

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
 Data File : BF090917.D
 Acq On : 28 Oct 2016 19:23
 Operator : UM/SJ
 Sample : H5411-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-02

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-BF102616.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	4.910	245	247	251	rBV	232178	295937	6.51%	0.918%
2	5.356	283	286	288	rBV	1865855	2156371	47.45%	6.691%
3	6.396	375	377	386	rBV	1150024	1422340	31.30%	4.413%
4	6.533	386	389	391	rBV	3113050	3848674	84.68%	11.941%
5	6.761	407	409	411	rBV	940787	867445	19.09%	2.691%
6	6.921	420	423	425	rBV	3074135	3540006	77.89%	10.984%
7	7.024	430	432	436	rVB2	33647	62065	1.37%	0.193%
8	7.184	441	446	449	rVB6	13799	46868	1.03%	0.145%
9	7.333	456	459	461	rBV	2387805	2841299	62.52%	8.816%
10	7.710	488	492	496	rBV5	23672	59845	1.32%	0.186%
11	7.790	496	499	503	rBV3	43680	87280	1.92%	0.271%
12	8.053	519	522	524	rBV	862073	1191910	26.23%	3.698%
13	8.430	551	555	556	rBV2	39315	70236	1.55%	0.218%
14	8.522	561	563	567	rVB5	48361	72345	1.59%	0.224%
15	8.613	570	571	575	rBV3	44478	52825	1.16%	0.164%
16	8.727	578	581	583	rBV4	20749	52949	1.17%	0.164%
17	8.910	594	597	599	rVB2	47362	83011	1.83%	0.258%
18	8.956	599	601	602	rBV	42058	58654	1.29%	0.182%
19	9.002	603	605	607	rBV3	39072	63210	1.39%	0.196%
20	9.047	607	609	613	rVB3	71596	154954	3.41%	0.481%
21	9.127	613	616	619	rBV	4639047	4544935	100.00%	14.102%
22	9.299	630	631	633	rBV2	44207	61180	1.35%	0.190%
23	9.390	637	639	641	rVB2	65474	90934	2.00%	0.282%
24	9.436	641	643	647	rBV4	83593	252739	5.56%	0.784%
25	9.527	648	651	653	rVB	281646	331795	7.30%	1.029%
26	9.665	661	663	665	rBV2	63427	107144	2.36%	0.332%
27	9.745	668	670	673	rBV4	46589	87595	1.93%	0.272%
28	9.802	673	675	677	rBV	1513789	1273674	28.02%	3.952%
