

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
 Data File : BF083754.D
 Acq On : 14 Dec 2015 3:14
 Operator : UM/IZ
 Sample : G4743-03
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WESTWALL-8

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-BF121315.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	2.224	10	12	16	rVB	44792	60315	1.67%	0.153%
2	5.116	262	265	270	rVB	771365	1100537	30.38%	2.790%
3	5.527	298	301	303	rBV	2563014	3272685	90.34%	8.298%
4	5.927	334	336	338	rBV	54409	49168	1.36%	0.125%
5	6.544	387	390	393	rVB	2423197	3175752	87.67%	8.052%
6	6.693	400	403	405	rBV	2629607	3622443	100.00%	9.185%
7	6.921	420	423	425	rBV	1675901	1637060	45.19%	4.151%
8	7.081	434	437	439	rVB	2398204	2890043	79.78%	7.328%
9	7.482	468	472	474	rBV	2117500	2460340	67.92%	6.238%
10	7.573	477	480	483	rVB	58586	85652	2.36%	0.217%
11	8.202	532	535	537	rBV	2235921	1961590	54.15%	4.974%
12	9.276	626	629	632	rVB	3441881	3418347	94.37%	8.667%
13	9.402	638	640	642	rVB	70260	74542	2.06%	0.189%
14	9.665	661	663	666	rBV	836370	819055	22.61%	2.077%
15	9.893	681	683	686	rBV	80905	62300	1.72%	0.158%
