

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
 Data File : BF094282.D
 Acq On : 7 Apr 2017 19:34
 Operator : SJ/MA
 Sample : I2595-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A2394

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	2.057	21	29	45	rVB	301322	560585	11.89%	1.830%
2	2.298	66	70	74	rVB	51459	61319	1.30%	0.200%
3	2.416	85	90	96	rBV	76639	94464	2.00%	0.308%
4	3.675	300	304	311	rBV	228012	262518	5.57%	0.857%
5	4.004	355	360	365	rBV	259964	278031	5.90%	0.908%
6	4.445	431	435	444	rVB	2048437	1948760	41.32%	6.362%
7	4.787	489	493	496	rVB	64013	55365	1.17%	0.181%
8	5.522	614	618	627	rBV	1216357	1258969	26.69%	4.110%
9	5.628	631	636	640	rBV	3428260	3484587	73.89%	11.376%
10	5.857	671	675	679	rBV	981972	902067	19.13%	2.945%
11	6.039	701	706	709	rBV	3393809	3486924	73.93%	11.383%
12	6.516	780	787	790	rBV	2423106	2746555	58.24%	8.966%
13	7.363	926	931	933	rBV	1311746	1226786	26.01%	4.005%
14	7.386	933	935	938	rVB	344014	287604	6.10%	0.939%
15	7.798	1001	1005	1009	rBV	65611	60058	1.27%	0.196%
16	8.692	1151	1157	1160	rVB	4356778	4716210	100.00%	15.396%
17	9.027	1206	1214	1222	rBV2	26951	61121	1.30%	0.200%
18	9.180	1237	1240	1245	rBV	45536	48395	1.03%	0.158%
19	9.351	1261	1269	1276	rVB	55001	106014	2.25%	0.346%
20	9.504	1291	1295	1299	rBV2	1229999	1178237	24.98%	3.846%
21	9.539	1299	1301	1306	rVB	104640	91295	1.94%	0.298%
22	10.486	1457	1462	1466	rBV	1759421	1979008	41.96%	6.461%
23	11.216	1583	1586	1593	rVB2	52460	80444	1.71%	0.263%
24	11.327	1601	1605	1609	rBV	1011088	986215	20.91%	3.220%
25	12.033	1720	1725	1728	rBV2	58905	79681	1.69%	0.260%
26	12.074	1728	1732	1734	rBV4	38983	63304	1.34%	0.207%
27	12.380	1780	1784	1790	rBV2	48390	74056	1.57%	0.242%
28	13.309	1937	1942	1946	rBV	2543485	2943098	62.40%	9.608%
29	14.586	2155	2159	2162	rBV	720772	761705	16.15%	2.487%
30	16.221	2433	2437	2443	rBV	605138	748832	15.88%	2.445%

