

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
 Data File : BF090977.D
 Acq On : 2 Nov 2016 14:08
 Operator : UM/SJ
 Sample : H5502-21
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-89-1.5-2.0

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-BF102616.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	4.876	242	244	257	rBV	636510	1113826	20.20%	2.249%
2	5.321	280	283	285	rBV	4138442	4752944	86.21%	9.598%
3	6.373	371	375	377	rBV	3517970	5055297	91.69%	10.208%
4	6.487	382	385	388	rBV	4194503	4389250	79.61%	8.863%
5	6.716	403	405	408	rBV	1025901	1040719	18.88%	2.102%
6	6.876	416	419	421	rBV	3819694	3471902	62.97%	7.011%
7	7.287	452	455	458	rBV	2708118	2922975	53.02%	5.902%
8	7.402	462	465	472	rVB	68955	120743	2.19%	0.244%
9	8.007	515	518	520	rBV	1662969	1552054	28.15%	3.134%
10	9.093	609	613	615	rBV	4469958	5513300	100.00%	11.133%
11	9.482	645	647	650	rBV	1030530	1162542	21.09%	2.348%
12	9.699	664	666	669	rBV	46415	59431	1.08%	0.120%
13	9.756	669	671	674	rBV	1381125	1736373	31.49%	3.506%
14	10.202	709	710	712	rVB	177303	144856	2.63%	0.293%
15	10.419	726	729	733	rBV	67321	130448	2.37%	0.263%
16	10.556	738	741	743	rBV	2982204	3703640	67.18%	7.479%
17	10.671	750	751	756	rVB	169030	278668	5.05%	0.563%
