

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
 Data File : BF093962.D
 Acq On : 28 Mar 2017 00:36
 Operator : SJ/MA
 Sample : I2409-09
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LIP-22

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-BF032217.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	4.075	368	372	379	rVB	226598	250972	4.76%	0.686%
2	4.469	434	439	442	rBV	2545512	2343464	44.43%	6.407%
3	5.528	614	619	622	rBV	1756520	1595969	30.26%	4.364%
4	5.681	639	645	648	rBV	3610935	3850545	73.00%	10.528%
5	5.934	684	688	692	rBV	965058	979934	18.58%	2.679%
6	6.116	714	719	723	rVB	3260550	3389467	64.26%	9.267%
7	6.586	792	799	802	rBV	2423274	2960435	56.12%	8.094%
8	7.139	884	893	898	rBV3	55960	103910	1.97%	0.284%
9	7.369	925	932	937	rVB7	80348	188393	3.57%	0.515%
10	7.439	938	944	948	rBV	1351823	1374836	26.06%	3.759%
11	7.610	969	973	979	rBV3	35521	59389	1.13%	0.162%
12	7.928	1021	1027	1031	rBV5	59432	113566	2.15%	0.311%
13	8.251	1075	1082	1086	rBV7	53897	97930	1.86%	0.268%
14	8.292	1086	1089	1092	rBV2	49409	67606	1.28%	0.185%
15	8.351	1095	1099	1105	rVV3	60005	107883	2.05%	0.295%
16	8.522	1122	1128	1132	rVB6	66966	153635	2.91%	0.420%
17	8.628	1139	1146	1150	rBV5	62851	133673	2.53%	0.365%
18	8.769	1162	1170	1173	rBV	4468312	5274737	100.00%	14.422%
19	8.957	1198	1202	1204	rBV4	42438	66381	1.26%	0.181%
20	8.986	1204	1207	1209	rBV3	51020	53206	1.01%	0.145%
21	9.086	1221	1224	1227	rBV2	75976	103424	1.96%	0.283%
22	9.169	1234	1238	1243	rVB5	74704	117671	2.23%	0.322%
23	9.263	1251	1254	1260	rVB	118366	177662	3.37%	0.486%
24	9.586	1304	1309	1313	rVB	1396533	1470155	27.87%	4.020%
25	10.045	1385	1387	1395	rVB7	60444	77272	1.46%	0.211%
