

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
 Data File : BF084488.D
 Acq On : 15 Jan 2016 13:58
 Operator : SJ/UM
 Sample : PB87825BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87825BL

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-BF123115.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	4.350	195	198	202	rVB	241896	333808	4.57%	0.562%
2	5.013	252	256	259	rBV	4099534	5315647	72.85%	8.956%
3	5.436	290	293	295	rBV	4761285	4657423	63.83%	7.847%
4	5.824	325	327	330	rBV	230147	259097	3.55%	0.437%
5	6.464	380	383	385	rBV	5127014	4678115	64.11%	7.882%
6	6.590	392	394	397	rBV	4959350	4304275	58.99%	7.252%
7	6.819	412	414	417	rVB	1777360	1698651	23.28%	2.862%
8	6.979	425	428	431	rBV	5602160	4835394	66.27%	8.147%
9	7.390	461	464	466	rBV	4395799	4417348	60.54%	7.443%
10	8.110	524	527	529	rBV	2779893	2395482	32.83%	4.036%
11	9.196	618	622	624	rBV	5656771	7296811	100.00%	12.295%
12	9.733	666	669	671	rBV2	35522	86754	1.19%	0.146%
13	9.779	671	673	678	rVB	76587	111860	1.53%	0.188%
14	9.870	678	681	683	rBV	2522112	2581698	35.38%	4.350%
15	10.076	686	699	700	rBV6	37716	173903	2.38%	0.293%
16	10.213	703	711	712	rBV9	25667	93988	1.29%	0.158%
17	10.659	747	750	752	rBV	2426477	2965056	40.63%	4.996%
18	11.093	786	788	790	rBV	246903	220677	3.02%	0.372%
19	11.356	808	811	813	rBV	1956781	2331282	31.95%	3.928%
20	11.939	860	862	864	rBV	115631	117160	1.61%	0.197%
21	12.945	947	950	952	rBV	5606033	6133639	84.06%	10.335%
