

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
 Data File : BF086791.D
 Acq On : 7 May 2016 23:28
 Operator : UM/SJ
 Sample : H2882-01
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MWHR3-14

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-BF050416.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	4.876	241	244	248	rBV	121436	187702	2.95%	0.443%
2	5.310	280	282	298	rBV	2561243	2857969	44.89%	6.748%
3	5.710	312	317	323	rBV	41652	70837	1.11%	0.167%
4	6.362	372	374	379	rBV	1852880	1861696	29.24%	4.395%
5	6.476	382	384	387	rBV	4629636	4512648	70.88%	10.654%
6	6.704	402	404	406	rBV	1003200	1120272	17.60%	2.645%
7	6.853	415	417	420	rBV	3055735	4191090	65.83%	9.895%
8	7.276	451	454	456	rBV	3501565	3824458	60.07%	9.029%
9	7.447	468	469	475	rVB2	76276	107378	1.69%	0.254%
10	7.985	514	516	519	rBV	1224645	1429163	22.45%	3.374%
11	8.579	565	568	571	rBV	60389	67518	1.06%	0.159%
12	9.070	607	611	613	rBV	5703375	6366692	100.00%	15.032%
13	9.733	666	669	672	rBV2	1455159	1754818	27.56%	4.143%
14	10.270	713	716	718	rBV	45886	65652	1.03%	0.155%
15	10.385	724	726	728	rBV	194681	169290	2.66%	0.400%
16	10.533	736	739	747	rBV2	3271609	4318546	67.83%	10.196%
17	10.831	763	765	773	rVB	94548	145496	2.29%	0.344%
18	11.219	796	799	801	rBV	1515020	1478874	23.23%	3.492%
19	12.625	920	922	925	rBV	167833	212307	3.33%	0.501%
20	12.705	925	929	935	rVB2	119787	148548	2.33%	0.351%
21	12.808	935	938	940	rBV	3655429	4996082	78.47%	11.796%
22	13.334	982	984	986	rBV	151039	137430	2.16%	0.324%
23	13.368	986	987	989	rBV	220496	252127	3.96%	0.595%
24	13.699	1014	1016	1021	rVB	65484	95471	1.50%	0.225%
25	13.848	1026	1029	1031	rBV	797014	1040679	16.35%	2.457%
