

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
 Data File : BF090403.D
 Acq On : 6 Oct 2016 2:02
 Operator : UM/SJ
 Sample : H5061-20
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B003-30-35

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-BF100516.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	3.468	97	99	113	rBV	79580	206494	3.09%	0.342%
2	5.206	248	251	254	rBV	1194453	1433783	21.49%	2.373%
3	5.606	283	286	289	rBV	4621948	6266066	93.90%	10.369%
4	6.623	372	375	377	rBV	5783104	6433205	96.40%	10.646%
5	6.772	385	388	390	rBV	5967751	6673232	100.00%	11.043%
6	7.000	406	408	410	rBV	1786846	1454524	21.80%	2.407%
7	7.160	419	422	424	rVB	5066516	4700094	70.43%	7.778%
8	7.560	454	457	459	rBV	3531701	3382263	50.68%	5.597%
9	7.640	459	464	465	rBV	93836	100750	1.51%	0.167%
10	8.292	518	521	523	rBV	1956435	1992576	29.86%	3.297%
11	9.366	612	615	618	rBV	6089741	5956539	89.26%	9.857%
12	9.766	647	650	651	rBV	1437802	1893785	28.38%	3.134%
13	10.052	672	675	677	rVB	2498648	2214926	33.19%	3.665%
14	10.486	709	713	714	rBV	110242	148847	2.23%	0.246%
15	10.703	729	732	735	rBV	49439	74947	1.12%	0.124%
16	10.841	741	744	746	rBV	4445461	4241305	63.56%	7.019%
17	10.955	752	754	761	rVB	183470	207045	3.10%	0.343%
18	11.401	792	793	795	rBV	79570	114178	1.71%	0.189%
19	11.538	803	805	808	rBV	2296158	2018039	30.24%	3.339%
20	11.835	829	831	833	rBV	96710	78880	1.18%	0.131%
21	12.064	849	851	865	rBV	556236	607243	9.10%	1.005%
22	12.772	909	913	918	rBV3	30941	80908	1.21%	0.134%