22	12.979	952	953	962	rVB4	293328	1045001	14.32%	1.761%
23	13.985	1040	1041	1044	rVB	1467333	1345806	18.44%	2.268%
24	15.414	1163	1166	1169	rBV	989653	1951325	26.74%	3.288%

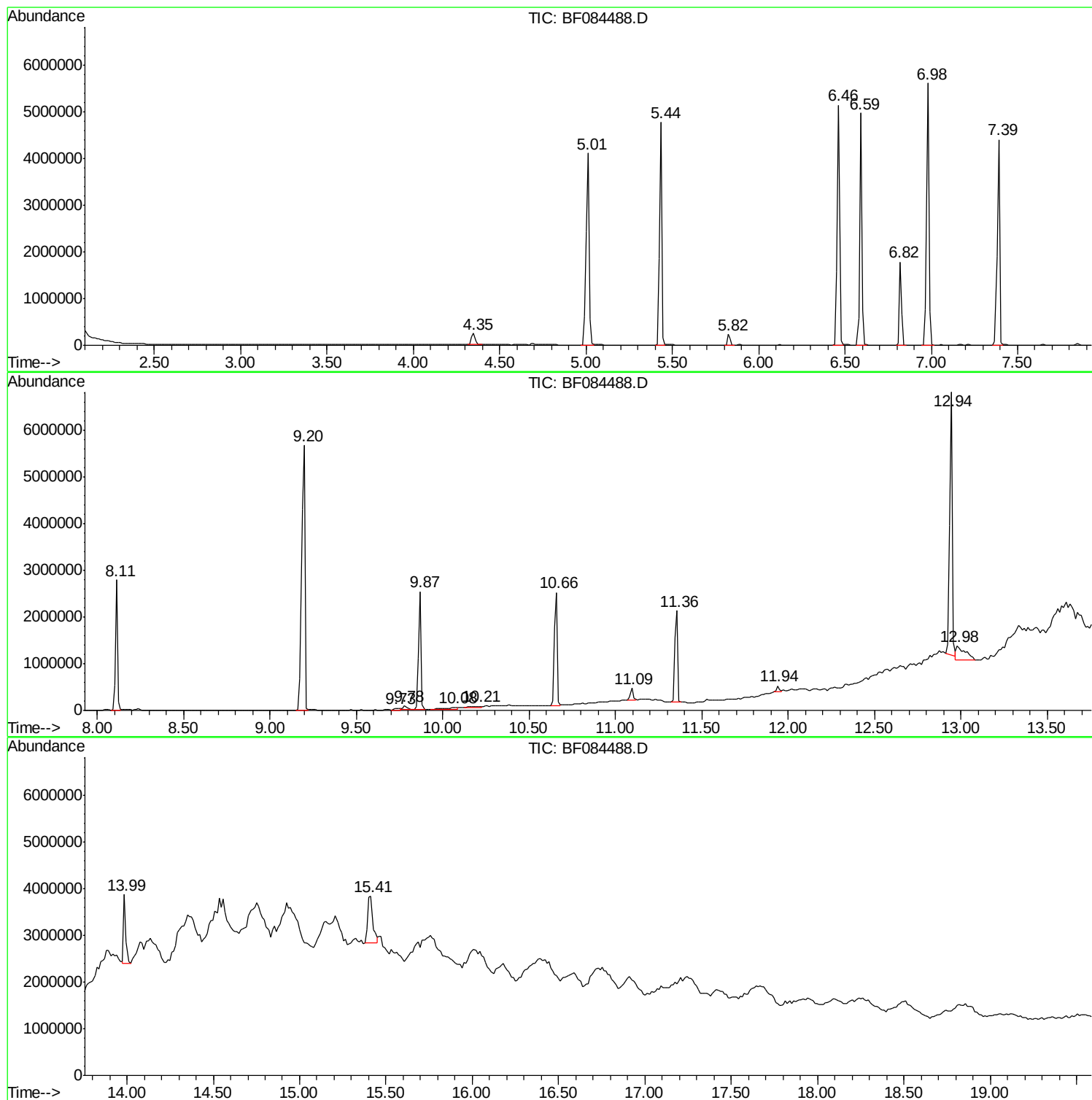
Sum of corrected areas: 59350200

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

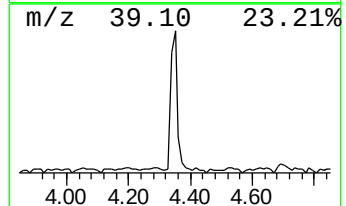
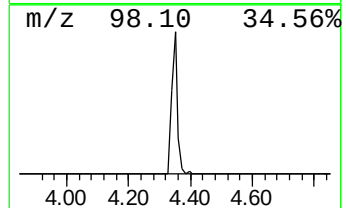
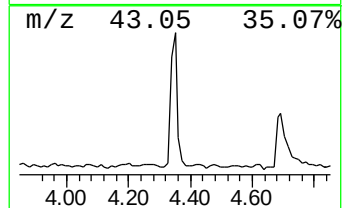
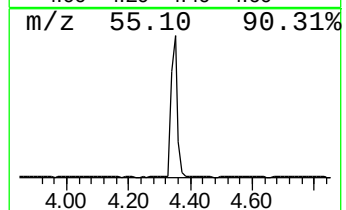
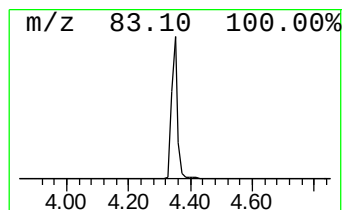
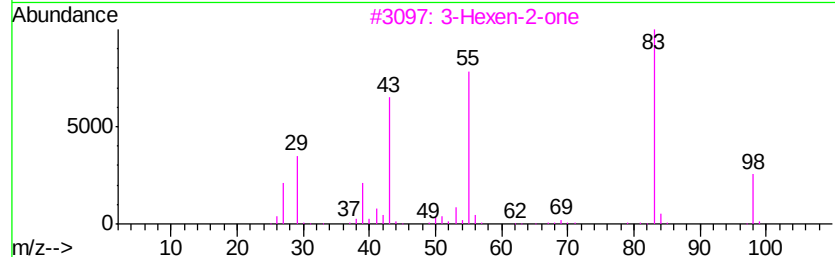
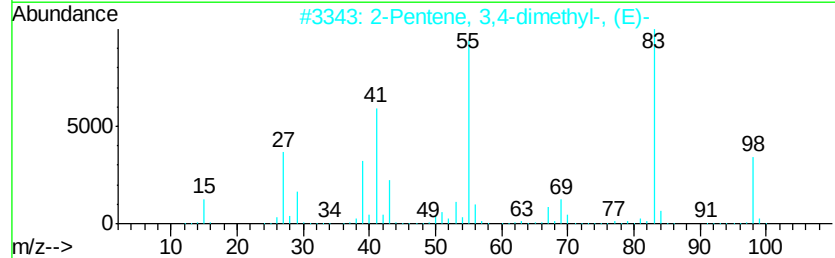
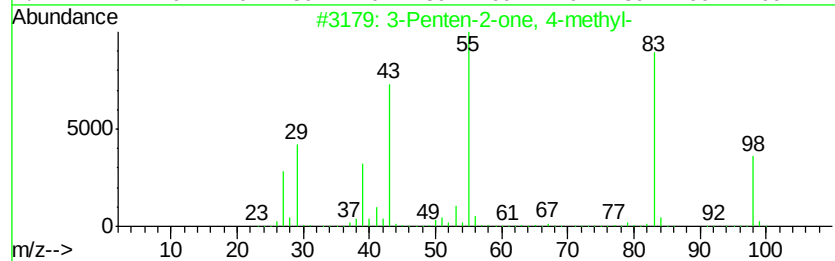
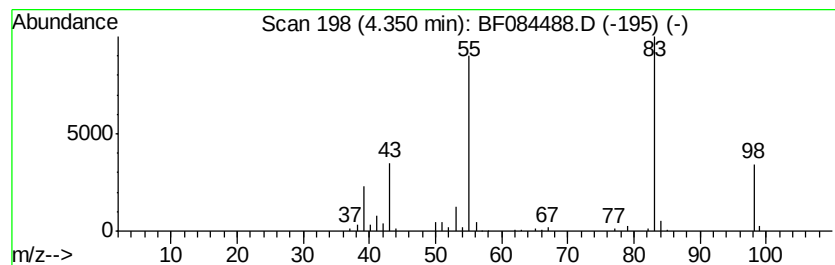
