

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
 Data File : BF096659.D
 Acq On : 11 Jul 2017 22:11
 Operator : SJ/JU
 Sample : I4126-07
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-GW-1

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	4.863	468	472	483	rVB	167023	197141	7.64%	1.078%
2	5.292	541	545	557	rVB	1514984	1405744	54.46%	7.684%
3	5.522	580	584	587	rBV	42871	36103	1.40%	0.197%
4	6.322	716	720	726	rVB	937371	852288	33.02%	4.659%
5	6.457	738	743	746	rBV	2314192	2247449	87.07%	12.286%
6	6.681	778	781	785	rBV	574086	522198	20.23%	2.855%
7	6.745	789	792	802	rVB	47935	42113	1.63%	0.230%
8	6.839	804	808	812	rBV	2093109	2049037	79.38%	11.201%
9	7.010	834	837	846	rVB	30572	30507	1.18%	0.167%
10	7.245	871	877	880	rBV	1702484	1749428	67.78%	9.563%
11	7.463	909	914	916	rBV	29950	27512	1.07%	0.150%
12	7.486	916	918	921	rVB	59053	42901	1.66%	0.235%
13	7.710	951	956	959	rBV2	85784	84567	3.28%	0.462%
14	7.963	995	999	1002	rBV	775448	696390	26.98%	3.807%
15	7.986	1002	1003	1007	rVB3	46305	38095	1.48%	0.208%
16	8.204	1035	1040	1043	rBV2	72322	81263	3.15%	0.444%
17	8.357	1063	1066	1068	rBV	37932	31274	1.21%	0.171%
18	8.439	1076	1080	1084	rBV2	30834	29976	1.16%	0.164%
19	8.675	1116	1120	1123	rVB3	24735	30291	1.17%	0.166%
20	8.775	1134	1137	1142	rBV	90953	90515	3.51%	0.495%
21	8.822	1142	1145	1152	rVB6	18741	32660	1.27%	0.179%
22	8.951	1164	1167	1174	rVB2	48897	47742	1.85%	0.261%
23	9.045	1178	1183	1186	rBV	2877182	2581206	100.00%	14.110%
24	9.433	1246	1249	1252	rBV	74916	57962	2.25%	0.317%
25	9.716	1293	1297	1301	rBV	737515	616269	23.88%	3.369%
26	10.498	1426	1430	1442	rVB	1245492	1225223	47.47%	6.698%
27	11.192	1544	1548	1555	rBV	591108	487021	18.87%	2.662%