23	12.852	918	920	926	rVV	256840	279451	4.19%	0.462%
24	13.138	942	945	947	rBV	5159070	6218062	93.18%	10.290%
25	14.030	1021	1023	1034	rBV	410206	554994	8.32%	0.918%
26	14.190	1034	1037	1039	rBV	1710429	1662993	24.92%	2.752%
27	14.670	1073	1079	1082	rBV5	24791	69875	1.05%	0.116%
28	15.058	1111	1113	1121	rVB	69739	98014	1.47%	0.162%
29	15.687	1165	1168	1171	rBV	839937	1198118	17.95%	1.983%
30	16.247	1214	1217	1222	rBV3	21979	69183	1.04%	0.114%

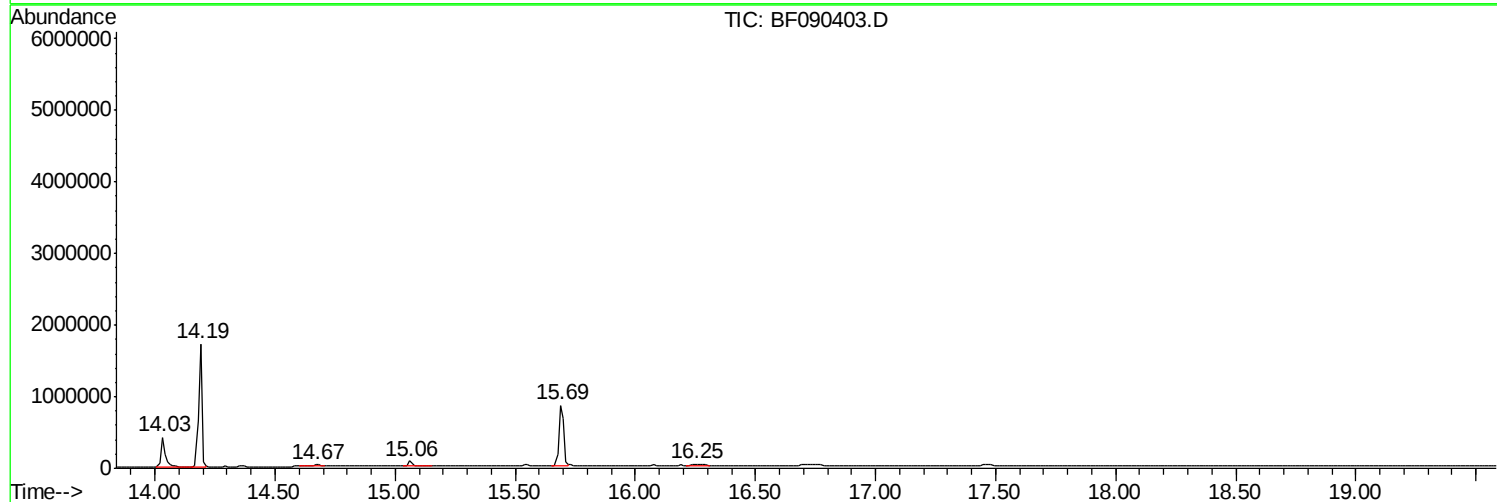
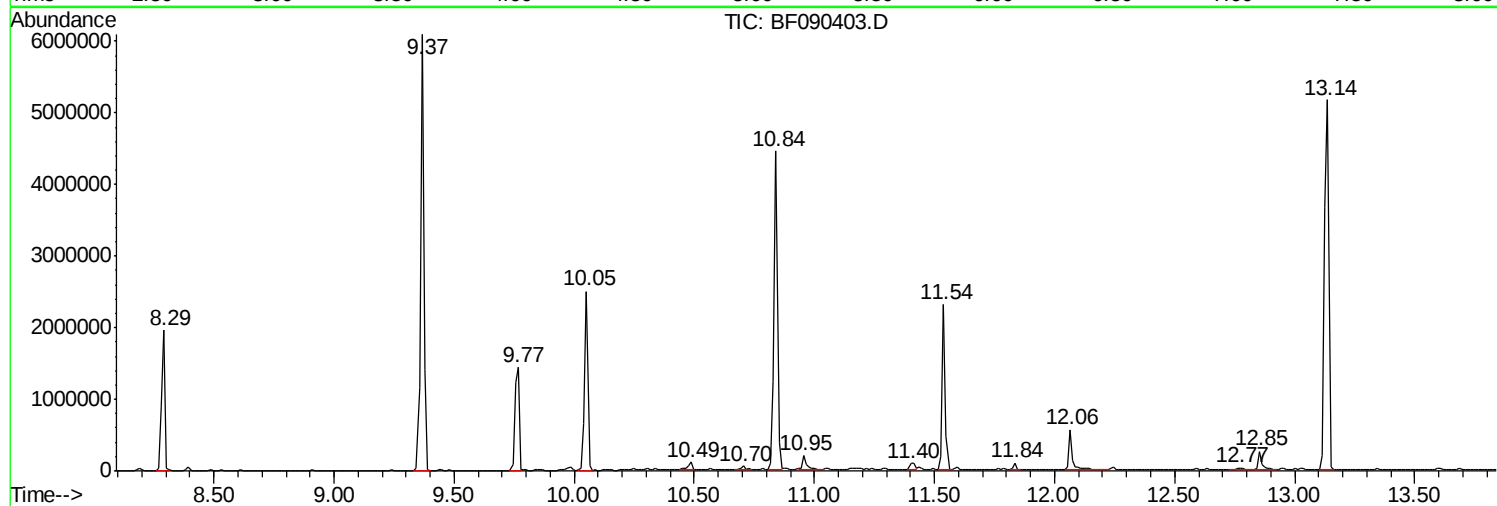
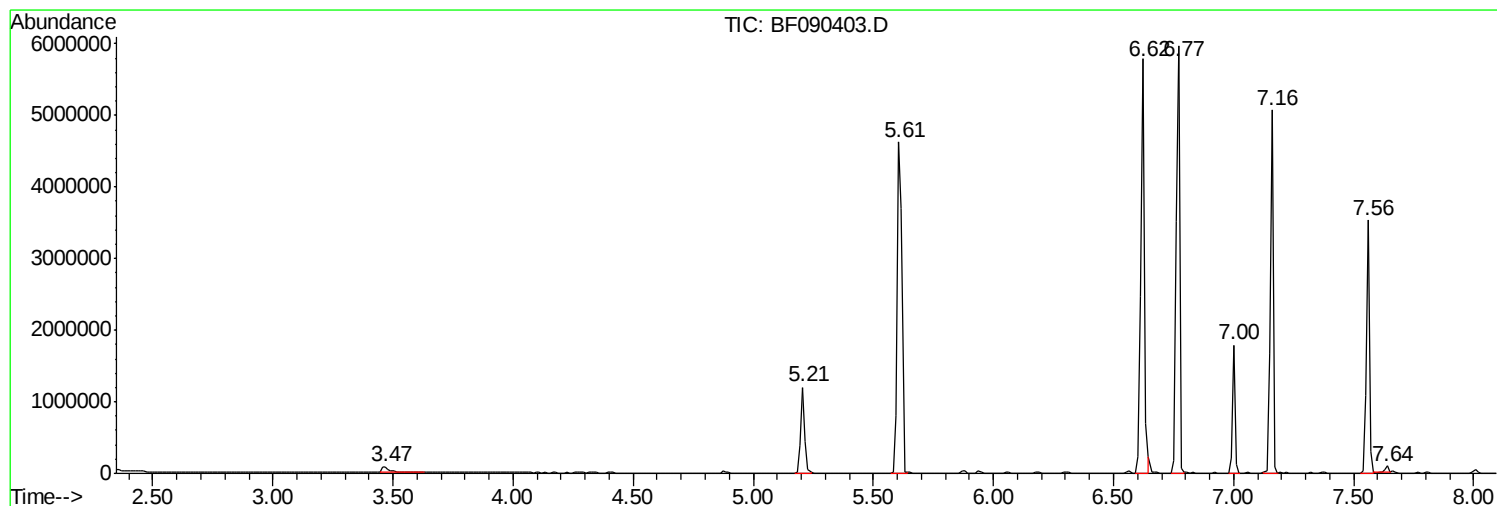
Sum of corrected areas: 60430319

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

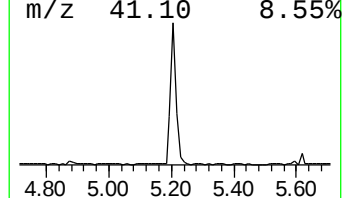
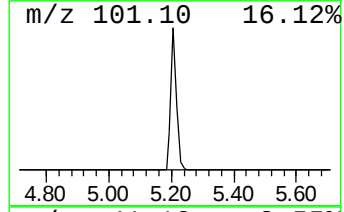
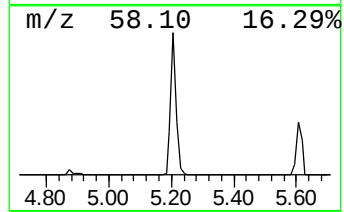