16	9.950	686	688	691	rVB	1615476	1923310	53.09%	4.877%
17	10.396	723	727	728	rVB	76702	105695	2.92%	0.268%
18	10.613	743	746	749	rBV	34732	48205	1.33%	0.122%
19	10.739	754	757	759	rBV	1956207	2033361	56.13%	5.156%
20	10.865	765	768	772	rBV	99984	127612	3.52%	0.324%
21	11.310	805	807	808	rBV	83981	65282	1.80%	0.166%
22	11.436	815	818	820	rBV	1632376	1713563	47.30%	4.345%
23	11.493	821	823	825	rBV3	25075	37991	1.05%	0.096%
24	11.665	835	838	840	rBV	267370	257592	7.11%	0.653%
25	11.733	842	844	847	rVB	45959	42871	1.18%	0.109%
26	11.962	862	864	866	rBV	59278	56484	1.56%	0.143%
27	11.996	866	867	869	rVB	51343	39099	1.08%	0.099%
28	12.133	876	879	882	rBV2	38624	73488	2.03%	0.186%
29	12.476	907	909	911	rBV	361011	314628	8.69%	0.798%
30	12.533	911	914	916	rVB2	47173	66627	1.84%	0.169%
31	12.636	921	923	925	rBV	47366	43605	1.20%	0.111%
32	12.842	939	941	944	rBV2	224985	230245	6.36%	0.584%
33	12.899	944	946	950	rVB2	94780	117785	3.25%	0.299%
34	13.014	954	956	959	rVB	2585450	2425963	66.97%	6.151%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.254	975	977	979	rVB	111672	97124	2.68%	0.246%
