

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
 Data File : BF082622.D
 Acq On : 31 Oct 2015 15:34
 Operator : UM/IZ
 Sample : G4200-01
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-22L

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	5.104	260	264	266	rBV	1730725	2845958	49.97%	4.887%
2	5.516	297	300	302	rBV	5315822	5695290	100.00%	9.780%
3	6.533	386	389	391	rBV	5021333	5262832	92.41%	9.037%
4	6.670	398	401	404	rVB	5482405	5131673	90.10%	8.812%
5	6.899	419	421	424	rBV	1266543	1511392	26.54%	2.595%
6	7.059	433	435	437	rVB	3946460	3696928	64.91%	6.348%
7	7.459	467	470	473	rBV	2491003	3653678	64.15%	6.274%
8	8.190	531	534	536	rBV	2560279	2079655	36.52%	3.571%
9	9.276	626	629	631	rBV	4721139	5645190	99.12%	9.694%
10	9.665	660	663	665	rBV	1491124	1256068	22.05%	2.157%
11	9.893	681	683	685	rBV	93300	79985	1.40%	0.137%
12	9.950	685	688	690	rBV	2465124	2307880	40.52%	3.963%
13	10.145	700	705	707	rBV2	23961	57560	1.01%	0.099%
14	10.396	723	727	728	rBV	98453	149931	2.63%	0.257%
15	10.613	743	746	749	rBV	53330	79773	1.40%	0.137%
16	10.728	754	756	759	rBV2	2633322	3721392	65.34%	6.390%
17	10.865	766	768	773	rVB	181040	199567	3.50%	0.343%