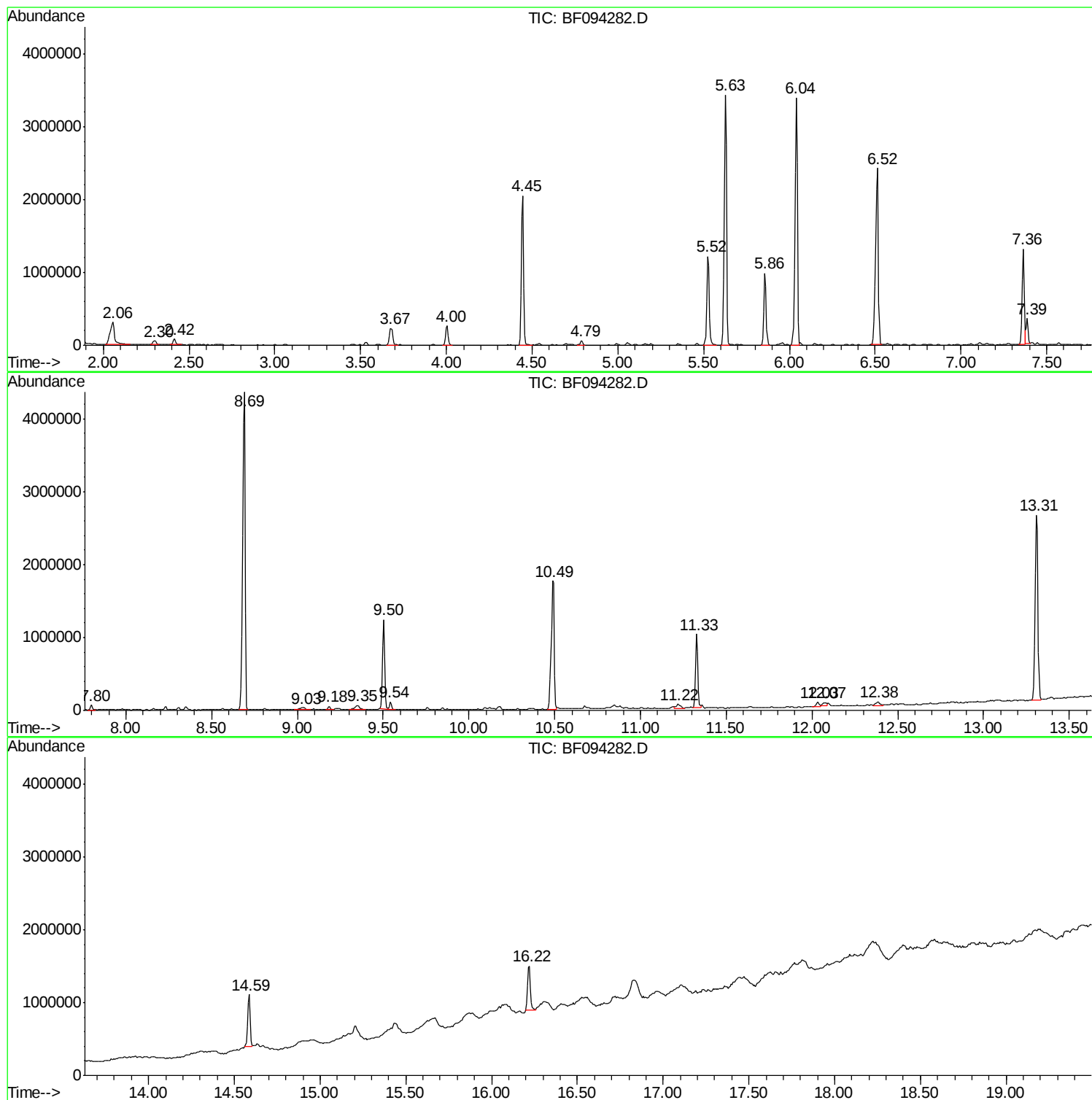
Sum of corrected areas: 30632207

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

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\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