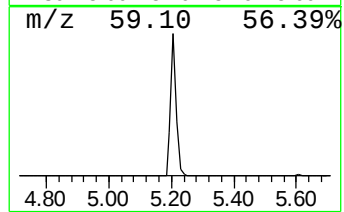
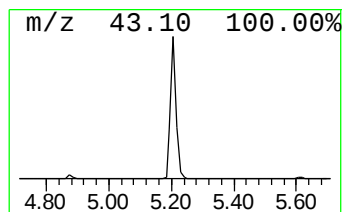
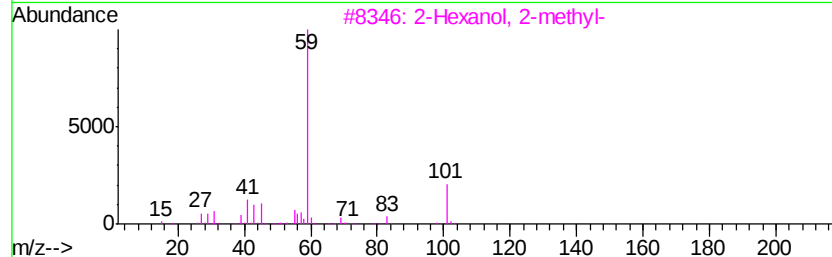
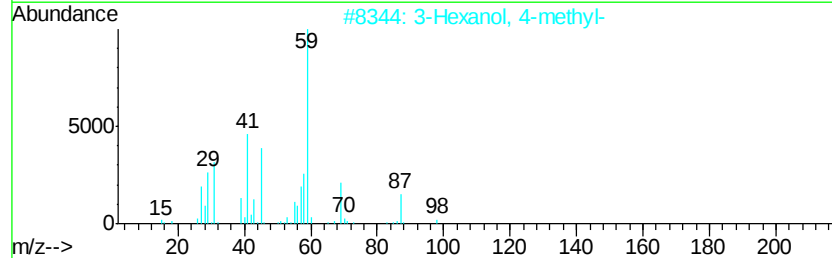
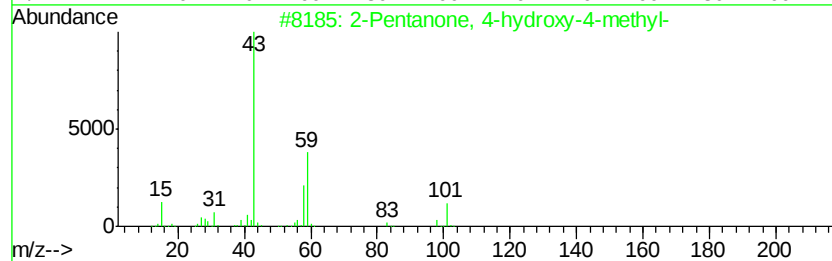
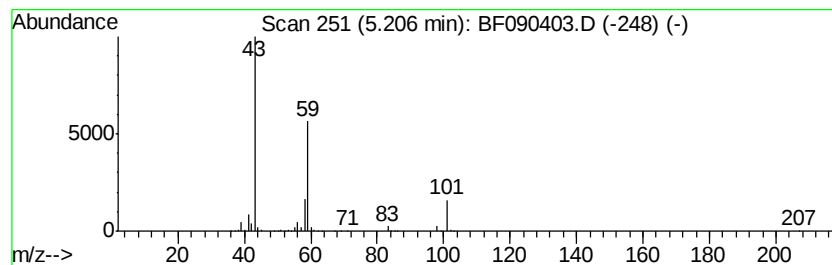
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	19.71 ng	1433780	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

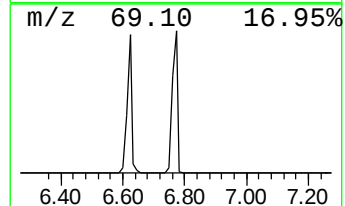
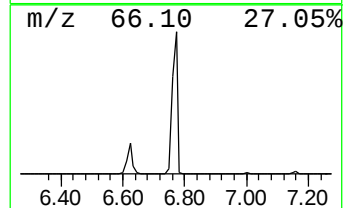
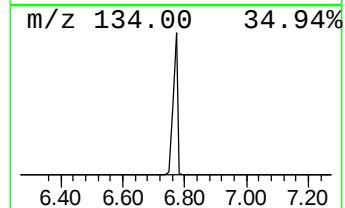
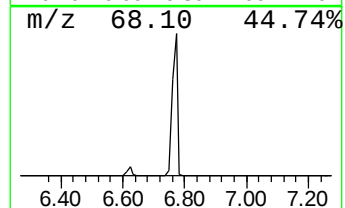
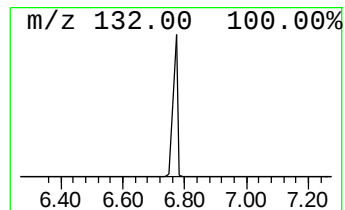
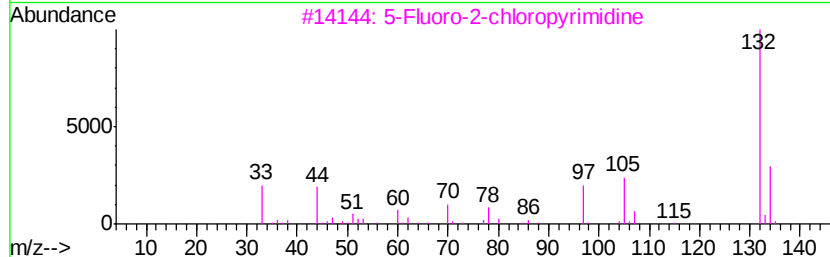
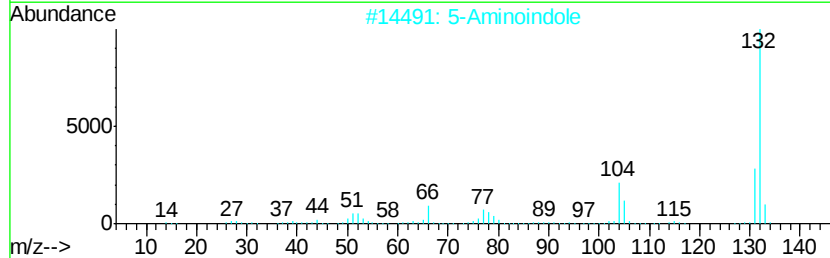
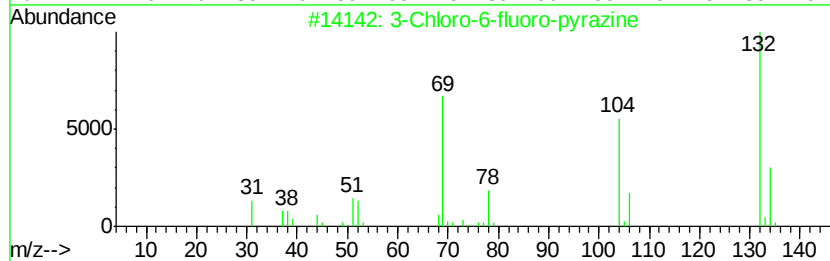
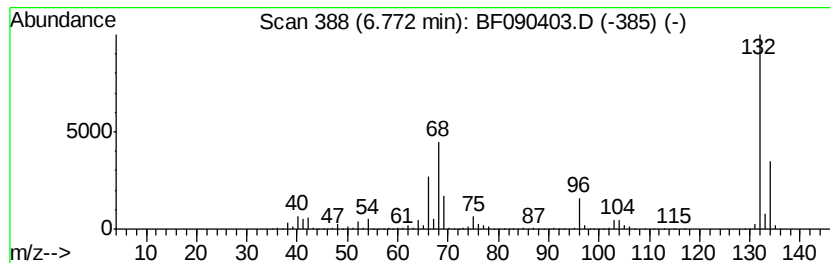