29	10.248	712	714	716	rBV	68561	78120	1.72%	0.242%
30	10.362	723	724	725	rBV	58731	50509	1.11%	0.157%
31	10.590	741	744	747	rBV	2325105	2381632	52.40%	7.390%
32	10.716	753	755	757	rVB	94083	109401	2.41%	0.339%
33	11.288	802	805	807	rBV	939521	969516	21.33%	3.008%
34	12.876	941	944	946	rBV	3483731	3047263	67.05%	9.455%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.779	1021	1023	1029	rVB	104784	134172	2.95%	0.416%
36	13.928	1033	1036	1038	rBV	550465	769651	16.93%	2.388%
37	15.334	1156	1159	1162	rBV	766264	910928	20.04%	2.826%

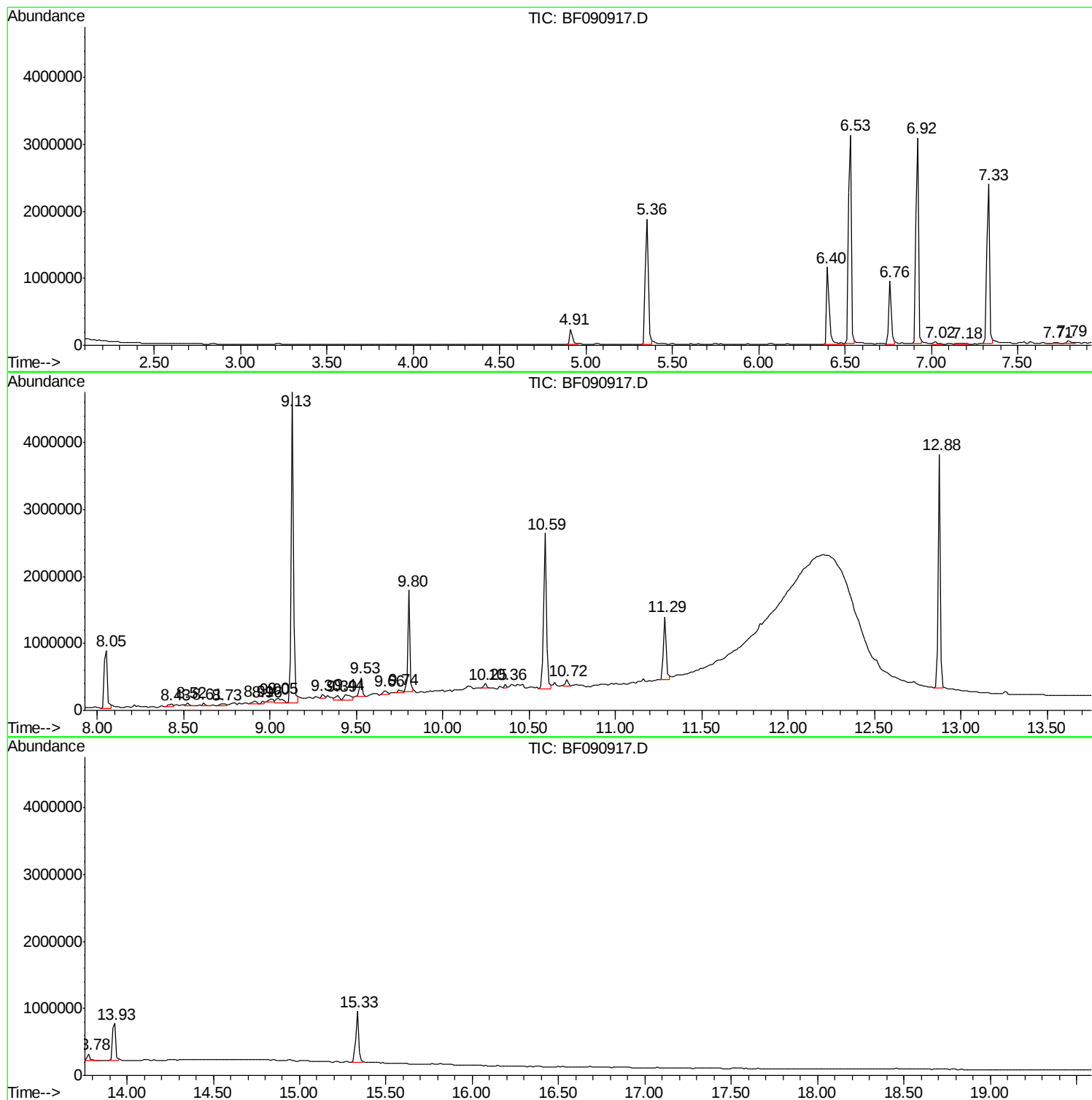
Sum of corrected areas: 32229412

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

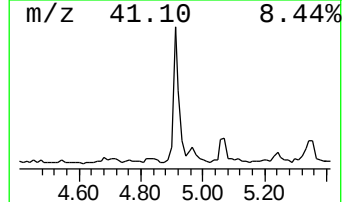
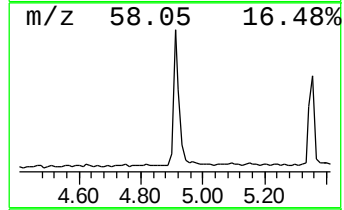
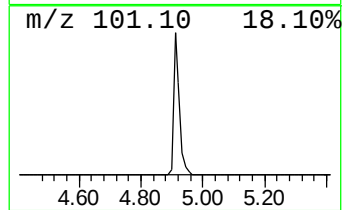
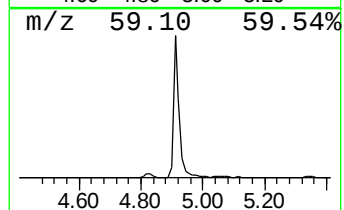
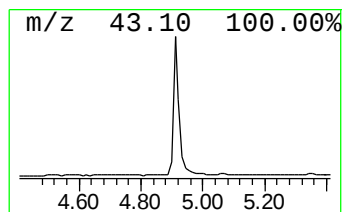
