

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
 Data File : BF081517.D
 Acq On : 6 Sep 2015 18:55
 Operator : UM/IZ
 Sample : G3561-02
 Misc :
 ALS Vial : 92 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SANDYLOAM

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-BF090115.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	4.387	242	245	257	rVB	363617	632709	49.78%	3.562%
2	4.901	288	290	302	rVB	1077288	1150218	90.50%	6.476%
3	6.033	386	389	391	rBV	1033734	1270924	100.00%	7.156%
4	6.124	395	397	399	rBV	1326706	1155693	90.93%	6.507%
5	6.353	415	417	420	rVB	342480	322557	25.38%	1.816%
6	6.513	428	431	433	rBV	1038301	880928	69.31%	4.960%
7	6.936	465	468	470	rBV	858753	789795	62.14%	4.447%
8	7.085	479	481	485	rBV	15085	16301	1.28%	0.092%
9	7.645	528	530	533	rBV	447572	399819	31.46%	2.251%
10	8.605	612	614	619	rBV	9966	13698	1.08%	0.077%
11	8.730	623	625	627	rBV	1346389	1126509	88.64%	6.342%
12	8.868	636	637	645	rVB	13676	18470	1.45%	0.104%
13	9.050	652	653	655	rBV2	12802	15182	1.19%	0.085%
14	9.130	658	660	663	rVV	181202	173012	13.61%	0.974%
15	9.245	667	670	673	rBV	35503	39366	3.10%	0.222%
16	9.359	678	680	681	rVV	19505	20753	1.63%	0.117%
17	9.382	681	682	684	rVV	303561	362177	28.50%	2.039%
18	9.416	684	685	688	rVV2	28293	28310	2.23%	0.159%
19	9.519	691	694	699	rBV2	6141	15361	1.21%	0.086%
20	9.588	699	700	702	rVB2	11139	13594	1.07%	0.077%
21	9.851	722	723	725	rVB	19791	16791	1.32%	0.095%
22	9.931	728	730	732	rVB	29207	28077	2.21%	0.158%
23	9.999	732	736	738	rVB4	5288	14579	1.15%	0.082%
24	10.091	738	744	748	rBV5	9347	29657	2.33%	0.167%
25	10.171	748	751	753	rBV	626635	575899	45.31%	3.242%
26	10.319	761	764	767	rBV	28451	46460	3.66%	0.262%
27	10.411	770	772	774	rBV2	13097	17716	1.39%	0.100%
28	10.765	800	803	804	rBV	22605	26789	2.11%	0.151%
29	10.856	808	811	814	rBV	254264	483587	38.05%	2.723%
30	10.925	814	817	818	rVV	84997	71684	5.64%	0.404%
31	10.948	818	819	822	rVB2	21982	25788	2.03%	0.145%
32	11.119	832	834	838	rVV	96392	131004	10.31%	0.738%
33	11.188	838	840	842	rVB	26641	29142	2.29%	0.164%
34	11.348	852	854	855	rBV2	34923	40240	3.17%	0.227%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
 Data File : BF081517.D
 Acq On : 6 Sep 2015 18:55
 Operator : UM/IZ
 Sample : G3561-02
 Misc :
 ALS Vial : 92 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SANDYLOAM

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-BF090115.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.382	855	857	859	rVV	35309	43542	3.43%	0.245%
36	11.428	859	861	862	rVV	126098	121327	9.55%	0.683%
37	11.451	862	863	867	rVV2	66376	114199	8.99%	0.643%
38	11.531	869	870	873	rVV3	17853	25811	2.03%	0.145%
39	11.588	873	875	877	rVV	25164	33154	2.61%	0.187%
40	11.668	878	882	885	rVB	36695	71936	5.66%	0.405%
41	11.828	894	896	899	rVB	14223	21867	1.72%	0.123%
42	11.896	900	902	903	rBV	36349	31142	2.45%	0.175%
43	11.931	903	905	908	rBV	286597	380070	29.91%	2.140%
44	12.045	913	915	918	rVB	245846	237557	18.69%	1.337%
45	12.114	918	921	922	rBV2	11864	17842	1.40%	0.100%
46	12.194	927	928	932	rBV4	15276	38649	3.04%	0.218%
47	12.274	932	935	936	rVV	200221	248719	19.57%	1.400%
48	12.342	939	941	944	rVB3	23054	31117	2.45%	0.175%
49	12.399	944	946	947	rBV	15039	15859	1.25%	0.089%
50	12.434	947	949	952	rVB	735519	676715	53.25%	3.810%
51	12.502	952	955	958	rVB3	21261	40606	3.19%	0.229%
52	12.605	958	964	966	rBV	53045	104567	8.23%	0.589%
53	12.674	966	970	971	rBV	36147	72912	5.74%	0.411%
54	12.697	971	972	974	rVB2	37369	47007	3.70%	0.265%
55	12.788	979	980	982	rBV	22391	27553	2.17%	0.155%
56	12.822	982	983	985	rVV	25046	27464	2.16%	0.155%
57	12.868	985	987	988	rVB2	13711	17606	1.39%	0.099%
58	12.902	988	990	992	rBV	43011	40871	3.22%	0.230%
59	13.005	997	999	1000	rVV2	14695	22637	1.78%	0.127%
60	13.039	1000	1002	1004	rVB2	21493	27631	2.17%	0.156%
61	13.165	1010	1013	1015	rBV3	11603	24684	1.94%	0.139%
62	13.211	1015	1017	1018	rBV2	29515	33811	2.66%	0.190%
63	13.257	1018	1021	1022	rVV2	19957	37059	2.92%	0.209%
64	13.371	1028	1031	1033	rBV2	73580	119686	9.42%	0.674%
65	13.462	1036	1039	1040	rBV2	355892	460840	36.26%	2.595%
66	13.565	1045	1048	1049	rBV2	26233	49233	3.87%	0.277%
67	13.851	1071	1073	1074	rVB	24391	27625	2.17%	0.156%
68	13.988	1082	1085	1089	rBV3	112537	217081	17.08%	1.222%
69	14.331	1113	1115	1118	rVB	30454	49674	3.91%	0.280%
70	14.445	1123	1125	1129	rBV	158170	245593	19.32%	1.383%
71	14.560	1133	1135	1138	rVB	508927	468654	36.88%	2.639%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.674	1144	1145	1148	rVB	65073	85116	6.70%	0.479%
73	14.731	1148	1150	1152	rBV	62901	106143	8.35%	0.598%
74	14.777	1152	1154	1158	rVV	153340	219307	17.26%	1.235%
75	14.845	1158	1160	1161	rVB	28834	26910	2.12%	0.152%
76	15.165	1185	1188	1191	rBV	483090	643061	50.60%	3.621%
77	15.600	1224	1226	1233	rVB4	47952	117326	9.23%	0.661%
78	15.851	1246	1248	1250	rBV2	28104	47085	3.70%	0.265%
79	15.943	1254	1256	1260	rVB	55846	106136	8.35%	0.598%
80	16.068	1265	1267	1269	rBV3	20759	35247	2.77%	0.198%
81	16.297	1282	1287	1291	rBV	122006	318721	25.08%	1.794%
82	16.503	1302	1305	1307	rBV3	21988	62072	4.88%	0.349%
83	16.594	1310	1313	1316	rVV	91756	260346	20.48%	1.466%
84	16.663	1316	1319	1323	rVB3	105203	269959	21.24%	1.520%
85	16.765	1324	1328	1331	rBV3	30912	67983	5.35%	0.383%
86	16.834	1331	1334	1341	rBV6	93393	403912	31.78%	2.274%
87	16.937	1341	1343	1346	rVV3	44735	101757	8.01%	0.573%
88	16.994	1346	1348	1354	rVB5	48339	136636	10.75%	0.769%
89	17.234	1363	1369	1375	rVB7	37224	161752	12.73%	0.911%
90	17.611	1398	1402	1407	rBV6	22515	80193	6.31%	0.452%
91	17.726	1407	1412	1420	rVB5	78465	256694	20.20%	1.445%

