

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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-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	243	244	251	rBV	67229	119003	1.84%	0.290%
2	5.299	279	281	297	rBV	2205901	2459806	37.99%	6.003%
3	6.350	372	373	382	rBV	1103618	1610507	24.88%	3.930%
4	6.476	382	384	386	rBV	4624698	4646339	71.77%	11.339%
5	6.705	401	404	406	rBV	988390	1111930	17.17%	2.714%
6	6.853	415	417	420	rBV	3098247	4108000	63.45%	10.026%
7	7.276	451	454	456	rBV	3573985	3846910	59.42%	9.388%
8	7.985	514	516	519	rBV	1239216	1382524	21.35%	3.374%
9	9.070	607	611	613	rBV	5846338	6474295	100.00%	15.801%
10	9.676	662	664	667	rBV	83897	84240	1.30%	0.206%
11	9.733	667	669	672	rBV2	1394528	1549738	23.94%	3.782%
12	10.179	705	708	709	rBV	114693	114701	1.77%	0.280%
13	10.533	736	739	741	rBV2	2581149	3934476	60.77%	9.602%
14	10.648	747	749	753	rVB	113425	132094	2.04%	0.322%
15	11.219	796	799	801	rBV	1416616	1477472	22.82%	3.606%
16	11.756	844	846	854	rBV	139368	179616	2.77%	0.438%
17	12.545	912	915	920	rBV	75801	145149	2.24%	0.354%
18	12.625	920	922	925	rVB	105828	137188	2.12%	0.335%
19	12.808	935	938	940	rBV	3720159	5055564	78.09%	12.338%
20	13.334	982	984	986	rBV	111220	94674	1.46%	0.231%
21	13.711	1014	1017	1024	rBV	119931	196198	3.03%	0.479%
22	13.837	1026	1028	1031	rBV	757747	1132165	17.49%	2.763%
23	14.328	1068	1071	1073	rBV	39824	65842	1.02%	0.161%
24	15.220	1146	1149	1156	rBV	673391	916690	14.16%	2.237%