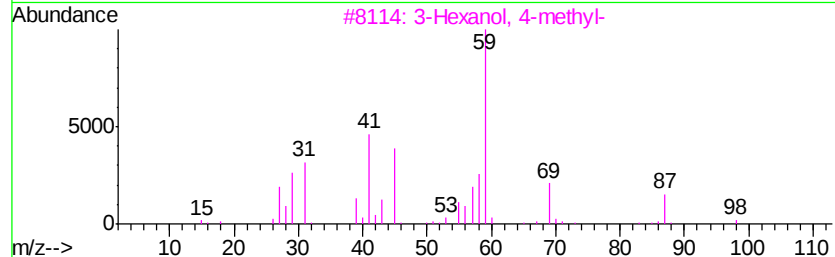
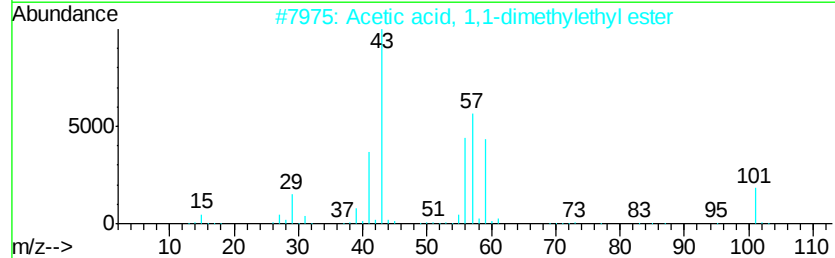
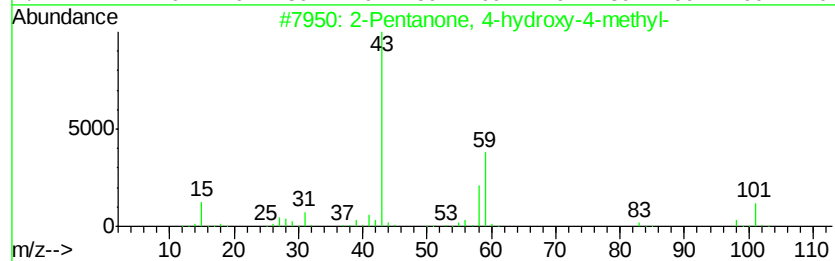
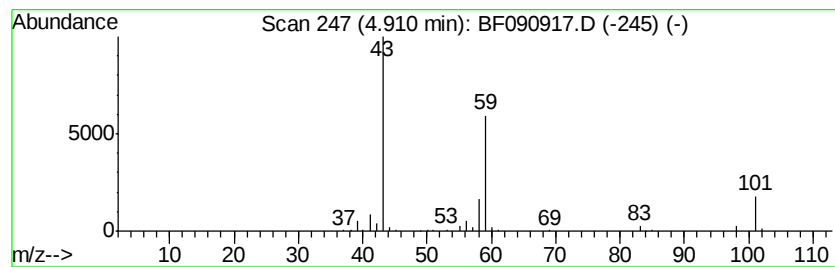
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	6.82 ng	295937	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

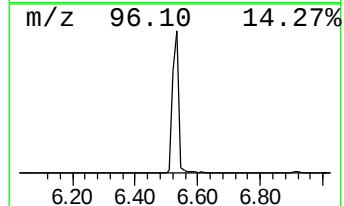
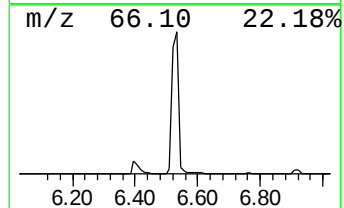
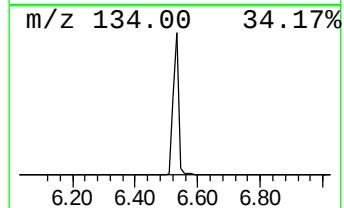
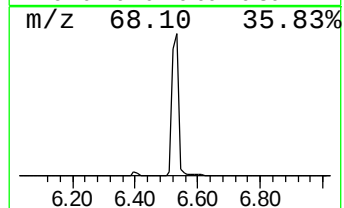
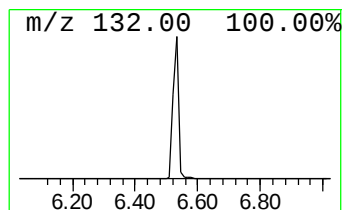
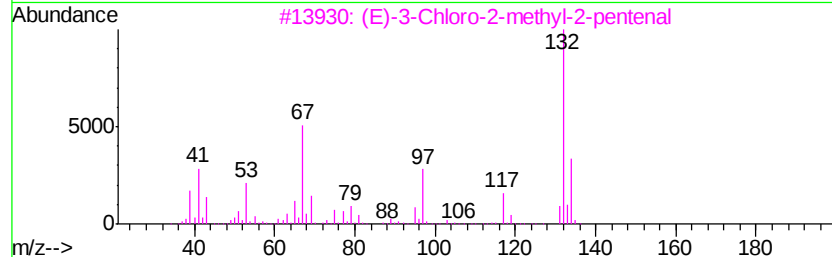
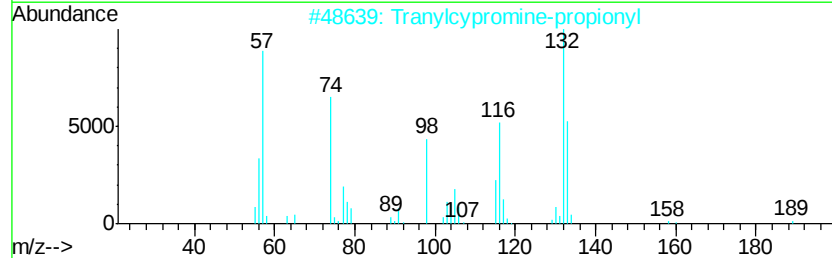
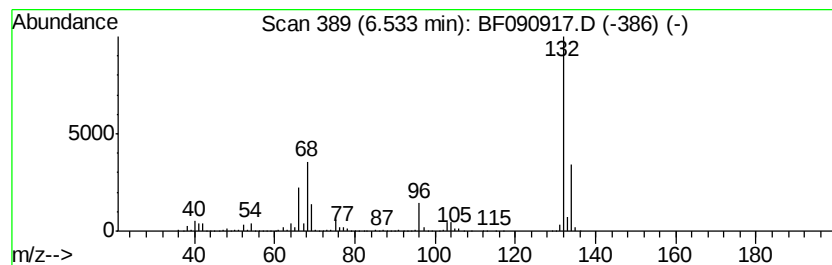
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	88.74 ng	3848670	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

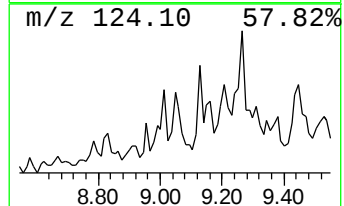
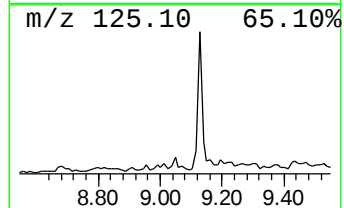
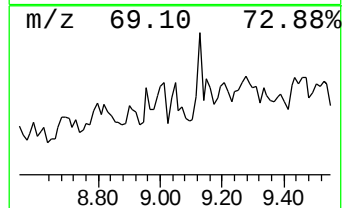
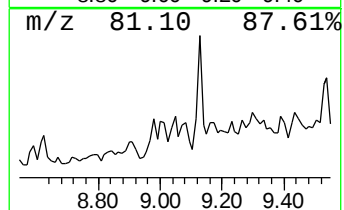