26	14.019	1042	1044	1046	rBV	75344	69936	1.10%	0.165%
27	15.220	1146	1149	1155	rBV	592832	872704	13.71%	2.060%

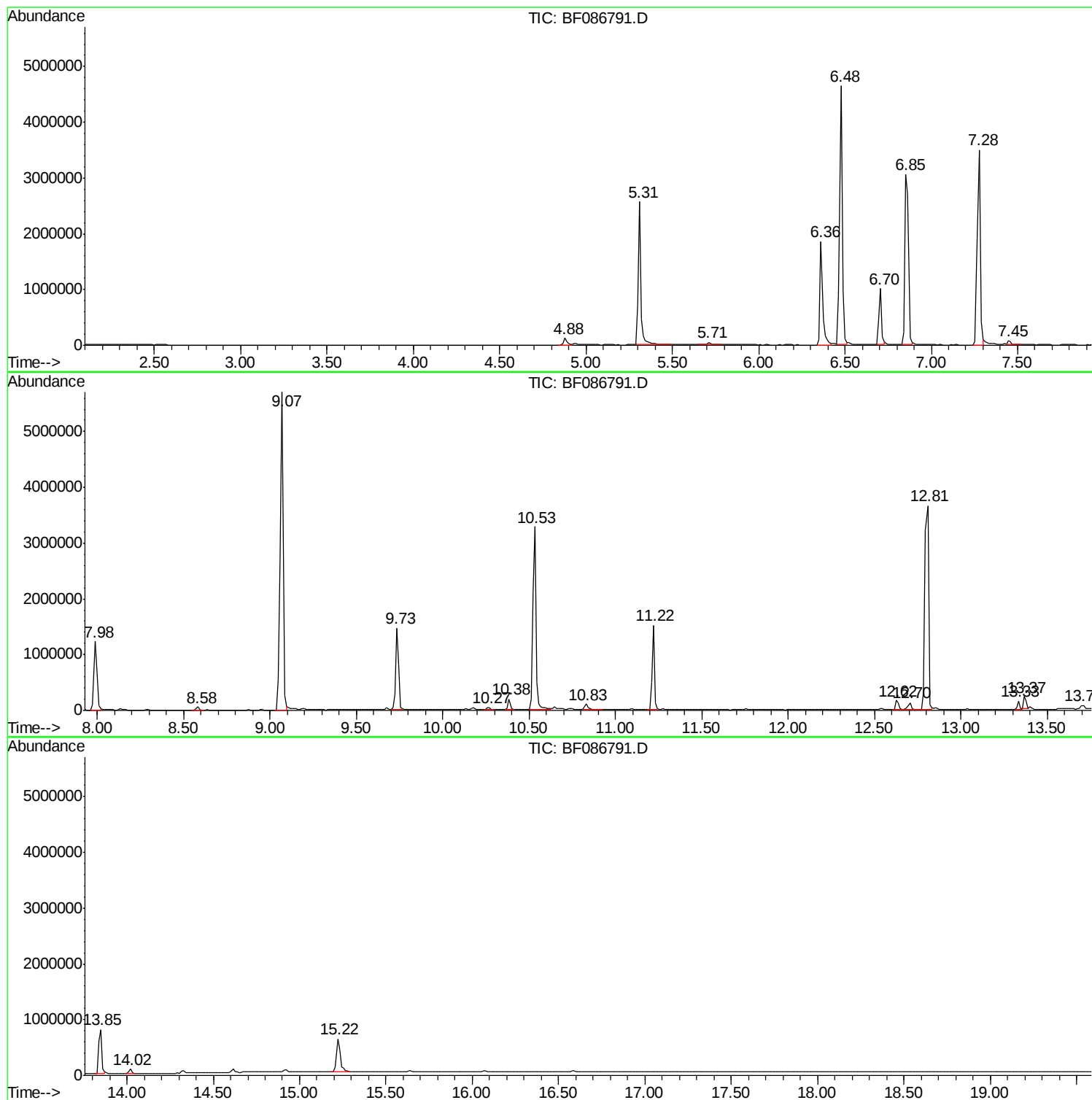
Sum of corrected areas: 42355383

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

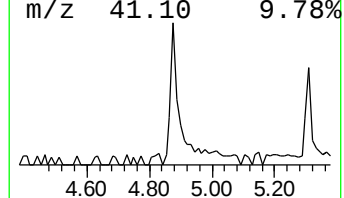
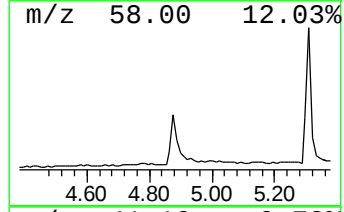
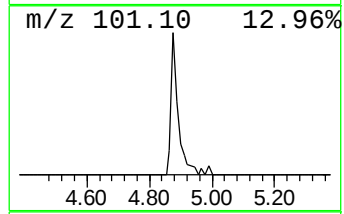
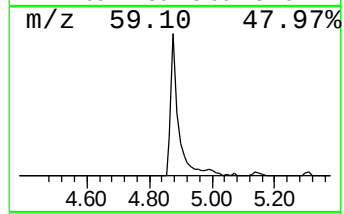
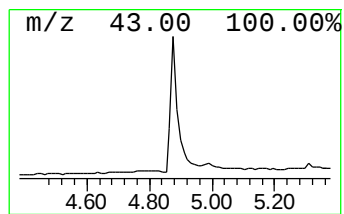
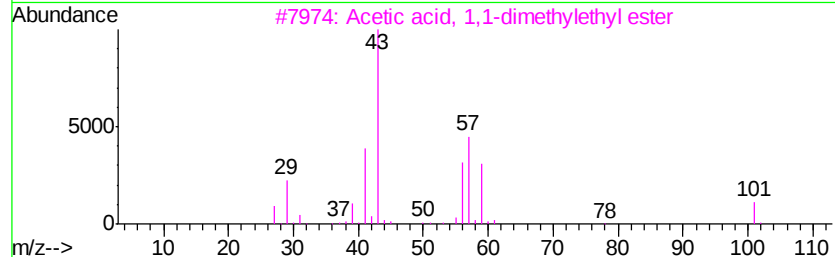
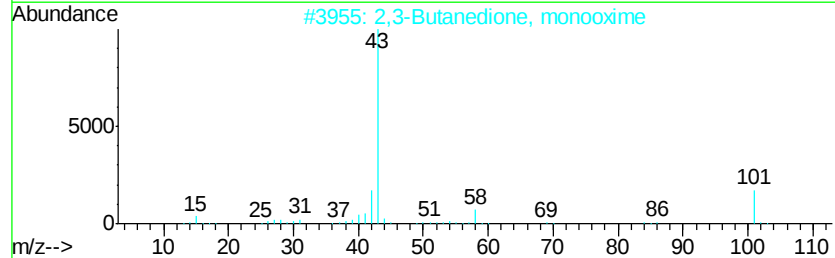
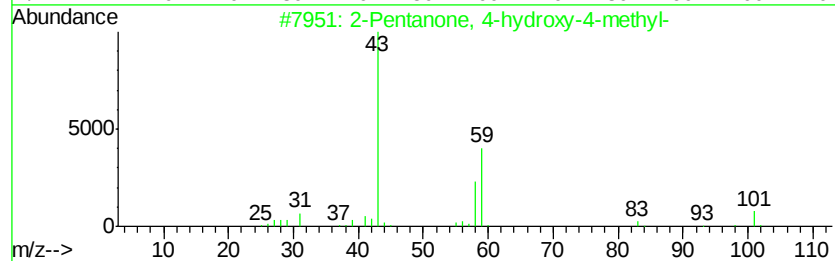
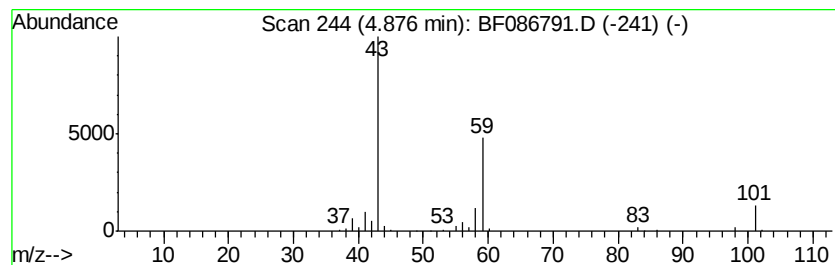
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	6.70 ng	187702	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2-Pentanone	86	C5H10O	000107-87-9	10
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

