

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
 Data File : BF082501.D
 Acq On : 24 Oct 2015 9:09
 Operator : UM/IZ
 Sample : G4116-13
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BT-02(0-2)

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-BF101015.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	4.914	240	243	251	rBV	740792	1080487	54.08%	5.034%
2	5.360	279	282	284	rBV	1193832	1714346	85.81%	7.987%
3	5.748	314	316	319	rVB	23630	22895	1.15%	0.107%
4	6.411	371	374	376	rBV	1345267	1770275	88.61%	8.248%
5	6.526	382	384	386	rBV	2113519	1930682	96.64%	8.995%
6	6.754	401	404	406	rBV	695701	621949	31.13%	2.898%
7	6.903	415	417	420	rBV	1184991	1474958	73.83%	6.872%
8	7.326	451	454	457	rBV	1164224	1091428	54.63%	5.085%
9	8.046	514	517	519	rBV	779367	798330	39.96%	3.719%
10	9.120	609	611	614	rBV	1883374	1997841	100.00%	9.308%
11	9.520	644	646	649	rBV	440700	406933	20.37%	1.896%
12	9.795	668	670	673	rBV	627163	881406	44.12%	4.106%
13	10.229	707	708	710	rVB	46540	33989	1.70%	0.158%
14	10.595	737	740	742	rBV	1152588	1125750	56.35%	5.245%
15	10.709	748	750	754	rVB	37110	61927	3.10%	0.289%
16	11.155	786	789	790	rBV	35881	36993	1.85%	0.172%
17	11.292	798	801	802	rBV	672812	798847	39.99%	3.722%
18	11.315	802	803	804	rVV	66546	53088	2.66%	0.247%
19	11.338	804	805	809	rVB3	15159	30242	1.51%	0.141%
20	11.555	820	824	825	rBV3	11893	22961	1.15%	0.107%
21	11.578	825	826	829	rVB2	33944	34741	1.74%	0.162%
22	11.783	842	844	846	rBV	73912	87230	4.37%	0.406%
23	11.818	846	847	850	rVV2	103011	140532	7.03%	0.655%
24	11.898	853	854	858	rVB	21669	30674	1.54%	0.143%
25	12.069	867	869	872	rVB	17682	22742	1.14%	0.106%
26	12.503	904	907	909	rBV	137444	143851	7.20%	0.670%
27	12.732	923	927	929	rBV	118684	136877	6.85%	0.638%
28	12.881	937	940	942	rBV	1587997	1548091	77.49%	7.213%
29	13.064	952	956	958	rBV	16939	32818	1.64%	0.153%
30	13.132	958	962	963	rVV3	16292	33163	1.66%	0.155%
31	13.166	963	965	969	rVB2	14742	32821	1.64%	0.153%
32	13.589	1000	1002	1004	rVB	24261	25052	1.25%	0.117%
33	13.726	1010	1014	1015	rBV2	14803	22134	1.11%	0.103%
34	13.829	1020	1023	1030	rBV3	56411	146391	7.33%	0.682%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.966	1030	1035	1042	rBV	735823	892229	44.66%	4.157%
36	14.481	1078	1080	1082	rBV3	27529	40241	2.01%	0.187%
37	14.527	1082	1084	1092	rBV8	45814	133419	6.68%	0.622%
38	14.812	1107	1109	1112	rBV3	17185	37484	1.88%	0.175%
39	14.892	1114	1116	1117	rVV	22679	26262	1.31%	0.122%
40	14.972	1120	1123	1125	rBV	88211	137509	6.88%	0.641%
41	15.075	1129	1132	1136	rBV	69369	154792	7.75%	0.721%
42	15.155	1136	1139	1140	rVV	44091	56372	2.82%	0.263%
43	15.212	1141	1144	1152	rVB2	100256	274267	13.73%	1.278%
44	15.361	1155	1157	1159	rVB	37277	40124	2.01%	0.187%
45	15.418	1160	1162	1165	rVB	50941	61001	3.05%	0.284%
46	15.475	1165	1167	1170	rBV	427006	665843	33.33%	3.102%
47	15.704	1185	1187	1189	rVB2	38479	50030	2.50%	0.233%
48	15.921	1203	1206	1210	rBV	100434	153385	7.68%	0.715%
49	16.664	1269	1271	1274	rBV4	20369	36439	1.82%	0.170%
50	16.892	1287	1291	1293	rBV	28687	88023	4.41%	0.410%
51	17.441	1336	1339	1344	rVB7	27524	75542	3.78%	0.352%
52	18.333	1414	1417	1426	rVB6	38766	148451	7.43%	0.692%

