

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
 Data File : BF081468.D
 Acq On : 5 Sep 2015 16:50
 Operator : UM/IZ
 Sample : G3559-02
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP226BR-40-42

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	243	245	254	rBV	385716	645524	54.67%	5.492%
2	4.902	288	290	303	rVB	1101491	1154190	97.74%	9.820%
3	6.022	385	388	390	rBV	1247388	1101593	93.29%	9.373%
4	6.125	395	397	399	rBV	1183411	1176654	99.64%	10.011%
5	6.353	415	417	420	rBV	407342	340388	28.83%	2.896%
6	6.513	429	431	433	rBV	847769	815442	69.05%	6.938%
7	6.936	465	468	470	rBV	670981	759634	64.33%	6.463%
8	7.645	528	530	532	rBV	535024	437029	37.01%	3.718%
9	8.730	622	625	627	rBV	1221780	1180865	100.00%	10.047%
10	9.131	658	660	663	rBV	256098	208715	17.67%	1.776%
11	9.382	680	682	685	rVB	491747	437863	37.08%	3.725%
12	9.851	722	723	725	rVB	15827	12074	1.02%	0.103%
13	10.171	748	751	753	rBV	610463	728630	61.70%	6.199%
14	10.319	762	764	769	rBV	26398	30529	2.59%	0.260%
15	10.765	801	803	804	rBV	22723	18847	1.60%	0.160%
16	10.845	808	810	813	rBV	439277	444317	37.63%	3.780%
17	11.188	838	840	843	rVB	13057	11925	1.01%	0.101%
18	11.428	859	861	865	rBV	31217	43381	3.67%	0.369%
19	12.285	934	936	939	rBV	64357	88625	7.51%	0.754%
20	12.365	942	943	946	rVB	26383	23786	2.01%	0.202%
21	12.434	946	949	951	rBV	1158474	1037831	87.89%	8.830%
22	12.994	995	998	999	rBV	65270	61320	5.19%	0.522%
23	13.040	999	1002	1003	rVB	15539	16001	1.36%	0.136%
24	13.360	1027	1030	1036	rBV	51851	92293	7.82%	0.785%
25	13.451	1036	1038	1041	rBV	365582	359877	30.48%	3.062%
26	13.680	1055	1058	1060	rBV	27999	28144	2.38%	0.239%
27	13.977	1082	1084	1086	rBV	25579	25120	2.13%	0.214%
28	14.240	1105	1107	1109	rBV	77112	84552	7.16%	0.719%
29	14.274	1109	1110	1112	rVV	24418	19158	1.62%	0.163%
30	14.331	1112	1115	1117	rVB	55923	48417	4.10%	0.412%
