

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030416\
 Data File : BF085229.D
 Acq On : 5 Mar 2016 3:35
 Operator : SJ/IZ
 Sample : H1676-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-004(0-2)

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-BF030316.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	2.938	55	57	61	rVB	126660	179057	3.44%	0.428%
2	3.716	122	125	129	rVB	37746	55349	1.06%	0.132%
3	4.481	190	192	197	rVB	49066	56937	1.09%	0.136%
4	4.573	197	200	203	rBV	641124	718531	13.80%	1.716%
5	5.190	251	254	261	rVB	695460	1076541	20.67%	2.571%
6	5.453	274	277	280	rBV	69226	81398	1.56%	0.194%
7	5.590	286	289	291	rBV	3688469	4034513	77.48%	9.635%
8	6.264	346	348	355	rBV	41126	52278	1.00%	0.125%
9	6.596	374	377	379	rBV	3457734	3681949	70.71%	8.793%
10	6.733	386	389	392	rBV	3054195	4415153	84.79%	10.544%
11	6.973	407	410	412	rBV	827017	937198	18.00%	2.238%
12	7.122	421	423	426	rVB	2607672	3536535	67.91%	8.446%
13	7.533	456	459	461	rVB	2866576	3116314	59.85%	7.442%
14	7.933	490	494	496	rBV2	28550	55249	1.06%	0.132%
15	7.968	496	497	501	rVB2	32513	55387	1.06%	0.132%
16	8.253	519	522	524	rBV	1439685	1426587	27.40%	3.407%
17	8.585	549	551	554	rBV	47113	66714	1.28%	0.159%
18	9.328	613	616	619	rBV	4264583	5038706	96.76%	12.033%
19	10.013	673	676	677	rBV	1175030	1429599	27.45%	3.414%
20	10.528	718	721	726	rBV2	25340	59258	1.14%	0.142%
21	10.802	741	745	747	rBV	2752960	3352318	64.38%	8.006%
22	11.488	803	805	808	rBV	1026617	1440059	27.65%	3.439%
