

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
 Data File : BF088394.D
 Acq On : 26 Jun 2016 1:42
 Operator : UM/SJ
 Sample : H3745-02
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-COMP

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-BF060716.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	1.678	6	8	9	rBV	18079	27804	1.59%	0.190%
2	1.701	9	10	51	rVB	712654	1458013	83.50%	9.980%
3	2.684	94	96	119	rBV	8323	47375	2.71%	0.324%
4	4.684	269	271	284	rBV	48253	84909	4.86%	0.581%
5	5.142	309	311	328	rBV	1051092	1344542	77.00%	9.204%
6	6.227	403	406	413	rBV	1176307	1354324	77.56%	9.271%
7	6.330	413	415	433	rVB	1466762	1487118	85.17%	10.180%
8	6.559	433	435	445	rBV	307172	335573	19.22%	2.297%
9	6.719	446	449	451	rBV	797375	1156428	66.23%	7.916%
10	7.130	483	485	502	rBV	549563	889675	50.95%	6.090%
11	7.850	546	548	550	rBV	367029	432005	24.74%	2.957%
12	8.925	639	642	652	rBV	1768111	1746149	100.00%	11.953%
13	9.325	675	677	680	rVB	93140	76473	4.38%	0.523%
14	9.588	698	700	703	rBV	528084	494080	28.30%	3.382%
15	10.376	767	769	779	rBV	718273	790793	45.29%	5.413%
16	10.502	779	780	787	rVB2	14102	22888	1.31%	0.157%
17	10.948	817	819	821	rBV	36969	35674	2.04%	0.244%
18	11.062	828	829	833	rBV	375657	409435	23.45%	2.803%
19	11.131	833	835	839	rVB	13392	26766	1.53%	0.183%
20	11.325	850	852	855	rBV	11469	21508	1.23%	0.147%
21	11.371	855	856	859	rVB	19249	19240	1.10%	0.132%
22	12.137	920	923	930	rBB	32571	74607	4.27%	0.511%
23	12.479	951	953	956	rBV2	50969	52012	2.98%	0.356%
24	12.651	965	968	970	rBV	1117484	1324001	75.82%	9.063%
25	13.188	1012	1015	1017	rBV	33473	47247	2.71%	0.323%