26	10.133	1399	1402	1406	rVB	194777	214847	4.07%	0.587%
27	10.563	1469	1475	1478	rVB	2512609	2897797	54.94%	7.923%
28	11.251	1589	1592	1597	rVB4	74041	88348	1.67%	0.242%
29	11.410	1615	1619	1623	rVB	1451596	1381142	26.18%	3.776%
30	11.868	1695	1697	1703	rVB	78030	78823	1.49%	0.216%
31	13.392	1950	1956	1960	rBV	3447125	4421671	83.83%	12.090%
32	14.127	2078	2081	2088	rVB	199073	194479	3.69%	0.532%
33	14.545	2149	2152	2160	rVB2	78317	101055	1.92%	0.276%
34	14.662	2167	2172	2177	rBV	1182134	1199774	22.75%	3.280%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.292	2445	2449	2457	rVB	736345	884284	16.76%	2.418%
----	--------	------	------	------	-----	--------	--------	--------	--------

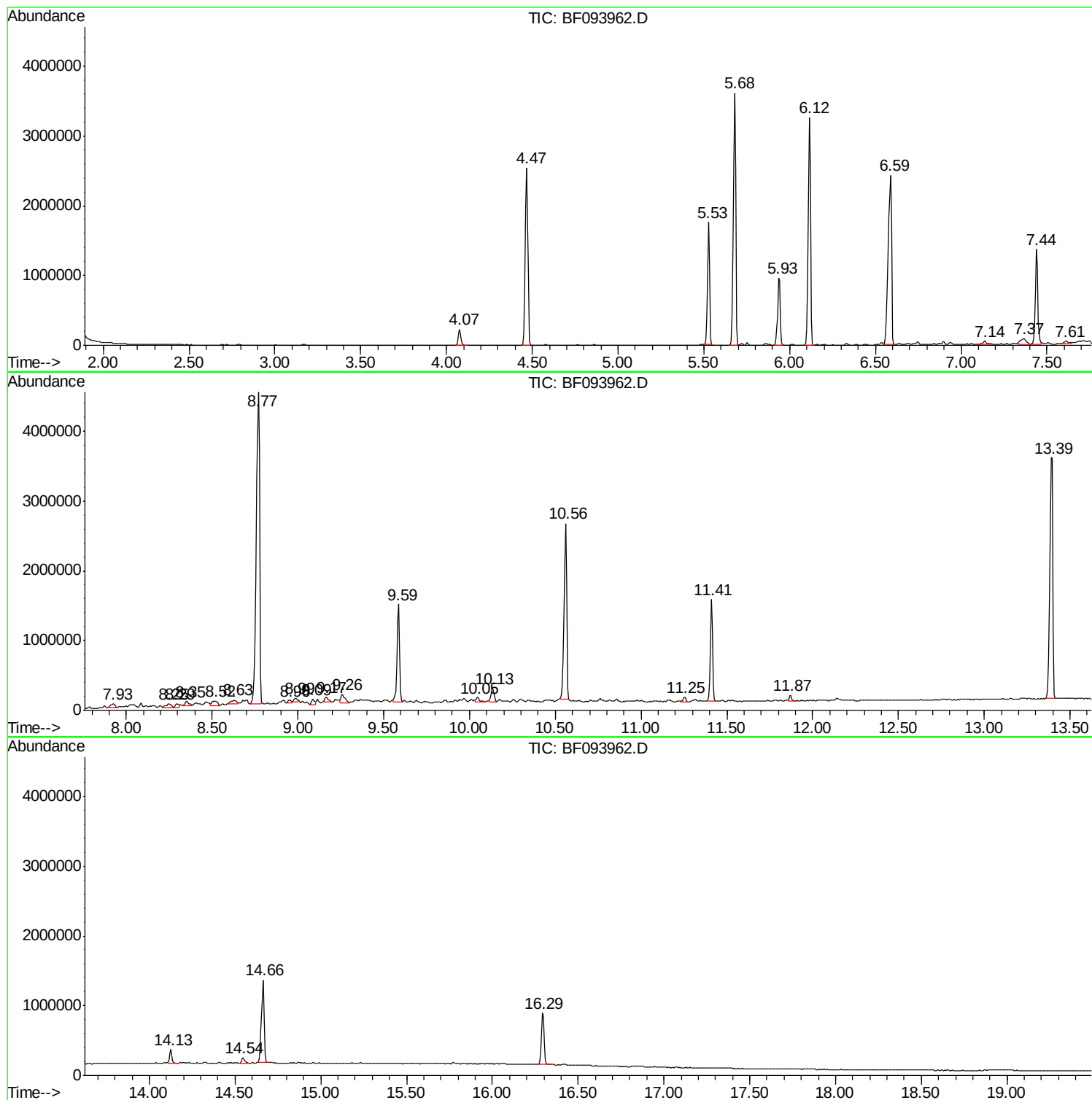
Sum of corrected areas: 36574335

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