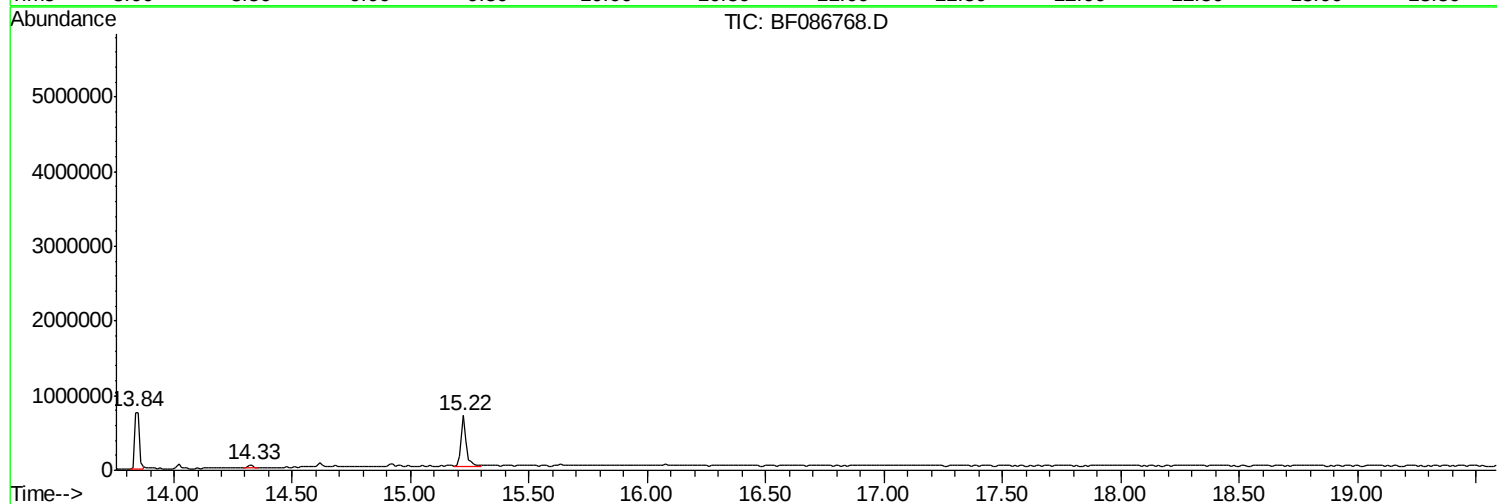
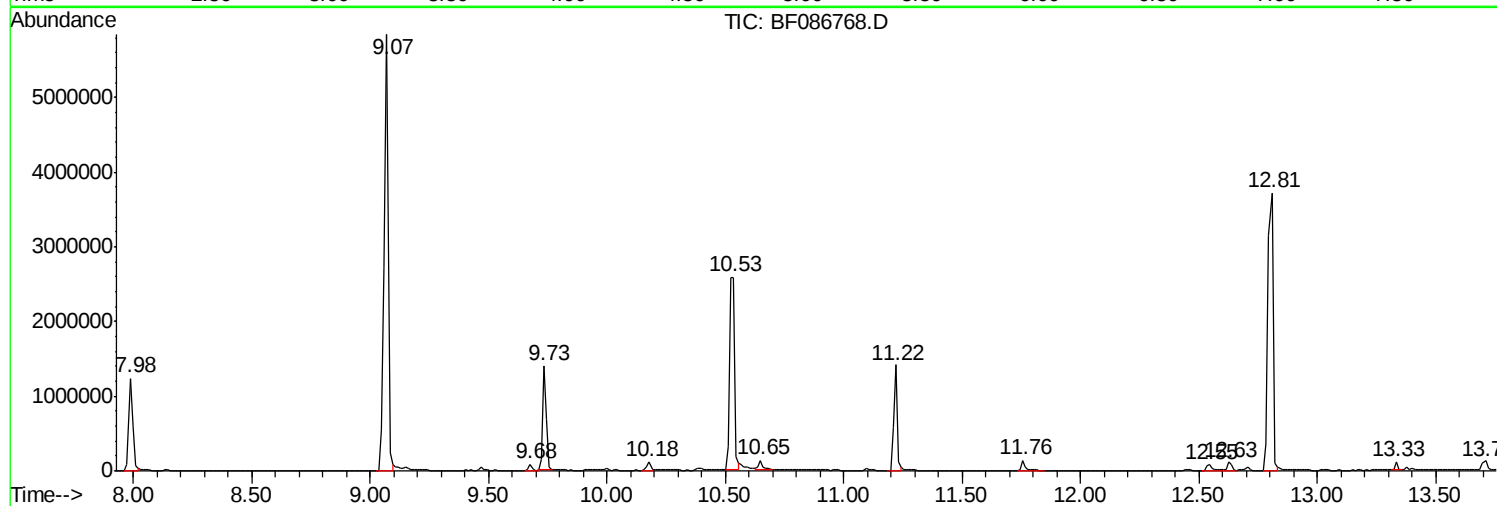
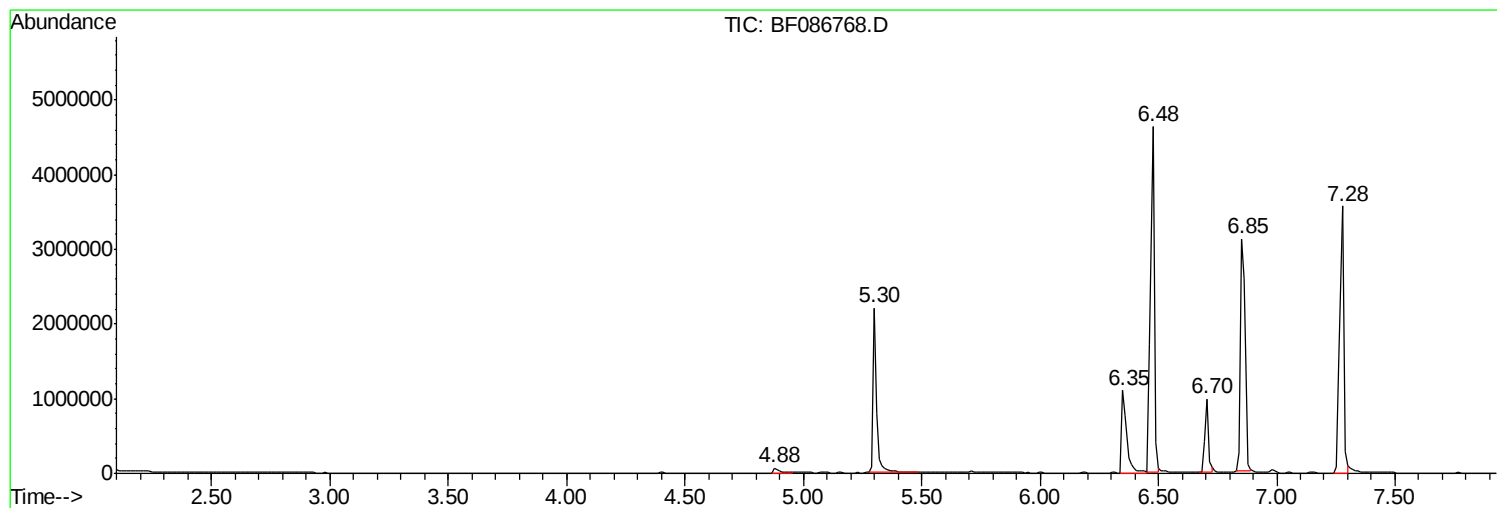
Sum of corrected areas: 40975121

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

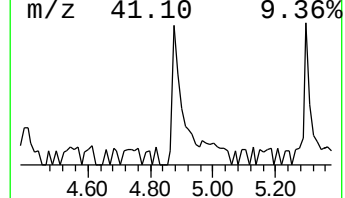
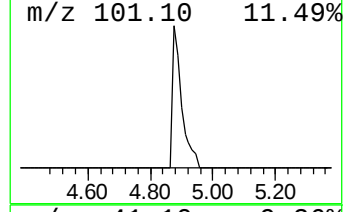
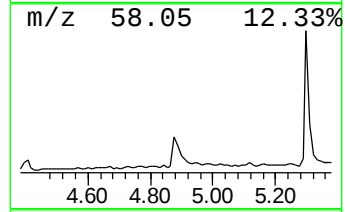
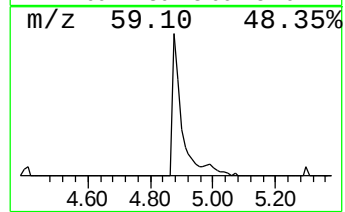
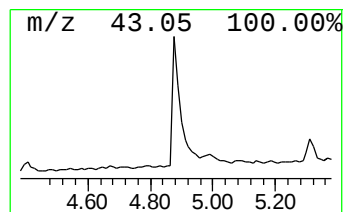
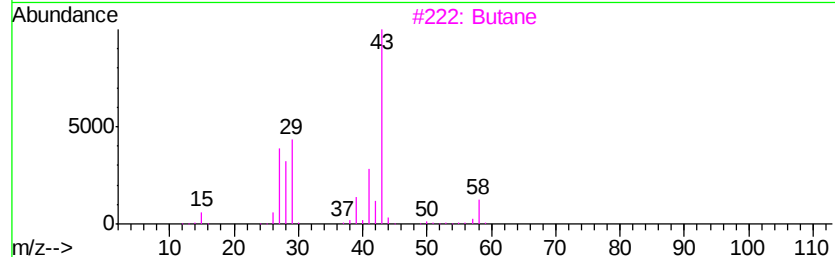
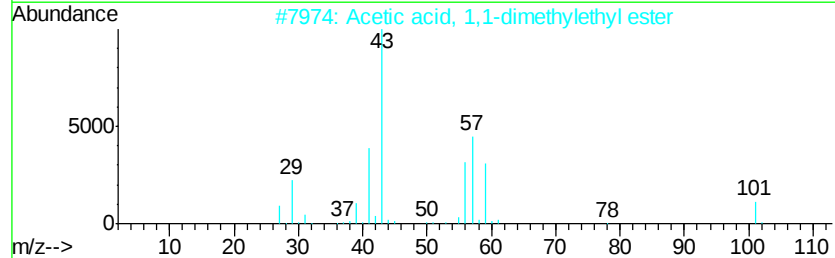
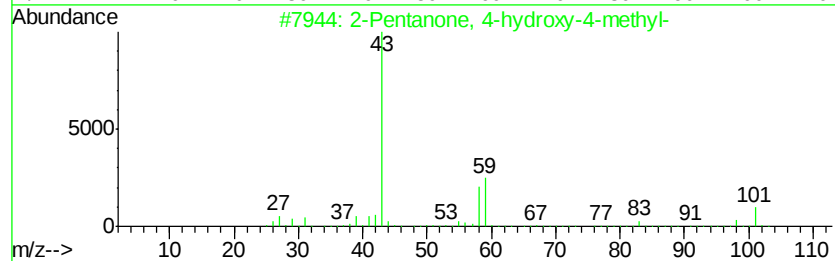
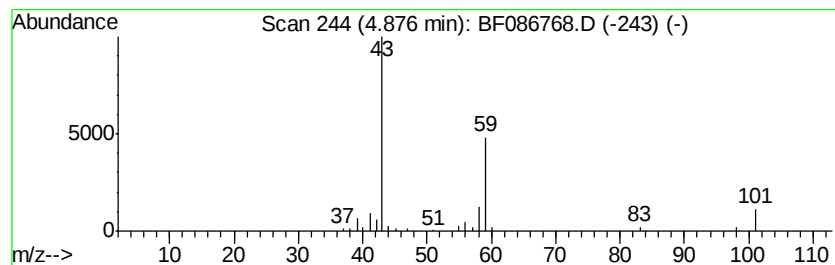
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	4.28 ng	119003	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	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	Butane	58	C4H10	000106-97-8	9		
