

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
 Data File : BF088589.D
 Acq On : 1 Jul 2016 22:40
 Operator : UM/SJ
 Sample : PB91760BL
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91760BL

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-BF063016.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	1.701	5	10	12	rBV	4079718	5783347	100.00%	14.339%
2	1.736	12	13	22	rVB	687228	997477	17.25%	2.473%
3	1.861	22	24	42	rVB	2234188	3943740	68.19%	9.778%
4	2.090	42	44	81	rVB2	121866	512753	8.87%	1.271%
5	4.993	295	298	304	rVB	170358	277101	4.79%	0.687%
6	5.416	331	335	337	rBV	2717491	3621655	62.62%	8.979%
7	6.445	421	425	427	rBV	2959231	3382747	58.49%	8.387%
8	6.582	434	437	439	rBV	2511149	3516833	60.81%	8.719%
9	6.810	454	457	459	rBV	850531	813011	14.06%	2.016%
10	6.970	468	471	473	rVB	2166139	2816793	48.71%	6.984%
11	7.370	503	506	508	rBV	1935843	2047743	35.41%	5.077%
12	8.090	566	569	571	rVB	1216193	1072900	18.55%	2.660%
13	9.176	660	664	666	rBV	2738290	3858292	66.71%	9.566%
14	9.839	720	722	725	rVB	1075867	1035024	17.90%	2.566%
15	10.628	788	791	793	rBV	1766048	1810641	31.31%	4.489%
16	11.314	849	851	854	rBV	667475	885424	15.31%	2.195%
17	12.902	987	990	993	rBV	2482467	2573120	44.49%	6.380%
18	13.942	1079	1081	1084	rBV	869986	745926	12.90%	1.849%
19	15.348	1201	1204	1206	rBV	387939	579109	10.01%	1.436%
20	16.251	1280	1283	1289	rBV2	22061	59759	1.03%	0.148%

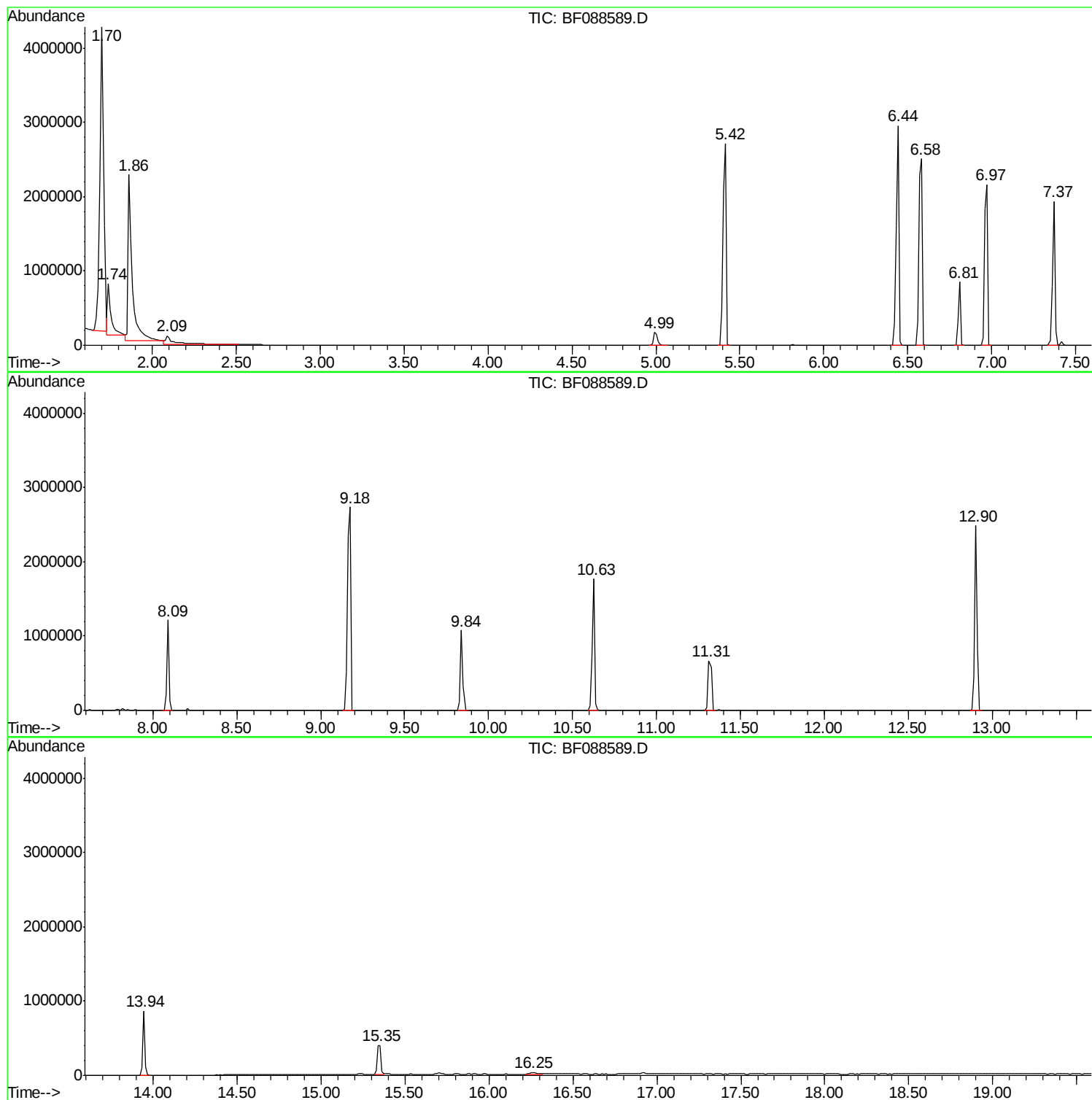