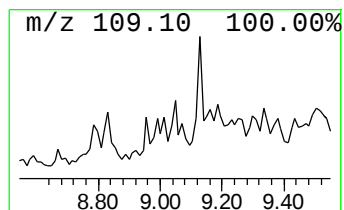
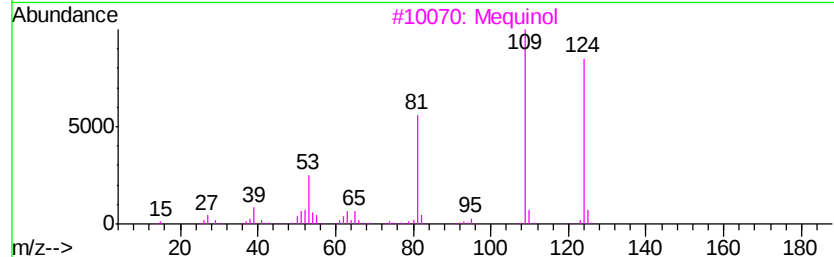
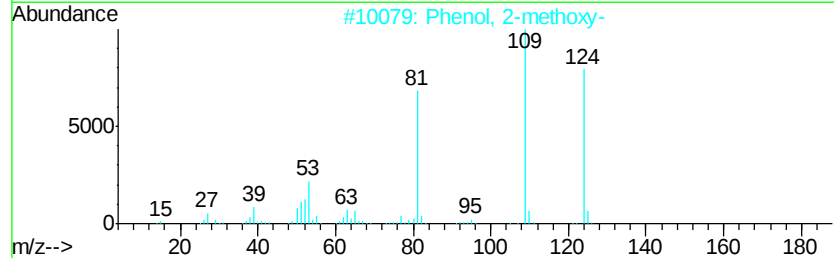
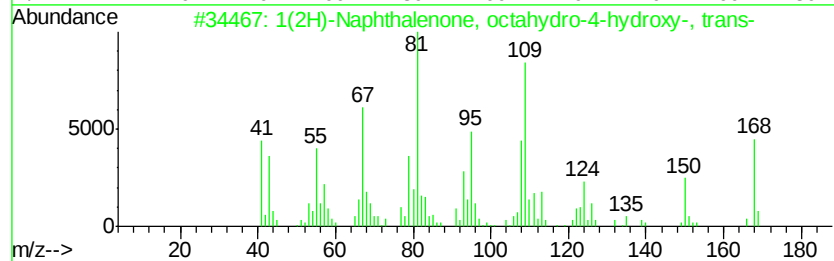
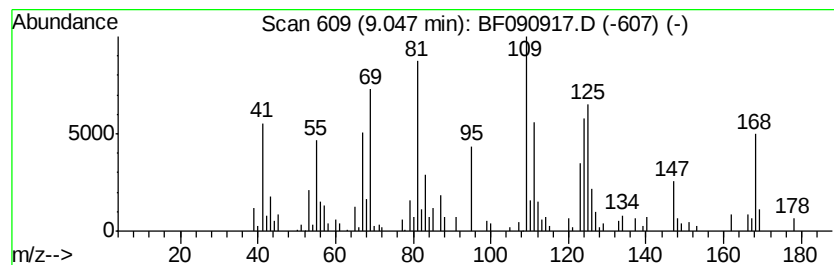
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1(2H)-Naphthalenone, octahy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	2.43 ng	154954	Acenaphthene-d10	9.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1(2H)-Naphthalenone, octahydro-4...	168	C10H16O2	021766-50-7	52
2		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	38
3		Mequinol	124	C7H8O2	000150-76-5	38
4		2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	38
5		Cyclohexene,1-propyl-	124	C9H16	002539-75-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TWP-02

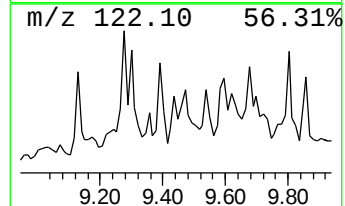
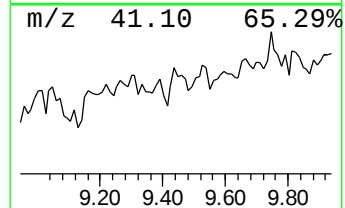
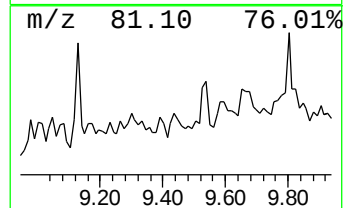