28	12.780	1813	1818	1821	rBV	1944425	1830874	70.93%	10.008%
29	13.680	1966	1971	1981	rBV	64438	82170	3.18%	0.449%
30	13.821	1991	1995	2001	rVB	611564	543922	21.07%	2.973%
31	15.221	2227	2233	2238	rBV	415481	503499	19.51%	2.752%

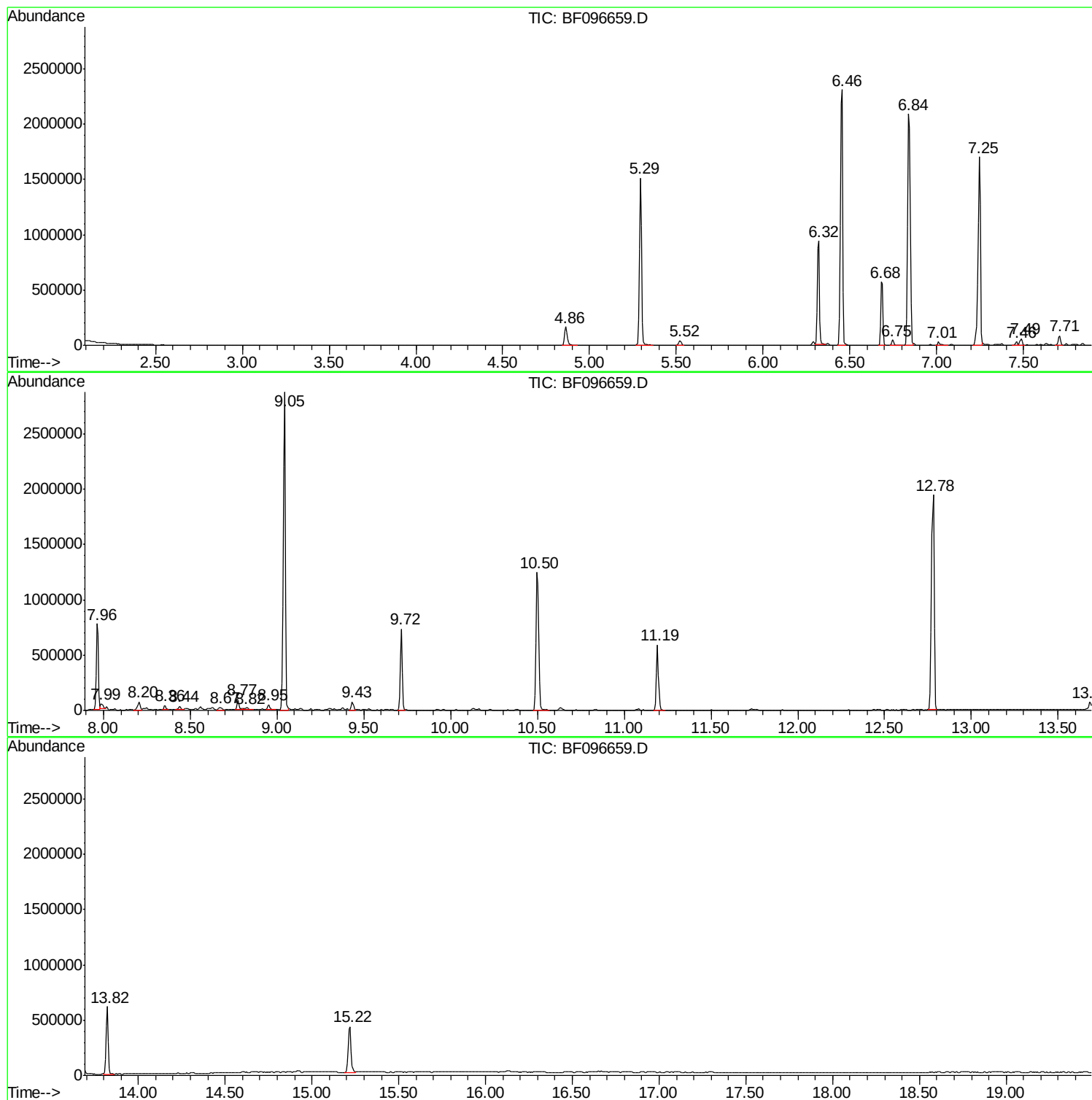
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ClientSampleId :
PP-GW-1

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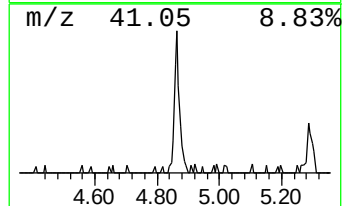
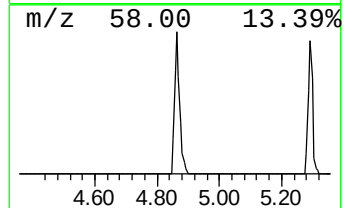
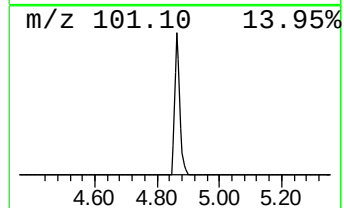
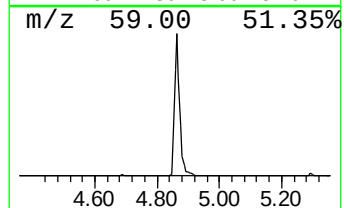
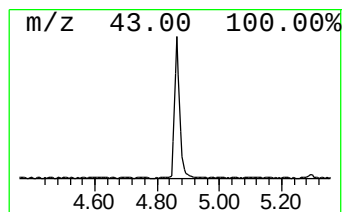
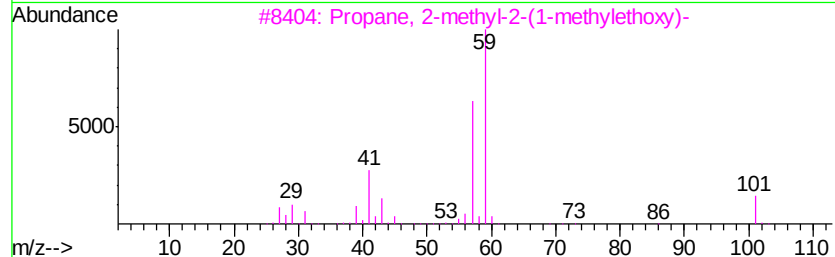
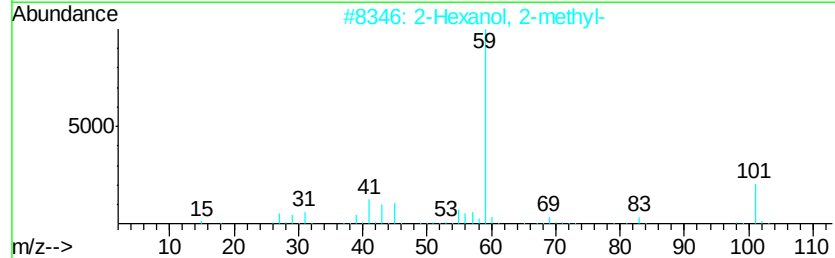
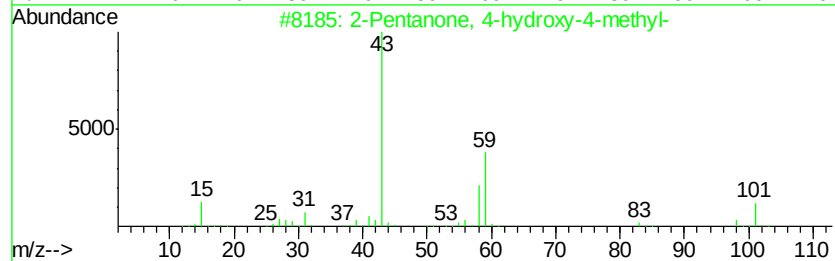
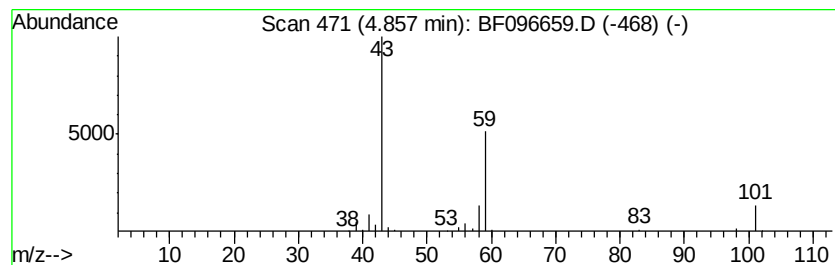