18	11.310	805	807	809	rVB	82638	70241	1.23%	0.121%
19	11.436	815	818	820	rBV	1703083	2169669	38.10%	3.726%
20	11.665	836	838	843	rBV	128112	155796	2.74%	0.268%
21	11.905	856	859	862	rBV2	54828	93138	1.64%	0.160%
22	11.962	862	864	870	rVV	298116	508437	8.93%	0.873%
23	12.145	877	880	882	rVB	80532	93547	1.64%	0.161%
24	12.293	892	893	896	rVB	132807	139275	2.45%	0.239%
25	12.488	908	910	913	rBV	810280	806199	14.16%	1.384%
26	12.533	913	914	917	rVB	59418	70467	1.24%	0.121%
27	12.636	921	923	925	rBV	51591	72456	1.27%	0.124%
28	12.693	926	928	930	rVV	194480	171604	3.01%	0.295%
29	12.751	931	933	940	rBV2	193302	261430	4.59%	0.449%
30	12.854	940	942	946	rVV2	192458	211975	3.72%	0.364%
31	13.025	954	957	959	rVB	5002719	4767114	83.70%	8.186%
32	13.162	967	969	971	rBV	347438	317770	5.58%	0.546%
33	13.482	991	997	999	rBV2	99240	138342	2.43%	0.238%
34	13.562	1002	1004	1006	rVV	132495	133108	2.34%	0.229%

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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 >
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35	13.608	1006	1008	1013	rVB4	26947	60063	1.05%	0.103%