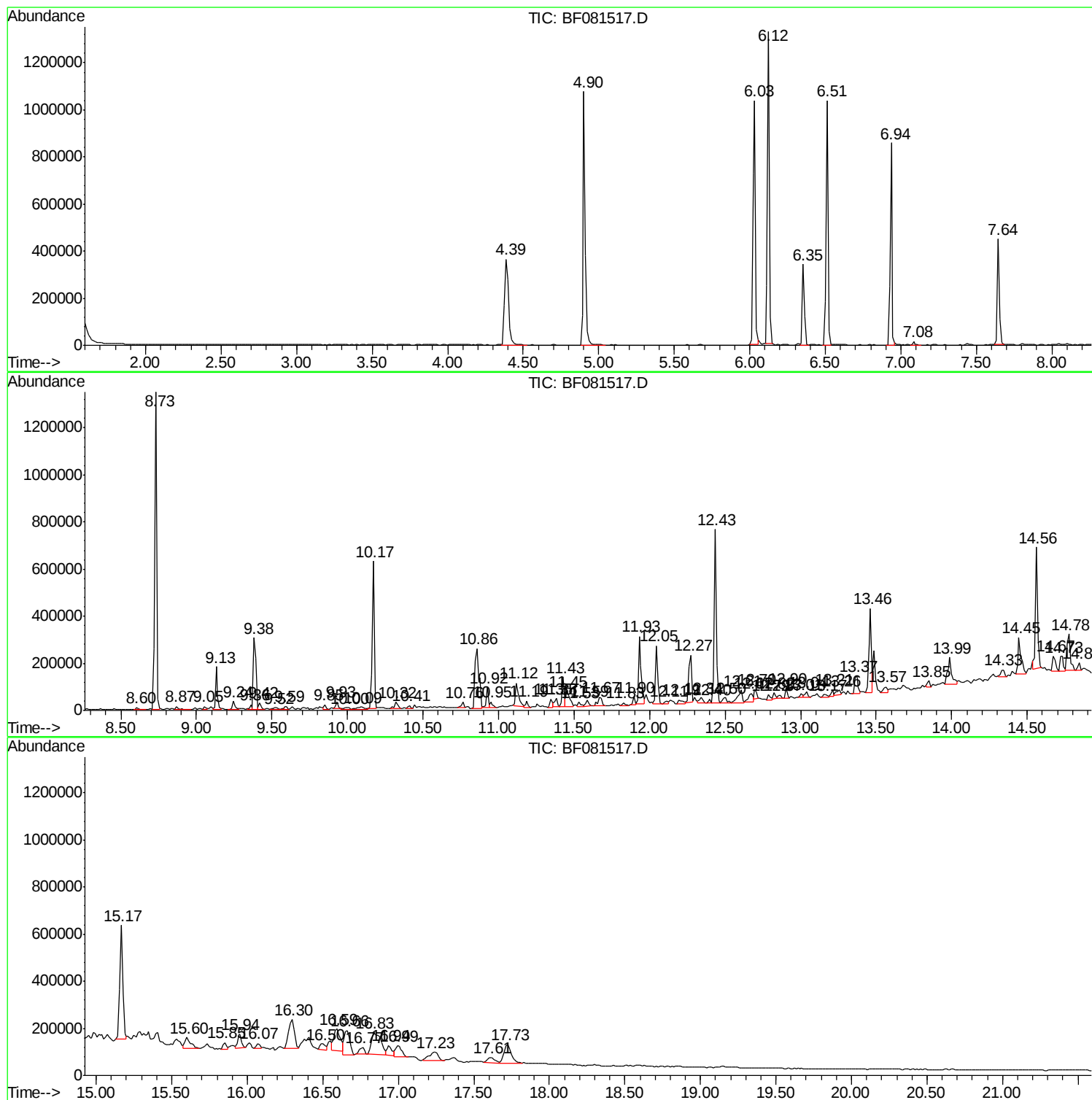
Sum of corrected areas: 17761445

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

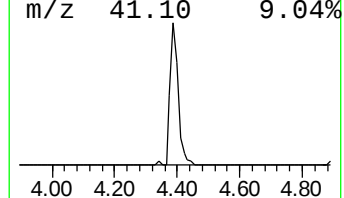
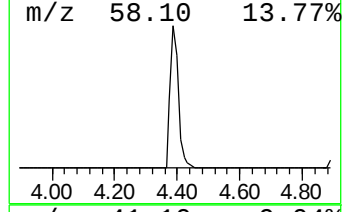
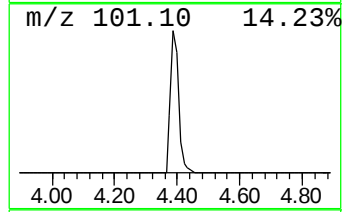
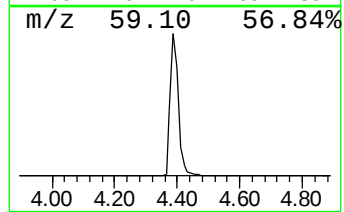
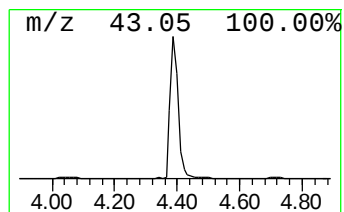
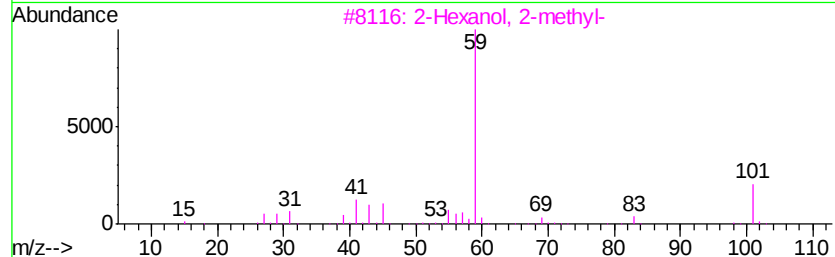
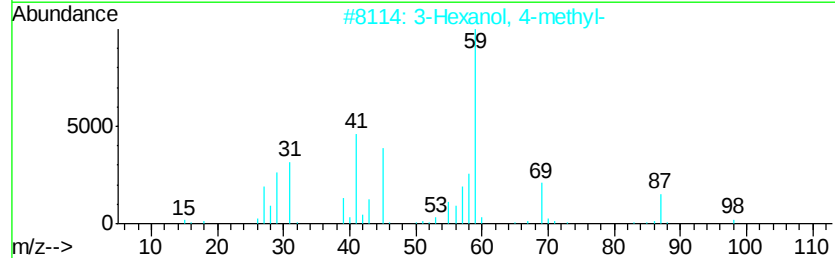
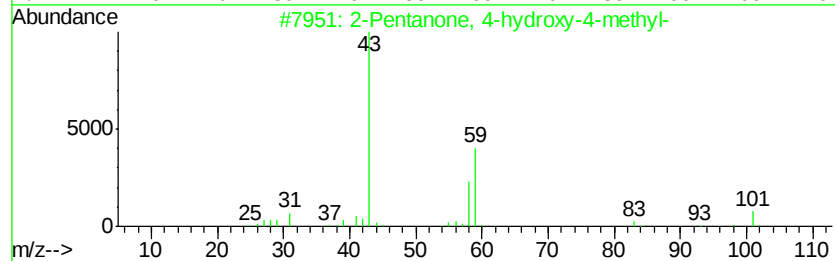
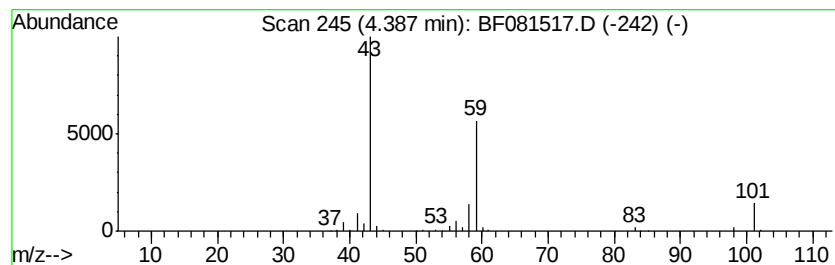
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	39.23 ng	632709	1,4-Dichlorobenzene-d4	6.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

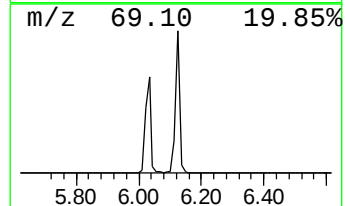
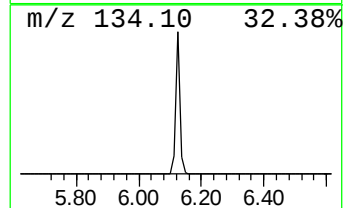
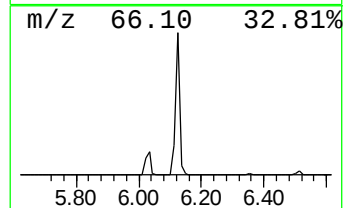
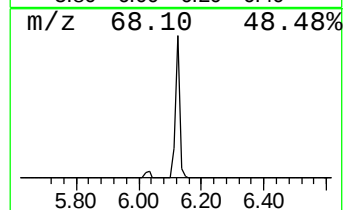
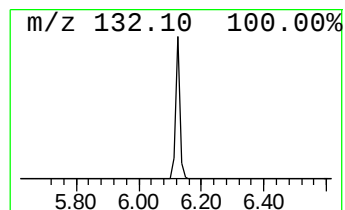
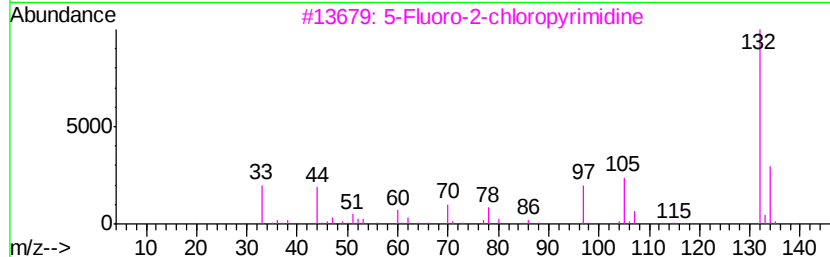
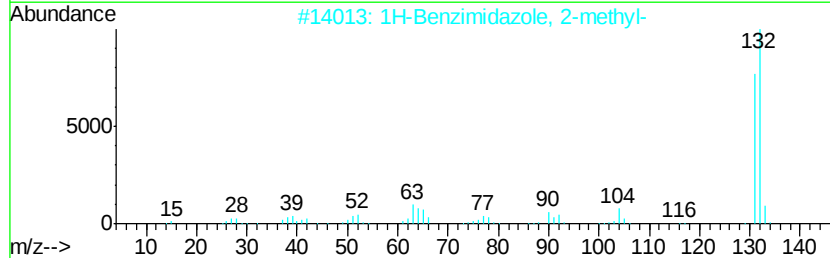
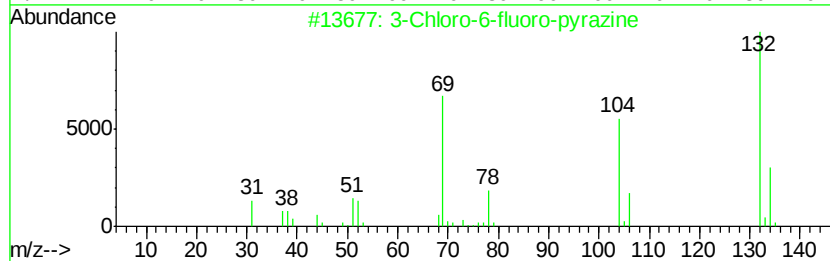
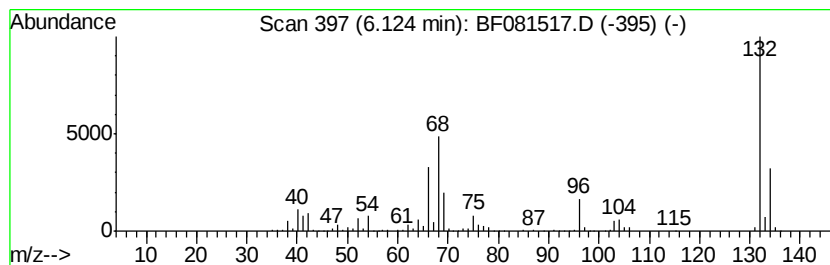
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	71.66 ng	1155690	1,4-Dichlorobenzene-d4	6.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

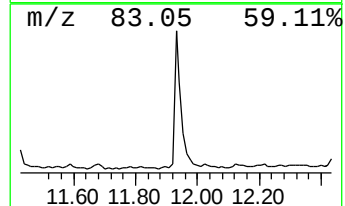
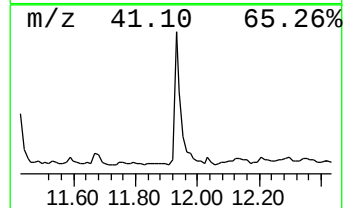
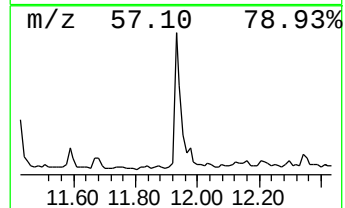
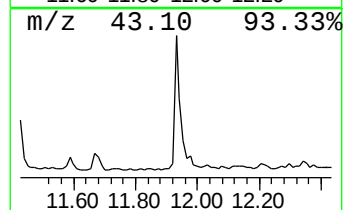
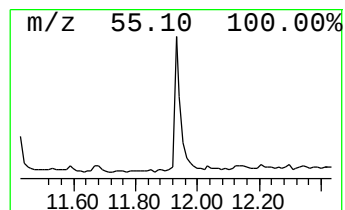
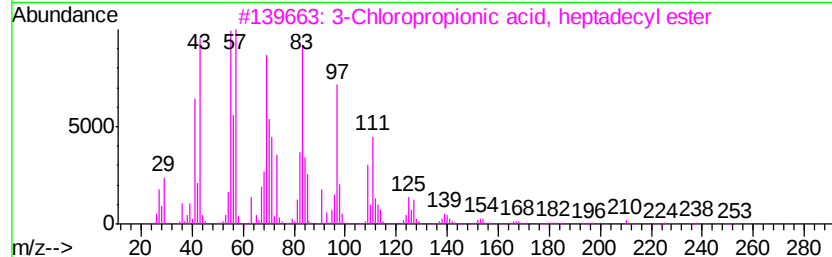
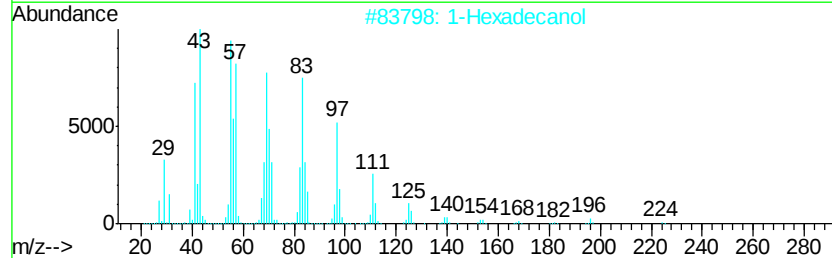
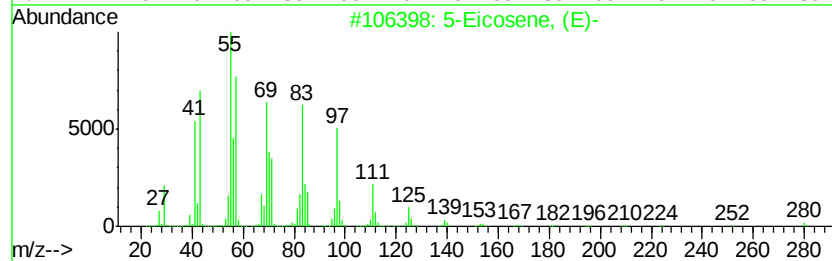
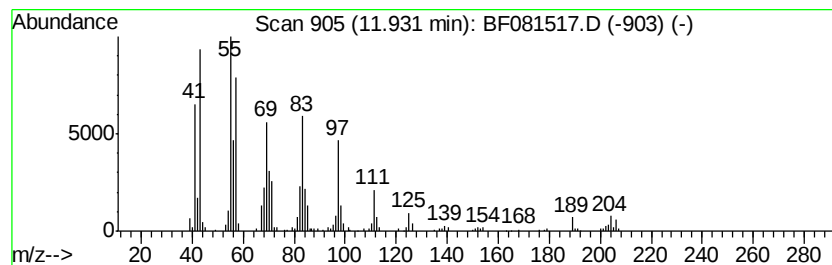
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 5-Eicosene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	15.72 ng	380070	Phenanthrene-d10	10.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4		1-Octadecene	252	C18H36	000112-88-9	87
5		1-Hexadecene	224	C16H32	000629-73-2	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