18	10.865	766	768	773	rBV	32990	80037	1.45%	0.162%
19	11.128	789	791	792	rBV	106570	129510	2.35%	0.262%
20	11.242	799	801	803	rVV	2012487	1817877	32.97%	3.671%
21	11.299	805	806	811	rVB3	32864	72188	1.31%	0.146%
22	11.482	819	822	826	rBV	76416	102953	1.87%	0.208%
23	12.454	904	907	909	rBV	89891	115420	2.09%	0.233%
24	12.682	917	927	929	rBV2	89113	310738	5.64%	0.627%
25	12.831	937	940	943	rBV	4411892	4706587	85.37%	9.504%
26	13.414	985	991	992	rBV4	36145	104763	1.90%	0.212%
27	13.734	1016	1019	1029	rBV2	376589	558518	10.13%	1.128%
28	13.882	1029	1032	1034	rVV	1090735	1550942	28.13%	3.132%
29	14.054	1045	1047	1050	rBV	47959	64082	1.16%	0.129%
30	14.362	1071	1074	1080	rBV	189169	297094	5.39%	0.600%
31	14.465	1081	1083	1086	rVB	75202	80200	1.45%	0.162%
32	14.579	1091	1093	1095	rBV	54398	62300	1.13%	0.126%
33	14.660	1096	1100	1104	rBV2	56111	118840	2.16%	0.240%
34	14.785	1110	1111	1114	rVB	63982	63866	1.16%	0.129%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.877	1117	1119	1124	rVB	31111	59803	1.08%	0.121%
36	14.968	1124	1127	1132	rBV2	81370	181507	3.29%	0.367%
37	15.208	1141	1148	1151	rBV2	67188	276362	5.01%	0.558%
38	15.277	1151	1154	1156	rVV	712341	1038082	18.83%	2.096%
39	15.311	1156	1157	1161	rVB	59930	64264	1.17%	0.130%