23	13.077	941	944	947	rBV	3670170	5207305	100.00%	12.436%
24	14.128	1033	1036	1038	rBV	1247275	1109423	21.31%	2.649%
25	15.591	1161	1164	1167	rBV	488588	692153	13.29%	1.653%

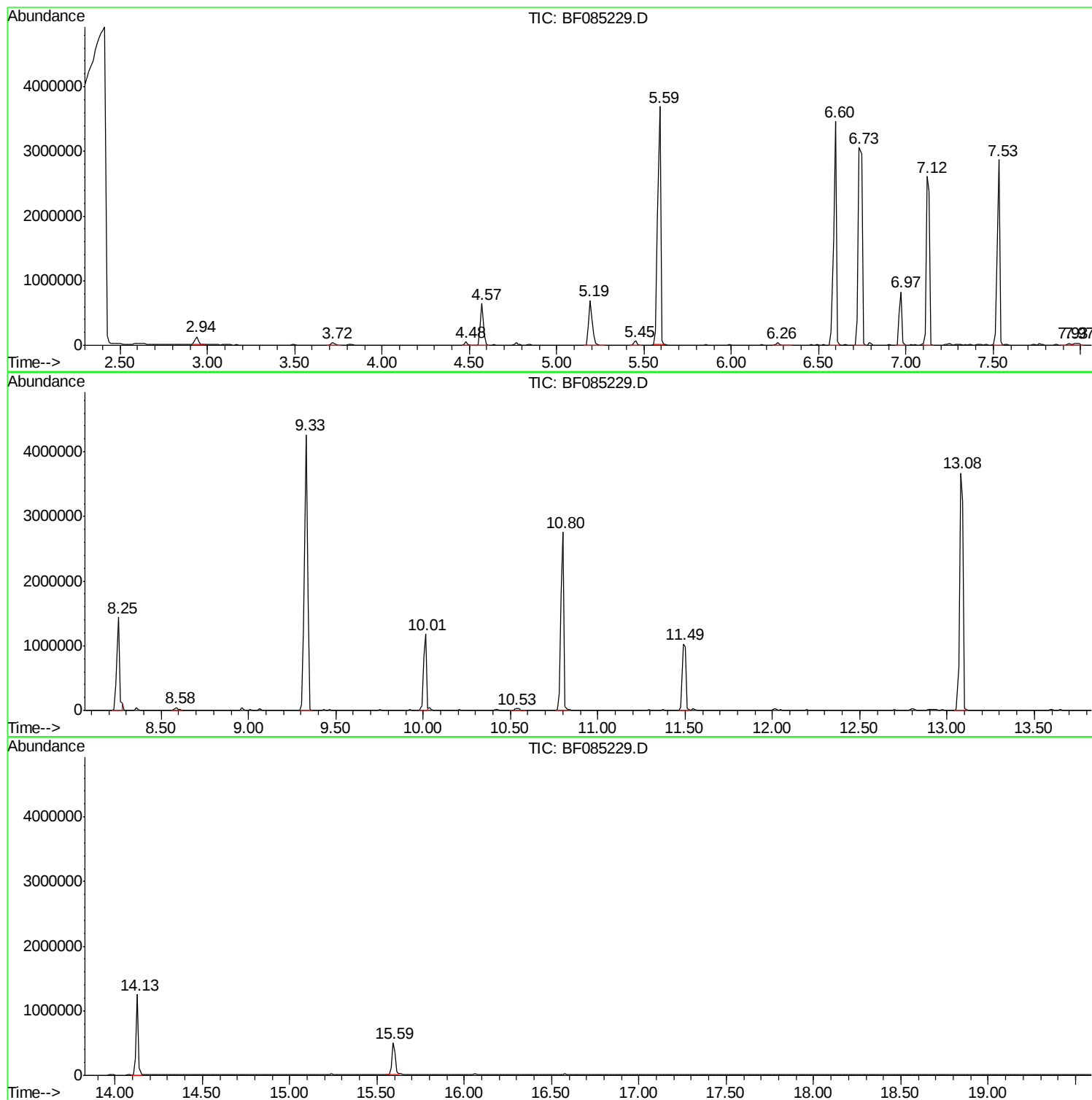
Sum of corrected areas: 41874511

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

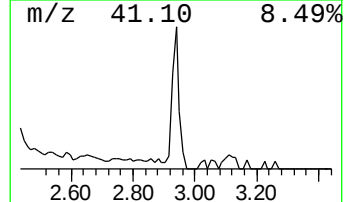
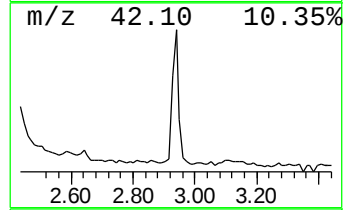
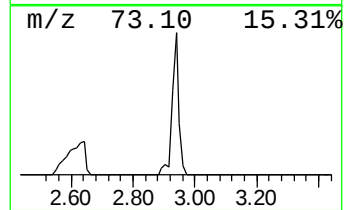
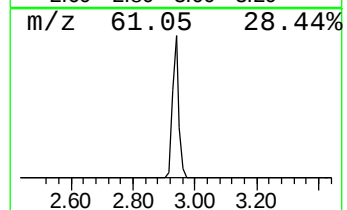
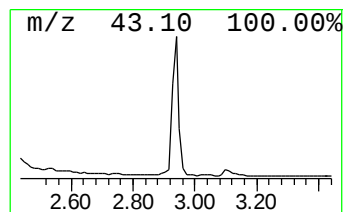
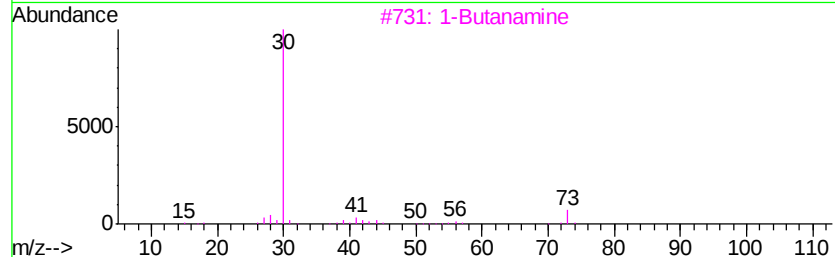
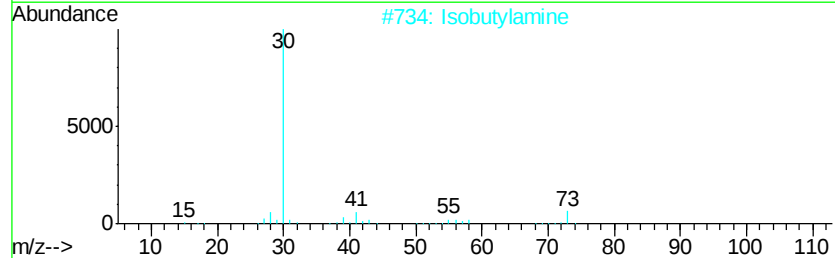
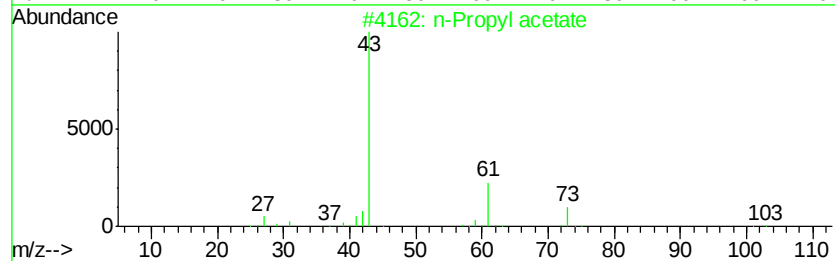
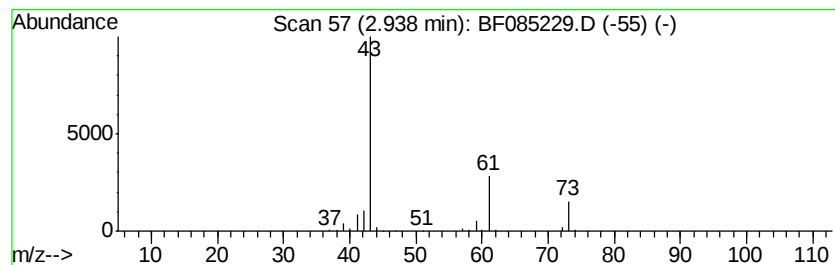
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	3.82 ng	179057	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Butanamine	73	C4H11N	000109-73-9	5
