

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
 Data File : BF082747.D
 Acq On : 6 Nov 2015 2:36
 Operator : UM/IZ
 Sample : G4282-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OCFNW1-10

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-BF103015.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	5.047	256	259	270	rVB	1396361	2288407	42.27%	4.985%
2	5.470	293	296	299	rBV	4144764	4329123	79.97%	9.431%
3	6.499	383	386	388	rBV	4499605	4792979	88.53%	10.442%
4	6.636	395	398	400	rBV	5197988	5299281	97.89%	11.545%
5	6.864	415	418	420	rBV	1258749	1038606	19.18%	2.263%
6	7.024	429	432	434	rBV	4476765	4037320	74.58%	8.796%
7	7.424	464	467	470	rBV	2857032	2953771	54.56%	6.435%
8	8.144	528	530	533	rBV	949960	1212361	22.39%	2.641%
9	9.230	622	625	627	rBV	6004195	5413723	100.00%	11.794%
10	9.619	657	659	662	rBV	1091410	917424	16.95%	1.999%
11	9.905	681	684	686	rBV	1739114	1480824	27.35%	3.226%
12	10.350	721	723	724	rVB	75799	62459	1.15%	0.136%
13	10.693	750	753	755	rBV	3331067	3386964	62.56%	7.379%
14	10.819	762	764	769	rVB	110598	127429	2.35%	0.278%
15	11.265	801	803	805	rBV	93069	82490	1.52%	0.180%
16	11.390	811	814	816	rVB	985351	1304028	24.09%	2.841%
17	11.928	859	861	863	rBV	104440	148189	2.74%	0.323%
18	12.979	950	953	955	rBV	3379996	4352698	80.40%	9.483%
19	13.871	1029	1031	1038	rBV	319693	411947	7.61%	0.897%
20	14.019	1041	1044	1046	rBV	1083487	995926	18.40%	2.170%
21	14.511	1083	1087	1093	rBV5	24755	58185	1.07%	0.127%