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	3.93 ng	333808	1,4-Dichlorobenzene-d4	6.82

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

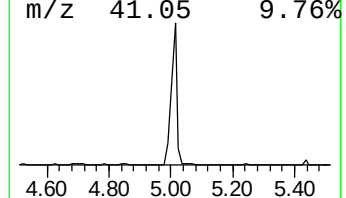
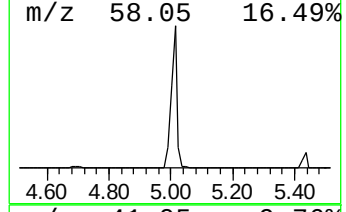
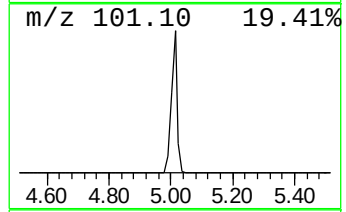
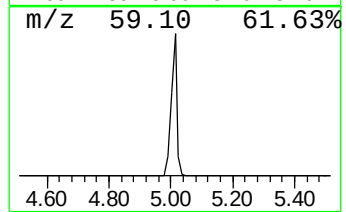
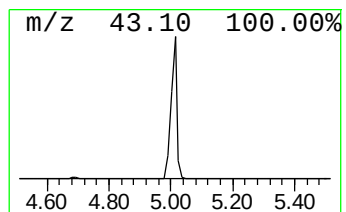
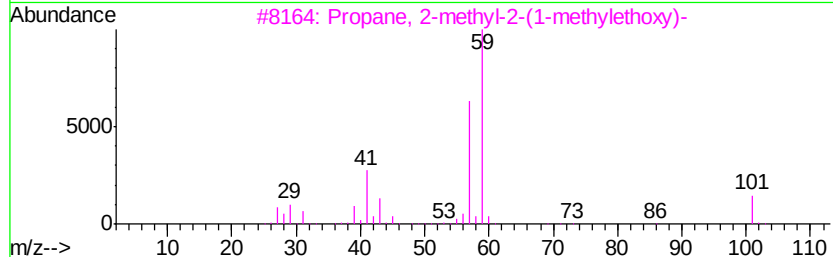
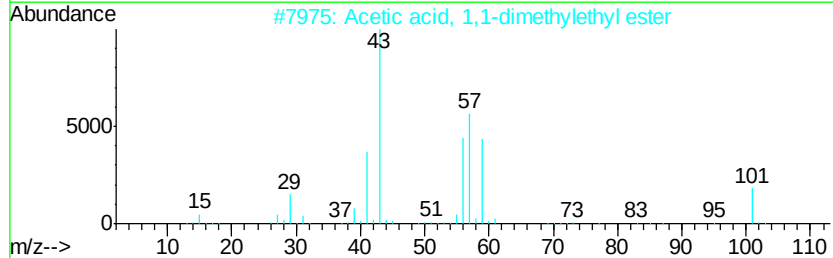
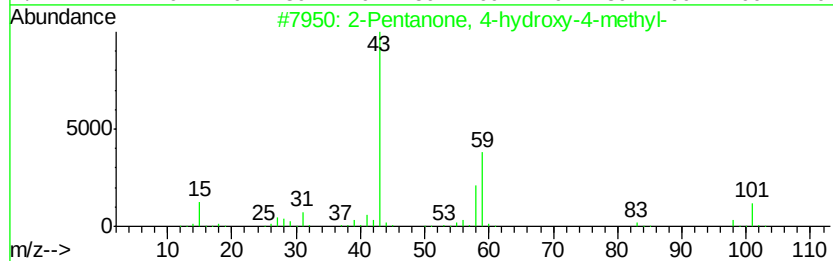
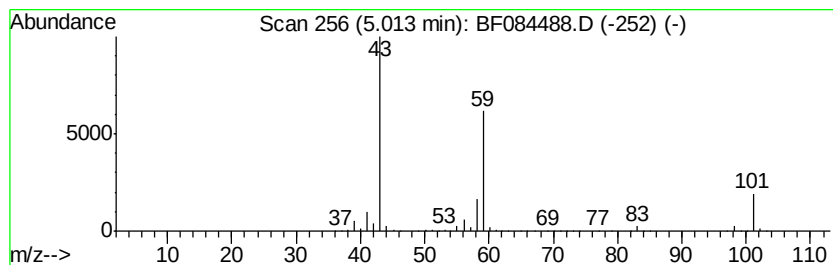
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	62.59 ng	5315650	1,4-Dichlorobenzene-d4	6.82

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

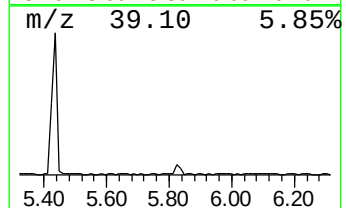
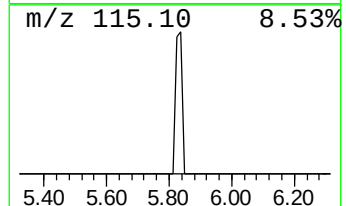
