

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
 Data File : BF083724.D
 Acq On : 12 Dec 2015 4:53
 Operator : UM/IZ
 Sample : G4648-09
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04(20-24)

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-BF121115.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	5.116	262	265	274	rVB	534494	753775	16.70%	2.087%
2	5.527	298	301	304	rBV	2639284	3504335	77.64%	9.702%
3	6.545	387	390	393	rBV	2662035	3277611	72.61%	9.074%
4	6.693	400	403	405	rBV	3495509	3748710	83.05%	10.379%
5	6.922	421	423	426	rVB	949069	786694	17.43%	2.178%
6	7.082	434	437	439	rBV	3271428	2942491	65.19%	8.147%
7	7.482	469	472	474	rBV	2238595	2247397	49.79%	6.222%
8	7.562	474	479	485	rVB	36313	55387	1.23%	0.153%
9	8.202	533	535	538	rBV	829351	985013	21.82%	2.727%
10	9.288	627	630	632	rBV	4088466	4513827	100.00%	12.497%
11	9.676	661	664	666	rBV	762384	687800	15.24%	1.904%
12	9.905	682	684	686	rVB	48079	46591	1.03%	0.129%
13	9.962	686	689	691	rBV	1180461	1141815	25.30%	3.161%
14	10.396	726	727	729	rVB	98069	86436	1.91%	0.239%
15	10.625	743	747	749	rBV	33322	61789	1.37%	0.171%
16	10.739	755	757	760	rBV2	2040725	2480233	54.95%	6.867%
17	10.876	767	769	772	rBV	86432	149919	3.32%	0.415%
18	11.059	783	785	788	rBV3	22564	52580	1.16%	0.146%