22	14.877	1117	1119	1121	rBV	122633	139754	2.58%	0.304%
23	15.448	1166	1169	1172	rBV	736908	906105	16.74%	1.974%
24	16.408	1249	1253	1259	rBV3	39782	102886	1.90%	0.224%
25	19.403	1510	1515	1521	rVB4	15535	58555	1.08%	0.128%

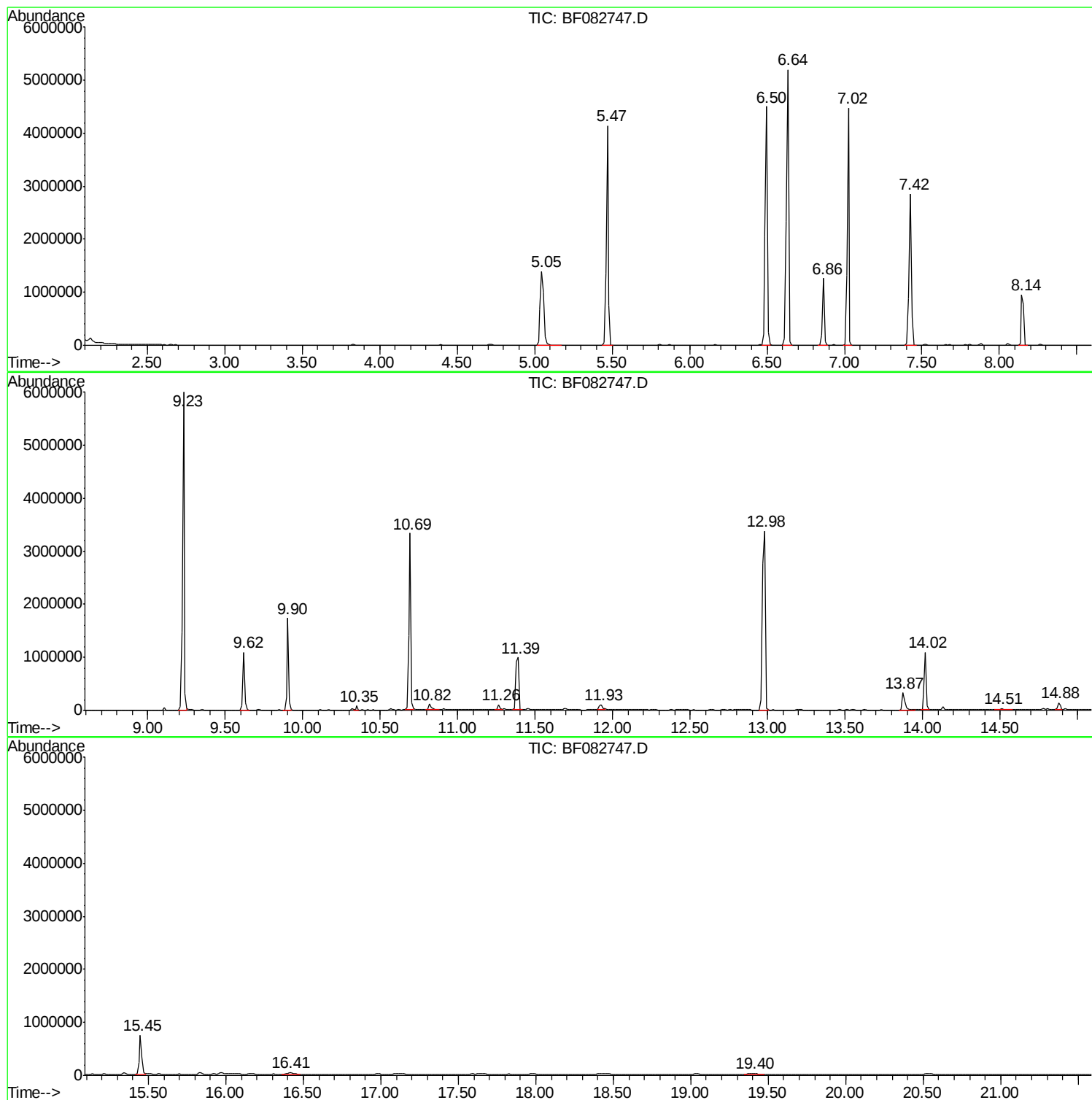
Sum of corrected areas: 45901434

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

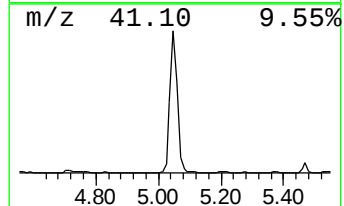
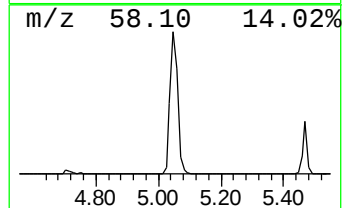
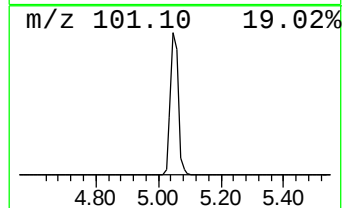
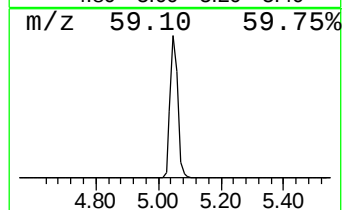
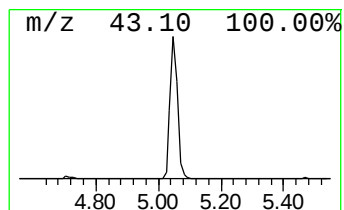
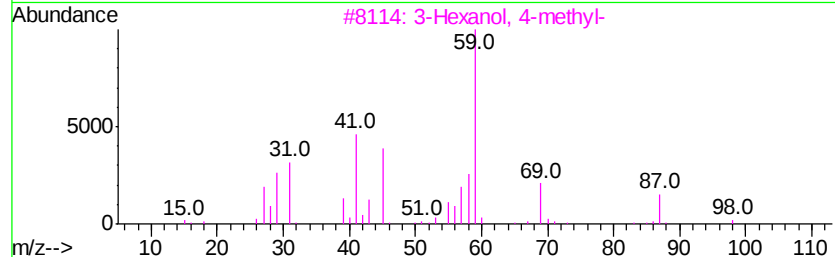
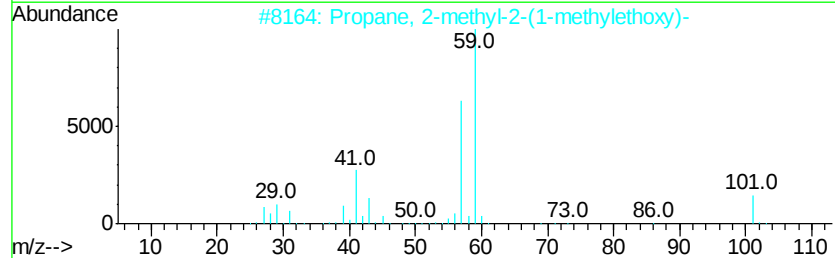
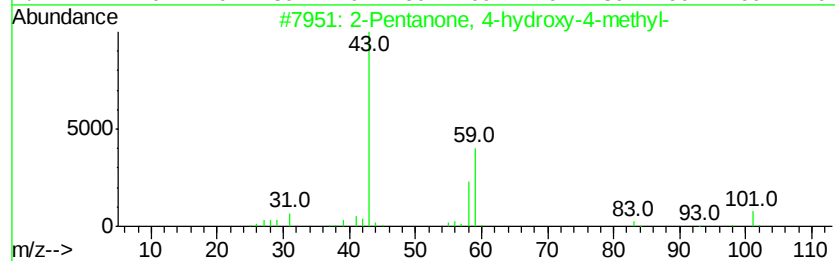