36	13.551	1001	1003	1005	rVV	152118	162105	4.48%	0.411%
37	13.596	1005	1007	1010	rVB	79918	93564	2.58%	0.237%
38	13.905	1032	1034	1040	rVB2	146656	249463	6.89%	0.633%
39	14.065	1045	1048	1050	rBV	1243947	1594917	44.03%	4.044%
40	14.236	1061	1063	1065	rBV	56315	63624	1.76%	0.161%
41	14.545	1088	1090	1091	rBV	57710	68550	1.89%	0.174%
42	14.842	1114	1116	1121	rVB	47394	54994	1.52%	0.139%
43	15.082	1134	1137	1143	rBV	28522	77547	2.14%	0.197%
44	15.174	1143	1145	1148	rVB2	35526	45724	1.26%	0.116%
45	15.368	1153	1162	1166	rVV4	90010	413498	11.41%	1.048%
46	15.505	1170	1174	1177	rVV	1209603	1692887	46.73%	4.292%
47	15.551	1177	1178	1187	rVB4	39879	101364	2.80%	0.257%
48	16.374	1246	1250	1253	rBV3	27636	78496	2.17%	0.199%
49	17.060	1306	1310	1314	rBV2	26189	75157	2.07%	0.191%
50	17.517	1347	1350	1355	rVB6	22169	49192	1.36%	0.125%
51	17.745	1367	1370	1376	rBV2	18703	42890	1.18%	0.109%
52	18.568	1436	1442	1448	rBV2	18047	64672	1.79%	0.164%

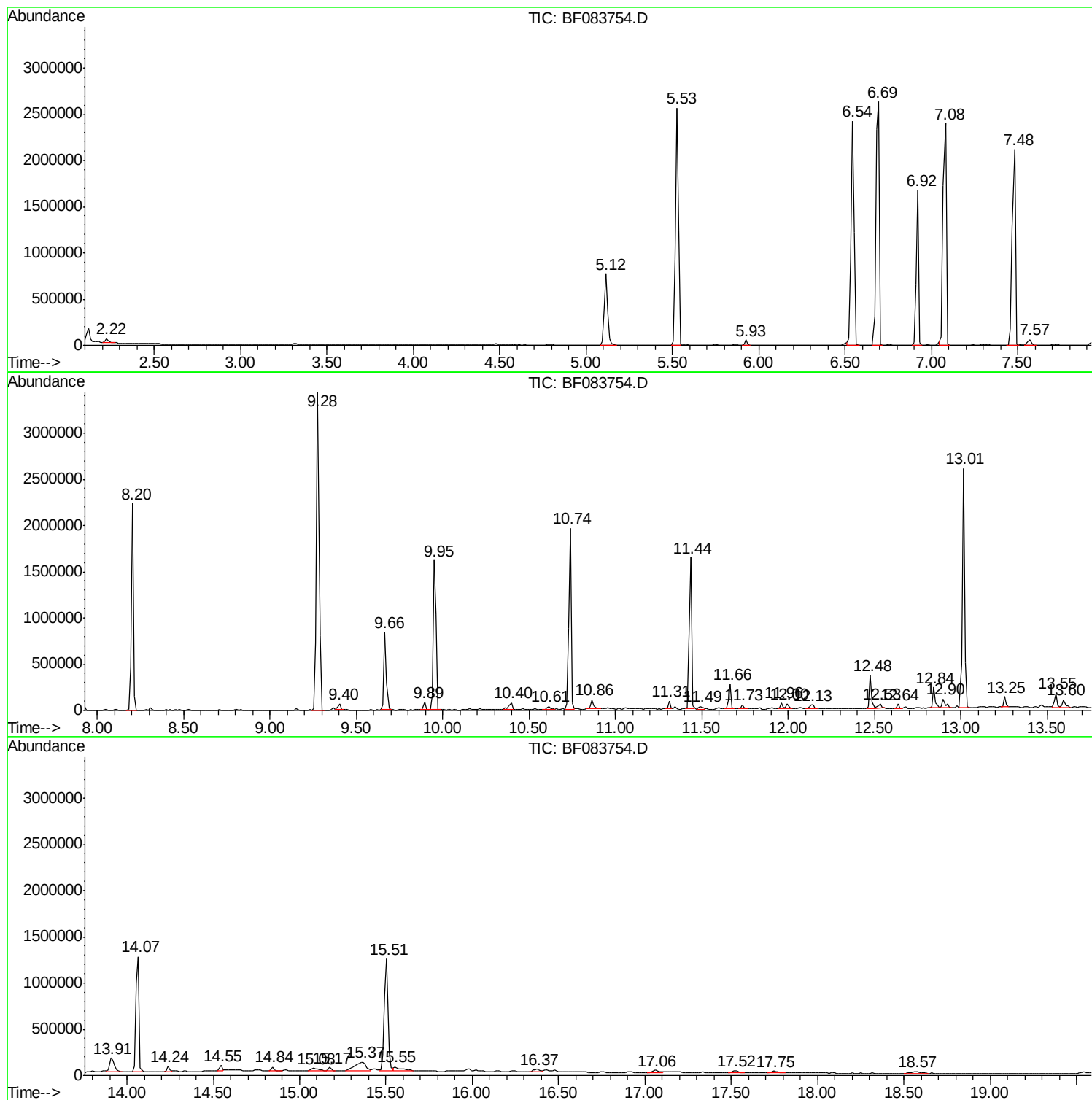
Sum of corrected areas: 39439003

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.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\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