40	15.700	1188	1191	1193	rBV	66858	109173	1.98%	0.220%
41	15.745	1193	1195	1199	rVB3	28532	63553	1.15%	0.128%
42	16.157	1228	1231	1238	rVB2	35736	79632	1.44%	0.161%
43	16.751	1279	1283	1289	rVB3	33454	130273	2.36%	0.263%
44	18.946	1471	1475	1486	rVB7	34086	134188	2.43%	0.271%

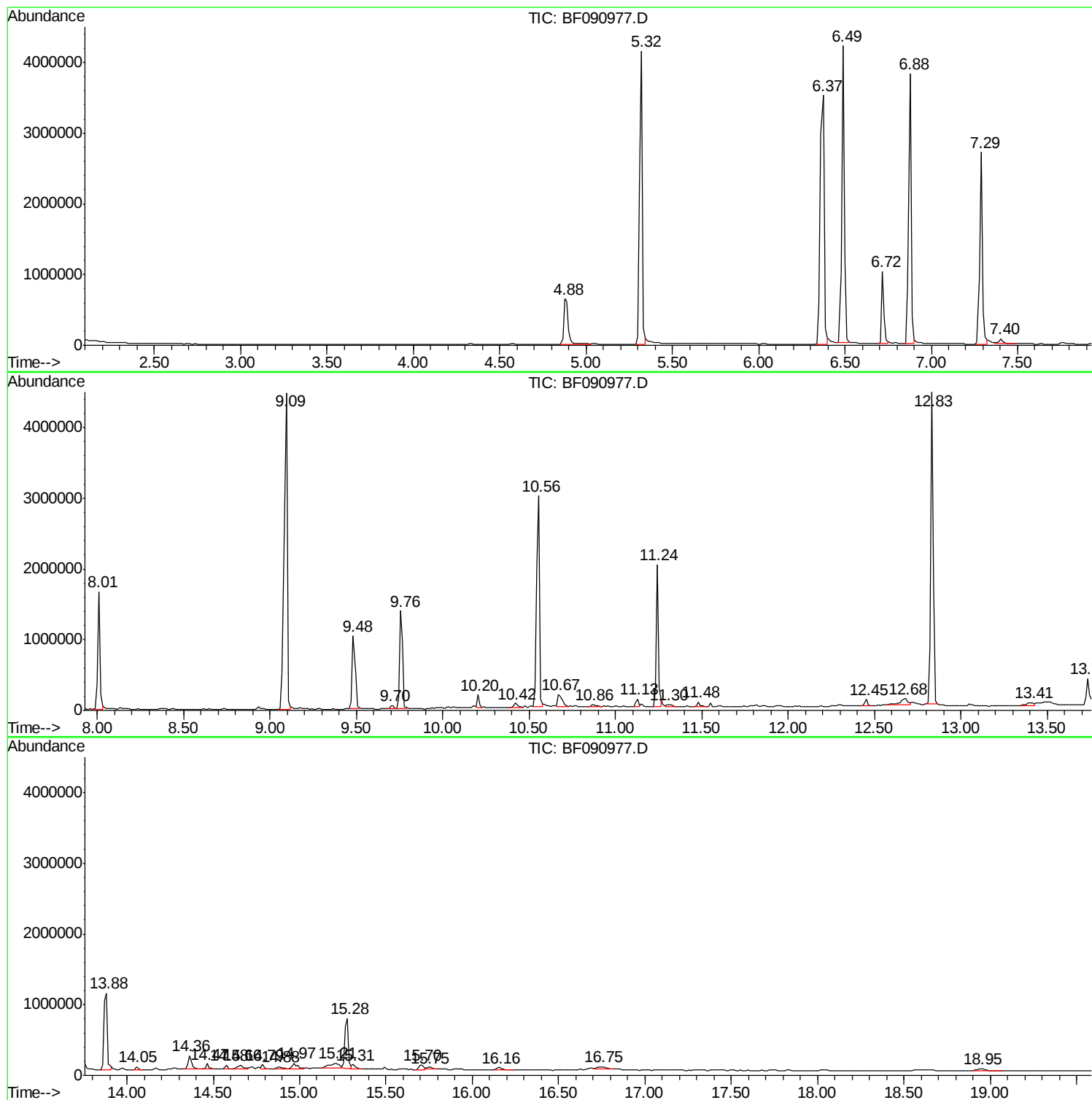
Sum of corrected areas: 49521720

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

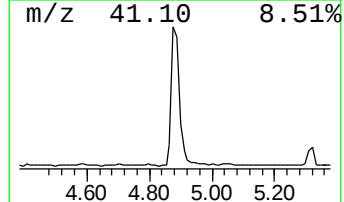
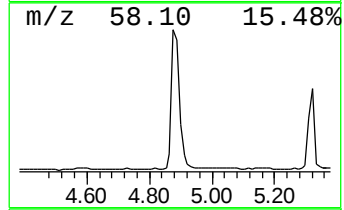
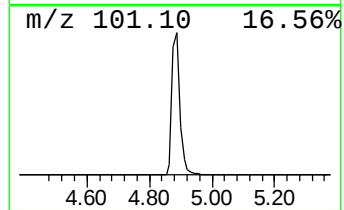
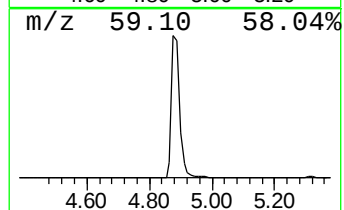
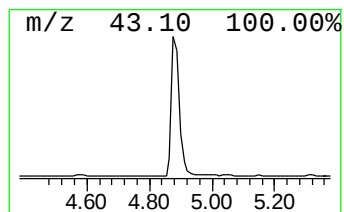
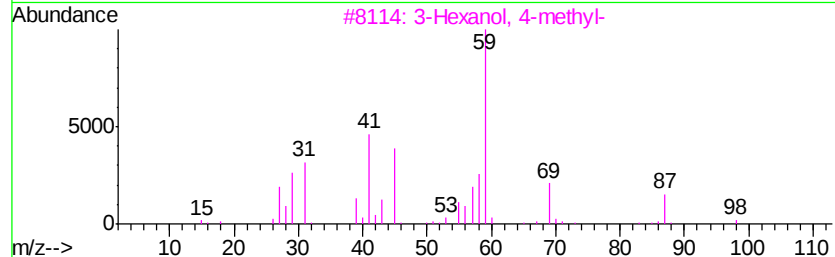
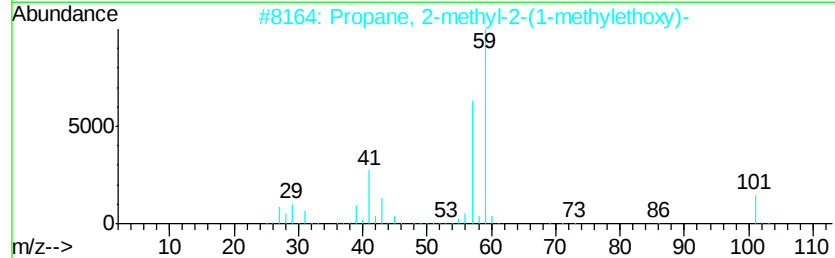
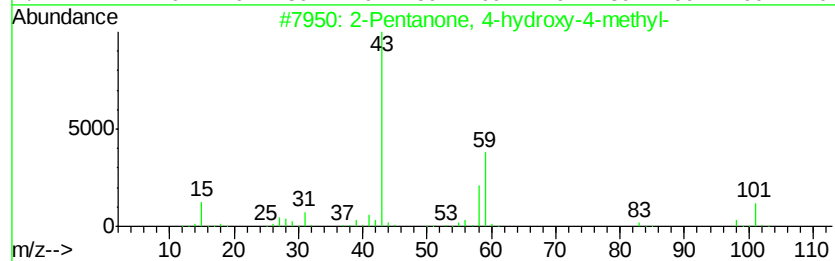
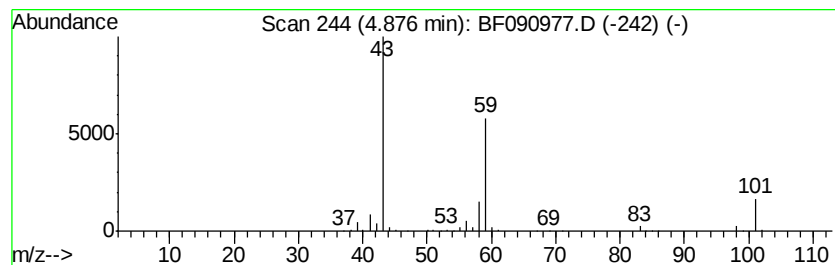
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.88	21.40 ng	1113830	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

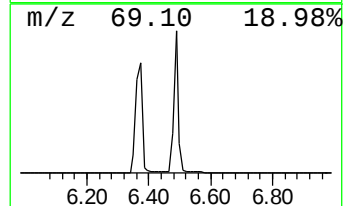
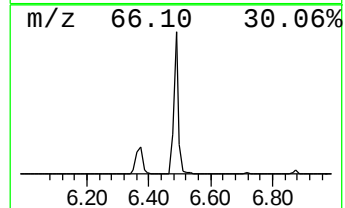
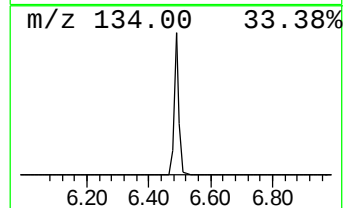
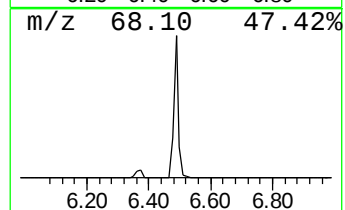
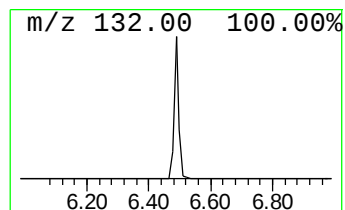
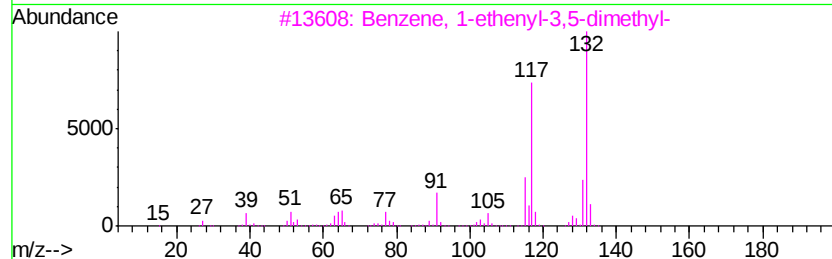
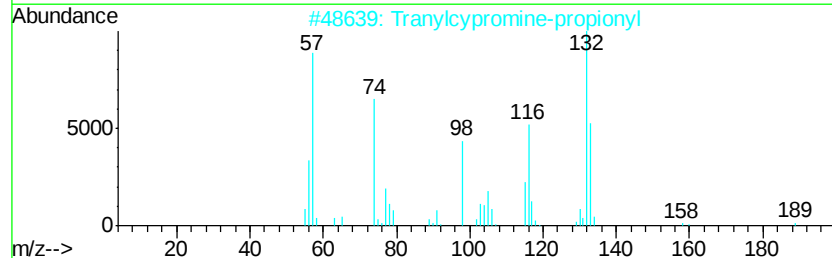
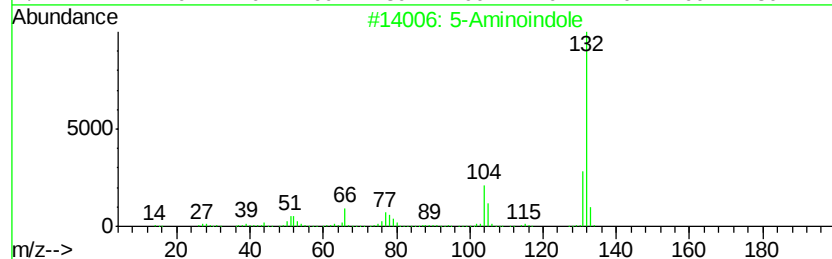