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.86	7.55 ng	197141	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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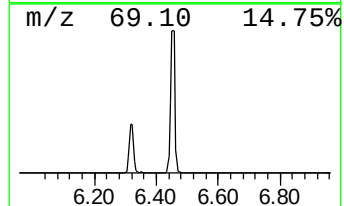
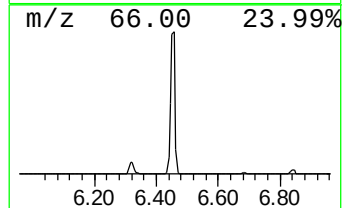
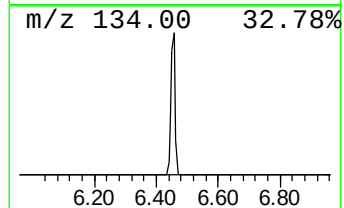
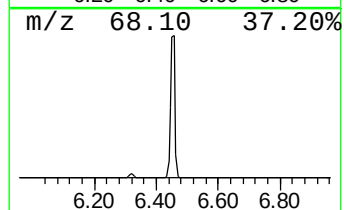
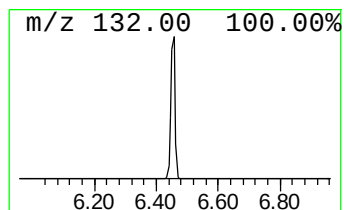
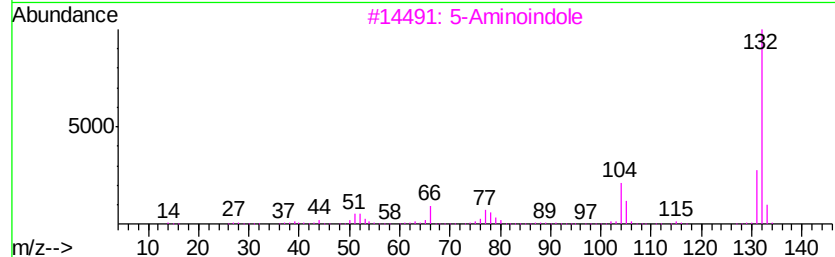
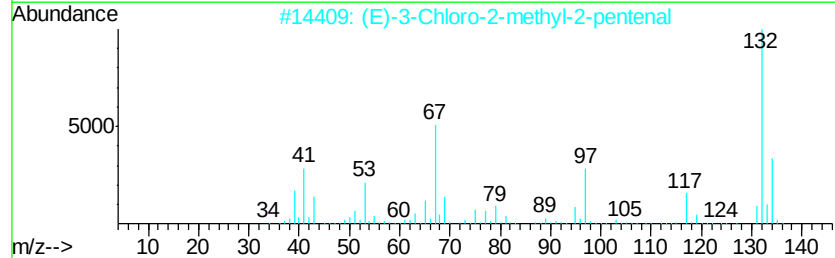
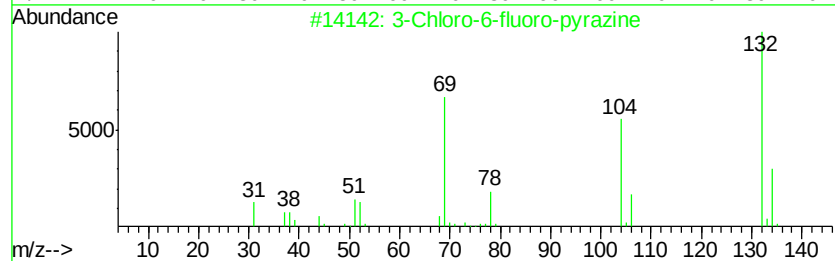
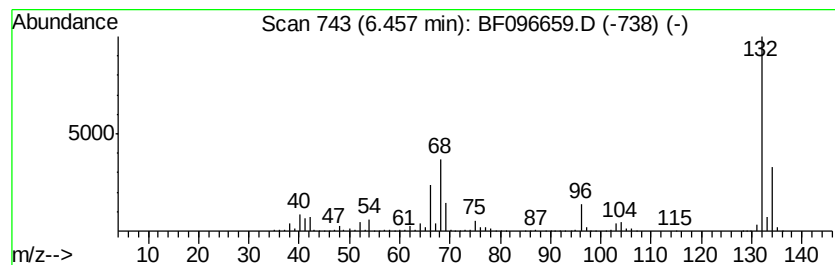
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Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	86.08 ng	2247450	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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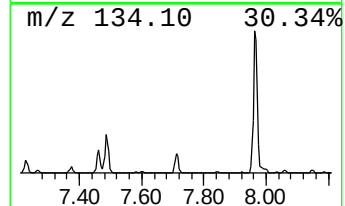
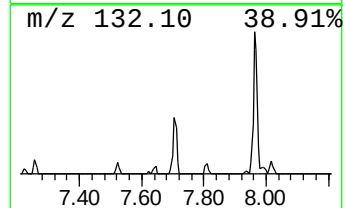
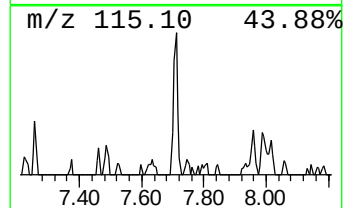
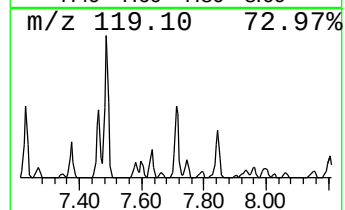