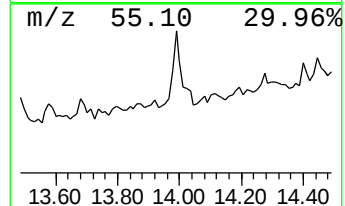
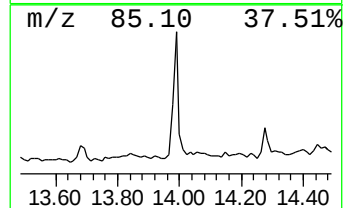
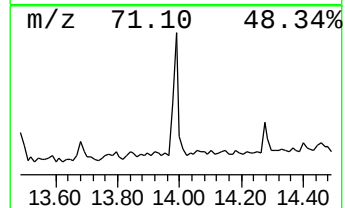
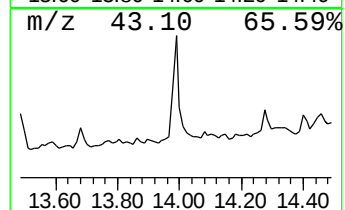
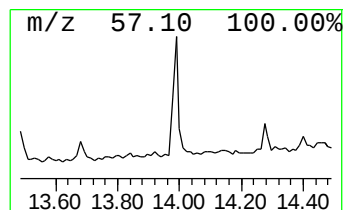
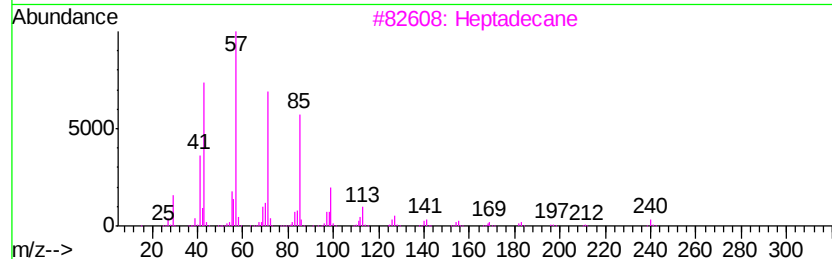
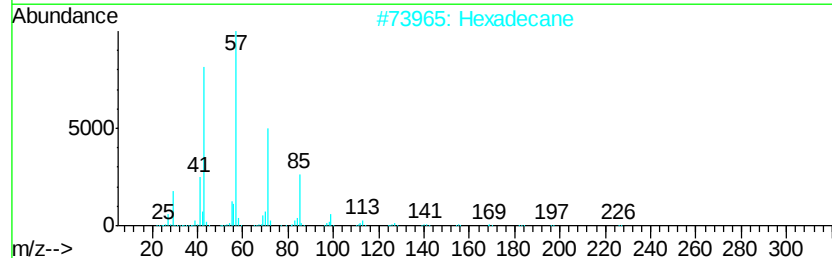
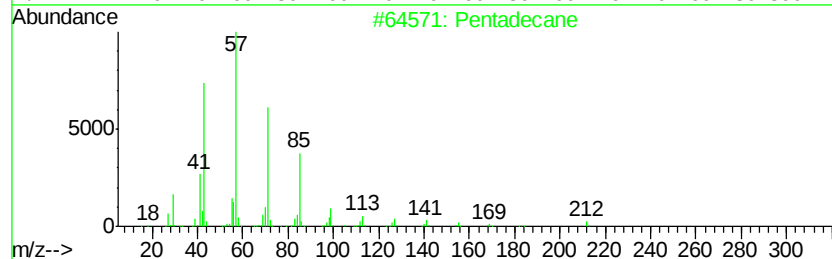
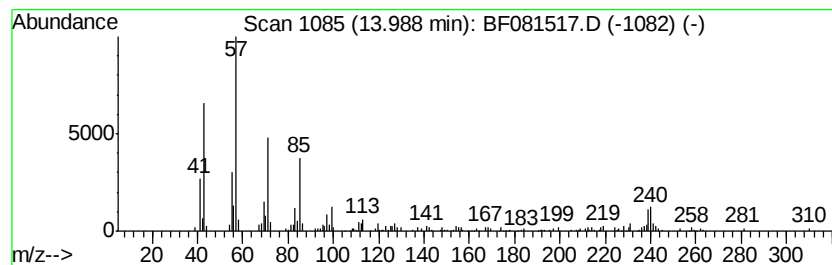
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	9.42 ng	217081	Chrysene-d12	13.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	96
2		Hexadecane	226	C16H34	000544-76-3	94
3		Heptadecane	240	C17H36	000629-78-7	94
4		Hexatriacontane	507	C36H74	000630-06-8	76
5		Tetracosane	338	C24H50	000646-31-1	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

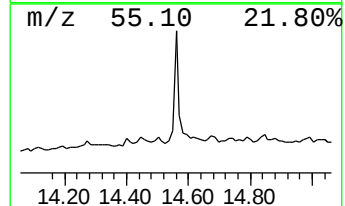
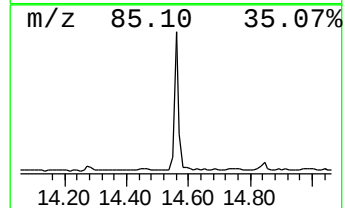
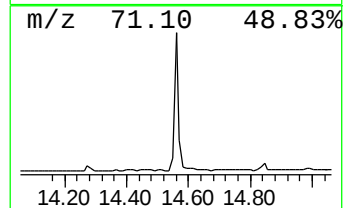
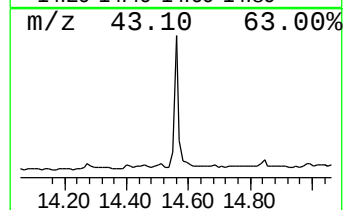
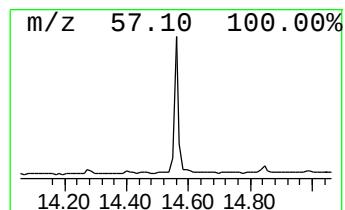
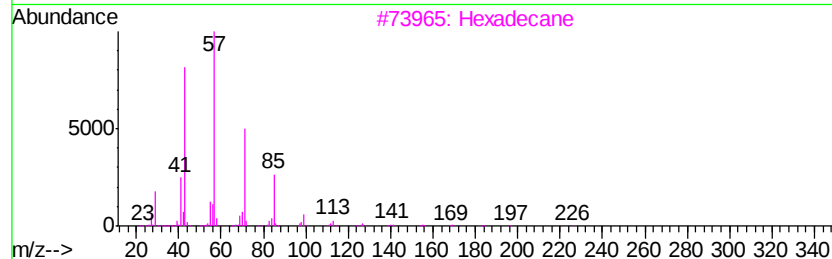
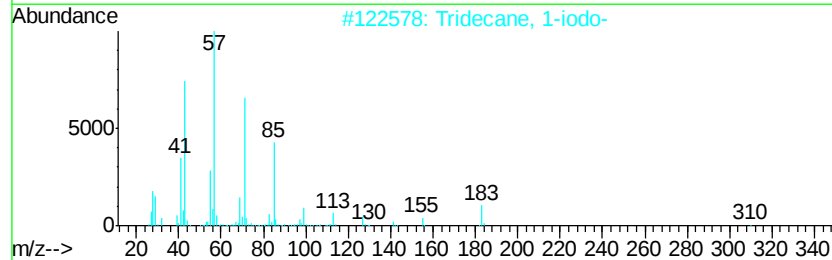
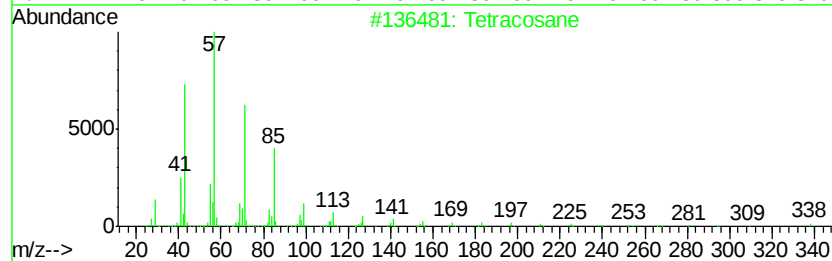
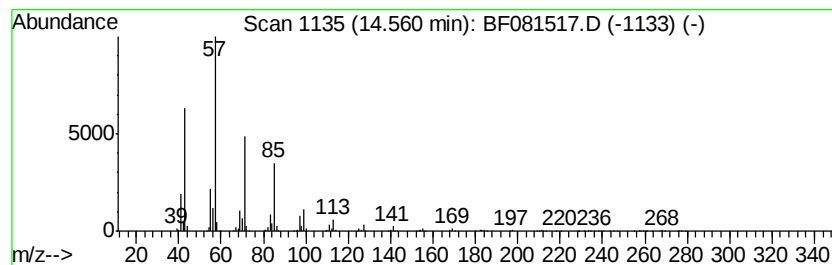
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	42.74 ng	468654	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

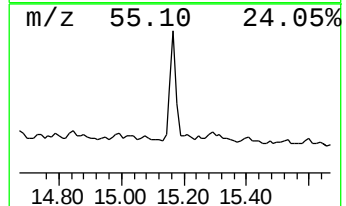
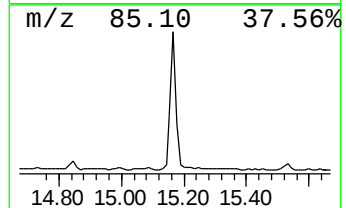
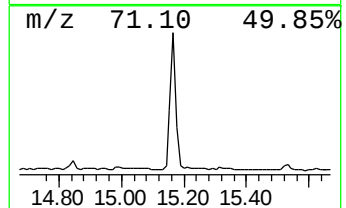
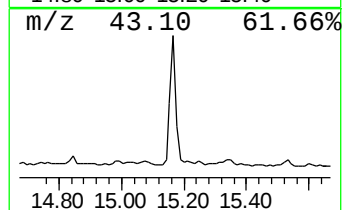
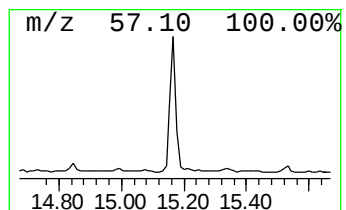
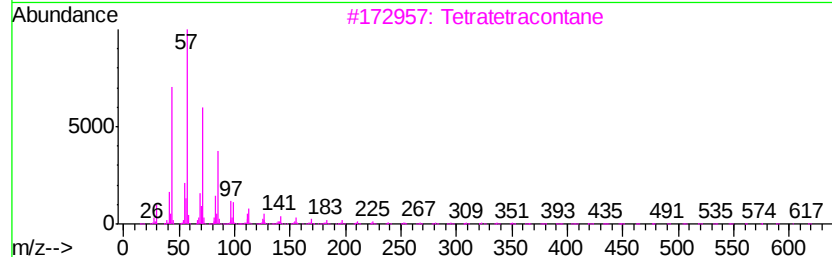
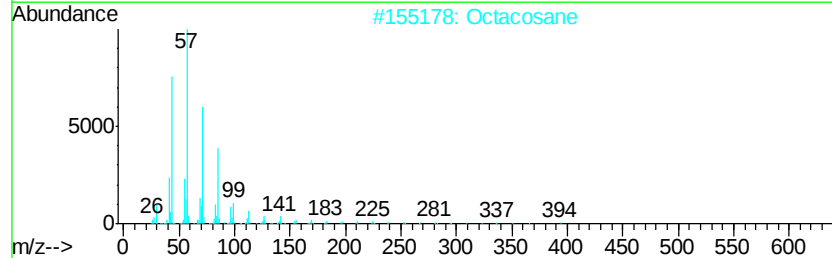
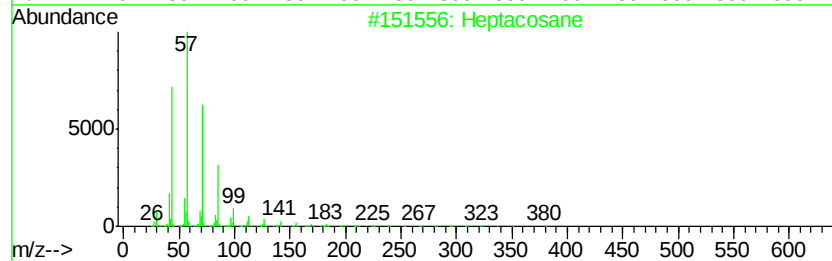
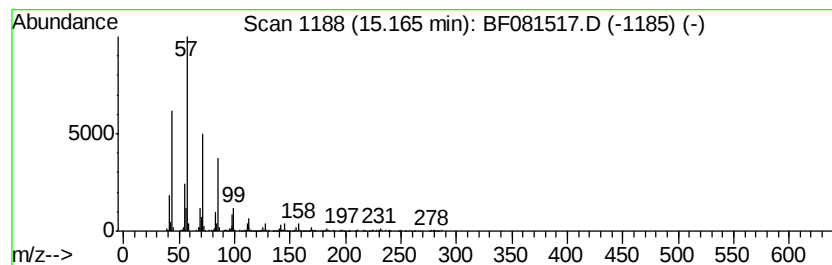
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	58.64 ng	643061	Perylene-d12	14.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Octacosane		394	C28H58	000630-02-4	87
3	Tetratetracontane		619	C44H90	007098-22-8	87
4	Tetratriacontane		479	C34H70	014167-59-0	86
5	Pentacosane		352	C25H52	000629-99-2	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