26	13.554	1045	1047	1056	rBV	36934	87877	5.03%	0.602%
27	13.691	1056	1059	1066	rVV	367433	394395	22.59%	2.700%
28	14.605	1136	1139	1144	rBV	5542	19309	1.11%	0.132%
29	15.040	1175	1177	1189	rBV	206255	307228	17.59%	2.103%
30	15.817	1243	1245	1252	rVB4	6561	18308	1.05%	0.125%
31	16.834	1328	1334	1340	rBV5	4474	22956	1.31%	0.157%

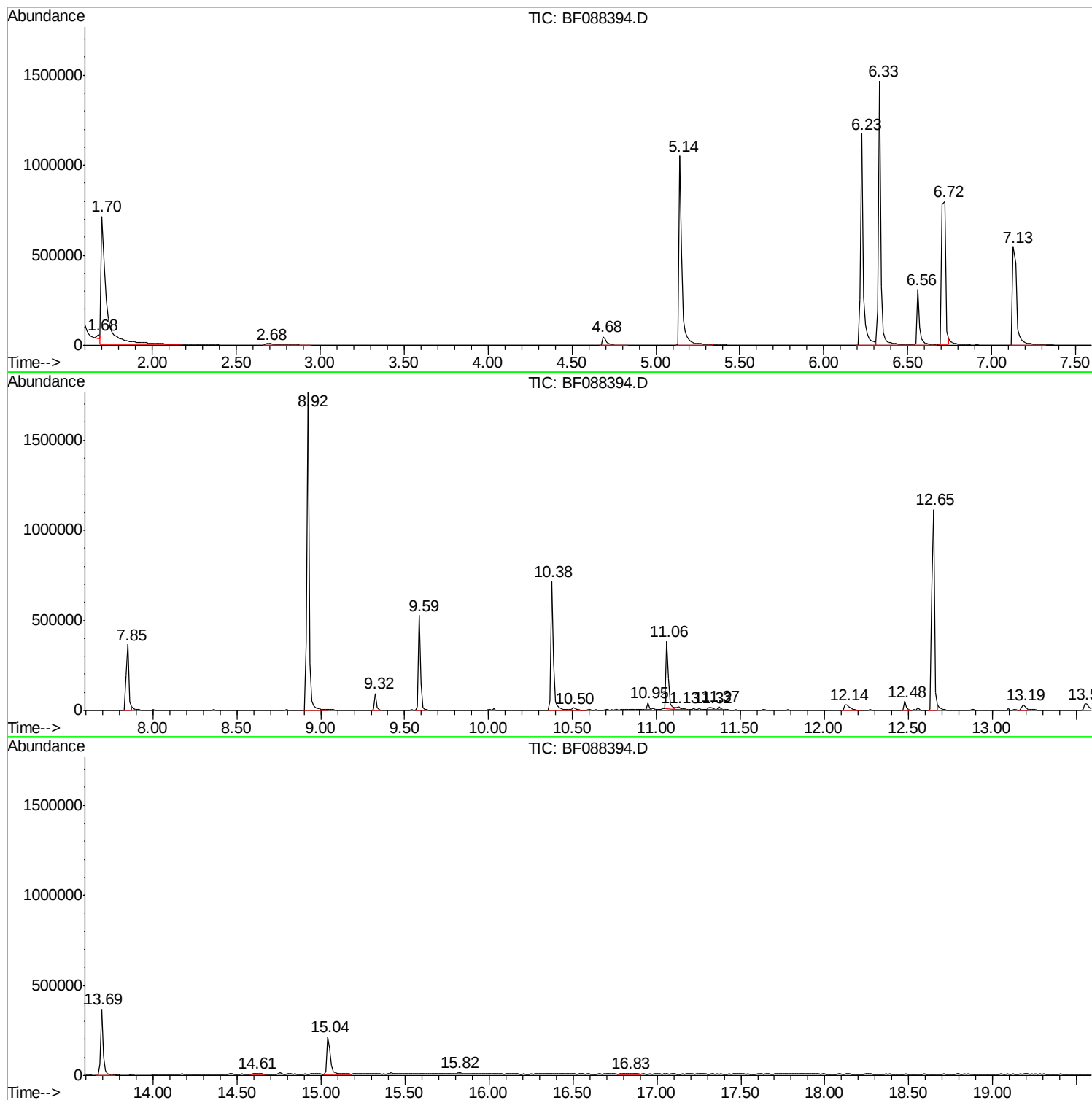
Sum of corrected areas: 14608712

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

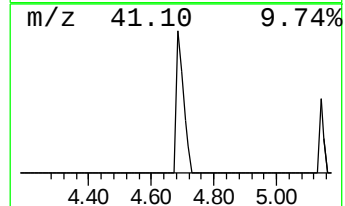
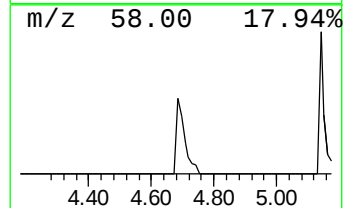
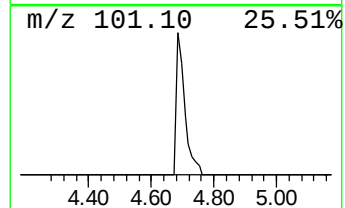
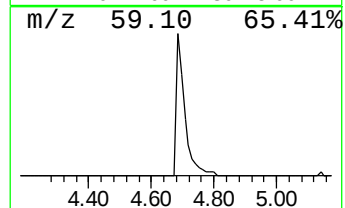
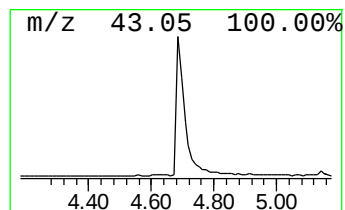
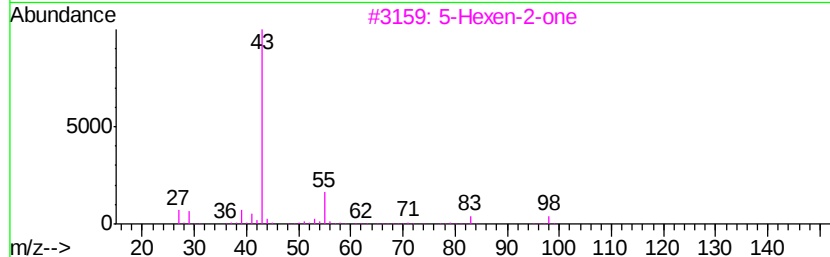
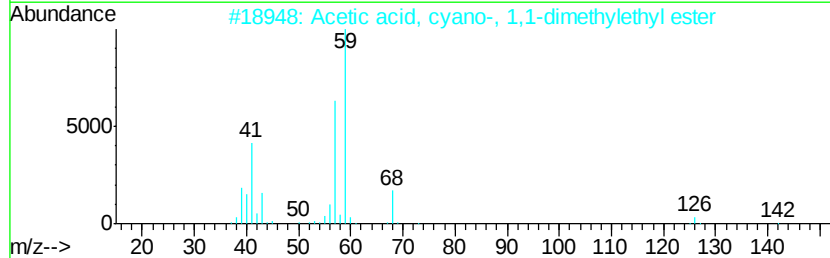
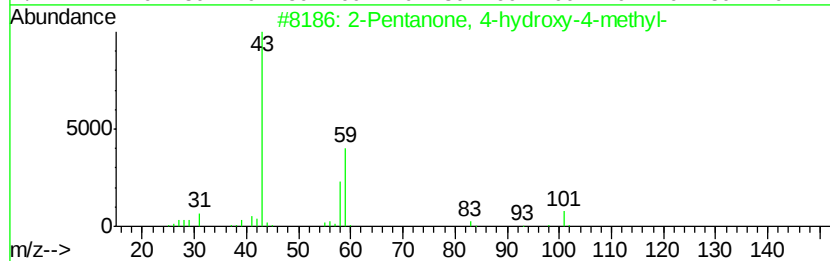
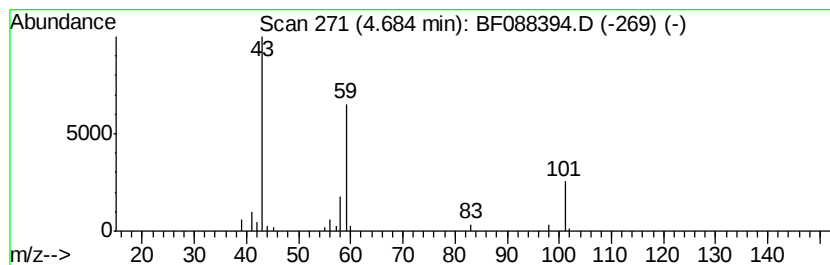