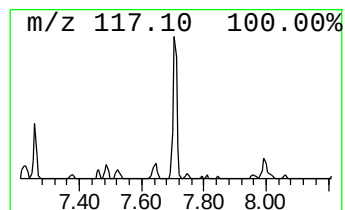
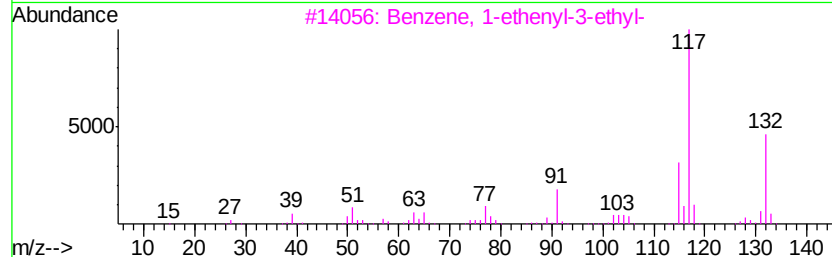
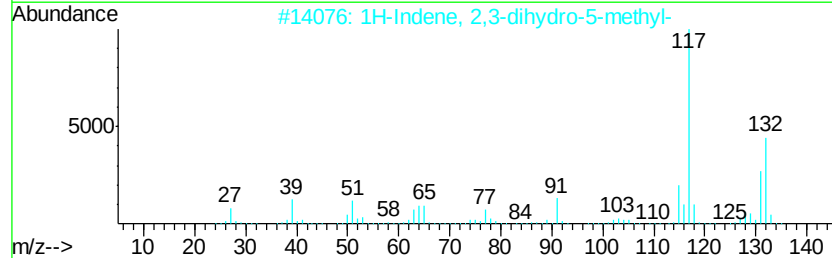
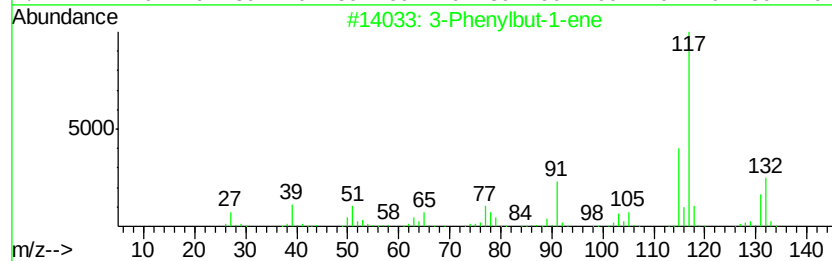
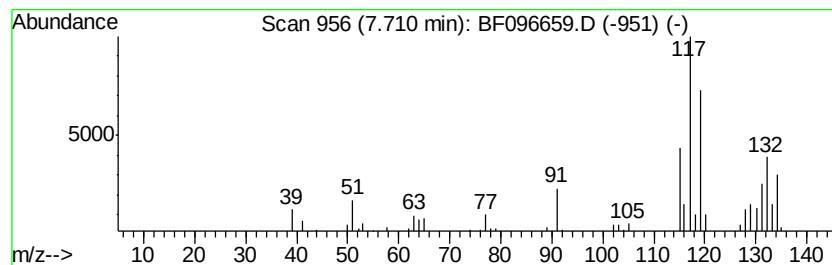
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Peak Number 4 3-Phenylbut-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	2.43 ng	84567	Napthalene-d8	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	49
3		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	49
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	49
5		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	46



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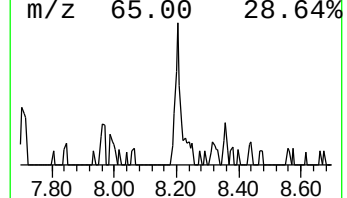
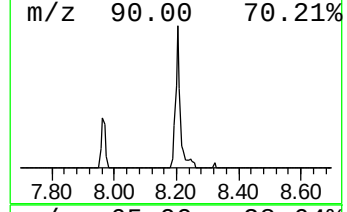
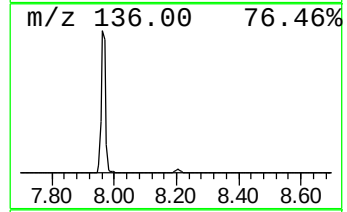
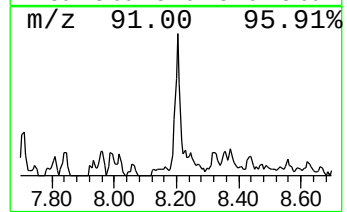
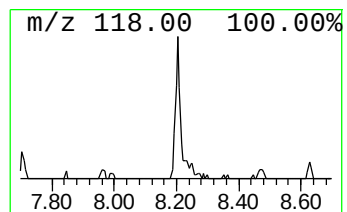