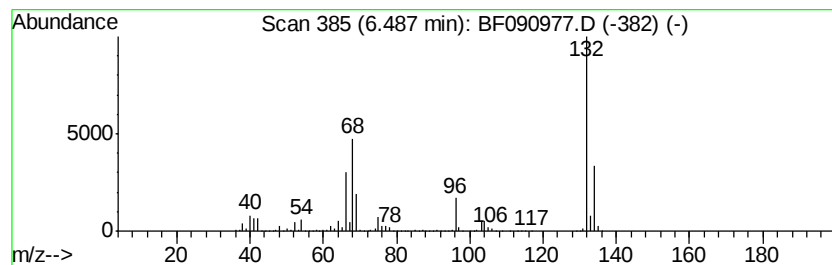
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.35 ng	4389250	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

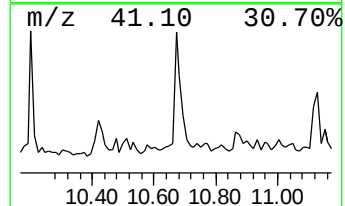
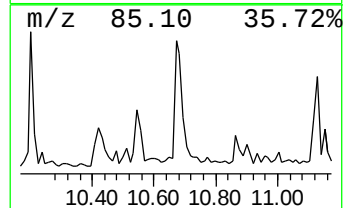
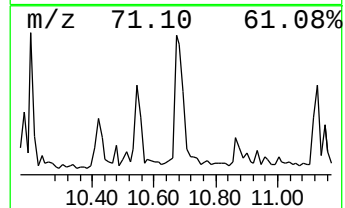
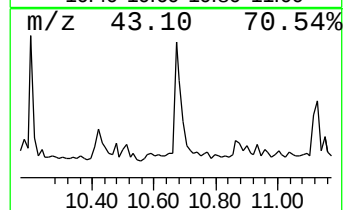
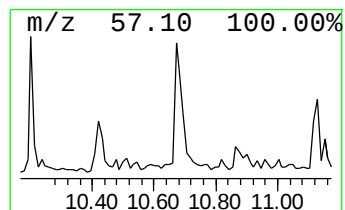
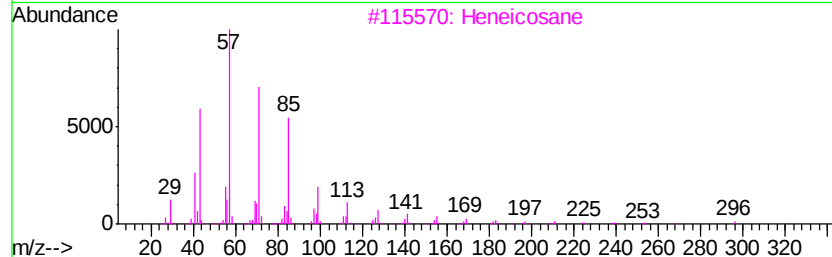
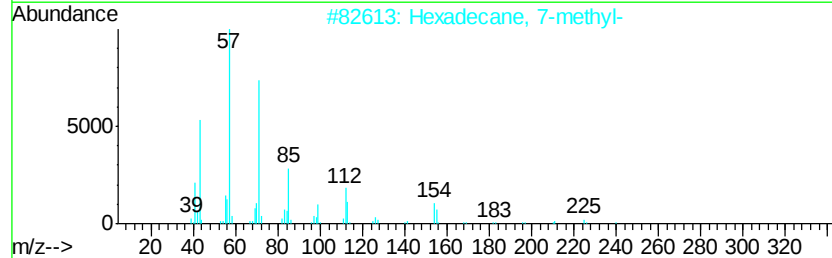
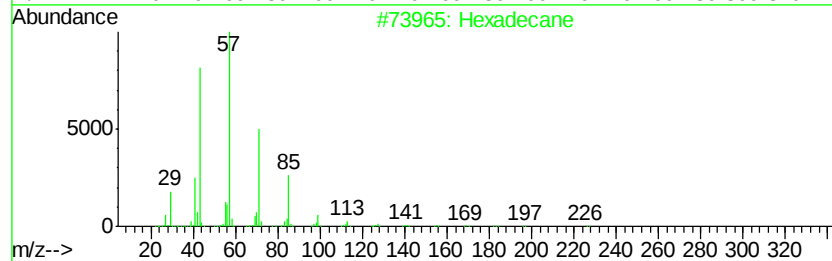
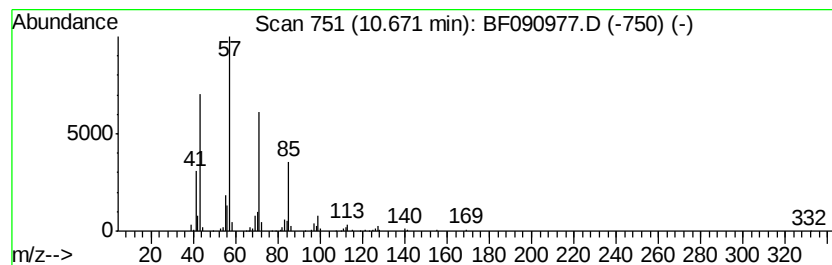
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.07 ng	278668	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Hexadecane, 7-methyl-		240	C17H36	026730-20-1	83
3	Heneicosane		296	C21H44	000629-94-7	83
4	Eicosane		282	C20H42	000112-95-8	74
5	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

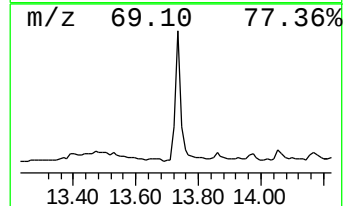
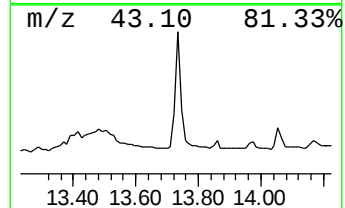
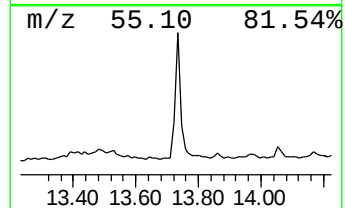
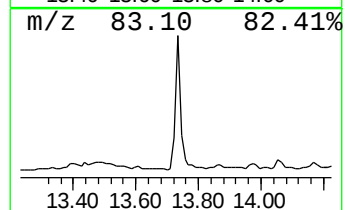
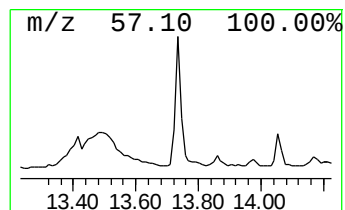
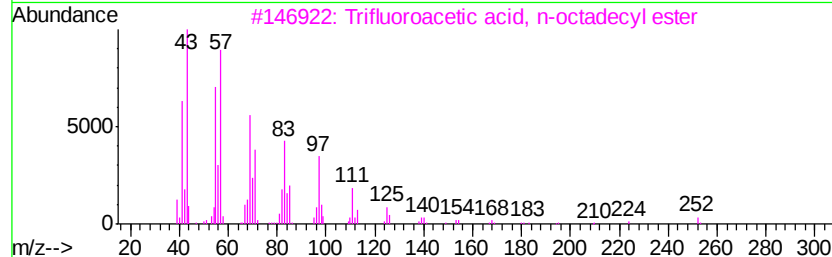
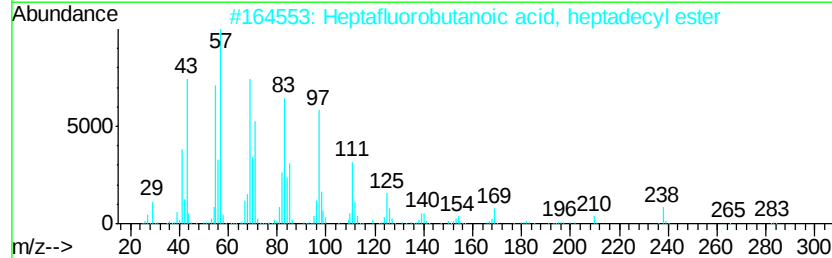
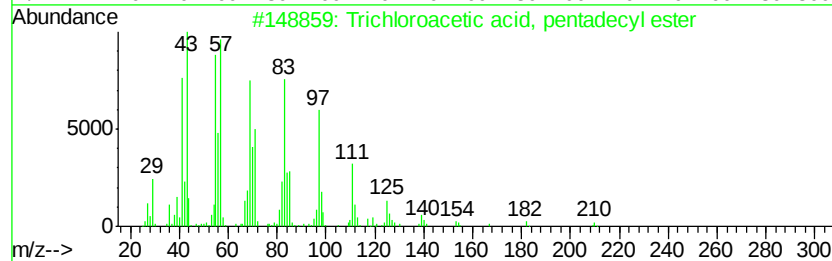
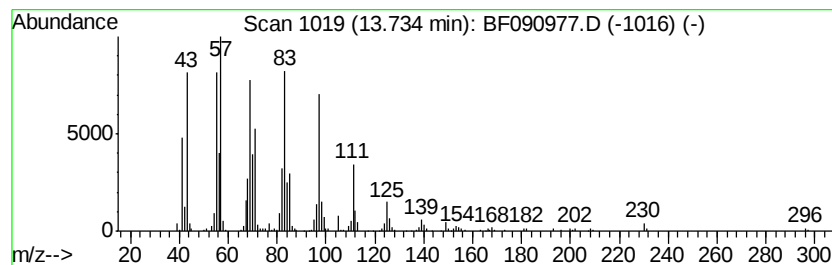
