

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
 Data File : BF083753.D
 Acq On : 14 Dec 2015 2:46
 Operator : UM/IZ
 Sample : G4758-01
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NCC-6

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	2.213	9	11	27	rVB	62151	168978	5.63%	0.434%
2	5.116	261	265	269	rVB	436840	704010	23.45%	1.807%
3	5.527	298	301	303	rBV	2751902	2949529	98.26%	7.569%
4	6.545	387	390	392	rBV	2570279	2738137	91.21%	7.027%
5	6.682	400	402	405	rBV	2418648	2893088	96.38%	7.424%
6	6.922	420	423	425	rBV	842809	912810	30.41%	2.342%
7	7.070	434	436	439	rVB	1780423	2473823	82.41%	6.348%
8	7.482	468	472	474	rBV	1565536	2052832	68.38%	5.268%
9	8.202	533	535	537	rBV	1369639	1221197	40.68%	3.134%
10	9.276	626	629	631	rBV	3320608	3001903	100.00%	7.704%
11	9.619	658	659	661	rVB	45384	32626	1.09%	0.084%
12	9.665	661	663	665	rBV	456732	361556	12.04%	0.928%
13	9.893	682	683	686	rVB	57045	36551	1.22%	0.094%
14	9.951	686	688	690	rBV	1310507	1170585	38.99%	3.004%
15	10.396	722	727	728	rBV	52691	75993	2.53%	0.195%
16	10.614	743	746	749	rBV2	30341	66922	2.23%	0.172%
17	10.739	754	757	759	rVV	1358655	1642164	54.70%	4.214%
18	10.865	765	768	772	rBV	106241	130562	4.35%	0.335%
19	11.311	803	807	809	rBV	60329	62610	2.09%	0.161%
20	11.425	815	817	820	rVV	670795	928625	30.93%	2.383%
21	11.471	820	821	825	rVB4	109997	166340	5.54%	0.427%
22	11.574	829	830	836	rVB3	32205	44248	1.47%	0.114%
23	11.654	836	837	840	rBV	39737	48864	1.63%	0.125%
24	11.894	855	858	859	rBV2	30991	45895	1.53%	0.118%
25	11.962	862	864	870	rVV3	141076	210914	7.03%	0.541%
26	12.134	875	879	882	rBV3	85248	127256	4.24%	0.327%
27	12.317	892	895	898	rBV4	19327	43838	1.46%	0.112%
28	12.477	907	909	911	rBV	29678	37502	1.25%	0.096%