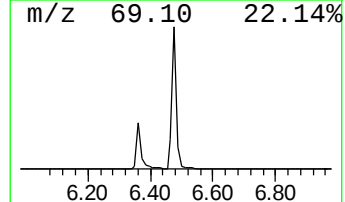
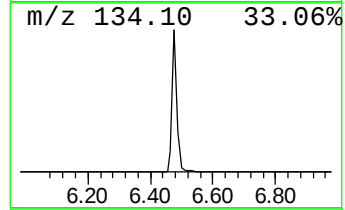
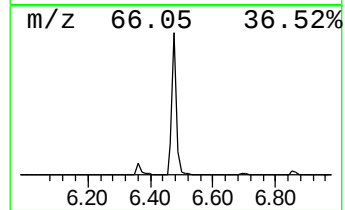
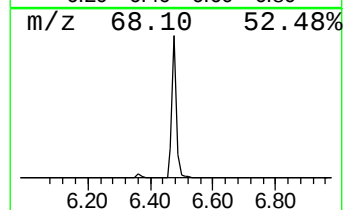
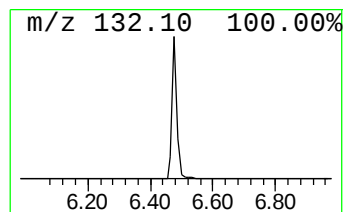
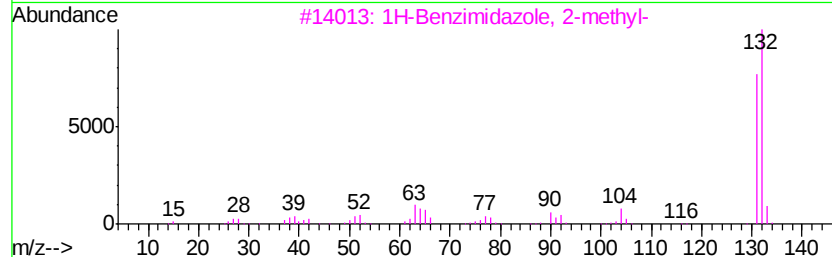
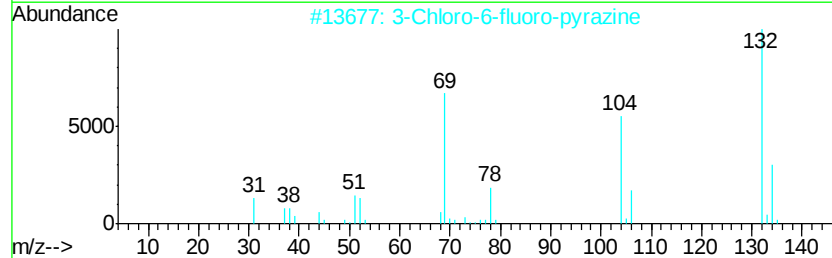
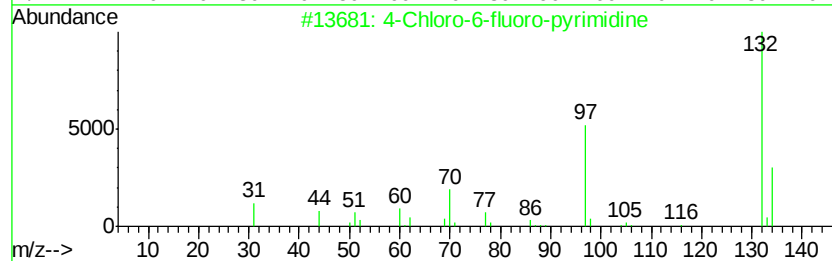
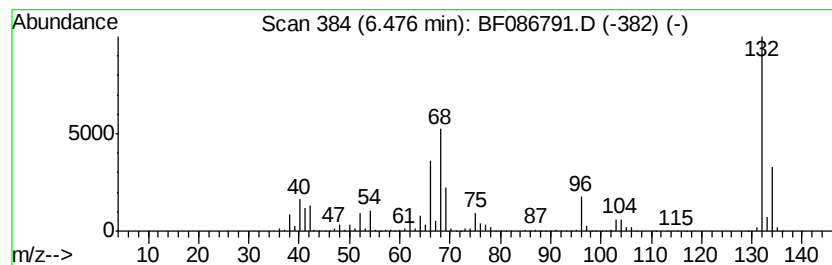
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	161.13 ng	4512650	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

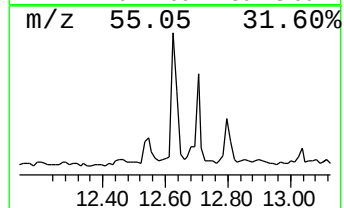
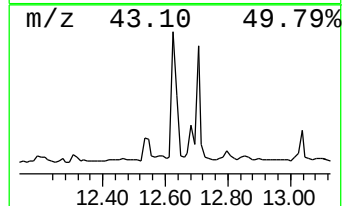
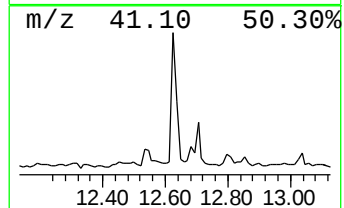
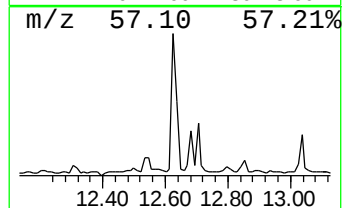
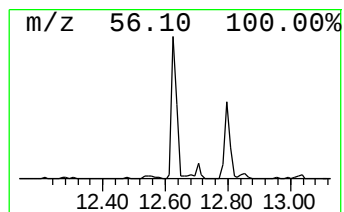
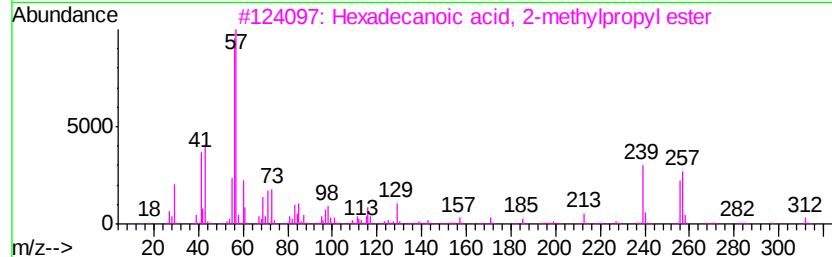
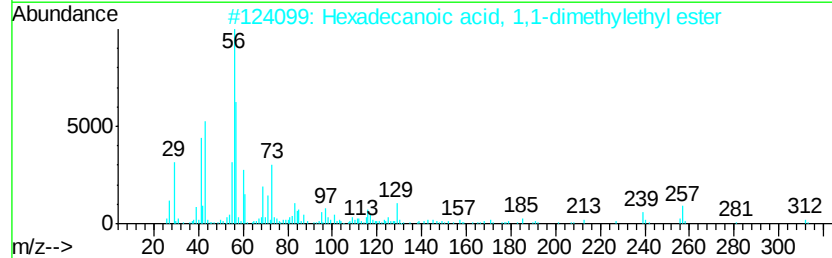
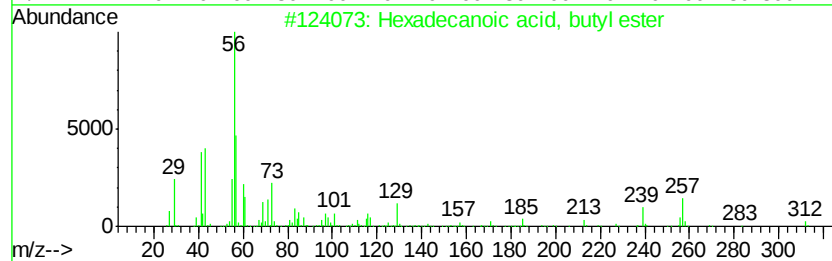
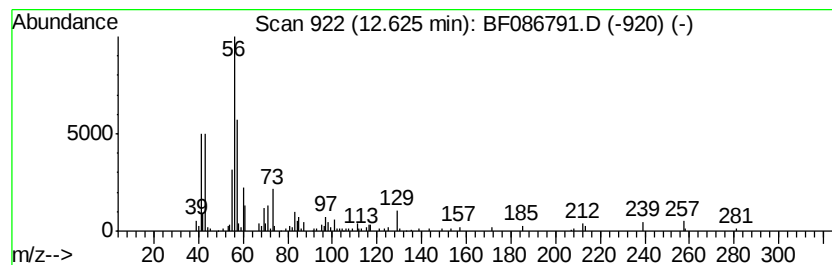