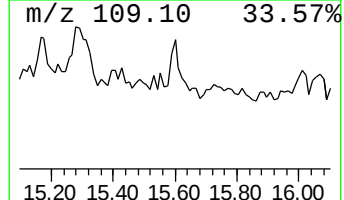
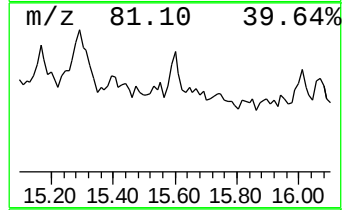
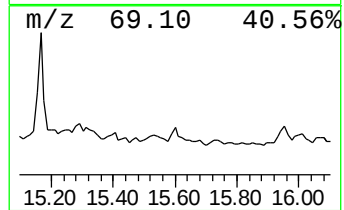
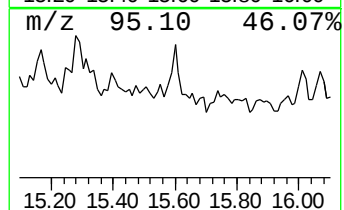
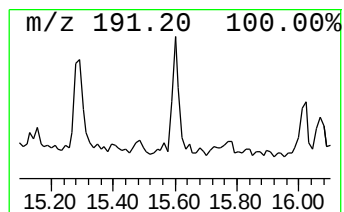
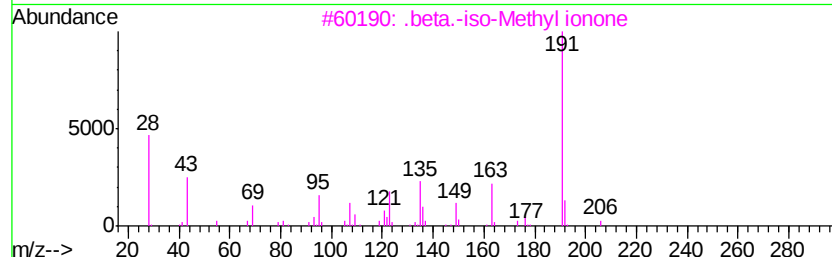
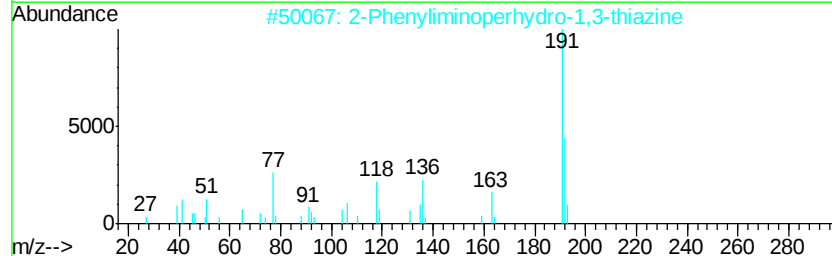
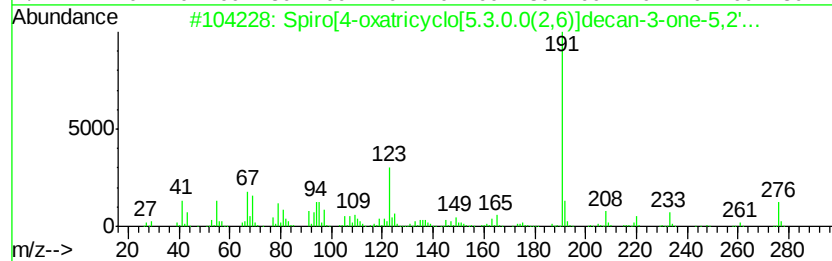
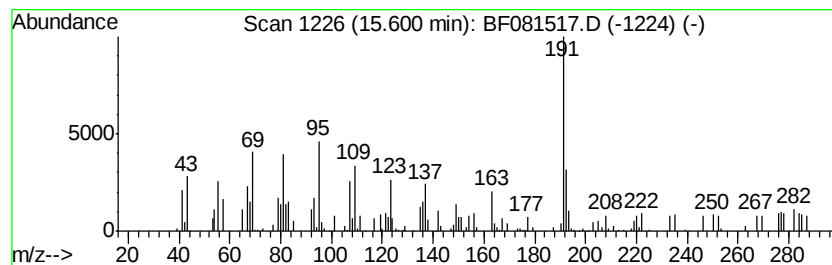
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.60 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	10.70 ng	117326	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Spino[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	43
2		2-Phenyliminoperhydro-1,3-thiazine	192	C10H12N2S	1000138-91-3	43
3		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	40
4		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
5		2-Fluoro-3-(trifluoromethyl)prop...	220	C10H8F4O	207986-23-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

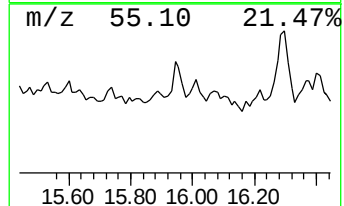
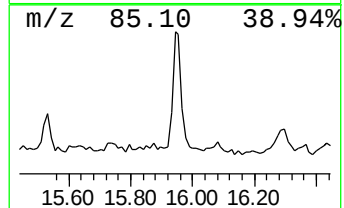
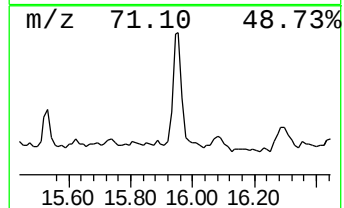
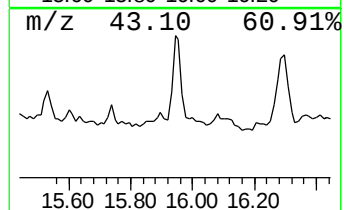
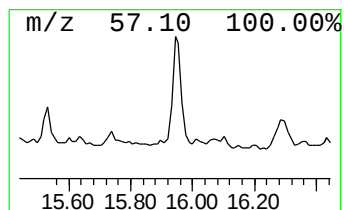
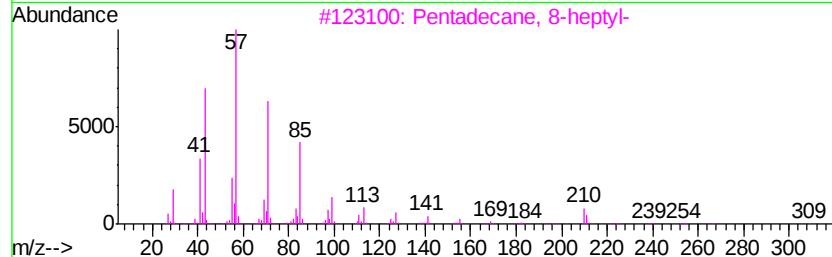
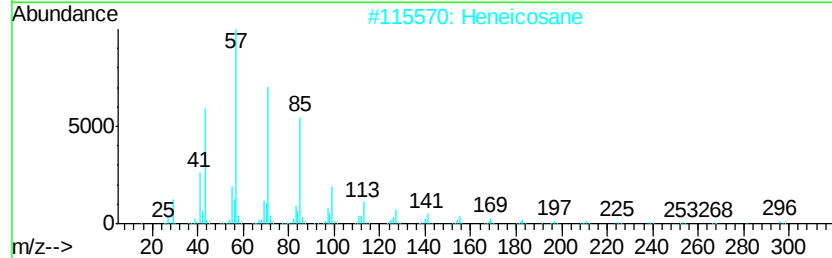
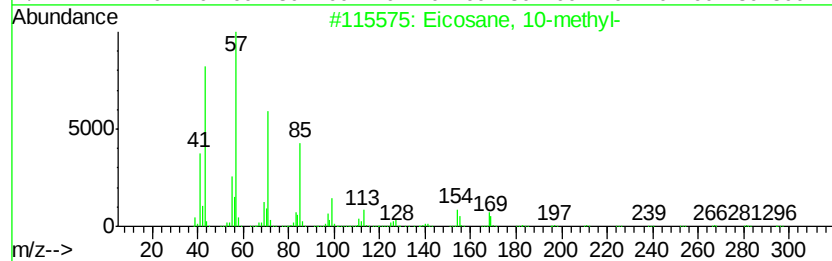
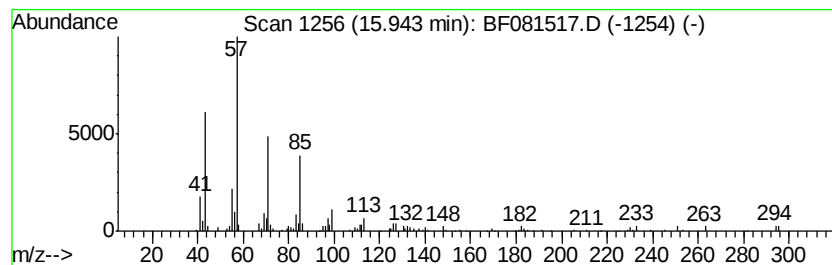
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	9.68 ng	106136	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
2		Heneicosane	296	C21H44	000629-94-7	74
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	72
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
5		Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