Sum of corrected areas: 40333395

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

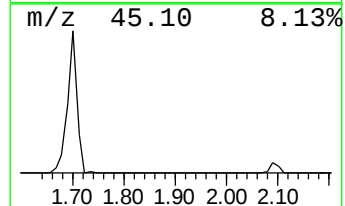
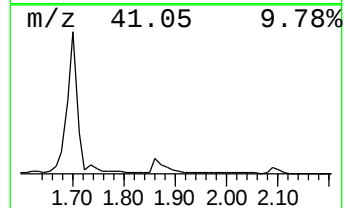
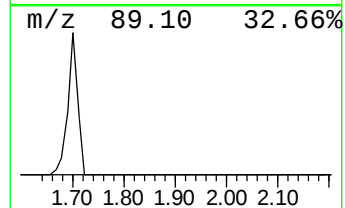
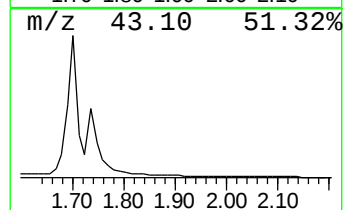
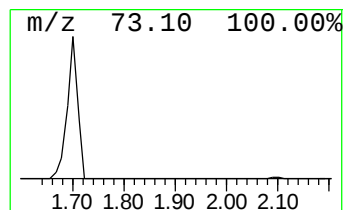
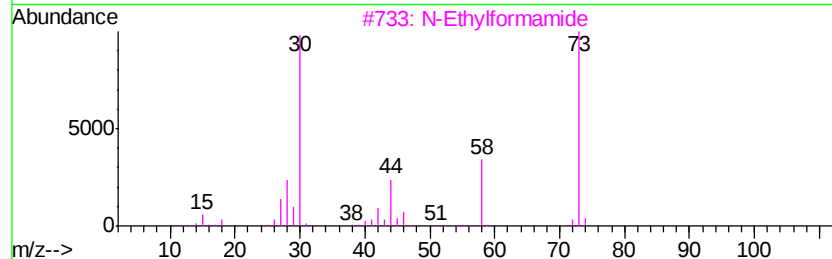
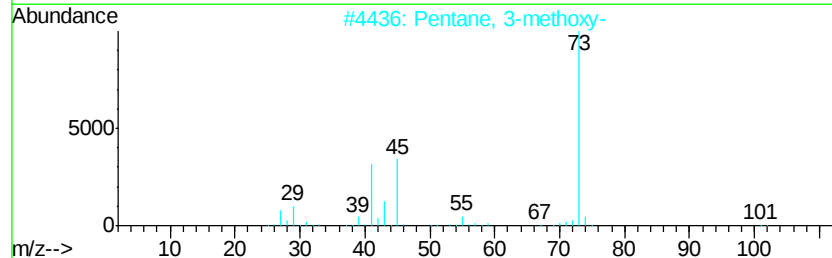
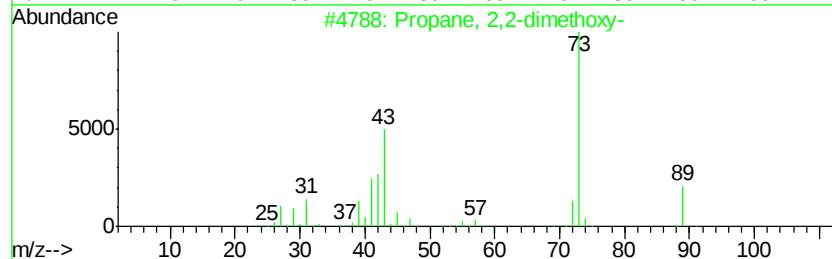
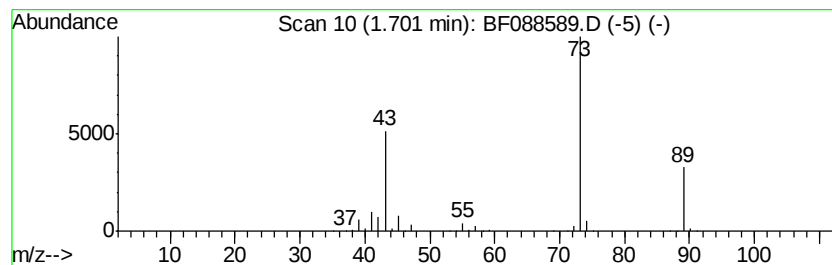
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	142.27 ng	5783350	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

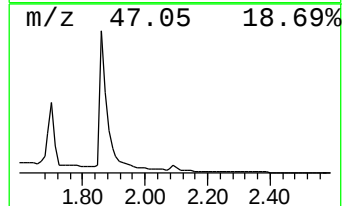
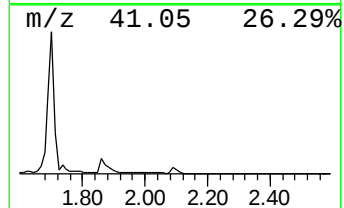
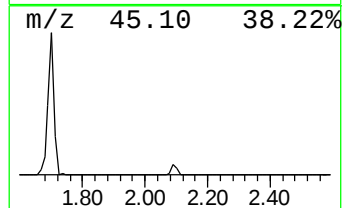
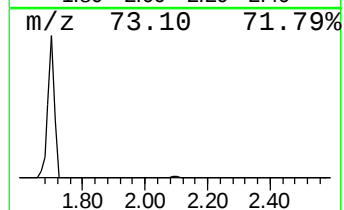
