

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
 Data File : BF080055.D
 Acq On : 19 Jun 2015 13:37
 Operator : TP/IZ
 Sample : PB84099BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84099BL

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-BF061715.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	4.961	162	164	168	rBB	40436	47069	2.48%	0.383%
2	5.544	213	215	218	rBV	688271	750030	39.56%	6.109%
3	5.944	248	250	252	rBV	1257164	1108412	58.47%	9.028%
4	6.344	283	285	287	rBB	58264	52299	2.76%	0.426%
5	6.927	334	336	339	rBV	924272	1032874	54.48%	8.413%
6	7.099	349	351	353	rBV	1398259	1190928	62.82%	9.700%
7	7.327	369	371	374	rBB	214692	235631	12.43%	1.919%
8	7.487	383	385	388	rBB	921154	860335	45.38%	7.007%
9	7.887	418	420	422	rBV	871806	701304	36.99%	5.712%
10	8.619	482	484	487	rBV	330918	327158	17.26%	2.665%
11	9.693	576	578	581	rBV	1029848	1392079	73.43%	11.338%
12	10.390	637	639	642	rBB2	345426	383960	20.25%	3.127%
13	11.191	707	709	711	rBV	1008024	911092	48.06%	7.421%
14	11.922	771	773	775	rBV	444546	437871	23.10%	3.566%
15	13.705	926	929	931	rBV	1977617	1895753	100.00%	15.441%
16	15.077	1046	1049	1052	rBV	413476	480530	25.35%	3.914%
17	17.088	1222	1225	1233	rBV	304606	470280	24.81%	3.830%

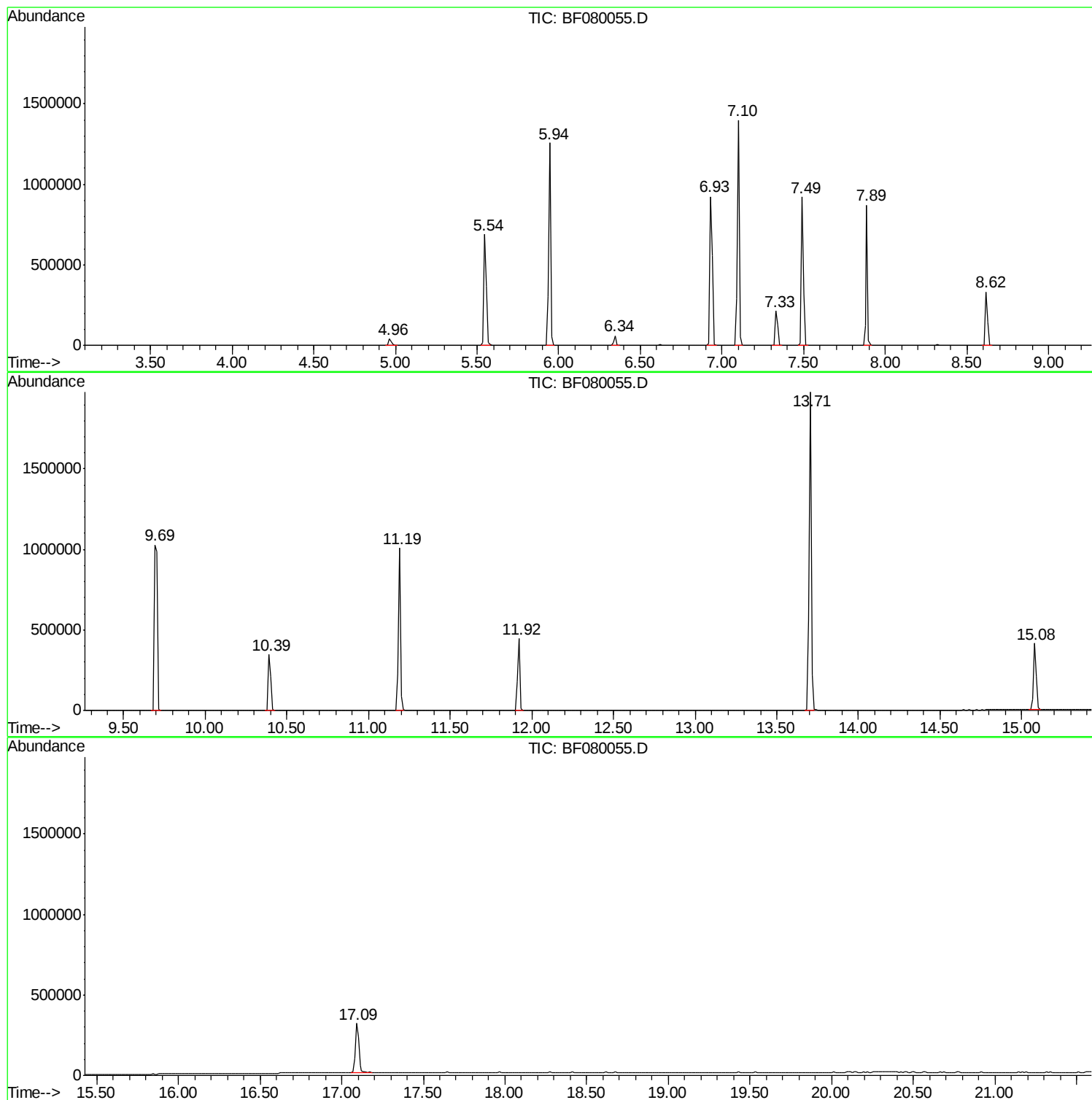
Sum of corrected areas: 12277605

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.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\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