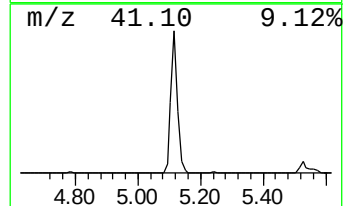
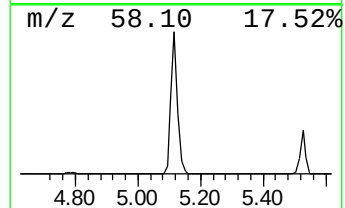
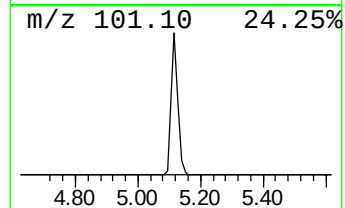
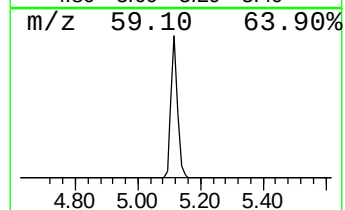
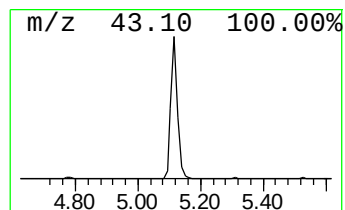
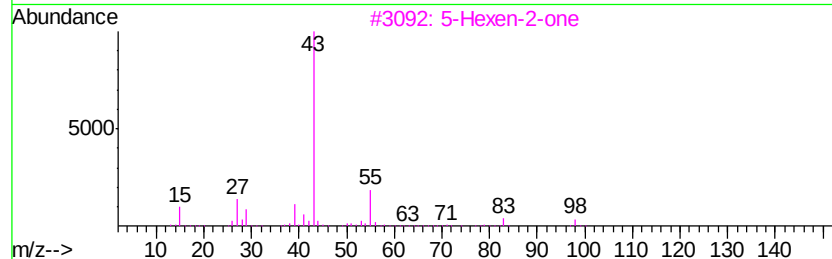
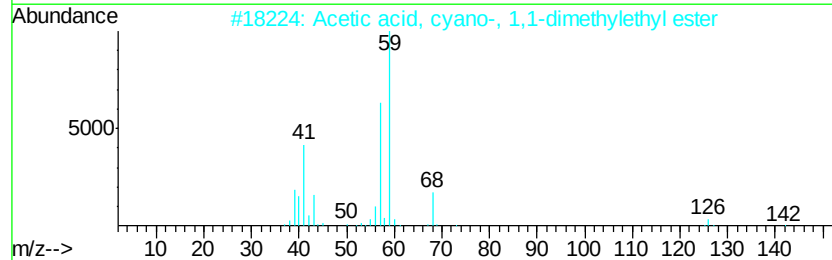
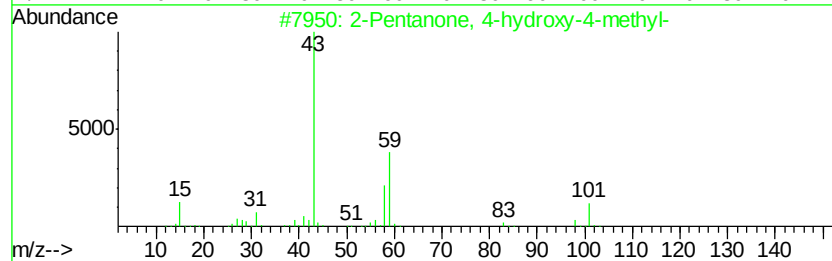
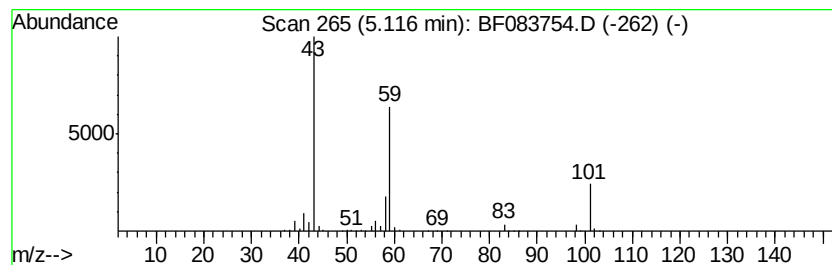
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	13.45 ng	1100540	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

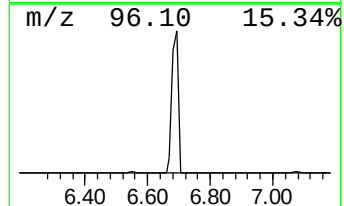
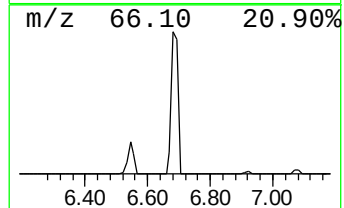
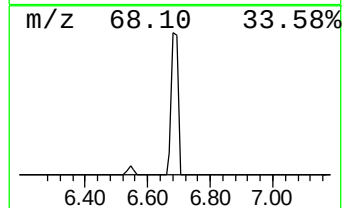
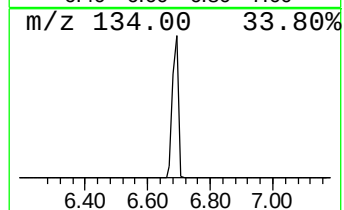
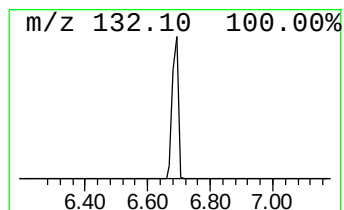
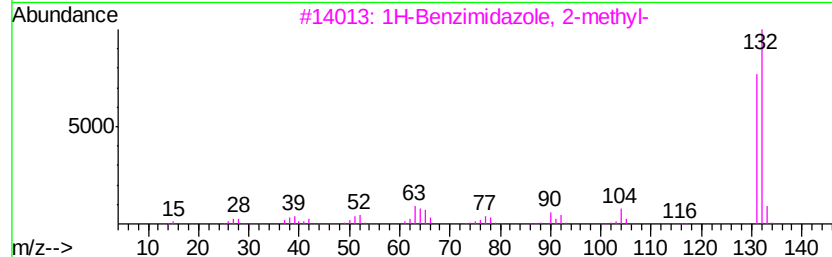
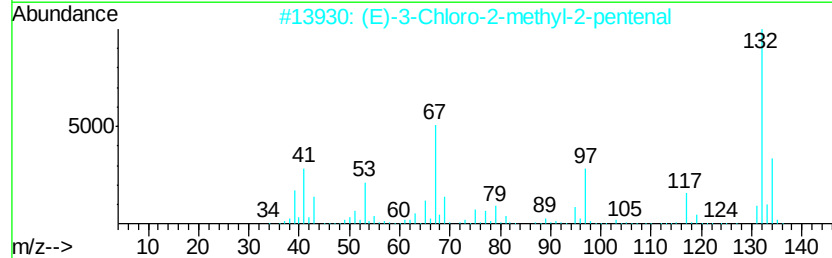
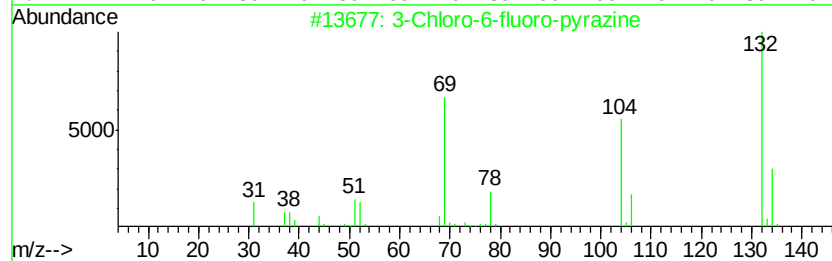
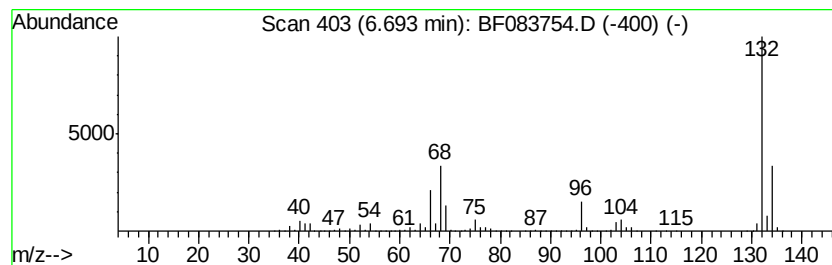
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	44.26 ng	3622440	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

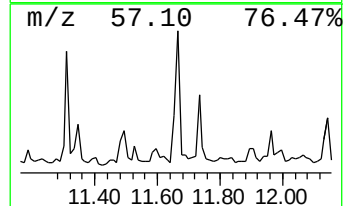