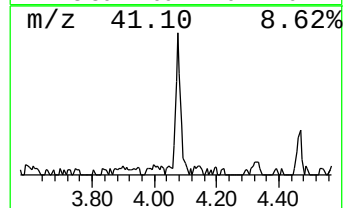
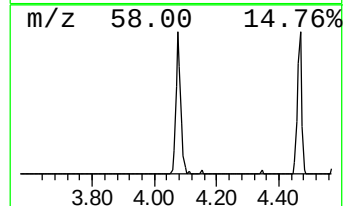
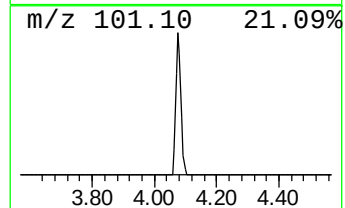
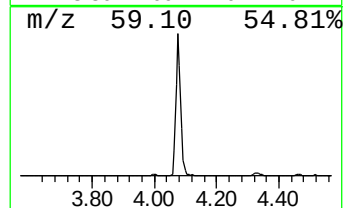
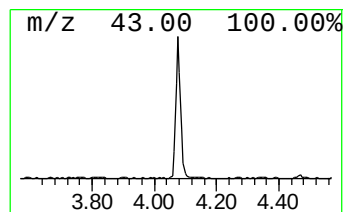
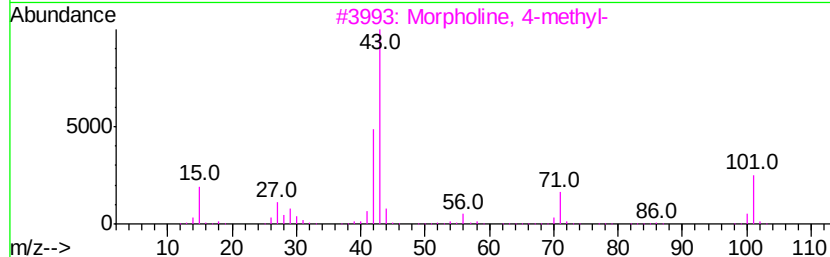
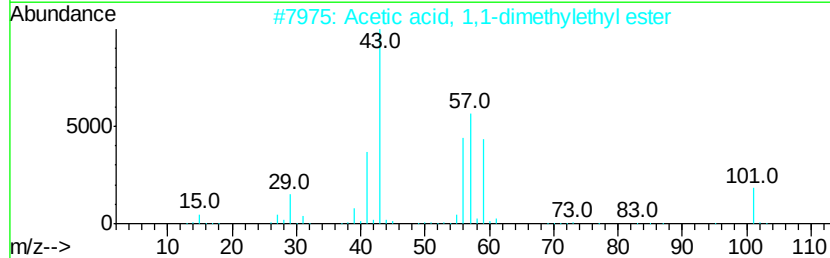
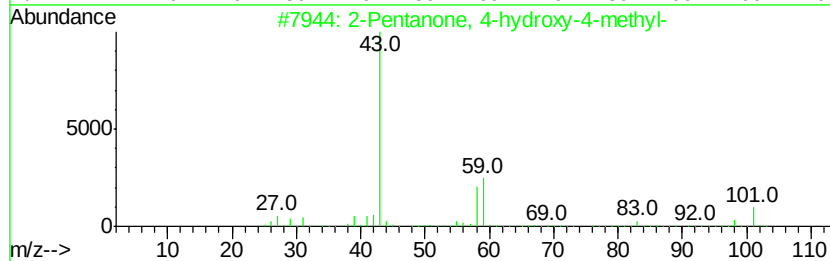
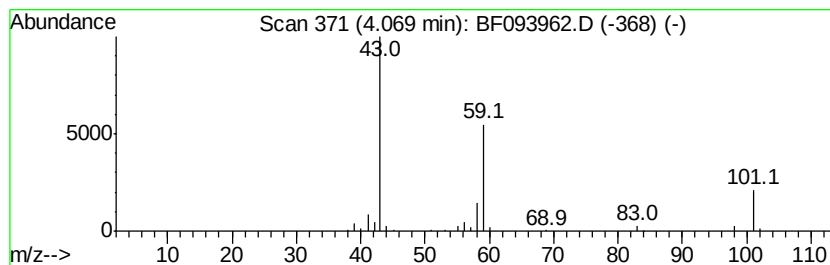
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.07	5.12 ng	250972	1,4-Dichlorobenzene-d4	5.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

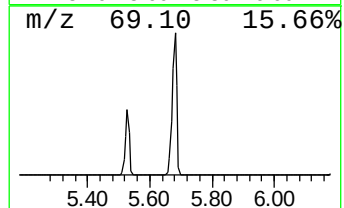
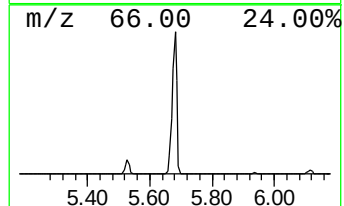
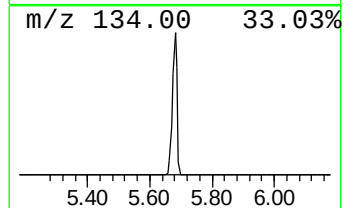
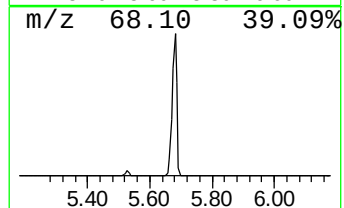
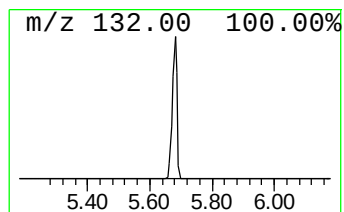
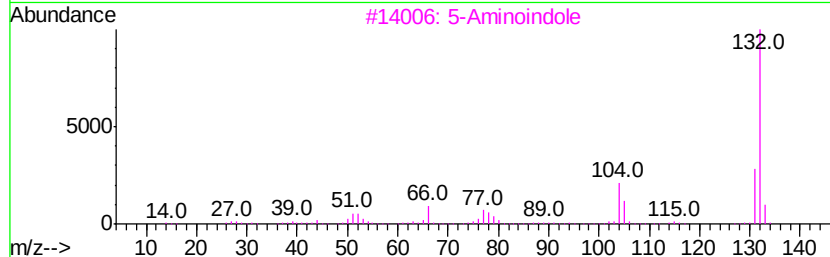
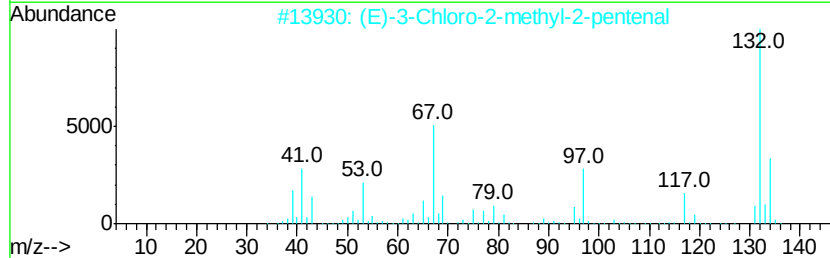