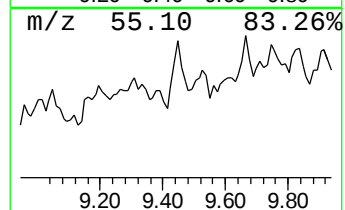
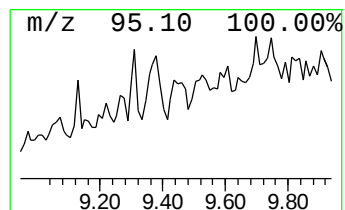
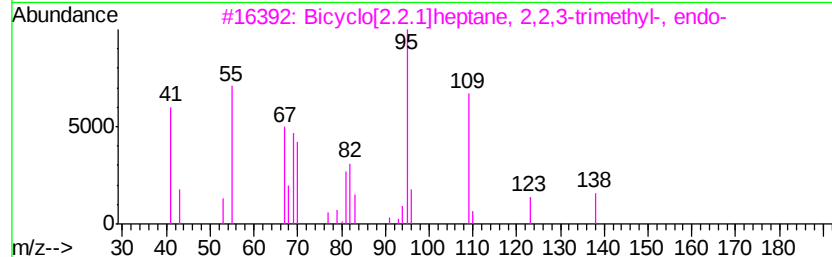
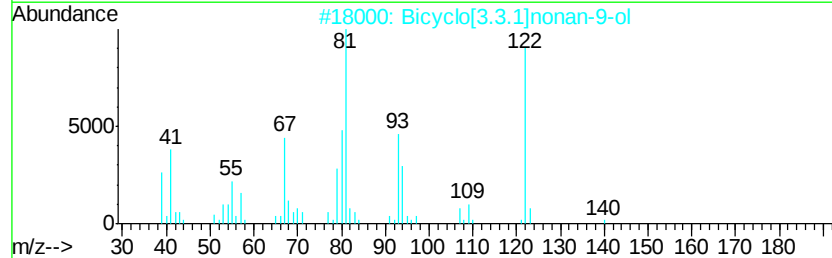
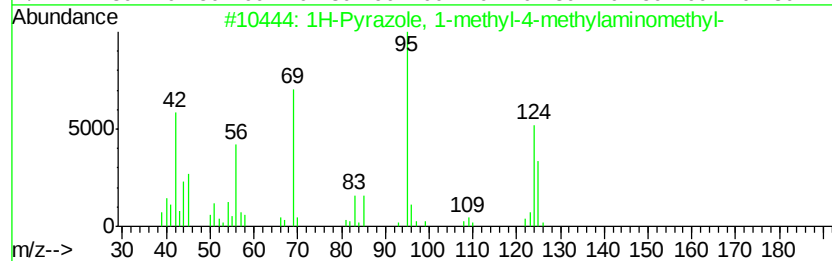
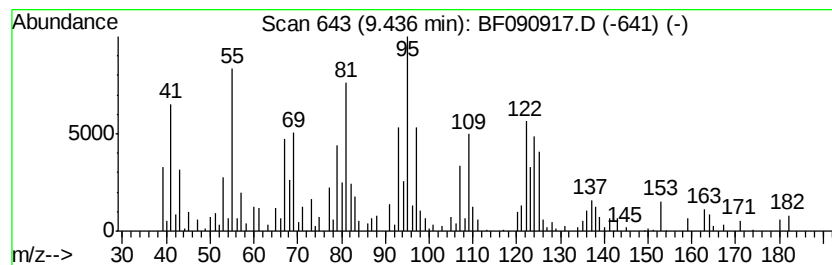
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.44 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	3.97 ng	252739	Acenaphthene-d10	9.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Pyrazole, 1-methyl-4-methylam...	125	C6H11N3	1000294-10-8	30
2		Bicyclo[3.3.1]nonan-9-ol	140	C9H16O	015598-80-8	22
3		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	20
4		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	18
5		2,3-Dimethyl-1,4-pentadiene	96	C7H12	000758-86-1	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

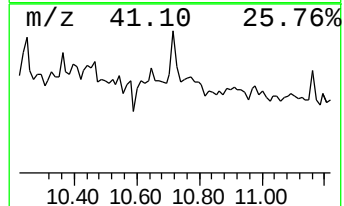
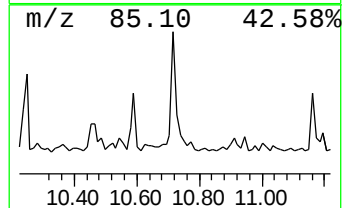
