rVB	85158	171597	2.06%	0.219%

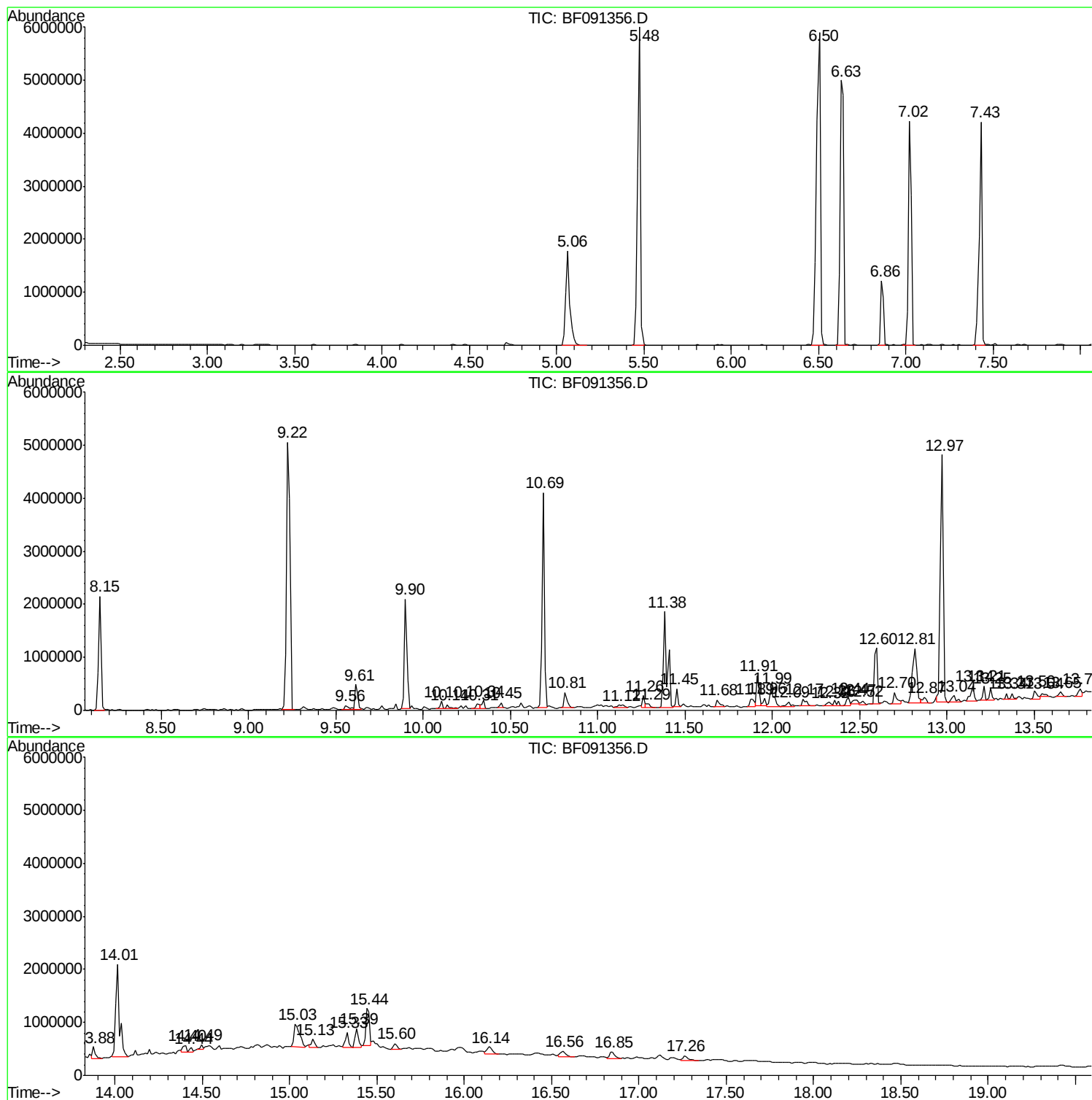
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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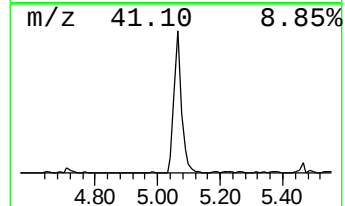
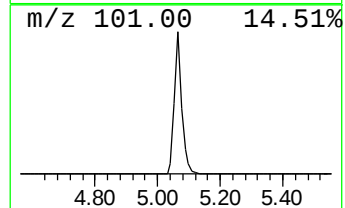
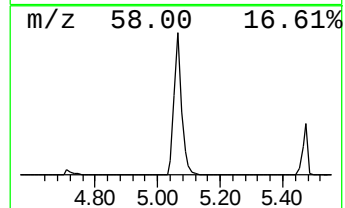
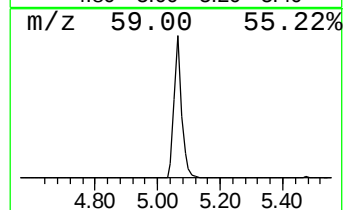
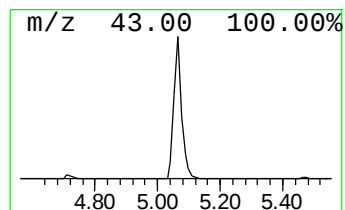
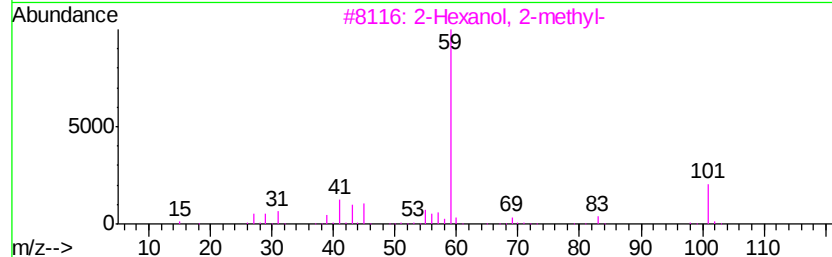
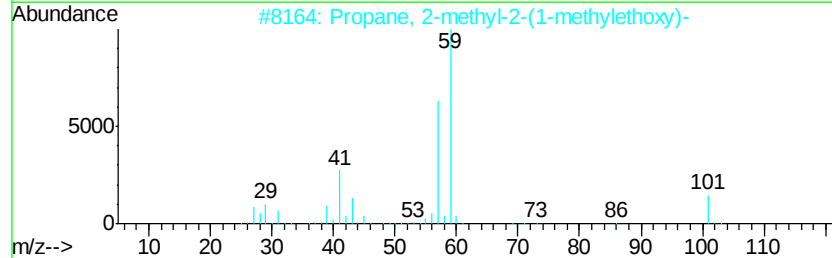
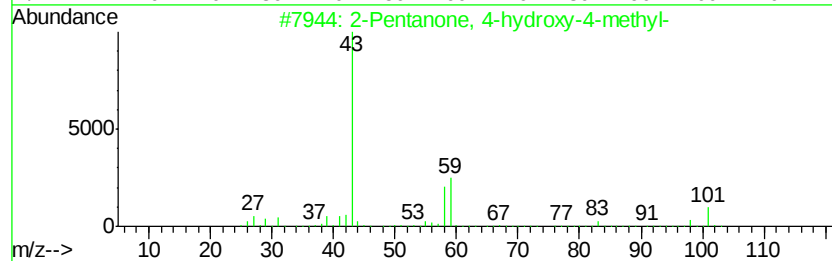
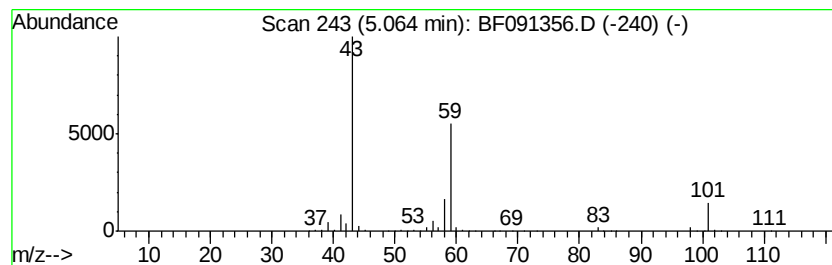
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.06	39.62 ng	2891760	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32



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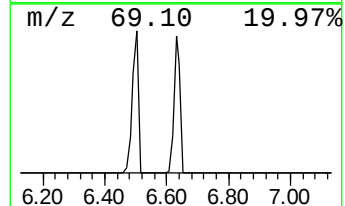
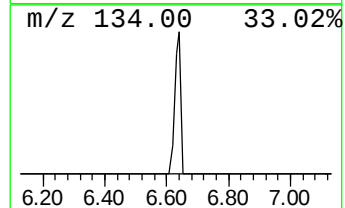
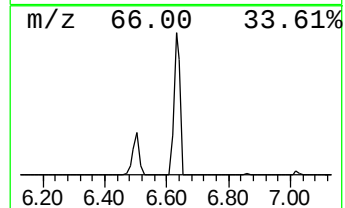
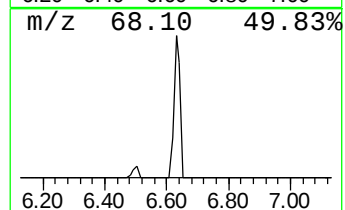
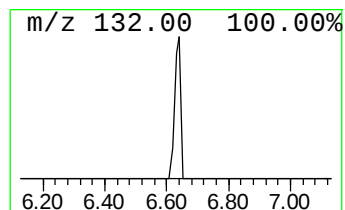
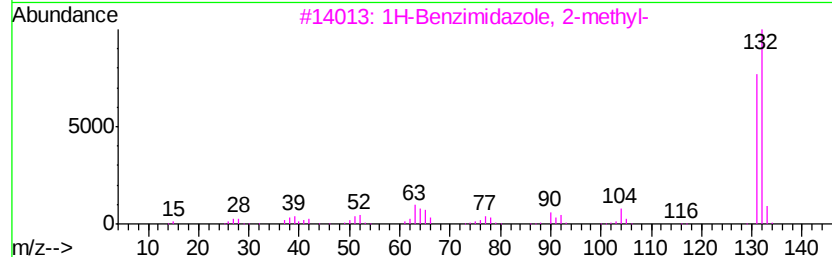
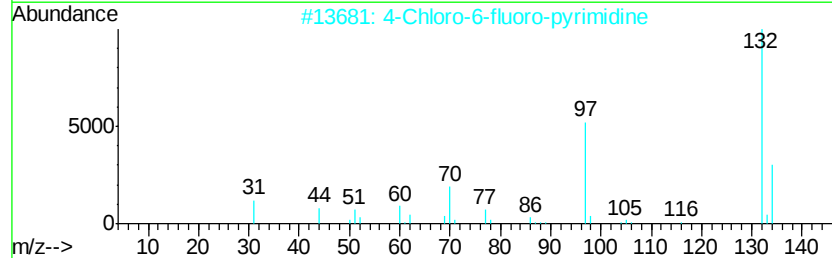
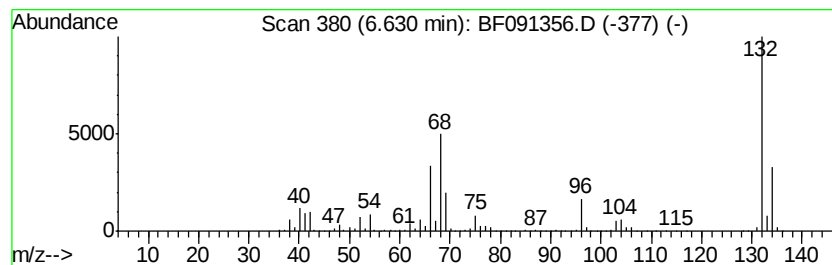
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	104.15 ng	7602070	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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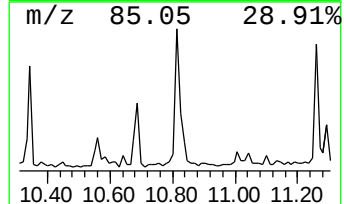