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.20 ng	558518	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

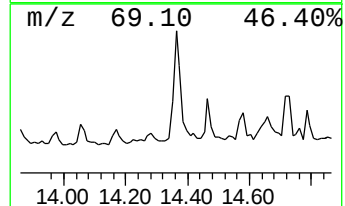
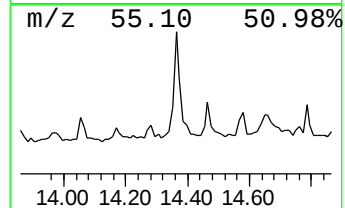
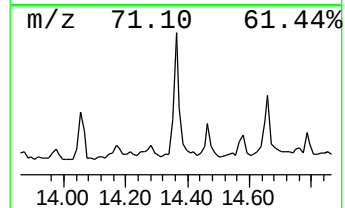
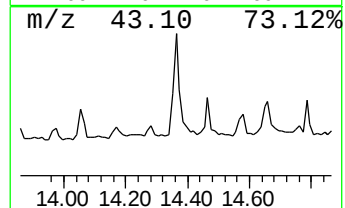
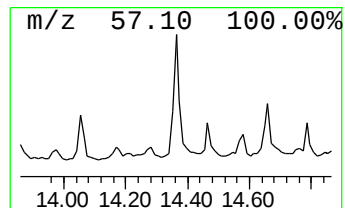
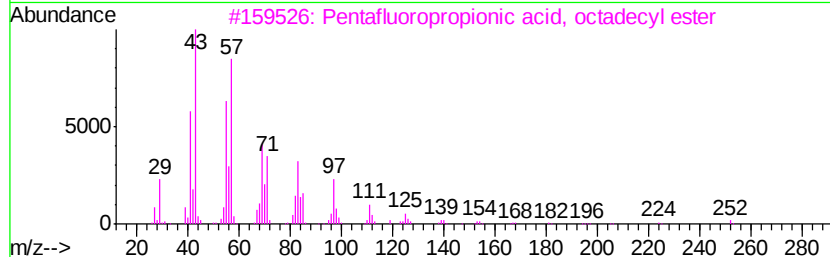
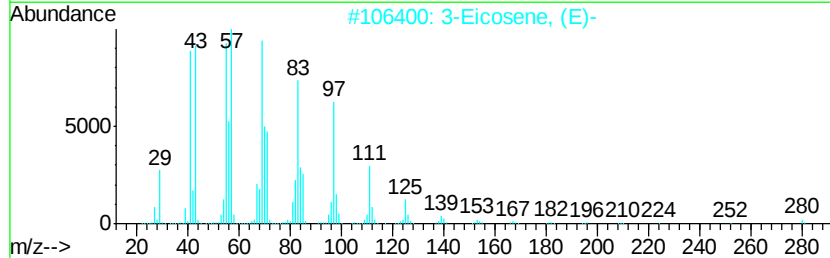
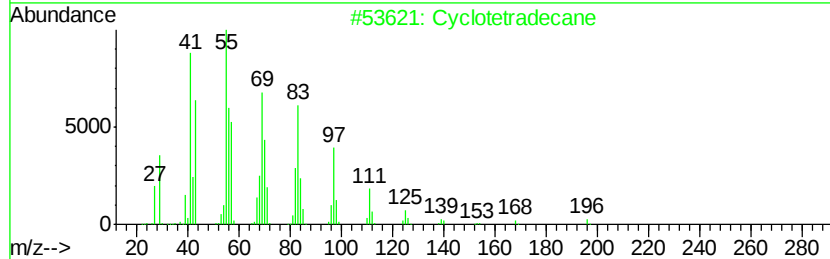
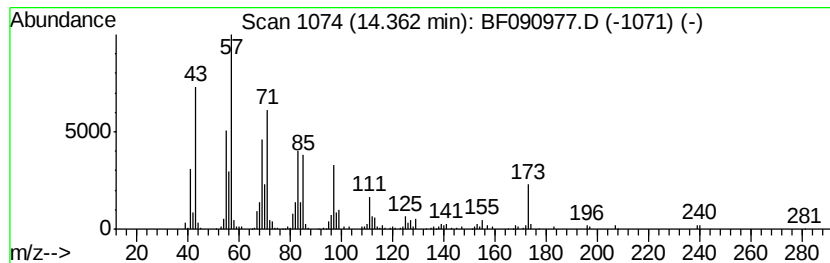
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.83 ng	297094	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	81
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	60
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	1000280-07-7	58
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	53
5		11-Tricosene	322	C23H46	052078-56-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

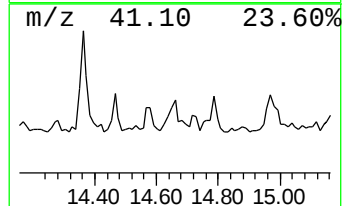
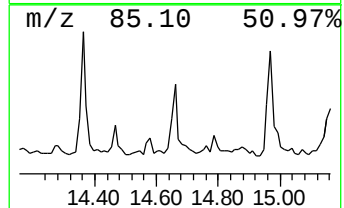
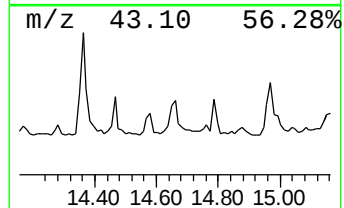
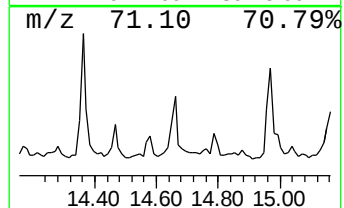
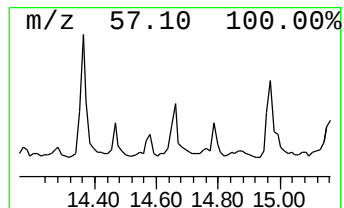
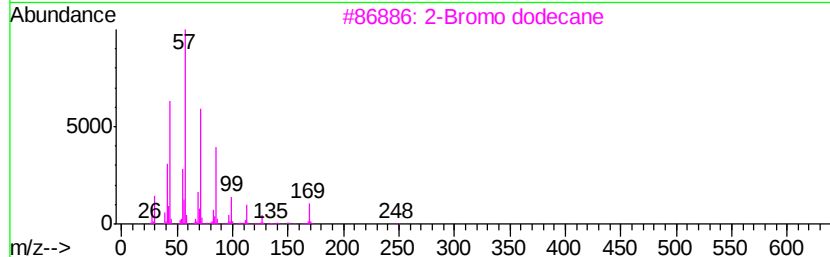
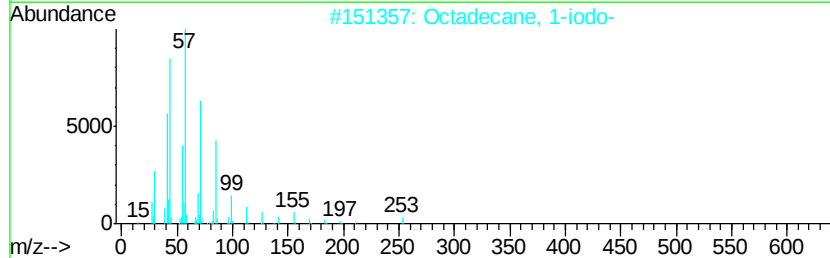
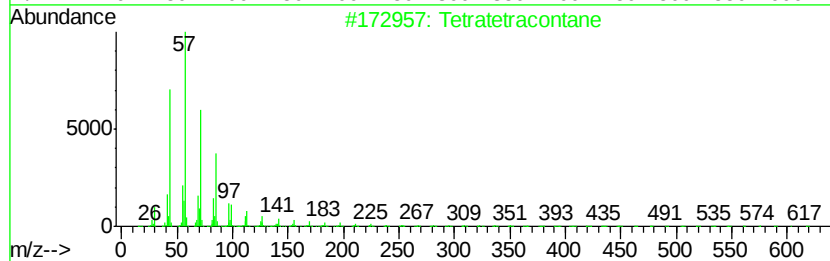
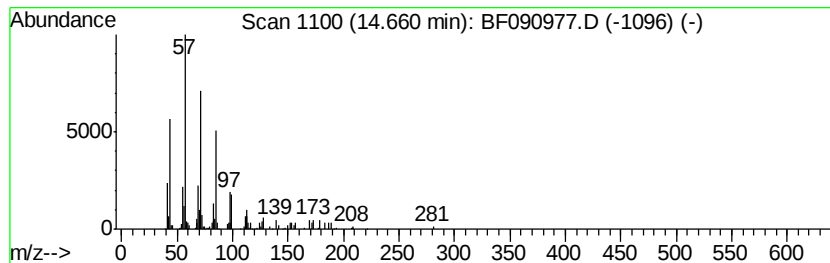
