

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
 Data File : BF089115.D
 Acq On : 19 Jul 2016 13:43
 Operator : UM/SJ
 Sample : PB92230BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB92230BL

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-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	1.735	11	13	45	rVB	669895	1156695	36.61%	6.966%
2	4.067	212	217	219	rBV	987916	1773620	56.14%	10.681%
3	4.810	275	282	284	rBV	1220684	3159096	100.00%	19.024%
4	5.221	316	318	320	rBV	1019884	943517	29.87%	5.682%
5	5.622	351	353	355	rBV	301618	270918	8.58%	1.631%
6	6.273	408	410	413	rBV	733303	902283	28.56%	5.434%
7	6.387	418	420	423	rBV	831842	942396	29.83%	5.675%
8	6.616	438	440	443	rBB	276792	318186	10.07%	1.916%
9	6.776	452	454	457	rBB	1084483	1037902	32.85%	6.250%
10	7.187	487	490	493	rBV	665784	849928	26.90%	5.118%
11	7.907	550	553	555	rBV	517897	442915	14.02%	2.667%
12	8.993	644	648	650	rBV	1366054	1743328	55.18%	10.498%
13	9.656	703	706	708	rBB	504025	453679	14.36%	2.732%
14	10.433	772	774	777	rBV2	386350	507714	16.07%	3.057%
15	11.131	832	835	837	rBV	405393	392900	12.44%	2.366%
16	12.708	971	973	976	rBV	869195	1149901	36.40%	6.925%
17	13.748	1061	1064	1066	rBV	357416	305137	9.66%	1.838%
18	15.097	1180	1182	1185	rBV	199211	255657	8.09%	1.540%

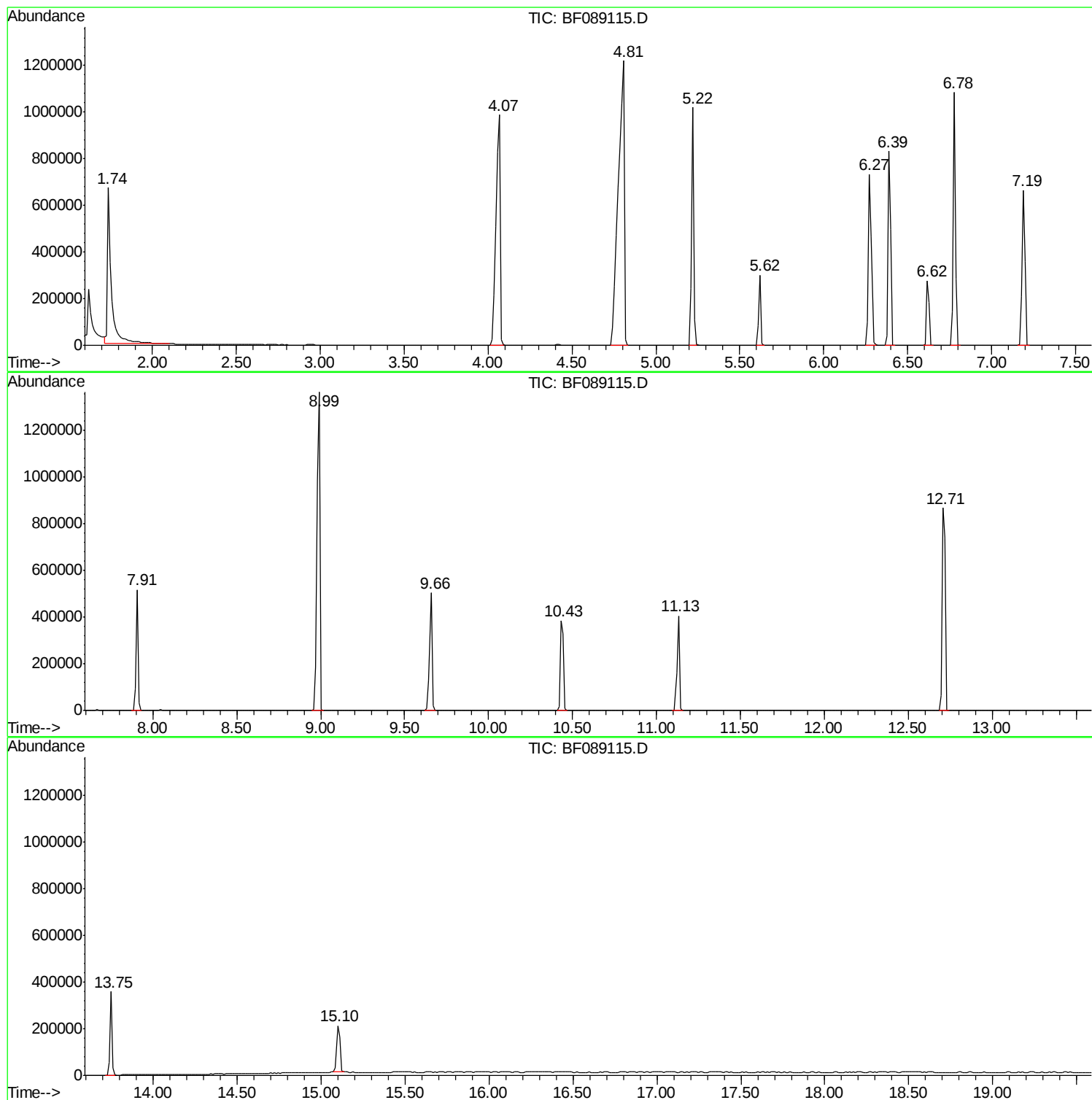
Sum of corrected areas: 16605772

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92230BL