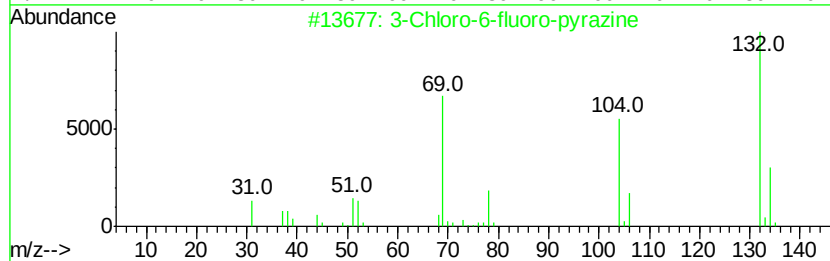
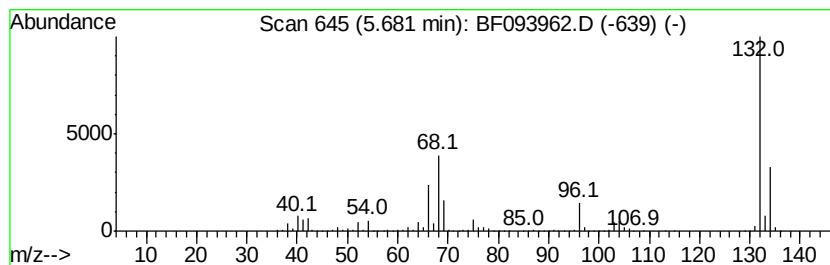
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	78.59 ng	3850550	1,4-Dichlorobenzene-d4	5.94

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	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
LIP-22

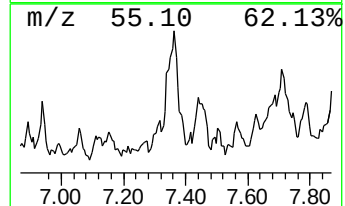
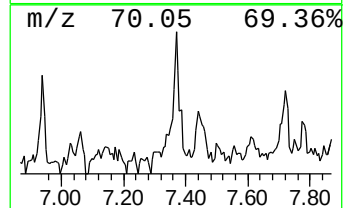
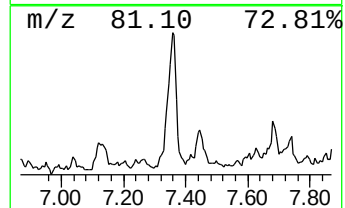
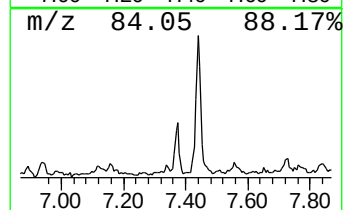
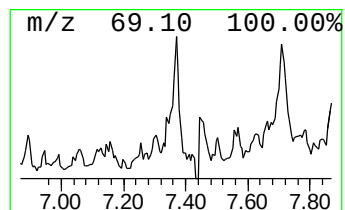
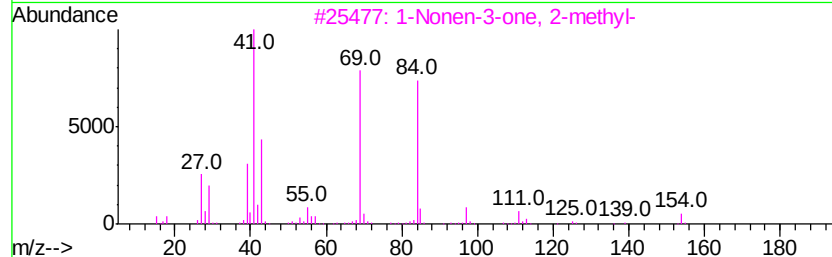
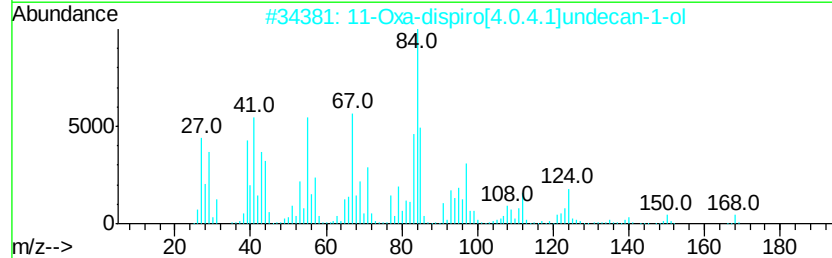
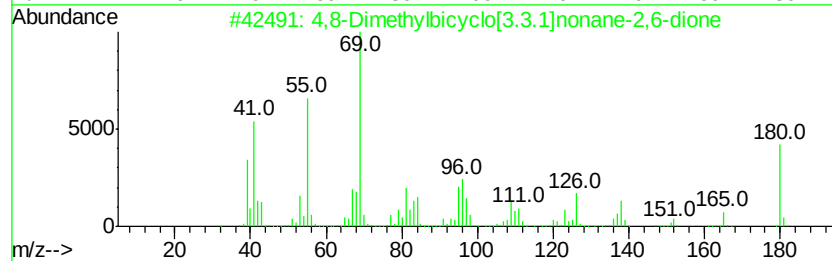
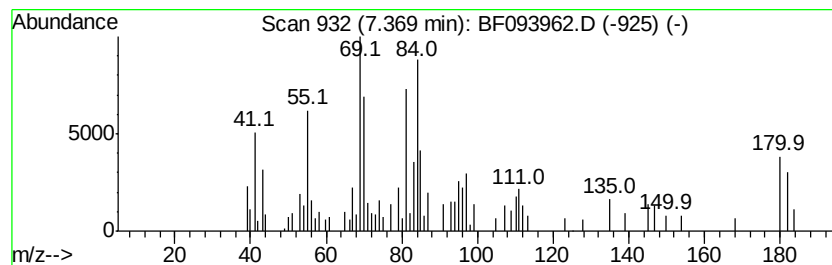
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.37 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	2.74 ng	188393	Napthalene-d8	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,8-Dimethylbicyclo[3.3.1]nonane...	180	C11H16O2	139914-54-8	38