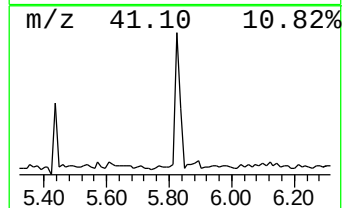
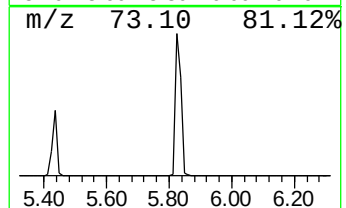
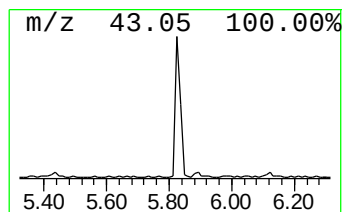
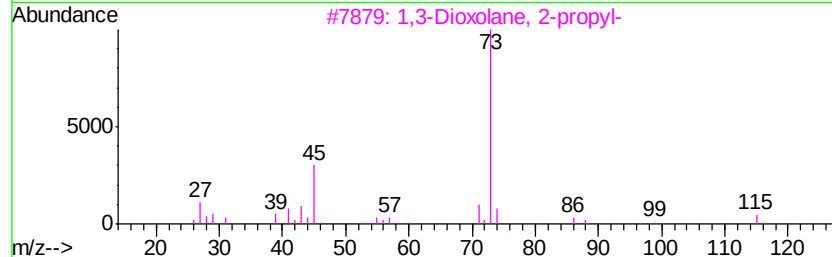
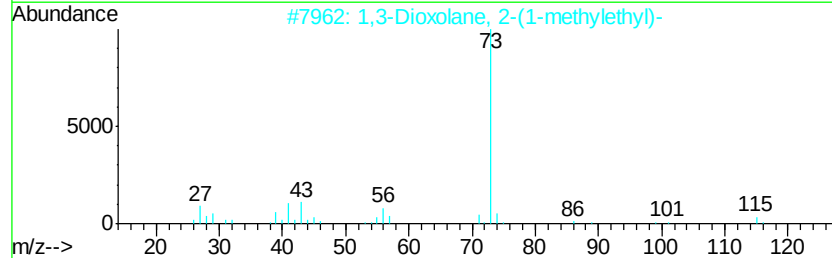
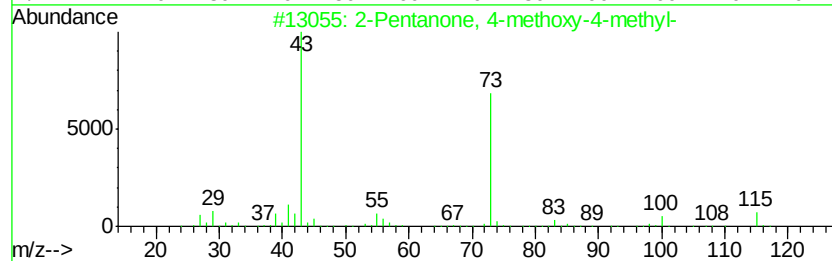
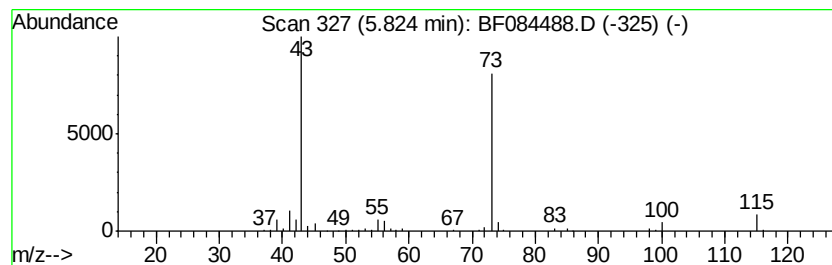
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	3.05 ng	259097	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
3		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

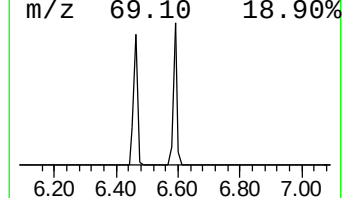
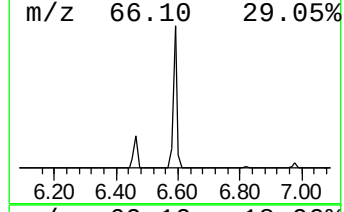
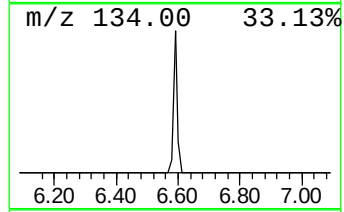
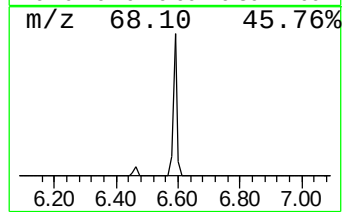
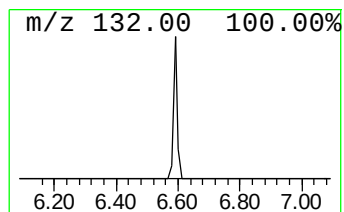
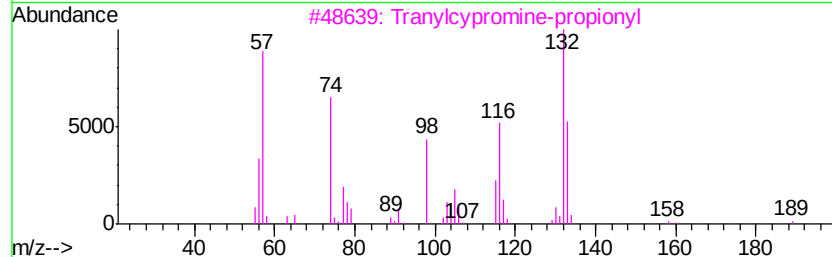