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\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92230BL

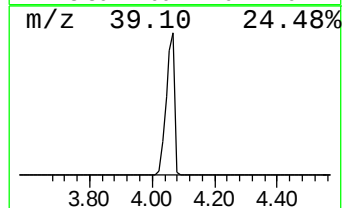
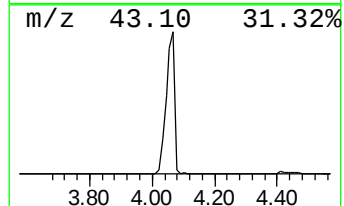
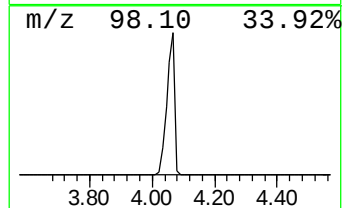
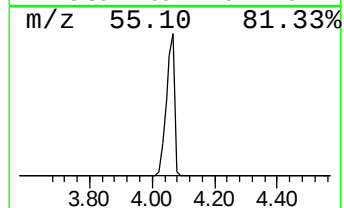
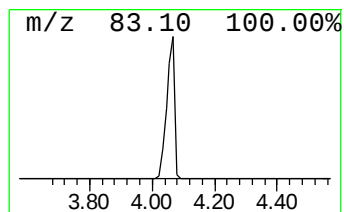
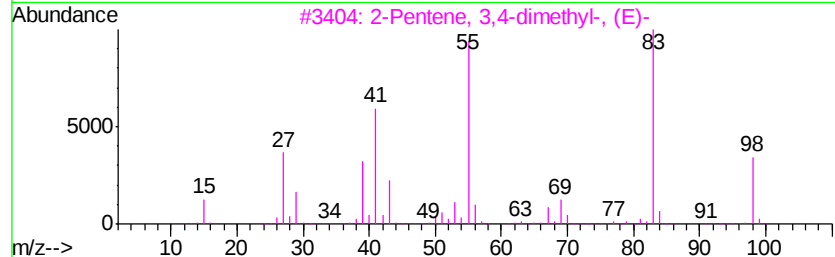
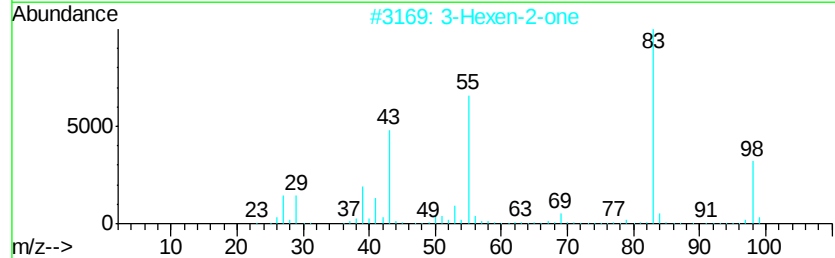
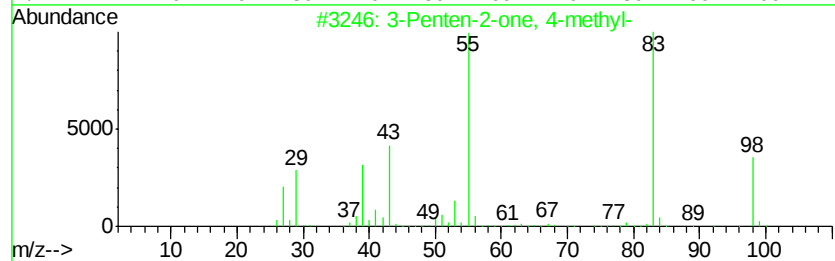
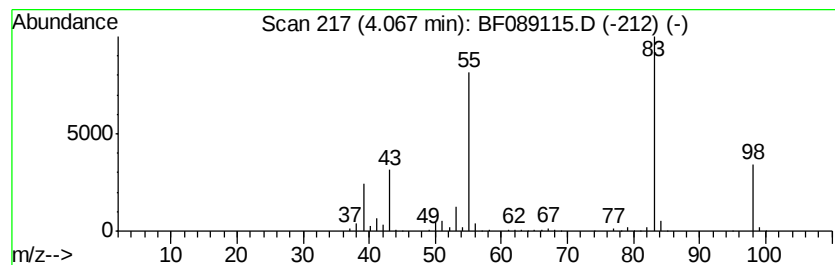
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	111.48 ng	1773620	1,4-Dichlorobenzene-d4	6.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB92230BL

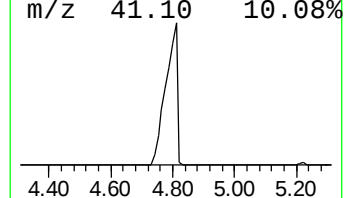