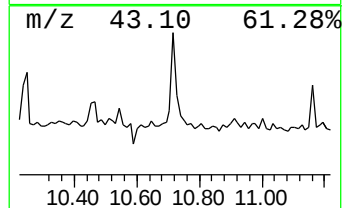
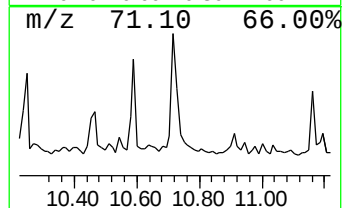
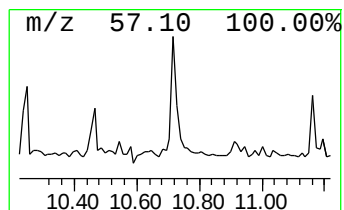
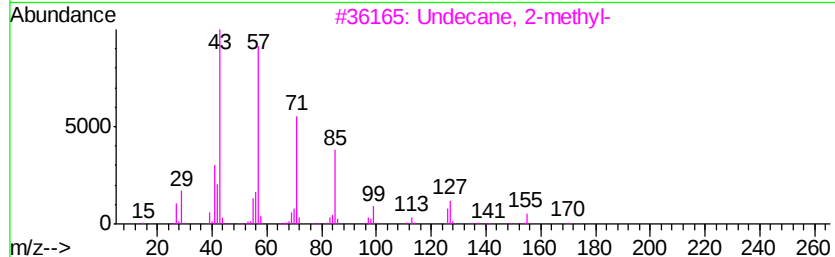
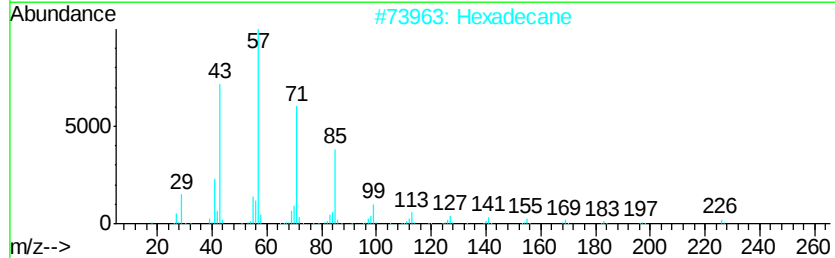
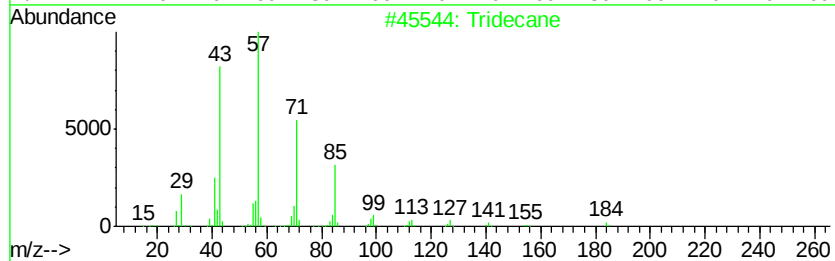
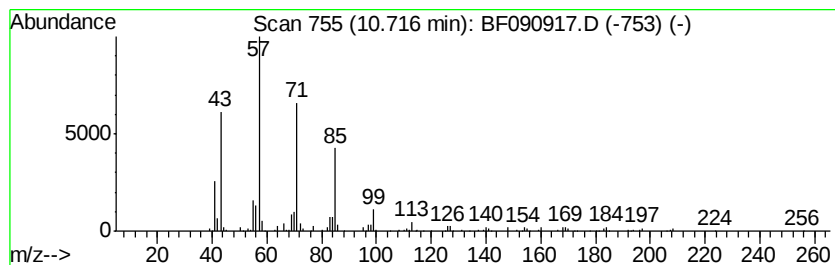
Instrument :
BNA_F
ClientSampleId :
TWP-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.72	2.26 ng	109401	Phenanthrene-d10		11.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	86
4	Dodecane	170	C12H26	000112-40-3	80
5	Tetradecane	198	C14H30	000629-59-4	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

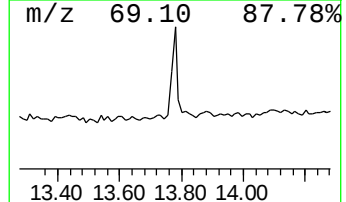
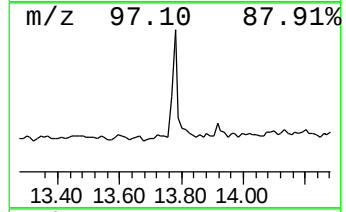
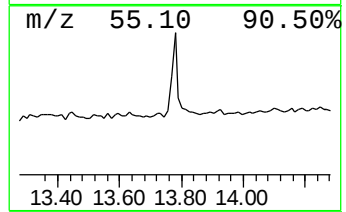
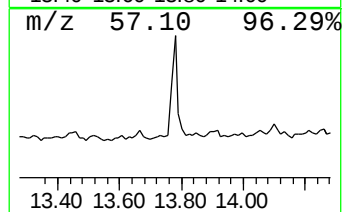
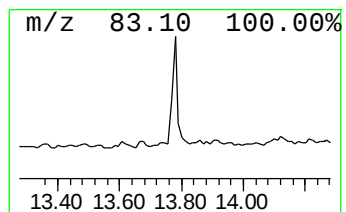
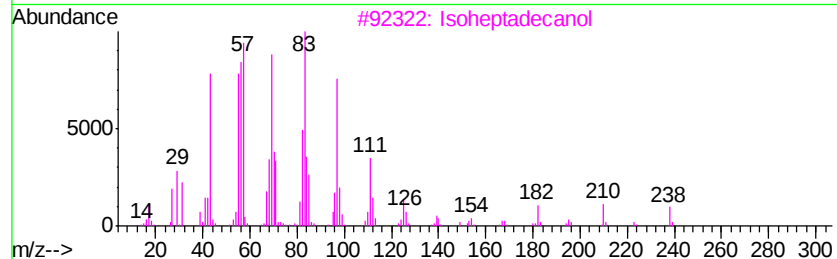
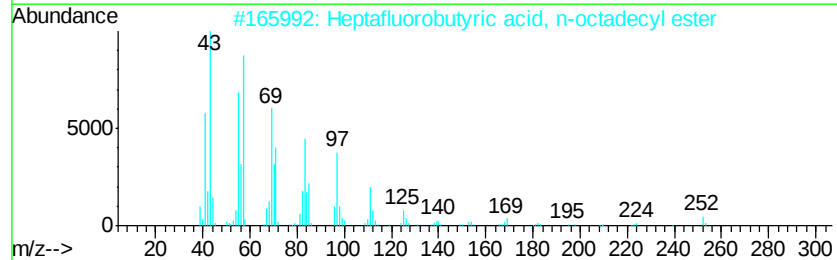