19	11.322	804	808	809	rBV	62846	73164	1.62%	0.203%
20	11.436	816	818	820	rBV	1355710	1122584	24.87%	3.108%
21	12.488	908	910	912	rBV	42955	47121	1.04%	0.130%
22	12.682	924	927	931	rVB	45950	61480	1.36%	0.170%
23	12.854	939	942	943	rBV2	83750	101781	2.25%	0.282%
24	13.025	954	957	959	rVB	4060477	4029729	89.28%	11.157%
25	13.185	969	971	972	rBV	59844	69259	1.53%	0.192%
26	13.505	997	999	1001	rVB	111840	120409	2.67%	0.333%
27	13.562	1001	1004	1006	rVV	115447	178138	3.95%	0.493%
28	13.654	1009	1012	1013	rVV	75318	119246	2.64%	0.330%
29	13.688	1013	1015	1016	rVV	122694	173948	3.85%	0.482%
30	13.722	1016	1018	1021	rVB	77246	105702	2.34%	0.293%
31	13.871	1027	1031	1034	rVB2	57783	108324	2.40%	0.300%
32	13.917	1034	1035	1038	rBV2	40453	61344	1.36%	0.170%
33	13.997	1039	1042	1044	rBV	175514	184659	4.09%	0.511%
34	14.065	1044	1048	1050	rBV	1022423	999267	22.14%	2.767%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

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-BF121115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.305	1066	1069	1070	rBV	66115	88244	1.95%	0.244%
36	14.340	1070	1072	1075	rVB2	33962	58430	1.29%	0.162%
37	14.602	1092	1095	1096	rBV	62175	82001	1.82%	0.227%
38	14.751	1104	1108	1109	rBV2	73388	122417	2.71%	0.339%