29	12.534	911	914	915	rVB3	32104	52773	1.76%	0.135%
30	12.579	916	918	921	rVB	58292	62784	2.09%	0.161%
31	12.637	921	923	924	rBV	65046	56299	1.88%	0.144%
32	12.682	924	927	931	rVB4	94335	136853	4.56%	0.351%
33	12.751	931	933	935	rBV3	24937	40414	1.35%	0.104%
34	12.842	940	941	944	rVV2	83171	122548	4.08%	0.314%

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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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.014	953	956	958	rBV	2109403	1862666	62.05%	4.780%
36	13.197	968	972	973	rBV2	20371	48217	1.61%	0.124%
37	13.265	976	978	979	rVV2	32069	39477	1.32%	0.101%
38	13.448	990	994	995	rBV2	122875	201784	6.72%	0.518%
39	13.471	995	996	1001	rVV3	74613	193880	6.46%	0.498%
40	13.551	1001	1003	1005	rVV2	76957	91252	3.04%	0.234%
41	13.642	1005	1011	1012	rVV3	22883	74958	2.50%	0.192%
42	13.711	1015	1017	1019	rVB3	25464	34949	1.16%	0.090%
43	13.802	1023	1025	1027	rBV2	30262	47844	1.59%	0.123%
44	13.905	1032	1034	1039	rBV	207460	346762	11.55%	0.890%
45	13.985	1039	1041	1043	rBV	120444	120667	4.02%	0.310%
46	14.054	1045	1047	1053	rVB2	785659	1089272	36.29%	2.795%
47	14.168	1053	1057	1059	rBV4	21542	55397	1.85%	0.142%
48	14.237	1061	1063	1066	rBV3	31133	53320	1.78%	0.137%
49	14.465	1080	1083	1085	rBV3	42785	84629	2.82%	0.217%
50	14.511	1085	1087	1088	rVV	45071	44911	1.50%	0.115%
51	14.545	1088	1090	1092	rVV	164915	188848	6.29%	0.485%
52	14.591	1092	1094	1096	rVB	50410	60688	2.02%	0.156%
53	14.820	1112	1114	1120	rBV	420168	501565	16.71%	1.287%
54	14.922	1120	1123	1125	rVB	132455	175216	5.84%	0.450%
55	15.083	1134	1137	1140	rBV	106432	233628	7.78%	0.600%
56	15.174	1143	1145	1150	rBV3	212725	335416	11.17%	0.861%