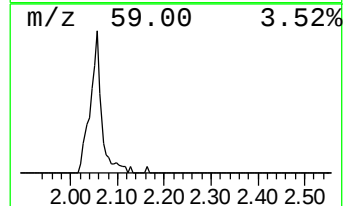
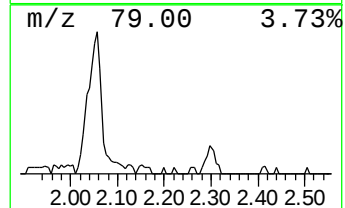
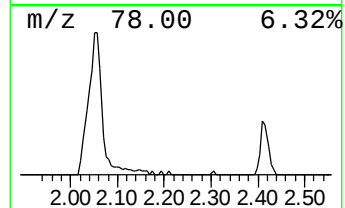
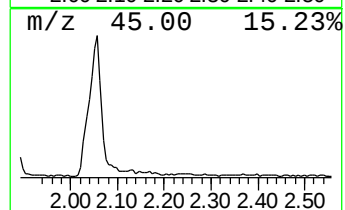
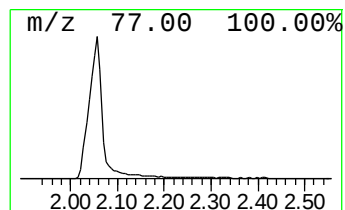
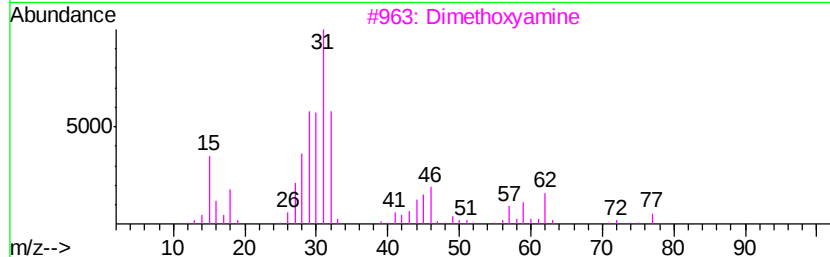
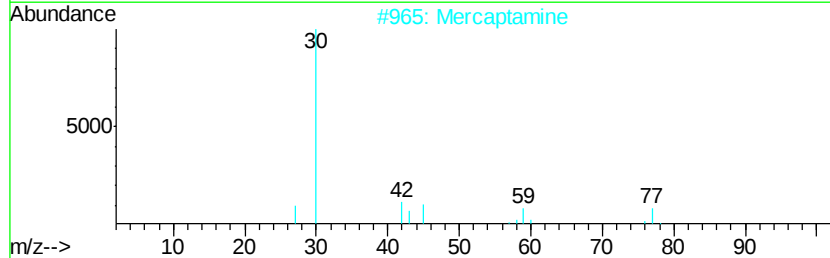
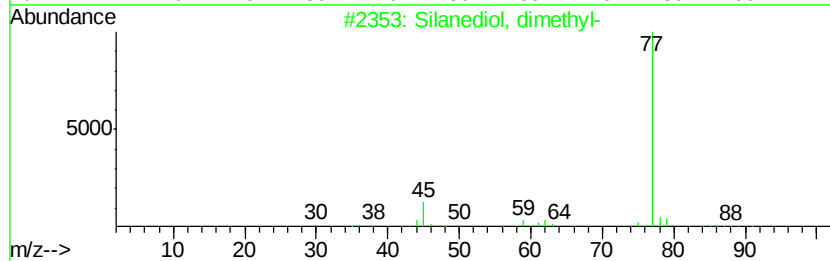
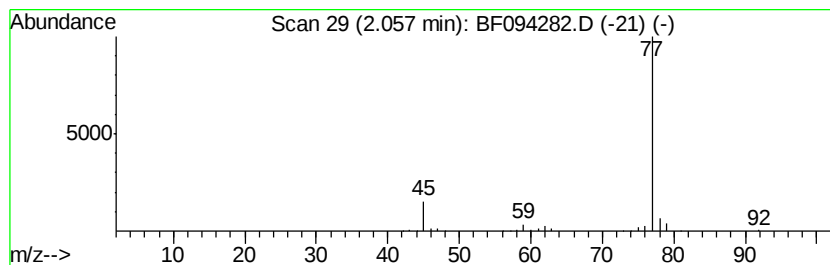
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.06 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	12.43 ng	560585	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silanediol, dimethyl-	92	C2H8O2Si	001066-42-8	43
2		Mercaptamine	77	C2H7NS	000060-23-1	2
3		Dimethoxvamine	77	C2H7NO2	007487-32-3	1
4		1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
5		Ethyl fluoroformate	92	C3H5FO2	000461-64-3	1