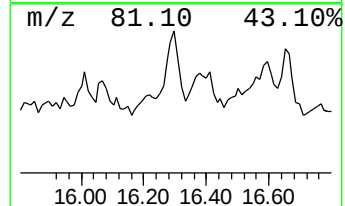
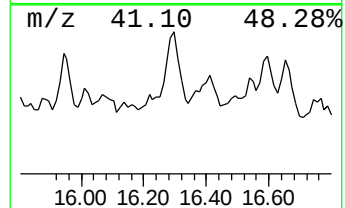
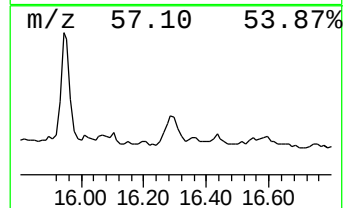
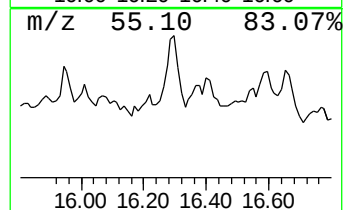
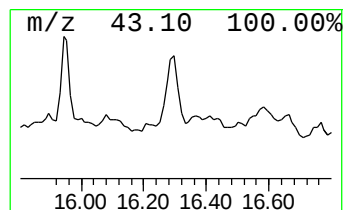
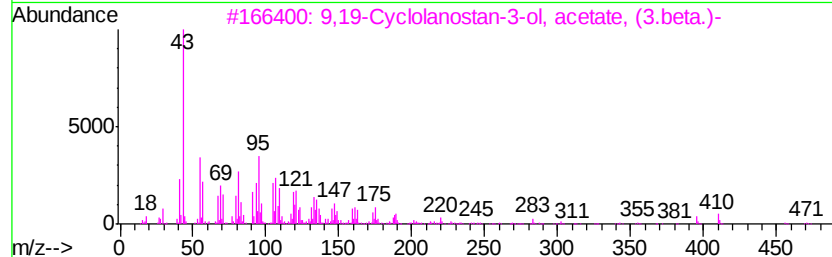
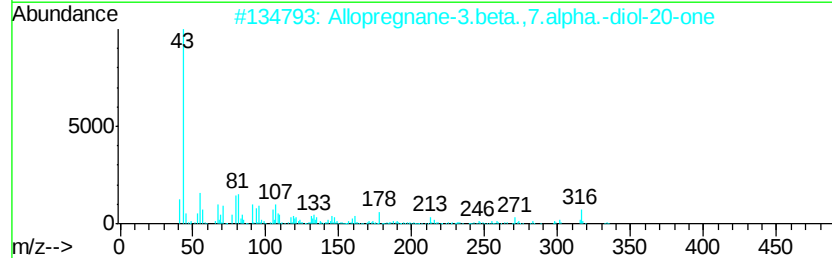
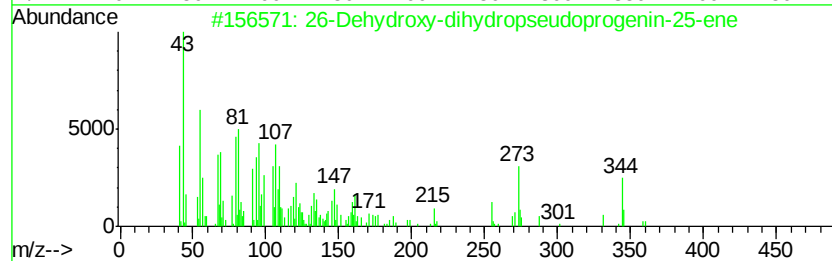
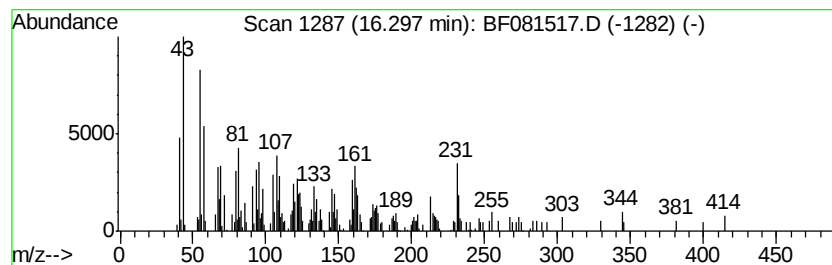
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	29.07 ng	318721	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	26-Dehydroxy-dihydropseudoprogen...	400	C27H44O2	1000255-22-7	38
2		Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	27
3		9,19-Cyclolanostan-3-ol, acetate...	470	C32H54O2	004575-74-0	22
4		5-.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	12
5		1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

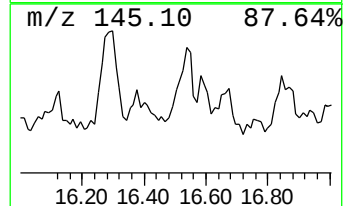
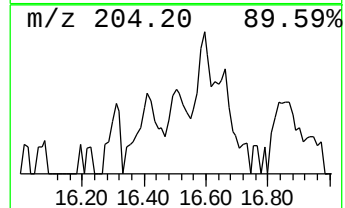
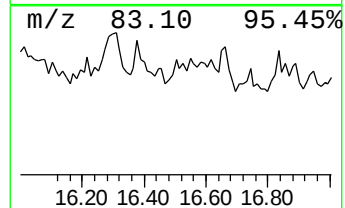
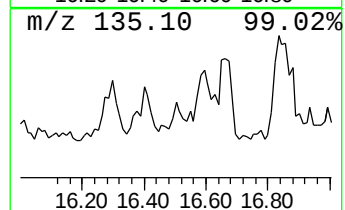
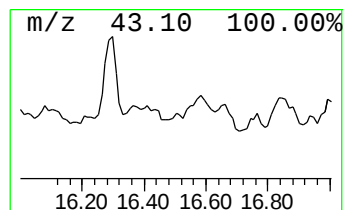
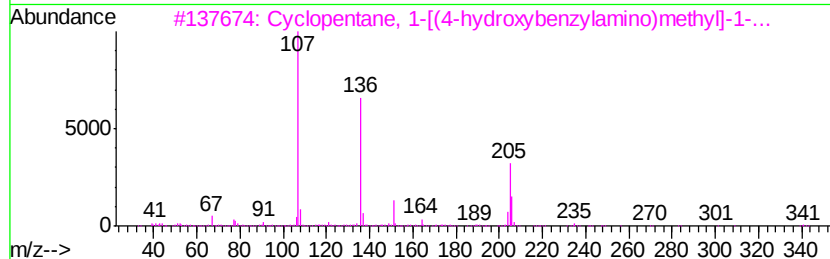
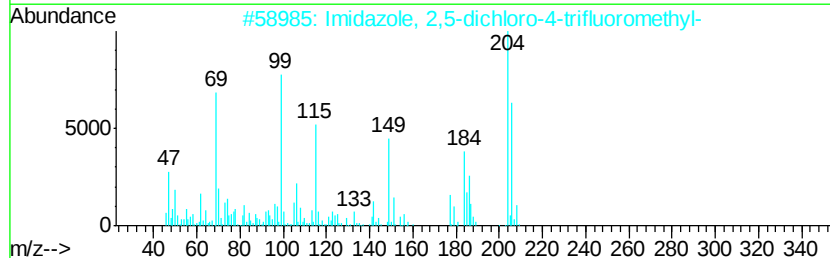
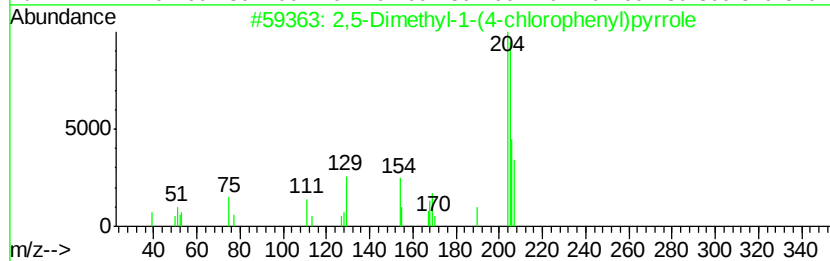
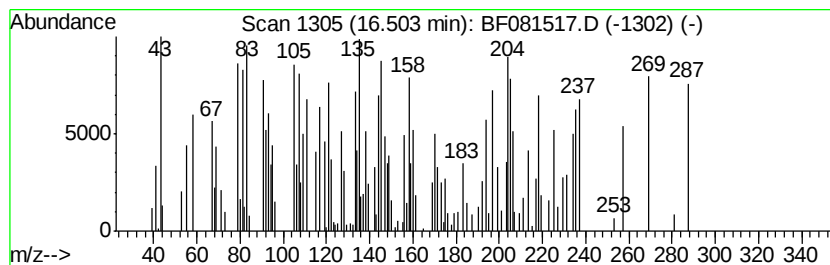
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.50 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	5.66 ng	62072	Perylene-d12	14.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dimethyl-1-(4-chlorophenyl)p...	205	C12H12ClN	005044-23-5	22		
2	Imidazole, 2,5-dichloro-4-triflu...	204	C4HCl2F3N2	219534-97-1	15		
3	Cyclopentane, 1-[(4-hydroxybenzy...	341	C21H27N03	1000264-64-8	10		
4	Phthalazine, 1-phenyl-	206	C14H10N2	007188-22-9	10		
5	1,2,3,4,6,7,8,9-Octahydrodipyrid...	205	C11H15N3O	111303-60-7	10		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

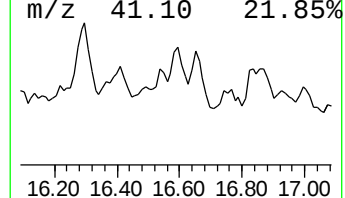
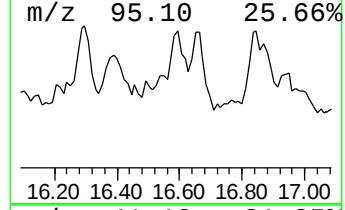
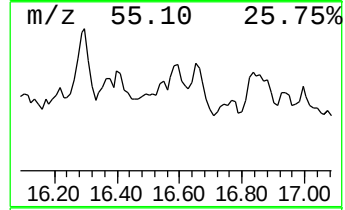
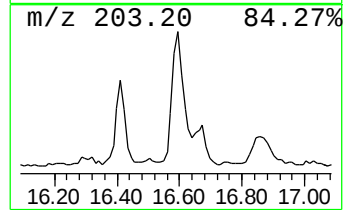
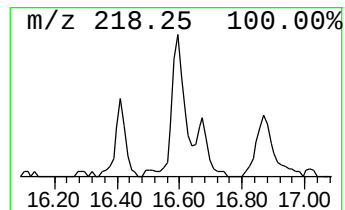
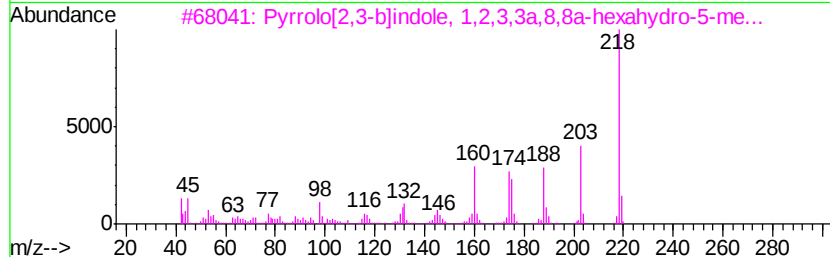
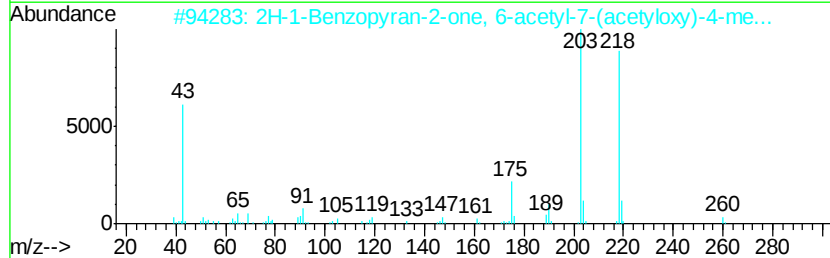
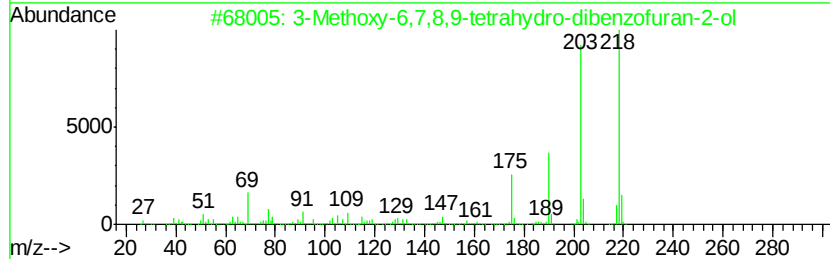
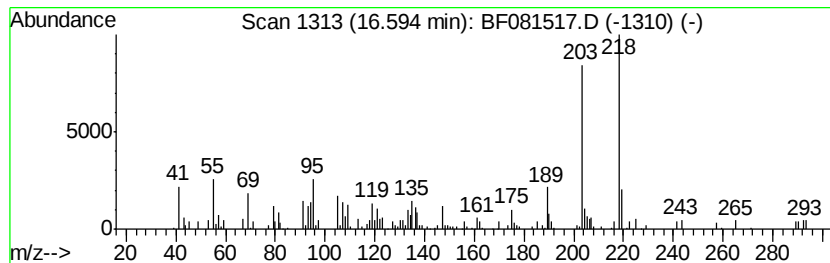
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 3-Methoxy-6,7,8,9-tetrahydr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	23.74 ng	260346	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	58
2		2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	53
3		Pyrrolo[2,3-b]indole, 1,2,3,3a,8...	218	C13H18N2O	046479-70-3	47
4		6,7,8,9-Tetrahydrodibenzo[b,d]fu...	260	C15H16O4	1000196-34-3	43
5		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