39	14.797	1109	1112	1116	rVB2	32356	58742	1.30%	0.163%
40	15.505	1171	1174	1177	rBV	518904	631294	13.99%	1.748%

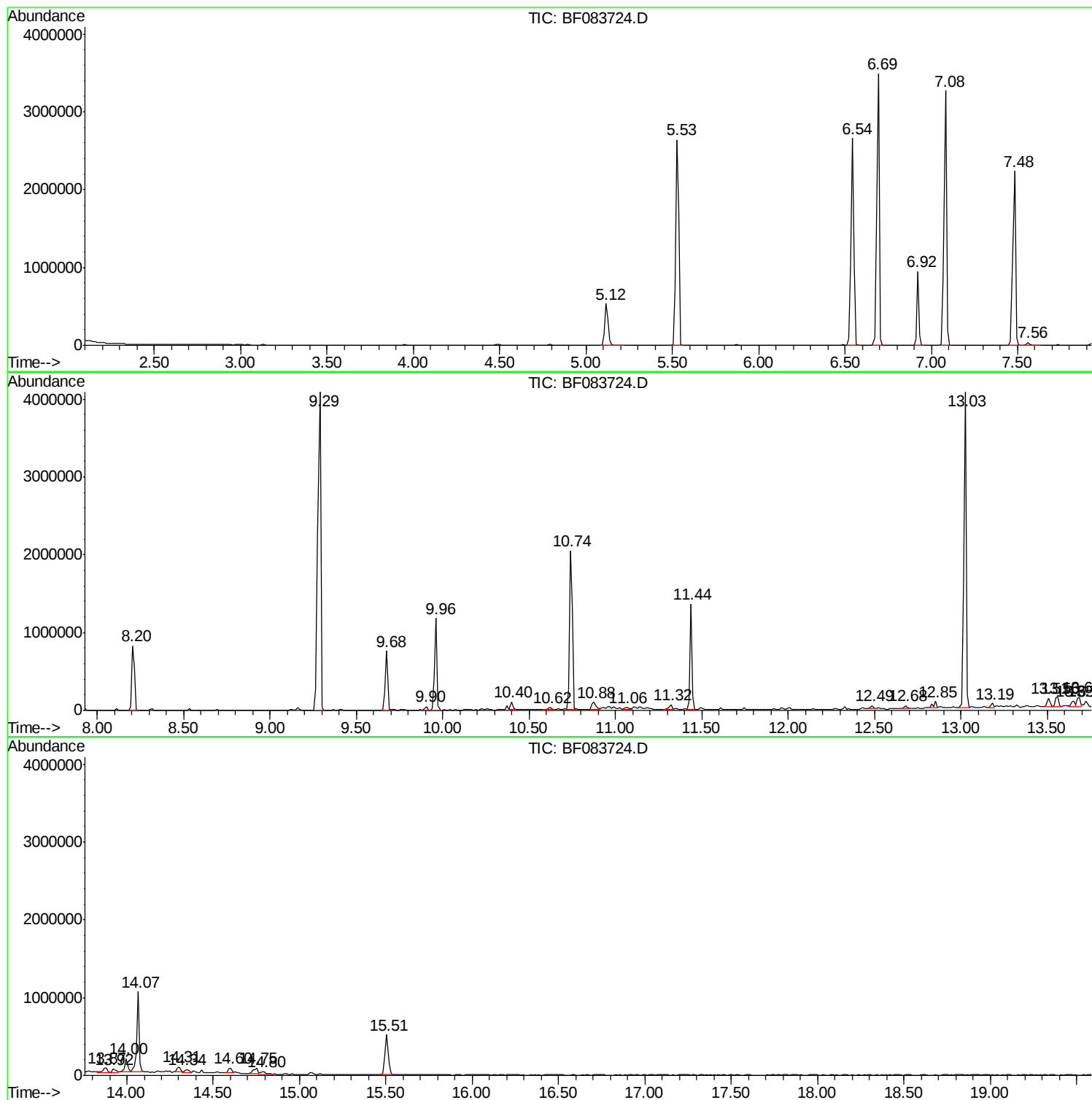
Sum of corrected areas: 36119686

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.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\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

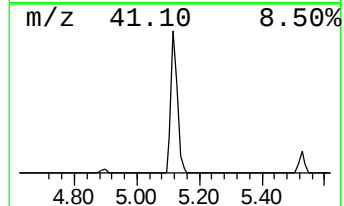
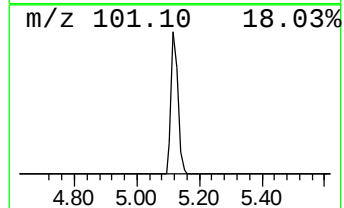
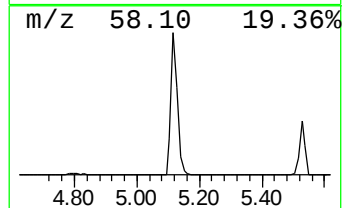
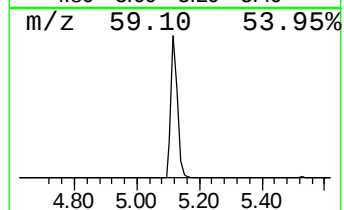
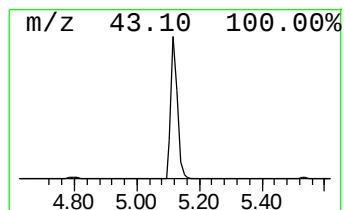
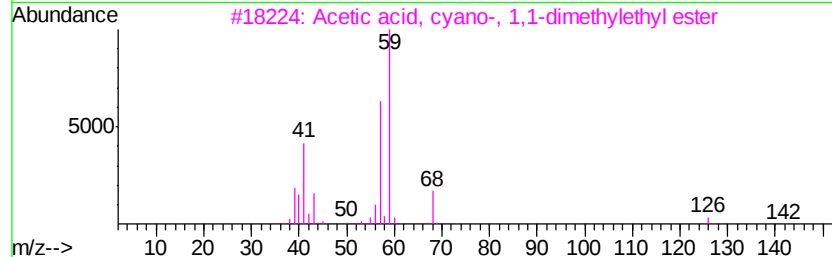
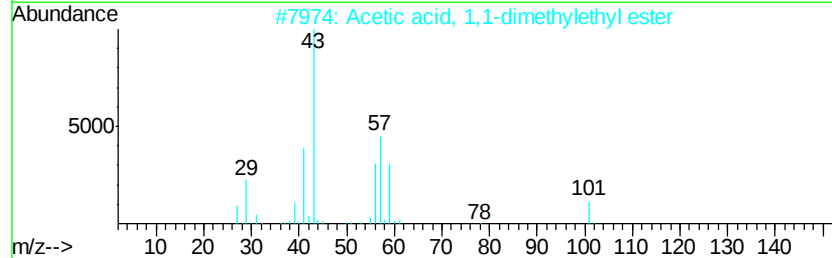
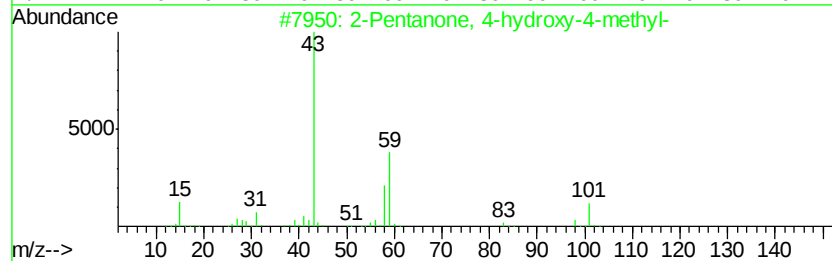
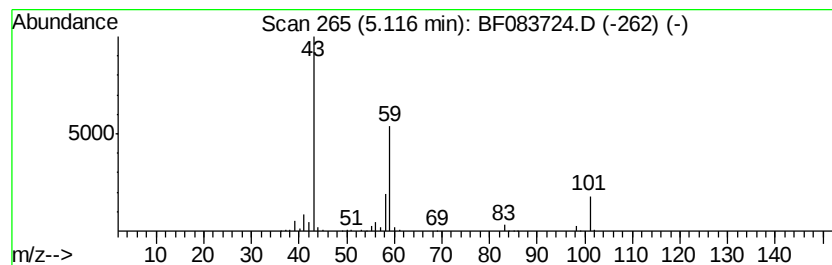
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	19.16 ng	753775	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

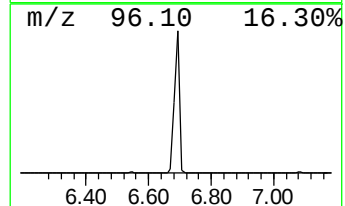
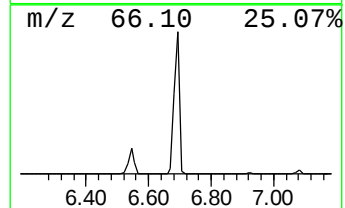
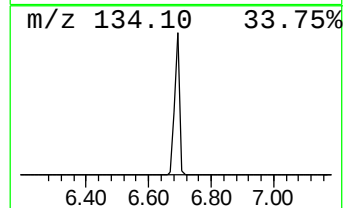
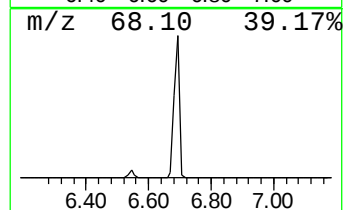
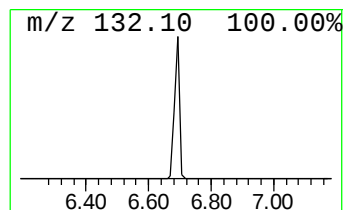
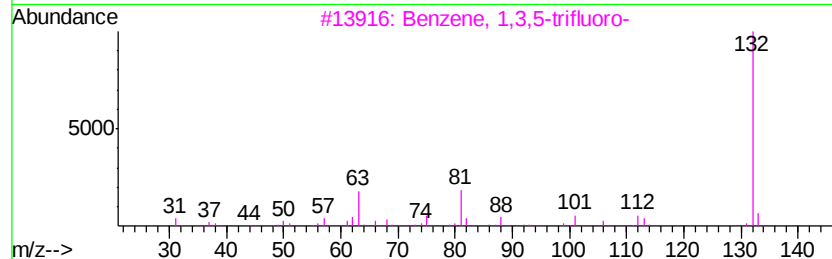
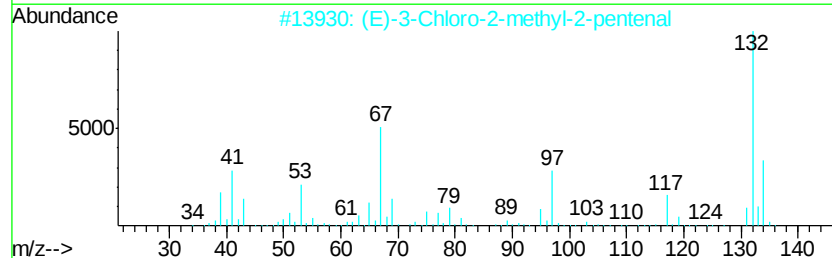
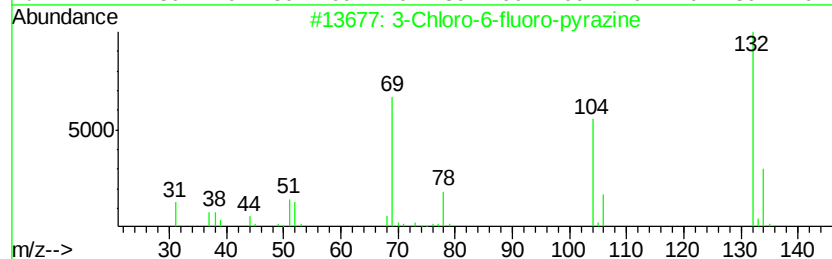
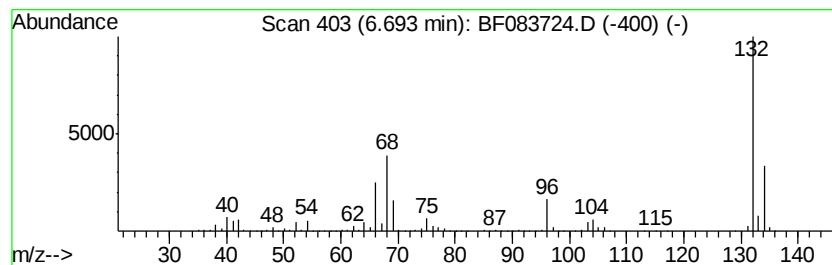
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	95.30 ng	3748710	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