57	15.380	1161	1163	1165	rBV	69337	99420	3.31%	0.255%
58	15.437	1165	1168	1170	rVB	56172	81258	2.71%	0.209%
59	15.494	1170	1173	1176	rBV	648924	974359	32.46%	2.500%
60	15.643	1184	1186	1190	rVB4	36866	83402	2.78%	0.214%
61	15.745	1193	1195	1197	rBV2	27742	47305	1.58%	0.121%
62	15.985	1213	1216	1218	rBV	174554	315699	10.52%	0.810%
63	16.020	1218	1219	1224	rVV3	87520	187298	6.24%	0.481%
64	16.134	1227	1229	1234	rVV5	58618	168591	5.62%	0.433%
65	16.237	1234	1238	1245	rVB3	101052	344095	11.46%	0.883%
66	16.637	1271	1273	1281	rVB5	47914	111048	3.70%	0.285%
67	16.923	1295	1298	1301	rBV2	35989	83166	2.77%	0.213%
68	17.071	1308	1311	1313	rBV	40711	92285	3.07%	0.237%
69	17.128	1313	1316	1321	rVB4	54459	157346	5.24%	0.404%
70	17.300	1328	1331	1333	rBV2	66463	129296	4.31%	0.332%
71	17.471	1343	1346	1347	rBV3	38713	75484	2.51%	0.194%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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72	17.540	1347	1352	1358	rBV2	433855	1571092	52.34%	4.032%
73	17.746	1363	1370	1374	rBV2	141815	491387	16.37%	1.261%
74	17.849	1377	1379	1382	rVB2	49891	97952	3.26%	0.251%
75	17.986	1387	1391	1393	rBV2	119542	302839	10.09%	0.777%
76	18.089	1397	1400	1408	rVB3	368511	1025551	34.16%	2.632%
77	18.226	1409	1412	1416	rVB2	55981	139585	4.65%	0.358%
78	18.317	1416	1420	1422	rBV2	252908	655153	21.82%	1.681%
79	18.466	1430	1433	1436	rVB3	71711	159824	5.32%	0.410%
80	18.534	1436	1439	1447	rVB4	102588	283490	9.44%	0.727%
81	18.820	1460	1464	1465	rBV4	30152	81092	2.70%	0.208%
82	19.392	1509	1514	1522	rVB2	148198	503628	16.78%	1.292%

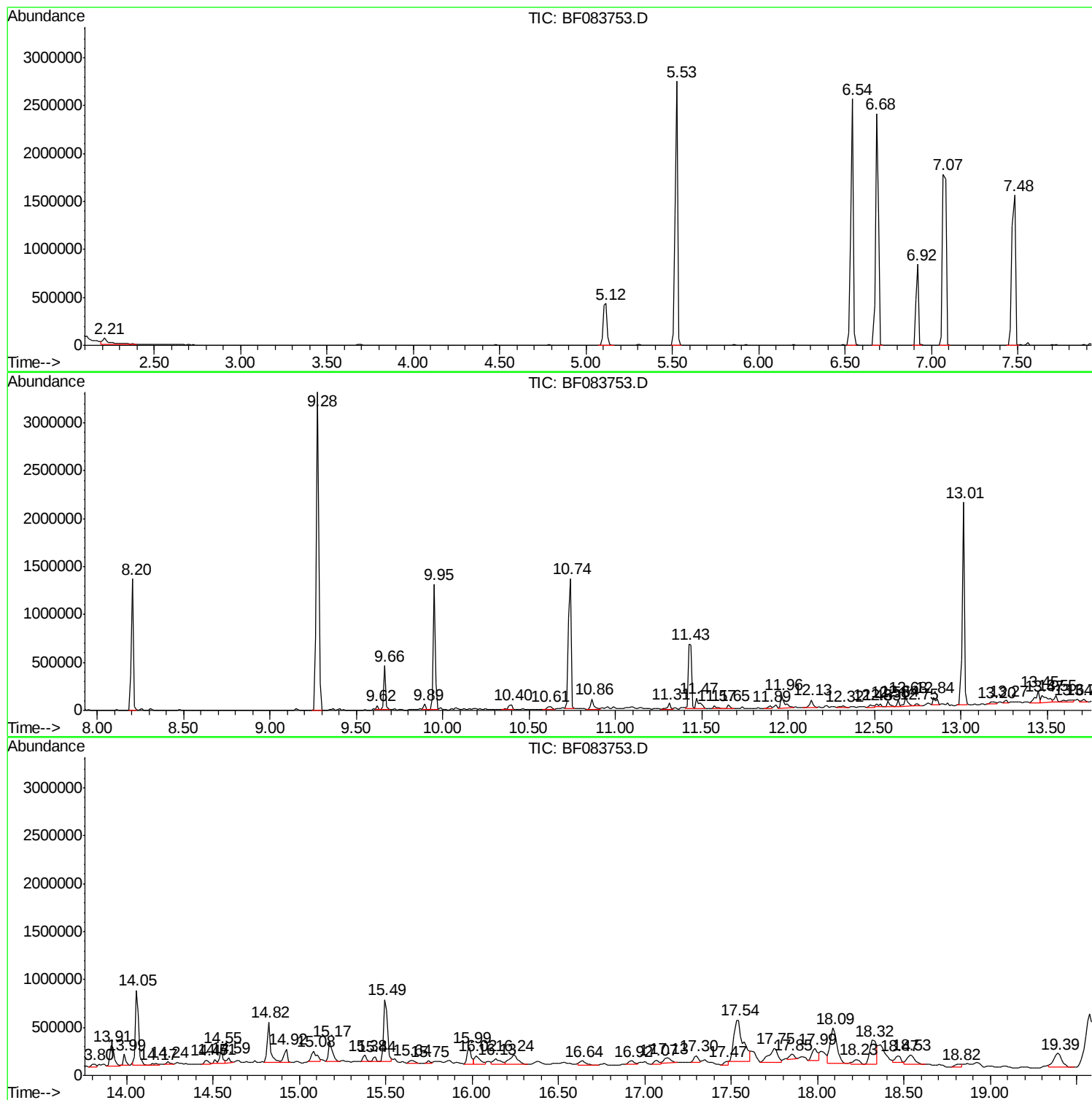
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF083753.D
Acq On : 14 Dec 2015 2:46
Operator : UM/IZ
Sample : G4758-01
Misc :