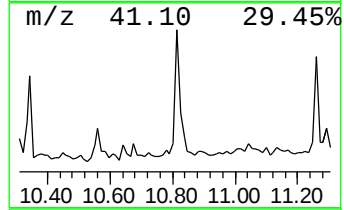
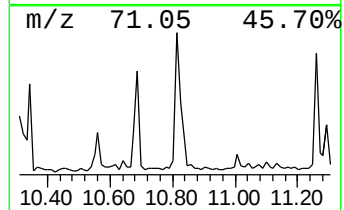
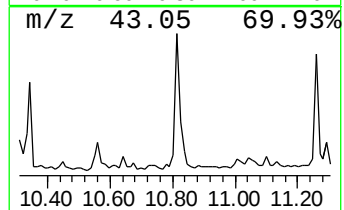
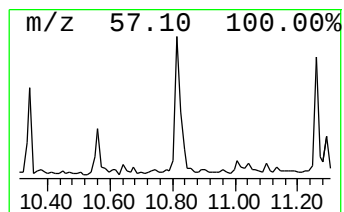
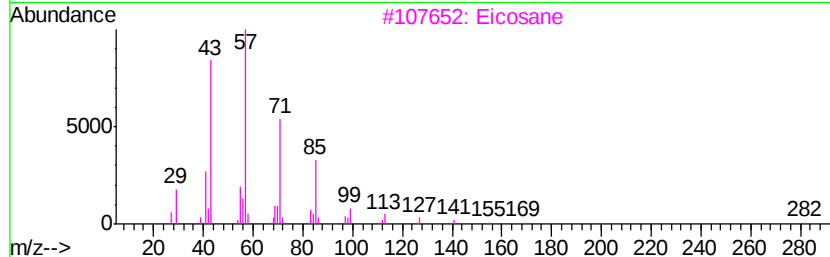
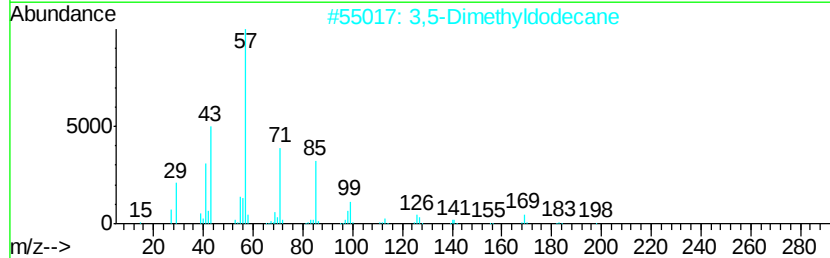
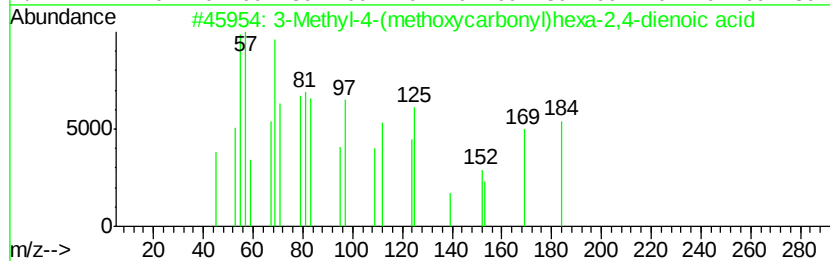
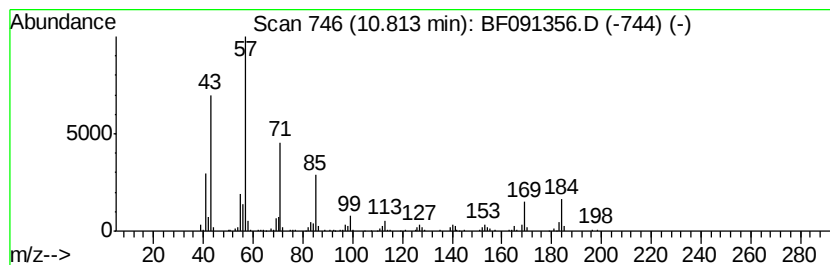
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ClientSampleId :
GRID-MM4-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Methyl-4-(methoxycarbonyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.81	2.44 ng	328747	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	90
2	3,5-Dimethyldodecane	198	C14H30	107770-99-0	81
3	Eicosane	282	C20H42	000112-95-8	70
4	Dodecane	170	C12H26	000112-40-3	64
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	58



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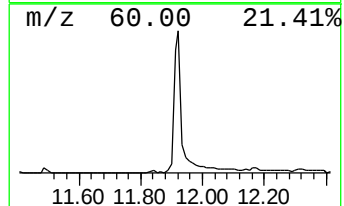
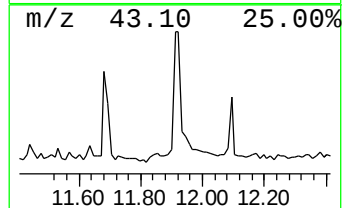
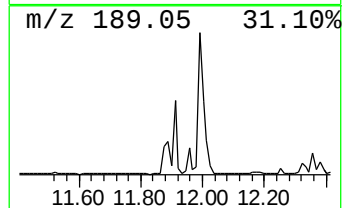
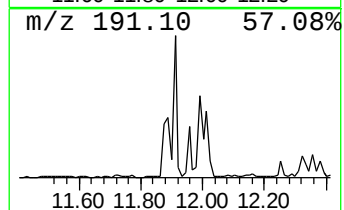
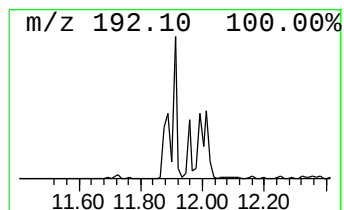
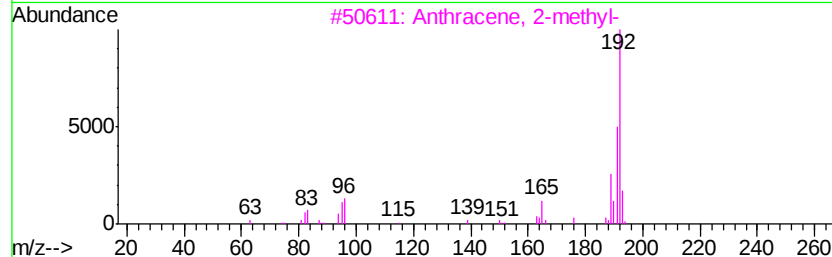
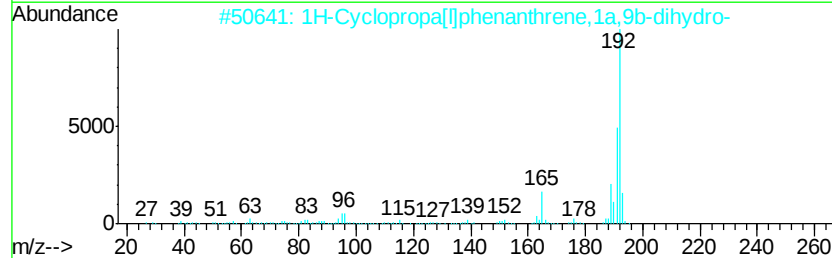