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
A2394

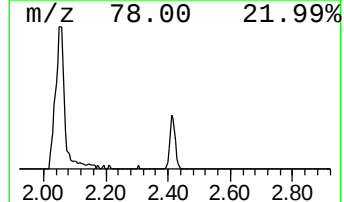
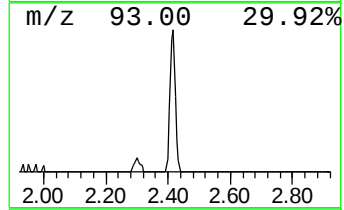
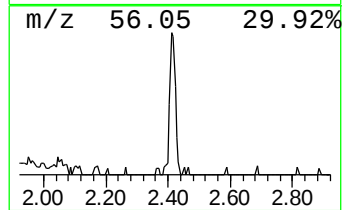
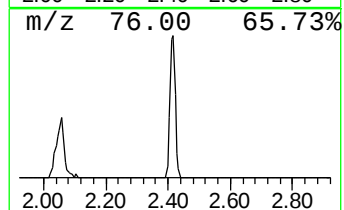
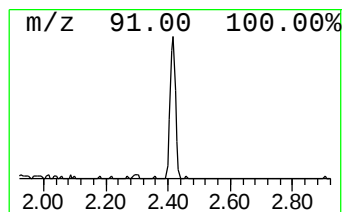
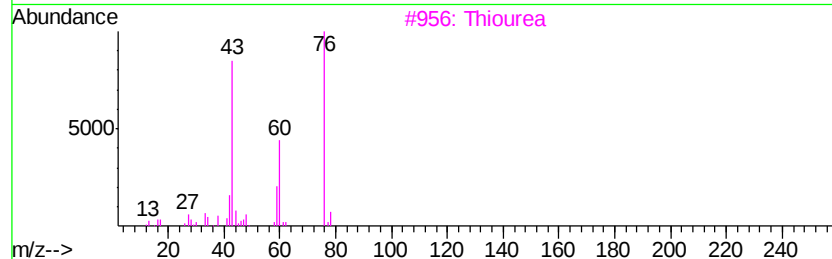
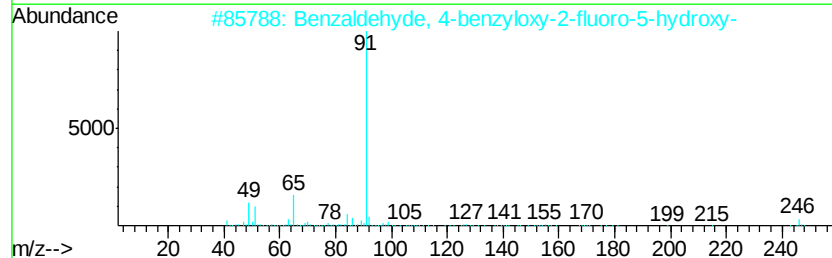
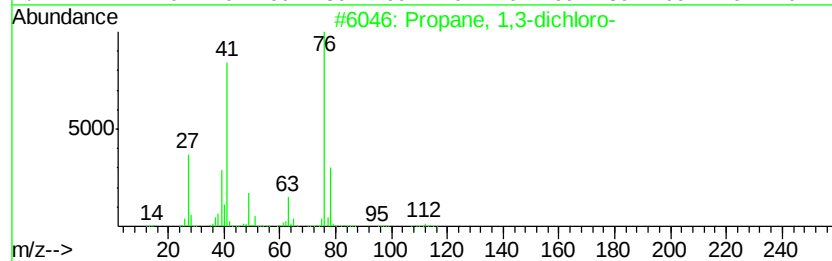
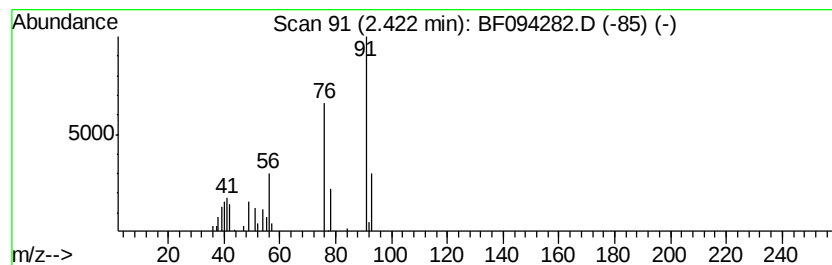
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.42 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	2.09 ng	94464	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	12
2		Benzaldehyde, 4-benzoyloxy-2-fluo...	246	C14H11F03	141523-16-2	9
3		Thiourea	76	CH4N2S	000062-56-6	5
4		Carbon disulfide	76	CS2	000075-15-0	4
5		Monobutyl carbonotrithioate	166	C5H10S3	044747-15-1	4