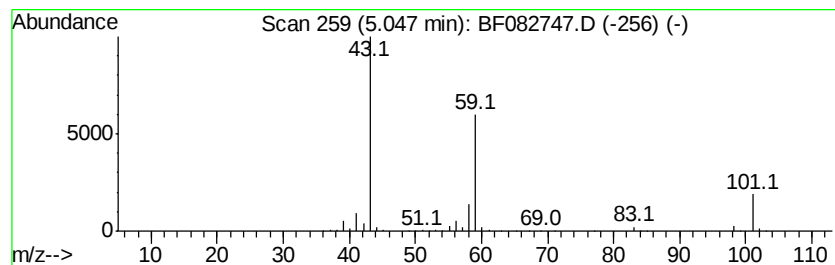
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	44.07 ng	2288410	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

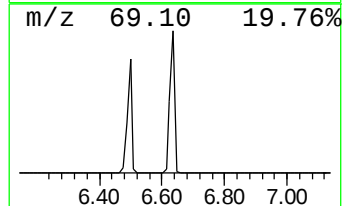
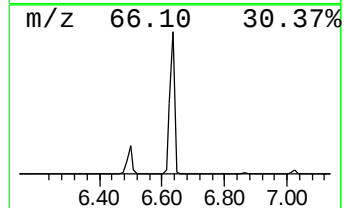
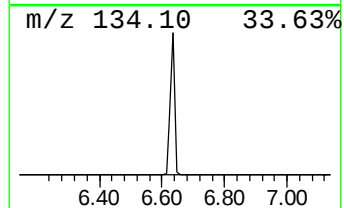
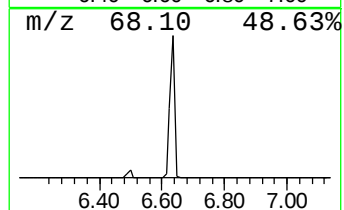
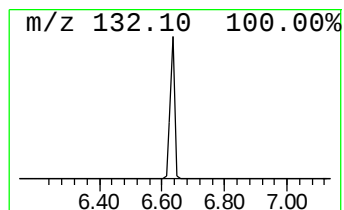
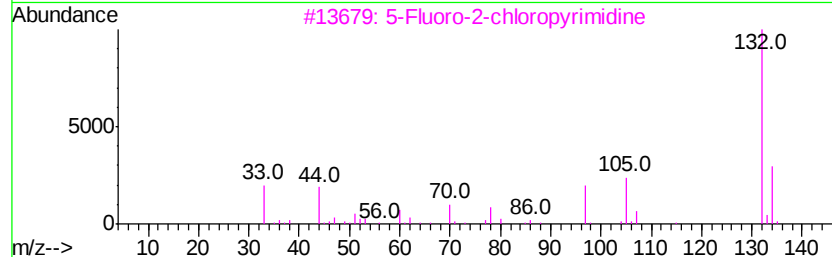
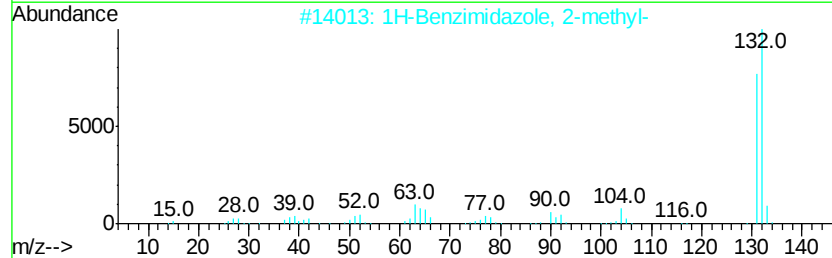
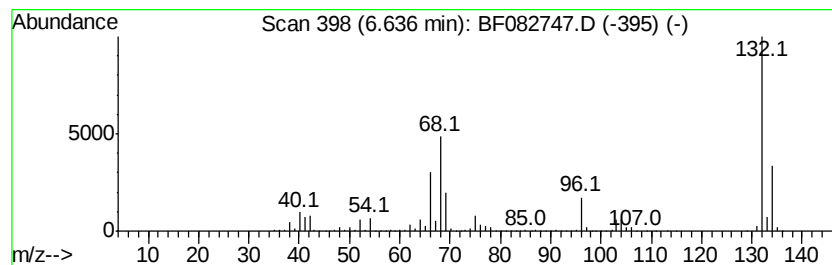
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	102.05 ng	5299280	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

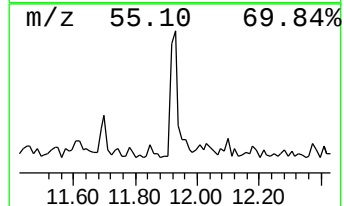
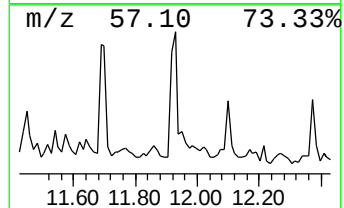
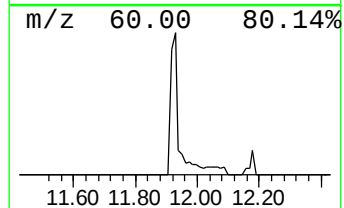