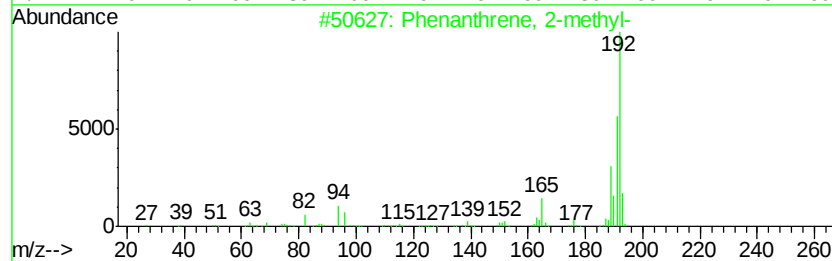
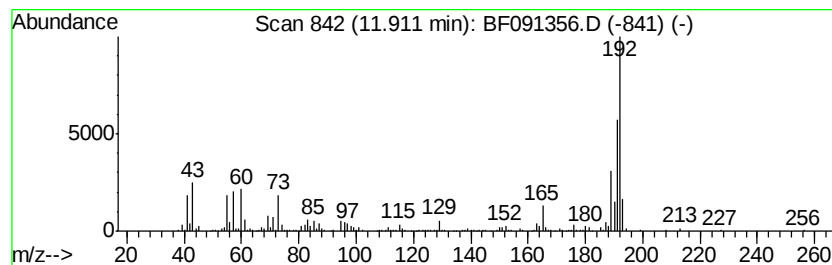
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.91	4.71 ng	633236	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93



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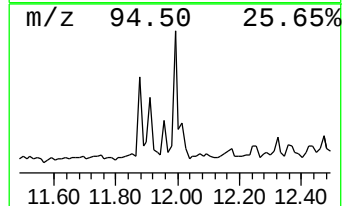
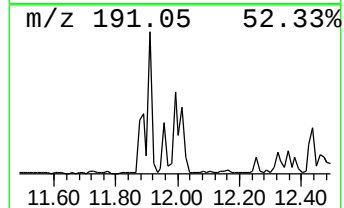
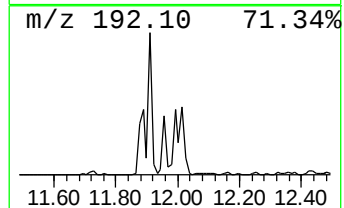
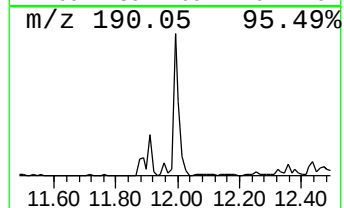
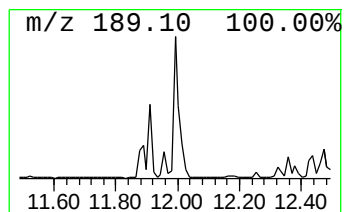
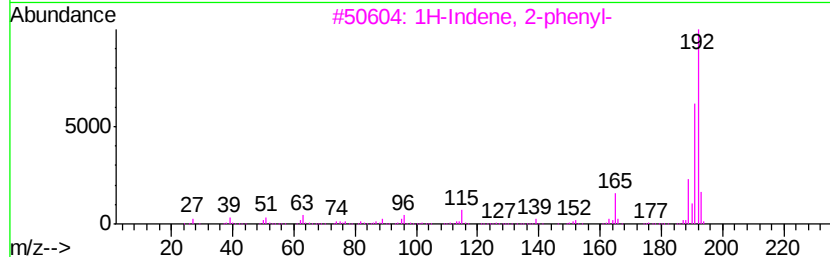
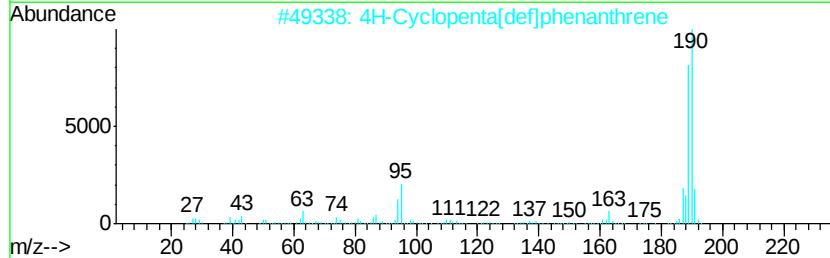
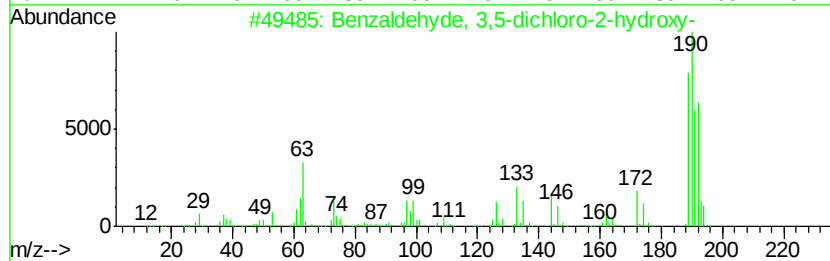
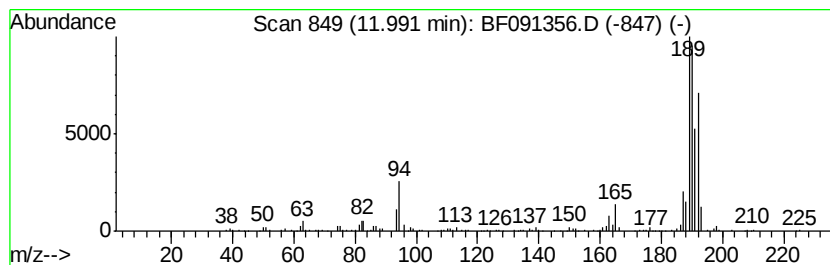
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	4.02 ng	541593	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzaldehydve, 3,5-dichloro-2-hvd...	190	C7H4Cl2O2	000090-60-8	72
2		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
3		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	30
5		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091356.D
Acq On : 30 Nov 2016 16:05
Operator : UM/SJ
Sample : H5749-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-MM4-4

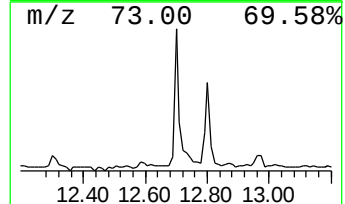
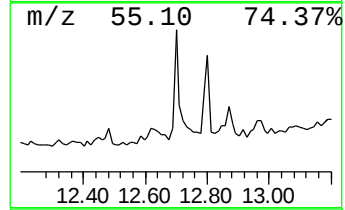