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

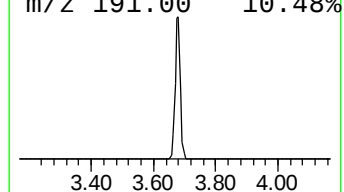
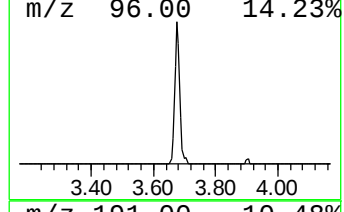
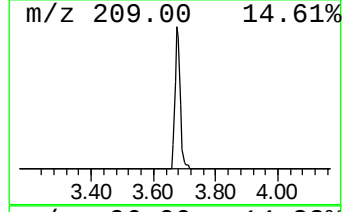
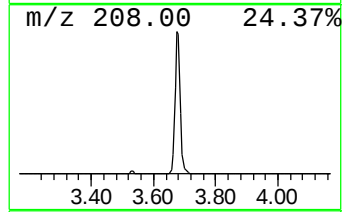
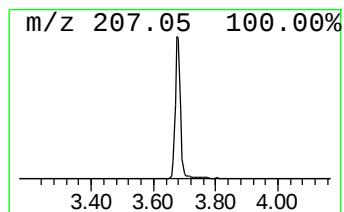
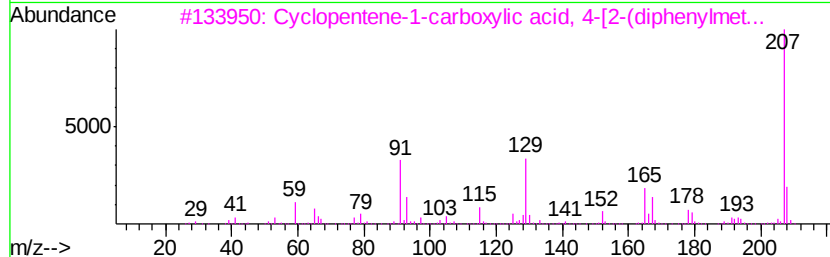
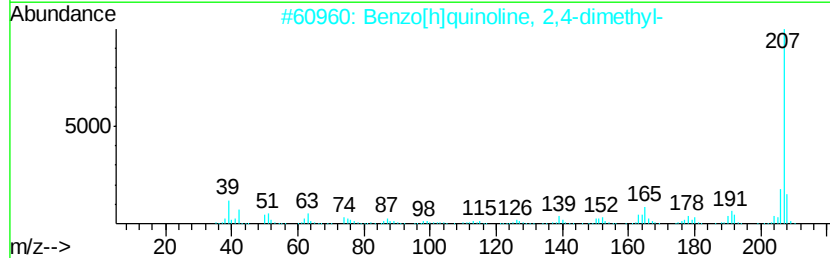
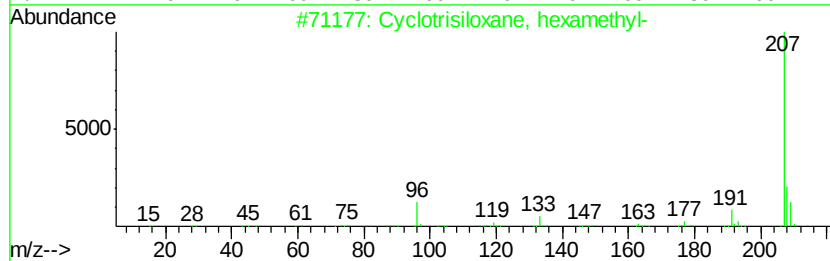
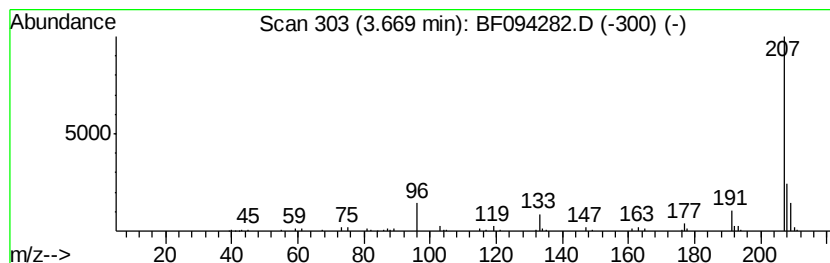
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.67	5.82 ng	262518	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2		Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
3		Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	38
4		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5		1H-Indole, 6-methyl-2-phenyl-	207	C15H13N	066354-87-8	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