31	14.548	1132	1134	1137	rVB	14229	18829	1.59%	0.160%
32	14.765	1150	1153	1155	rBV	218860	260740	22.08%	2.218%
33	14.834	1157	1159	1163	rVB	13739	14317	1.21%	0.122%
34	15.154	1185	1187	1189	rBV	10744	13813	1.17%	0.118%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

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

35	15.508	1214	1218	1221	rBV2	6215	12740	1.08%	0.108%
----	--------	------	------	------	------	------	-------	-------	--------

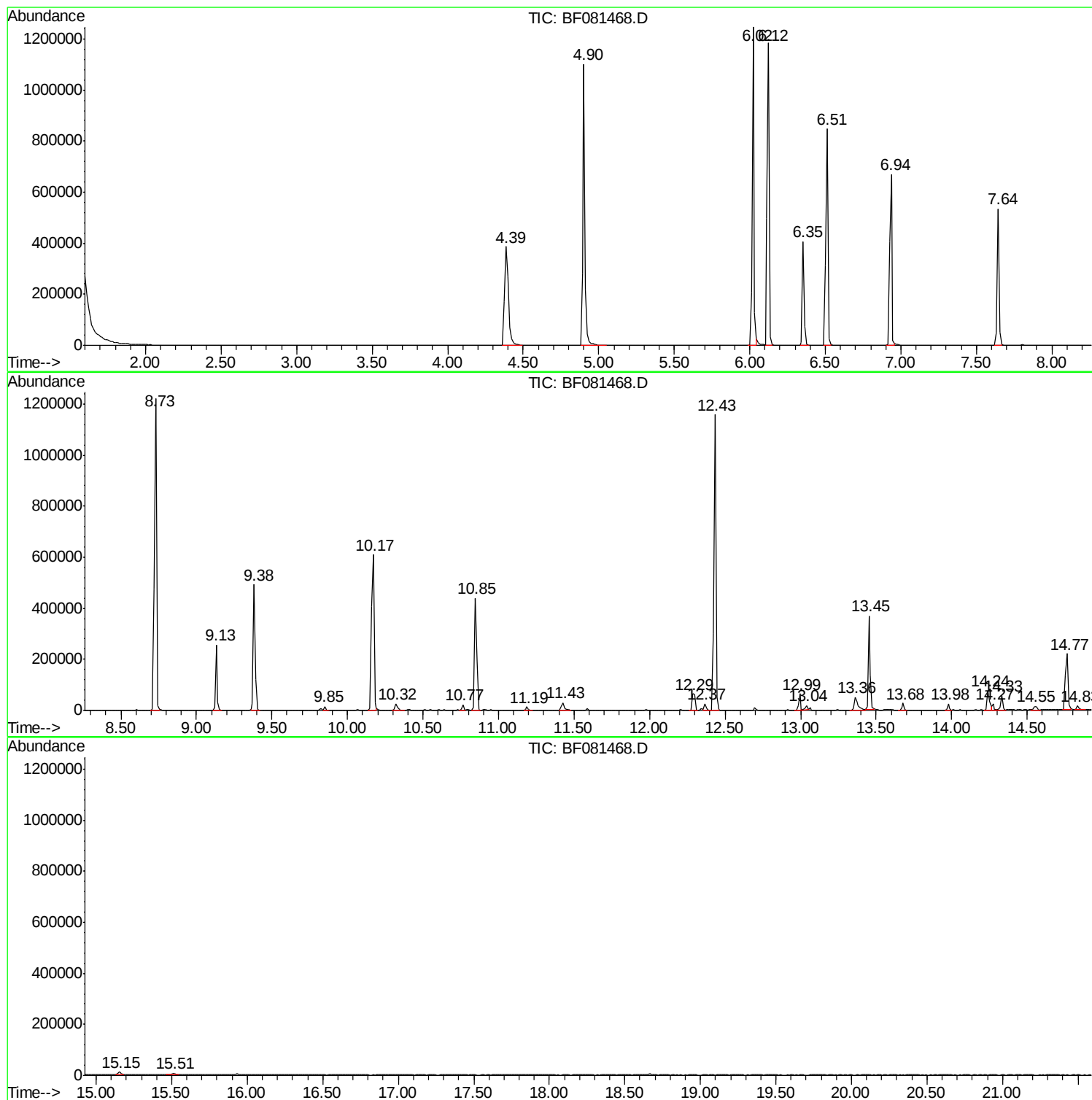
Sum of corrected areas: 11753163

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

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\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

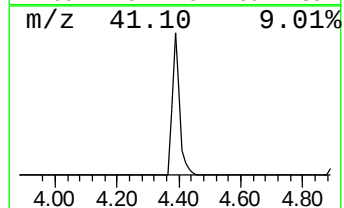
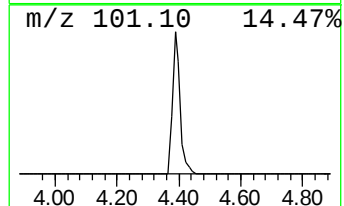
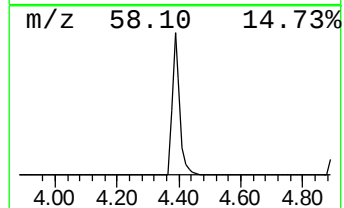
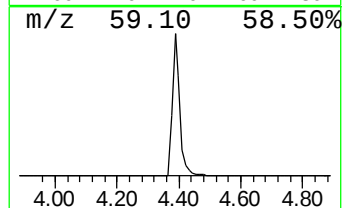
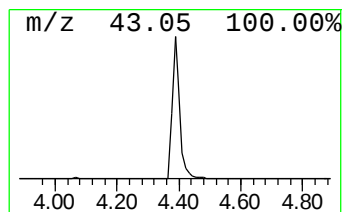