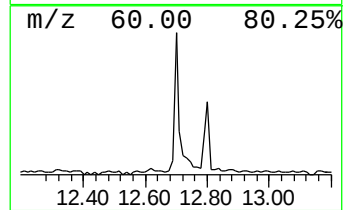
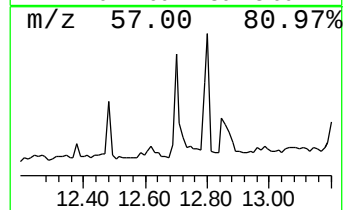
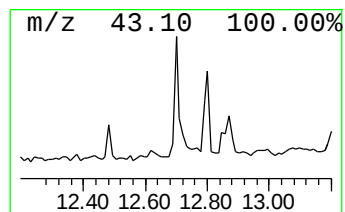
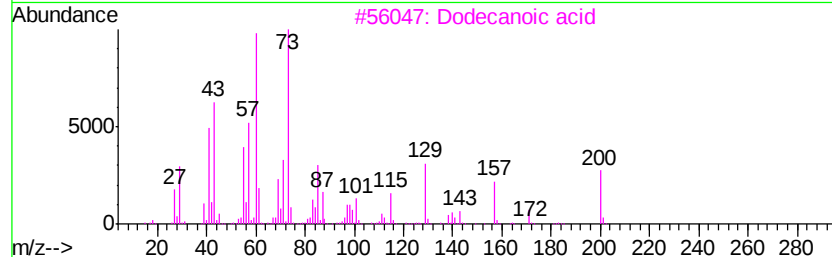
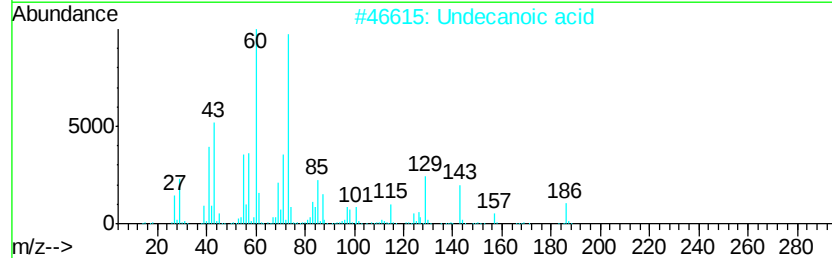
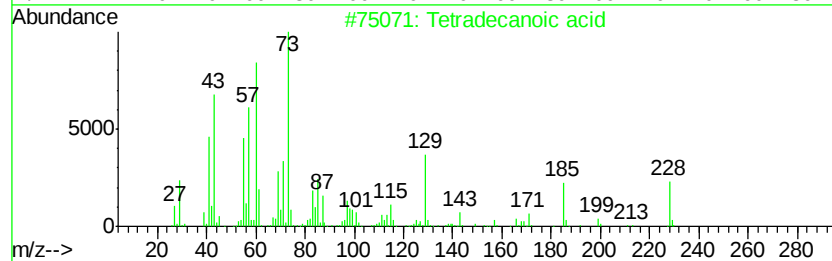
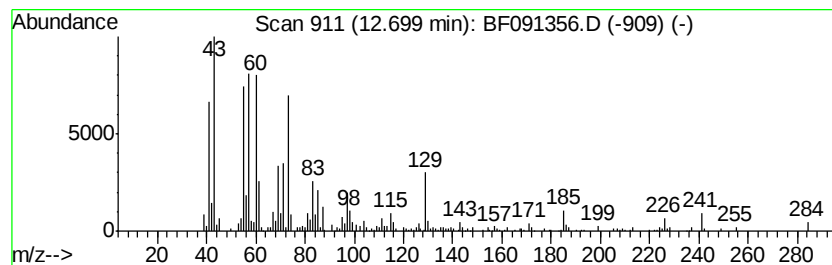
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetradecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.16 ng	290509	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
2		Undecanoic acid	186	C11H22O2	000112-37-8	58
3		Dodecanoic acid	200	C12H24O2	000143-07-7	53
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091356.D
Acq On : 30 Nov 2016 16:05
Operator : UM/SJ
Sample : H5749-07
Misc :
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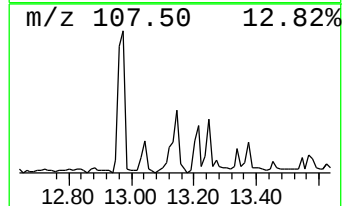
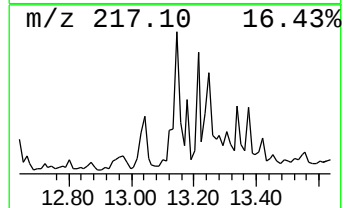
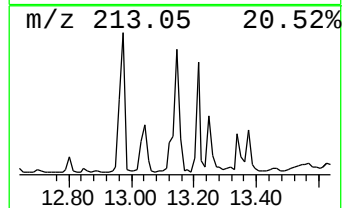
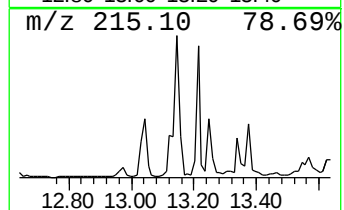
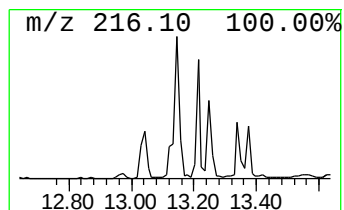
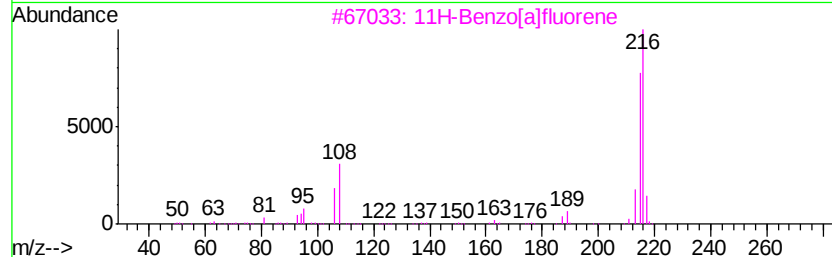
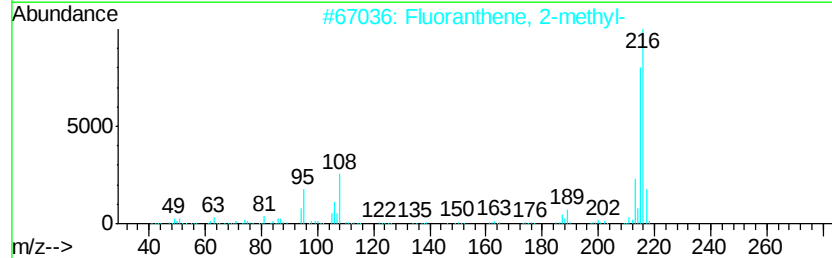
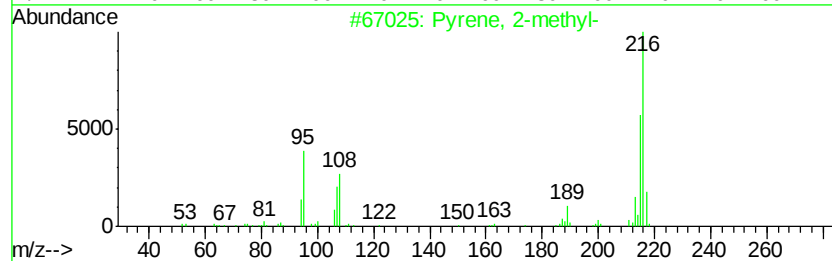
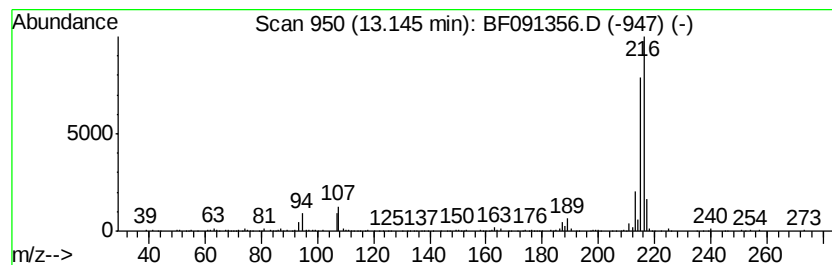