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	91.76 ng	6673230	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
4	2H-Cyclopenta[d]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine			132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

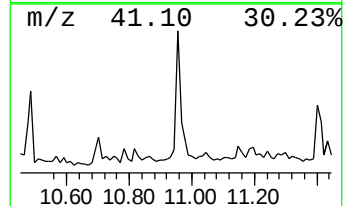
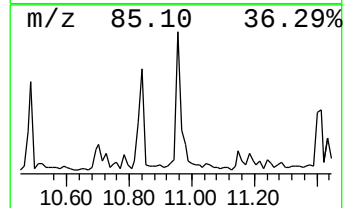
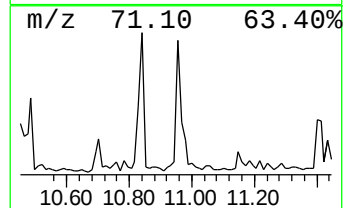
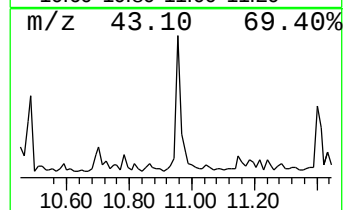
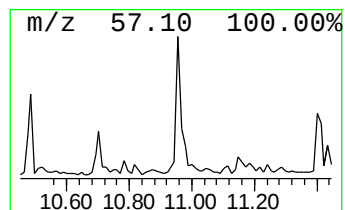
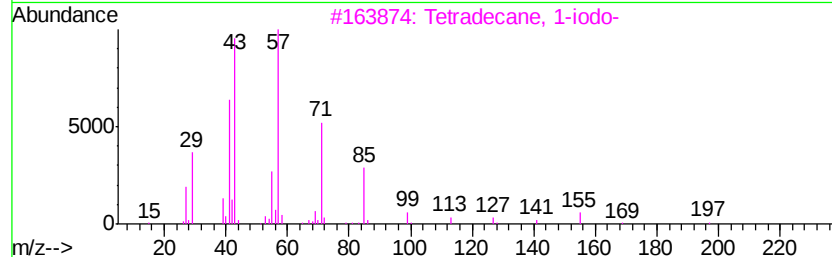
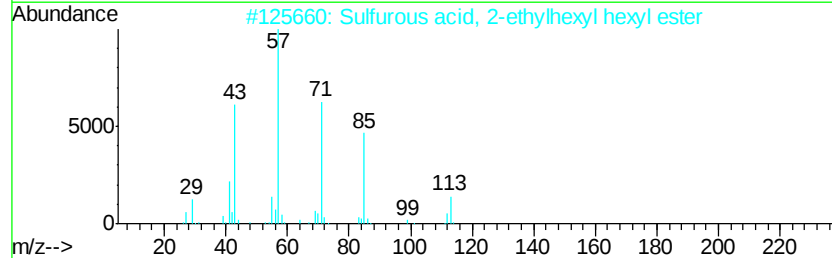
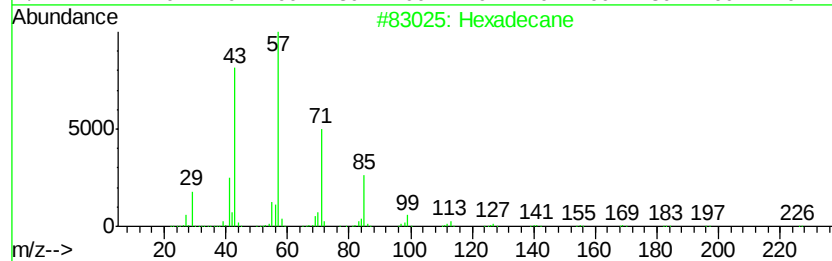
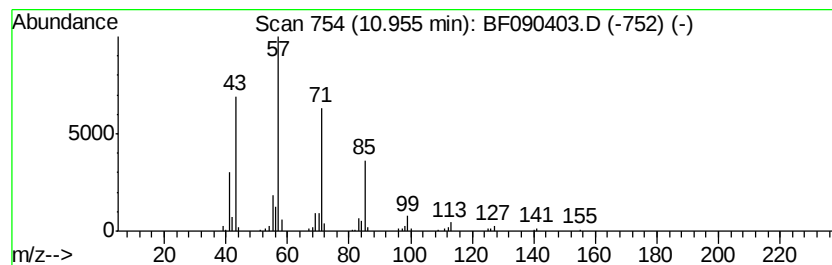
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.05 ng	207045	Phenanthrene-d10	11.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	90