2		11-Oxa-dispiro[4.0.4.1]undecan-1-ol	168	C10H16O2	1000190-18-5	38
3		1-Nonen-3-one, 2-methyl-	154	C10H18O	051756-19-5	38
4		2(3H)-Furanone, 4,5-dihydro-4-(2...	168	C10H16O2	1000153-91-4	38
5		2-Pentene, 3-methyl-	84	C6H12	000922-61-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

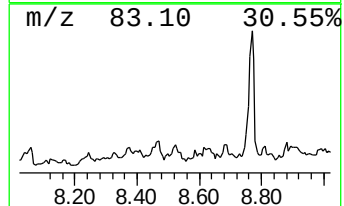
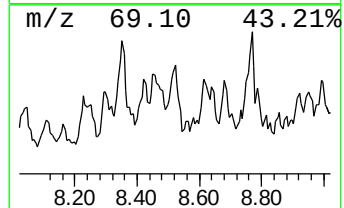
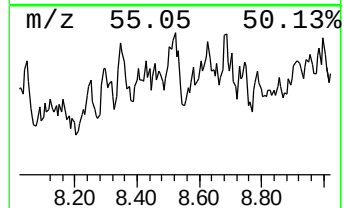
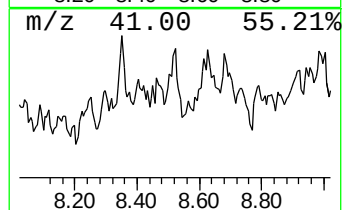
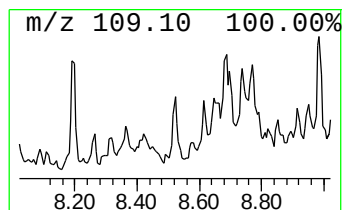
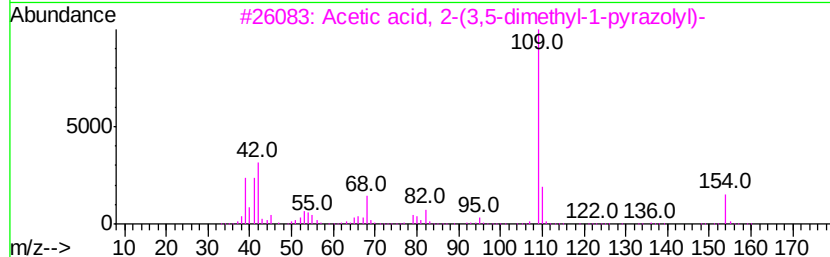
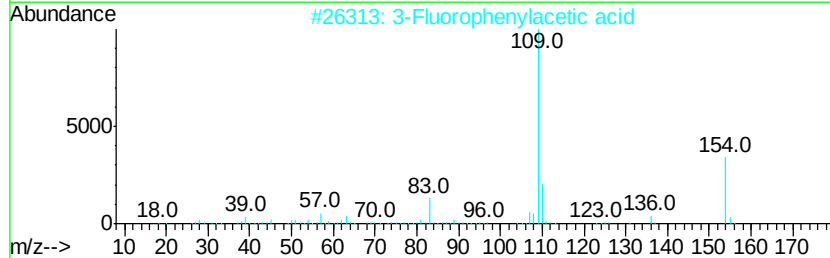
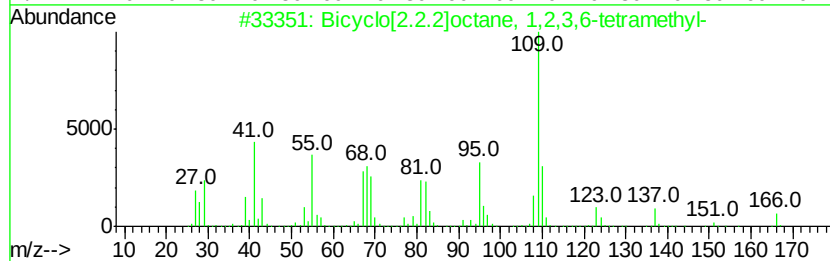
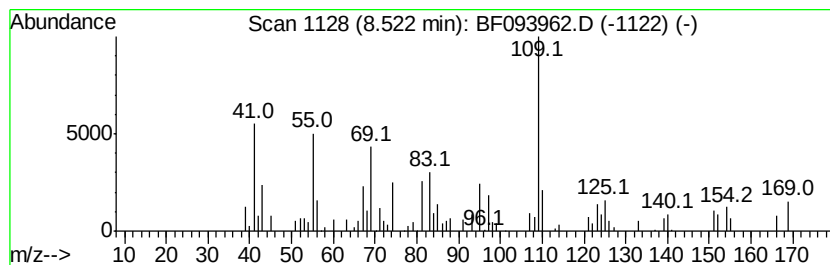
Instrument :
BNA_F