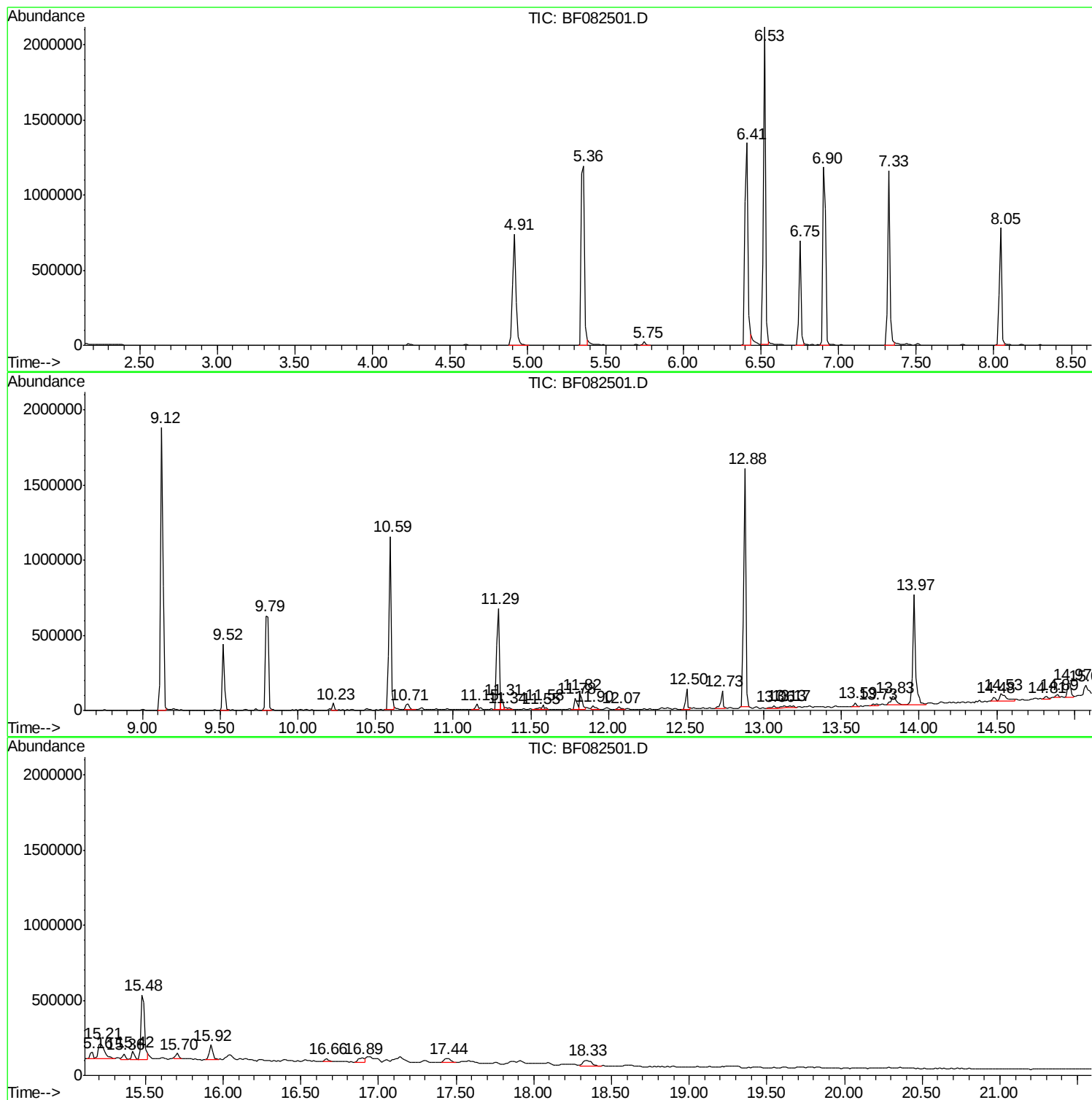
Sum of corrected areas: 21463857

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

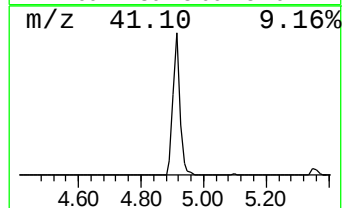
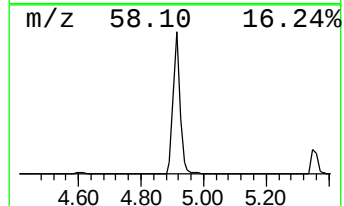
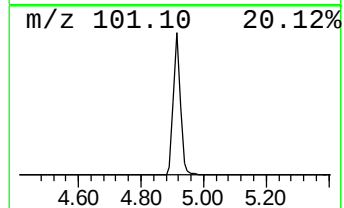
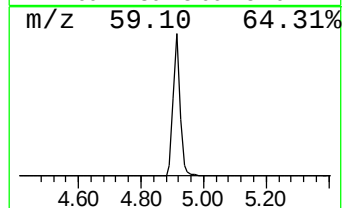
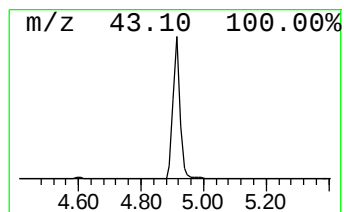
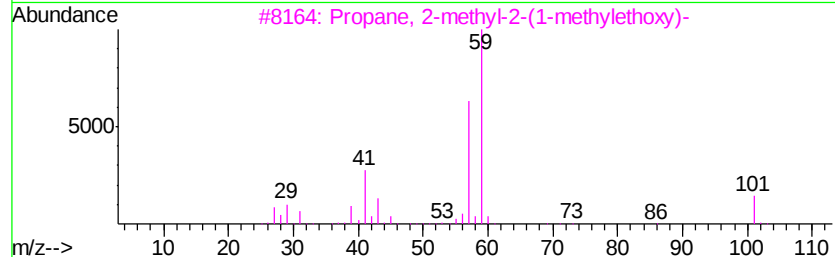
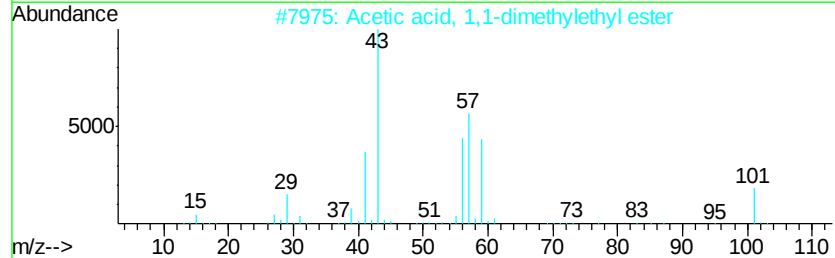
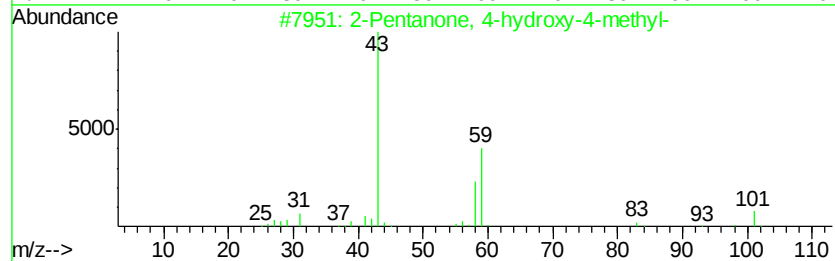
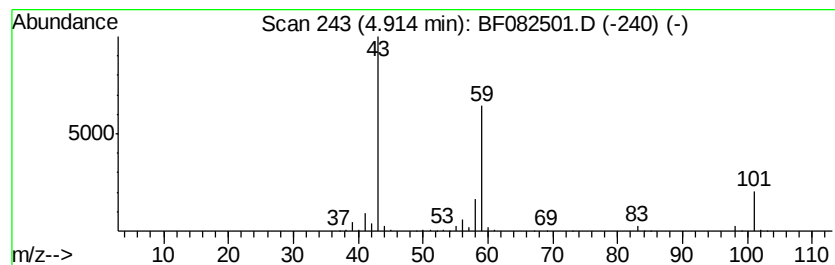
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	34.75 ng	1080490	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
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	36
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\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