4	Diacetamide	101	C4H7NO2	000625-77-4	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

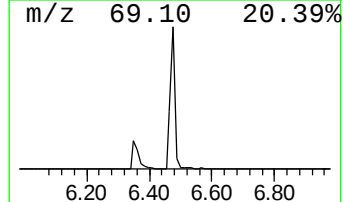
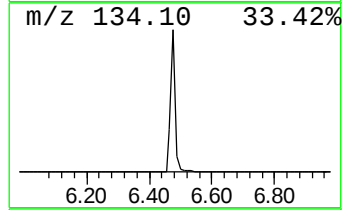
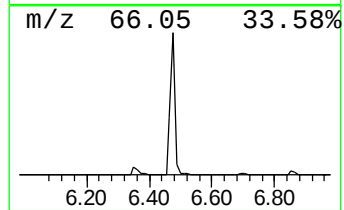
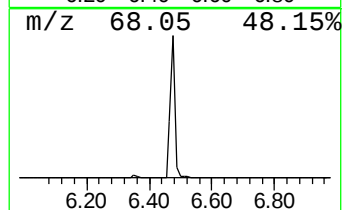
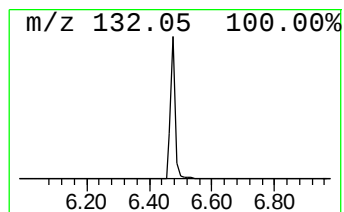
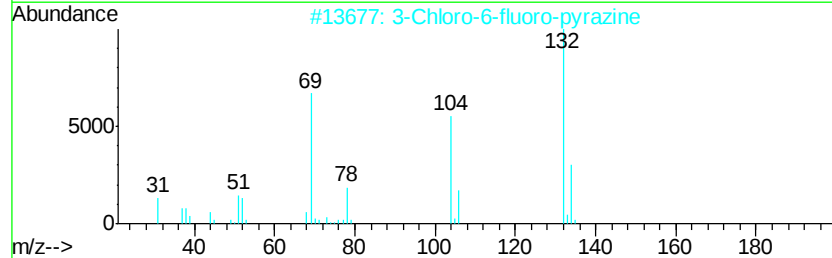
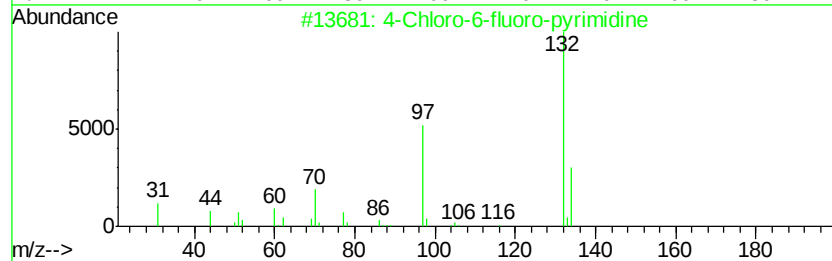
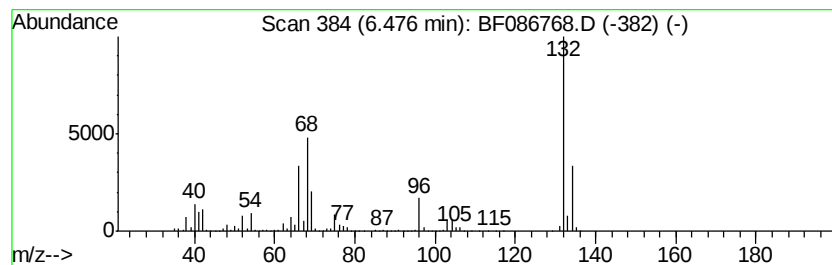
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	167.15 ng	4646340	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

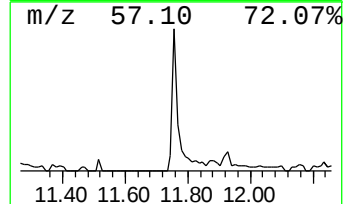
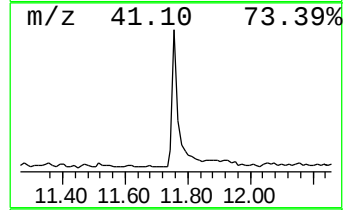