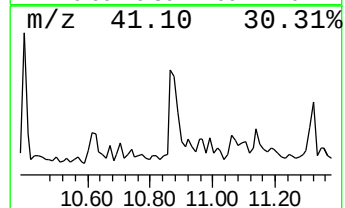
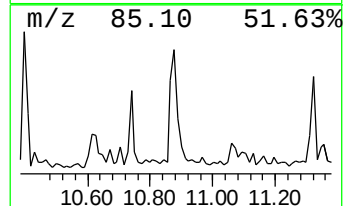
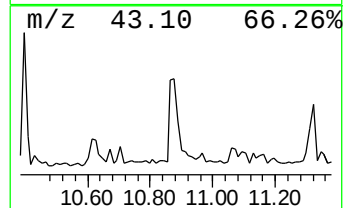
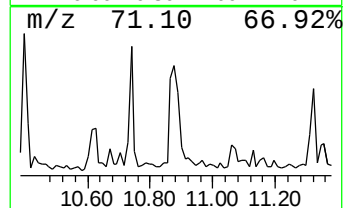
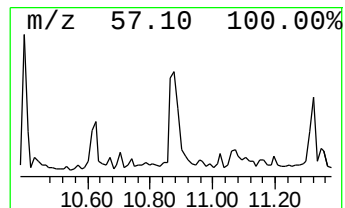
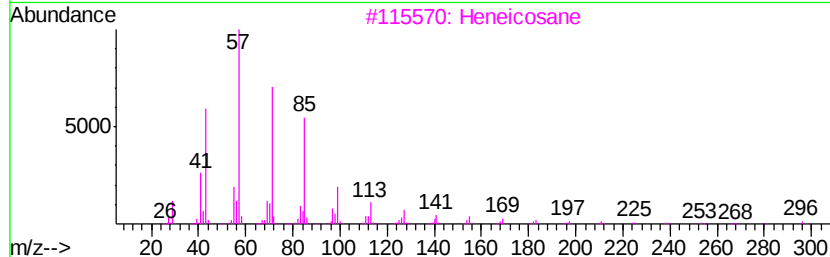
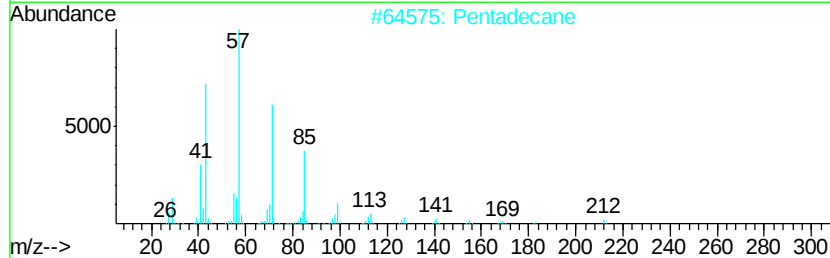
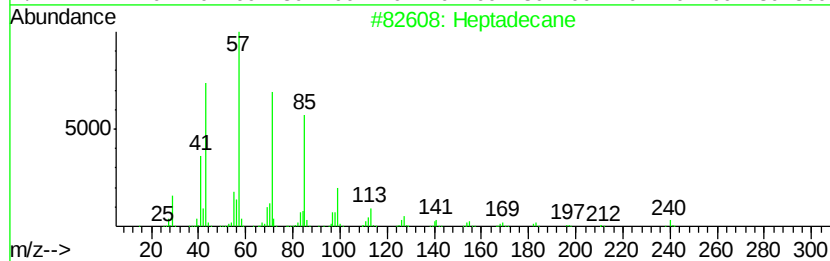
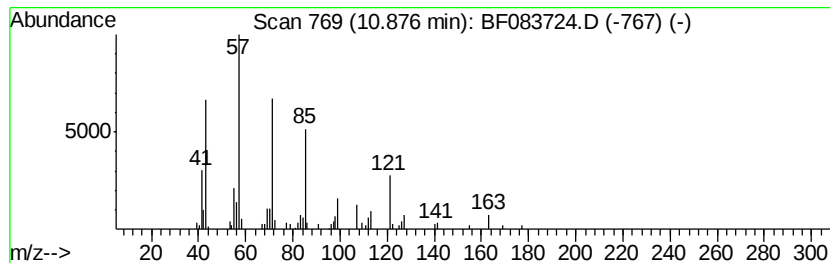
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.67 ng	149919	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	87
2	Pentadecane		212	C15H32	000629-62-9	86
3	Heneicosane		296	C21H44	000629-94-7	83
4	Octadecane		254	C18H38	000593-45-3	80
5	Hexadecane		226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

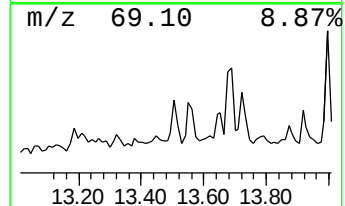
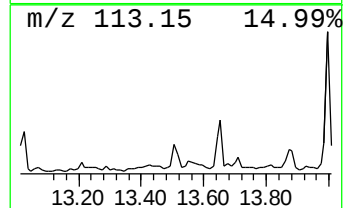
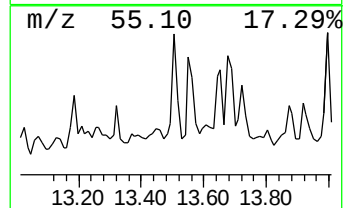
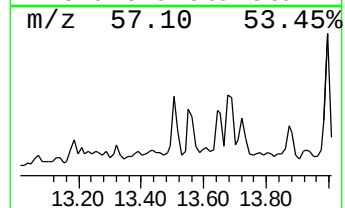
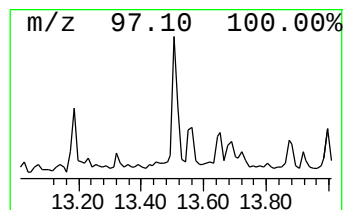
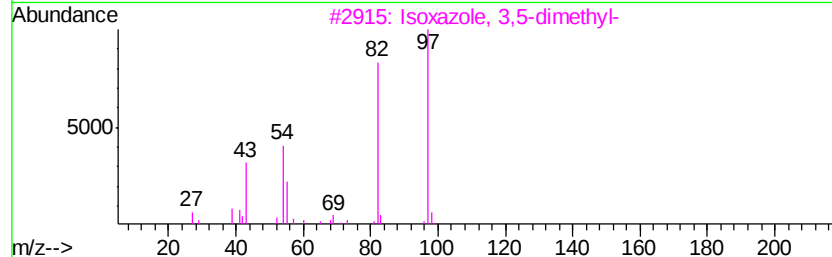
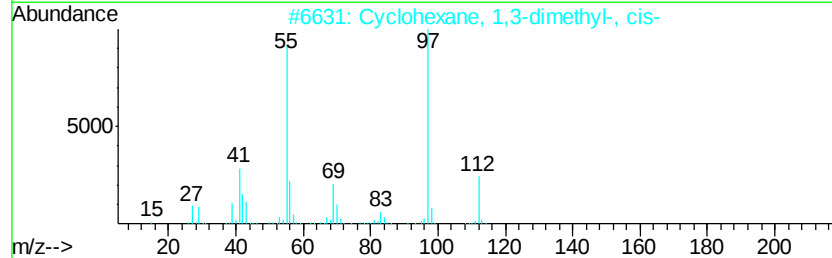
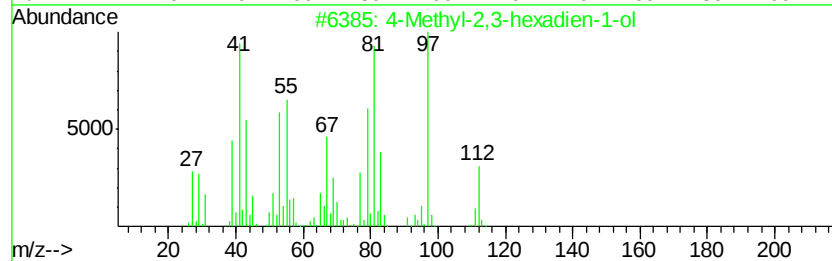
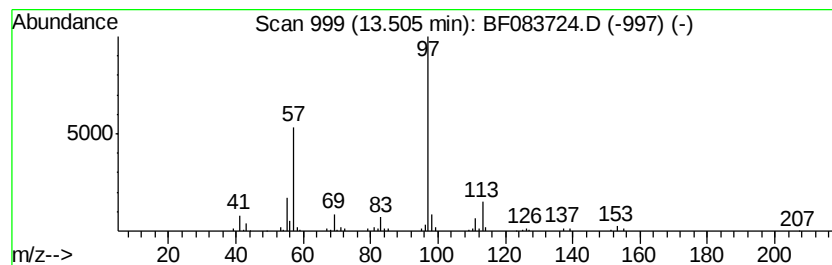
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4-Methyl-2,3-hexadien-1-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	2.41 ng	120409	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	53