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	5.06 ng	84909	1,4-Dichlorobenzene-d4	6.56

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		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

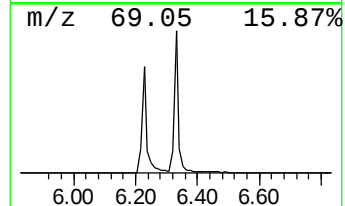
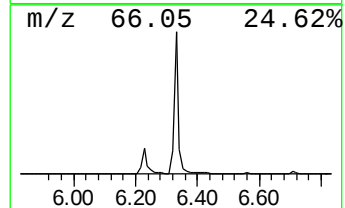
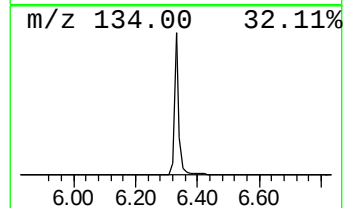
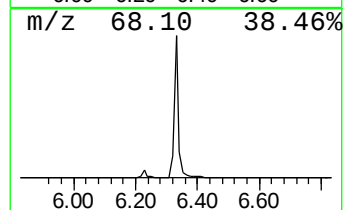
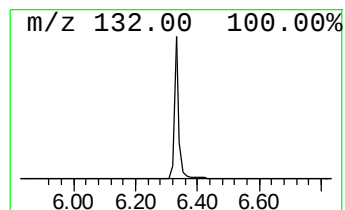
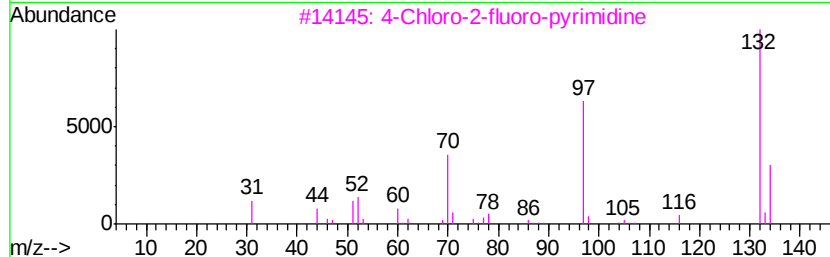
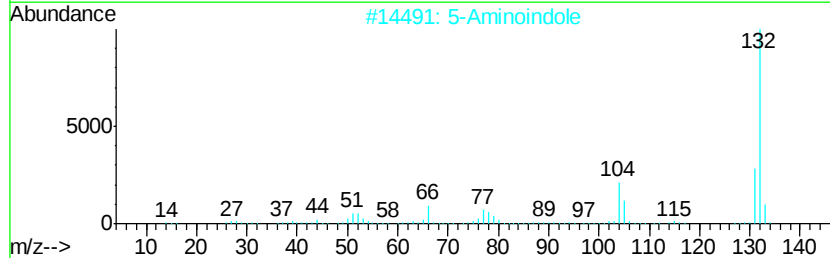
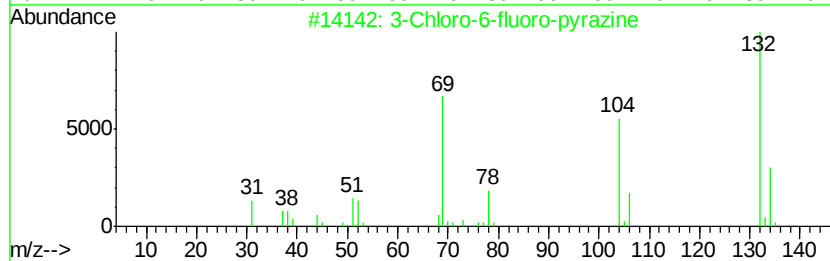
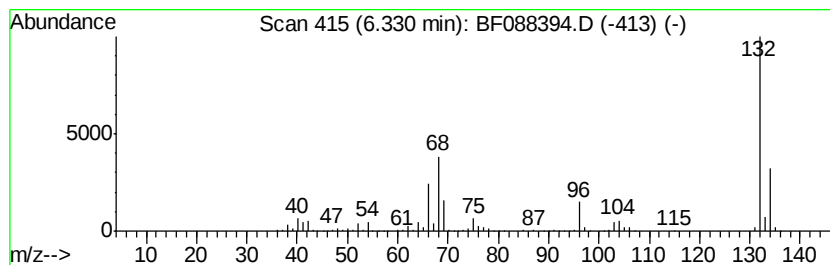
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	88.63 ng	1487120	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

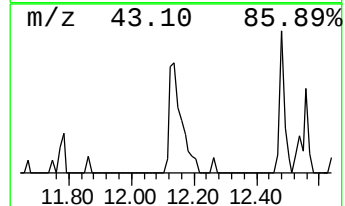
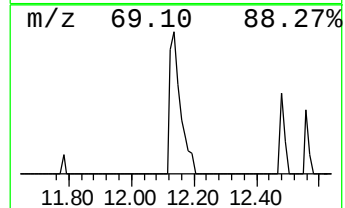
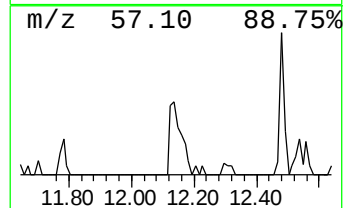