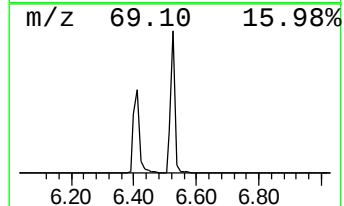
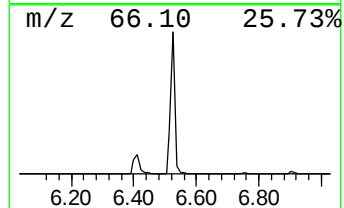
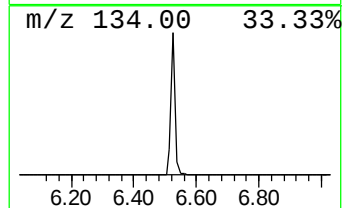
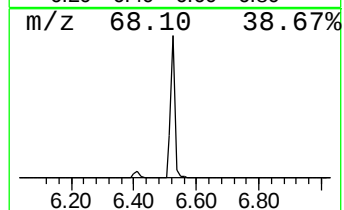
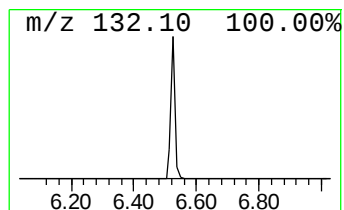
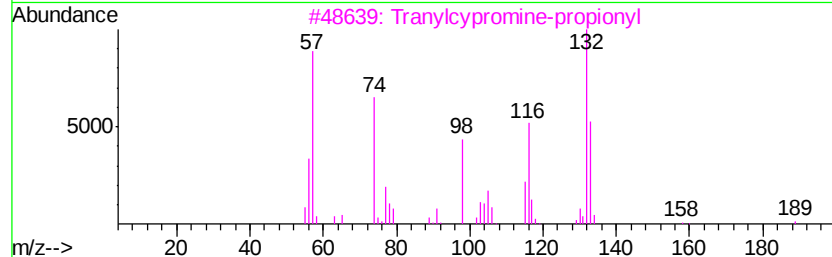
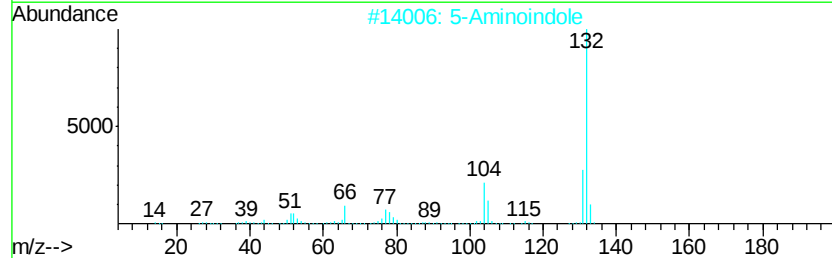
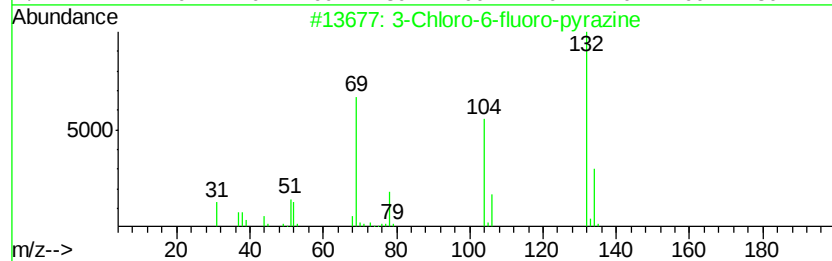
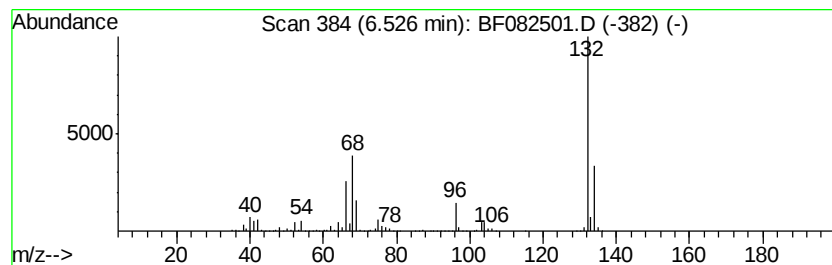
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	62.08 ng	1930680	1,4-Dichlorobenzene-d4	6.75

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

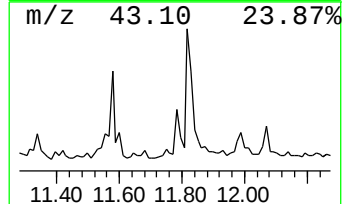
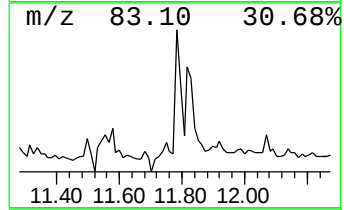
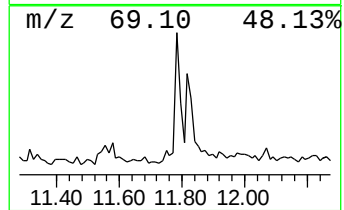
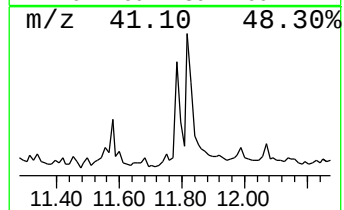
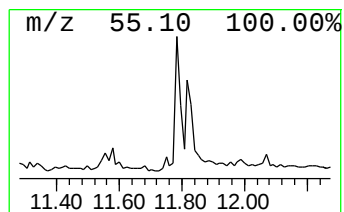
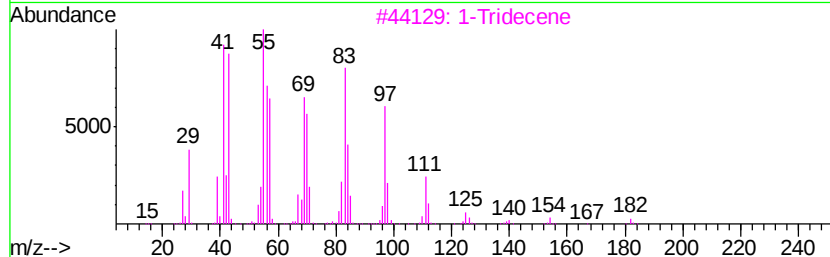
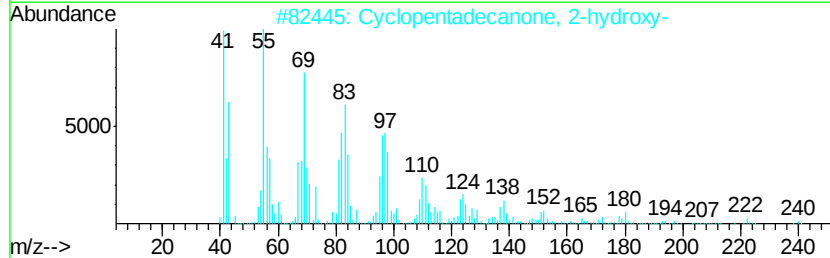
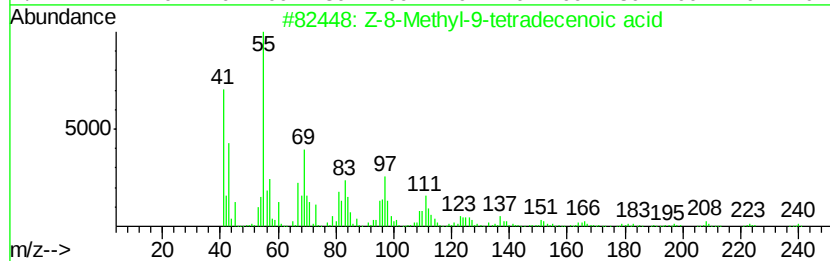
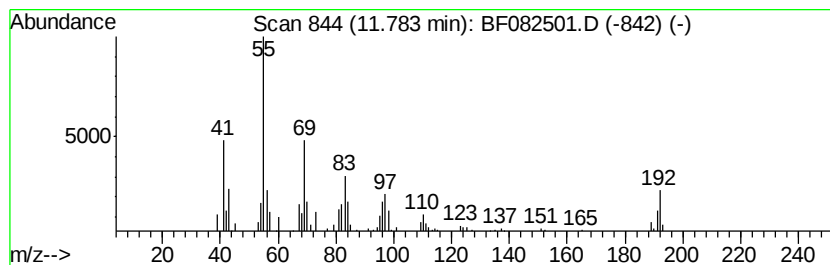
Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown11.78 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	2.18 ng	87230	Phenanthrene-d10		11.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	47
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	43
3	1-Tridecene	182	C13H26	002437-56-1	35
4	13-Tetradecenal	210	C14H26O	085896-31-7	27
5	1-Dodecanol	186	C12H26O	000112-53-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