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pyrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.14	2.64 ng	373690	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	11H-Benzo[al]fluorene	216	C17H12	000238-84-6	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091356.D
Acq On : 30 Nov 2016 16:05
Operator : UM/SJ
Sample : H5749-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

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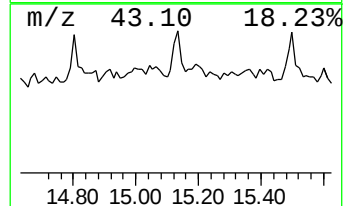
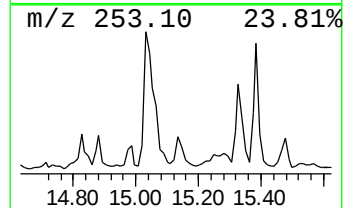
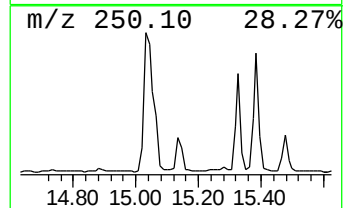
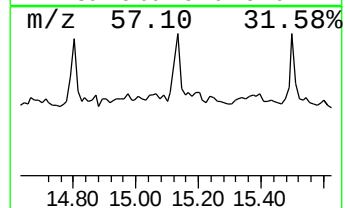
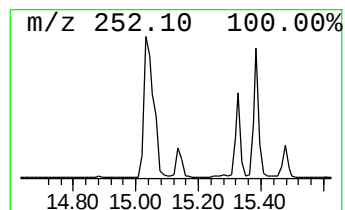
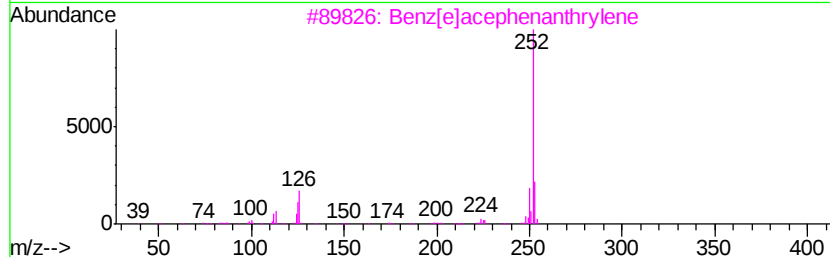
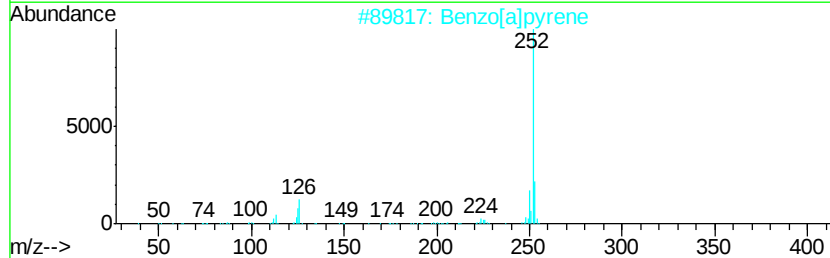
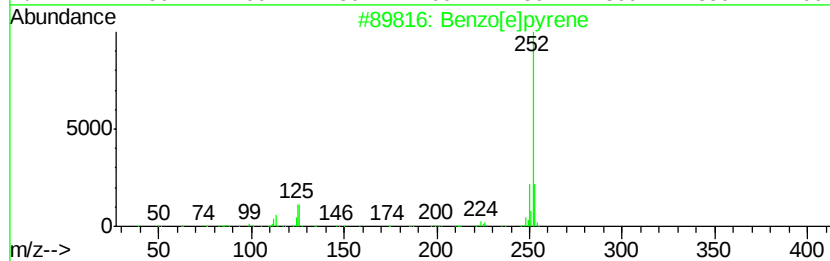
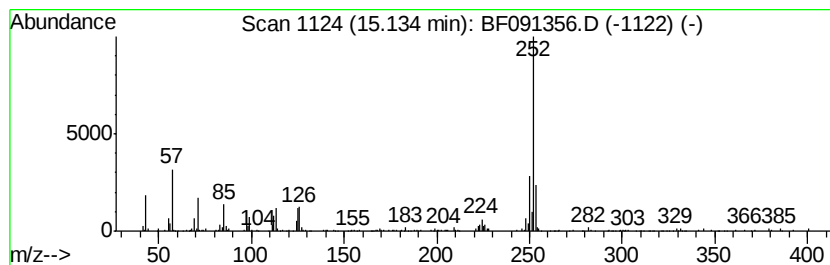
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	3.55 ng	183546	Perylene-d12	15.45

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	91
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	90
4		Perylene	252	C20H12	000198-55-0	81
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091356.D
Acq On : 30 Nov 2016 16:05
Operator : UM/SJ
Sample : H5749-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

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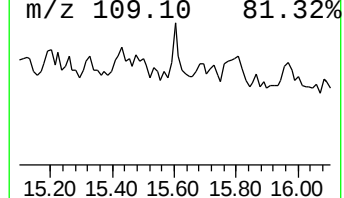