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Instrument :
BNA_F
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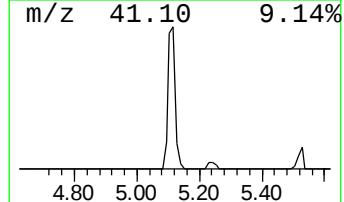
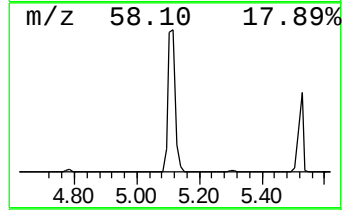
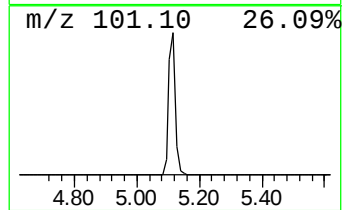
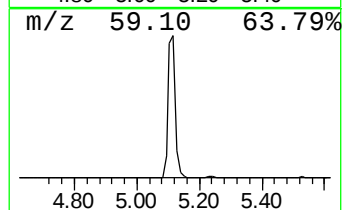
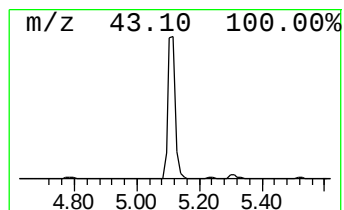
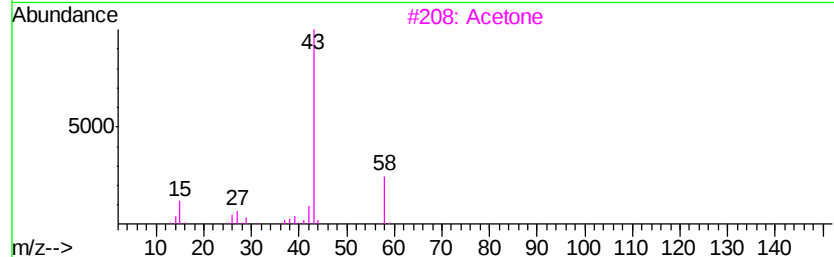
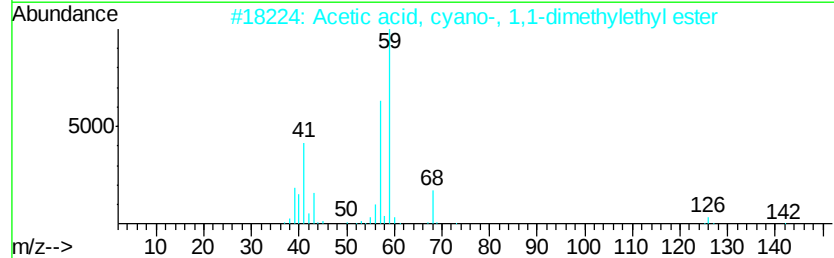
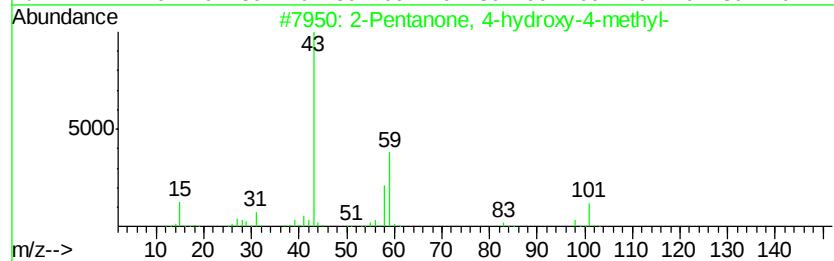
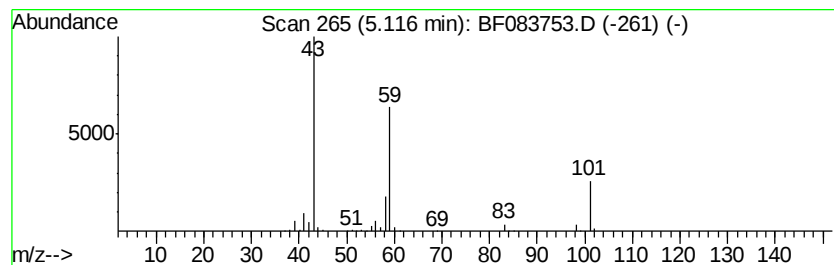
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	15.43 ng	704010	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	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Acetone	58	C3H6O	000067-64-1	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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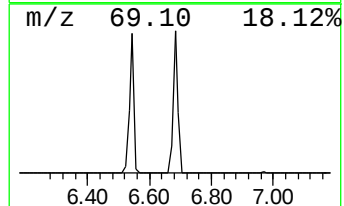
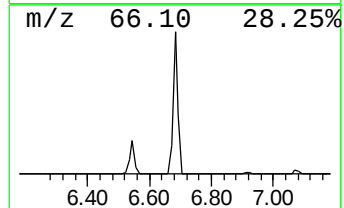
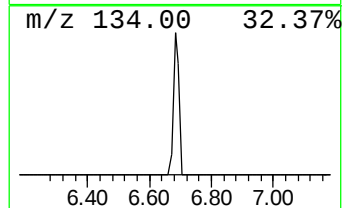
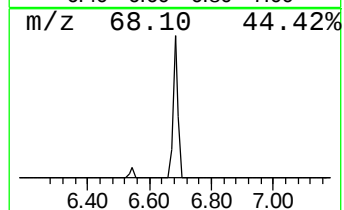
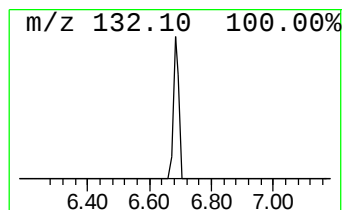
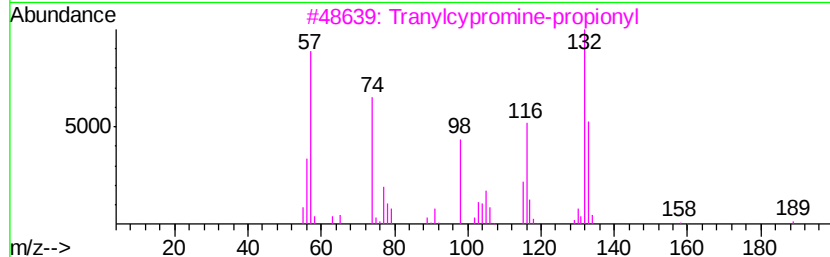
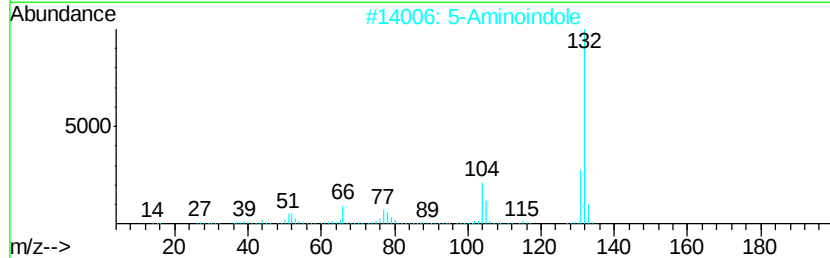
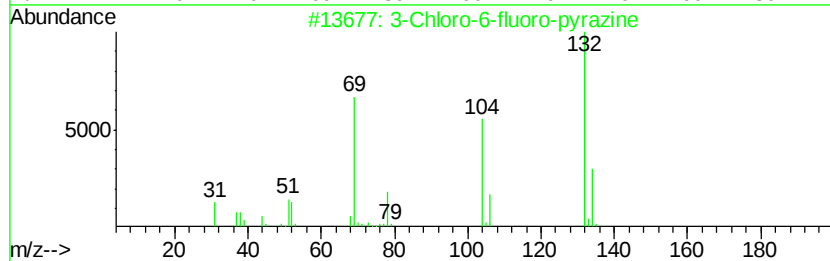
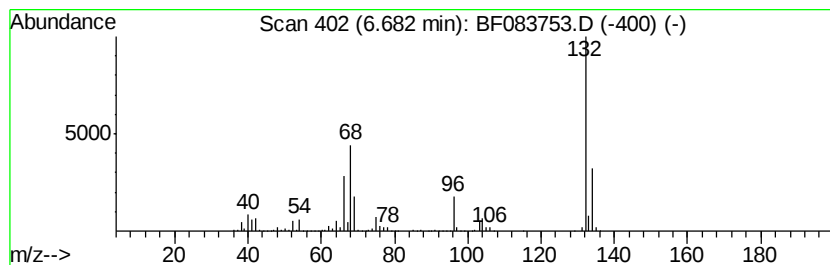
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	63.39 ng	2893090	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-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



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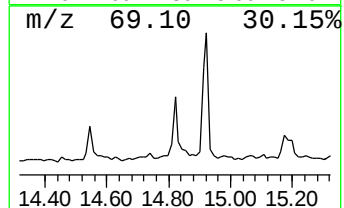
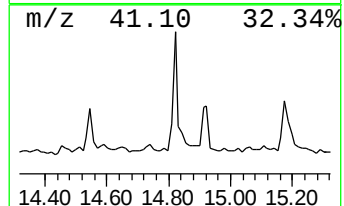
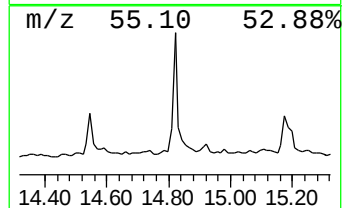
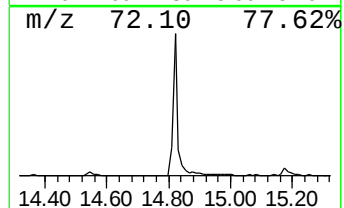
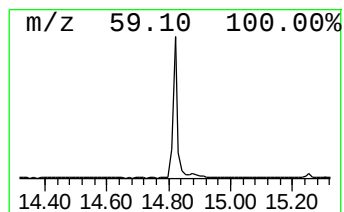
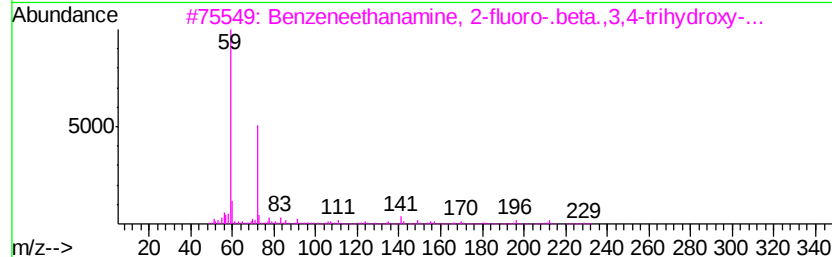
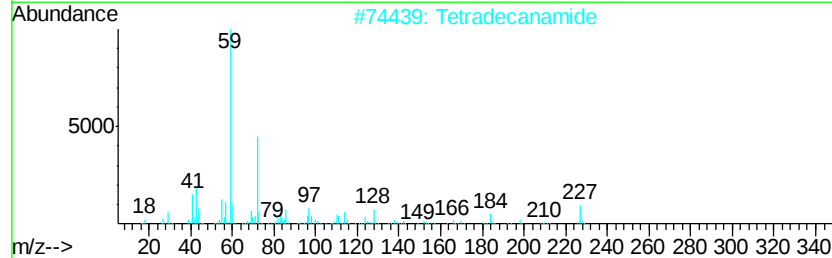
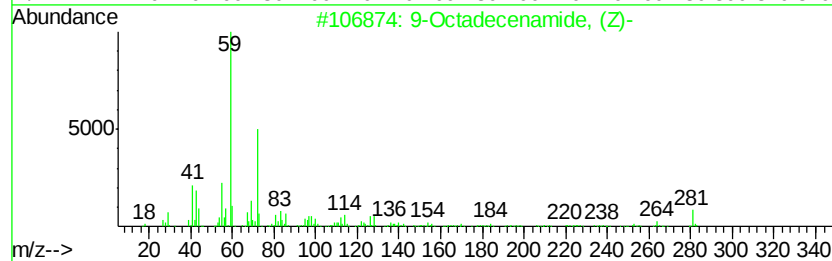