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	8.16 ng	212307	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	72
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	47
5		Oxan-4-one, 2-trifluoromethyl-2-...	212	C8H11F3O3	212615-80-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

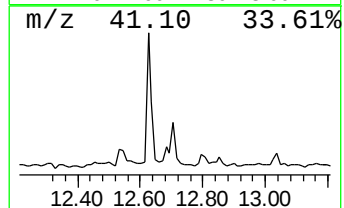
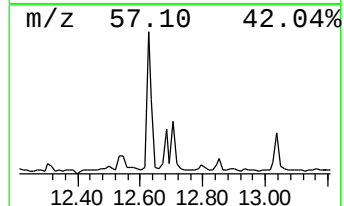
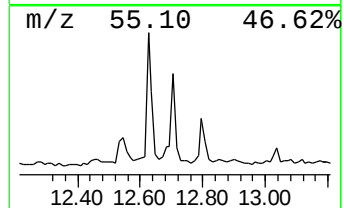
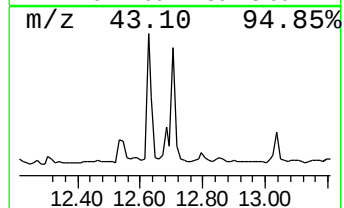
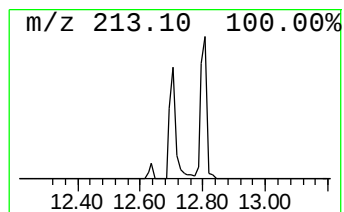
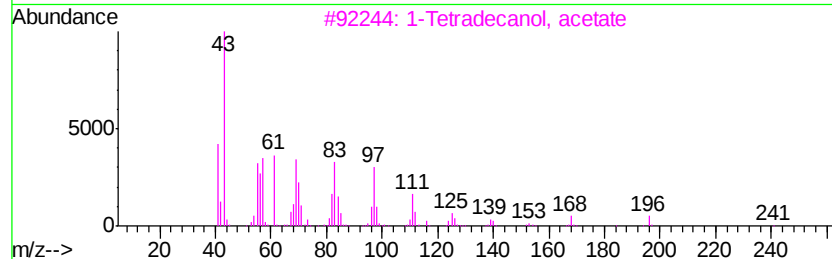
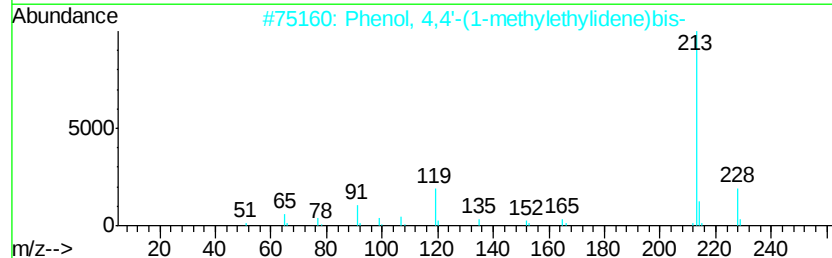
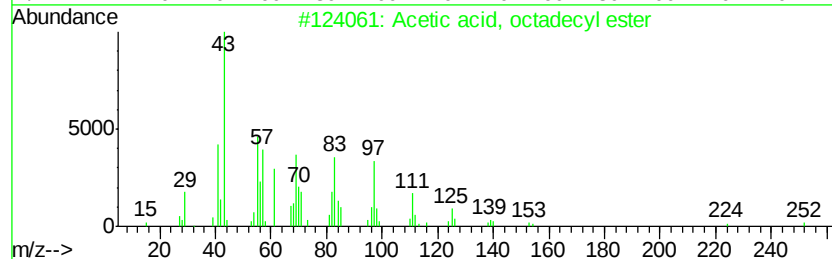
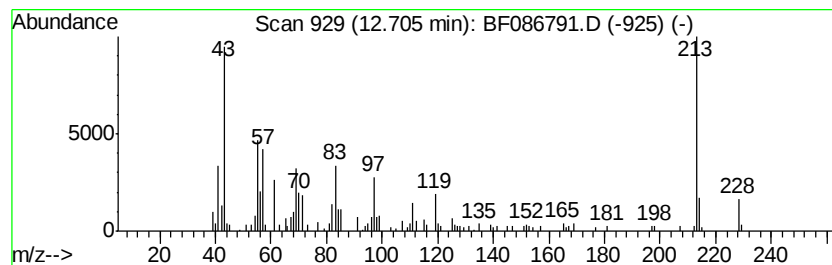
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Acetic acid, octadecyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	5.71 ng	148548	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	80