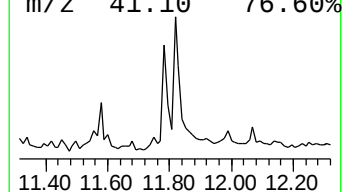
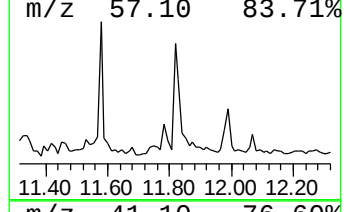
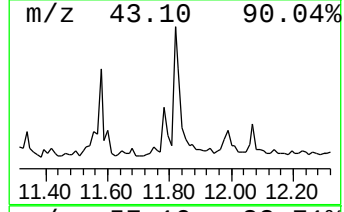
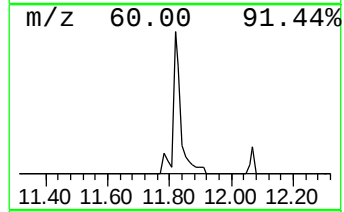
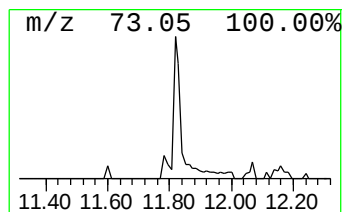
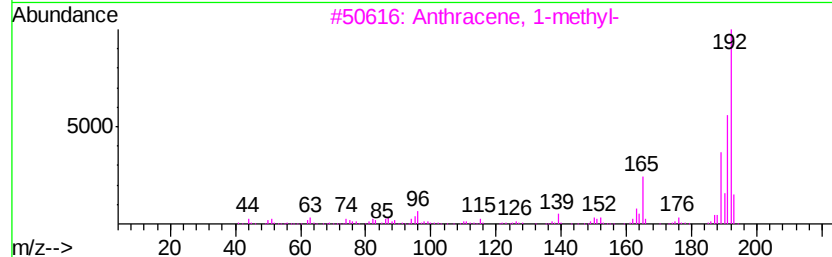
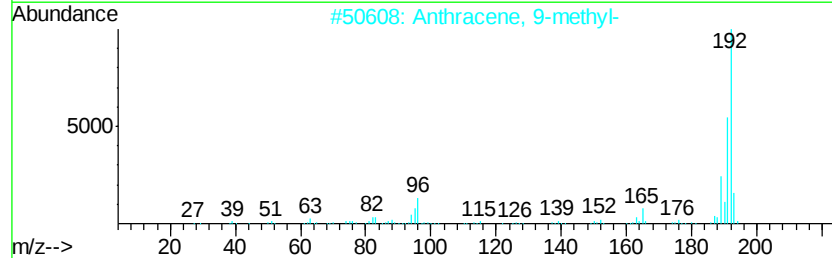
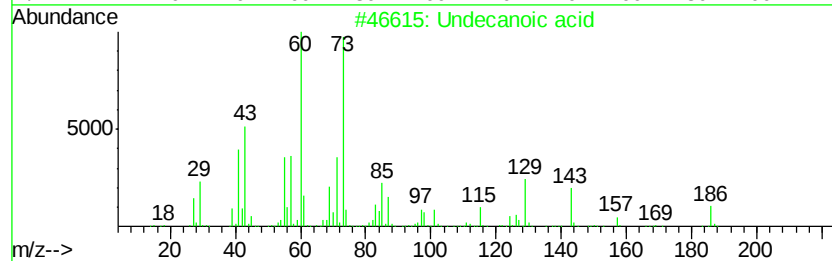
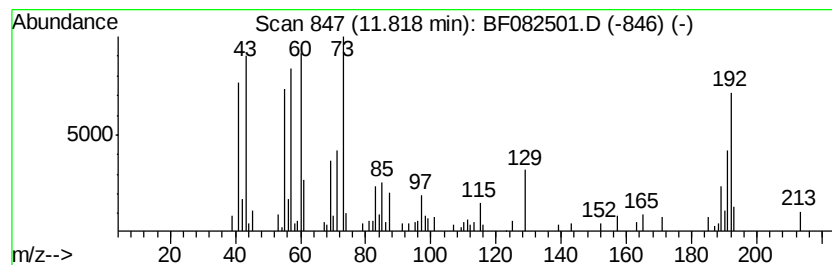
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	3.52 ng	140532	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	50
2	Anthracene, 9-methyl-		192	C15H12	000779-02-2	25
3	Anthracene, 1-methyl-		192	C15H12	000610-48-0	25
4	Anthracene, 2-methyl-		192	C15H12	000613-12-7	18
5	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