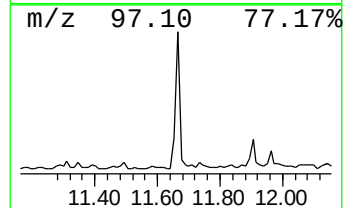
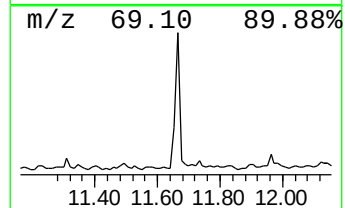
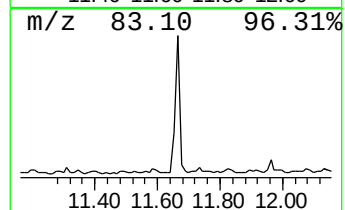
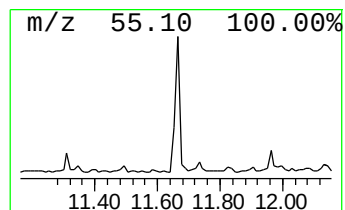
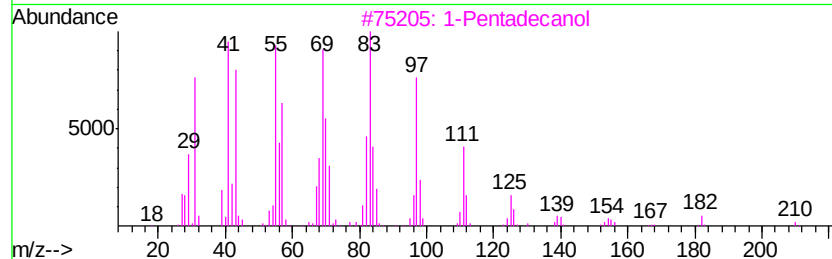
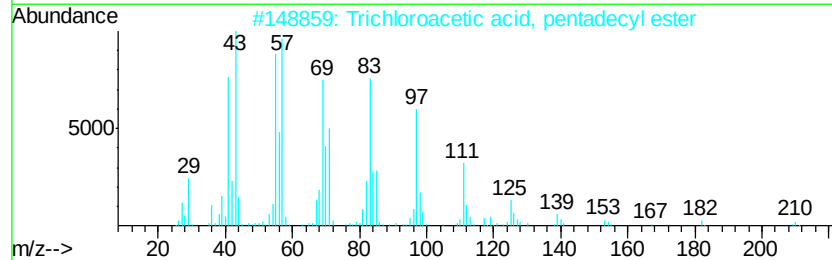
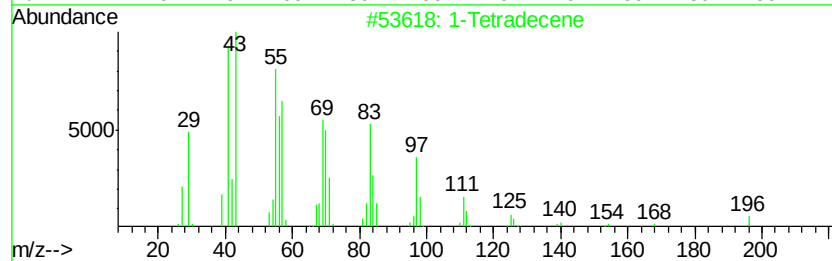
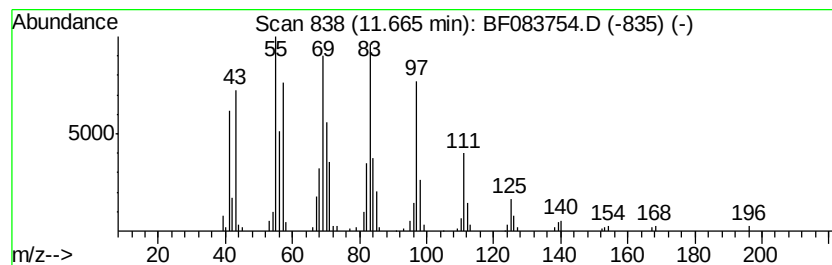
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Tetradecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.01 ng	257592	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetradecene	196	C14H28	001120-36-1	96
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		1-Pentadecanol	228	C15H32O	000629-76-5	91
4		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

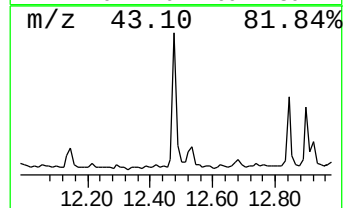
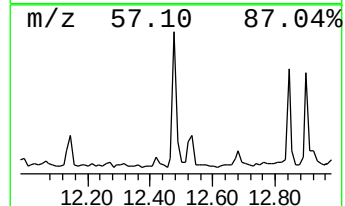
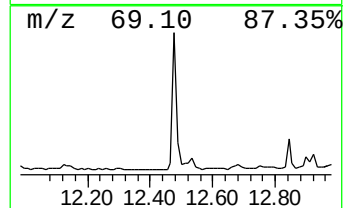
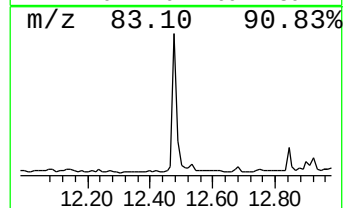
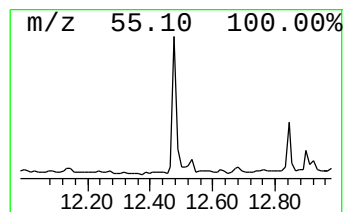
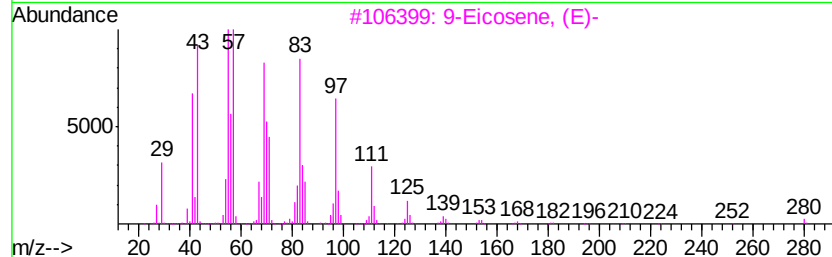
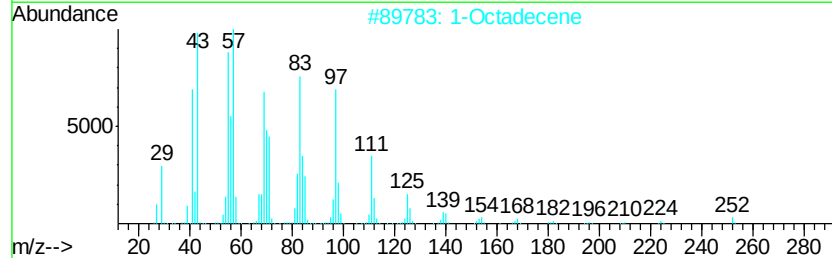
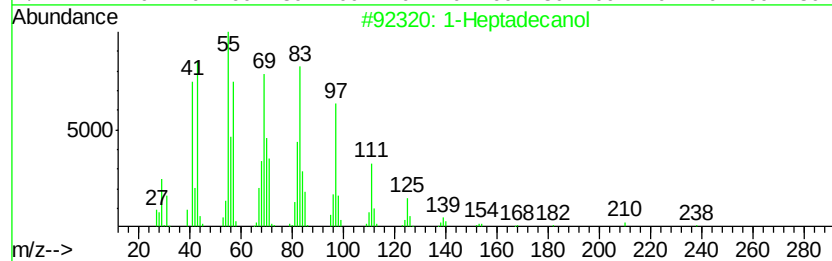
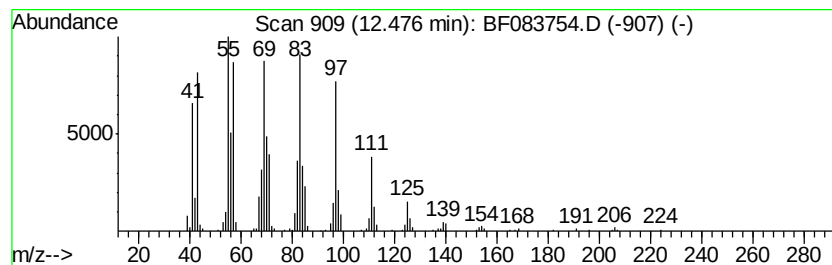
Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heptadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.48	3.67 ng	314628	Phenanthrene-d10		11.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecanol	256	C17H36O	001454-85-9	95
2	1-Octadecene	252	C18H36	000112-88-9	93
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

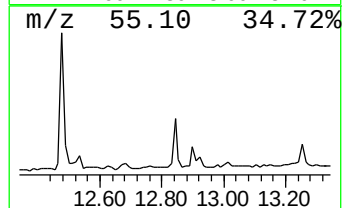
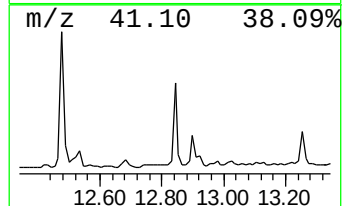
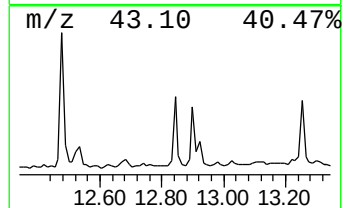
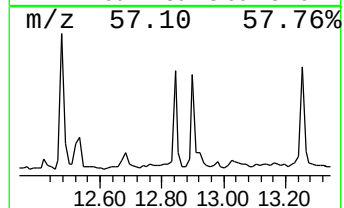
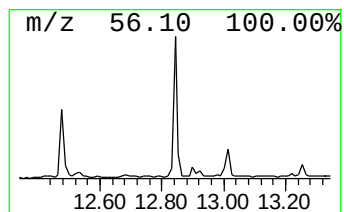
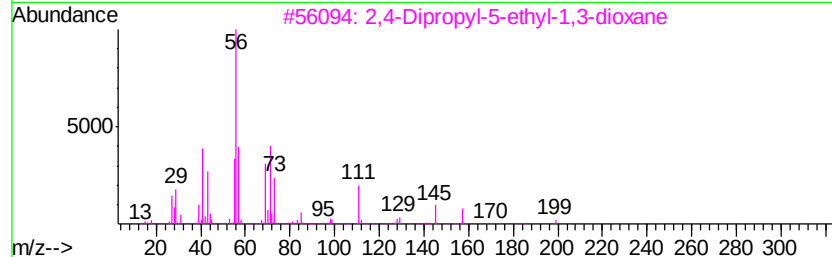
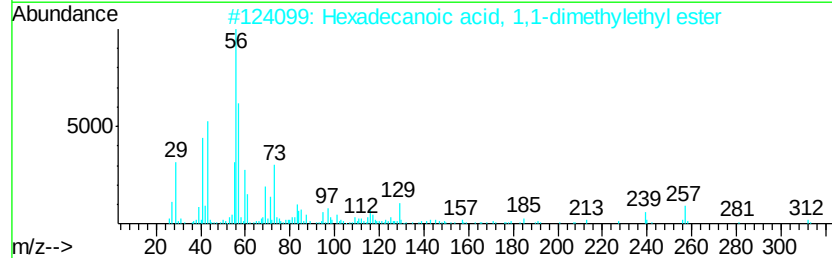
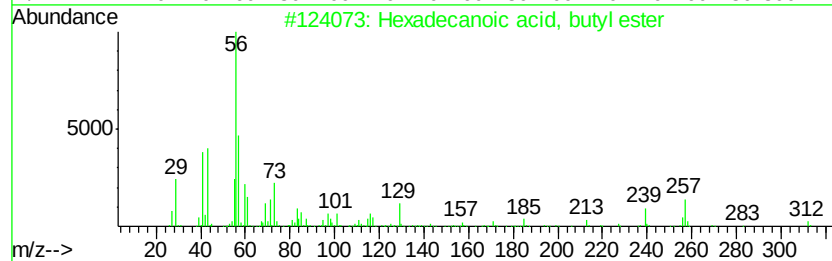
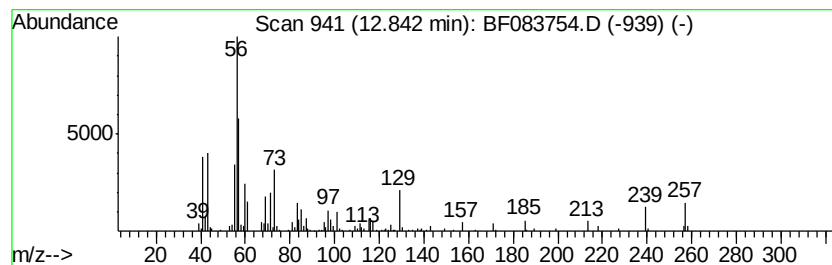
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.89 ng	230245	Chrysene-d12	14.07

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		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

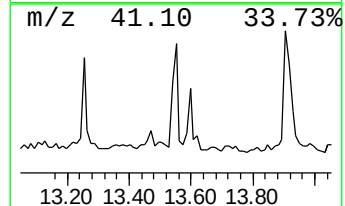
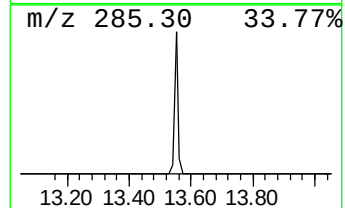
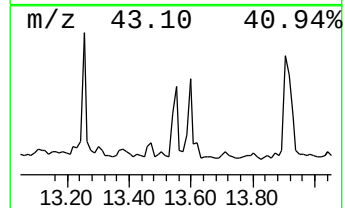
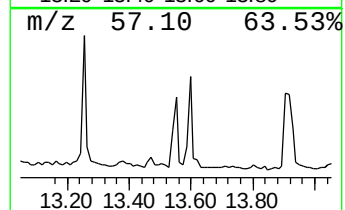
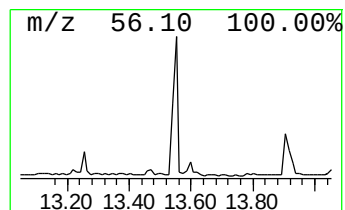
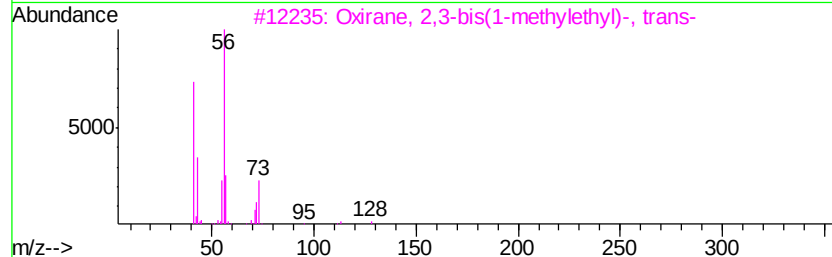