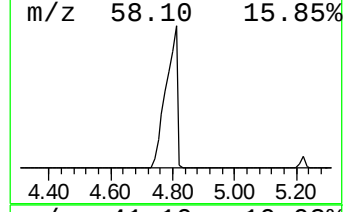
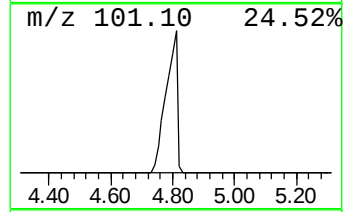
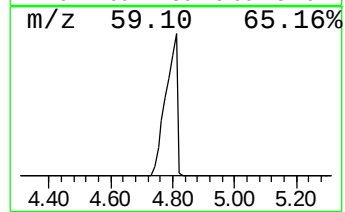
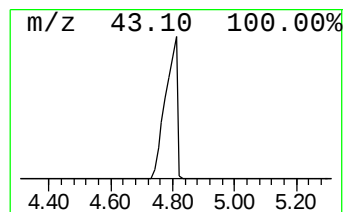
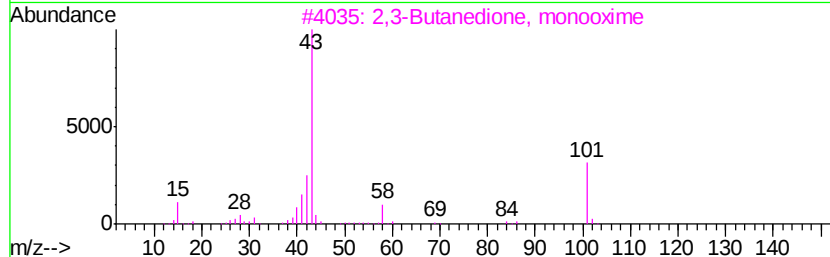
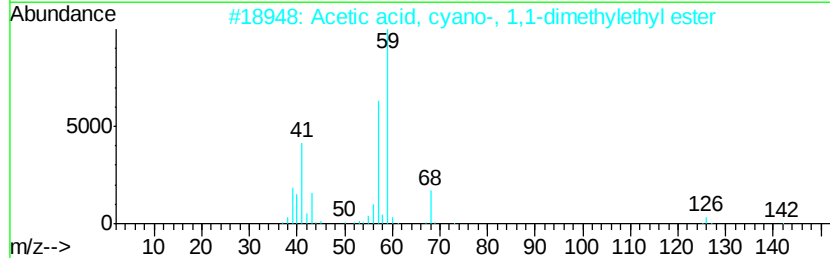
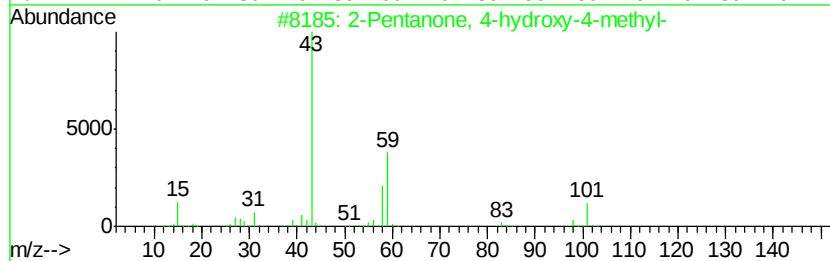
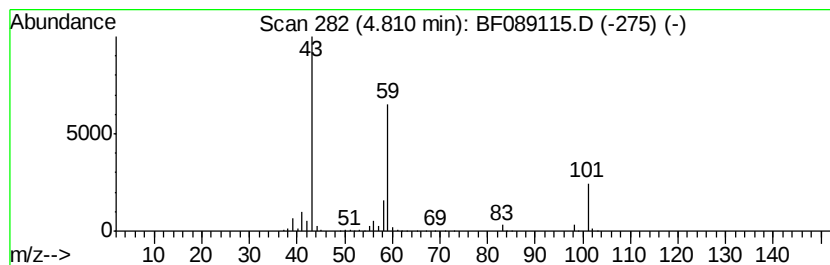
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	198.57 ng	3159100	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetone	58	C3H6O	000067-64-1	10
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB92230BL

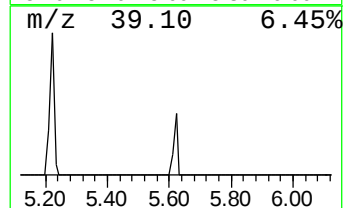
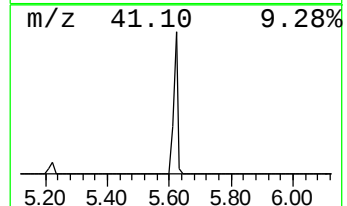
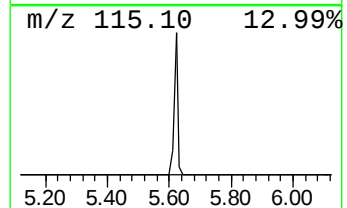
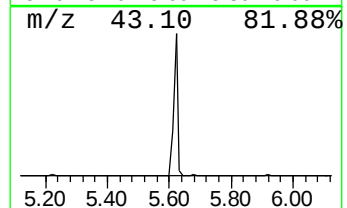