3	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	80
4	Pentadecane		212	C15H32	000629-62-9	78
5	Octacosane		394	C28H58	000630-02-4	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

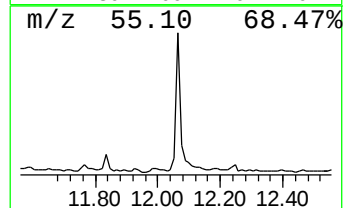
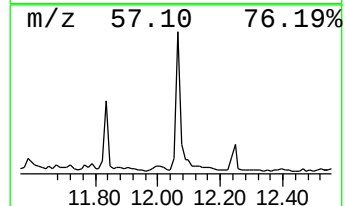
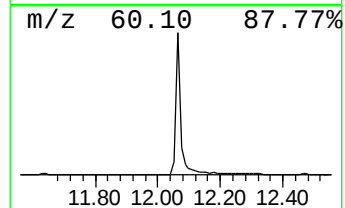
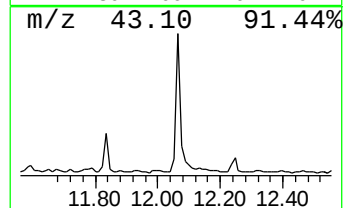
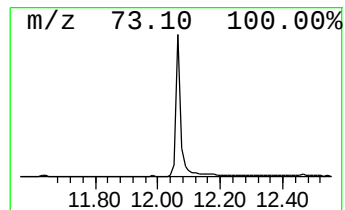
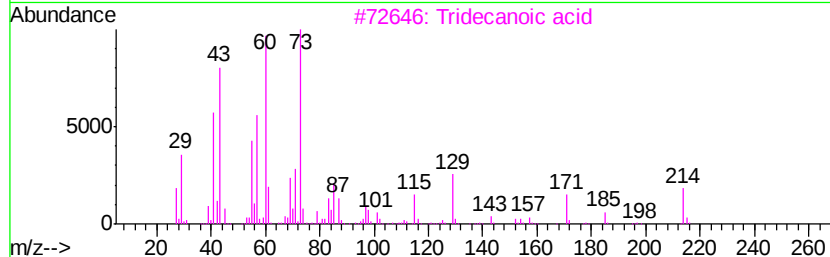
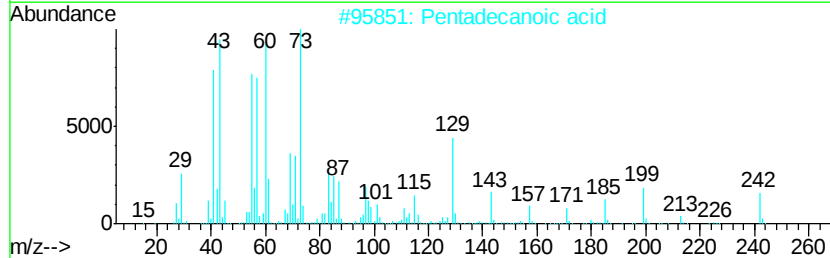
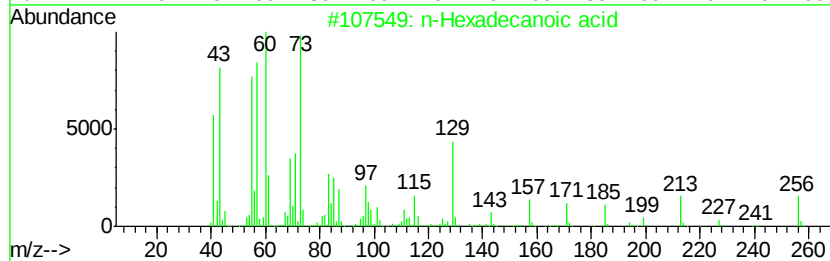
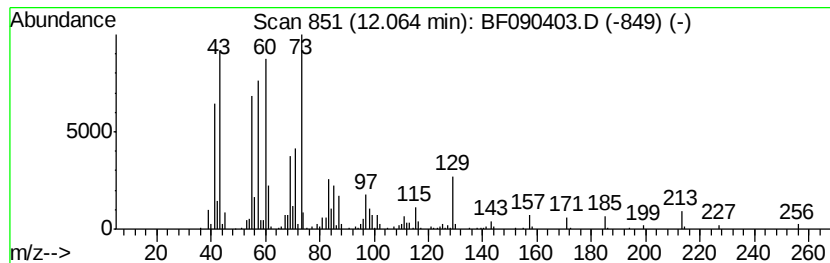
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	6.02 ng	607243	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

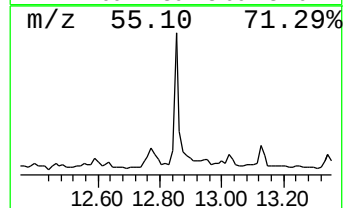
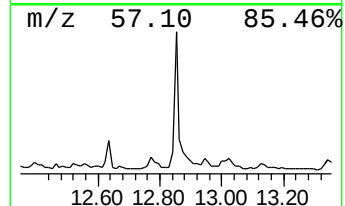