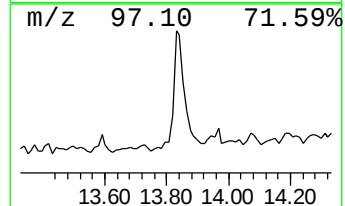
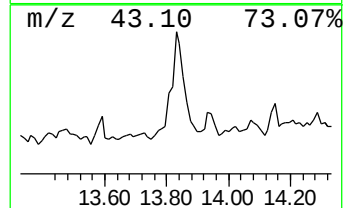
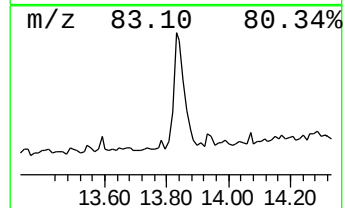
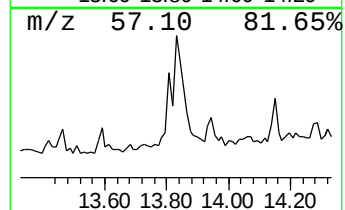
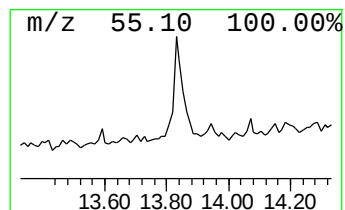
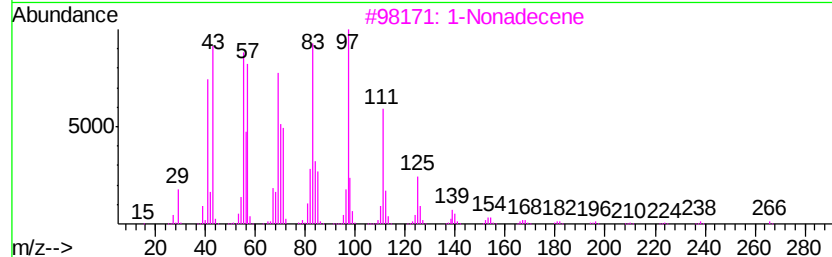
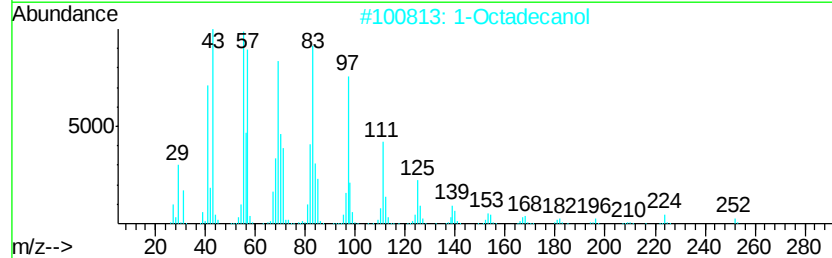
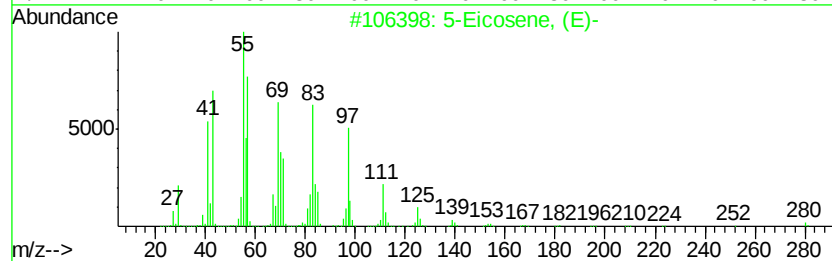
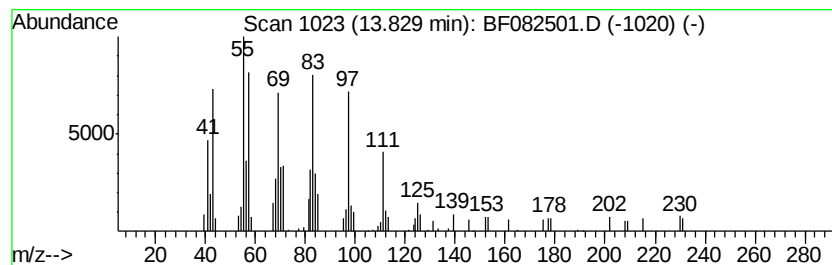
Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.83	3.28 ng	146391	Chrysene-d12		13.97		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-			280	C20H40	074685-30-6	87
2	1-Octadecanol			270	C18H38O	000112-92-5	87
3	1-Nonadecene			266	C19H38	018435-45-5	83
4	Trichloroacetic acid, tetradecyl...			358	C16H29Cl3O2	074339-52-9	81
5	1-Pentadecanol			228	C15H32O	000629-76-5	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

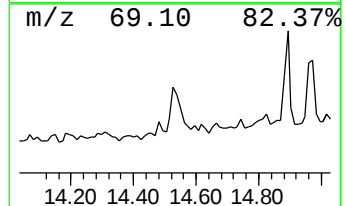
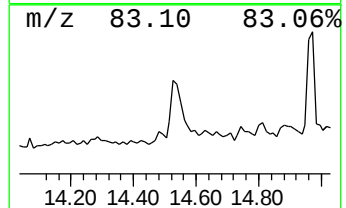
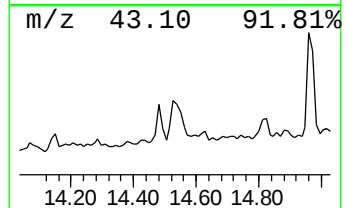
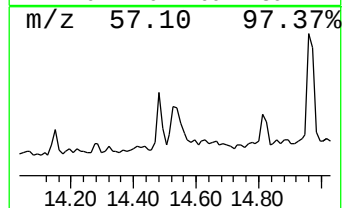
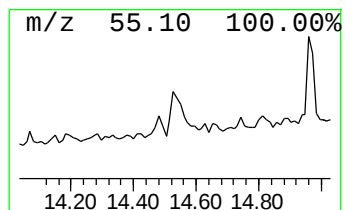
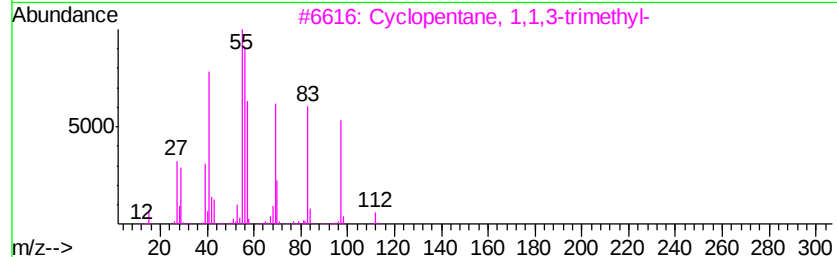
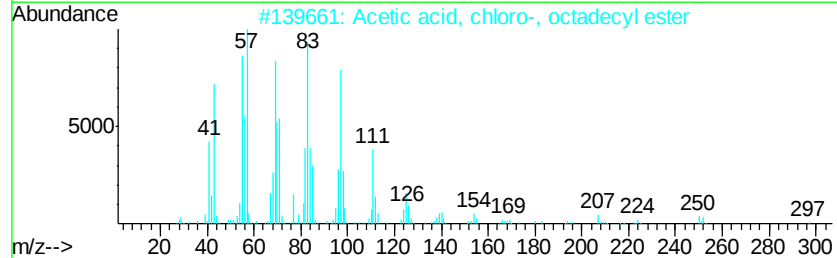
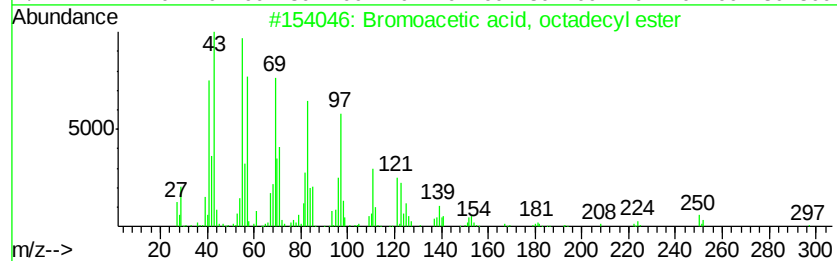
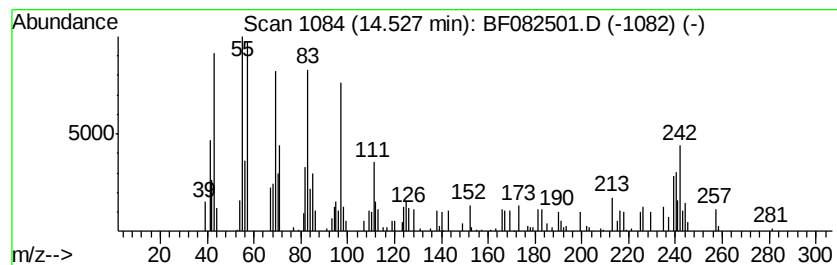
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.99 ng	133419	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	70
2		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	70
3		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52
4		17-Pentatriacontene	491	C35H70	006971-40-0	43
5		Diisoamylene	140	C10H20	054063-09-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