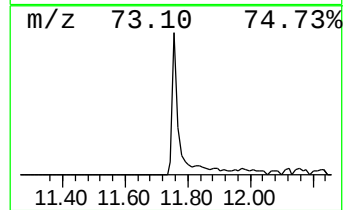
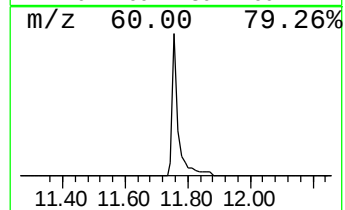
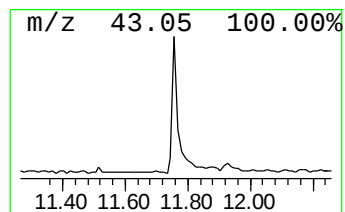
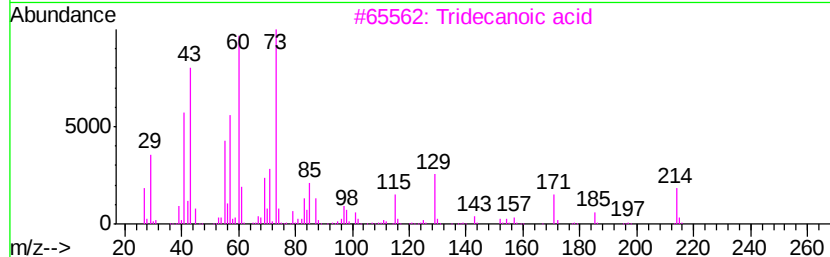
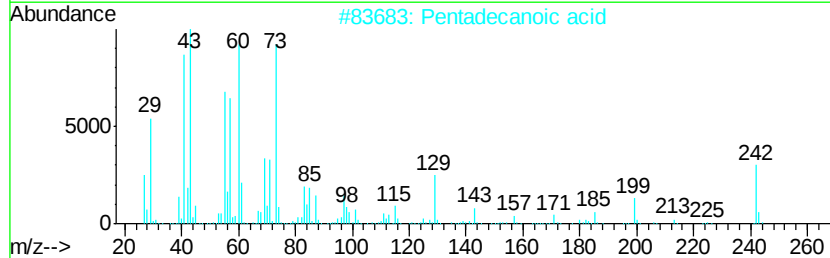
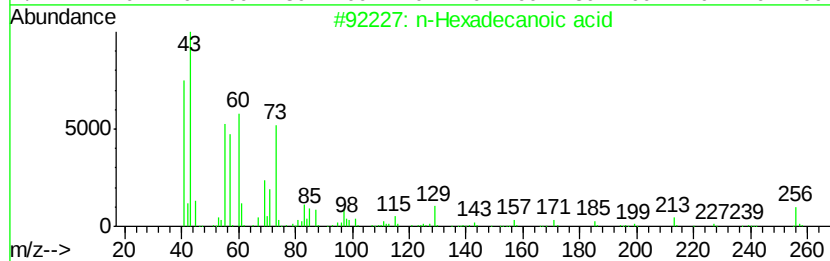
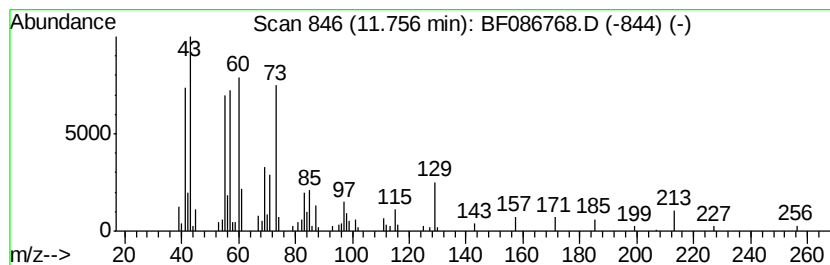
Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.76	4.86 ng	179616	Phenanthrene-d10	11.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

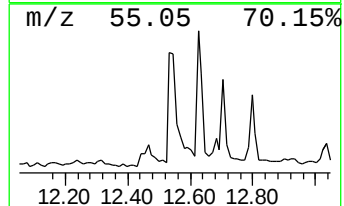
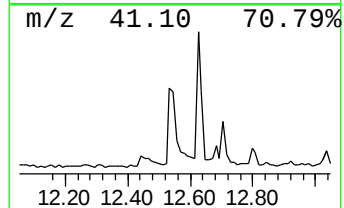
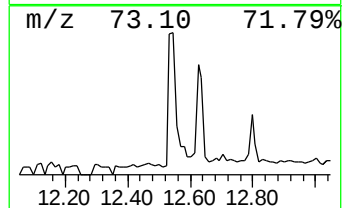
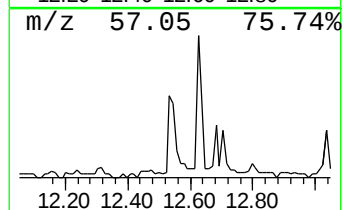
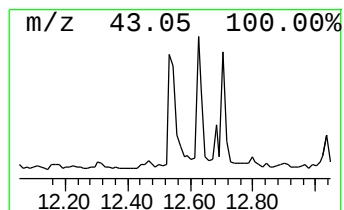
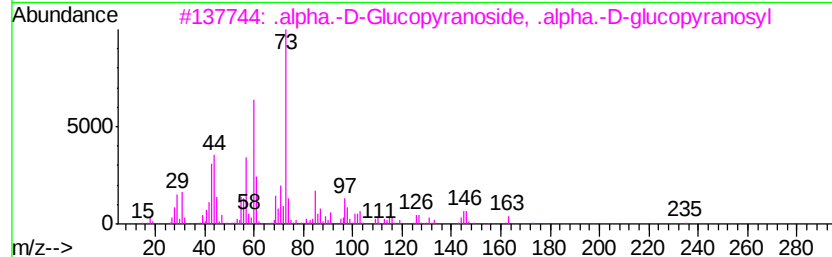
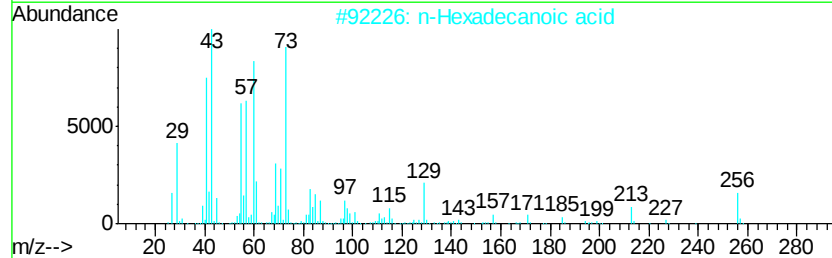