36	13.814	1022	1026	1028	rBV3	36936	64381	1.13%	0.111%
37	13.928	1033	1036	1040	rBV	320865	461552	8.10%	0.793%
38	14.076	1046	1049	1051	rBV	1153896	1586208	27.85%	2.724%
39	14.579	1090	1093	1100	rBV2	124135	245335	4.31%	0.421%
40	15.219	1147	1149	1150	rBV	69039	80553	1.41%	0.138%
41	15.528	1173	1176	1179	rBV	897057	1291370	22.67%	2.217%
42	16.077	1222	1224	1229	rBV4	36527	76264	1.34%	0.131%
43	16.820	1284	1289	1294	rVB5	25608	64619	1.13%	0.111%
44	17.414	1337	1341	1346	rVB	126144	258342	4.54%	0.444%
45	17.585	1351	1356	1361	rBV3	77692	229747	4.03%	0.395%
46	19.608	1529	1533	1537	rVB6	24914	72260	1.27%	0.124%
47	20.397	1596	1602	1609	rBV9	50088	190712	3.35%	0.327%

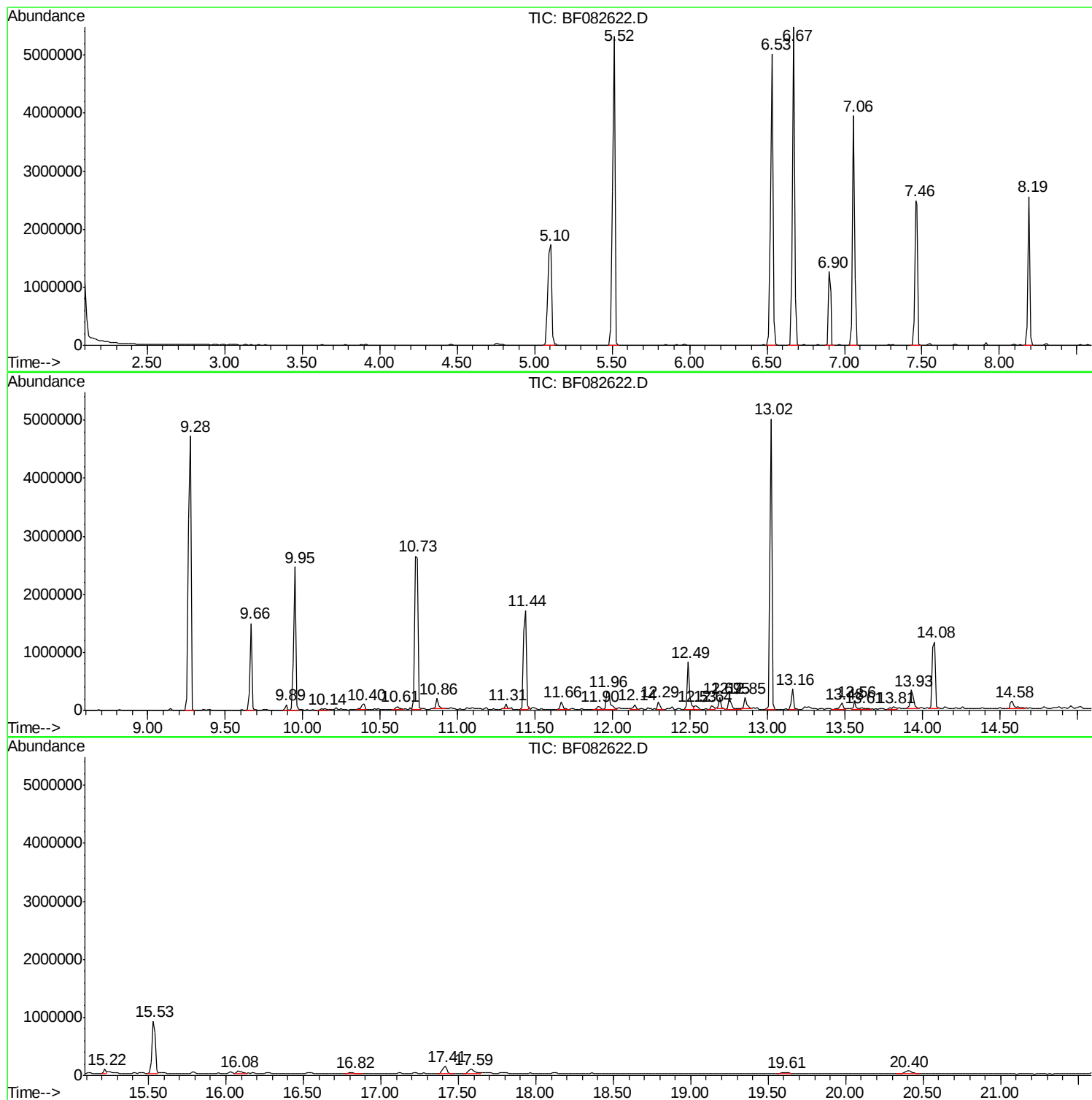
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : UM/IZ
Sample : G4200-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

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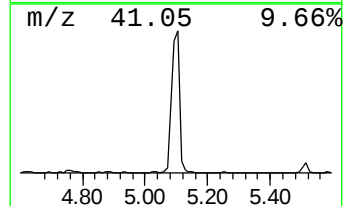
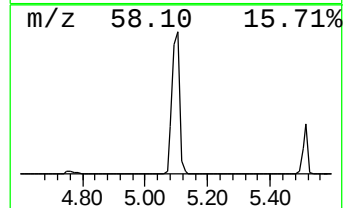
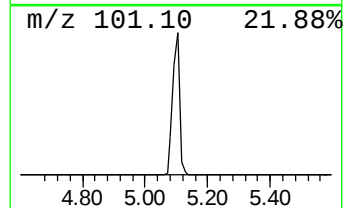
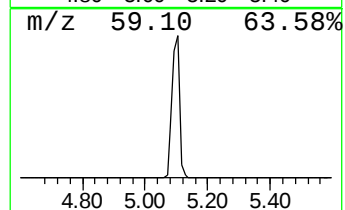
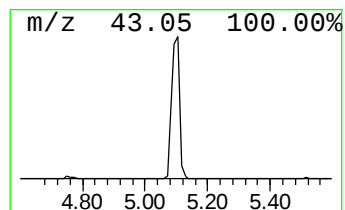
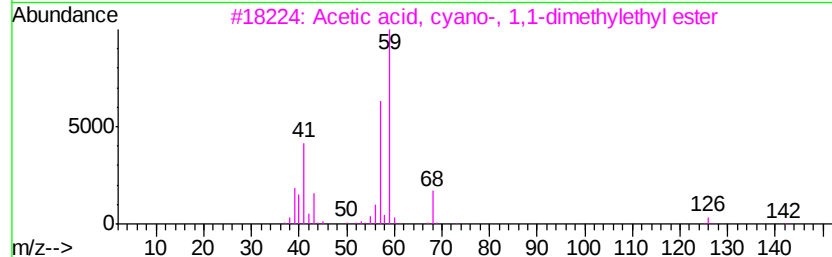