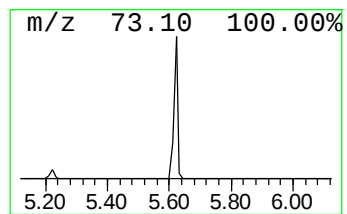
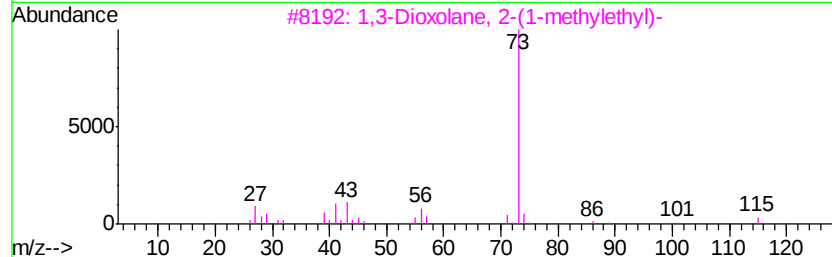
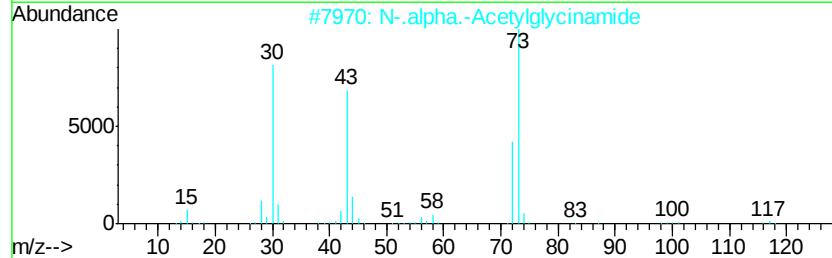
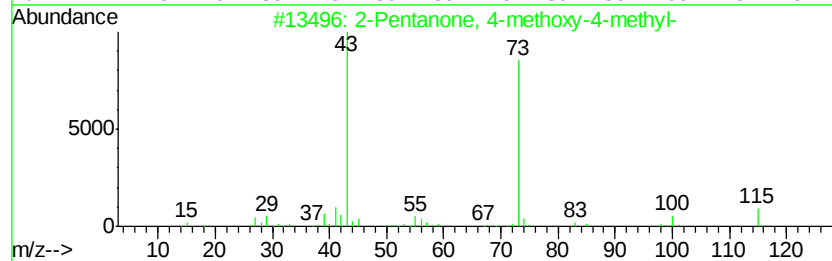
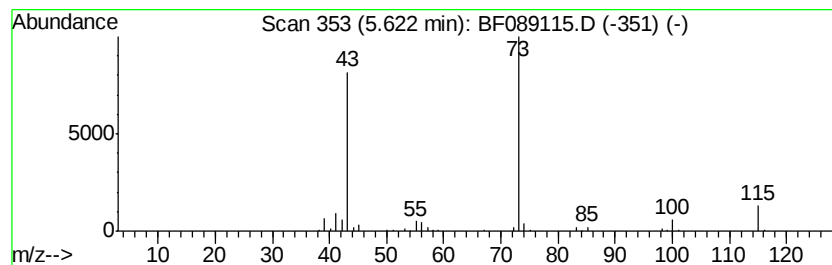
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.62	17.03 ng	270918	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4		Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	10
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92230BL

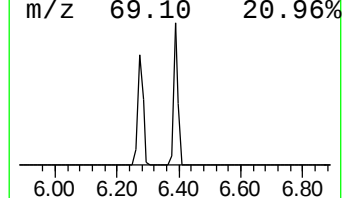
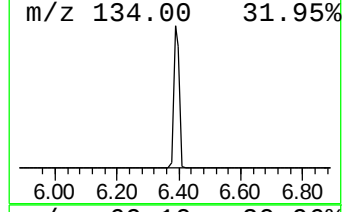
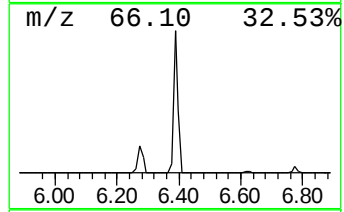
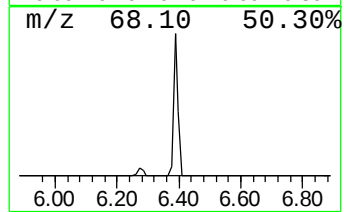
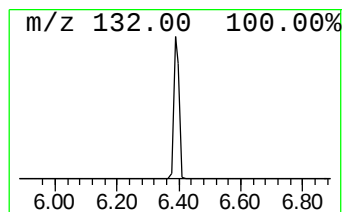
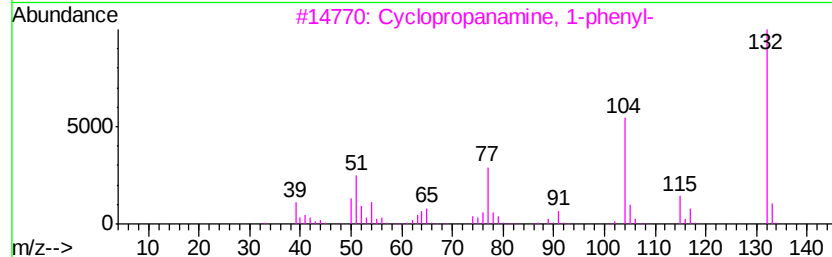