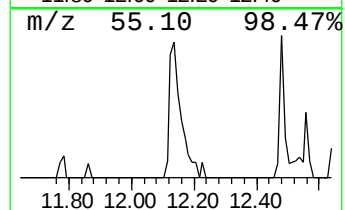
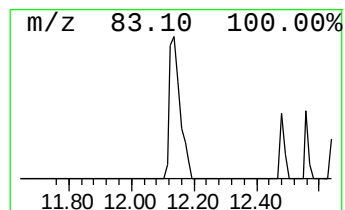
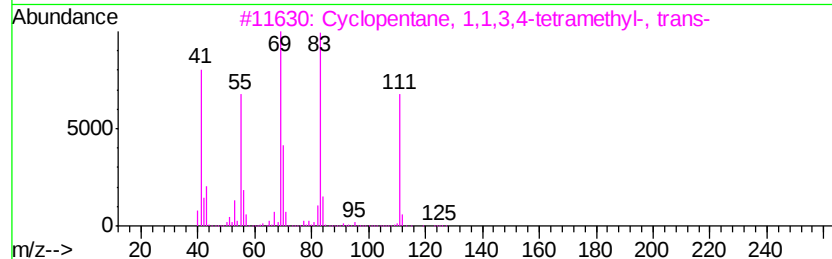
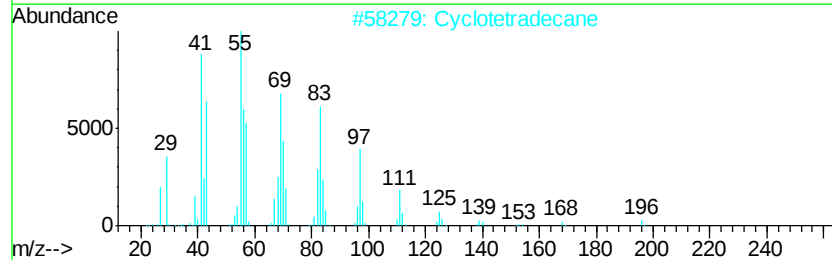
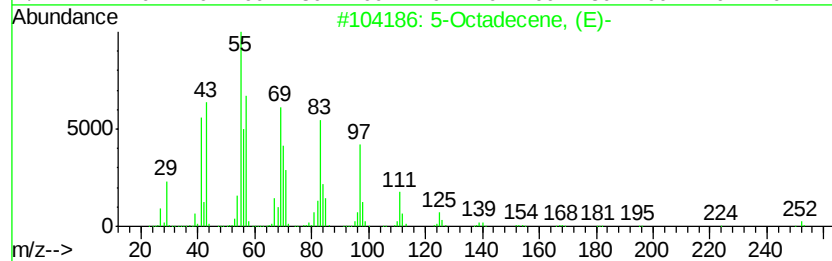
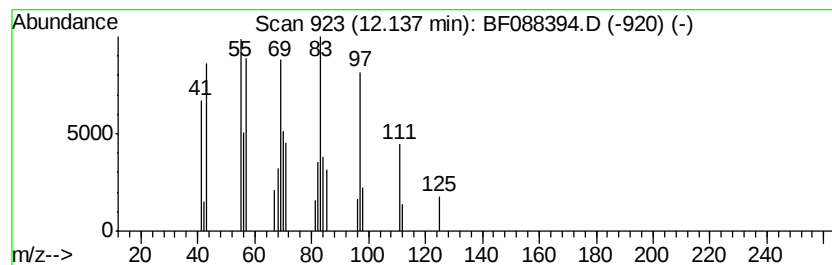
Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.14	3.64 ng	74607	Phenanthrene-d10	11.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	Cyclotetradecane	196	C14H28	000295-17-0	50
3	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	43
4	Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	38
5	3-Chloropropionic acid, hexadecy...	332	C19H37ClO2	053312-70-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

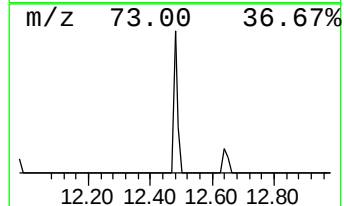
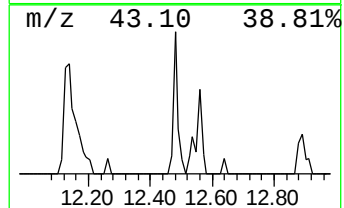
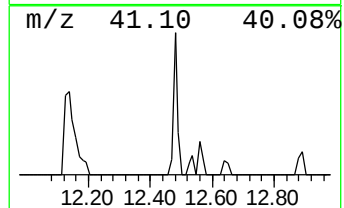
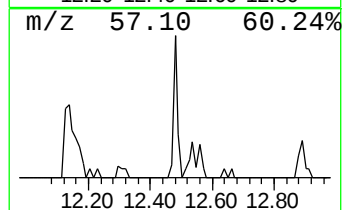