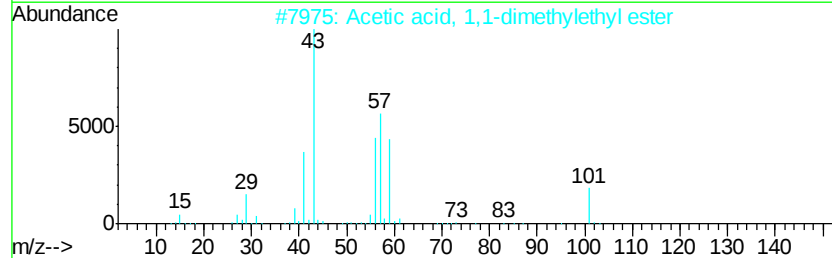
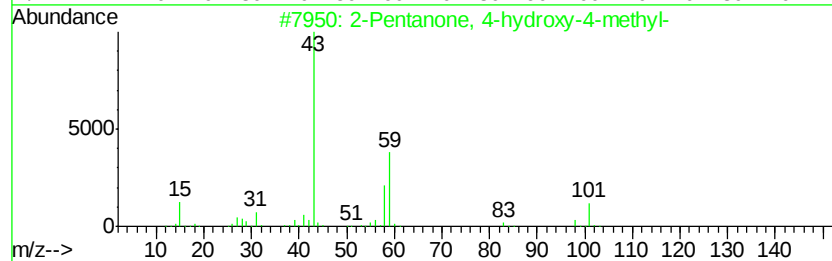
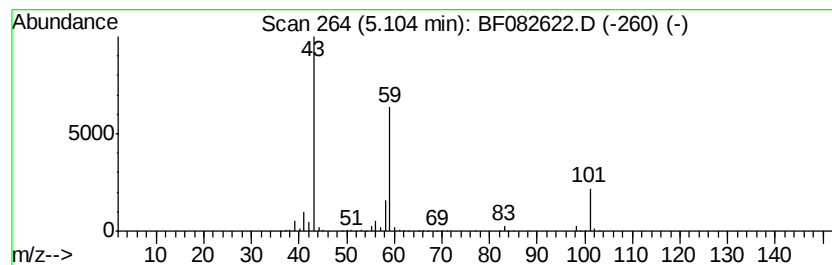
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	37.66 ng	2845960	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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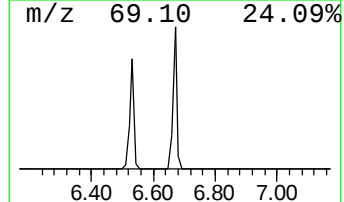
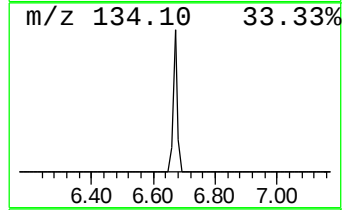
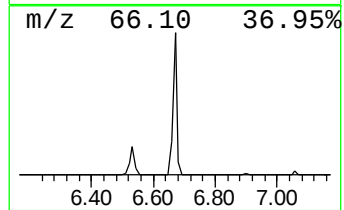
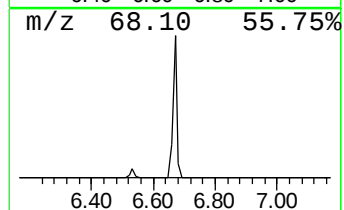
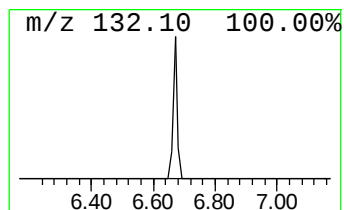
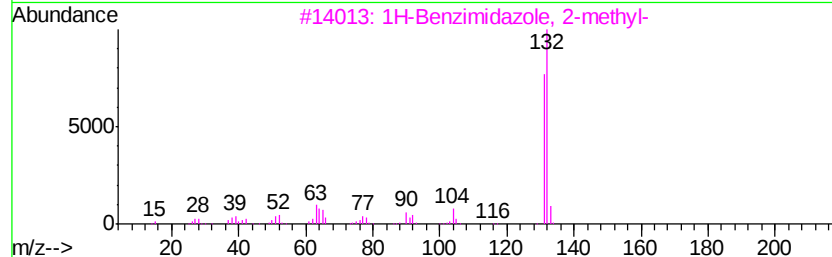
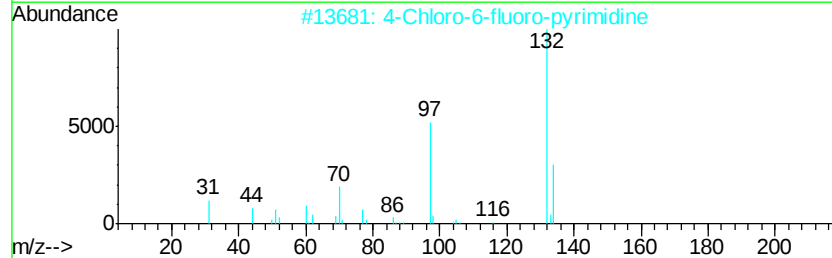
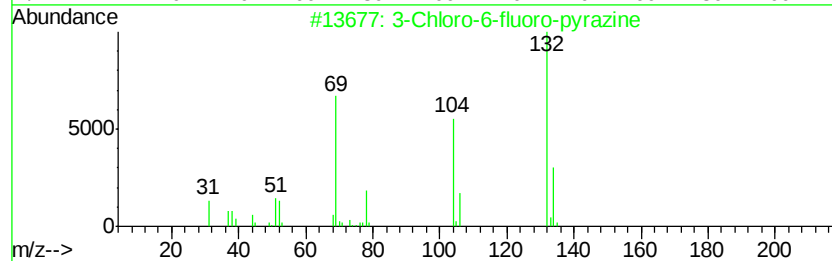
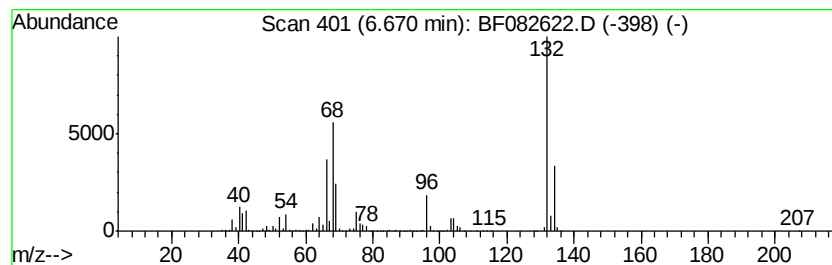
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	67.91 ng	5131670	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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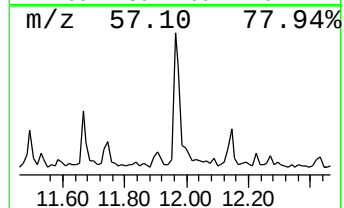
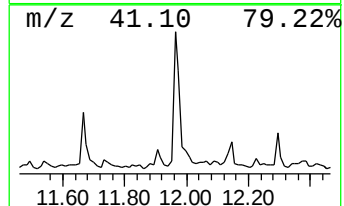
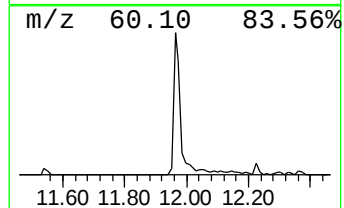
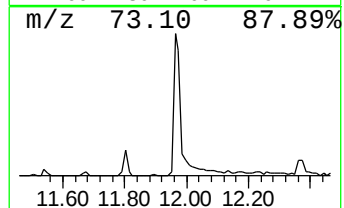
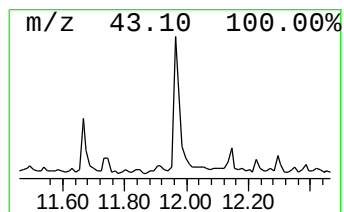
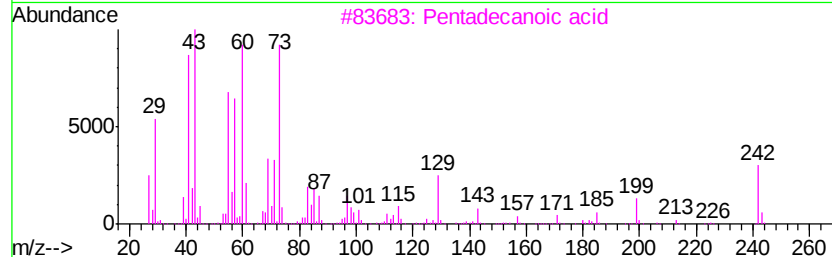
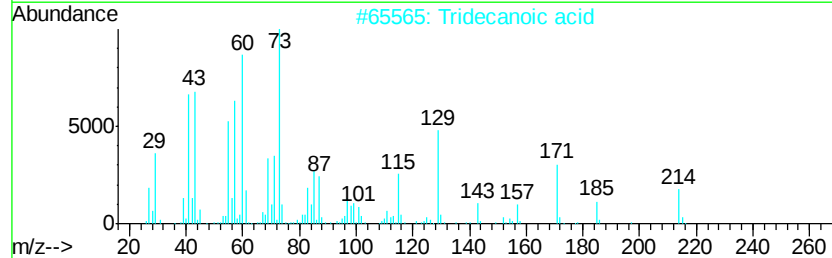