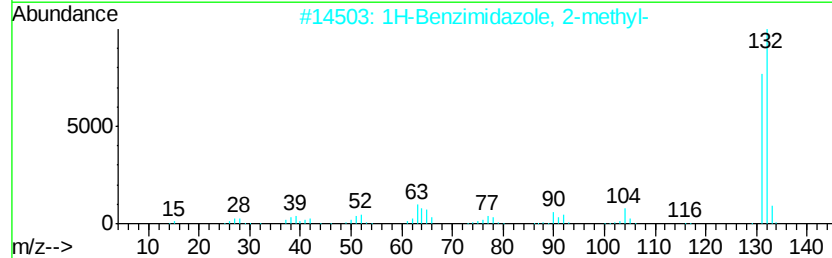
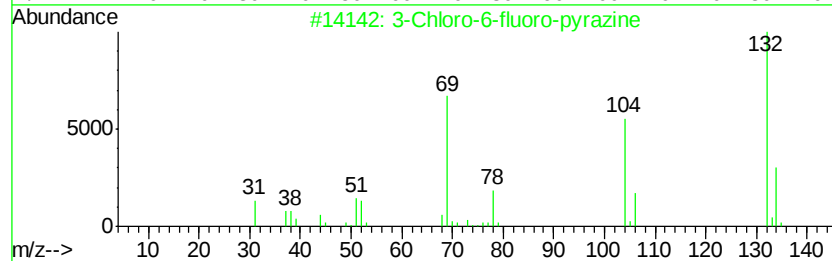
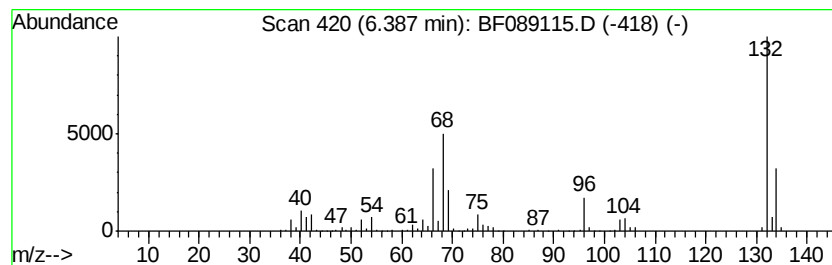
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.39 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	59.24 ng	942396	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089115.D
Acq On : 19 Jul 2016 13:43
Operator : UM/SJ
Sample : PB92230BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92230BL

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
3-Penten-2-one, 4...	4.07	111.5	ng	1773620	1	6.62	318186	20.0
2-Pentanone, 4-hy...	4.81	198.6	ng	3159100	1	6.62	318186	20.0
2-Pentanone, 4-me...	5.62	17.0	ng	270918	1	6.62	318186	20.0
unknown6.39	6.39	59.2	ng	942396	1	6.62	318186	20.0