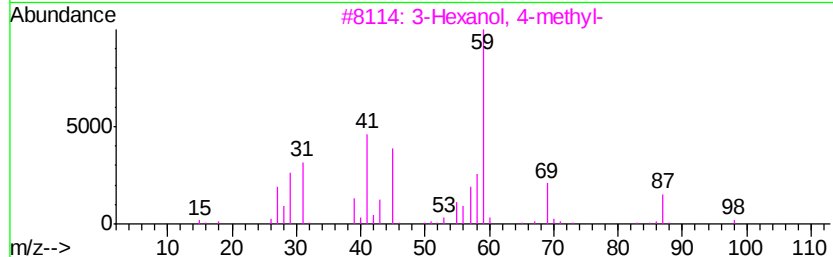
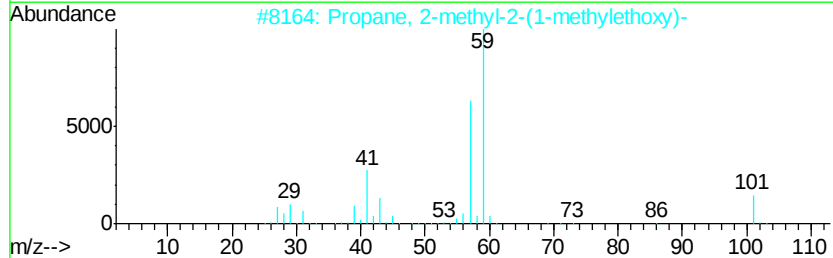
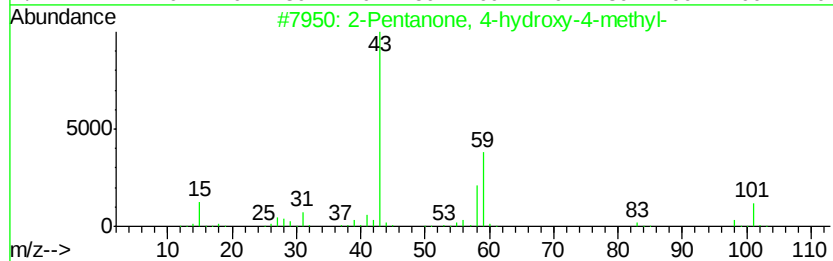
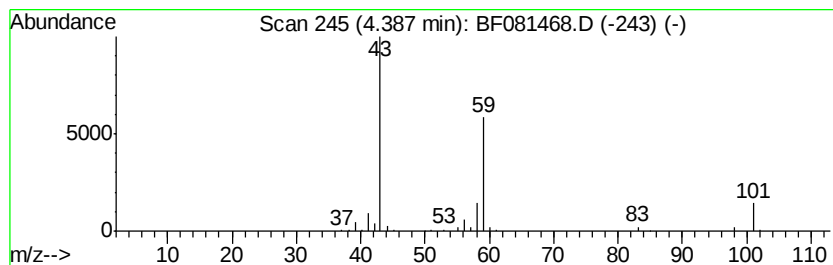
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	37.93 ng	645524	1,4-Dichlorobenzene-d4	6.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

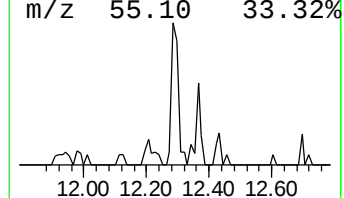
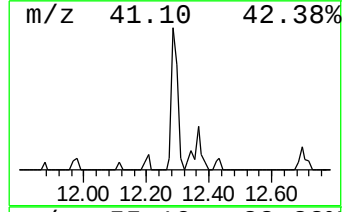
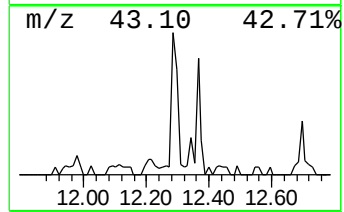
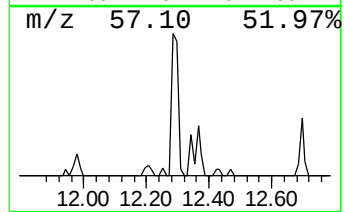
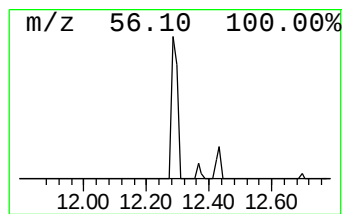
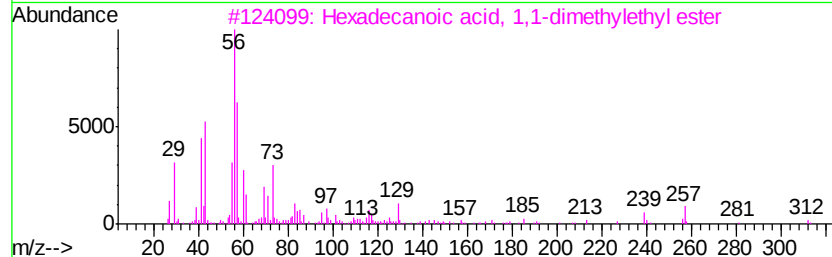
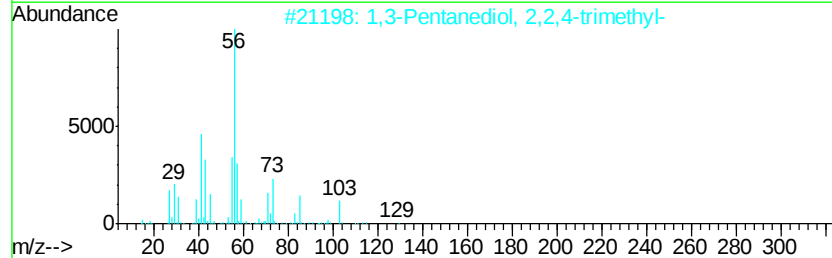
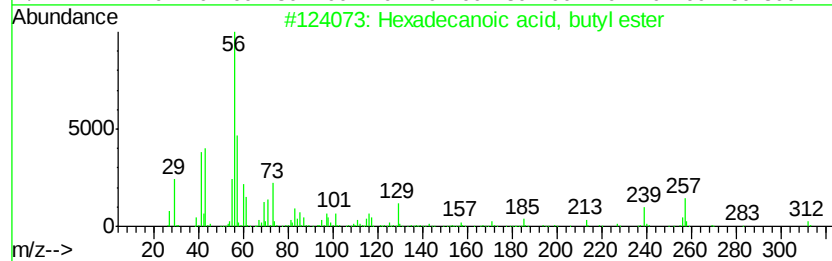
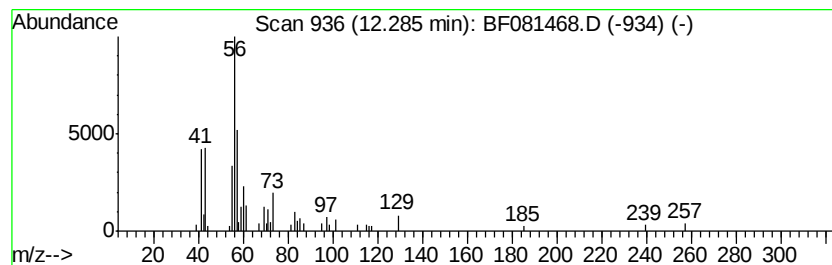
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	4.93 ng	88625	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
2		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	47
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	43