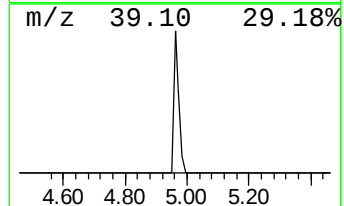
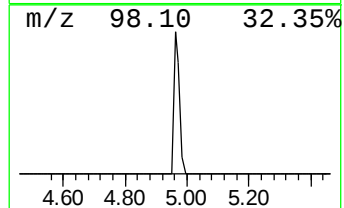
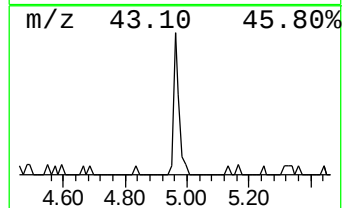
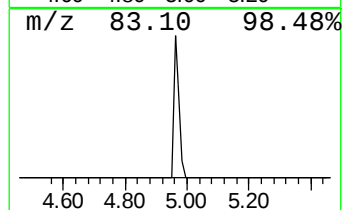
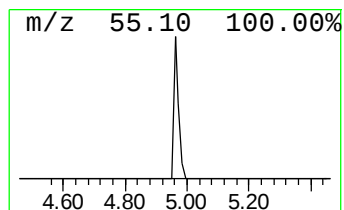
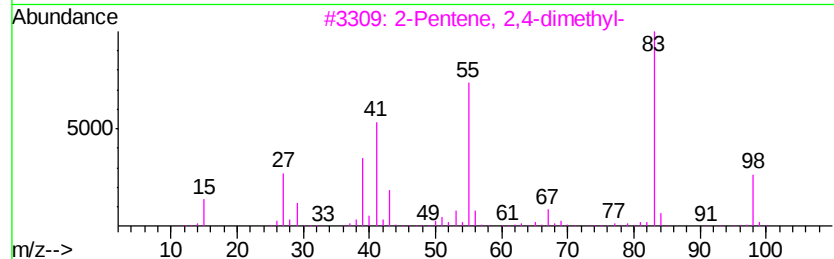
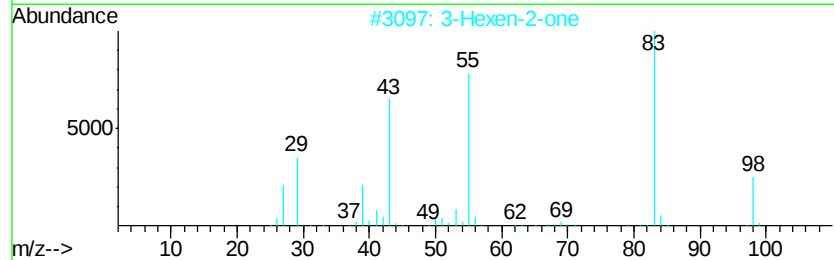
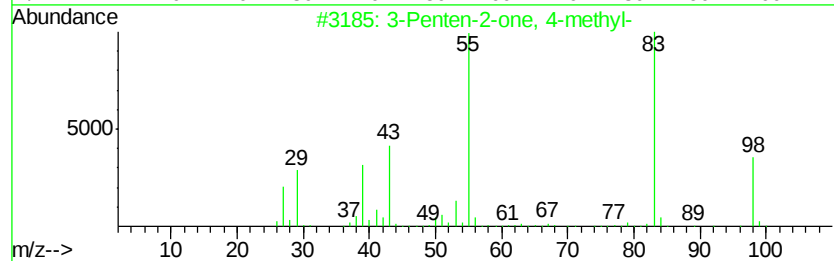
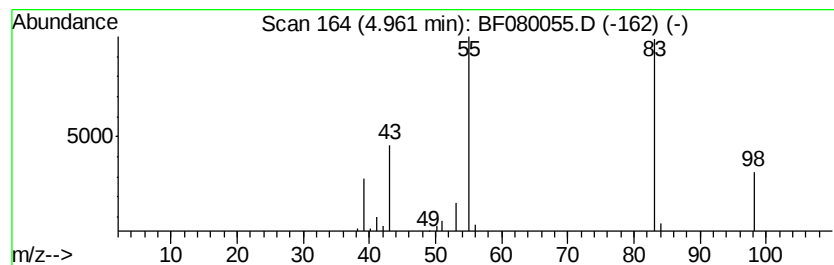
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.00 ng	47069	1,4-Dichlorobenzene-d4	7.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

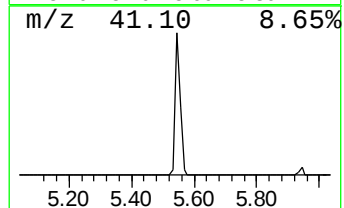
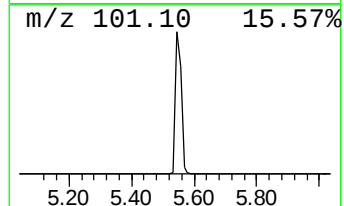
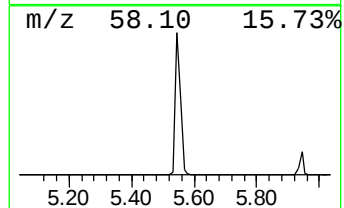