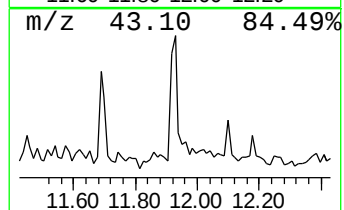
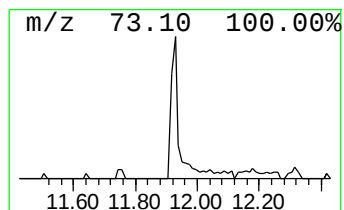
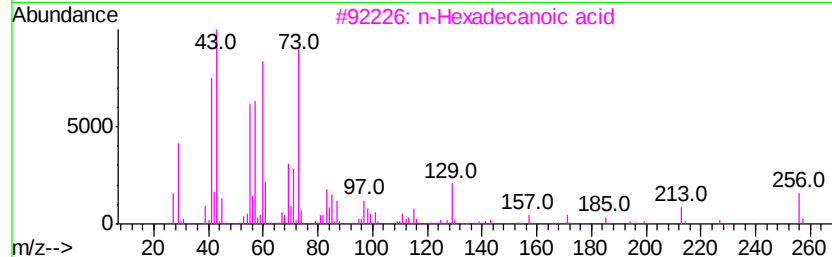
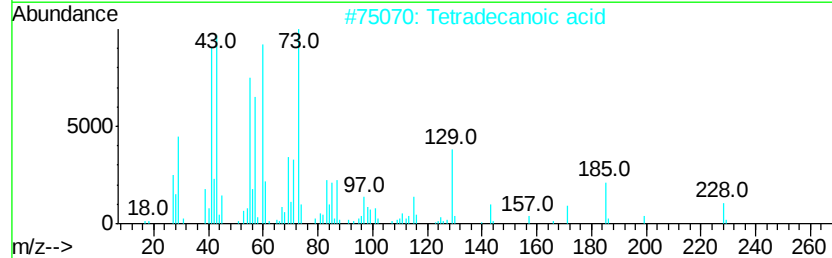
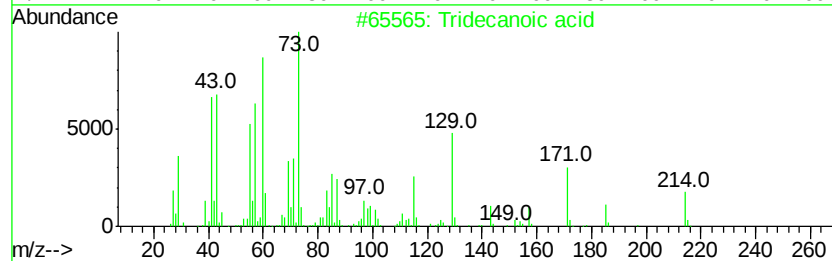
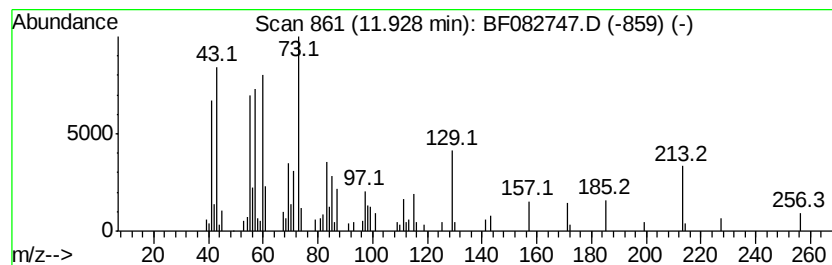
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.27 ng	148189	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

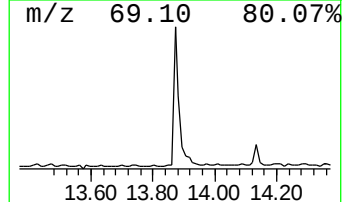
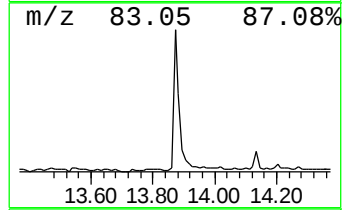
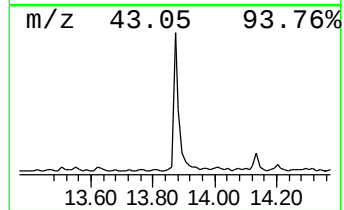
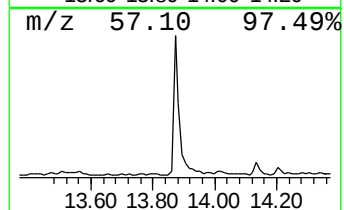
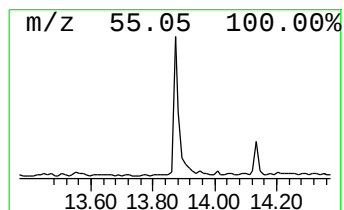
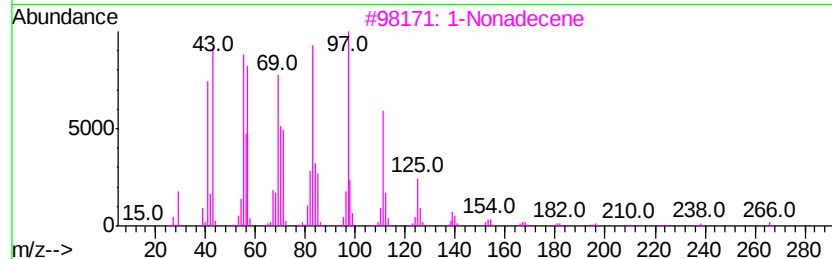
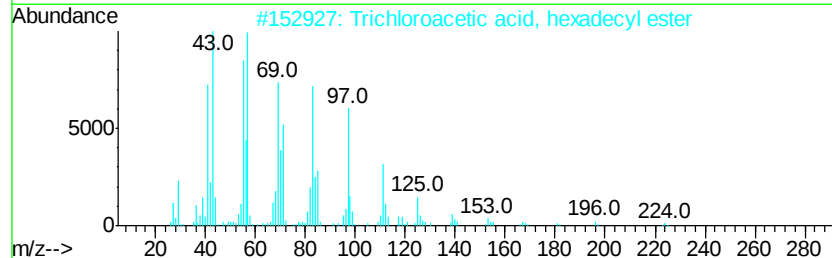
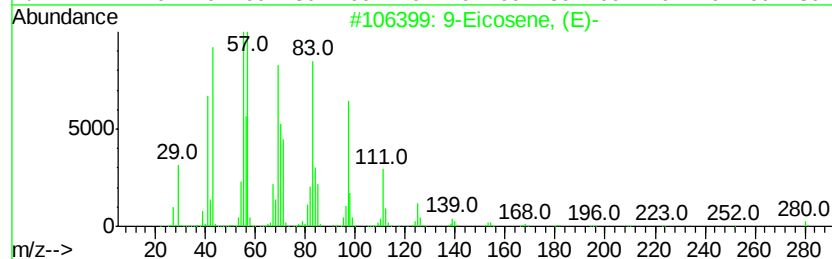