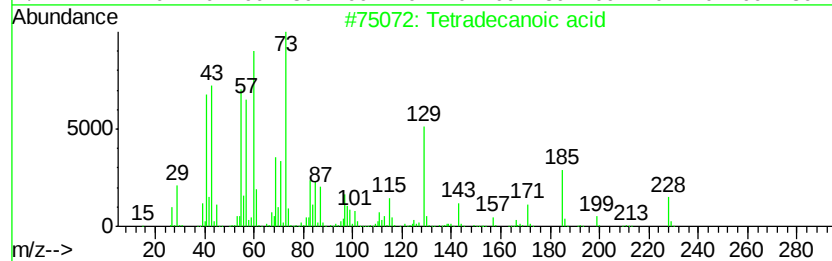
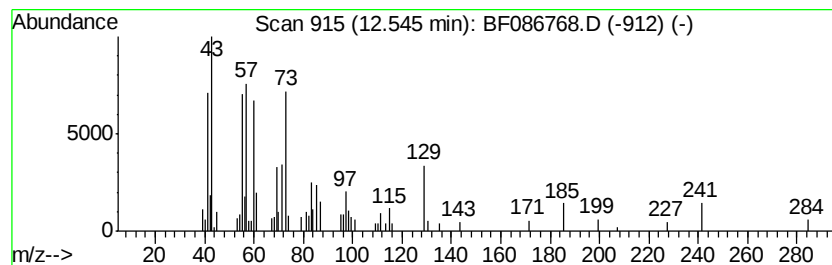
Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	5.13 ng	145149	Chrysene-d12	13.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecanoic acid	228 C14H28O2	000544-63-8 72
2		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 50
3		.alpha.-D-Glucopyranoside, .alph...	342 C12H22O11	000099-20-7 43
4		n-Decanoic acid	172 C10H20O2	000334-48-5 43
5		D-Glucose, 4-O-.alpha.-D-glucopy...	342 C12H22O11	000069-79-4 35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

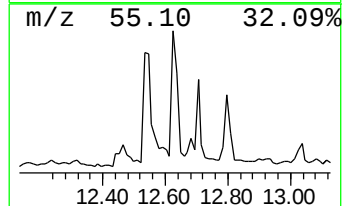
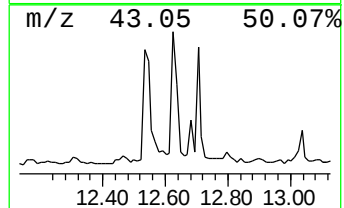
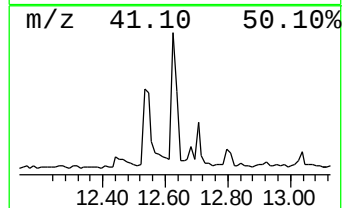
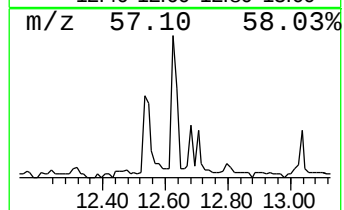