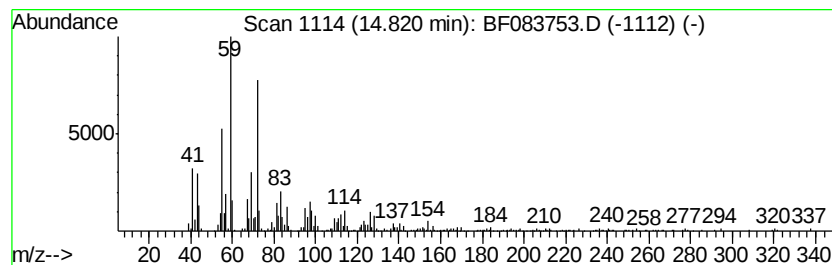
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	10.30 ng	501565	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2		Tetradecanamide	227	C14H29NO	000638-58-4	50
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43
5		Dodecanamide	199	C12H25NO	001120-16-7	38



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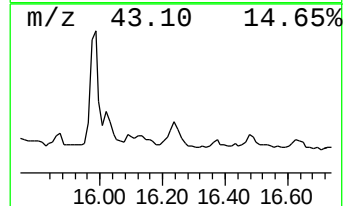
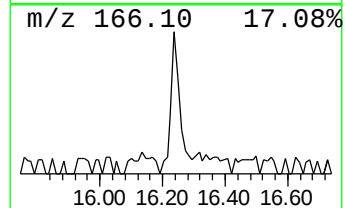
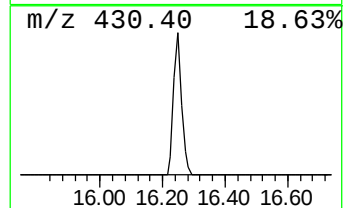
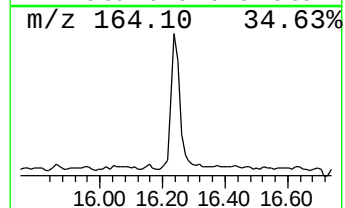
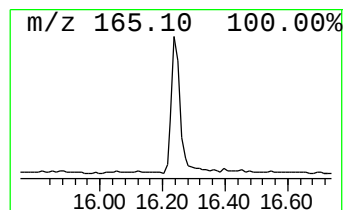
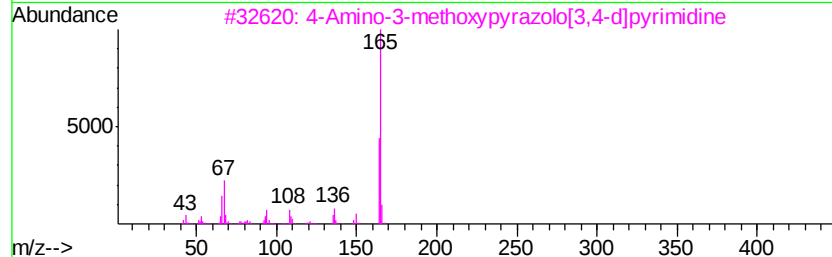
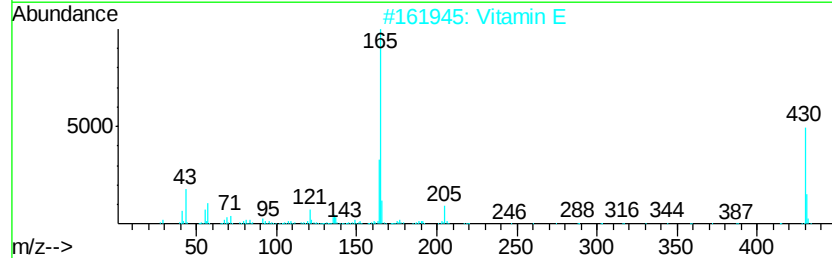
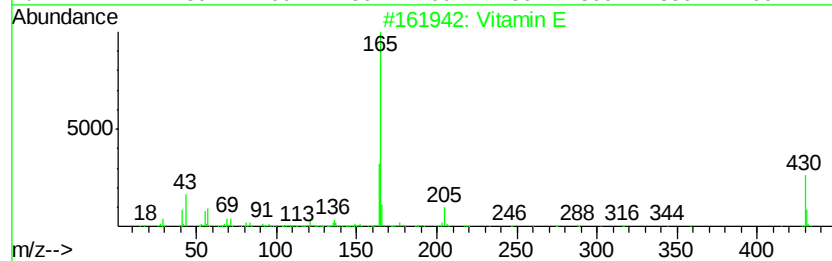
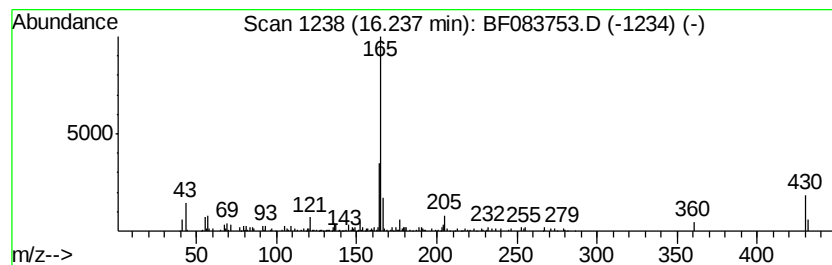
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Vitamin E Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	7.06 ng	344095	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vitamin E	430	C29H50O2	010191-41-0	94
2		Vitamin E	430	C29H50O2	000059-02-9	93
3		4-Amino-3-methoxypprazolo[3,4-d]...	165	C6H7N5O	111375-22-5	59
4		Stannane, ethyltrimethyl-	194	C5H14Sn	003531-44-0	42
5		Benzoic amide, 2,5-dimethoxy-N-[...	253	C13H19NO4	1000126-74-4	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083753.D
Acq On : 14 Dec 2015 2:46
Operator : UM/IZ
Sample : G4758-01
Misc :
ALS Vial : 43 Sample Multiplier: 1

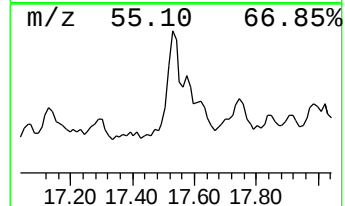
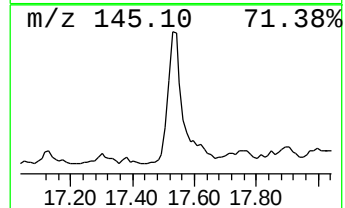
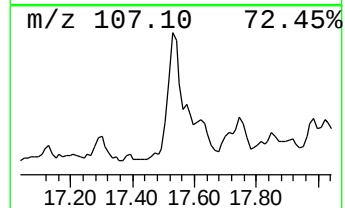
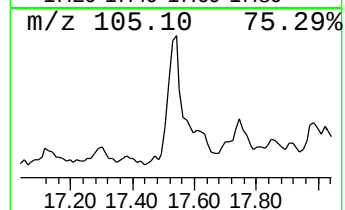
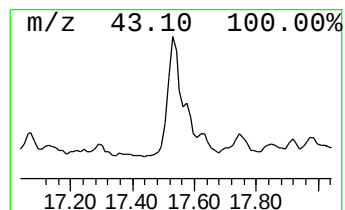
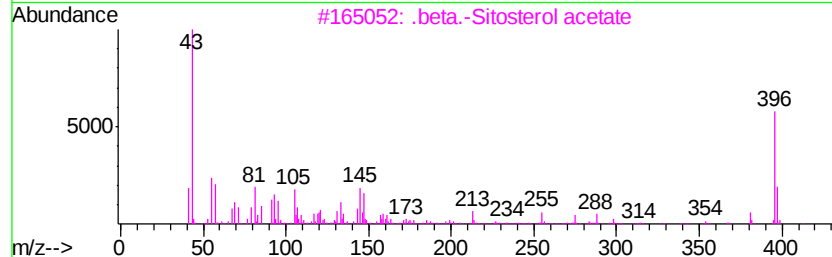
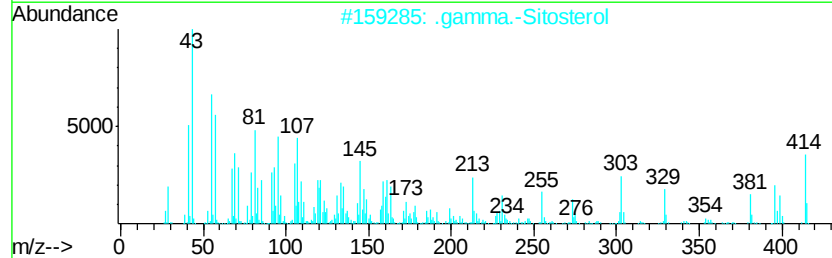
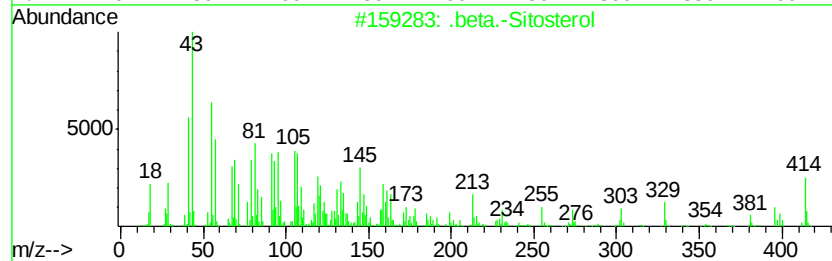
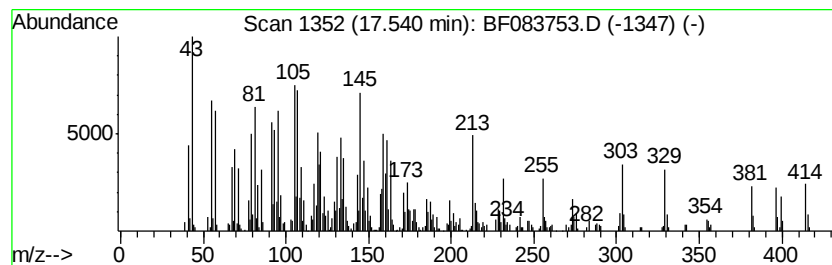