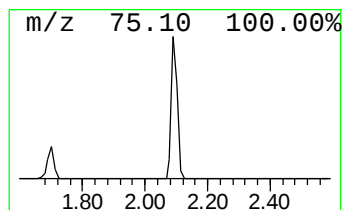
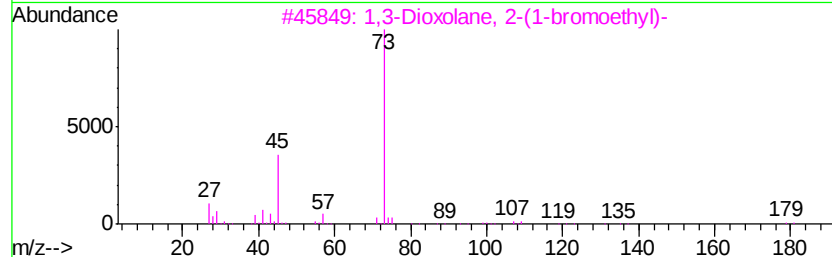
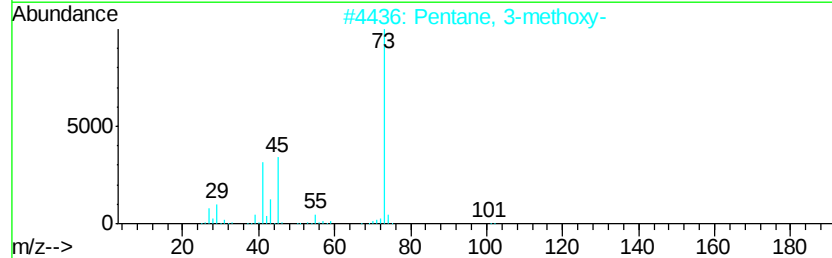
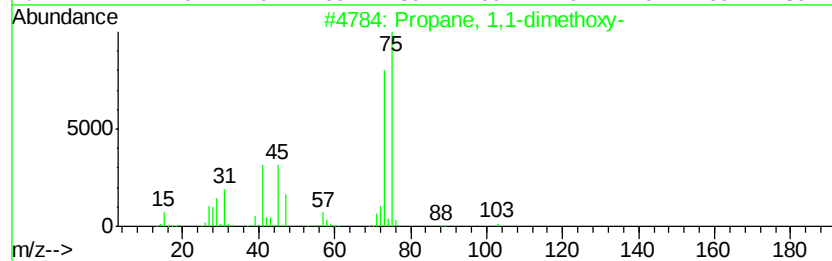
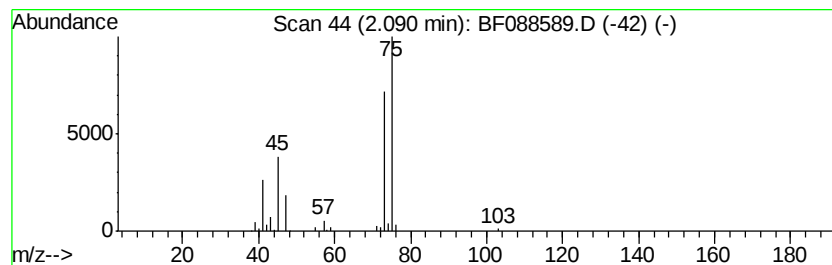
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	12.61 ng	512753	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
4		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

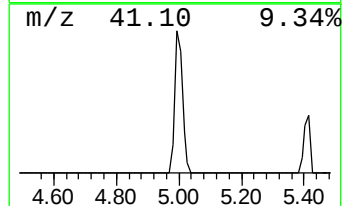
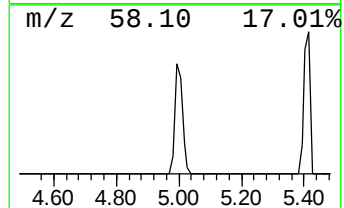
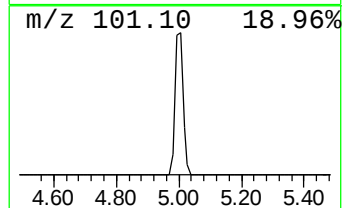
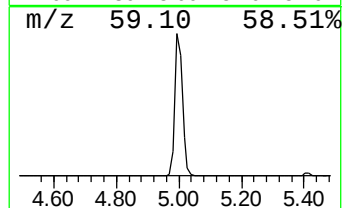
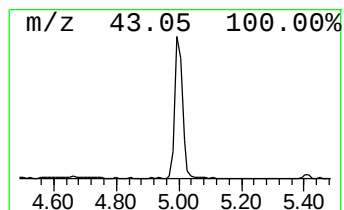
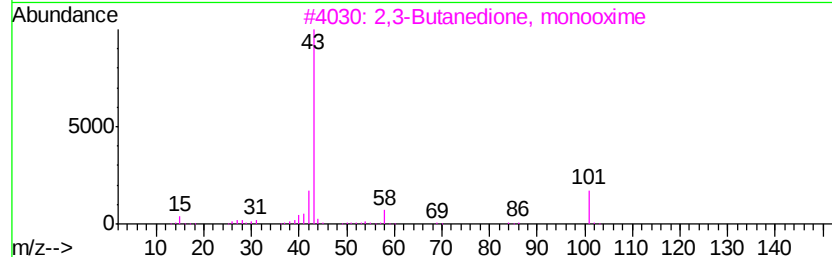
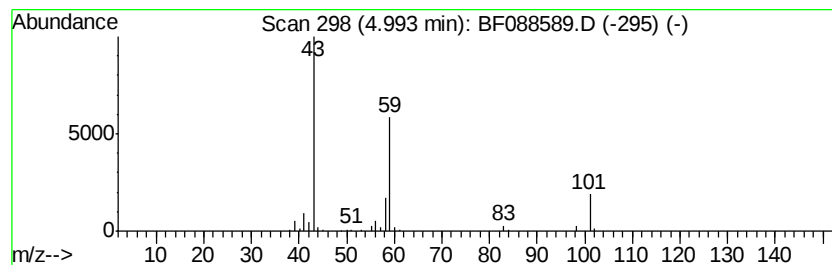