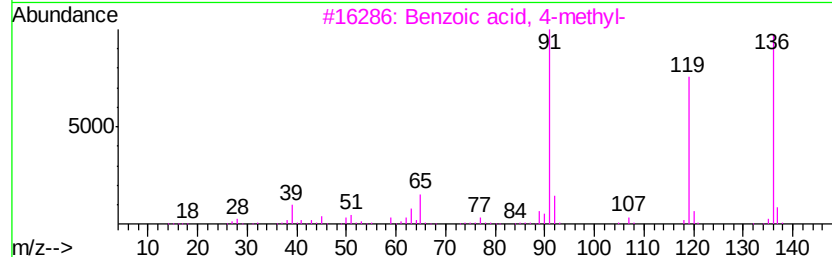
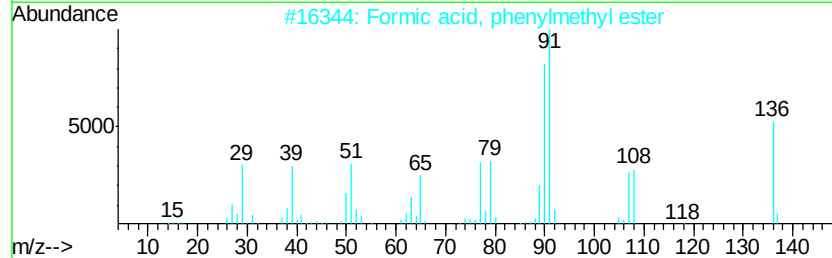
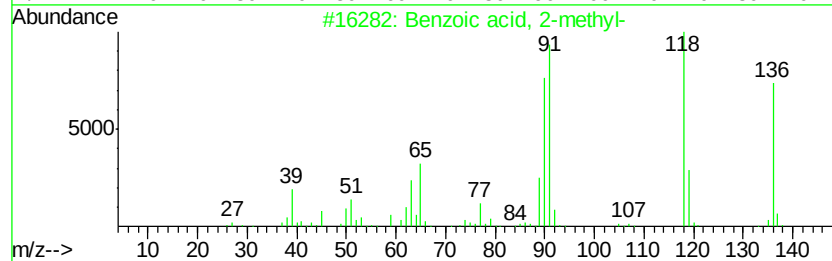
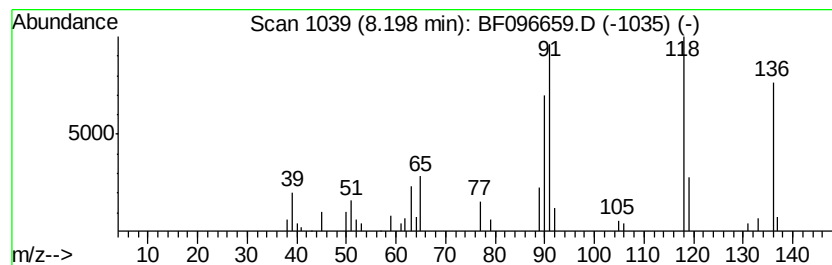
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	2.33 ng	81263	Napthalene-d8	7.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 2-methyl-	136	C8H8O2	000118-90-1	98
2		Formic acid, phenylmethyl ester	136	C8H8O2	000104-57-4	76
3		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	25
4		3-Pyridineacetonitrile	118	C7H6N2	006443-85-2	20
5		1H-Pyrrolo(2,3-c)pyridine	118	C7H6N2	000271-29-4	18



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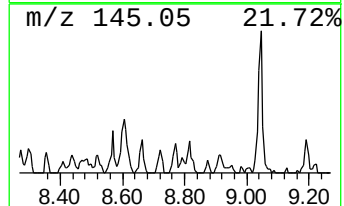
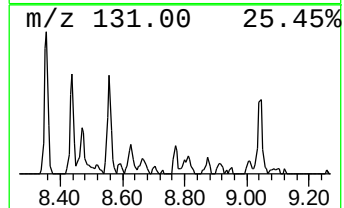
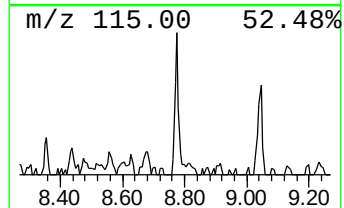
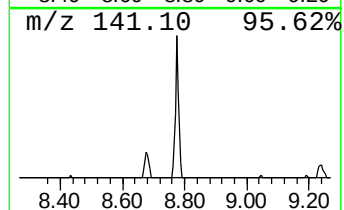
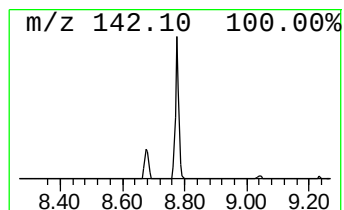
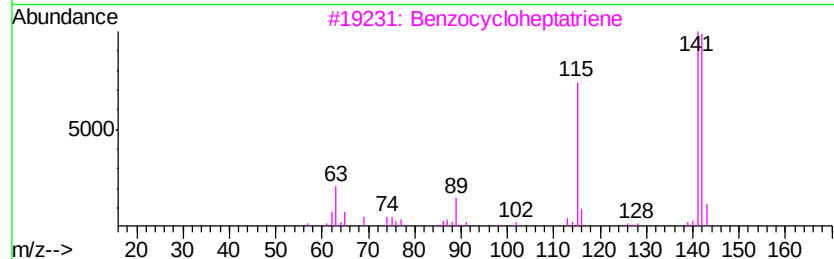