4			Isobutane	58	C4H10	000075-28-5	4
5			Pentane	72	C5H12	000109-66-0	4



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

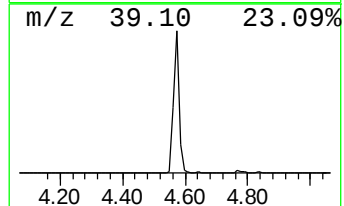
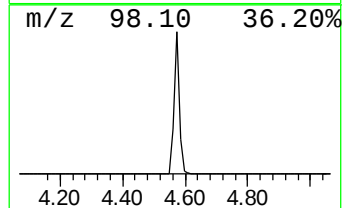
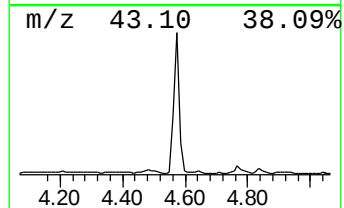
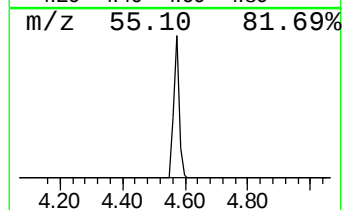
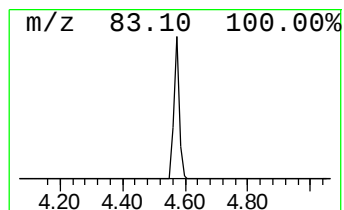
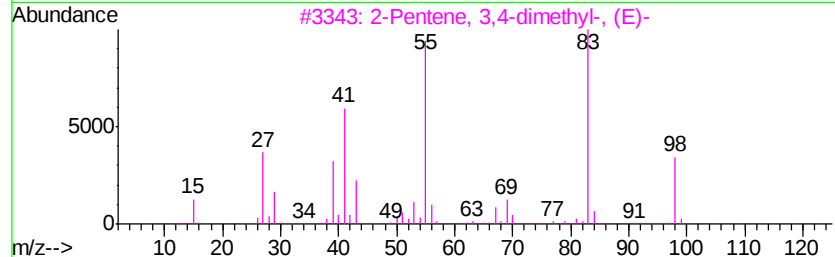
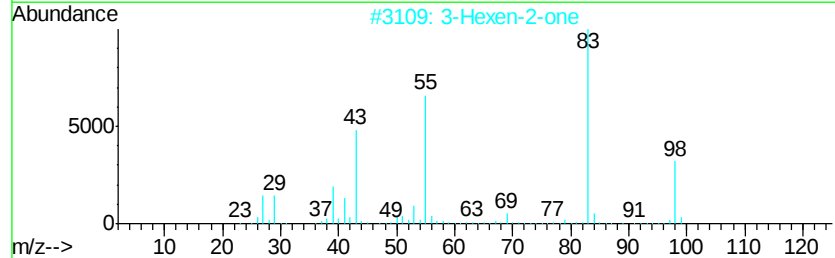
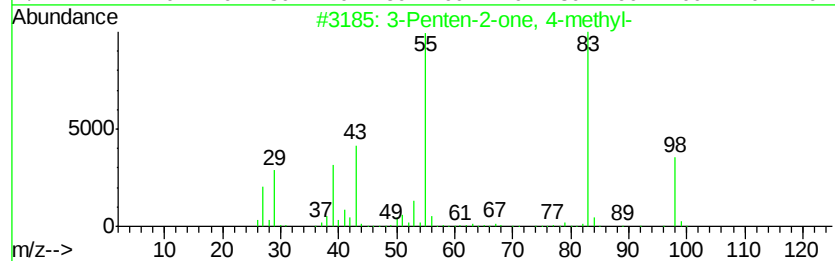
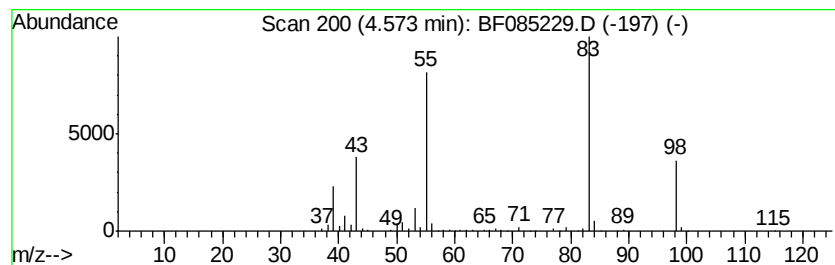
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	15.33 ng	718531	1,4-Dichlorobenzene-d4	6.97

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	90