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	6.82 ng	277101	1,4-Dichlorobenzene-d4	6.81

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, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O		000625-23-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

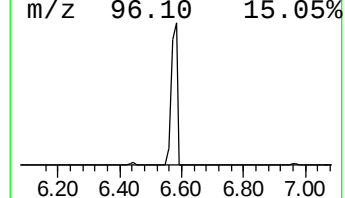
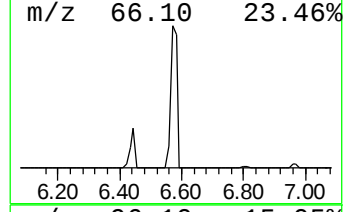
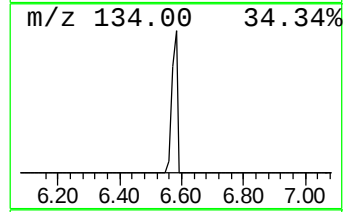
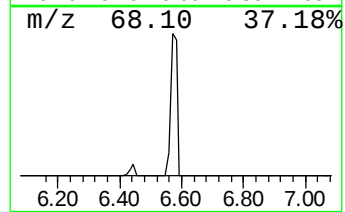
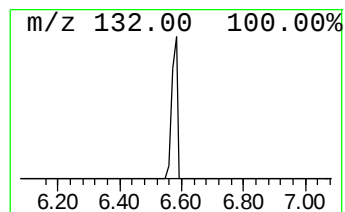
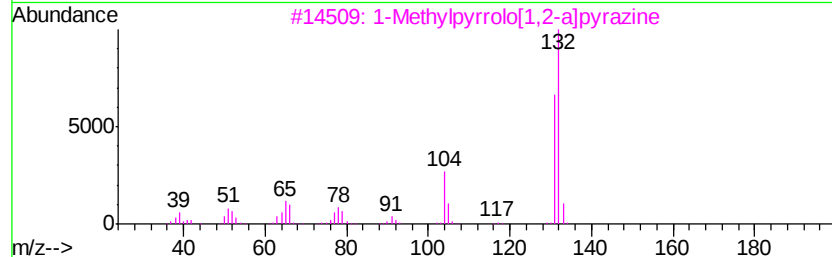
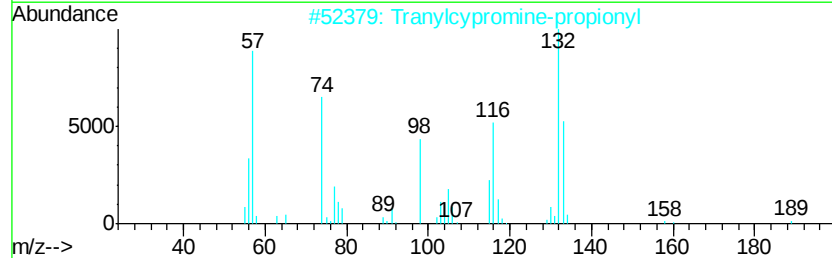
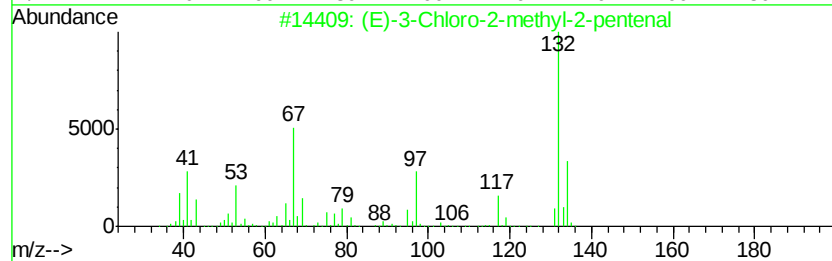
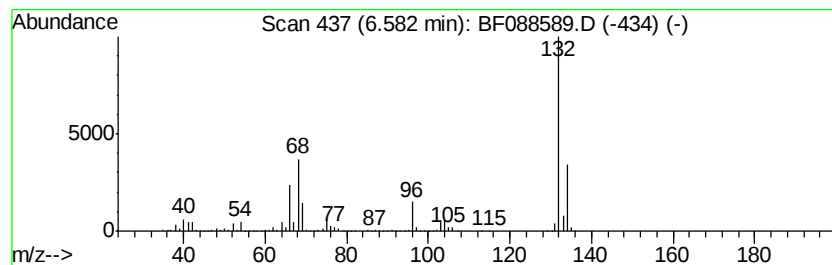
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	86.51 ng	3516830	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranlylcypropine-propionyl	189	C12H15NO	1000123-86-3	16