2		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	70
3		1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	42
4		Trichloroacetic acid, pentadecyl-	372	C17H31Cl3O2	074339-53-0	38
5		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

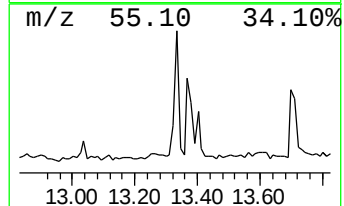
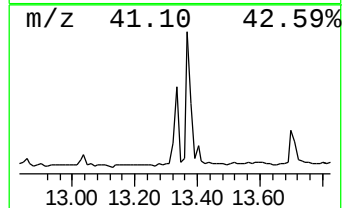
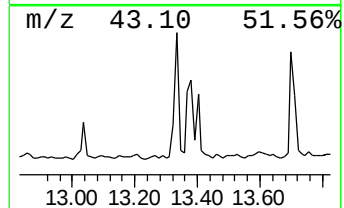
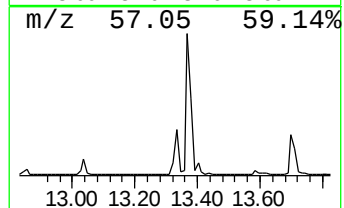
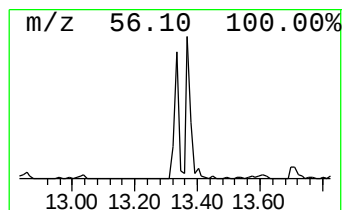
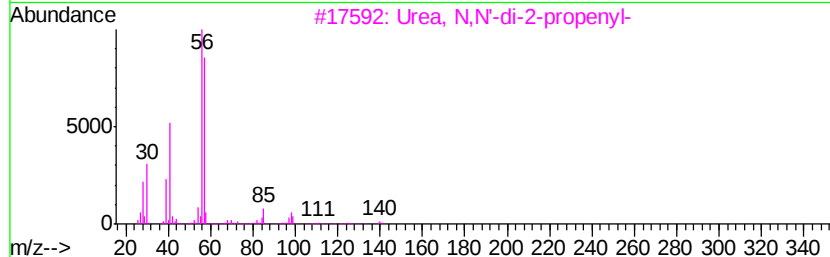
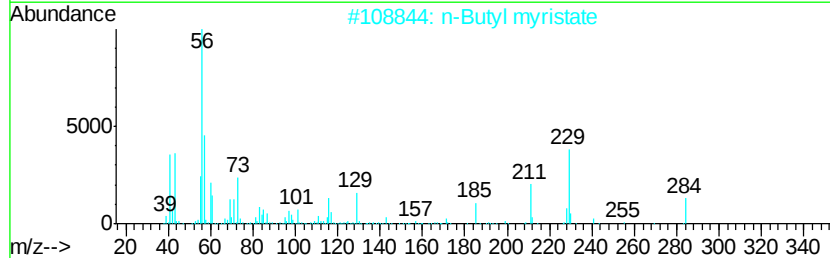
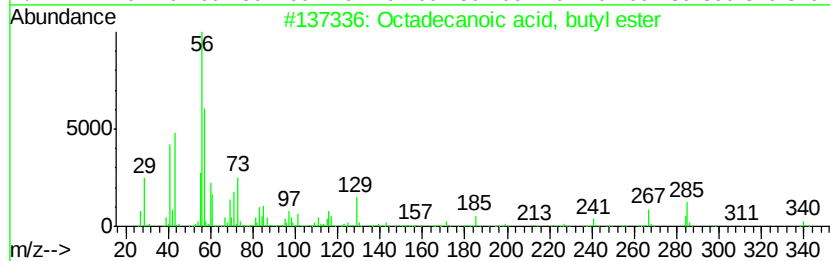
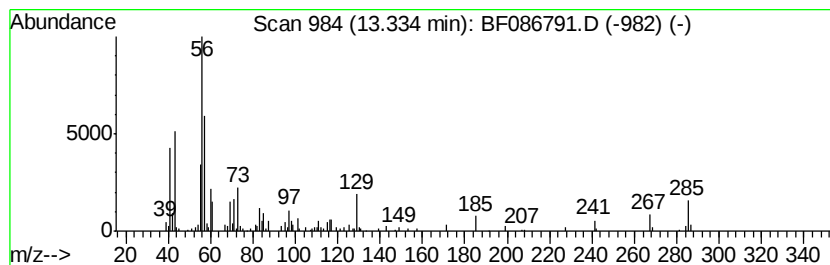
Instrument :
BNA_F
ClientSampleId :
MWHR3-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.33	5.28 ng	137430	Chrysene-d12		13.85		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2			n-Butyl myristate	284	C18H36O2	000110-36-1	86