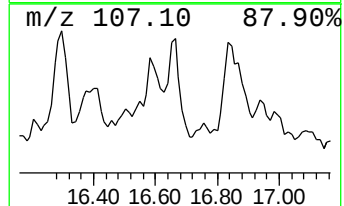
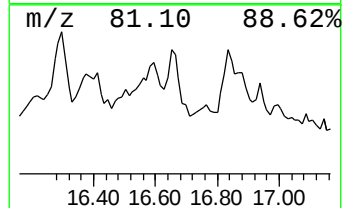
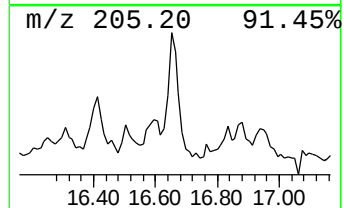
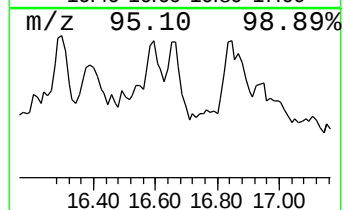
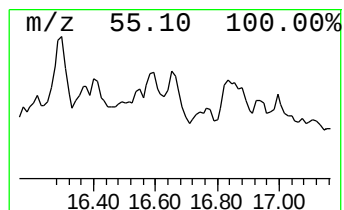
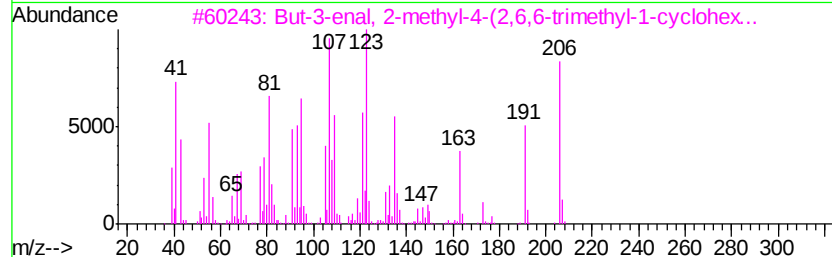
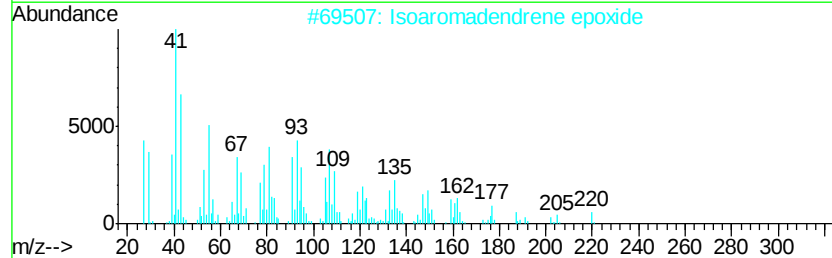
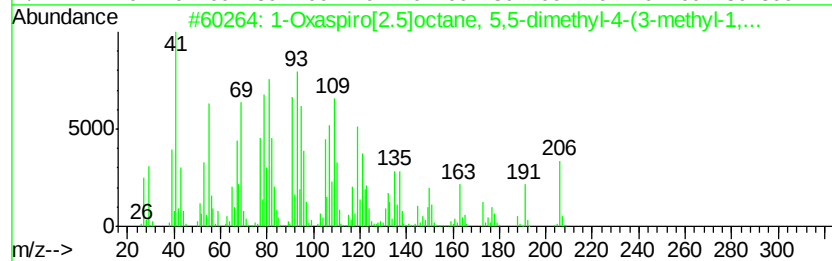
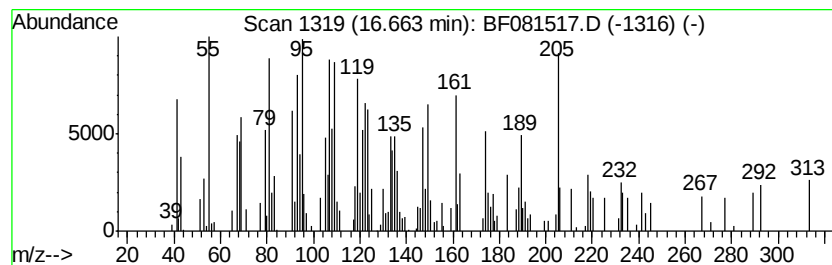
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Oxaspiro[2.5]octane, 5,5-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	24.62 ng	269959	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	52
2		Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	38
3		But-3-enal, 2-methyl-4-(2,6,6-tr...	206	C14H22O	104900-59-6	30
4		2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	27
5		Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

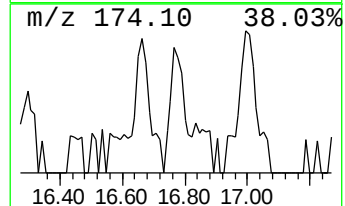
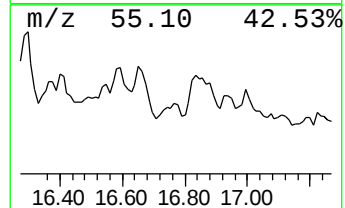
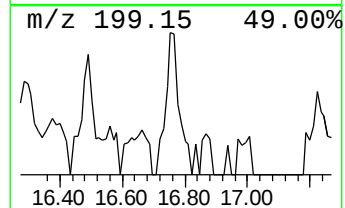
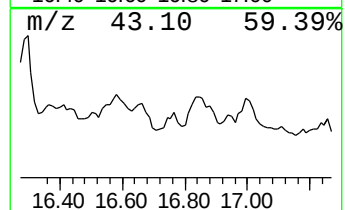
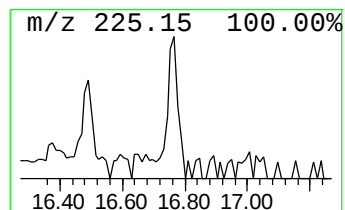
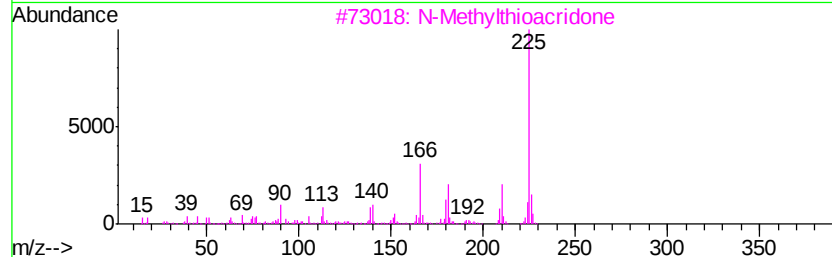
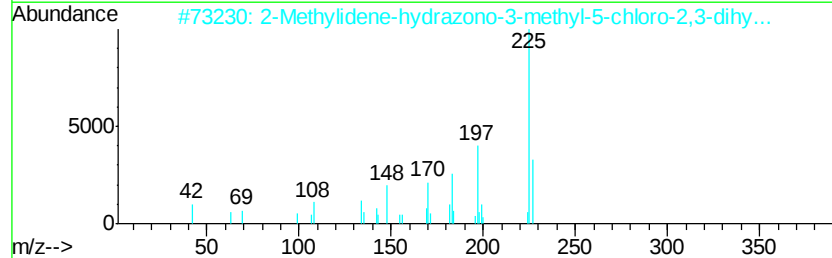
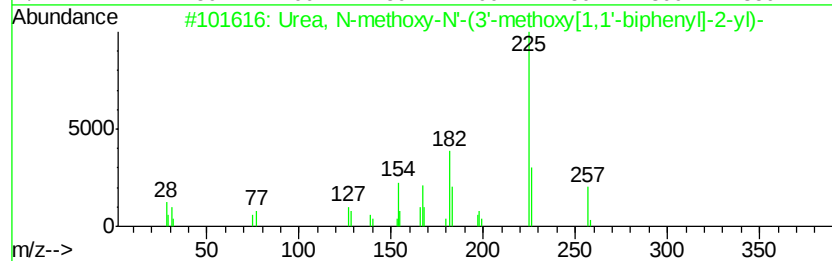
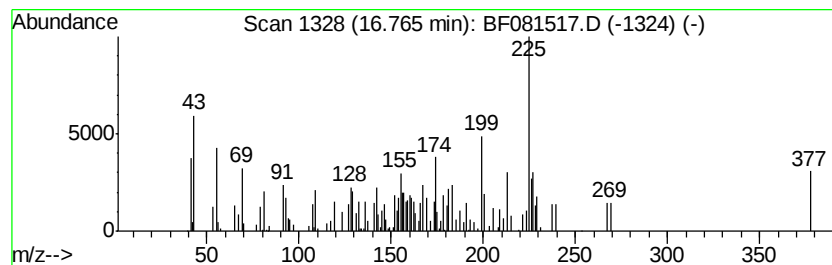
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.77 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	6.20 ng	67983	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Urea, N-methoxy-N'-(3'-methoxy[1...	272	C15H16N2O3	056666-85-4	35
2		2-Methylidene-hydrazono-3-methyl...	225	C9H8ClN3S	1000147-91-3	32
3		N-Methylthioacridone	225	C14H11NS	017435-19-7	27
4		6-n-Butyl-2-methyl-3-n-propyl-4-...	267	C19H25N	073669-41-7	27
5		Thiazole-2-hydrazine, 4-(4-chlor...	225	C9H8ClN3S	061323-64-6	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