2		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
3		Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
4		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	50
5		1H-Pyrazole, 4,5-dihydro-3-methy...	126	C7H14N2	026964-49-8	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

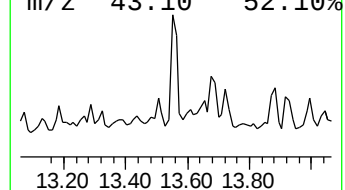
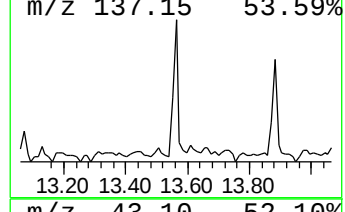
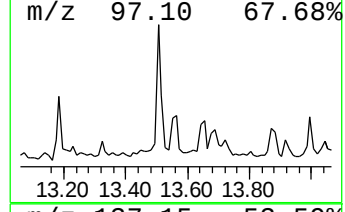
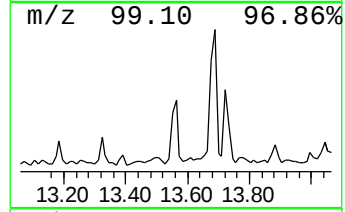
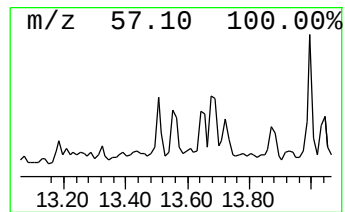
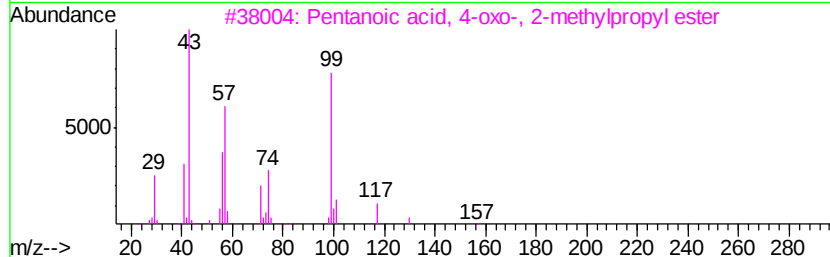
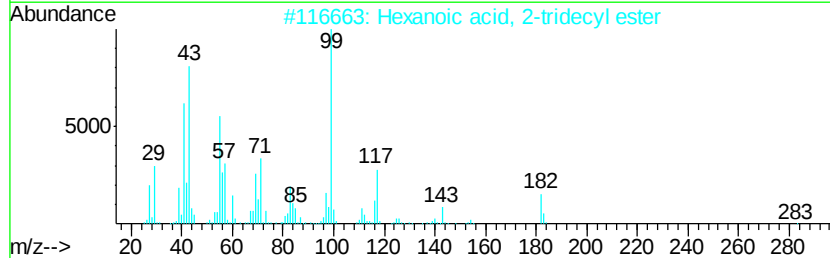
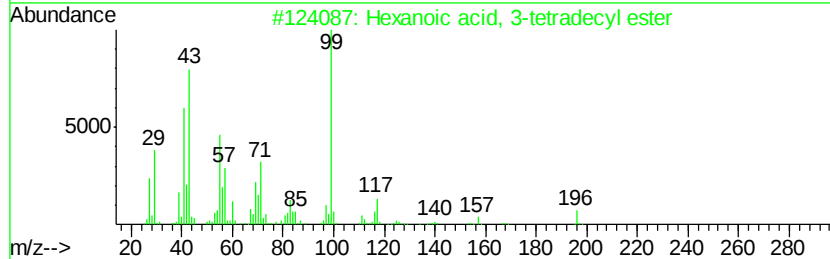
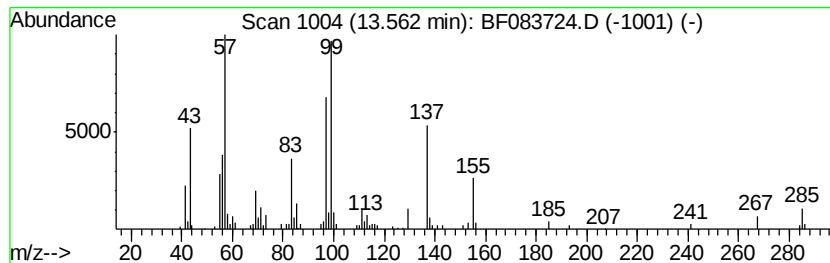
Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.56 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.56	3.57 ng	178138	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1000279-29-7	27
2	Hexanoic acid, 2-tridecyl ester	298	C19H38O2	055193-20-9	27
3	Pentanoic acid, 4-oxo-, 2-methyl...	172	C9H16O3	003757-32-2	25
4	1,4-Dioxaspiro[4.5]decan-8-one, ...	186	C9H14O4	108177-20-4	22
5	2-Propylthiazole	127	C6H9NS	017626-75-4	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

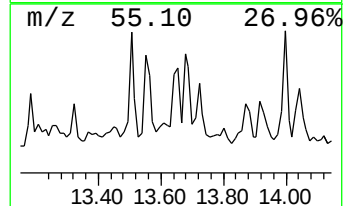
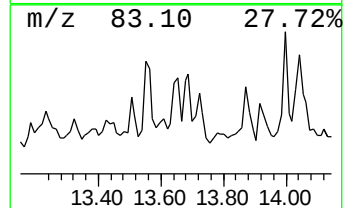
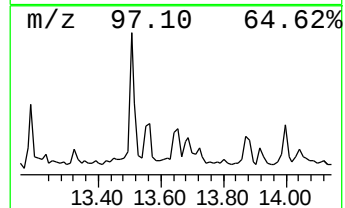