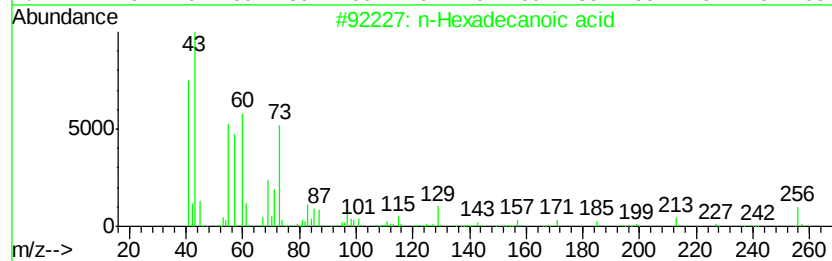
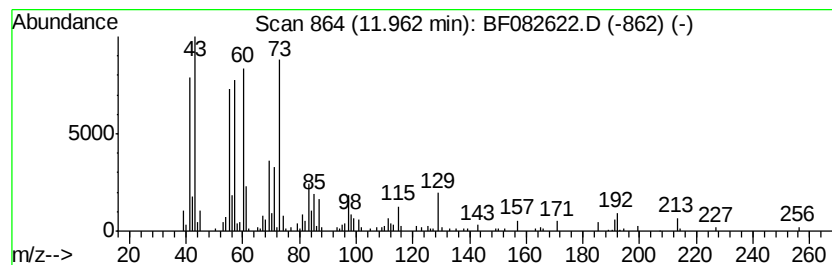
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	4.69 ng	508437	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



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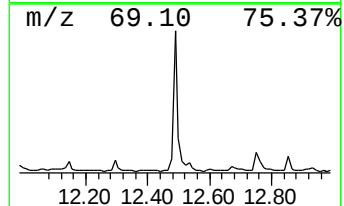
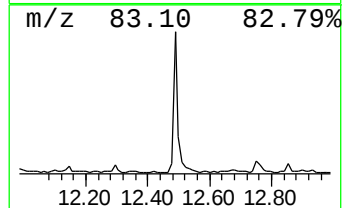
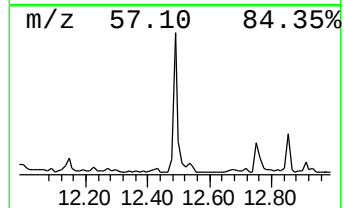
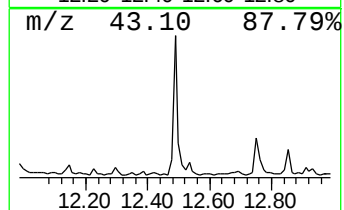
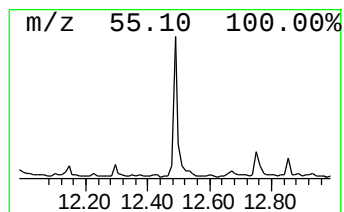
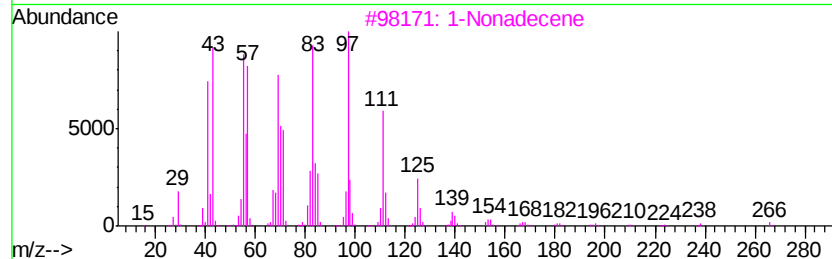
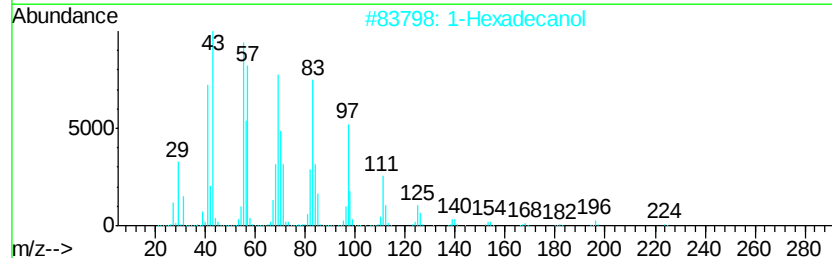
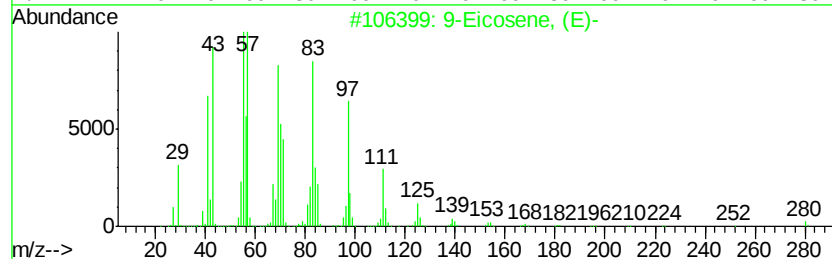
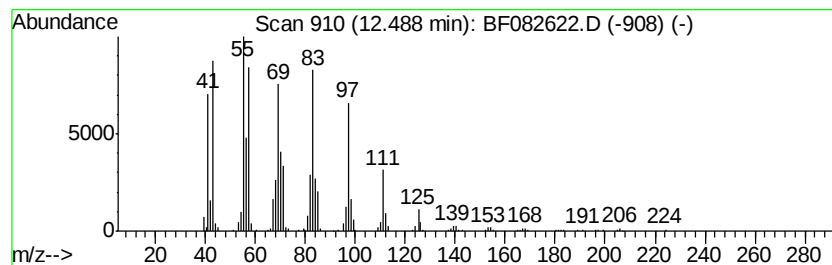
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	7.43 ng	806199	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Cyclohexadecane	224	C16H32	000295-65-8	91
5		9-Octadecene, (E)-	252	C18H36	007206-25-9	91



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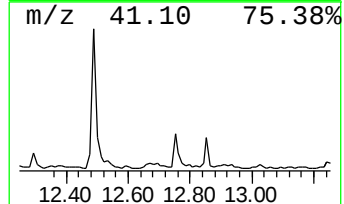
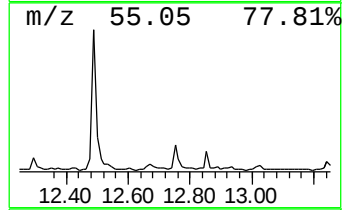
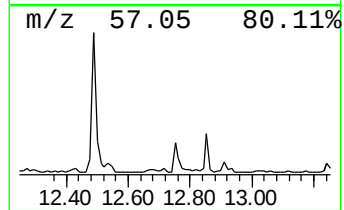
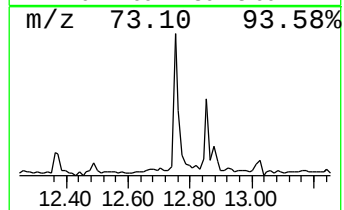
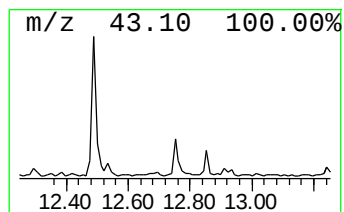
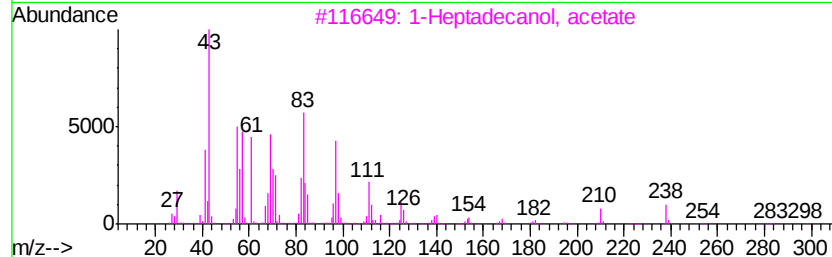