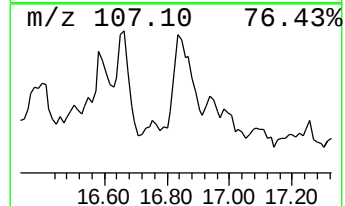
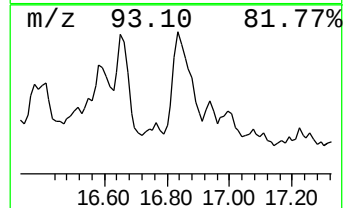
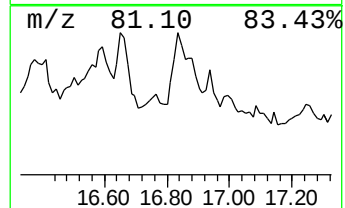
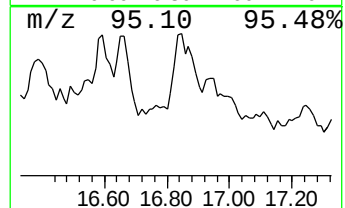
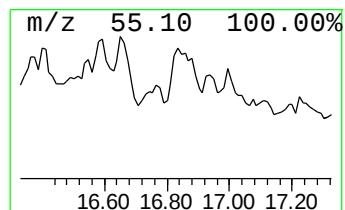
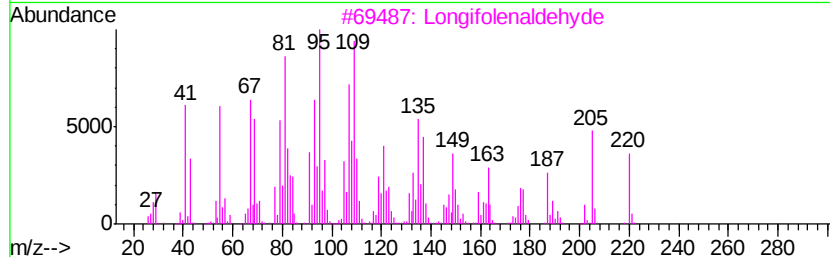
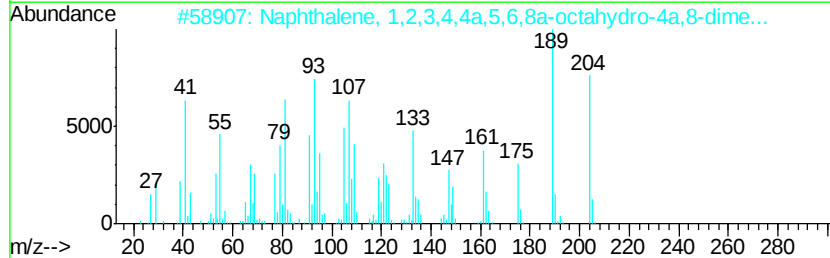
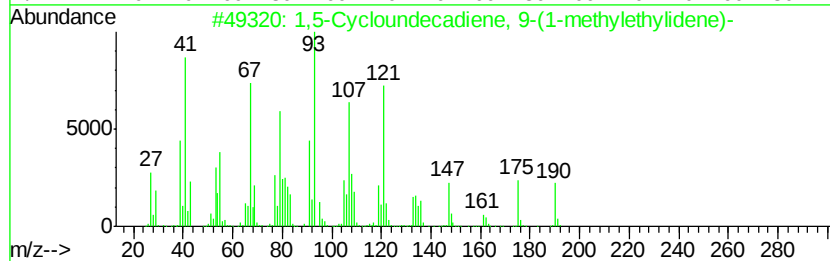
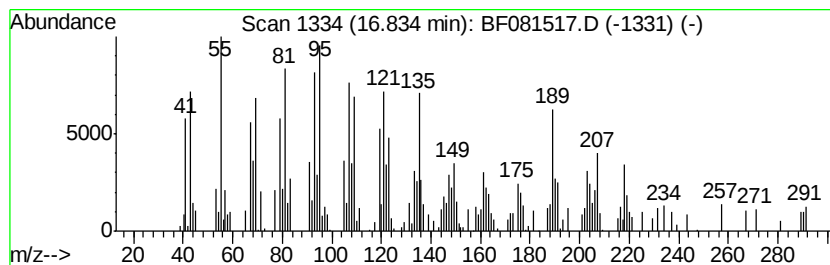
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1,5-Cycloundecadiene, 9-(1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	36.84 ng	403912	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	70
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	60
3		Longifolenaldehyde	220	C15H24O	019890-84-7	56
4		Spiro[4.5]dec-6-en-8-one, 1,7-di...	220	C15H24O	039510-36-6	55
5		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

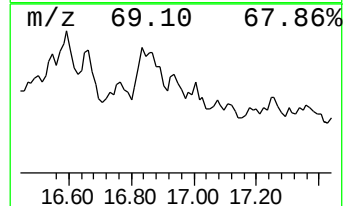
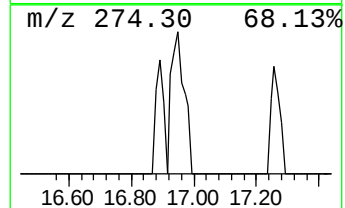
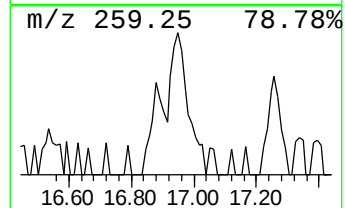
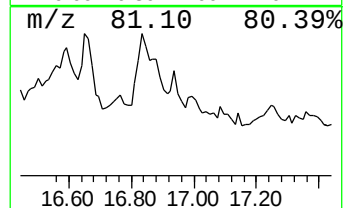
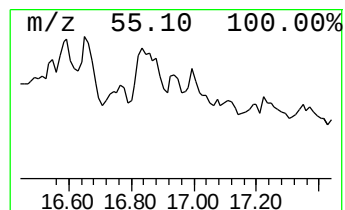
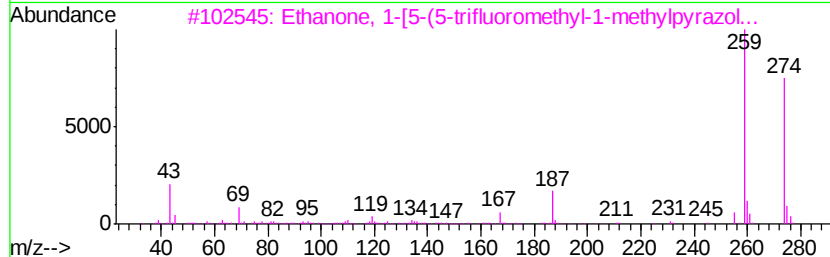
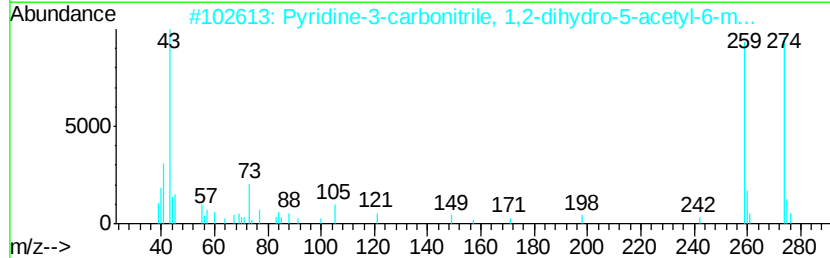
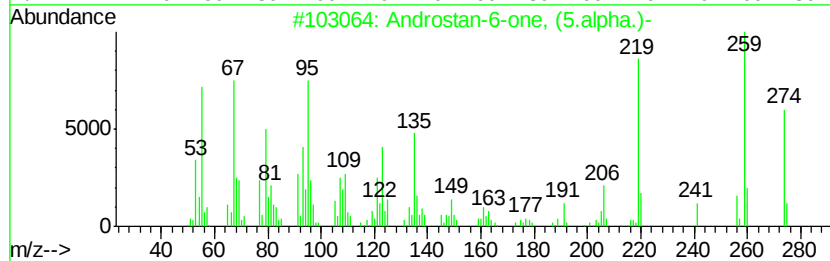
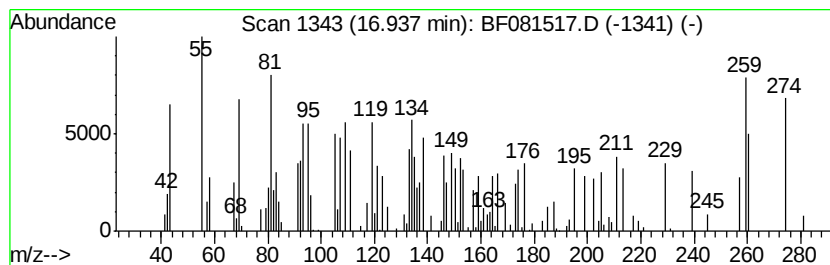
Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.94 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.94	9.28 ng	101757	Perylene-d12	14.78		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Androstan-6-one, (5.alpha.)-	274	C19H30O	003676-06-0	16
2		Pyridine-3-carbonitrile, 1,2-dih...	274	C13H10N2OS2	179088-20-1	14
3		Ethanone, 1-[5-(5-trifluoromethy...	274	C11H9F3N2OS	1000266-44-5	14
4		Propionitrile, 3-(4-butoxybenzyl...	259	C14H17N3O2	314753-98-5	14
5		2-Methyl-3-trans-propenylpyrazine	134	C8H10N2	232255-41-3	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

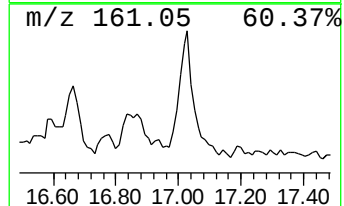
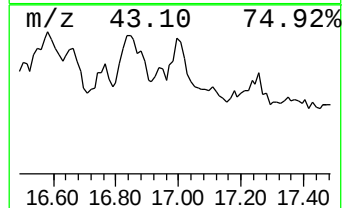
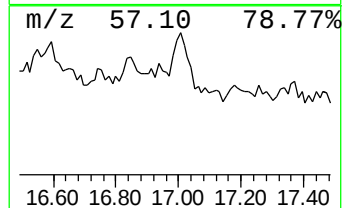
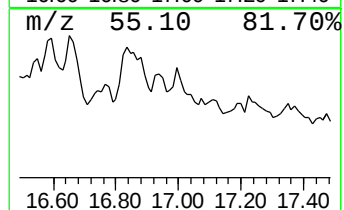
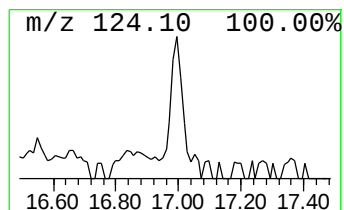
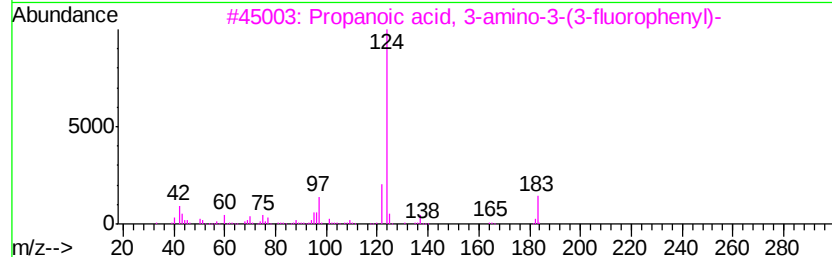
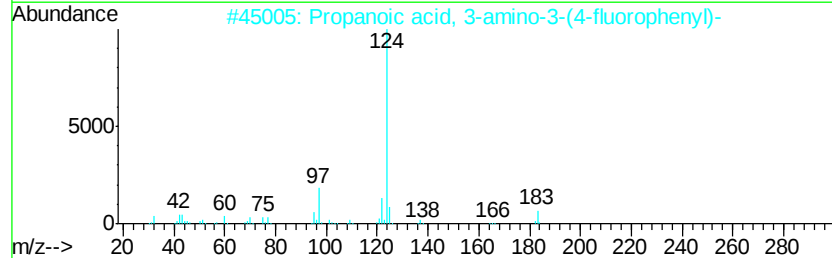
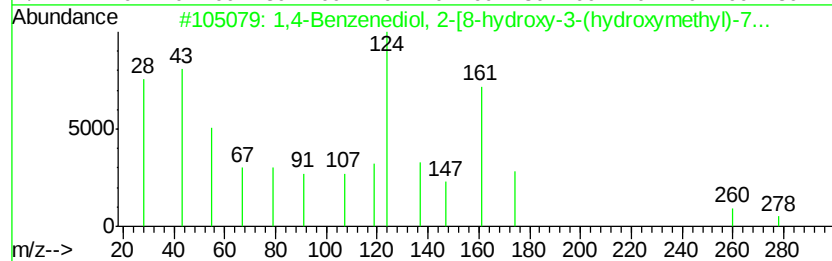
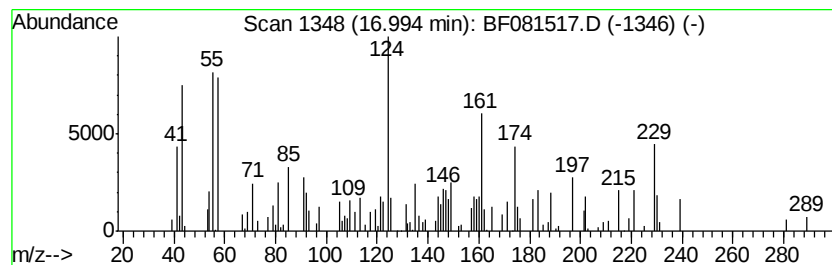
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.99 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	12.46 ng	136636	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2-[8-hydroxy-3-...	278	C16H22O4	077828-64-9	25
2		Propanoic acid, 3-amino-3-(4-flu...	183	C9H10FN02	000325-89-3	14
3		Propanoic acid, 3-amino-3-(3-flu...	183	C9H10FN02	117391-51-2	14
4		3-Diphenyl(methyl)silyloxypropene	254	C16H18OSi	017933-45-8	10
5		2-Methyl-4,5-pyrimidinediamine	124	C5H8N4	015579-63-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