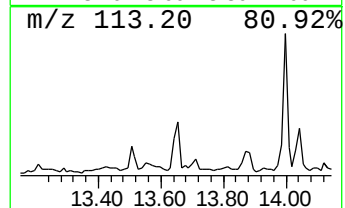
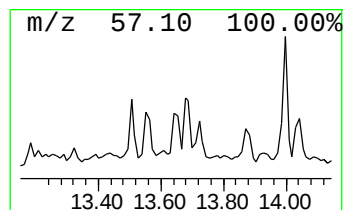
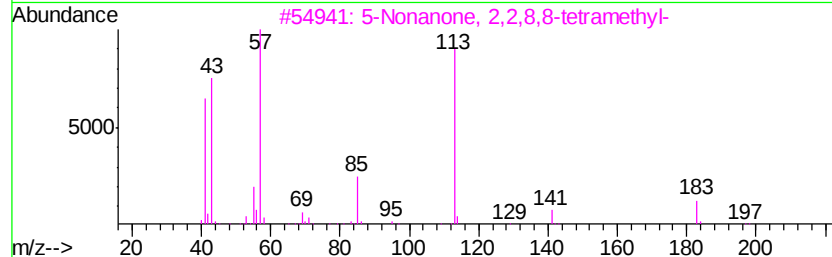
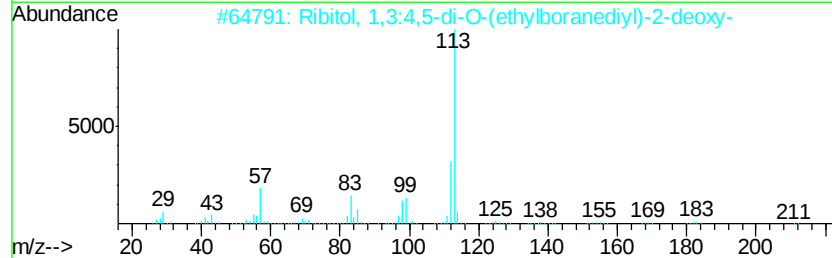
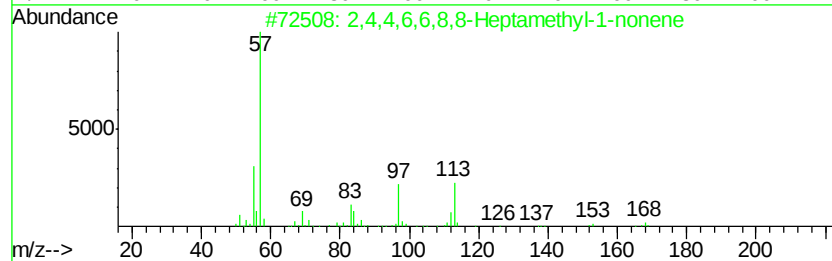
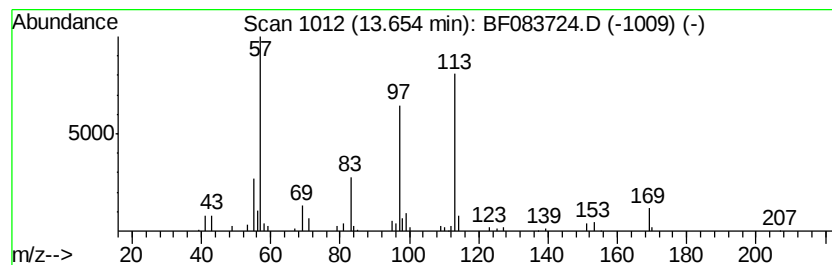
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	2.39 ng	119246	Chrysene-d12	14.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	72
2			Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	42
3			5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32
4			Propanenitrile, 3-(dichloromethyl-...	167	C4H7Cl2NSi	001071-21-2	32
5			1-[2-(3-Chloro-phenoxy)-ethyl]-4...	254	C13H19ClN2O	337312-00-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

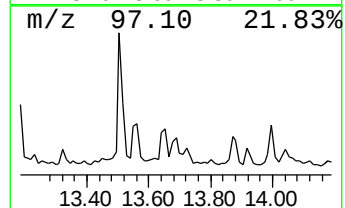
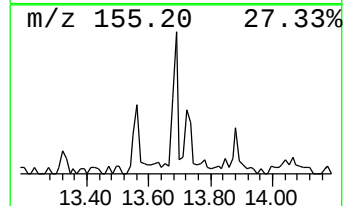
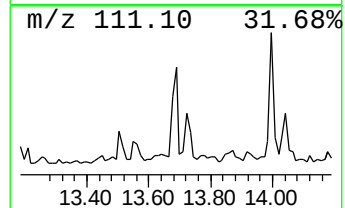
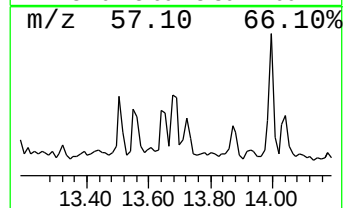
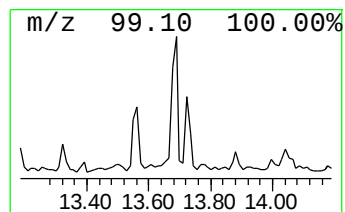
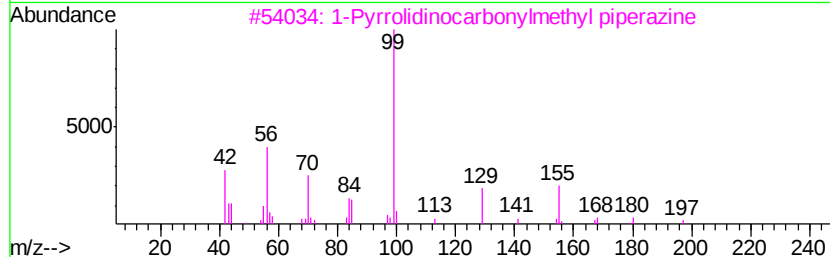
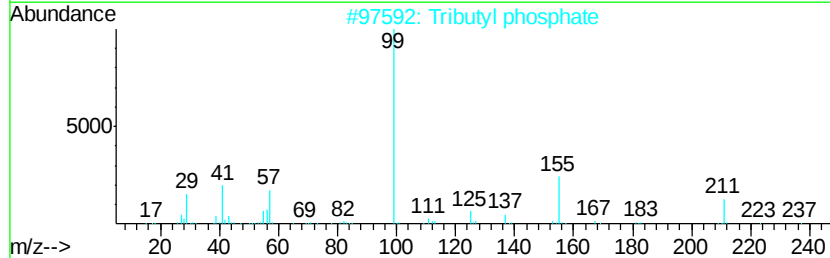
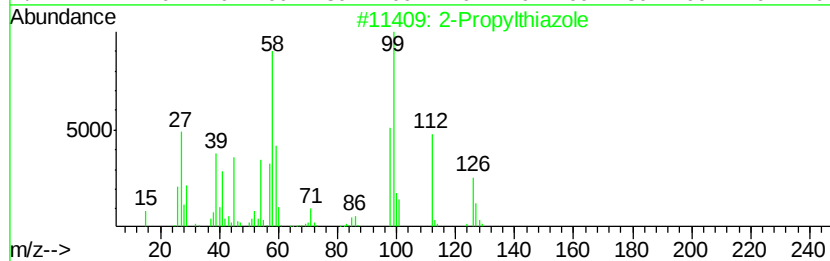
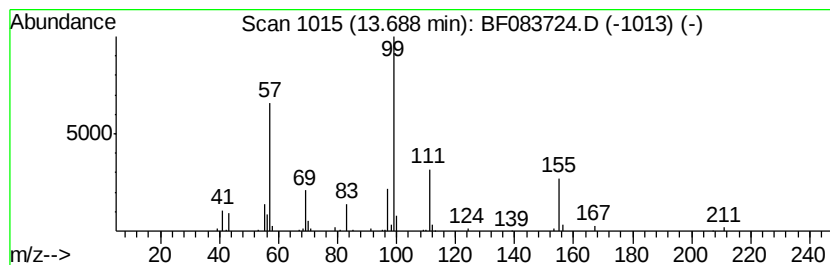
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.48 ng	173948	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propylthiazole		127	C6H9NS	017626-75-4	35
2	Tributyl phosphate		266	C12H27O4P	000126-73-8	33