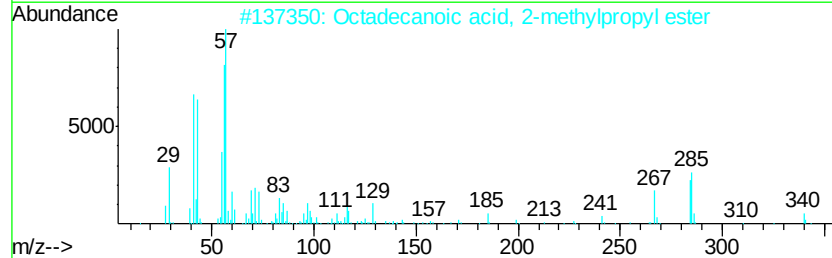
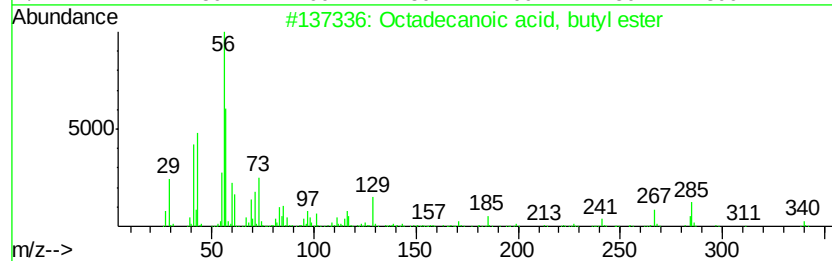
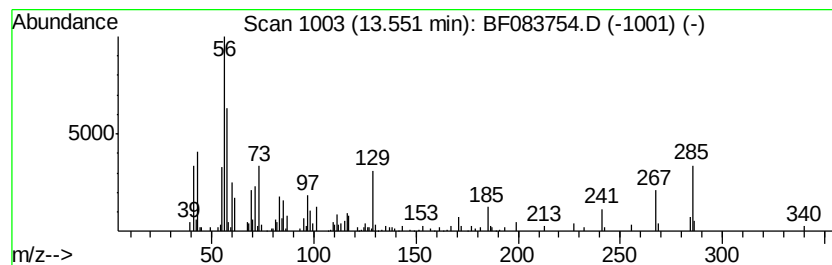
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.03 ng	162105	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	80
3		Oxirane, 2,3-bis(1-methylethyl)-, trans-	128	C8H16O	054644-32-5	35
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

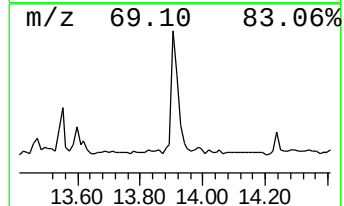
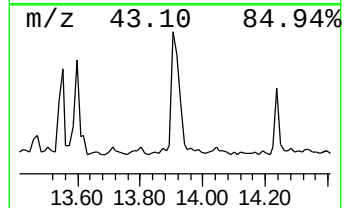
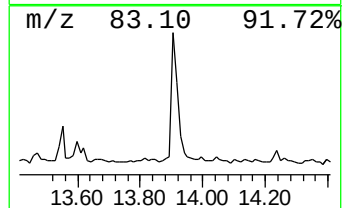
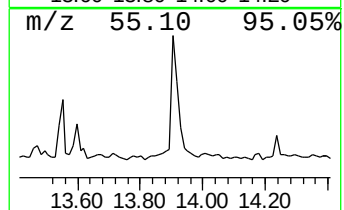
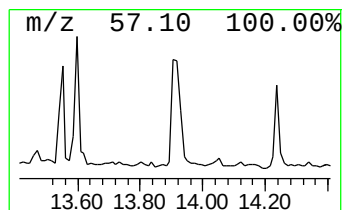
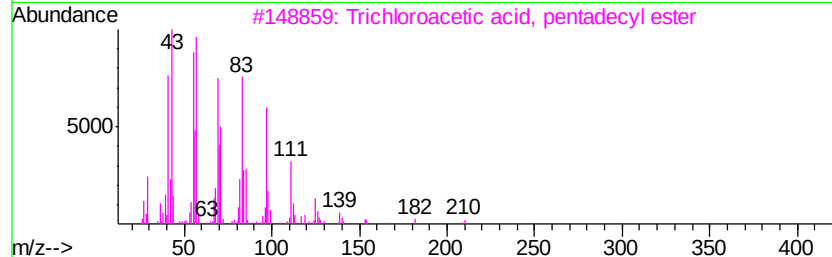
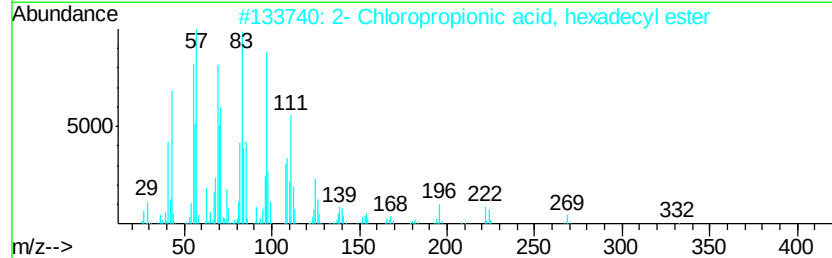
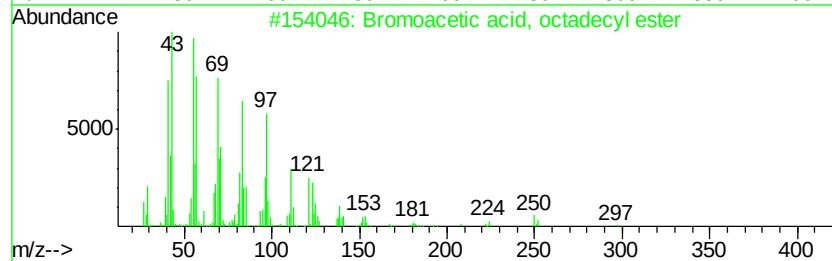
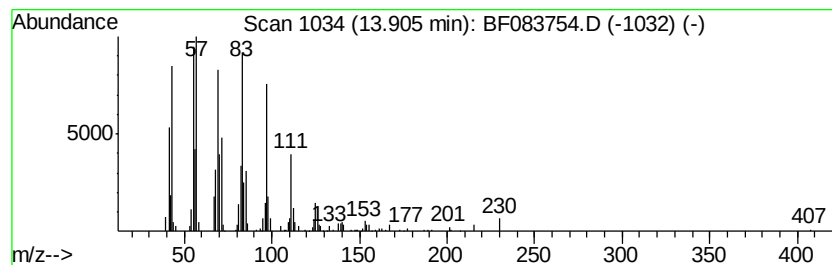
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.13 ng	249463	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

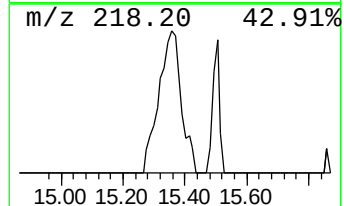
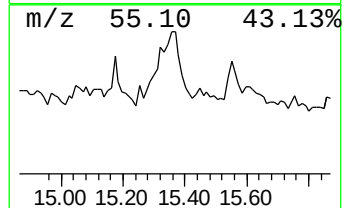
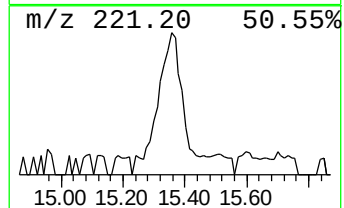
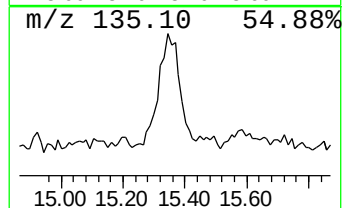
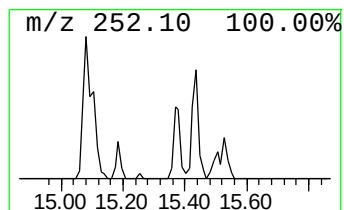
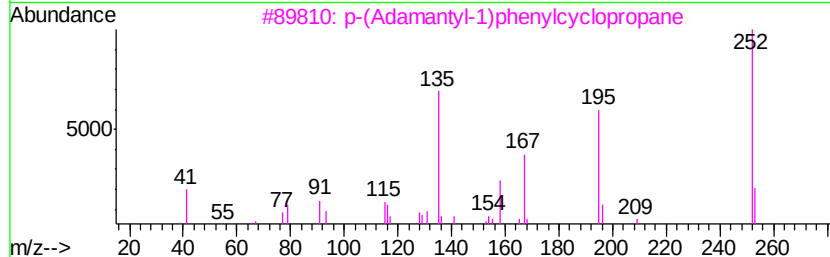