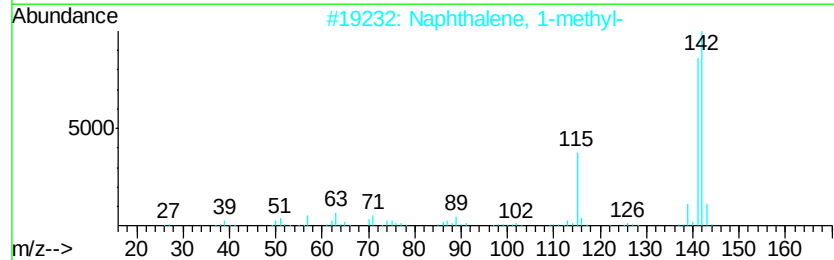
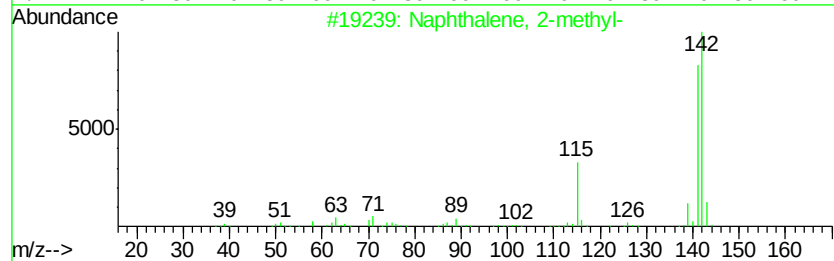
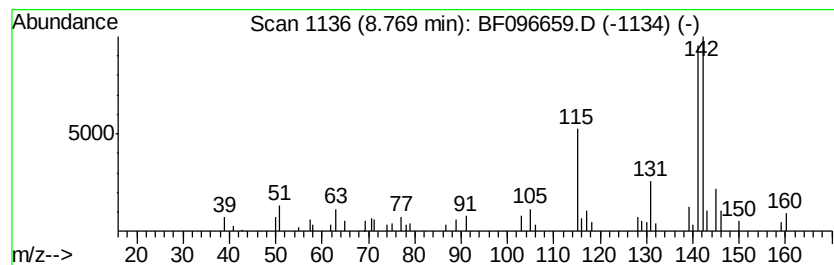
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	2.60 ng	90515	Naphthalene-d8	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3		Benzocycloheptatriene	142	C11H10	000264-09-5	91
4		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87
5		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87



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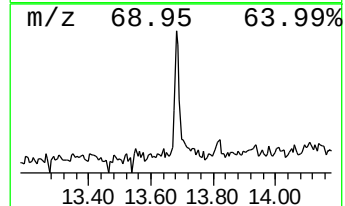
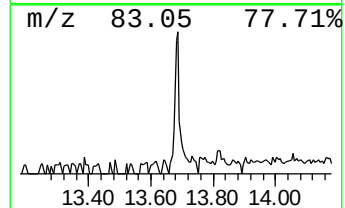
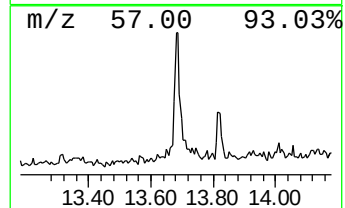
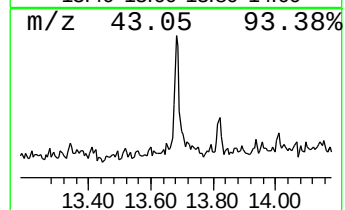
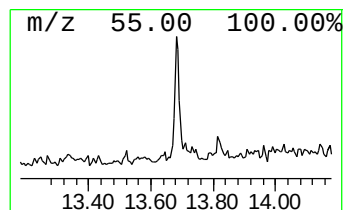
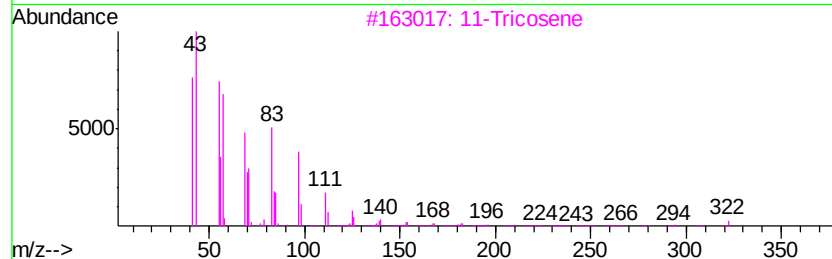
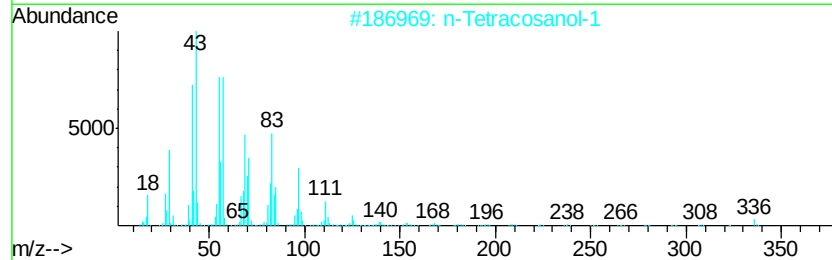
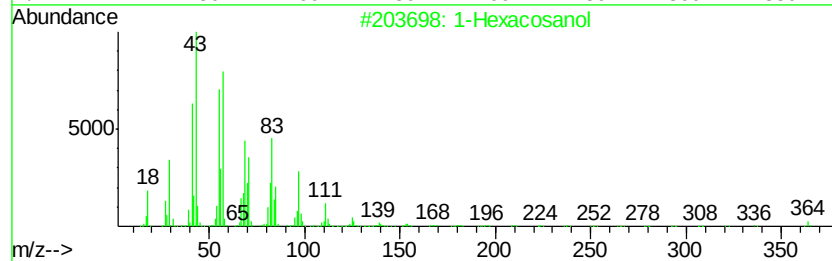
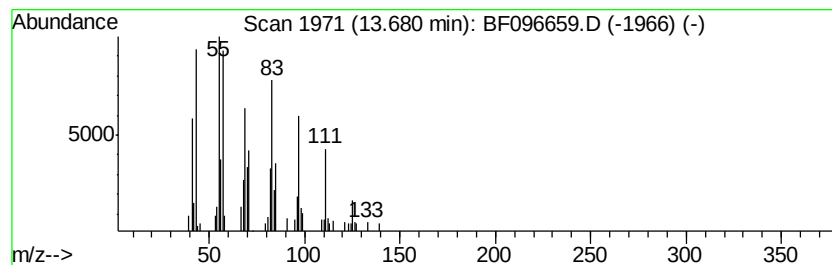
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.02 ng	82170	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexacosanol	382	C26H54O	000506-52-5	87
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	83
3		11-Tricosene	322	C23H46	052078-56-5	80
4		1-Eicosanol	298	C20H42O	000629-96-9	80
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096659.D
Acq On : 11 Jul 2017 22:11
Operator : SJ/JU
Sample : I4126-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-GW-1

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...	4.86	7.5	ng	197141	1	6.69	522198	20.0
unknown6.46	6.46	86.1	ng	2247450	1	6.69	522198	20.0
3-Phenylbut-1-ene	7.71	2.4	ng	84567	2	7.96	696390	20.0
Benzoic acid, 2-m...	8.20	2.3	ng	81263	2	7.96	696390	20.0
Naphthalene, 1-me...	8.77	2.6	ng	90515	2	7.96	696390	20.0
1-Hexacosanol	13.68	3.0	ng	82170	5	13.82	543922	20.0