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		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

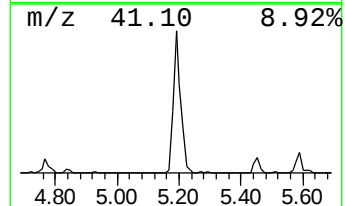
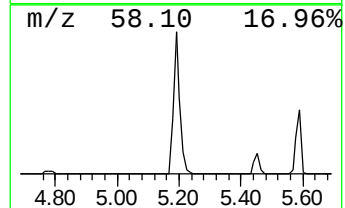
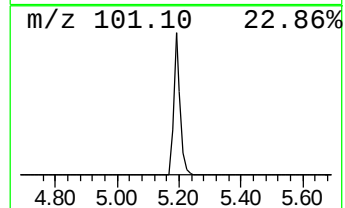
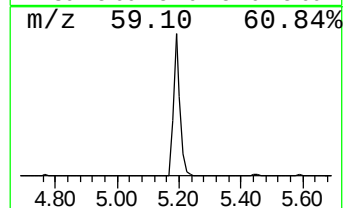
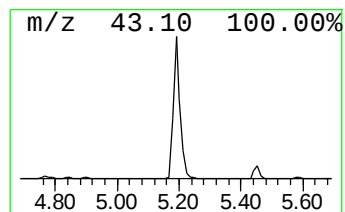
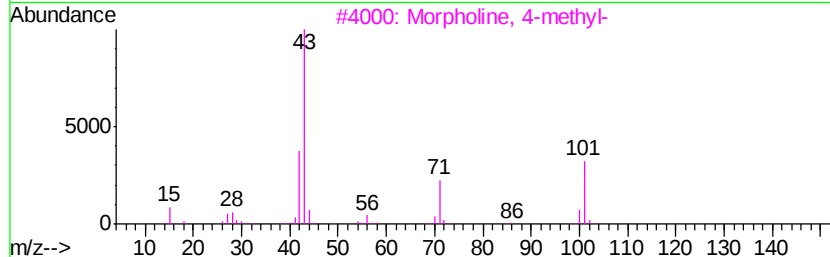
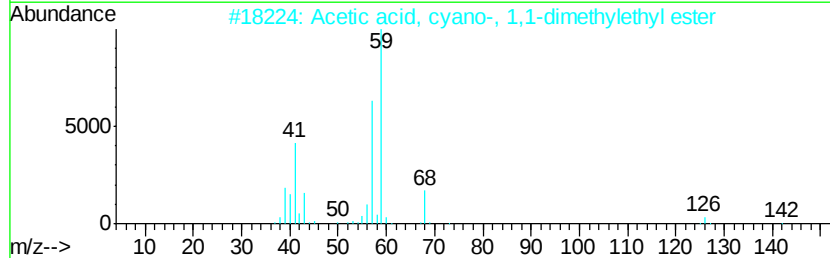
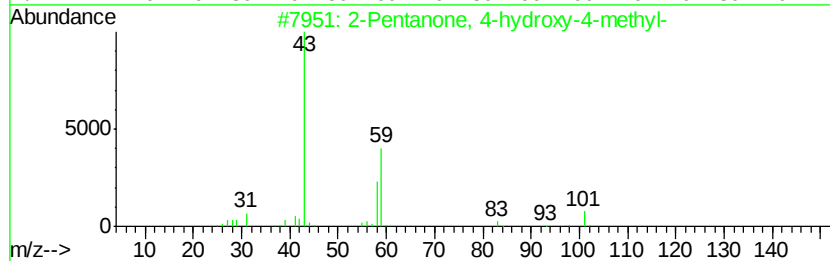
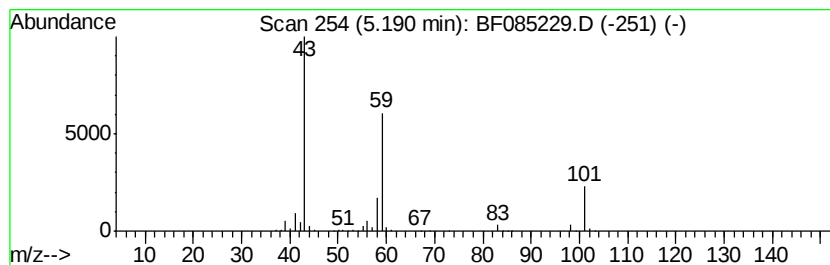
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	22.97 ng	1076540	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

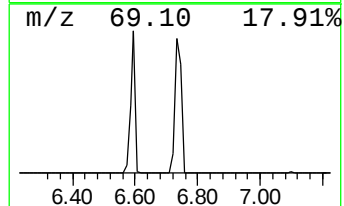
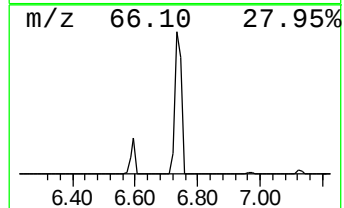
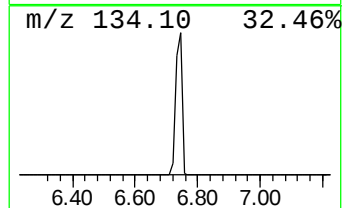
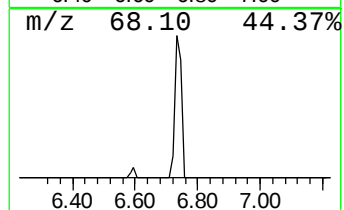