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

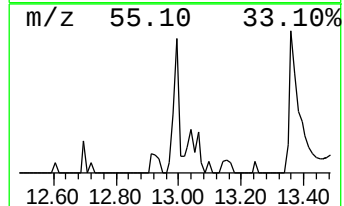
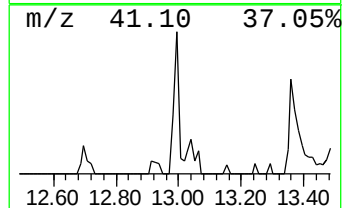
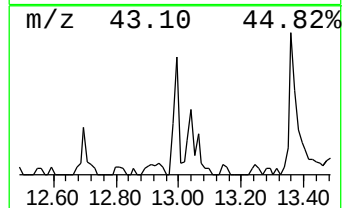
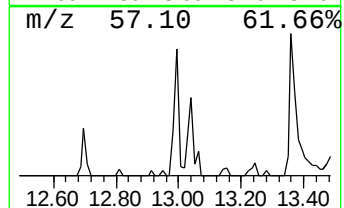
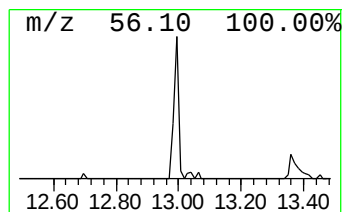
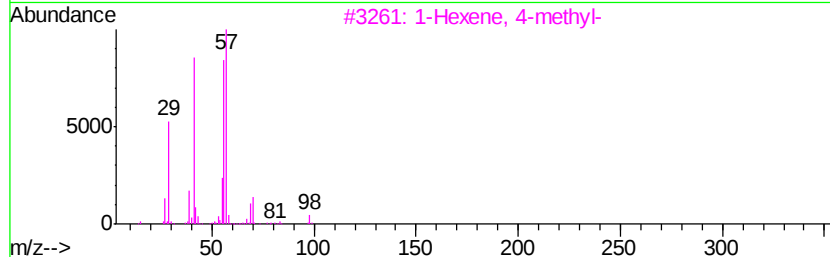
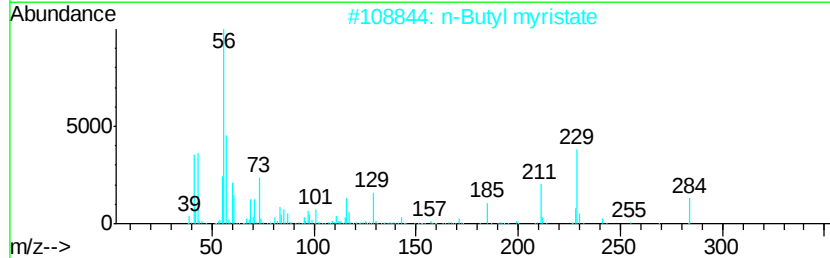
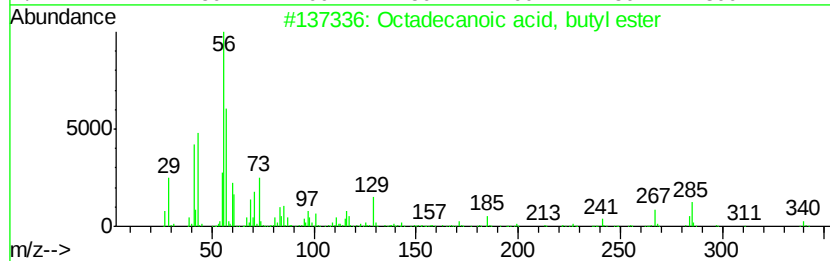
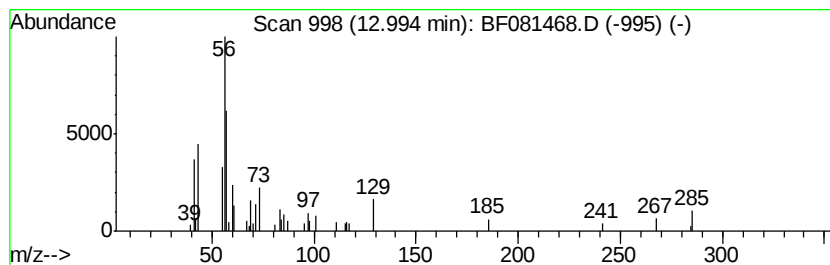
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	3.41 ng	61320	Chrysene-d12	13.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2		n-Butyl myristate	284	C18H36O2	000110-36-1	56
3		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38
4		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
5		Undecane, 5-methylene-	168	C12H24	005698-48-6	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

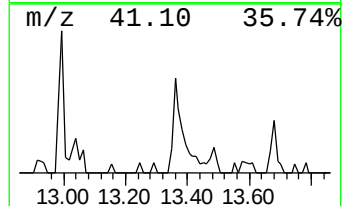
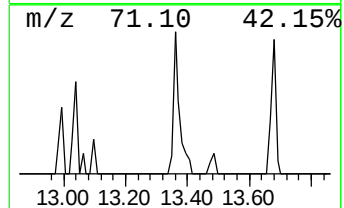