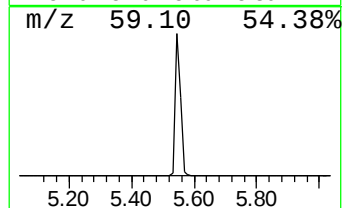
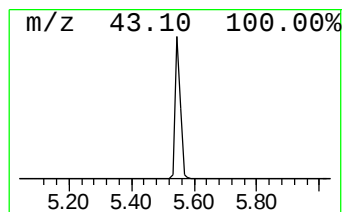
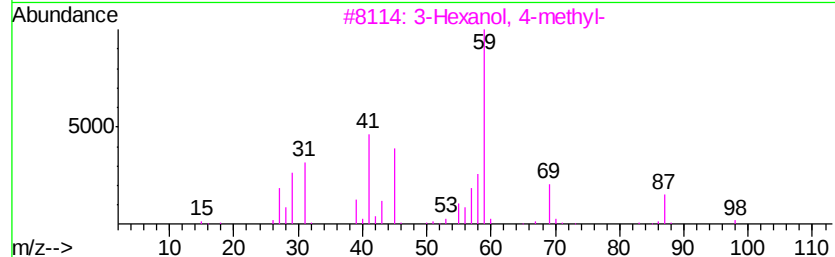
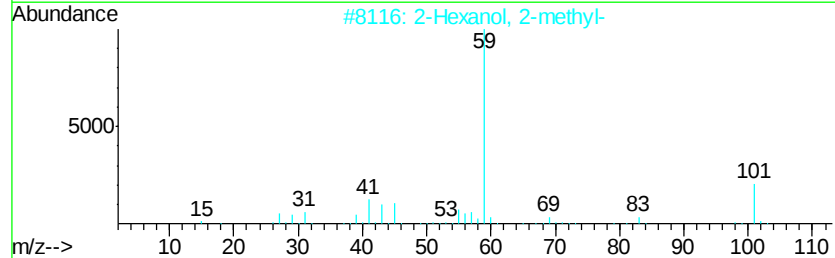
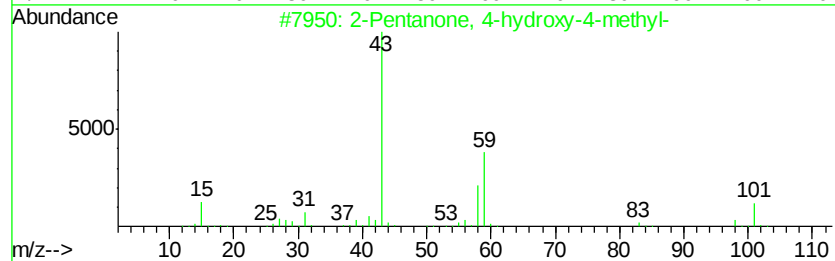
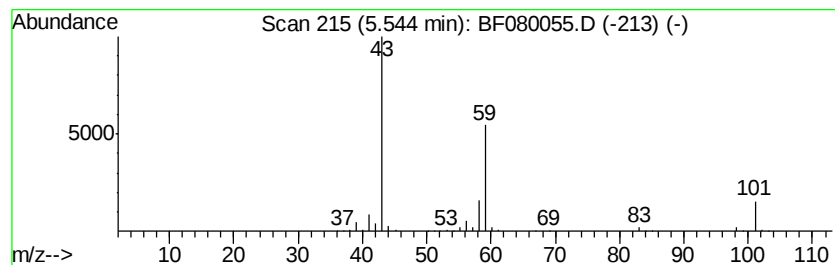
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	63.66 ng	750030	1,4-Dichlorobenzene-d4	7.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

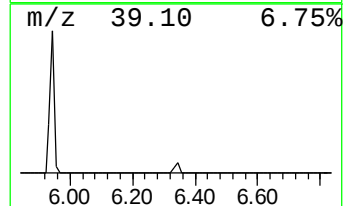
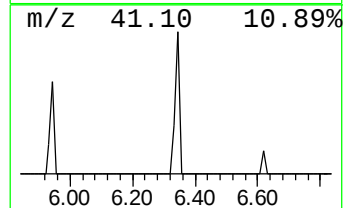
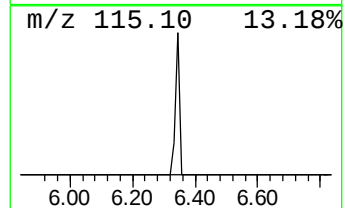
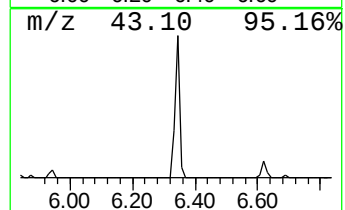
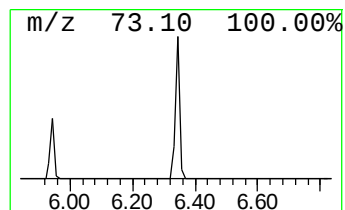
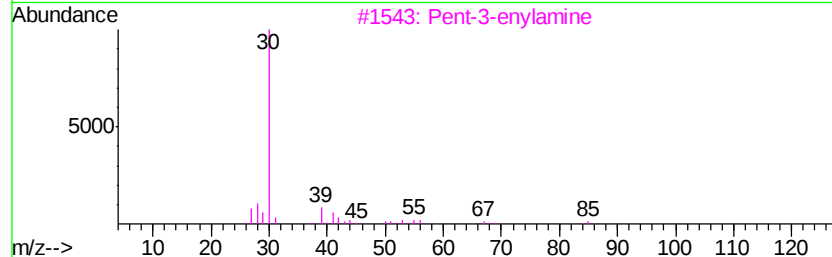
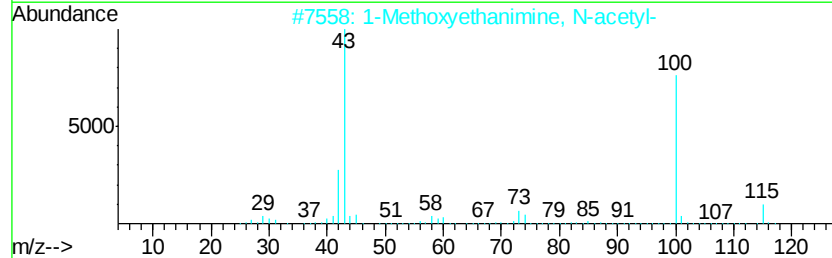
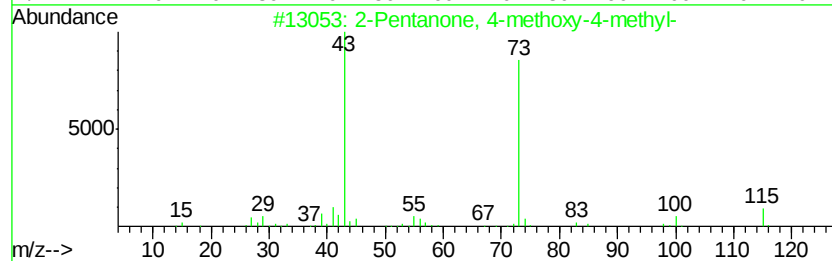