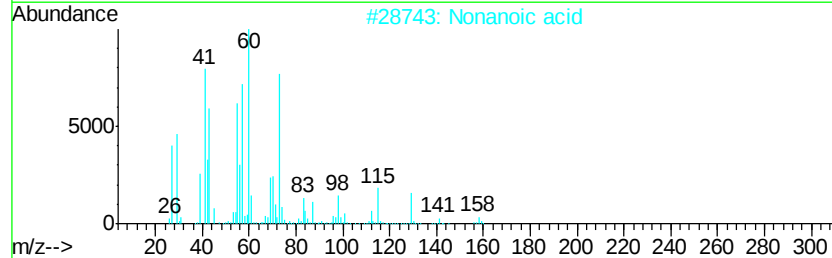
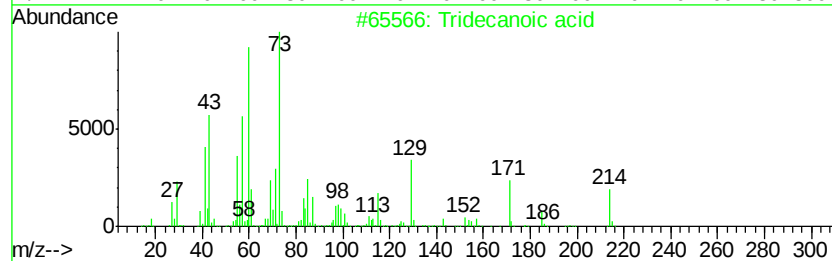
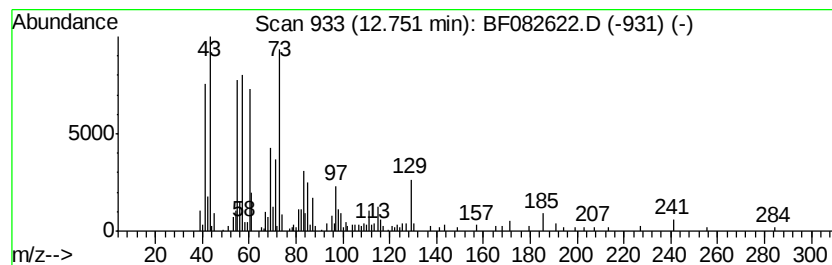
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.41 ng	261430	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	80
2		Nonanoic acid	158	C9H18O2	000112-05-0	27
3		1-Heptadecanol, acetate	298	C19H38O2	000822-20-8	25
4		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	14
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082622.D
Acq On : 31 Oct 2015 15:34
Operator : UM/IZ
Sample : G4200-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-22L

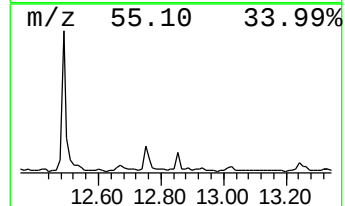
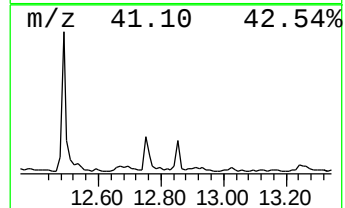
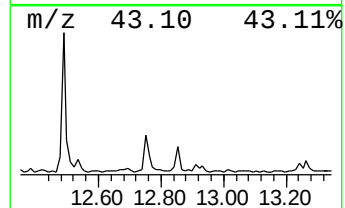
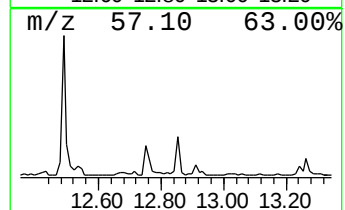
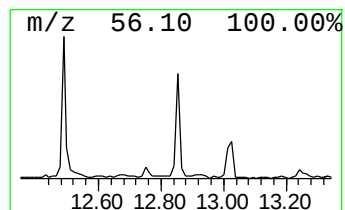
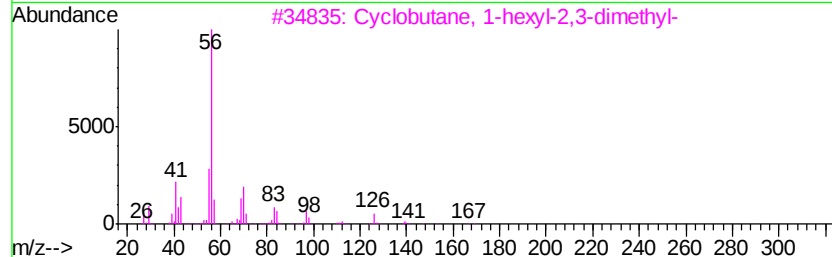
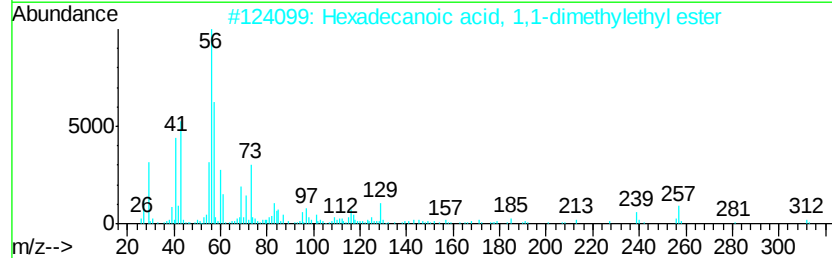
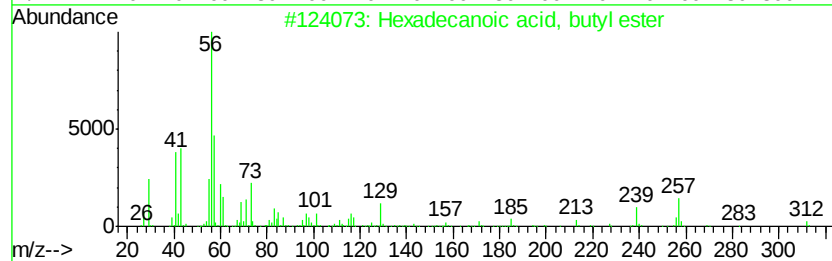
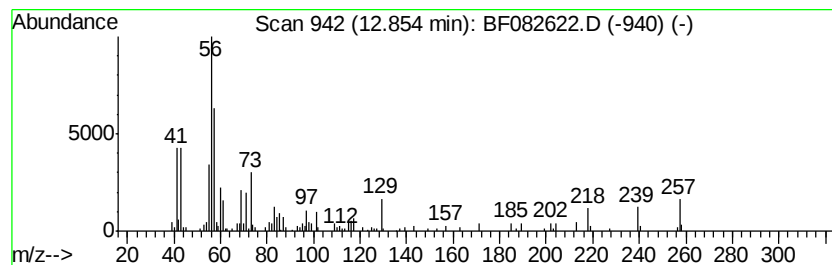
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.67 ng	211975	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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Sample : G4200-01