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Bicyclo[2.2.2]octane, 1,2,3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.52	2.09 ng	153635	Acenaphthene-d10	9.59		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.2]octane, 1,2,3,6-te...	166	C12H22	062338-45-8	58
2		3-Fluorophenylacetic acid	154	C8H7FO2	000331-25-9	49
3		Acetic acid, 2-(3,5-dimethyl-1-p...	154	C7H10N2O2	016034-49-4	47
4		trans-3(10)-Caren-2-ol	152	C10H16O	1000151-66-5	47
5		Benzene, 1-fluoro-2-(2-methoxyet...	152	C9H9FO	054533-36-7	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

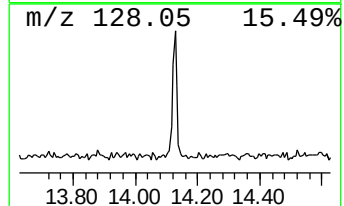
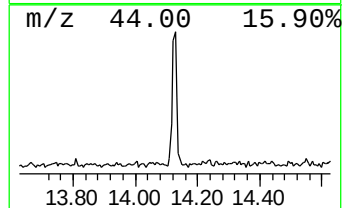
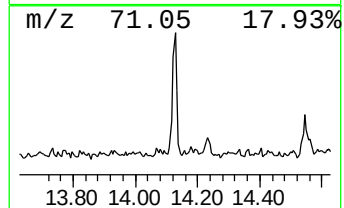
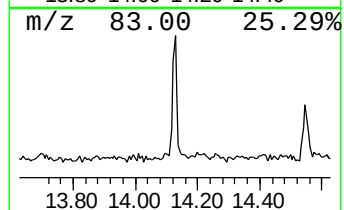
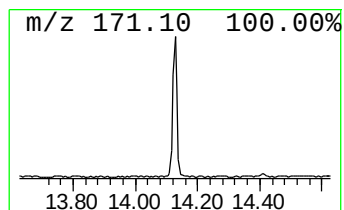
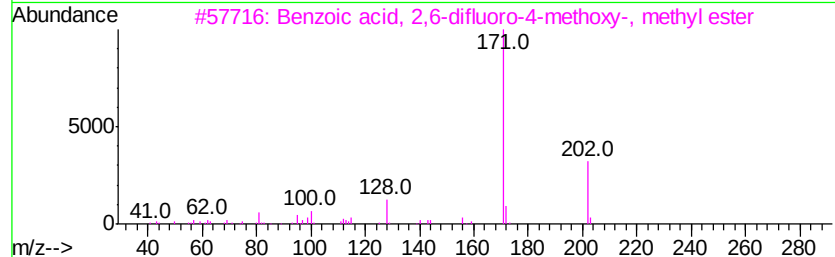
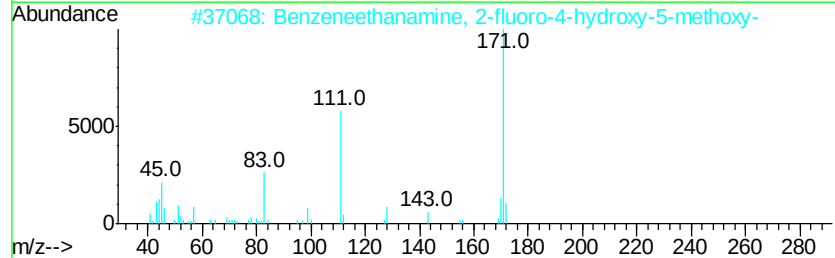
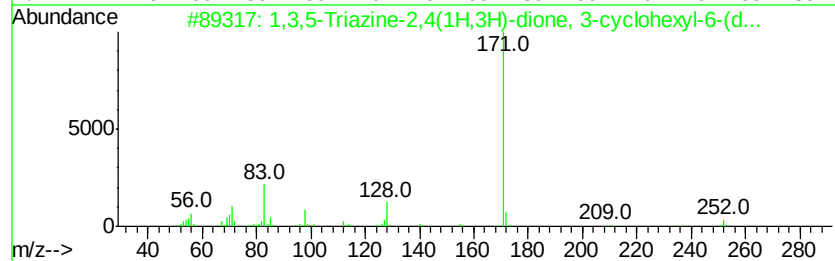