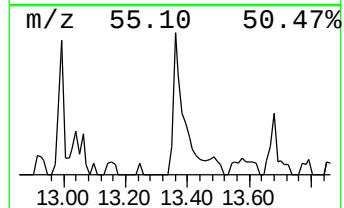
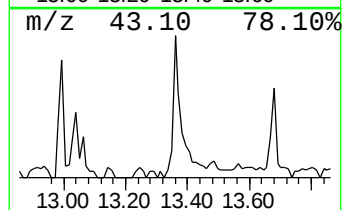
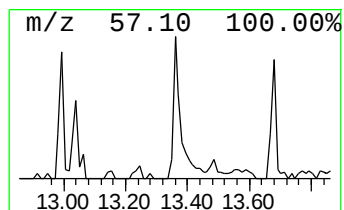
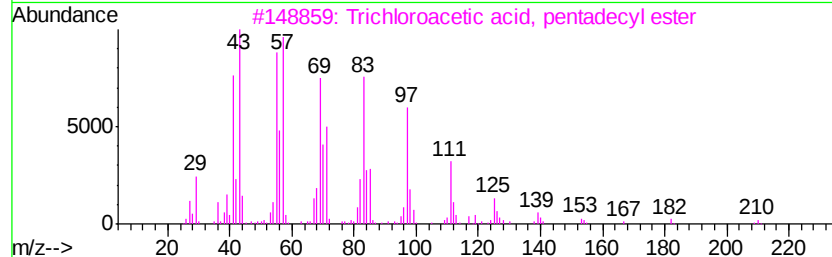
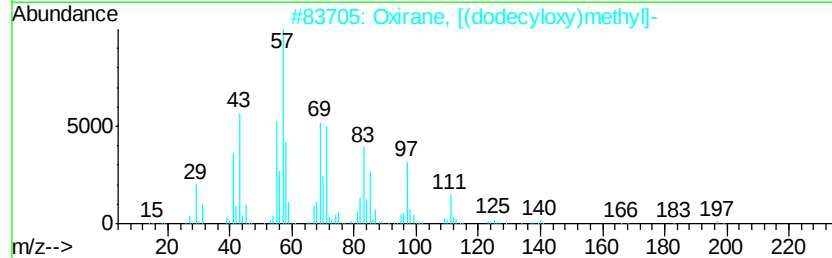
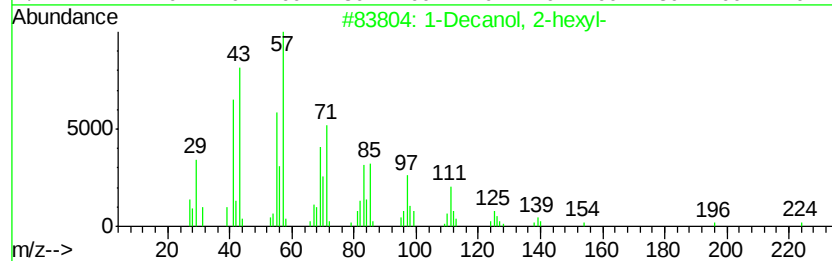
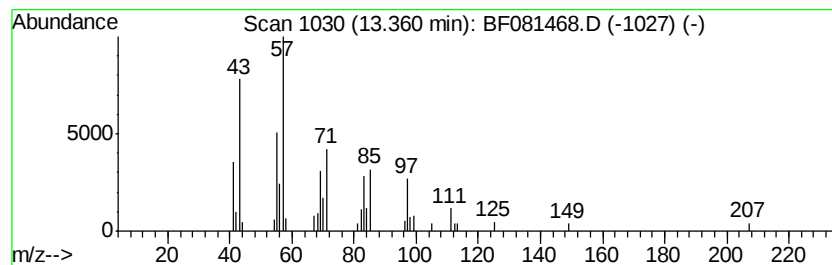
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Decanol, 2-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	5.13 ng	92293	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	80
2		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	64
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49
4		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	46
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

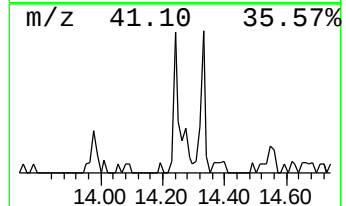
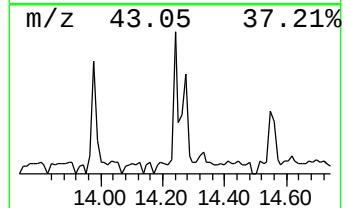
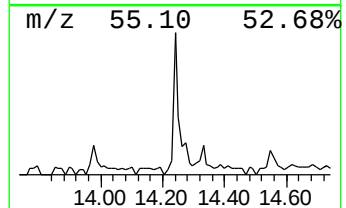
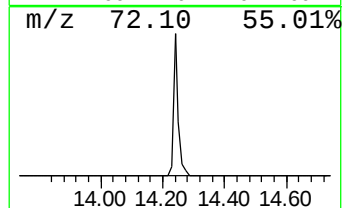
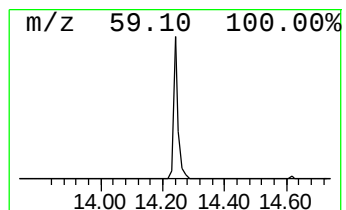
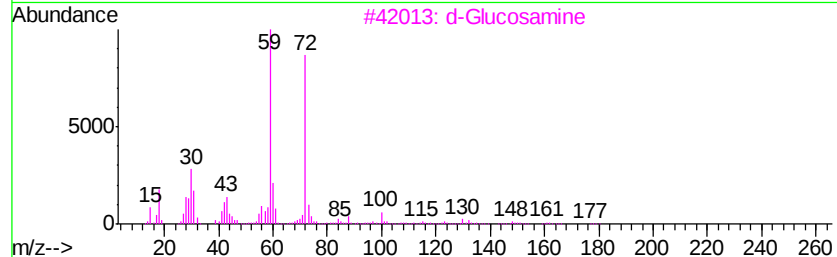