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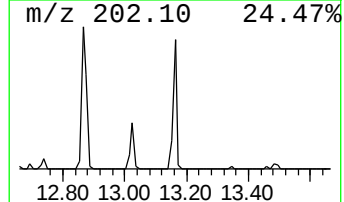
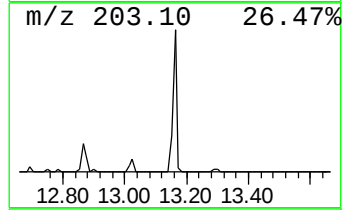
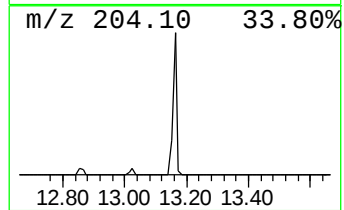
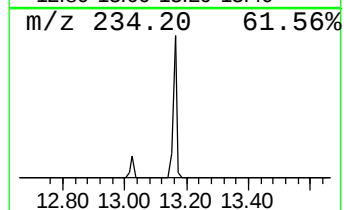
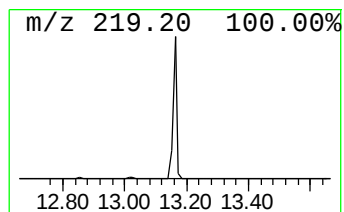
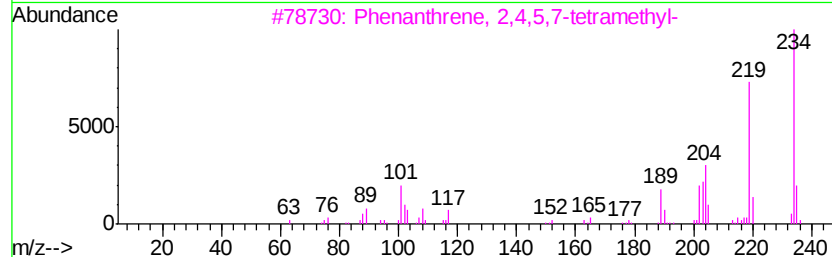
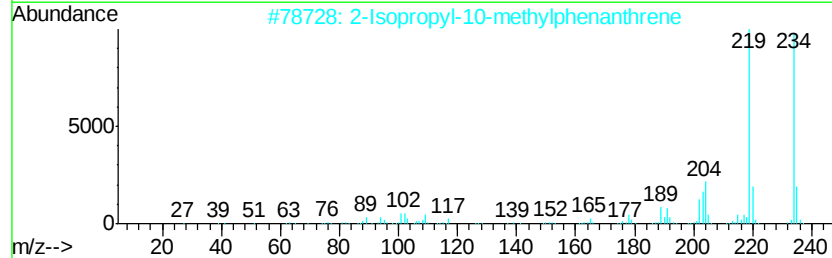
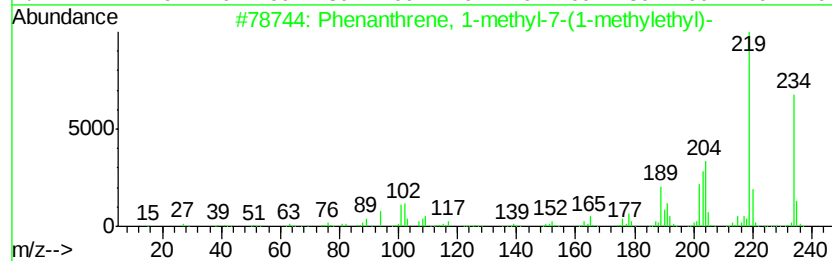
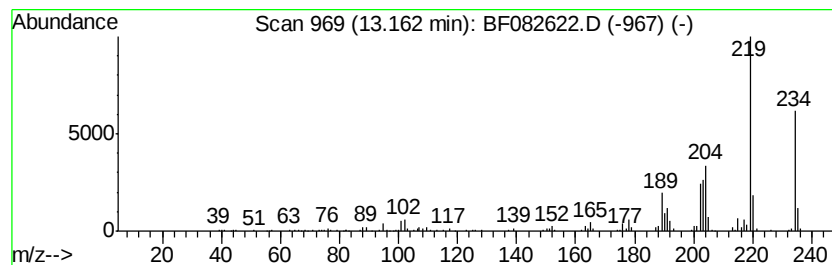
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenanthrene, 1-methyl-7-(1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.16	4.01 ng	317770	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-7-(1-meth...	234	C18H18	000483-65-8	98
2	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	68
4	2,5-Diphenyl-2,4-hexadiene	234	C18H18	016819-47-9	64
5	Ethanone, 1-(4,6-dihydroxy-2,3,5...	234	C13H14O4	021987-07-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082622.D
Acq On : 31 Oct 2015 15:34
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Sample : G4200-01
Misc :
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Instrument :
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ClientSampleId :