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.54	32.25 ng	1571090	Perylene-d12	15.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 97
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 91
3		.beta.-Sitosterol acetate	456 C31H52O2	000915-05-9 38
4		Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H50O	000986-19-6 35
5		Isocholesteryl methyl ether	400 C28H48O	029944-53-4 35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083753.D
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ClientSampleId :
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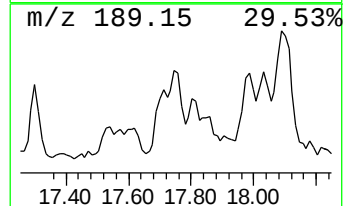
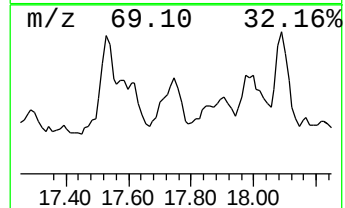
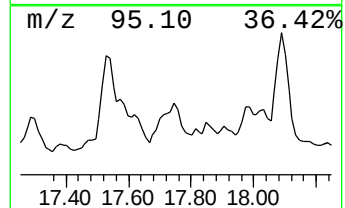
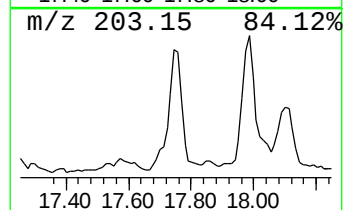
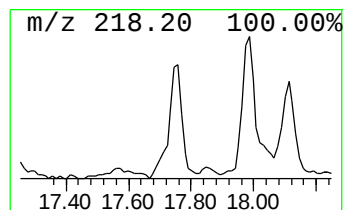
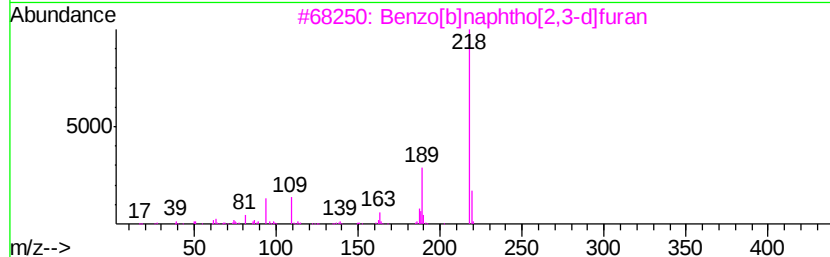
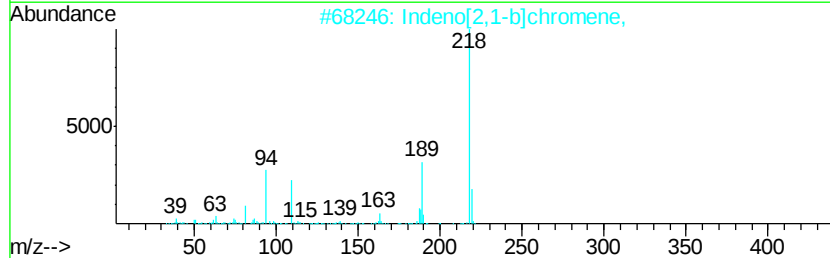
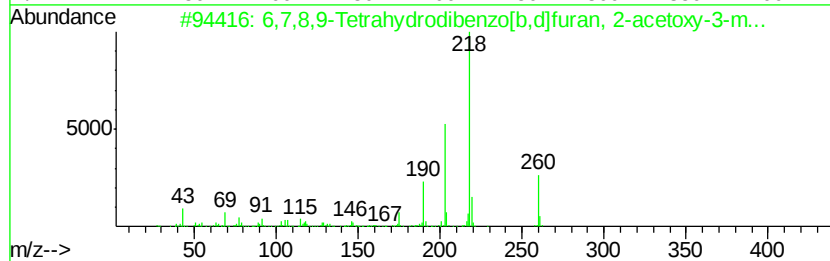
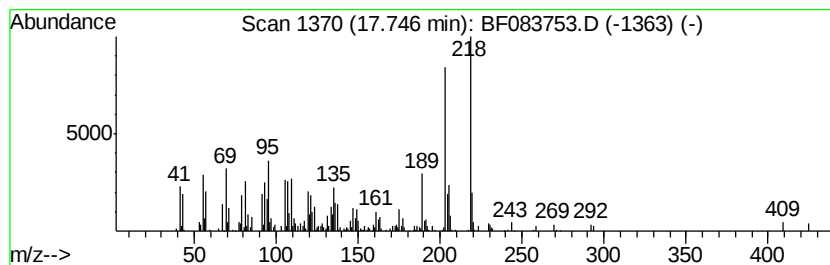
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	10.09 ng	491387	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6,7,8,9-Tetrahydrodibenzo[b,d]fu...	260	C15H16O4	1000196-34-3	38
2		Indeno[2,1-b]chromene,	218	C16H10O	000243-24-3	38
3		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	38
4		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	38
5		1-Pyrrolin-2-amine, N-(1-adamant...	218	C14H22N2	300695-00-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083753.D
Acq On : 14 Dec 2015 2:46
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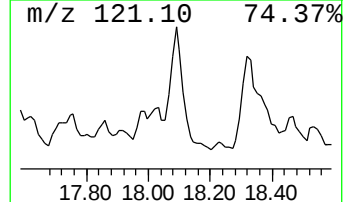
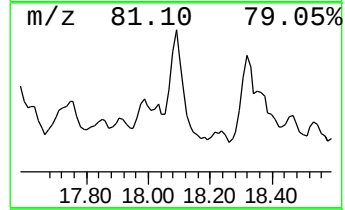
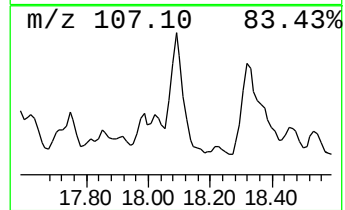
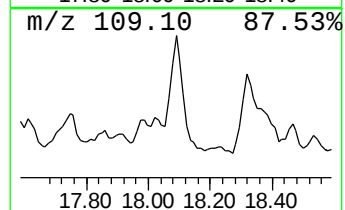
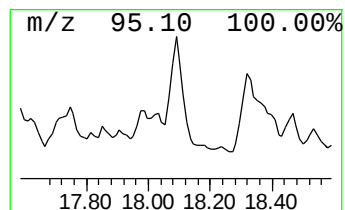