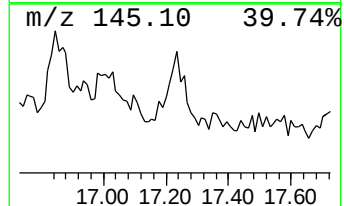
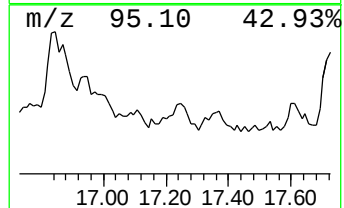
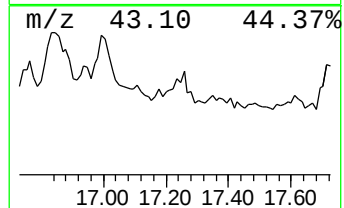
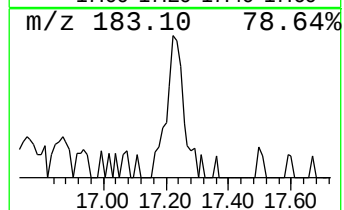
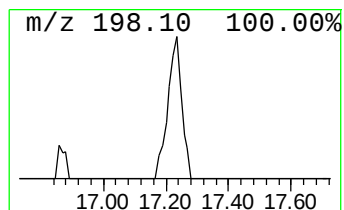
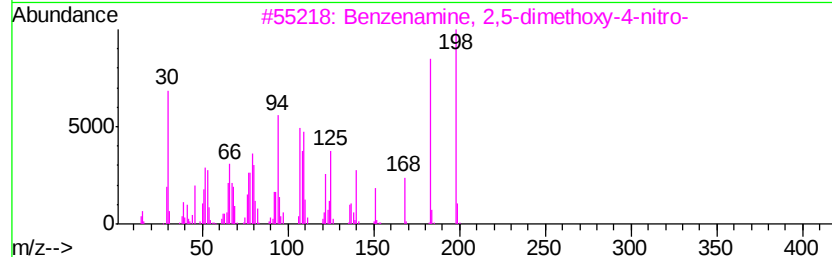
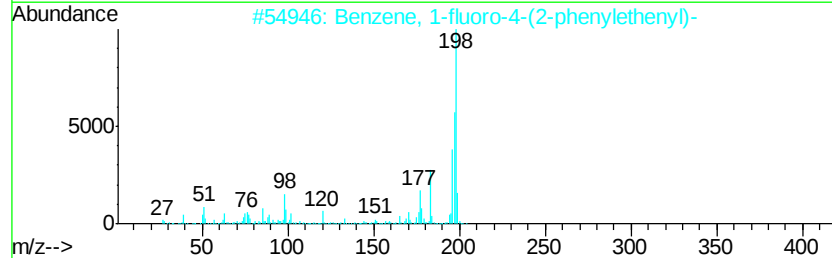
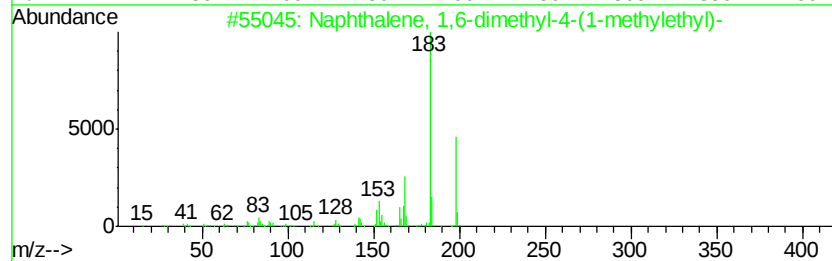
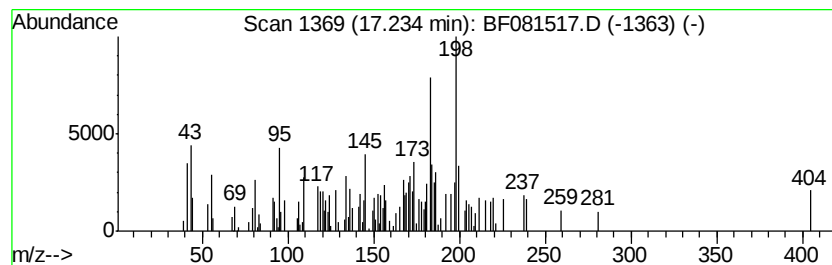
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.23 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	14.75 ng	161752	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	46
2		Benzene, 1-fluoro-4-(2-phenyleth...	198	C14H11F	017404-69-2	45
3		Benzenamine, 2,5-dimethoxy-4-nitro-	198	C8H10N2O4	006313-37-7	38
4		3-Hydroxy-4,5-dimethoxybenzoic acid	198	C9H10O5	001916-08-1	38
5		Benzene, 1,1'-(1-fluoro-1,2-ethe...	198	C14H11F	000671-19-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081517.D
Acq On : 6 Sep 2015 18:55
Operator : UM/IZ
Sample : G3561-02
Misc :
ALS Vial : 92 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SANDYLOAM

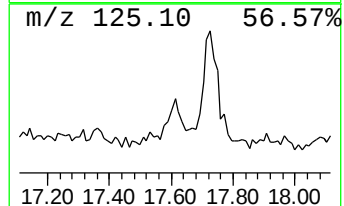
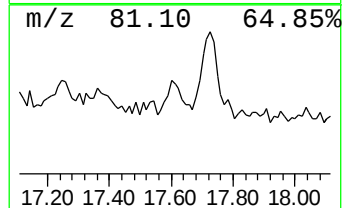
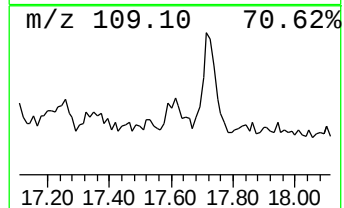
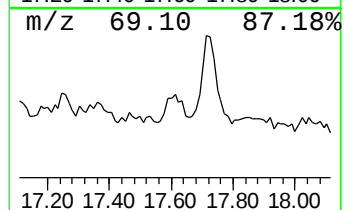
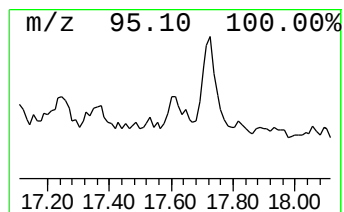
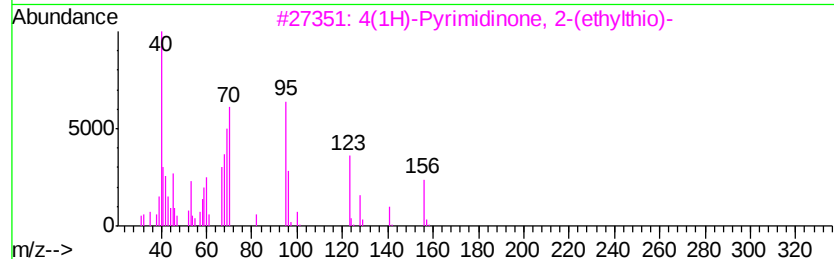
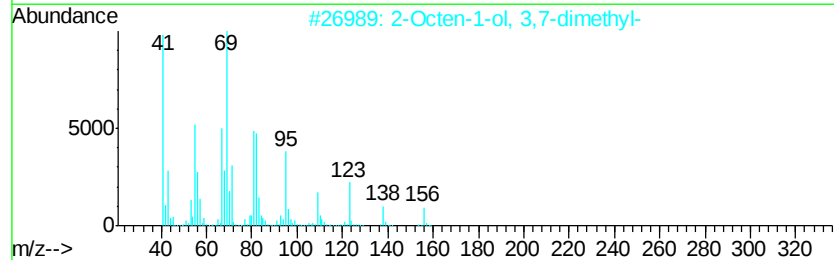
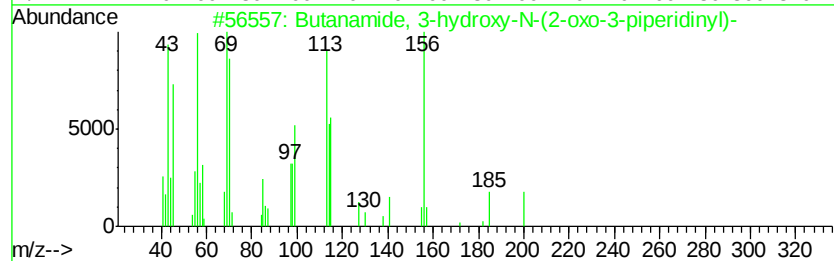
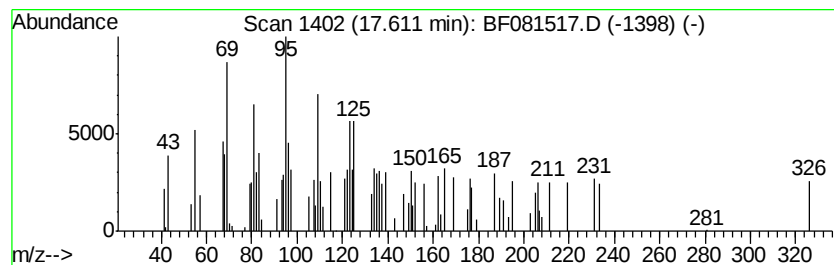
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Butanamide, 3-hydroxy-N-(2-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	7.31 ng	80193	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanamide, 3-hydroxy-N-(2-oxo-3...	200	C9H16N2O3	034655-85-1	53
2		2-Octen-1-ol, 3,7-dimethyl-	156	C10H20O	040607-48-5	40
3		4(1H)-Pyrimidinone, 2-(ethylthio)-	156	C6H8N2OS	006965-19-1	35
4		2,3-5,6-Bis(1,5-octanediyl)-2,5-...	300	C18H30B2O2	1000159-33-1	32
5		4-(1,5-Dimethylhex-4-enyl)cycloh...	206	C14H22O	001723-80-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
 Data File : BF081517.D
 Acq On : 6 Sep 2015 18:55
 Operator : UM/IZ
 Sample : G3561-02
 Misc :
 ALS Vial : 92 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SANDYLOAM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.39	39.2	ng	632709	1	6.35	322557	20.0
unknown6.12	6.12	71.7	ng	1155690	1	6.35	322557	20.0
5-Eicosene, (E)-	11.93	15.7	ng	380070	4	10.86	483587	20.0
Pentadecane	13.99	9.4	ng	217081	5	13.46	460840	20.0
Tetracosane	14.56	42.7	ng	468654	6	14.78	219307	20.0
Heptacosane	15.17	58.6	ng	643061	6	14.78	219307	20.0
unknown15.60	15.60	10.7	ng	117326	6	14.78	219307	20.0
Eicosane, 10-methyl-	15.94	9.7	ng	106136	6	14.78	219307	20.0
unknown16.30	16.30	29.1	ng	318721	6	14.78	219307	20.0
unknown16.50	16.50	5.7	ng	62072	6	14.78	219307	20.0
3-Methoxy-6,7,8,9...	16.59	23.7	ng	260346	6	14.78	219307	20.0
1-Oxaspiro[2.5]oc...	16.66	24.6	ng	269959	6	14.78	219307	20.0
unknown16.77	16.77	6.2	ng	67983	6	14.78	219307	20.0
1,5-Cycloundecadi...	16.83	36.8	ng	403912	6	14.78	219307	20.0
unknown16.94	16.94	9.3	ng	101757	6	14.78	219307	20.0
unknown16.99	16.99	12.5	ng	136636	6	14.78	219307	20.0
unknown17.23	17.23	14.8	ng	161752	6	14.78	219307	20.0
Butanamide, 3-hyd...	17.61	7.3	ng	80193	6	14.78	219307	20.0
Longifolenaldehyde	17.73	23.4	ng	256694	6	14.78	219307	20.0