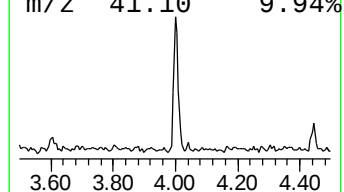
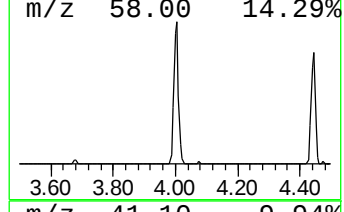
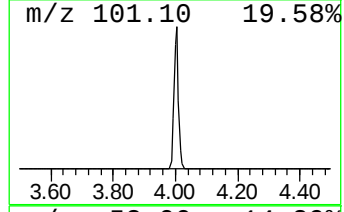
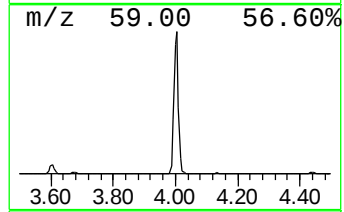
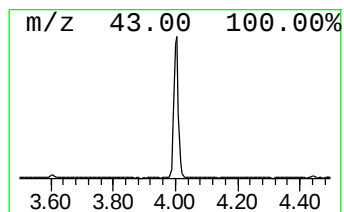
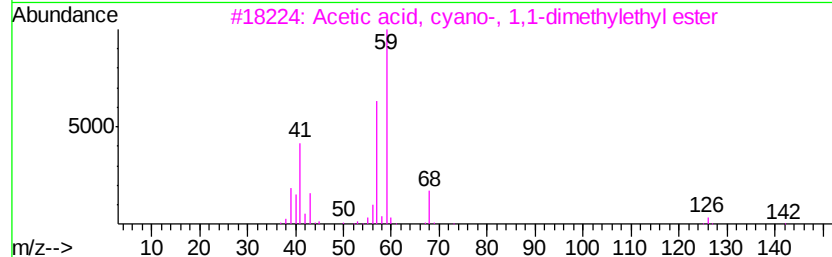
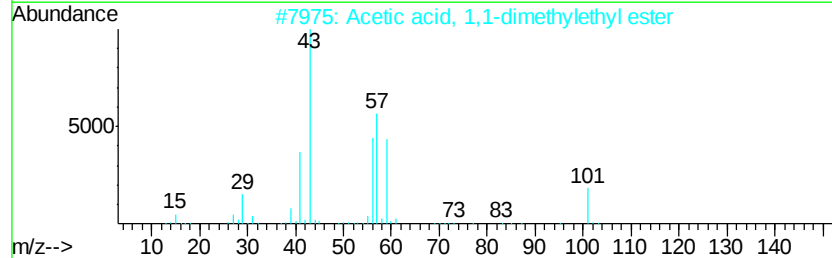
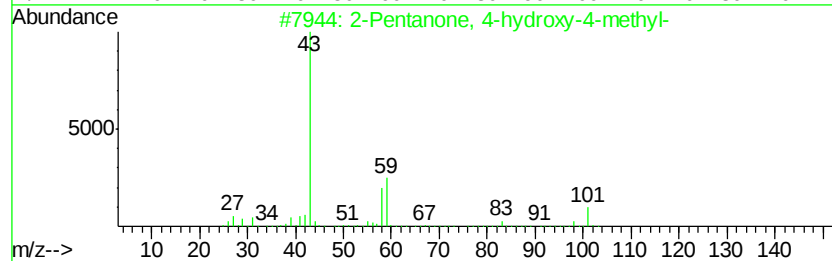
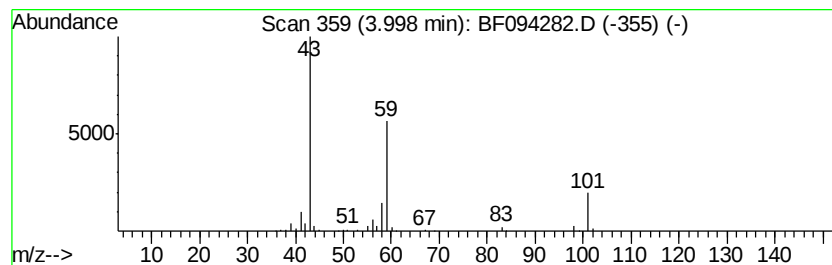
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	6.16 ng	278031	1,4-Dichlorobenzene-d4	5.86

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	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