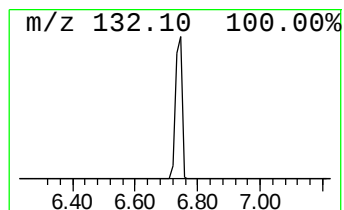
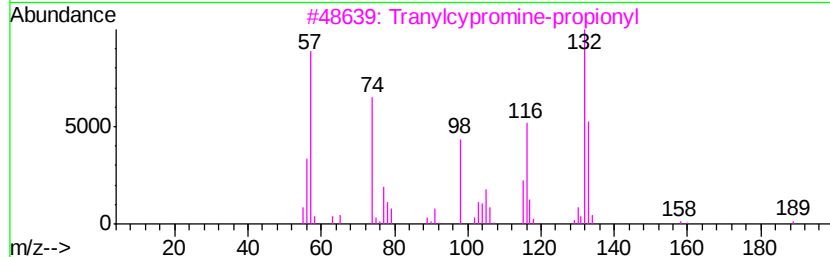
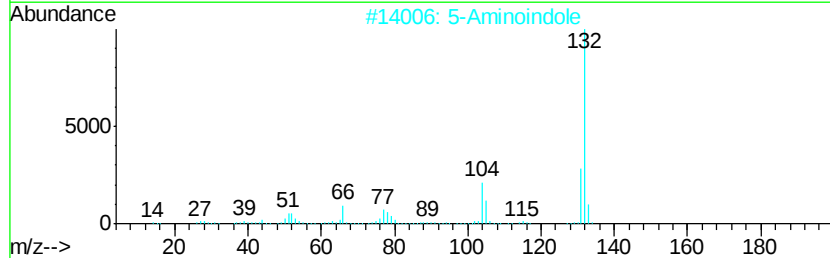
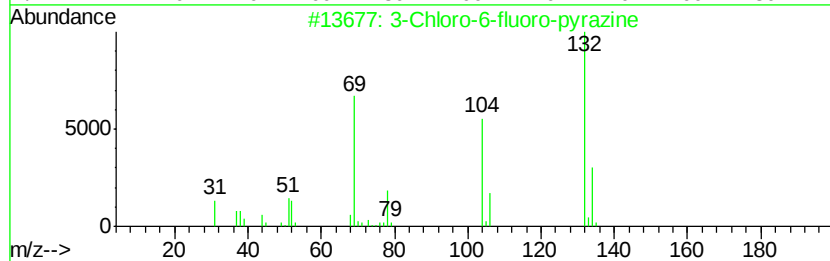
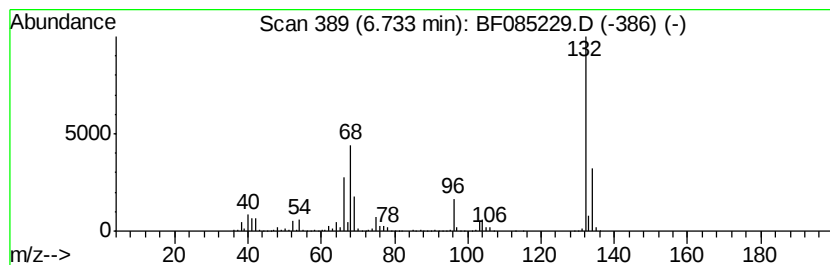
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	94.22 ng	4415150	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030416\
Data File : BF085229.D
Acq On : 5 Mar 2016 3:35
Operator : SJ/IZ
Sample : H1676-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-004(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
n-Propyl acetate	2.94	3.8	ng	179057	1	6.97	937198	20.0
3-Penten-2-one, 4...	4.57	15.3	ng	718531	1	6.97	937198	20.0
2-Pentanone, 4-hy...	5.19	23.0	ng	1076540	1	6.97	937198	20.0
unknown6.73	6.73	94.2	ng	4415150	1	6.97	937198	20.0