3	1-Pyrrolidinocarbonylmethyl pipe...		197	C10H19N3O	039890-45-4	33
4	4-Butoxy-2,4-dimethyl-2-pentene		170	C11H22O	1000159-08-7	33
5	2,5-Pyrrolidinedione		99	C4H5NO2	000123-56-8	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

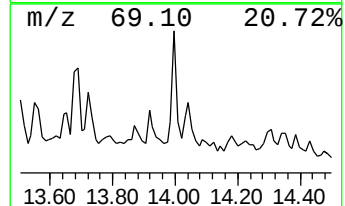
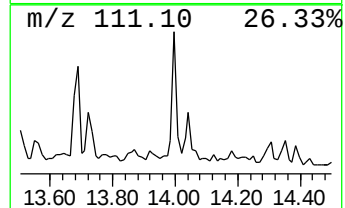
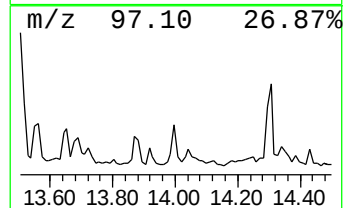
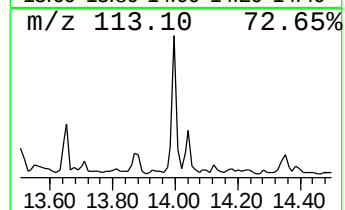
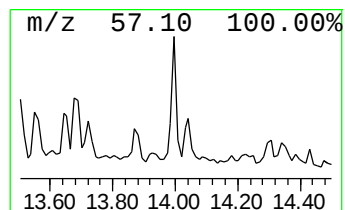
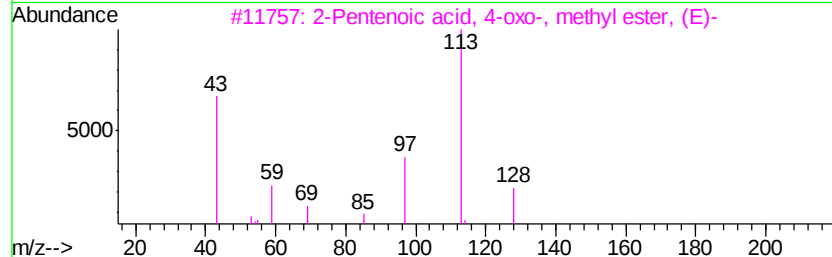
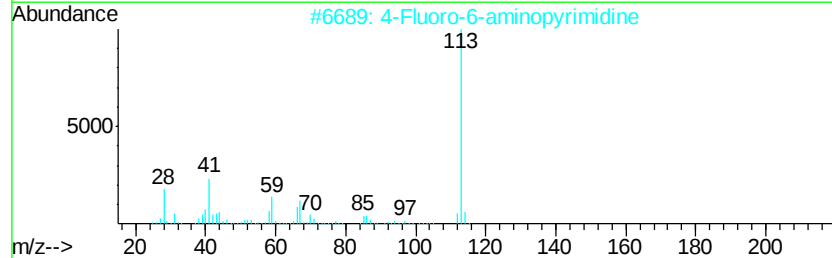
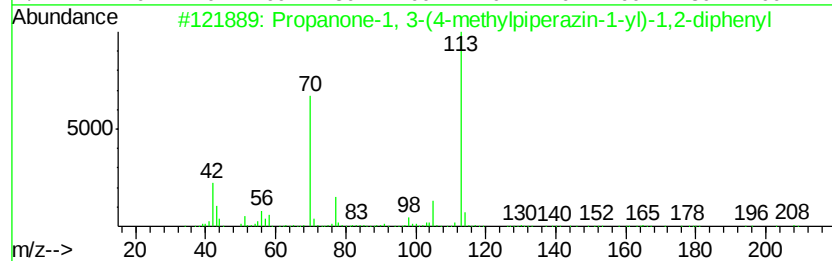
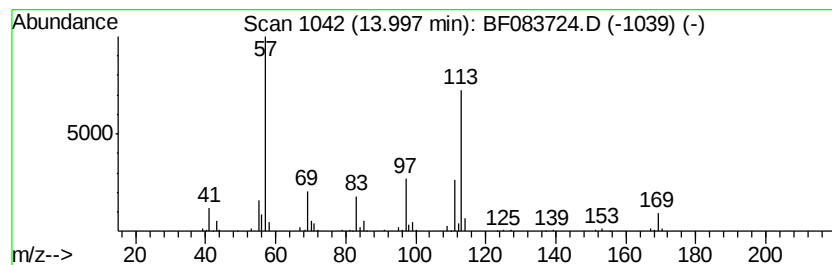
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	3.70 ng	184659	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanone-1, 3-(4-methylpiperazi...	308	C20H24N2O	053756-76-6	27
2		4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	27
3		2-Pentenoic acid, 4-oxo-, methyl...	128	C6H8O3	002833-24-1	23
4		Dibutyl itaconate	242	C13H22O4	002155-60-4	23
5		Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

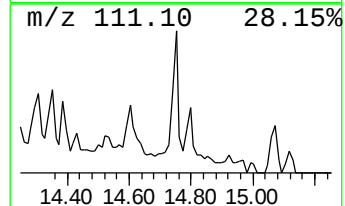
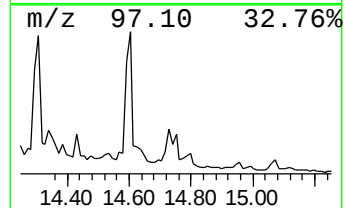
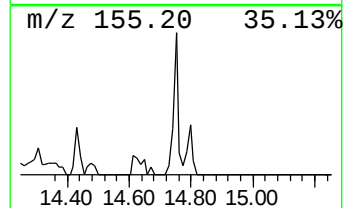
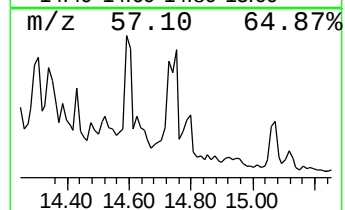
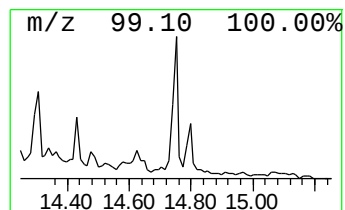
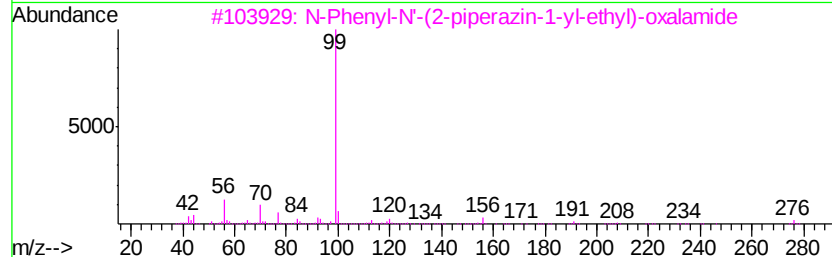