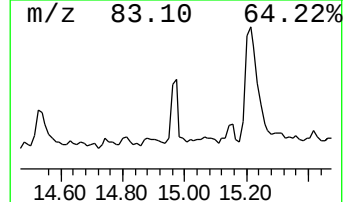
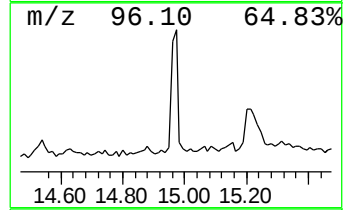
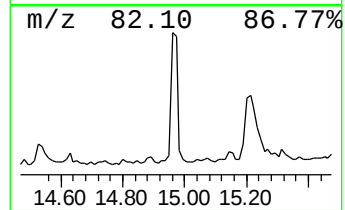
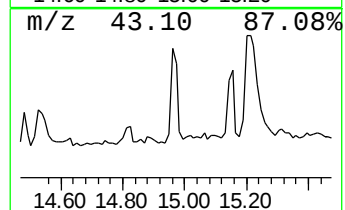
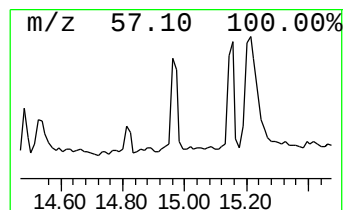
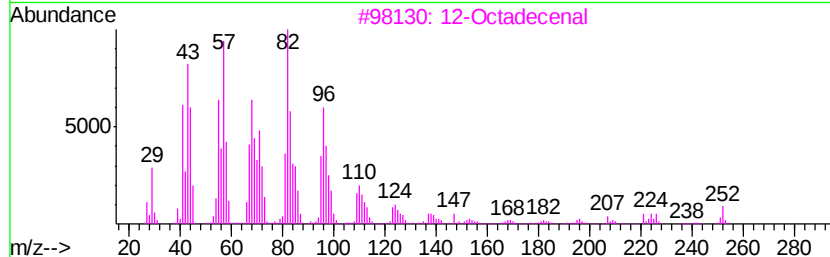
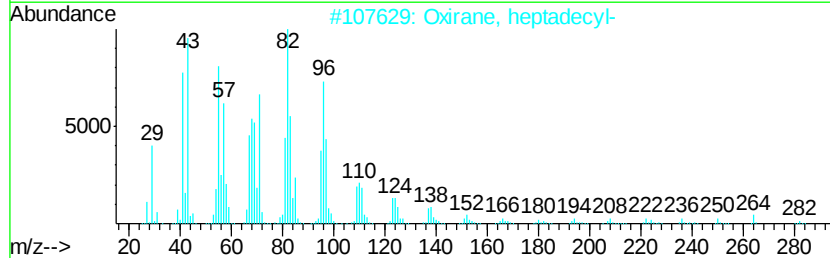
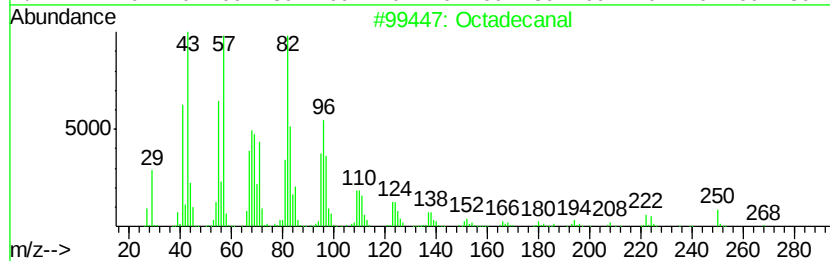
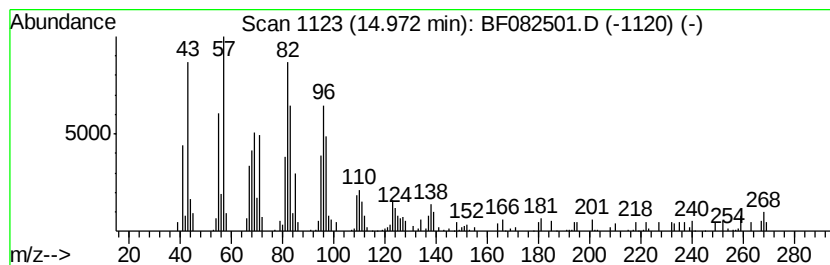
Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.97	4.13 ng	137509	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3	12-Octadecenal	266	C18H34O	056554-91-7	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5	2-Heptadecenal	252	C17H32O	1000143-48-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