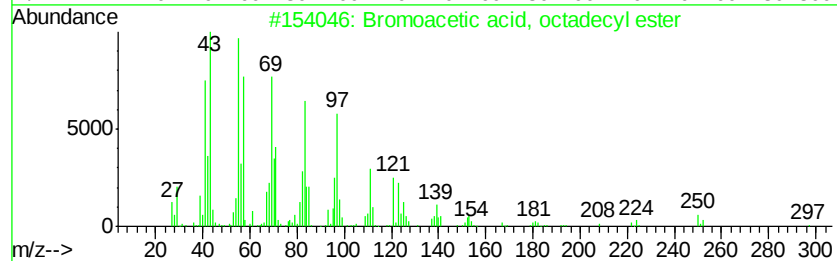
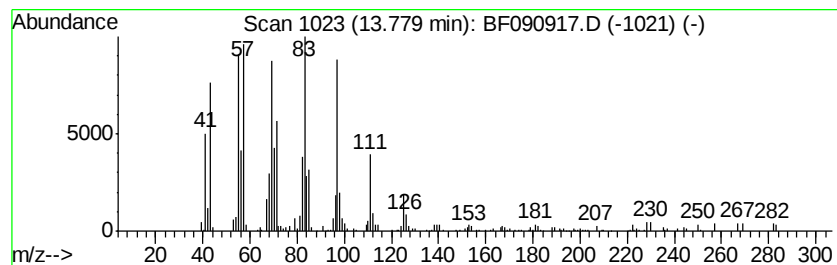
Instrument :
BNA_F
ClientSampleId :
TWP-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	3.49 ng	134172	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
3	Isoheptadecanol	256	C17H36O	057289-07-3	86
4	Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	83
5	1-Heptadecanol	256	C17H36O	001454-85-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102816\
Data File : BF090917.D
Acq On : 28 Oct 2016 19:23
Operator : UM/SJ
Sample : H5411-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.91	6.8	ng	295937	1	6.76	867445	20.0
unknown6.53	6.53	88.7	ng	3848670	1	6.76	867445	20.0
1(2H)-Naphthaleno...	9.05	2.4	ng	154954	3	9.80	1273670	20.0
unknown9.44	9.44	4.0	ng	252739	3	9.80	1273670	20.0
Tridecane	10.72	2.3	ng	109401	4	11.29	969516	20.0
Bromoacetic acid,...	13.78	3.5	ng	134172	5	13.93	769651	20.0