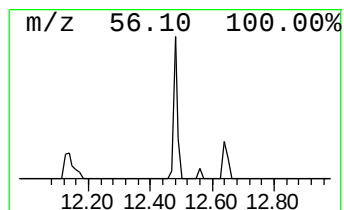
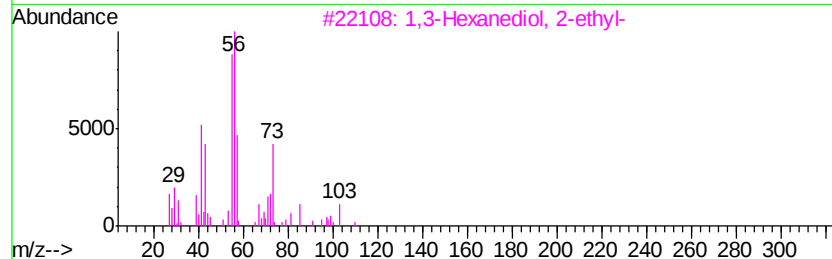
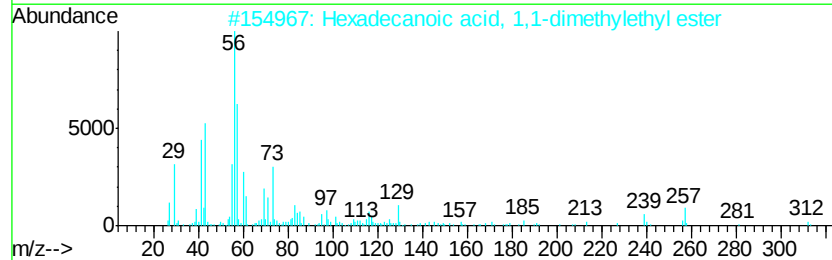
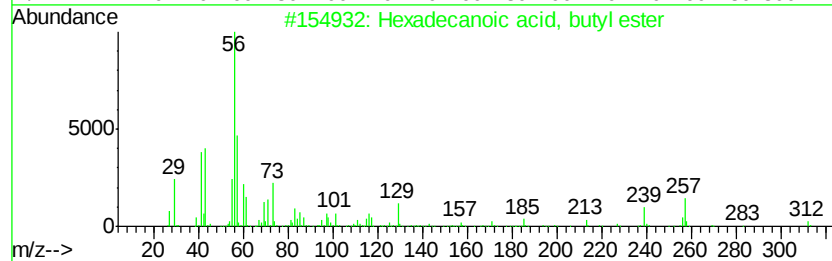
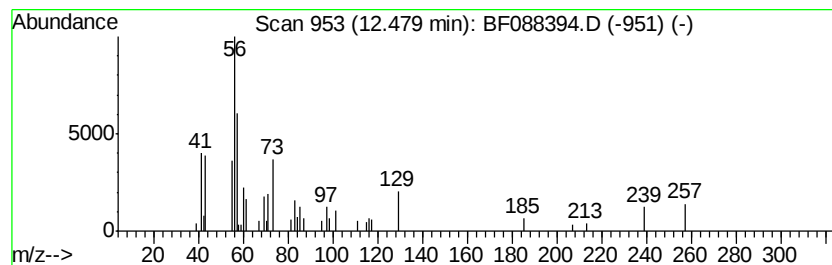
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.64 ng	52012	Chrysene-d12	13.69

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	74
3		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	40
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

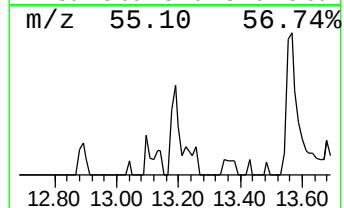
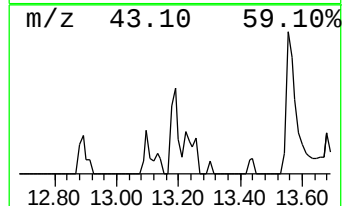
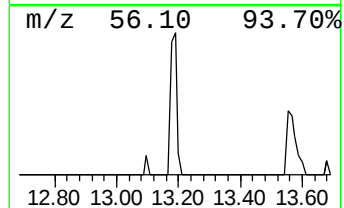
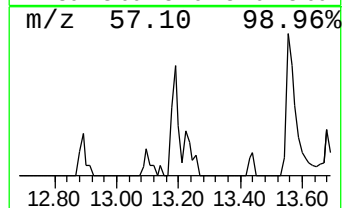
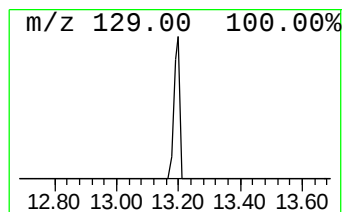
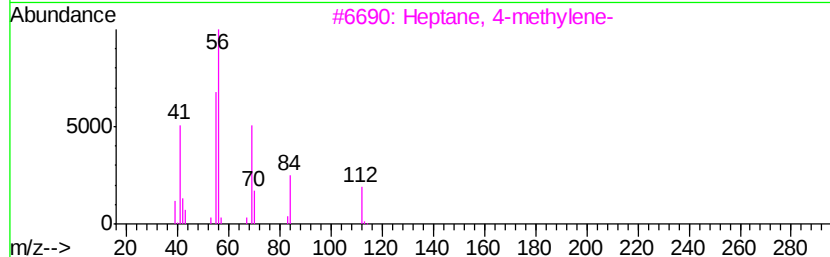
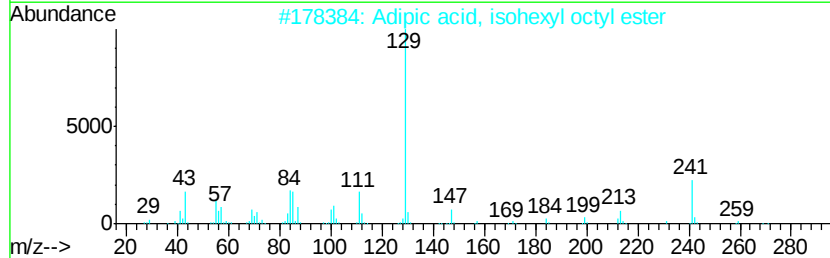
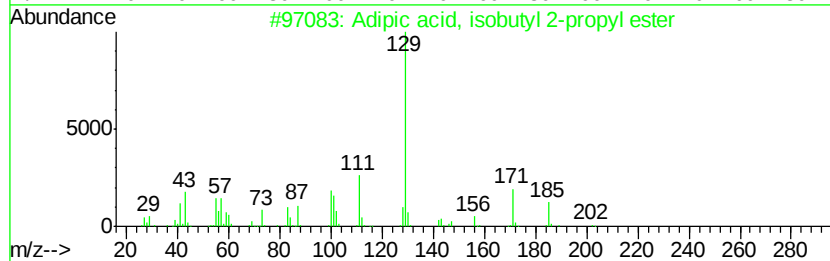