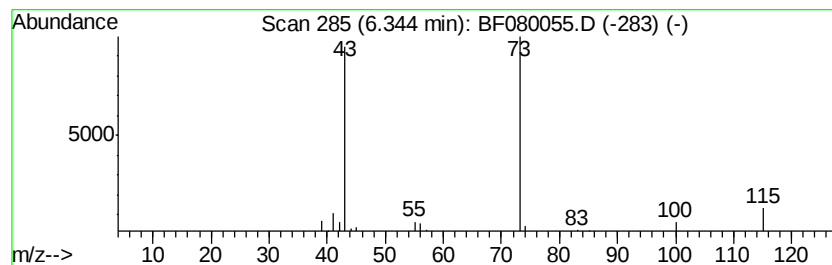
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.34 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.44 ng	52299	1,4-Dichlorobenzene-d4	7.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25	
3	Pent-3-enylamine	85	C5H11N	087156-70-5	9	
4	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9	
5	2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

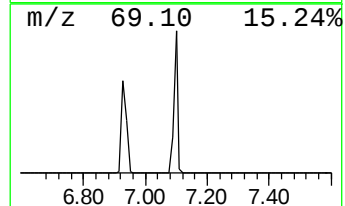
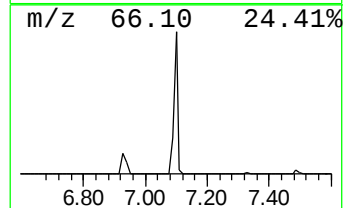
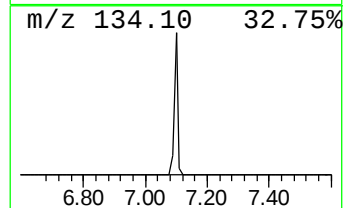
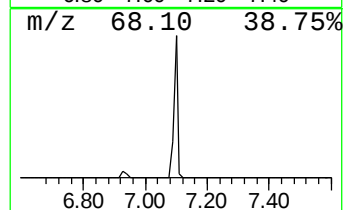
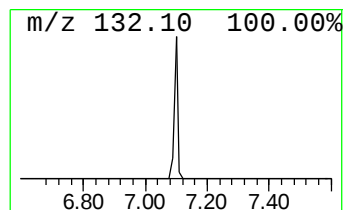
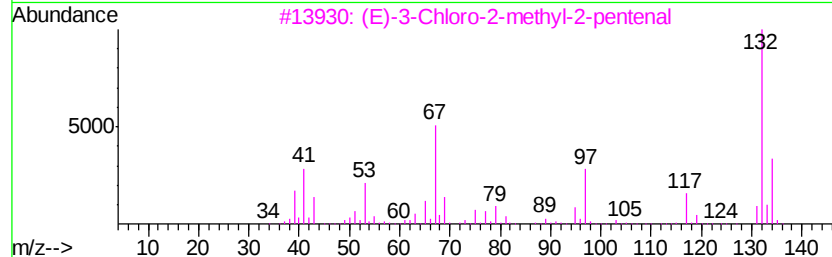
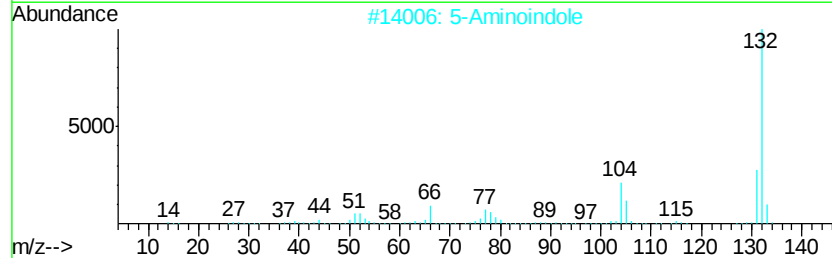