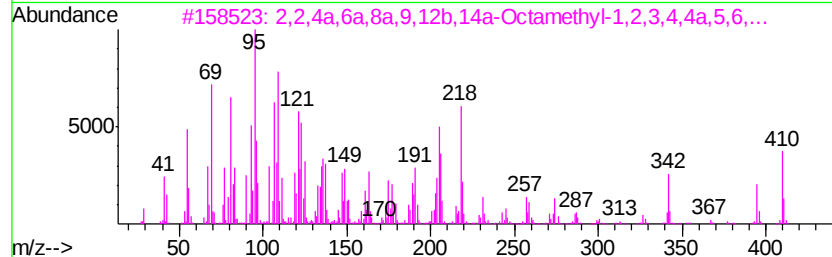
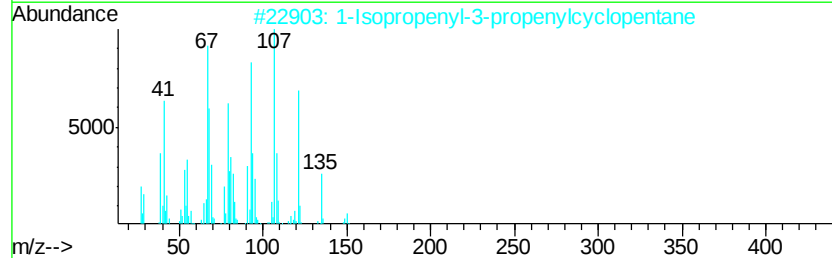
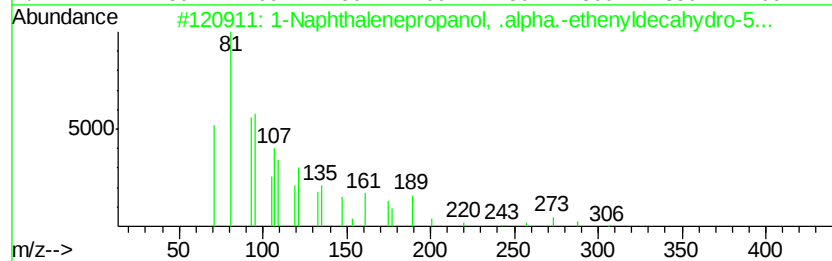
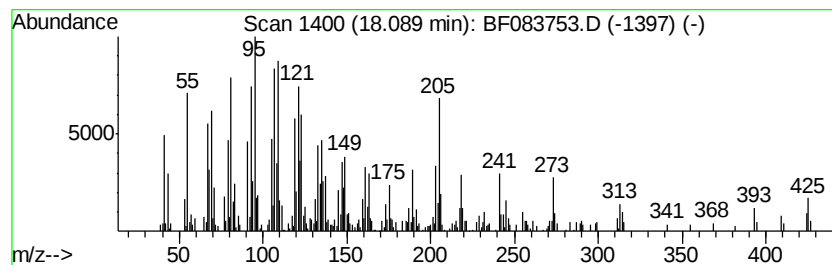
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Naphthalenepropanol, .alp... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	21.05 ng	1025550	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	004549-12-6	68
2		1-Isopropenyl-3-propenylcyclopent...	150	C11H18	1000192-81-2	49
3		2,2,4a,6a,8a,9,12b,14a-Octamethv...	410	C30H50	053013-35-7	47
4		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	44
5		13,15-Octacosadiyne	386	C28H50	024643-46-7	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
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Acq On : 14 Dec 2015 2:46
Operator : UM/IZ
Sample : G4758-01
Misc :
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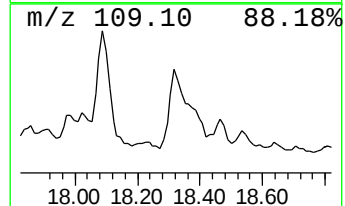
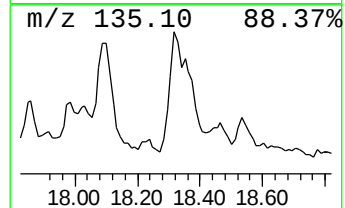
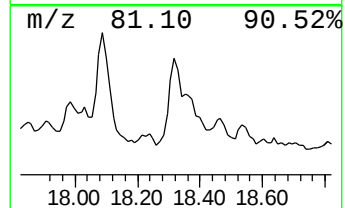
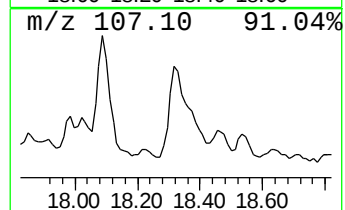
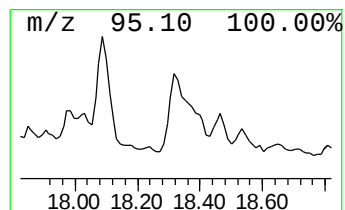
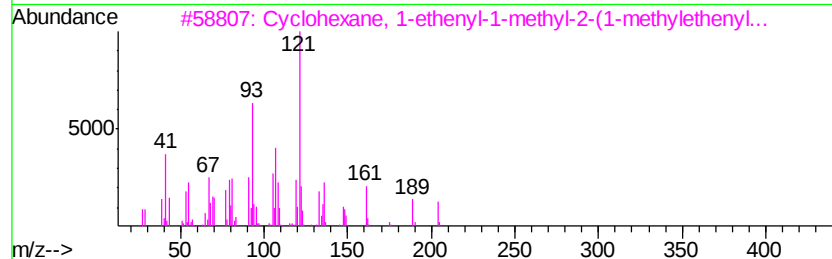
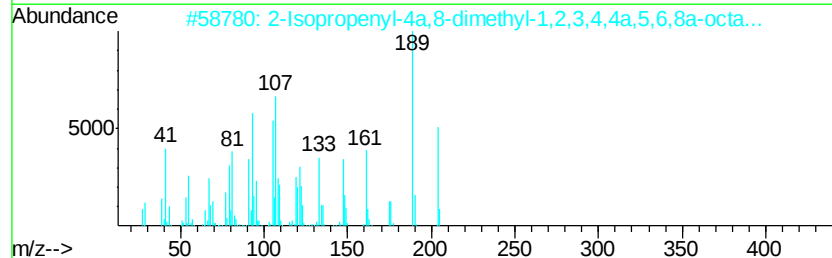
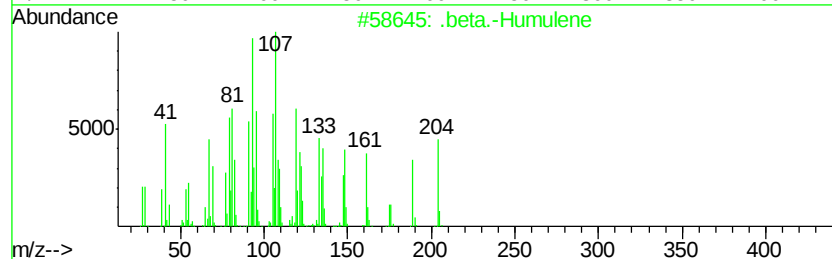
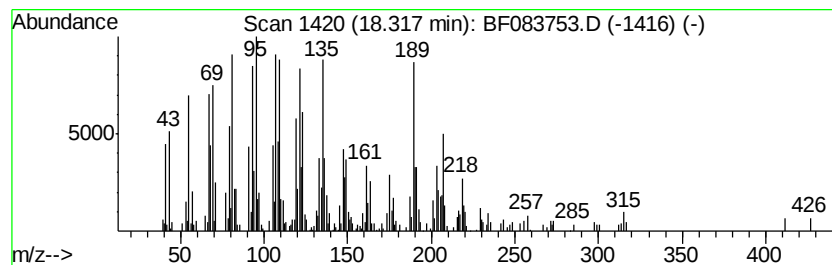
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-Humulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	13.45 ng	655153	Perylene-d12	15.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Humulene	204 C15H24	000116-04-1 74
2		2-Isopropenyl-4a,8-dimethyl-1,2,...	204 C15H24	1000193-57-0 49
3		Cyclohexane, 1-ethenyl-1-methyl-...	204 C15H24	003242-08-8 46
4		.gamma.-Elemene	204 C15H24	030824-67-0 46
5		Hop-22(29)-en-3.beta.-ol	426 C30H50O	058801-23-3 46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083753.D