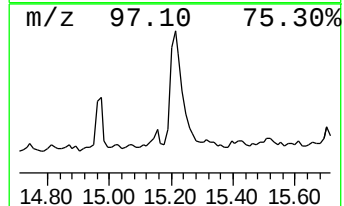
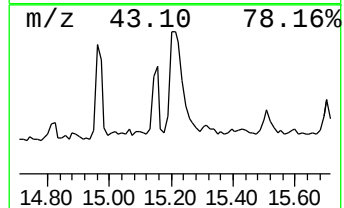
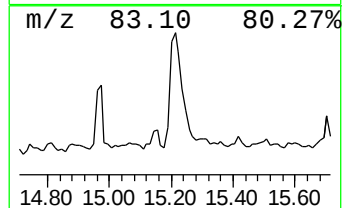
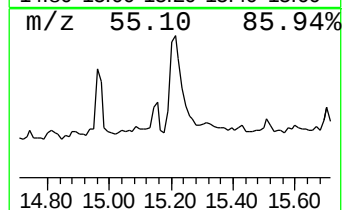
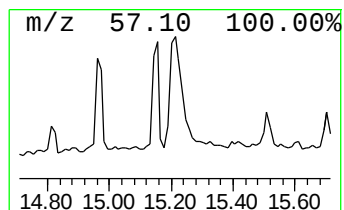
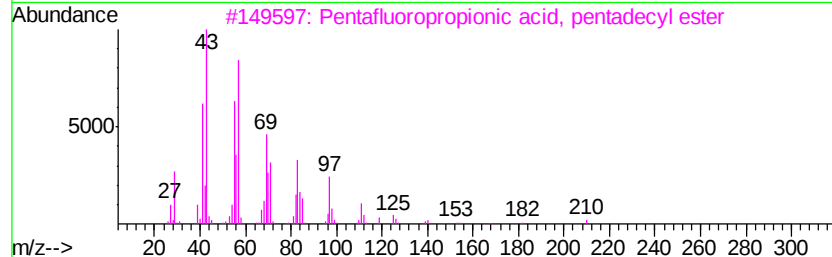
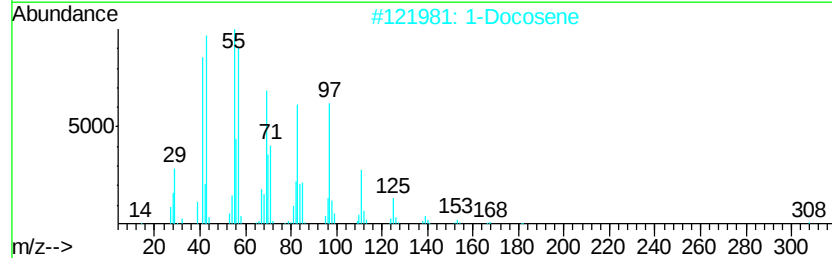
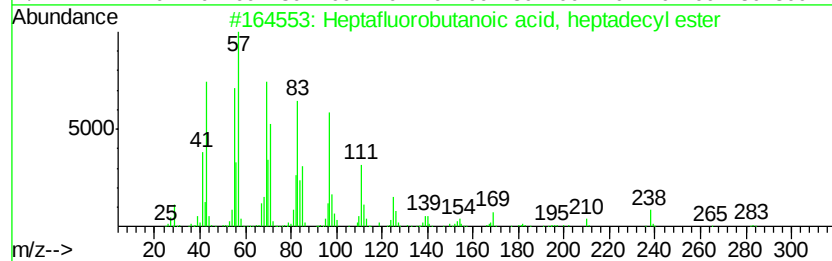
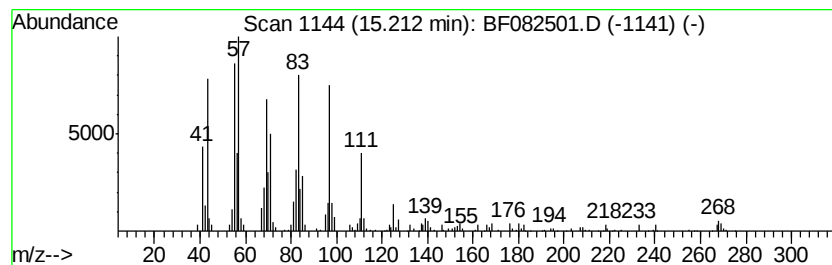
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	8.24 ng	274267	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2		1-Docosene	308	C22H44	001599-67-3	87
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	86
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	80
5		1-Heptadecene	238	C17H34	006765-39-5	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

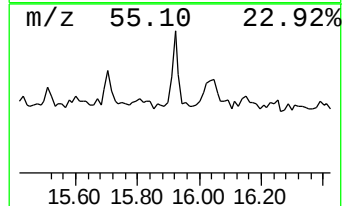
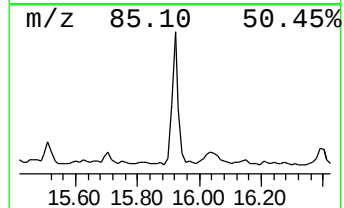
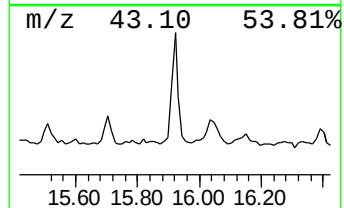
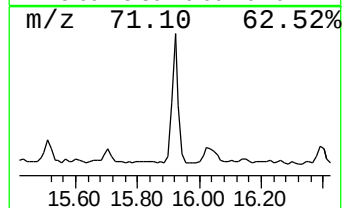
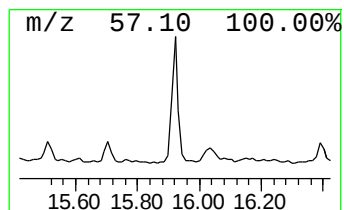
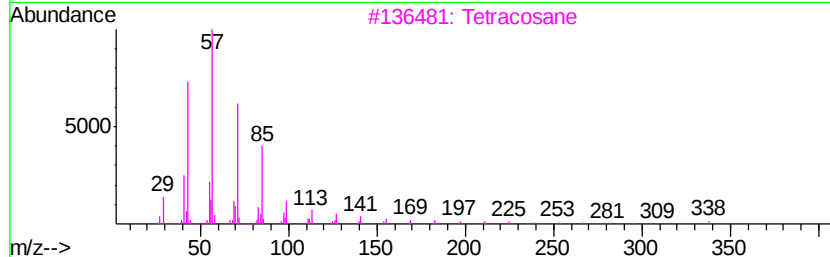
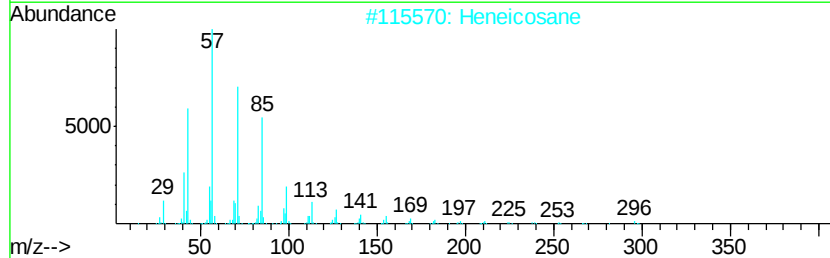
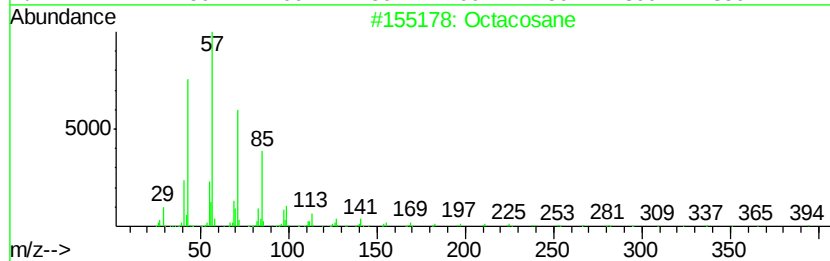
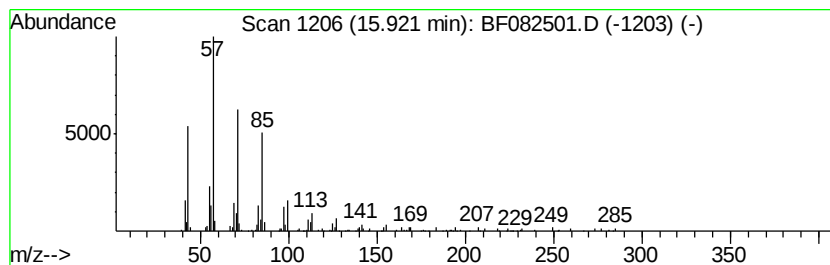
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	4.61 ng	153385	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tetracosane	338	C24H50	000646-31-1	87
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	87
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