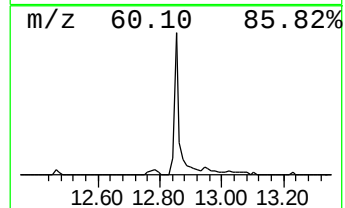
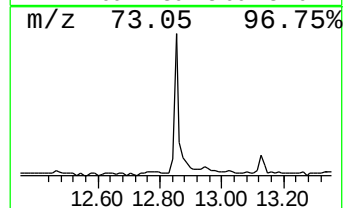
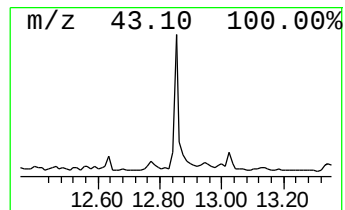
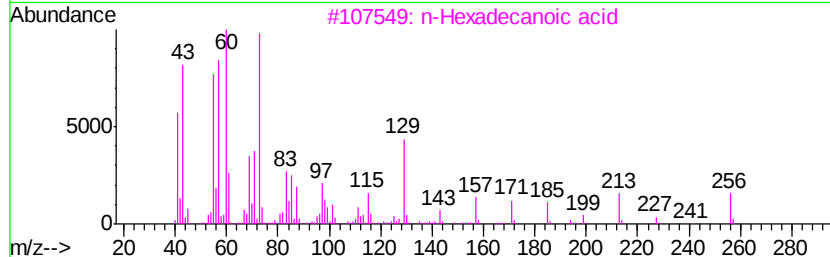
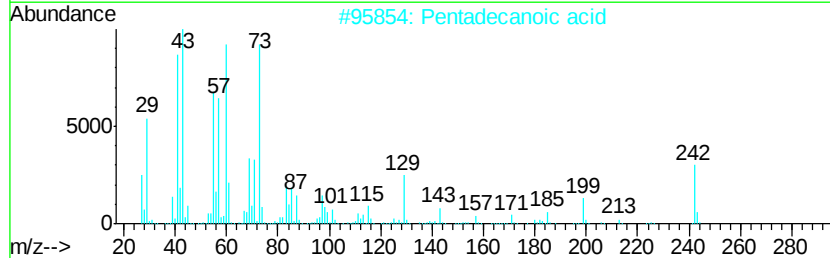
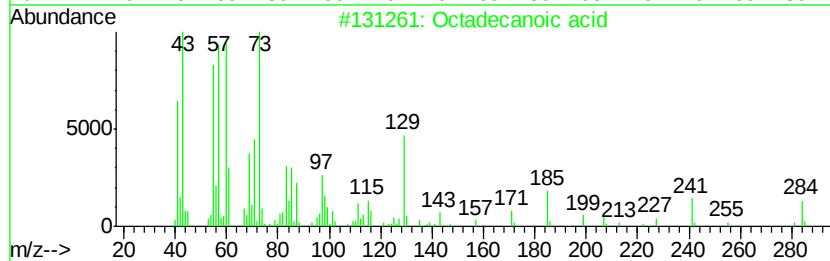
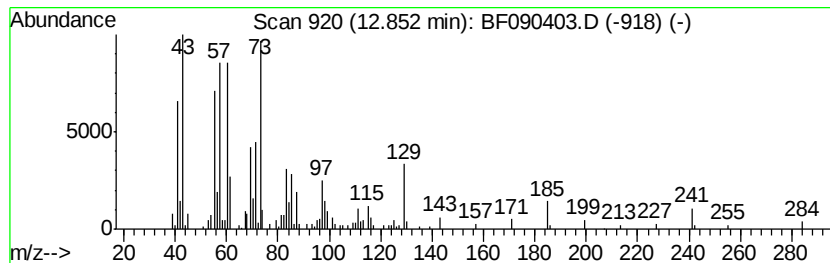
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.77 ng	279451	Phenanthrene-d10	11.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4		n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

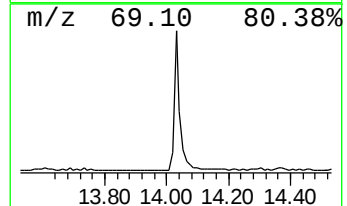
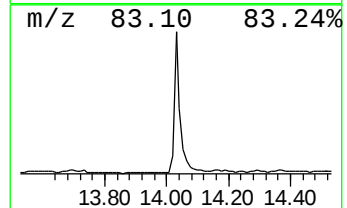
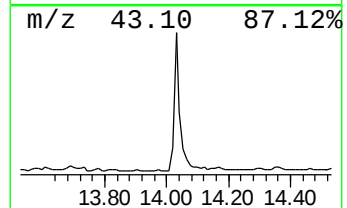
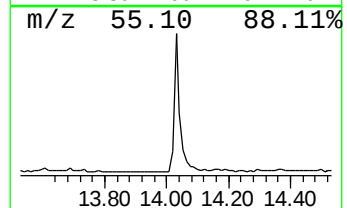
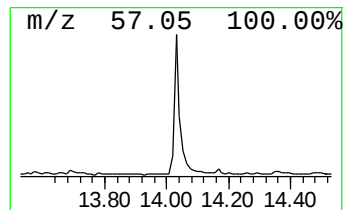
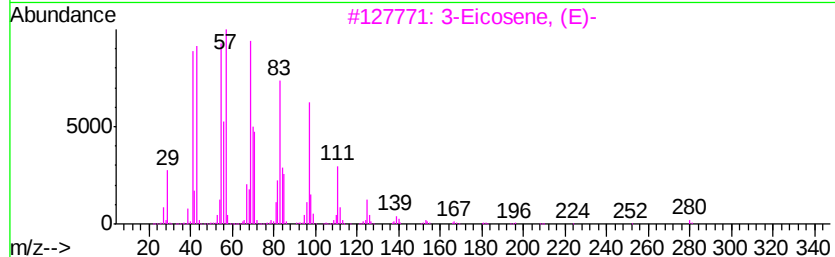
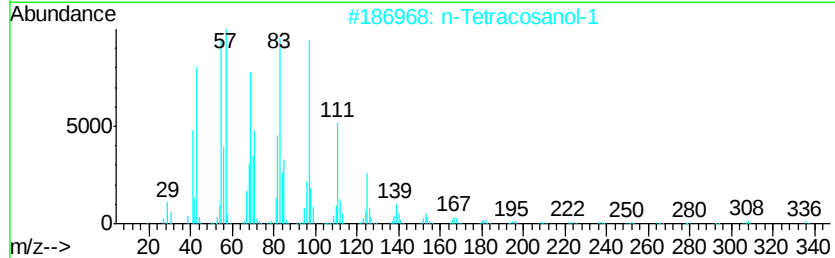