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.29 ng	118840	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	72
2		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	64
4		Octacosane	394	C28H58	000630-02-4	64
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

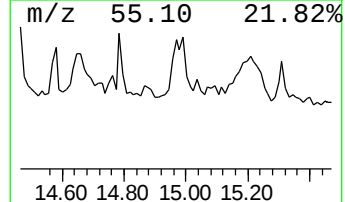
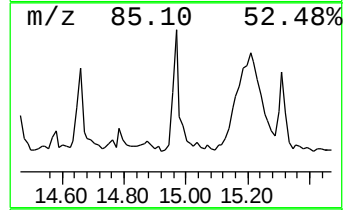
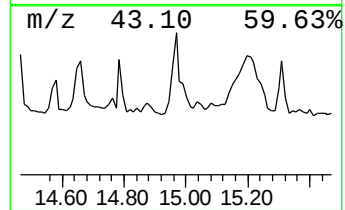
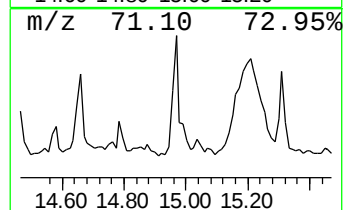
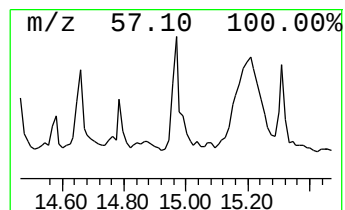
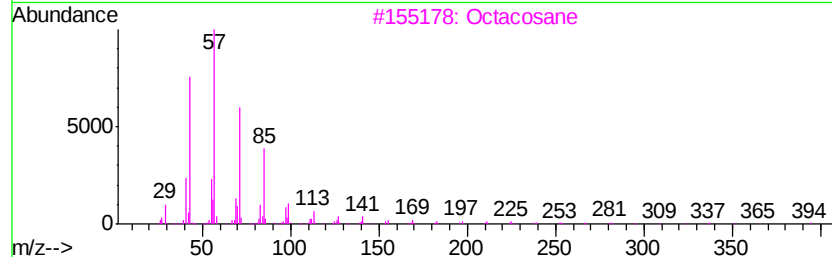
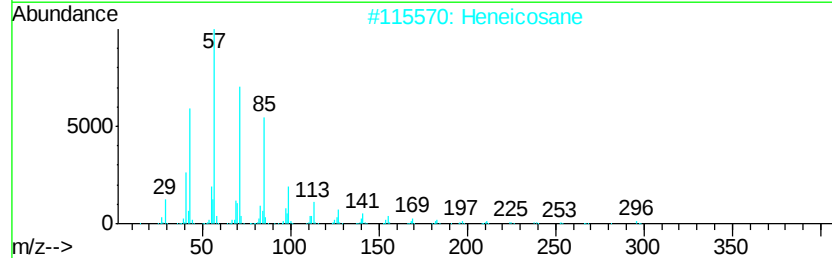
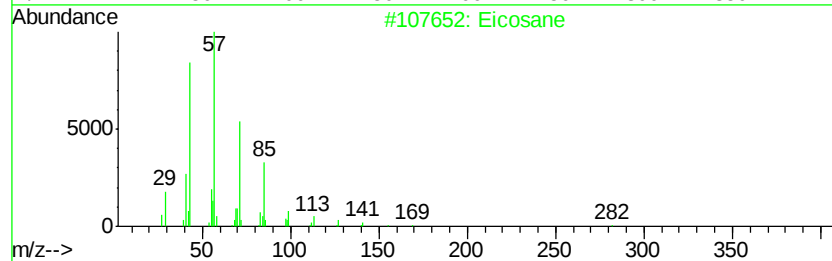
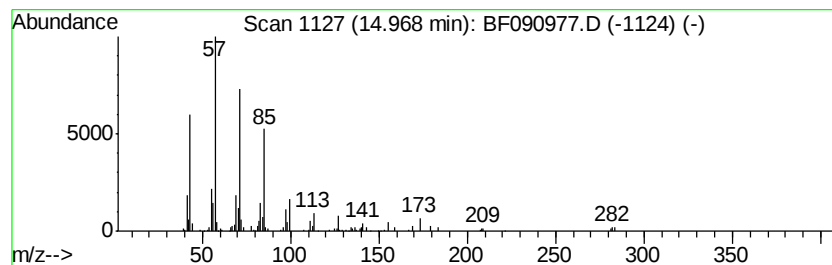
Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.97	3.50 ng	181507	Perylene-d12		15.28
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

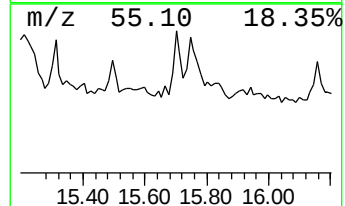
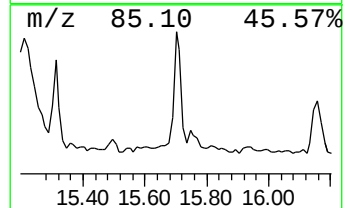
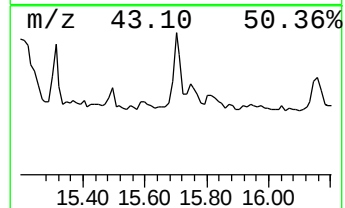
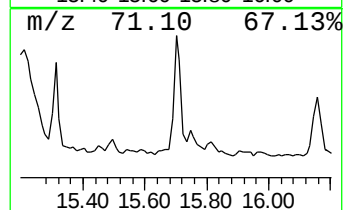
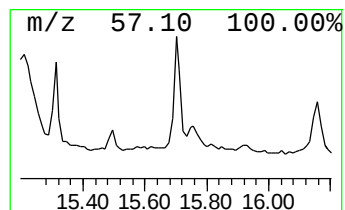
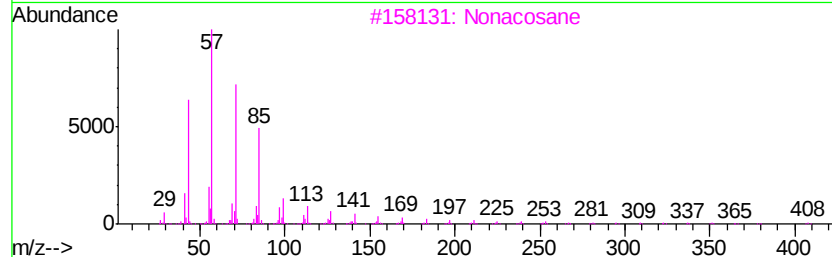
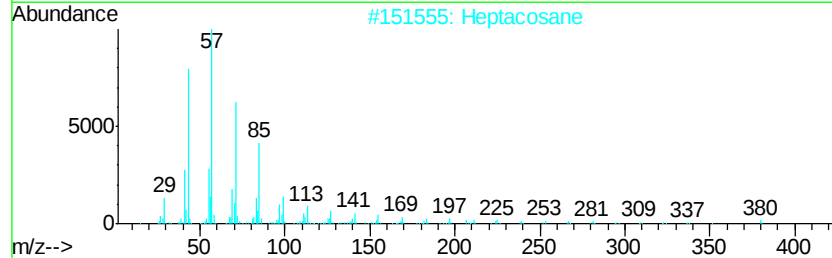
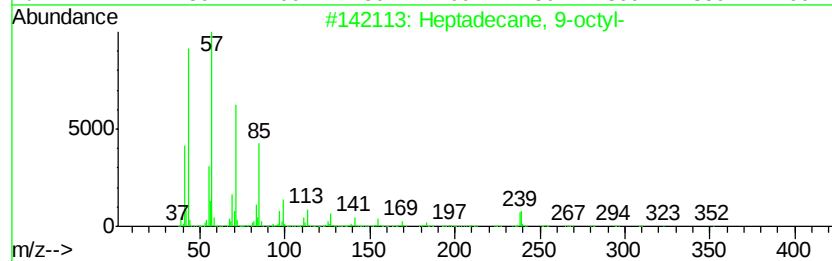
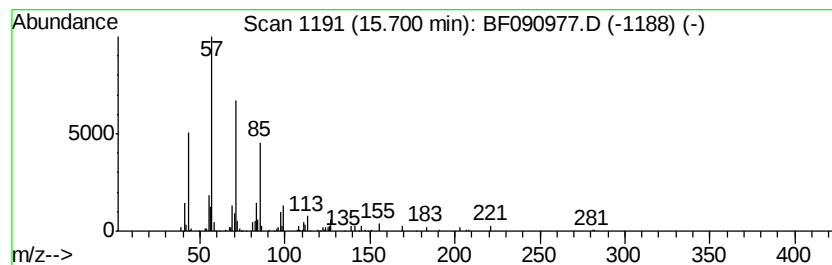
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.10 ng	109173	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heptacosane	380	C27H56	000593-49-7	90