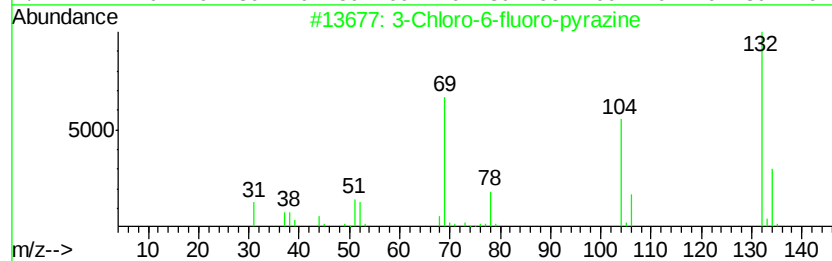
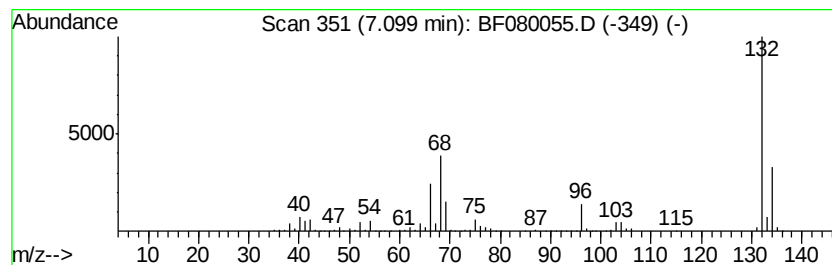
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	101.08 ng	1190930	1,4-Dichlorobenzene-d4	7.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061915\
Data File : BF080055.D
Acq On : 19 Jun 2015 13:37
Operator : TP/IZ
Sample : PB84099BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84099BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.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
3-Penten-2-one, 4...	4.96	4.0	ng	47069	1	7.33	235631	20.0
2-Pentanone, 4-hy...	5.54	63.7	ng	750030	1	7.33	235631	20.0
unknown6.34	6.34	4.4	ng	52299	1	7.33	235631	20.0
unknown7.10	7.10	101.1	ng	1190930	1	7.33	235631	20.0