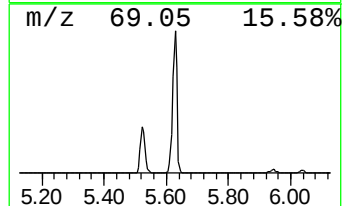
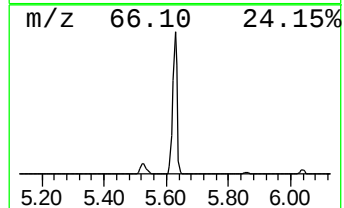
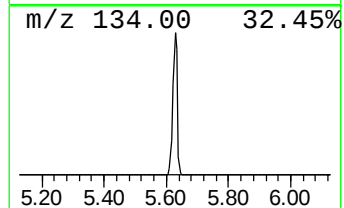
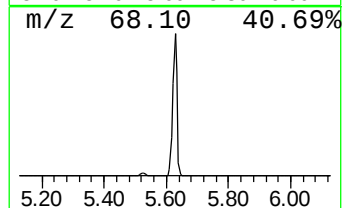
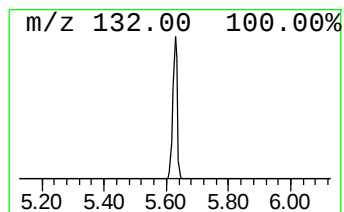
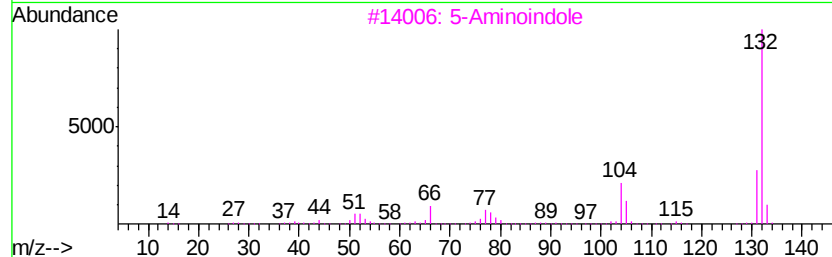
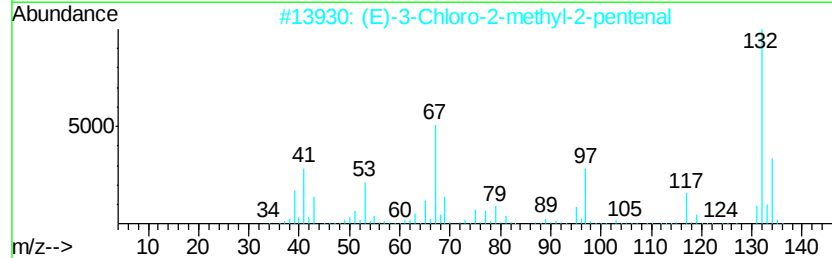
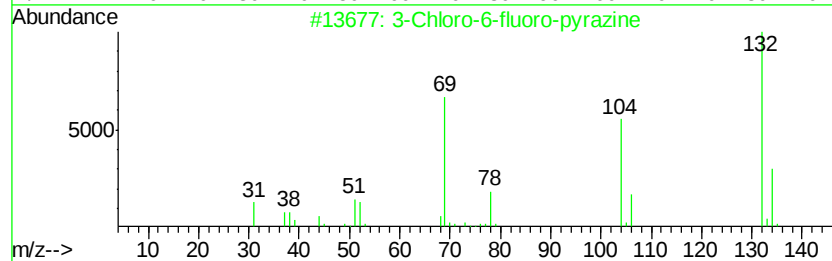
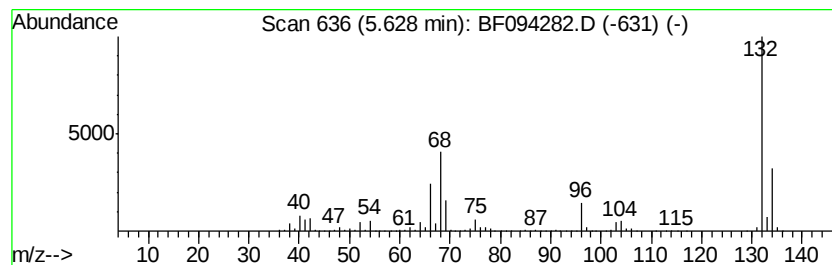
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown5.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	77.26 ng	3484590	1,4-Dichlorobenzene-d4	5.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	16
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
Data File : BF094282.D
Acq On : 7 Apr 2017 19:34
Operator : SJ/MA
Sample : I2595-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2394

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
unknown2.06	2.06	12.4	ng	560585	1	5.86	902067	20.0
unknown2.42	2.42	2.1	ng	94464	1	5.86	902067	20.0
Cyclotrisiloxane,...	3.67	5.8	ng	262518	1	5.86	902067	20.0
2-Pentanone, 4-hy...	4.00	6.2	ng	278031	1	5.86	902067	20.0
unknown5.63	5.63	77.3	ng	3484590	1	5.86	902067	20.0