3		Nonacosane	408	C29H60	000630-03-5	90
4		Tetratriacontane	479	C34H70	014167-59-0	90
5		Eicosane, 9-octyl-	394	C28H58	013475-77-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

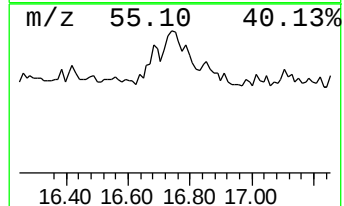
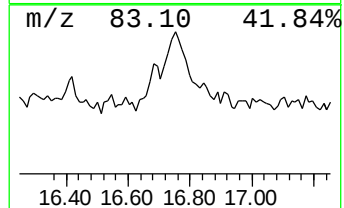
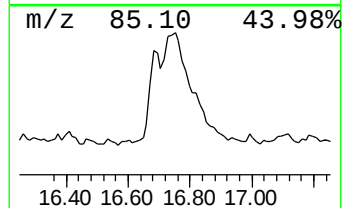
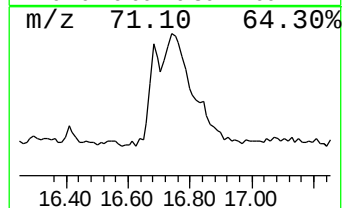
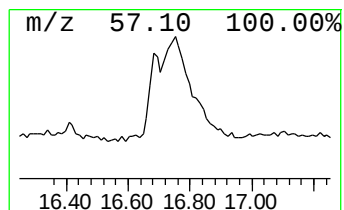
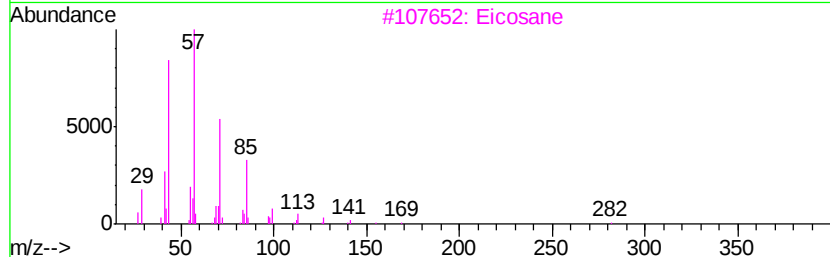
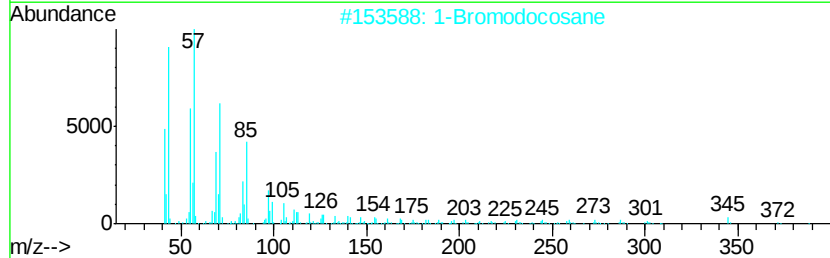
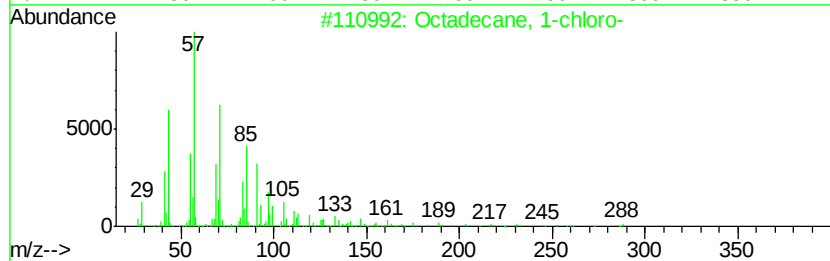
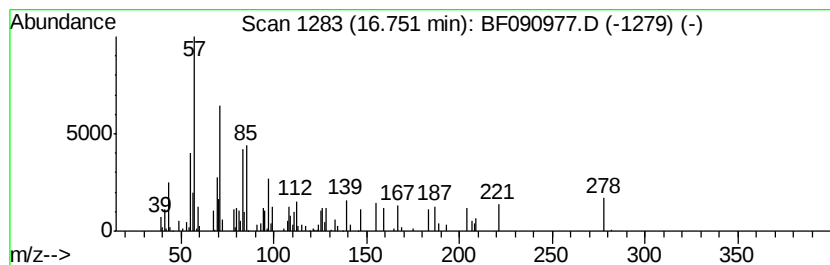
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.75 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.51 ng	130273	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	47
2			1-Bromodocosane	388	C22H45Br	006938-66-5	43
3			Eicosane	282	C20H42	000112-95-8	41
4			Tetratetracontane	619	C44H90	007098-22-8	38
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

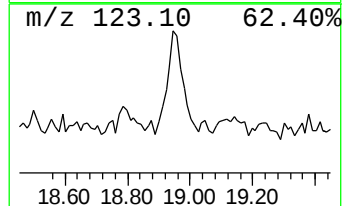
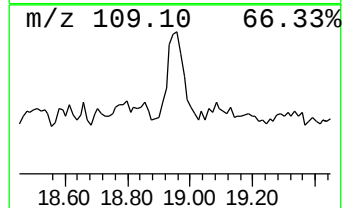
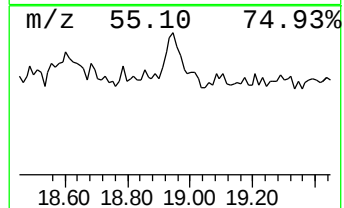
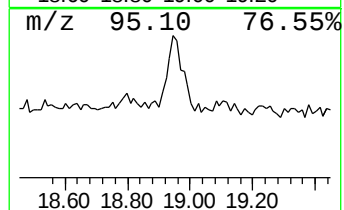
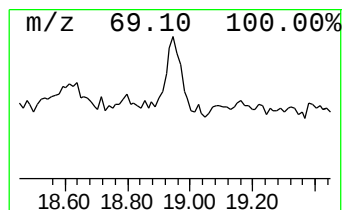
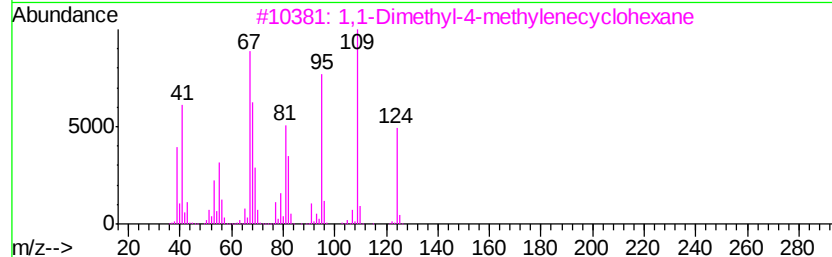
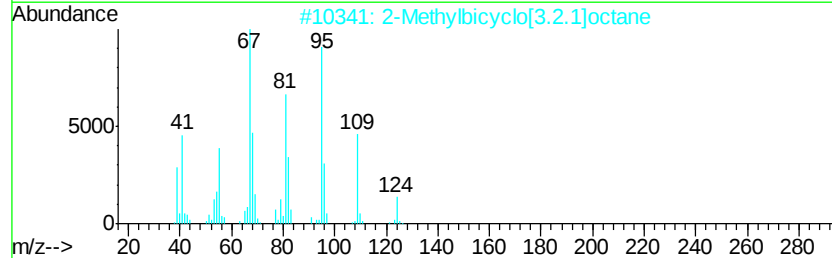