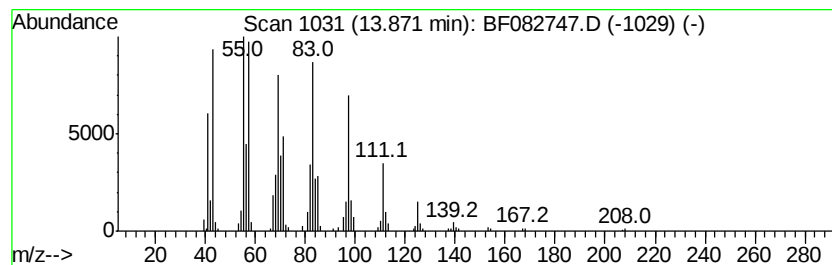
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.27 ng	411947	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		1-Heptadecanol	256	C17H36O	001454-85-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

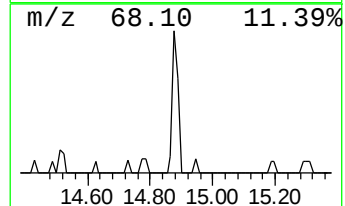
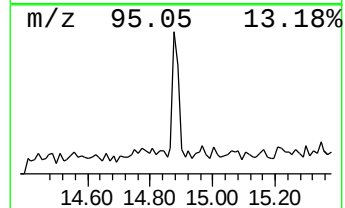
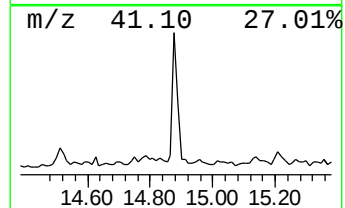
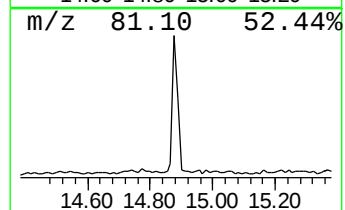
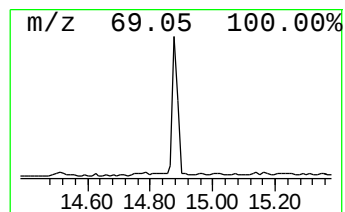
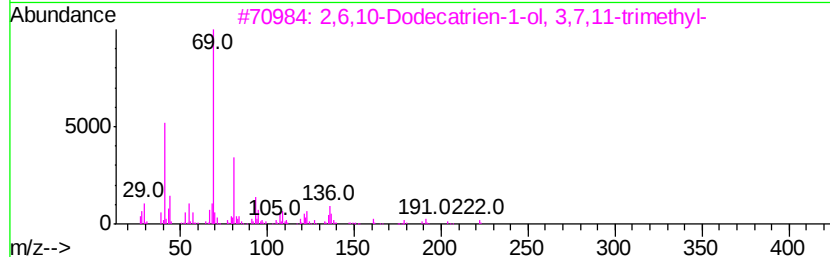
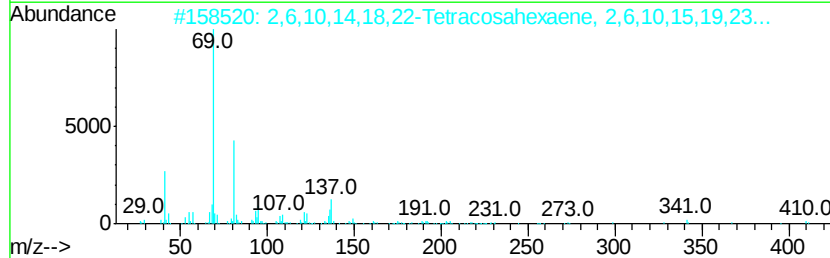
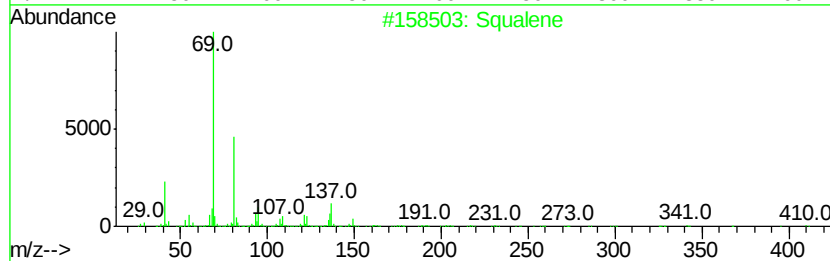
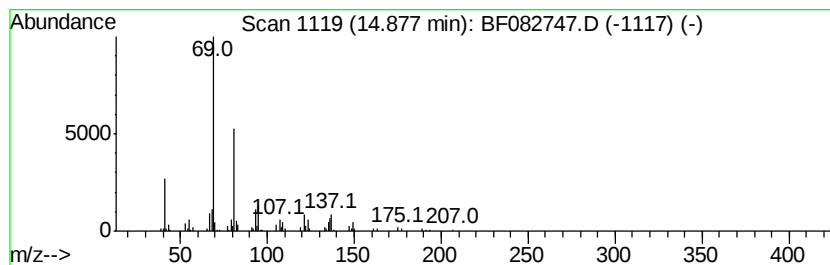
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	3.08 ng	139754	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