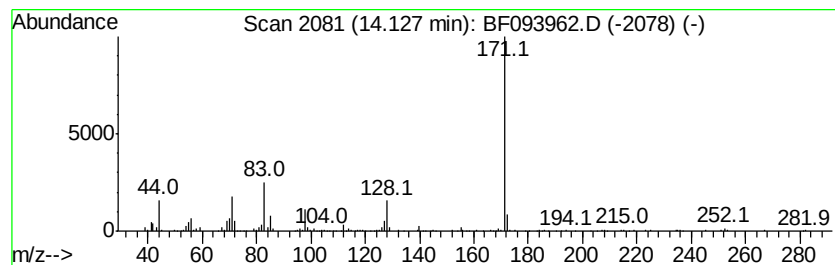
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.24 ng	194479	Chrysene-d12	14.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	94
2		Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	64
3		Benzoic acid, 2,6-difluoro-4-met...	202	C9H8F2O3	084937-82-6	53
4		2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	40
5		1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
Data File : BF093962.D
Acq On : 28 Mar 2017 00:36
Operator : SJ/MA
Sample : I2409-09
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	4.07	5.1	ng	250972	1	5.94	979934	20.0
unknown5.68	5.68	78.6	ng	3850550	1	5.94	979934	20.0
unknown7.37	7.37	2.7	ng	188393	2	7.44	1374840	20.0
Bicyclo[2.2.2]oct...	8.52	2.1	ng	153635	3	9.59	1470160	20.0
1,3,5-Triazine-2,...	14.13	3.2	ng	194479	5	14.66	1199770	20.0