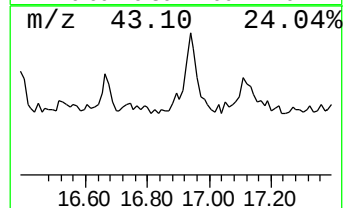
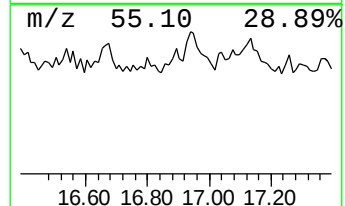
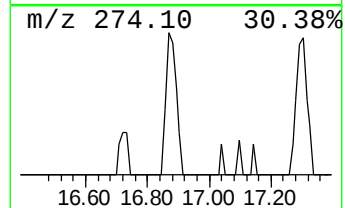
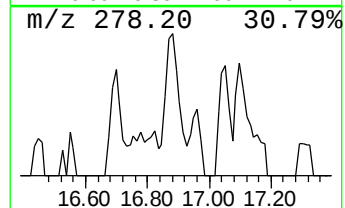
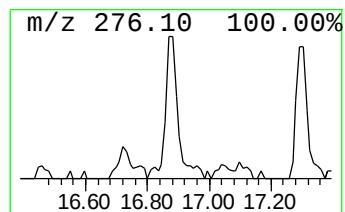
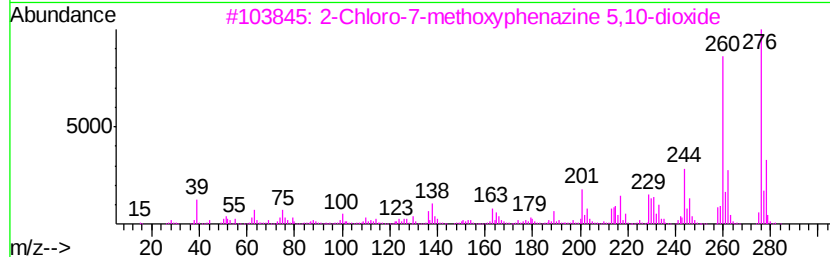
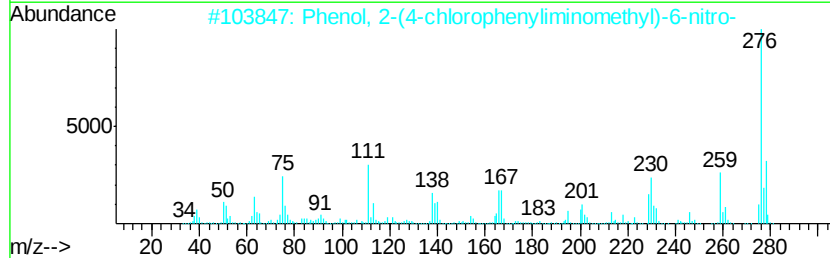
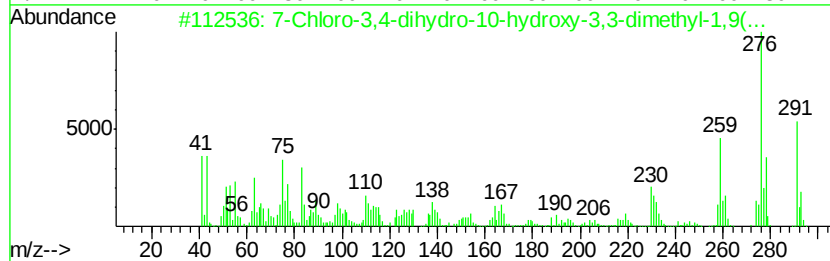
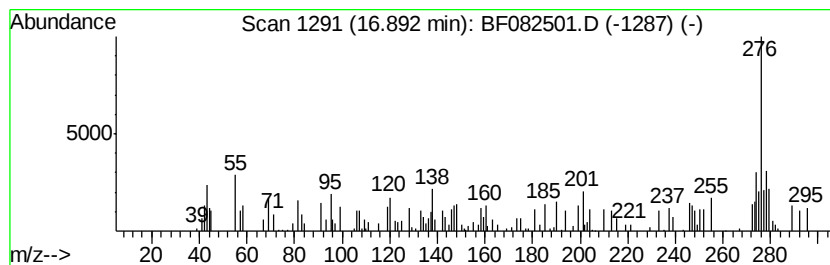
Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 7-Chloro-3,4-dihydro-10-hyd... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.89	2.64 ng	88023	Perylene-d12	15.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Chloro-3,4-dihydro-10-hydroxy-...	291	C15H14ClN03	055579-63-0	50	
2	Phenol, 2-(4-chlorophenyliminome...	276	C13H9ClN2O3	1000262-90-3	47	
3	2-Chloro-7-methoxyphenazine 5,10...	276	C13H9ClN2O3	023677-04-5	47	
4	1-Naphthalenecarboxylic acid, 2-...	276	C18H12O3	038119-11-8	46	
5	Indophenol	276	C18H16N2O	000132-31-0	46	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082501.D
Acq On : 24 Oct 2015 9:09
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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...	4.91	34.8	ng	1080490	1	6.75	621949	20.0
unknown6.53	6.53	62.1	ng	1930680	1	6.75	621949	20.0
unknown11.78	11.78	2.2	ng	87230	4	11.29	798847	20.0
Undecanoic acid	11.82	3.5	ng	140532	4	11.29	798847	20.0
5-Eicosene, (E)-	13.83	3.3	ng	146391	5	13.97	892229	20.0
Bromoacetic acid,...	14.53	3.0	ng	133419	5	13.97	892229	20.0
Octadecanal	14.97	4.1	ng	137509	6	15.49	665843	20.0
Heptafluorobutano...	15.21	8.2	ng	274267	6	15.49	665843	20.0
Octacosane	15.92	4.6	ng	153385	6	15.49	665843	20.0
7-Chloro-3,4-dihy...	16.89	2.6	ng	88023	6	15.49	665843	20.0