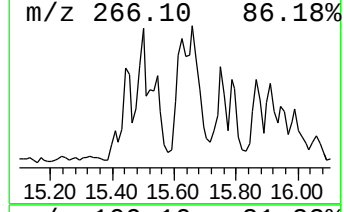
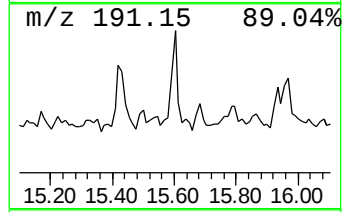
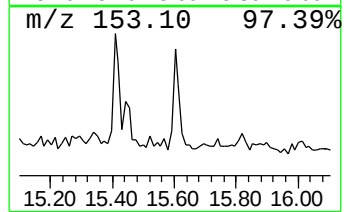
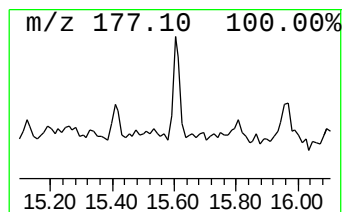
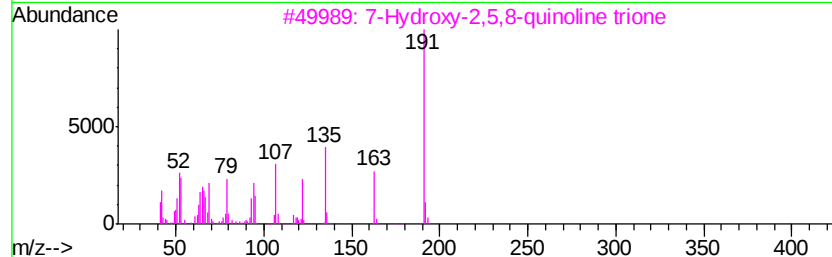
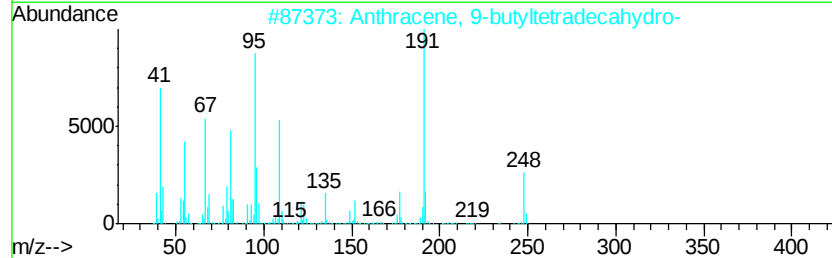
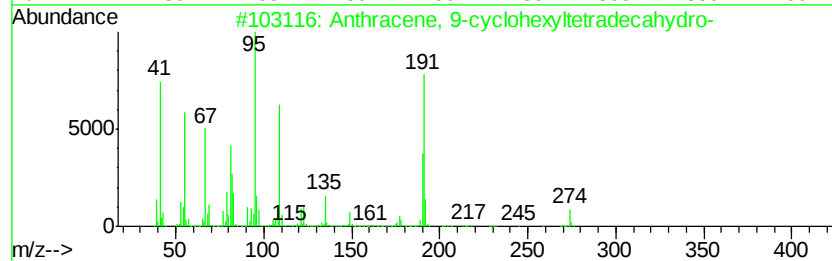
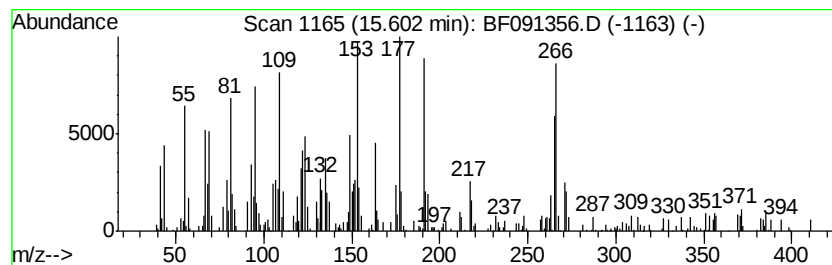
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.60 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	3.26 ng	168625	Perylene-d12	15.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	14
2			Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	12
3			7-Hydroxy-2,5,8-quinoline trione	191	C9H5NO4	015544-54-4	11
4			Cyclohexane, 1,1-dimethyl-2,4-bi...	192	C14H24	062337-98-8	10
5			Cyclohexane, 3,4-bis(1-methyleth...	192	C14H24	061142-74-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
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Acq On : 30 Nov 2016 16:05
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Sample : H5749-07
Misc :
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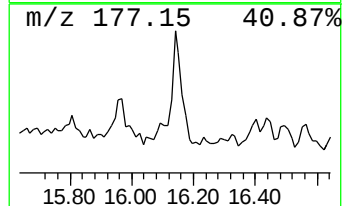
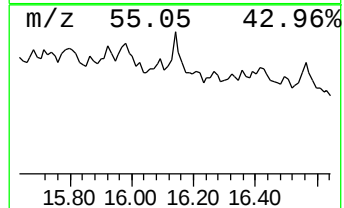
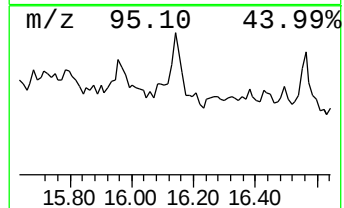
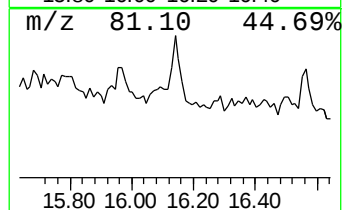