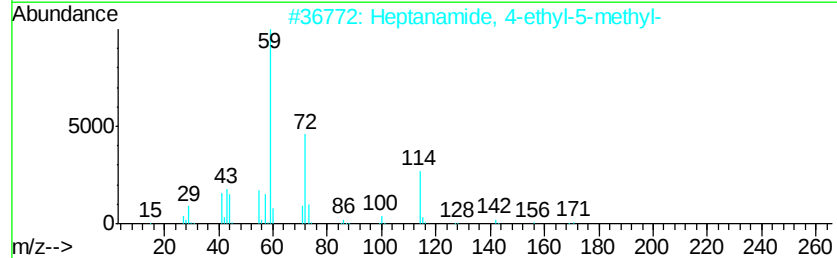
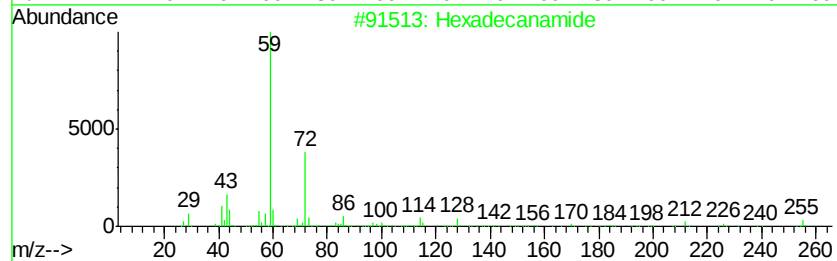
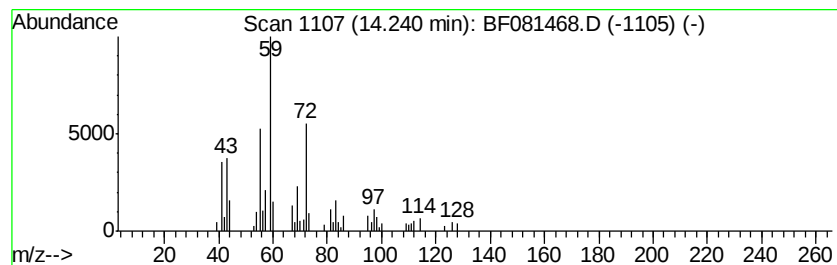
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	6.49 ng	84552	Perylene-d12	14.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide		255	C16H33NO	000629-54-9	72
2	Heptanamide, 4-ethyl-5-methyl-		171	C10H21NO	054789-40-1	64
3	d-Glucosamine		179	C6H13NO5	000090-77-7	50
4	Mannosamine hydrochloride		179	C6H13NO5	1000127-68-8	43
5	Nonanamide		157	C9H19NO	001120-07-6	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

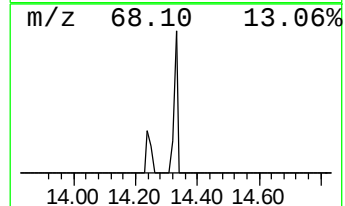
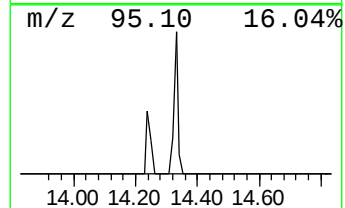
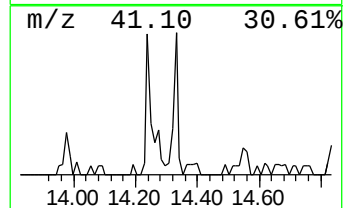
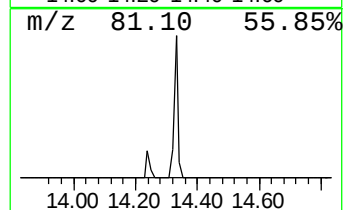
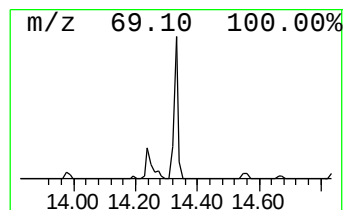
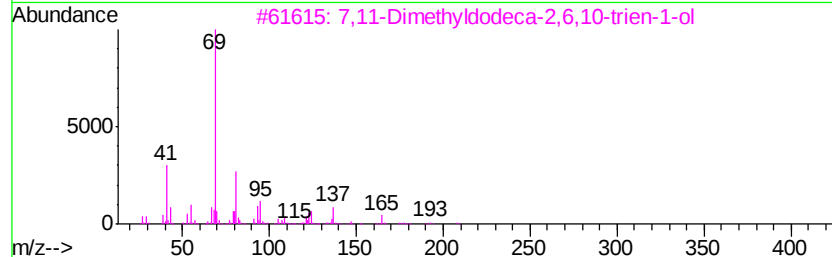
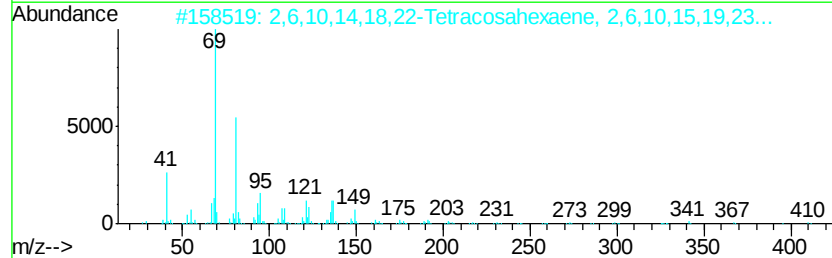
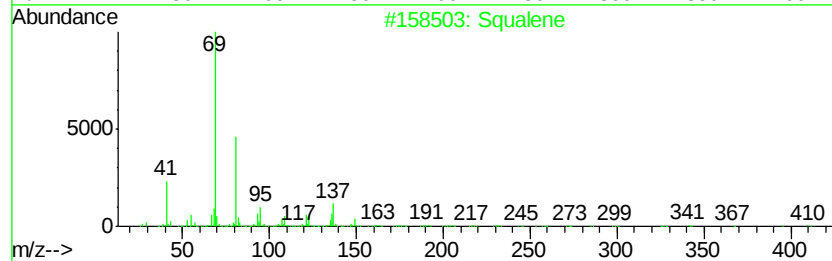
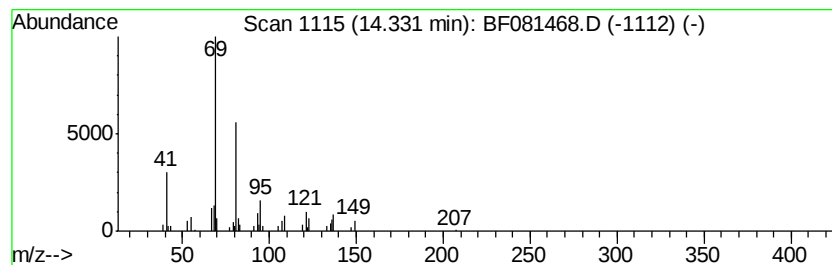
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	3.71 ng	48417	Perylene-d12	14.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	90
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H240	125529-10-4	64
4		.beta.-D-Mannofuranoside, farnesyl-	384	C21H3606	1000155-15-5	64
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H280	066408-55-7	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081468.D
Acq On : 5 Sep 2015 16:50
Operator : UM/IZ
Sample : G3559-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-40-42

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	37.9	ng	645524	1	6.35	340388	20.0
Hexadecanoic acid...	12.29	4.9	ng	88625	5	13.45	359877	20.0
Octadecanoic acid...	12.99	3.4	ng	61320	5	13.45	359877	20.0
1-Decanol, 2-hexyl-	13.36	5.1	ng	92293	5	13.45	359877	20.0
Hexadecanamide	14.24	6.5	ng	84552	6	14.77	260740	20.0
Squalene	14.33	3.7	ng	48417	6	14.77	260740	20.0