3			Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
4			2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
5			2-Methyl-1-octadecene	266	C19H38	061868-20-0	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

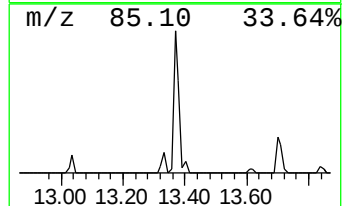
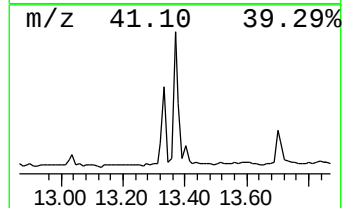
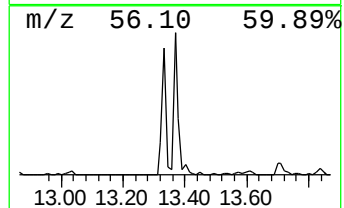
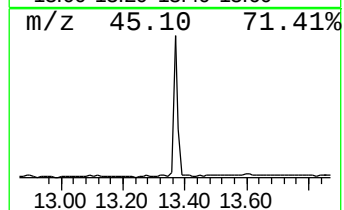
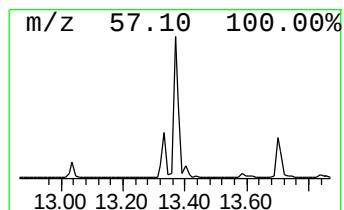
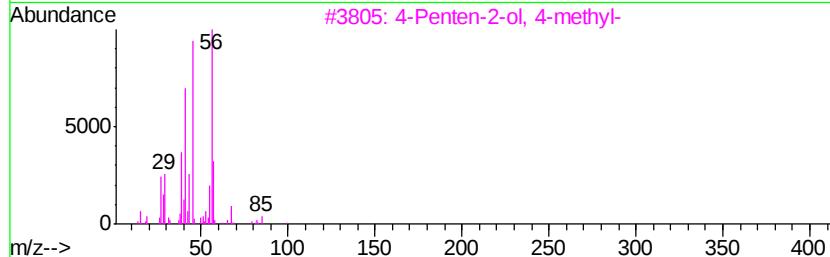
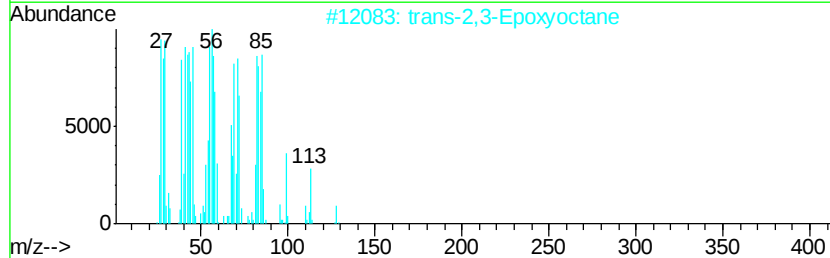
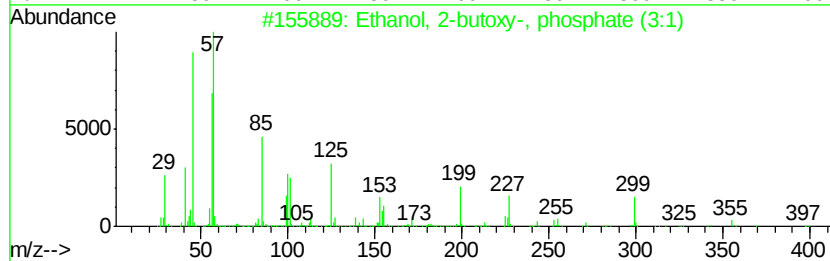
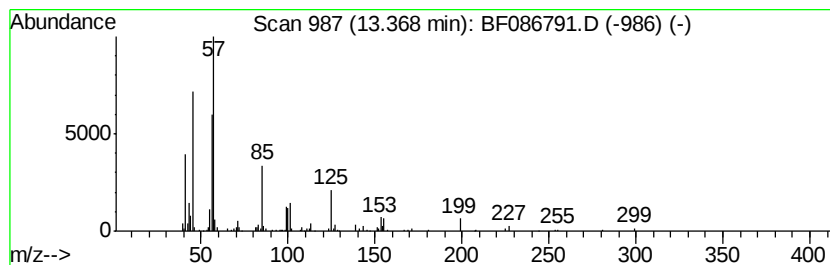
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-butoxy-, phospho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	9.69 ng	252127	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	59
2		trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	43
3		4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	38
4		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	38
5		Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086791.D
Acq On : 7 May 2016 23:28
Operator : UM/SJ
Sample : H2882-01
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR3-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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
2-Pentanone, 4-hy...	4.88	6.7	ng	187702	1	6.70	1120270	40.0
unknown6.48	6.48	161.1	ng	4512650	1	6.70	1120270	40.0
Hexadecanoic acid...	12.63	8.2	ng	212307	5	13.85	1040680	40.0
Acetic acid, octa...	12.71	5.7	ng	148548	5	13.85	1040680	40.0
Octadecanoic acid...	13.33	5.3	ng	137430	5	13.85	1040680	40.0
Ethanol, 2-butoxy...	13.37	9.7	ng	252127	5	13.85	1040680	40.0