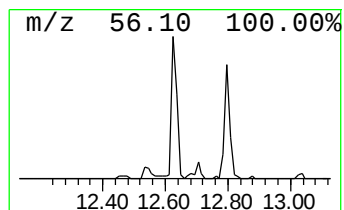
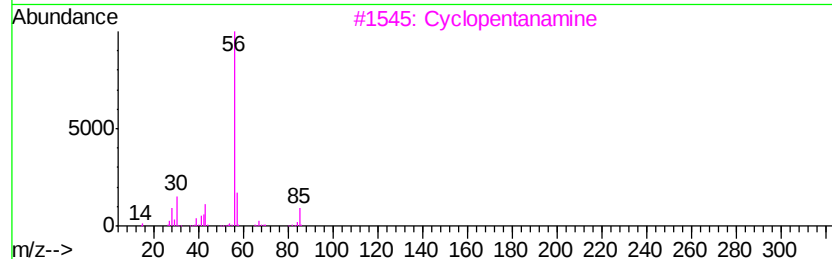
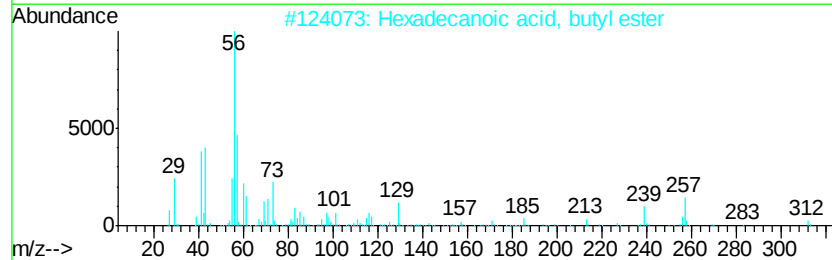
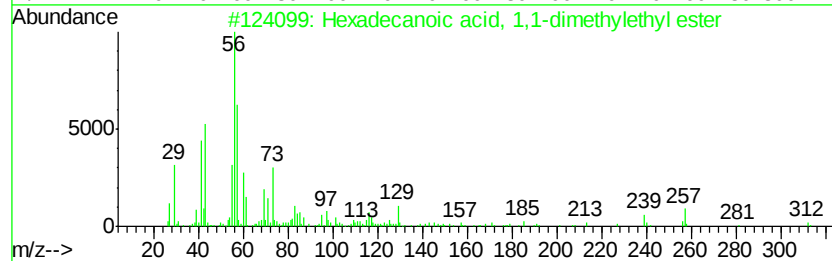
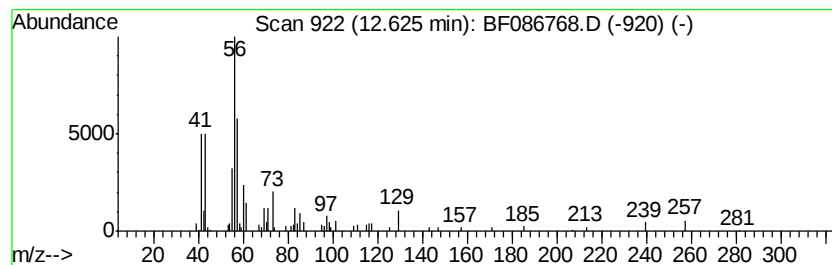
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	4.85 ng	137188	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
3		Cyclopentanamine	85	C5H11N	001003-03-8	38
4		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

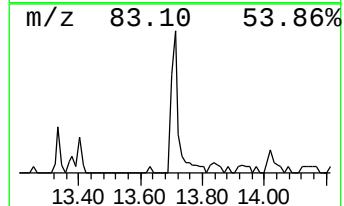
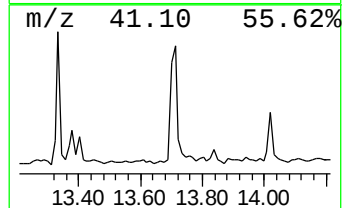
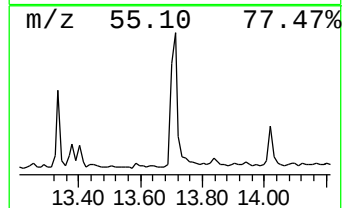
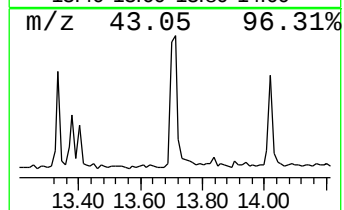
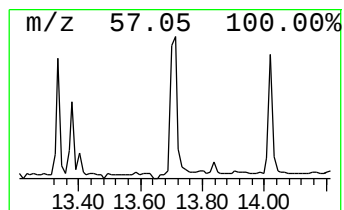
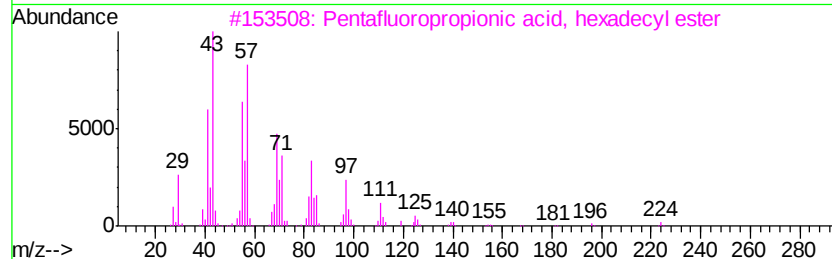
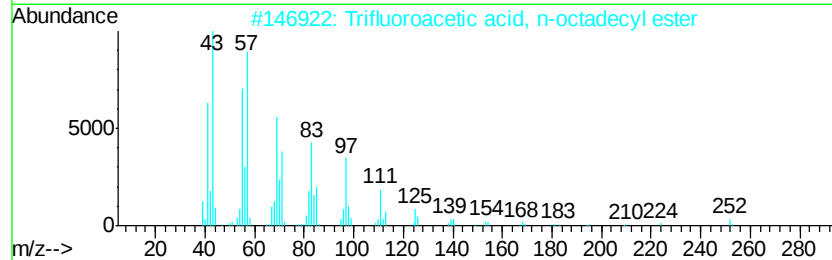