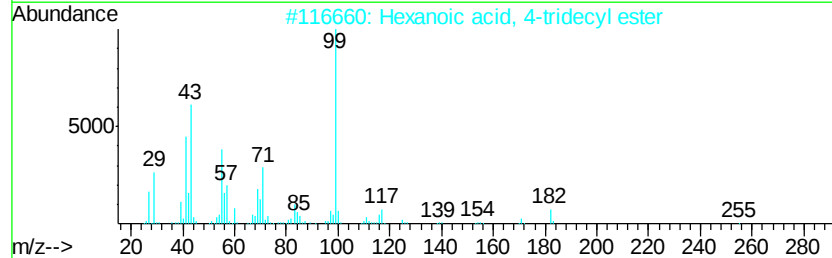
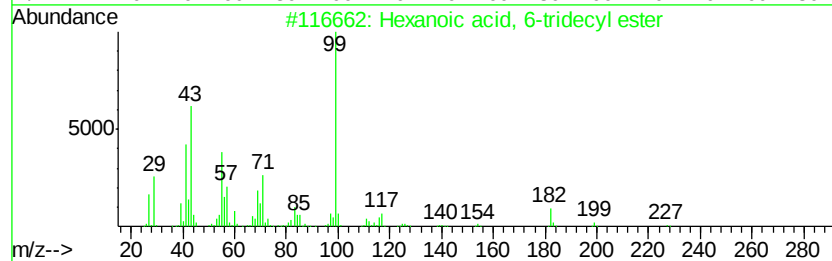
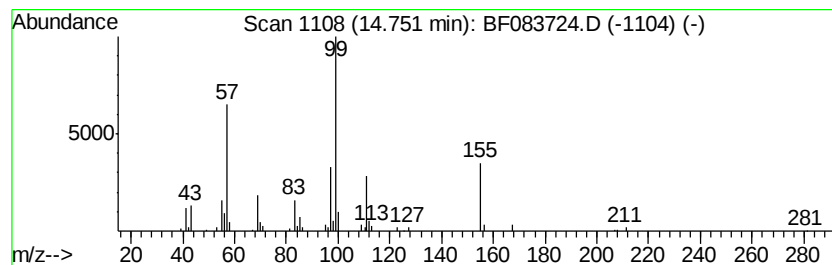
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.75 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.45 ng	122417	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
2		Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	47
3		N-Phenvl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	43
4		2-Propylthiazole	127	C6H9NS	017626-75-4	43
5		cis-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121115\
Data File : BF083724.D
Acq On : 12 Dec 2015 4:53
Operator : UM/IZ
Sample : G4648-09
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(20-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121115.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	19.2	ng	753775	1	6.92	786694	20.0
unknown6.69	6.69	95.3	ng	3748710	1	6.92	786694	20.0
Heptadecane	10.88	2.7	ng	149919	4	11.44	1122580	20.0
4-Methyl-2,3-hexa...	13.51	2.4	ng	120409	5	14.07	999267	20.0
unknown13.56	13.56	3.6	ng	178138	5	14.07	999267	20.0
2,4,4,6,6,8,8-Hep...	13.65	2.4	ng	119246	5	14.07	999267	20.0
unknown13.69	13.69	3.5	ng	173948	5	14.07	999267	20.0
unknown14.00	14.00	3.7	ng	184659	5	14.07	999267	20.0
unknown14.75	14.75	2.5	ng	122417	5	14.07	999267	20.0