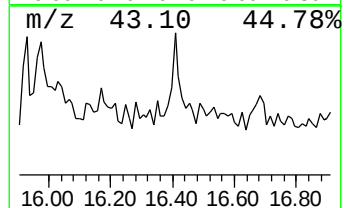
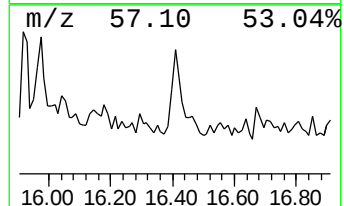
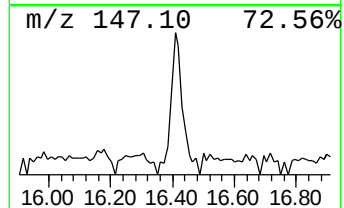
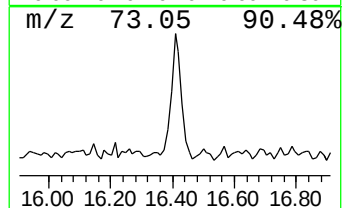
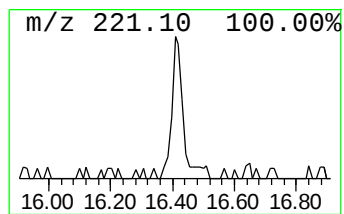
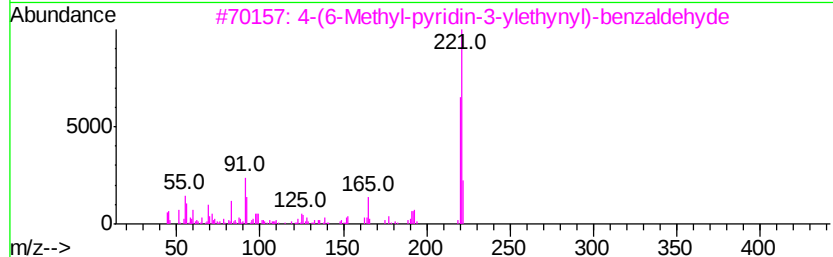
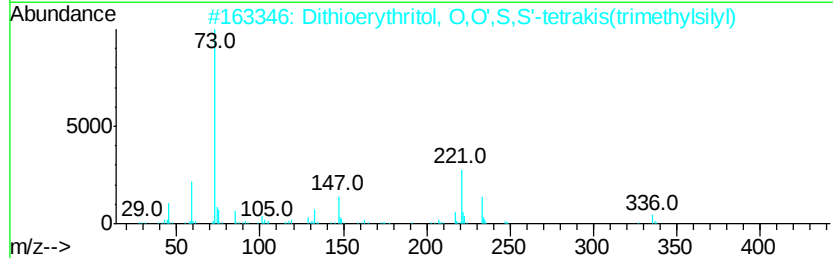
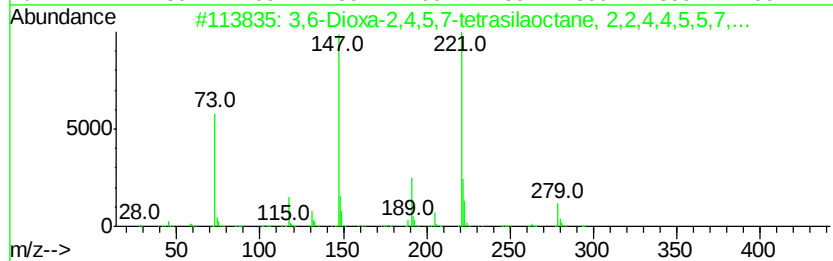
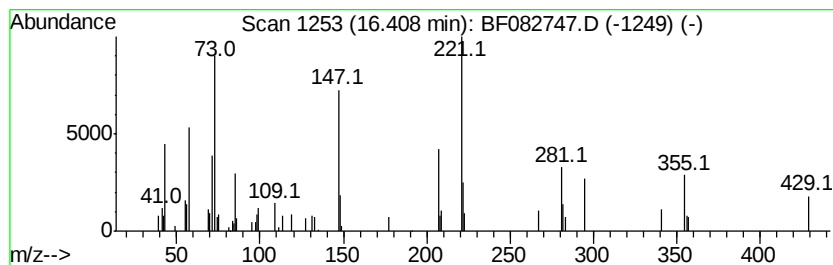
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.41 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.27 ng	102886	Perylene-d12	15.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	23		
2	Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	23		
3	4-(6-Methyl-pyridin-3-ylethynyl)...	221	C15H11NO	1000297-32-9	22		
4	2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	16		
5	2-(Trifluoromethyl)-7H-1,3,4-thi...	221	C6H2F3N3OS	094605-13-7	14		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082747.D
Acq On : 6 Nov 2015 2:36
Operator : UM/IZ
Sample : G4282-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OCFNW1-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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...	5.05	44.1	ng	2288410	1	6.86	1038610	20.0
unknown6.64	6.64	102.1	ng	5299280	1	6.86	1038610	20.0
Tridecanoic acid	11.93	2.3	ng	148189	4	11.39	1304030	20.0
9-Eicosene, (E)-	13.87	8.3	ng	411947	5	14.02	995926	20.0
Squalene	14.88	3.1	ng	139754	6	15.45	906105	20.0
unknown16.41	16.41	2.3	ng	102886	6	15.45	906105	20.0