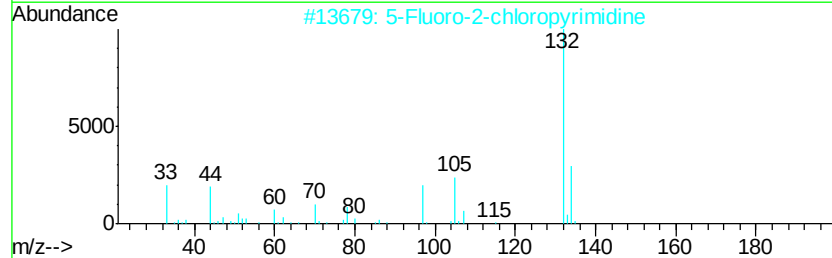
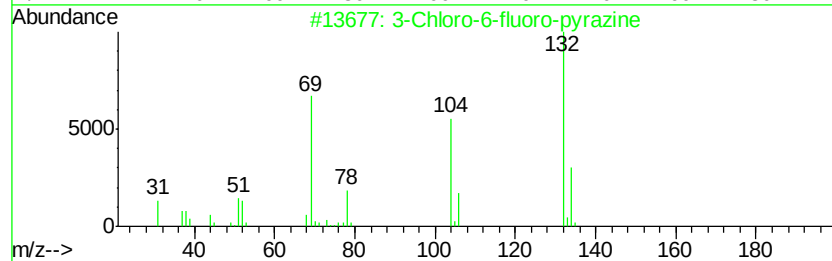
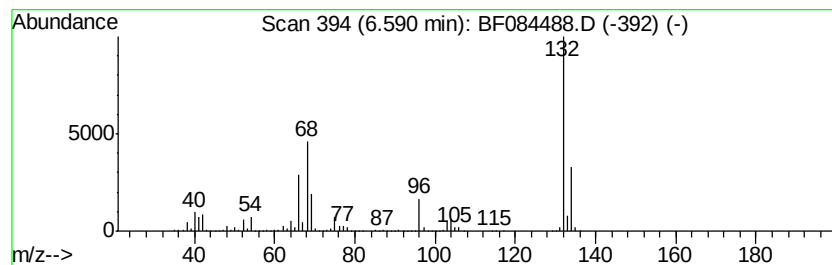
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	50.68 ng	4304280	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
Data File : BF084488.D
Acq On : 15 Jan 2016 13:58
Operator : SJ/UM
Sample : PB87825BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB87825BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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...	4.35	3.9	ng	333808	1	6.82	1698650	20.0
2-Pentanone, 4-hy...	5.01	62.6	ng	5315650	1	6.82	1698650	20.0
2-Pentanone, 4-me...	5.82	3.0	ng	259097	1	6.82	1698650	20.0
unknown6.59	6.59	50.7	ng	4304280	1	6.82	1698650	20.0