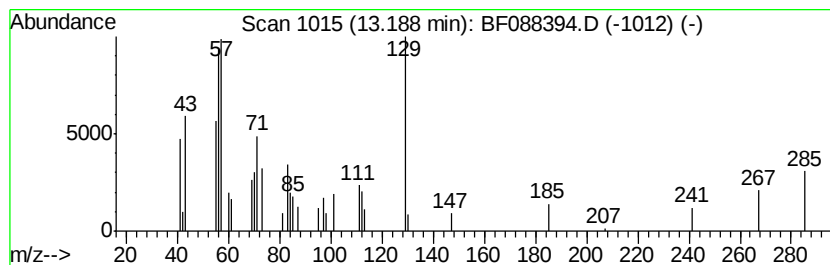
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.40 ng	47247	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adipic acid, isobutyl 2-propyl e...	244	C13H24O4	1000324-42-9	27
2		Adipic acid, isohexyl octyl ester	342	C20H38O4	1000324-47-0	27
3		Heptane, 4-methylene-	112	C8H16	015918-08-8	22
4		3-Undecene, 7-methyl-, (Z)-	168	C12H24	074630-49-2	22
5		2-Heptene, 5-methyl-	112	C8H16	022487-87-2	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

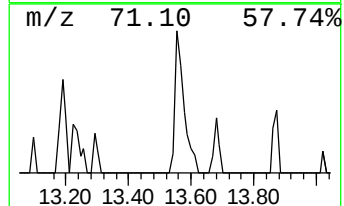
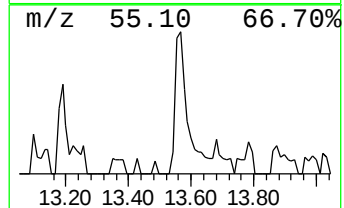
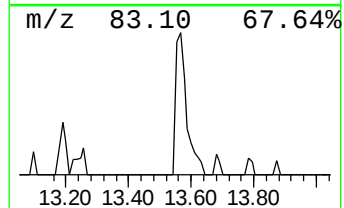
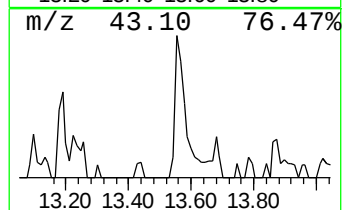
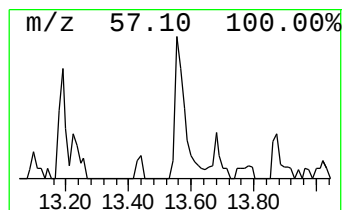
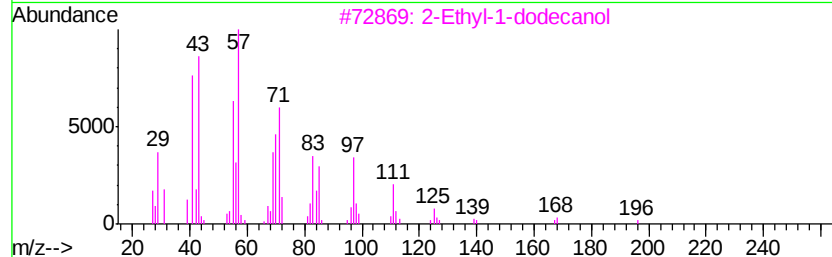
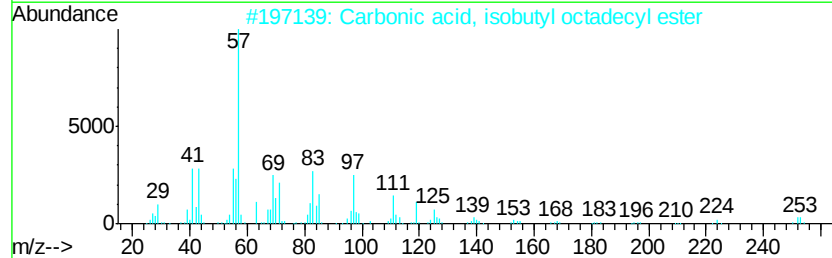
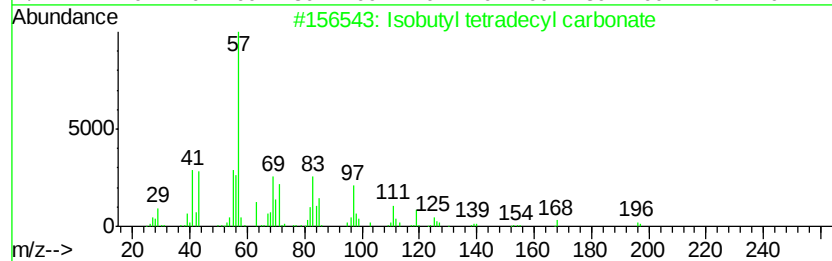