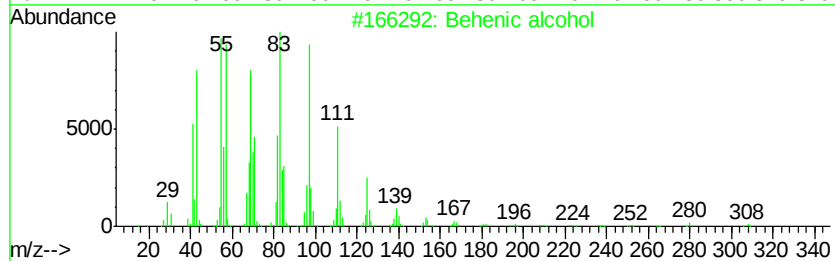
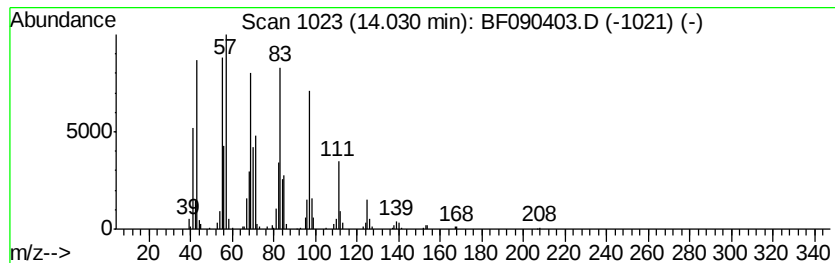
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	6.67 ng	554994	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090403.D
Acq On : 6 Oct 2016 2:02
Operator : UM/SJ
Sample : H5061-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-30-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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...	5.21	19.7	ng	1433780	1	7.00	1454520	20.0
unknown6.77	6.77	91.8	ng	6673230	1	7.00	1454520	20.0
Hexadecane	10.95	2.0	ng	207045	4	11.54	2018040	20.0
n-Hexadecanoic acid	12.06	6.0	ng	607243	4	11.54	2018040	20.0
Octadecanoic acid	12.85	2.8	ng	279451	4	11.54	2018040	20.0
Behenic alcohol	14.03	6.7	ng	554994	5	14.19	1662990	20.0