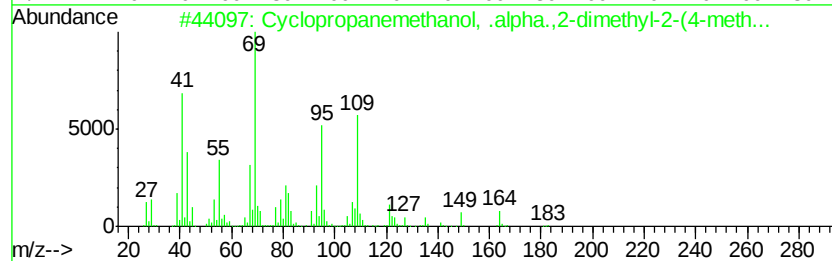
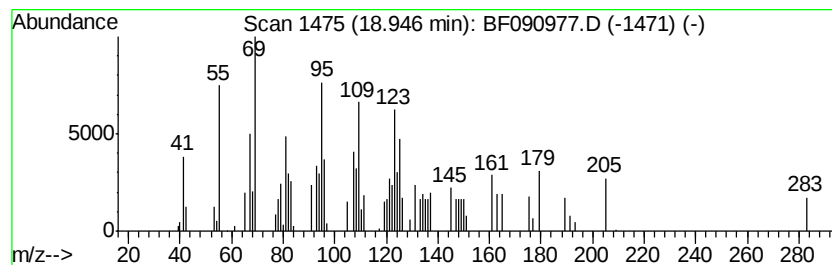
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.95 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.95	2.59 ng	134188	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	38
2		2-Methylbicyclo[3.2.1]octane	124	C9H16	1000215-28-0	35
3		1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	20
4		[2-(1-butenyl)-2,2-dimethylcyclo...	163	C11H17N	1000111-15-4	15
5		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090977.D
Acq On : 2 Nov 2016 14:08
Operator : UM/SJ
Sample : H5502-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-89-1.5-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.88	21.4	ng	1113830	1	6.72	1040720	20.0
unknown6.49	6.49	84.3	ng	4389250	1	6.72	1040720	20.0
Hexadecane	10.67	3.1	ng	278668	4	11.24	1817880	20.0
Trichloroacetic a...	13.73	7.2	ng	558518	5	13.88	1550940	20.0
Cyclotetradecane	14.36	3.8	ng	297094	5	13.88	1550940	20.0
Tetratetracontane	14.66	2.3	ng	118840	6	15.28	1038080	20.0
Eicosane	14.97	3.5	ng	181507	6	15.28	1038080	20.0
Heptadecane, 9-oc...	15.70	2.1	ng	109173	6	15.28	1038080	20.0
unknown16.75	16.75	2.5	ng	130273	6	15.28	1038080	20.0
unknown18.95	18.95	2.6	ng	134188	6	15.28	1038080	20.0