Acq On : 14 Dec 2015 2:46
Operator : UM/IZ
Sample : G4758-01
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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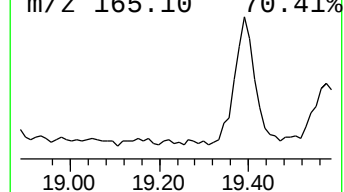
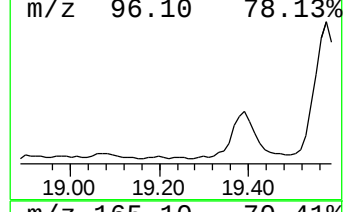
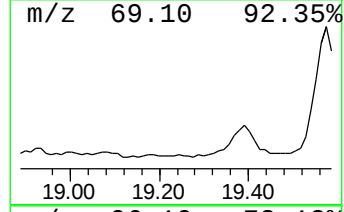
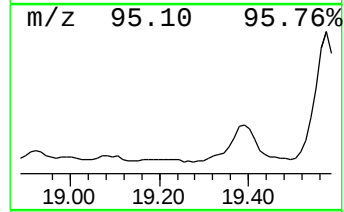
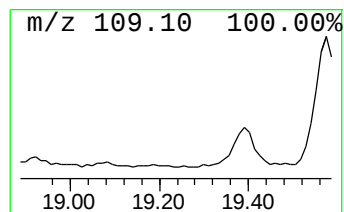
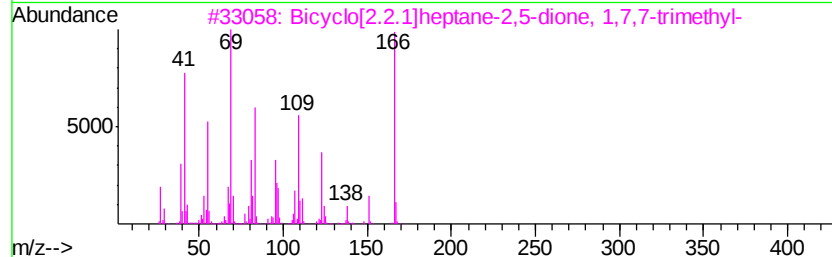
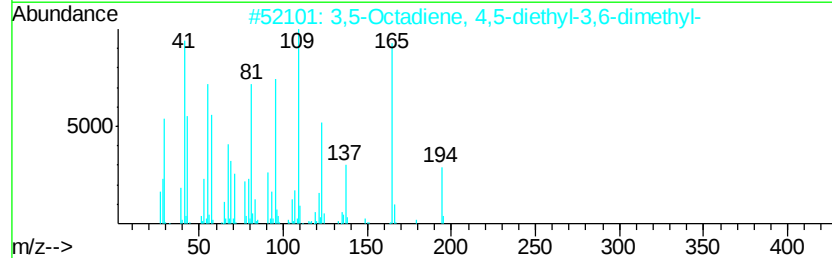
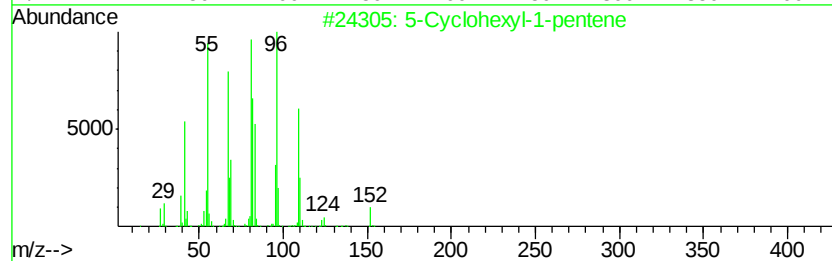
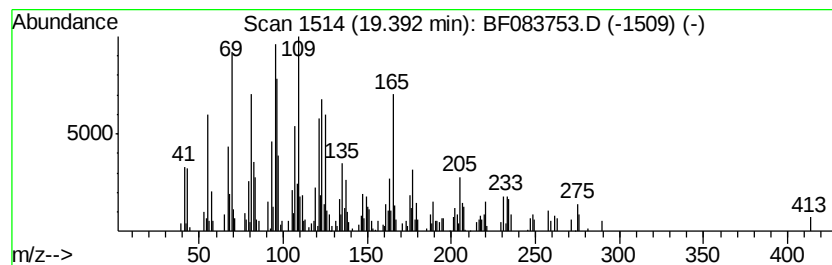
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Cyclohexyl-1-pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	10.34 ng	503628	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	53
2		3,5-Octadiene, 4,5-diethyl-3,6-d...	194	C14H26	061233-79-2	41
3		Bicyclo[2.2.1]heptane-2,5-dione,...	166	C10H14O2	004230-32-4	38
4		Naphthalene, decahydro-1,2-dimet...	166	C12H22	003604-14-6	38
5		(7,7-Dimethyl-2-oxobicyclo[2.2.1...	246	C11H18O4S	1000197-55-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083753.D
Acq On : 14 Dec 2015 2:46
Operator : UM/IZ
Sample : G4758-01
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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unknown6.68	6.68	63.4	ng	2893090	1	6.92	912810	20.0
9-Octadecenamide, ...	14.82	10.3	ng	501565	6	15.49	974359	20.0
Vitamin E	16.24	7.1	ng	344095	6	15.49	974359	20.0
.beta.-Sitosterol	17.54	32.3	ng	1571090	6	15.49	974359	20.0
unknown17.75	17.75	10.1	ng	491387	6	15.49	974359	20.0
1-Naphthaleneprop...	18.09	21.1	ng	1025550	6	15.49	974359	20.0
.beta.-Humulene	18.32	13.4	ng	655153	6	15.49	974359	20.0
5-Cyclohexyl-1-pe...	19.39	10.3	ng	503628	6	15.49	974359	20.0