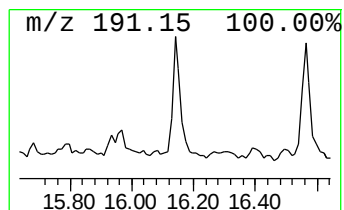
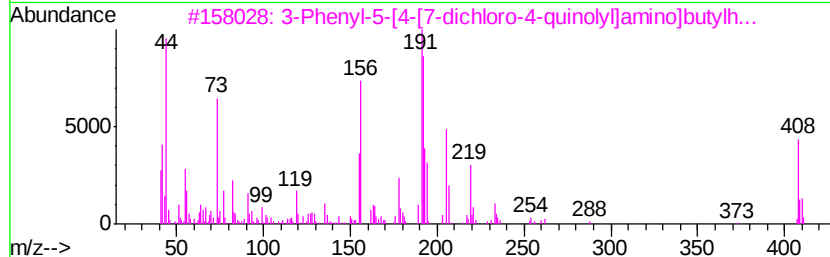
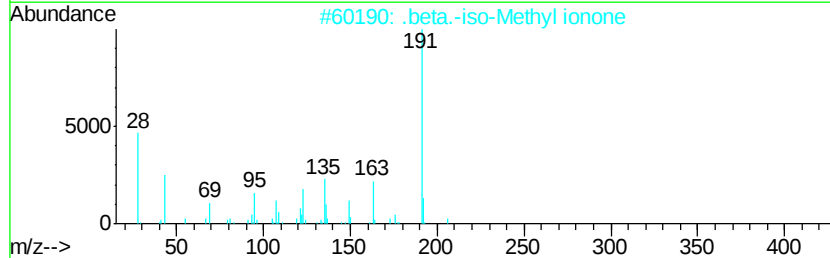
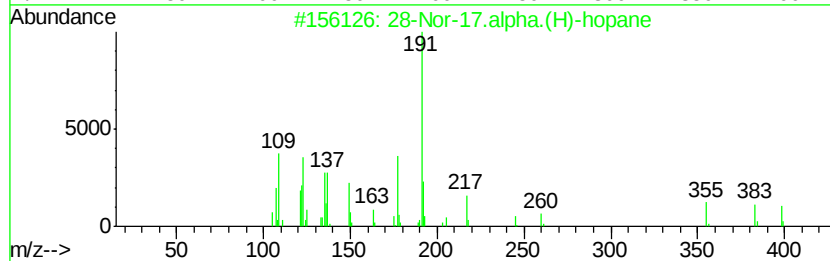
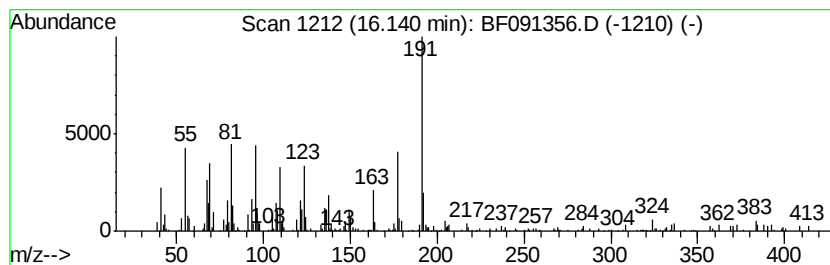
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 28-Nor-17.alpha.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	5.66 ng	292513	Perylene-d12	15.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4 59
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2 58
3	3-Phenyl-5-[4-[7-dichloro-4-quin...	408	C22H21ClN4O2	1000252-32-2 42
4	5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8 40
5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7 32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
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Sample : H5749-07
Misc :
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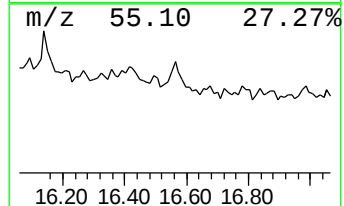
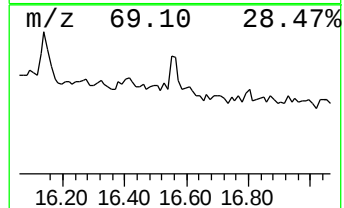
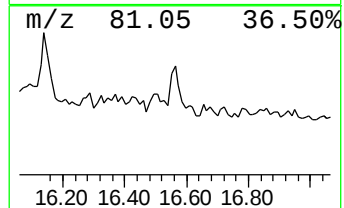
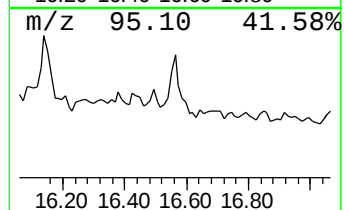
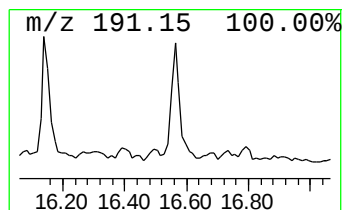
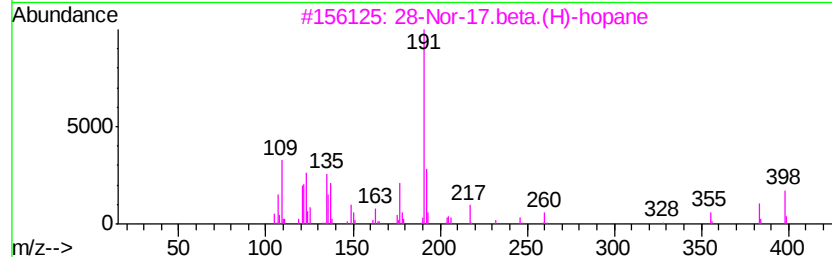
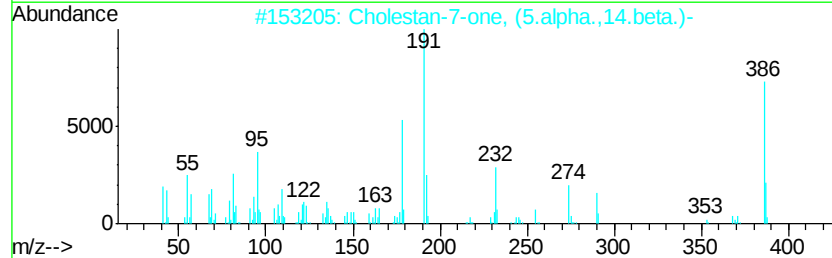
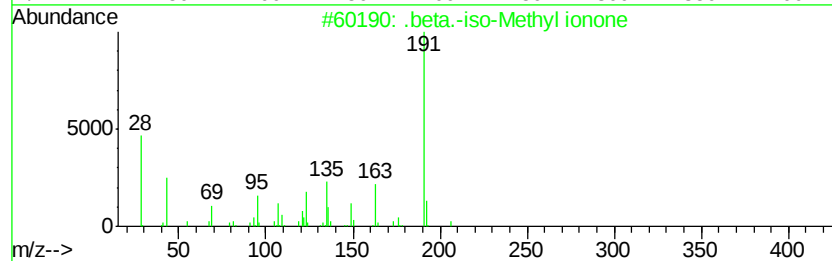