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

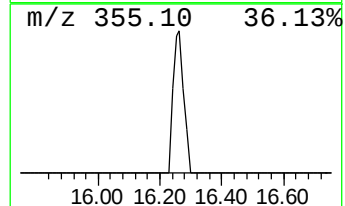
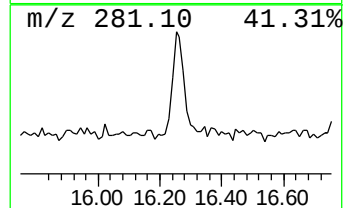
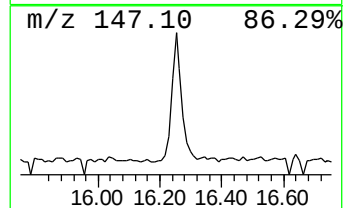
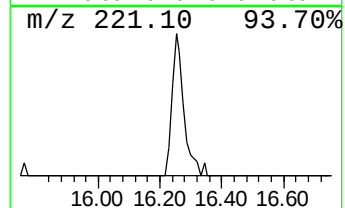
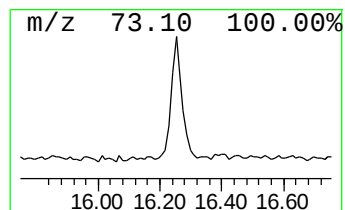
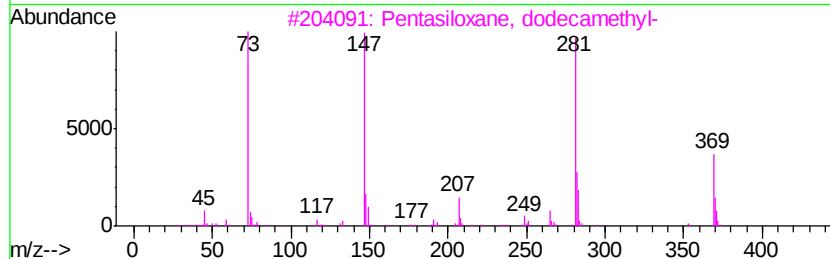
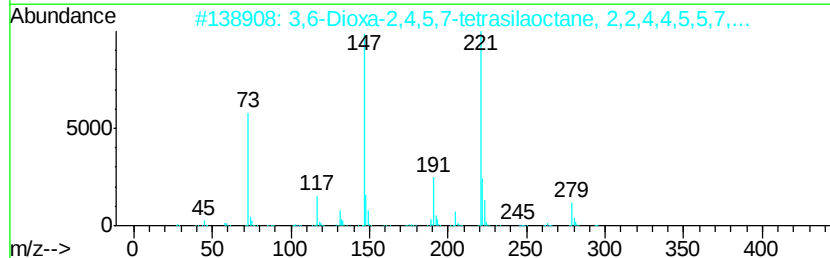
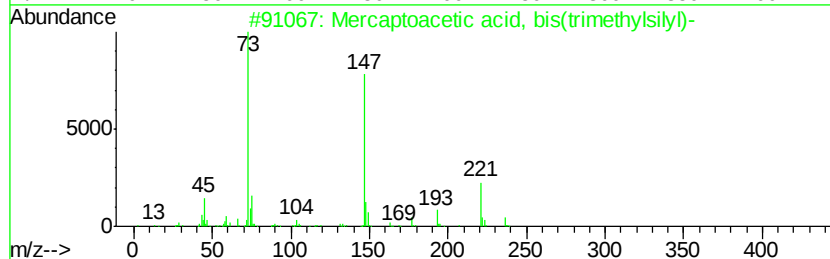
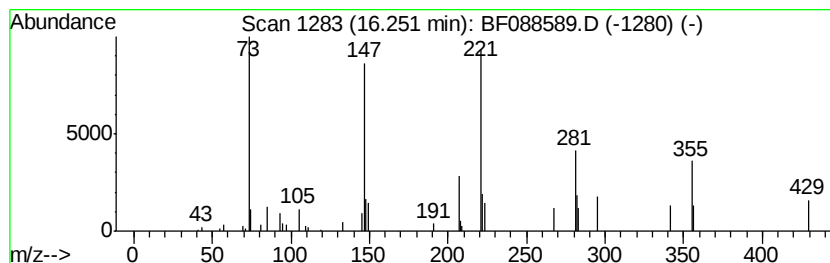
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.25 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.06 ng	59759	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	38
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	38
3		Pentasiloxane, dodecamethyl-	384	C12H3604Si5	000141-63-9	35
4		1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15N03	1000124-33-0	22
5		2-tert-Butyl-6-methylphenol, tri...	236	C14H240Si	1000333-48-3	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088589.D
Acq On : 1 Jul 2016 22:40
Operator : UM/SJ
Sample : PB91760BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91760BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
unknown1.70	1.70	142.3	ng	5783350	1	6.81	813011	20.0
Propane, 1,1-dime...	2.09	12.6	ng	512753	1	6.81	813011	20.0
2-Pentanone, 4-hy...	4.99	6.8	ng	277101	1	6.81	813011	20.0
unknown6.58	6.58	86.5	ng	3516830	1	6.81	813011	20.0
unknown16.25	16.25	2.1	ng	59759	6	15.35	579109	20.0