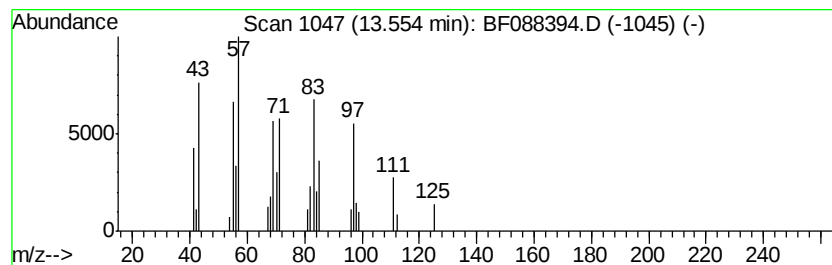
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.46 ng	87877	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
2		Carbonic acid, isobutyl octadecyl ester	370	C23H46O3	1000314-61-5	86
3		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	62
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
Data File : BF088394.D
Acq On : 26 Jun 2016 1:42
Operator : UM/SJ
Sample : H3745-02
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
2-Pentanone, 4-hy...	4.68	5.1	ng	84909	1	6.56	335573	20.0
unknown6.33	6.33	88.6	ng	1487120	1	6.56	335573	20.0
5-Octadecene, (E)-	12.14	3.6	ng	74607	4	11.06	409435	20.0
Hexadecanoic acid...	12.48	2.6	ng	52012	5	13.69	394395	20.0
unknown13.19	13.19	2.4	ng	47247	5	13.69	394395	20.0
Isobutyl tetradec...	13.55	4.5	ng	87877	5	13.69	394395	20.0