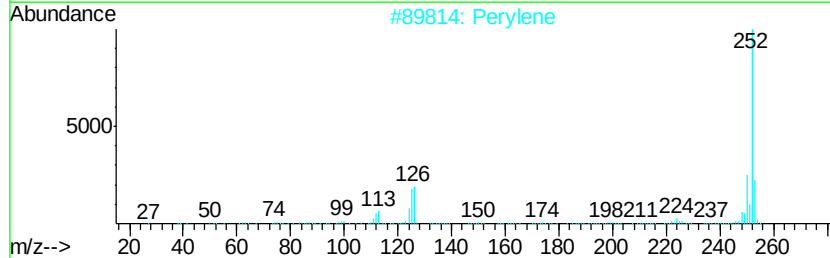
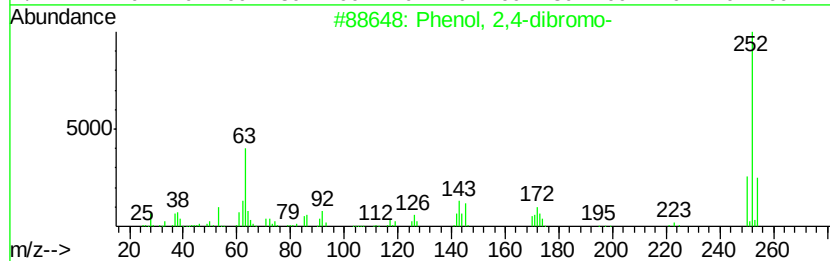
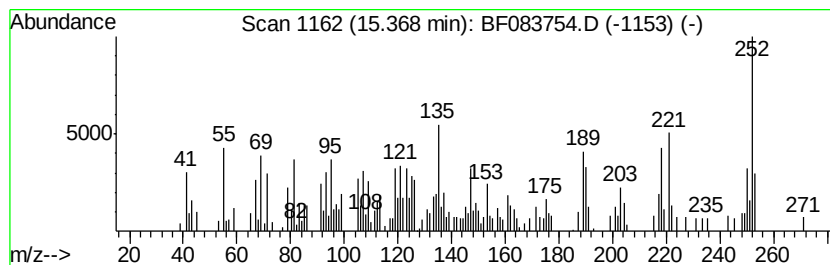
Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.37	4.89 ng	413498	Perylene-d12	15.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	38
2	Perylene	252	C20H12	000198-55-0	38
3	p-(Adamantyl-1)phenylcyclopropane	252	C19H24	1000140-46-1	30
4	Dibenzo[b,E][1,4]dioxin, 2,7-dic...	252	C12H6Cl2O2	033857-26-0	27
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083754.D
Acq On : 14 Dec 2015 3:14
Operator : UM/IZ
Sample : G4743-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WESTWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.12	13.4	ng	1100540	1	6.92	1637060	20.0
unknown6.69	6.69	44.3	ng	3622440	1	6.92	1637060	20.0
1-Tetradecene	11.66	3.0	ng	257592	4	11.44	1713560	20.0
1-Heptadecanol	12.48	3.7	ng	314628	4	11.44	1713560	20.0
Hexadecanoic acid...	12.84	2.9	ng	230245	5	14.07	1594920	20.0
Octadecanoic acid...	13.55	2.0	ng	162105	5	14.07	1594920	20.0
Bromoacetic acid,...	13.91	3.1	ng	249463	5	14.07	1594920	20.0
unknown15.37	15.37	4.9	ng	413498	6	15.51	1692890	20.0