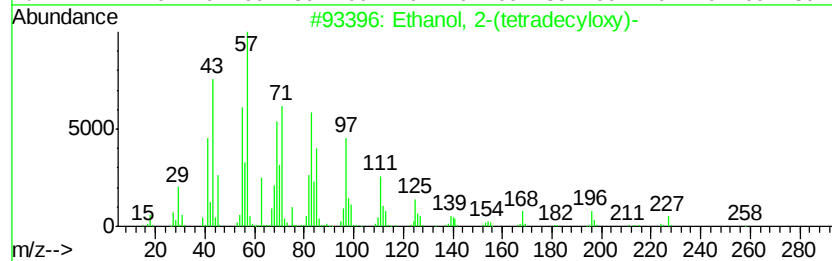
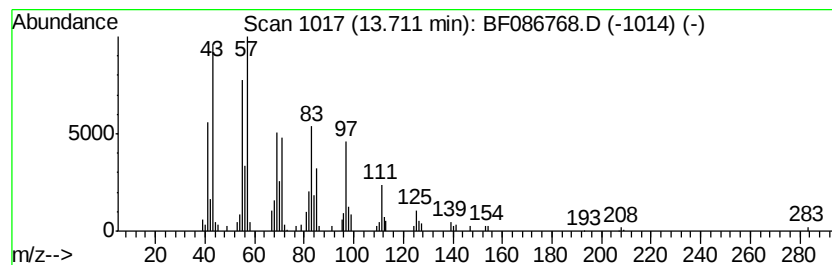
Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	6.93 ng	196198	Chrysene-d12	13.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086768.D
Acq On : 7 May 2016 12:22
Operator : UM/SJ
Sample : H2858-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR(2-10)

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	4.3	ng	119003	1	6.70	1111930	40.0
unknown6.48	6.48	167.2	ng	4646340	1	6.70	1111930	40.0
n-Hexadecanoic acid	11.76	4.9	ng	179616	4	11.22	1477470	40.0
Tetradecanoic acid	12.55	5.1	ng	145149	5	13.85	1132170	40.0
Hexadecanoic acid...	12.63	4.8	ng	137188	5	13.85	1132170	40.0
Ethanol, 2-(tetra...	13.71	6.9	ng	196198	5	13.85	1132170	40.0