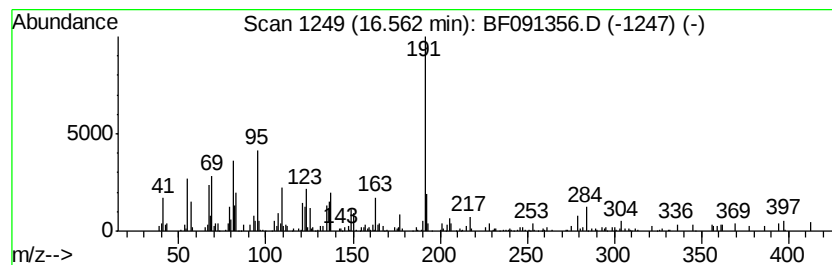
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.56	4.65 ng	240517	Perylene-d12	15.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	59
2	Cholestan-7-one, (5.alpha.,14.be...	386	C27H46O	040072-53-5	45
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	37
4	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	37
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091356.D
Acq On : 30 Nov 2016 16:05
Operator : UM/SJ
Sample : H5749-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-MM4-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	39.6	ng	2891760	1	6.86	1459800	20.0
unknown6.63	6.63	104.2	ng	7602070	1	6.86	1459800	20.0
3-Methyl-4-(metho...	10.81	2.4	ng	328747	4	11.38	2691690	20.0
Phenanthrene, 2-m...	11.91	4.7	ng	633236	4	11.38	2691690	20.0
Benzaldehyde, 3,5...	11.99	4.0	ng	541593	4	11.38	2691690	20.0
Tetradecanoic acid	12.70	2.2	ng	290509	4	11.38	2691690	20.0
Pyrene, 2-methyl-	13.14	2.6	ng	373690	5	14.01	2830430	20.0
Benzo[e]pyrene	15.13	3.5	ng	183546	6	15.45	1033870	20.0
unknown15.60	15.60	3.3	ng	168625	6	15.45	1033870	20.0
28-Nor-17.alpha.(...	16.14	5.7	ng	292513	6	15.45	1033870	20.0
.beta.-iso-Methyl...	16.56	4.7	ng	240517	6	15.45	1033870	20.0