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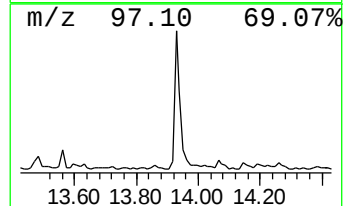
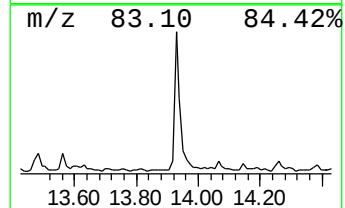
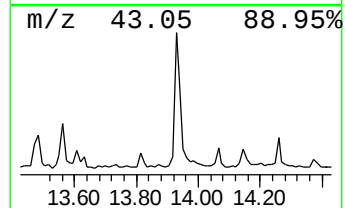
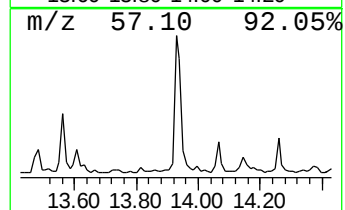
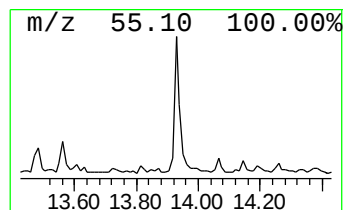
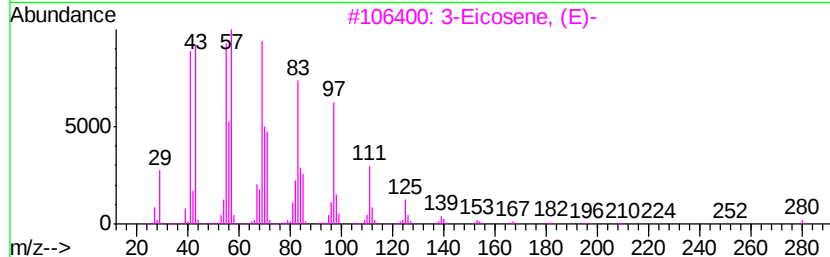
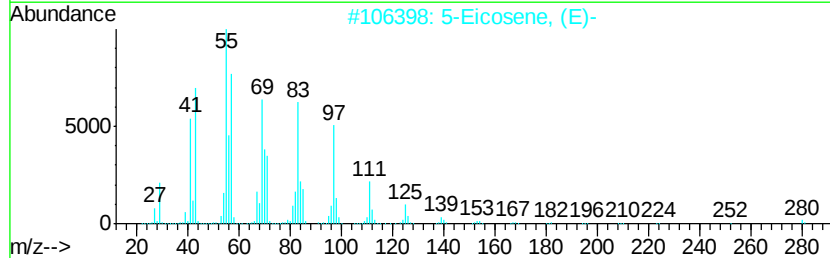
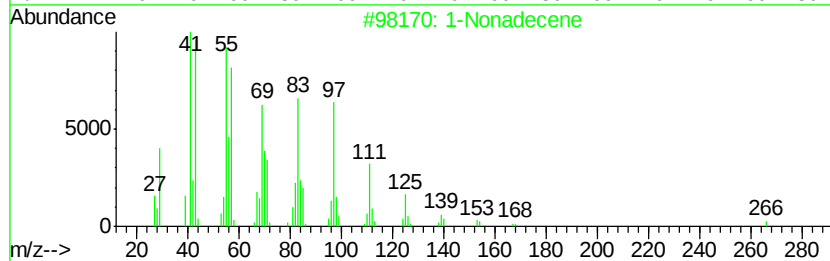
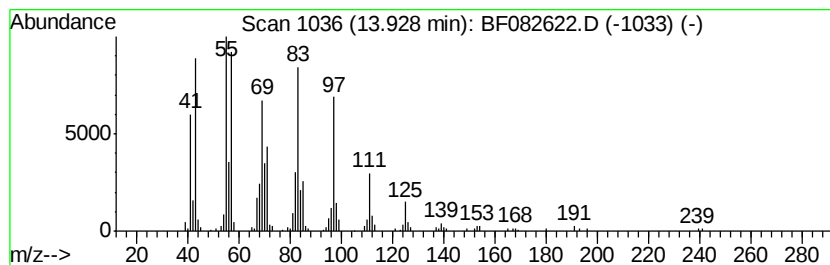
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	5.82 ng	461552	Chrysene-d12	14.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	5-Eicosene, (E)-		280	C20H40	074685-30-6	83
3	3-Eicosene, (E)-		280	C20H40	074685-33-9	76
4	1-Docosene		308	C22H44	001599-67-3	76
5	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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Acq On : 31 Oct 2015 15:34
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Sample : G4200-01
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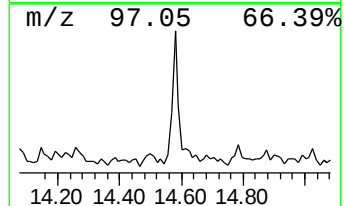
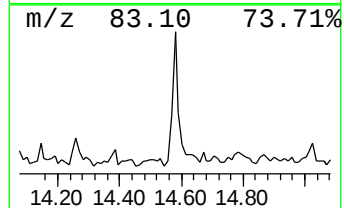
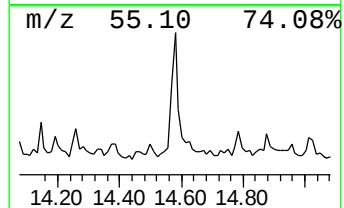
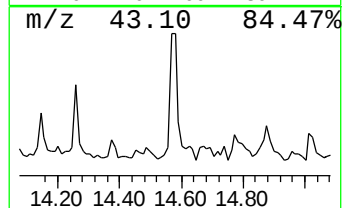
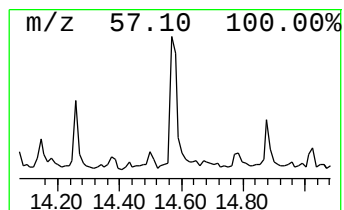
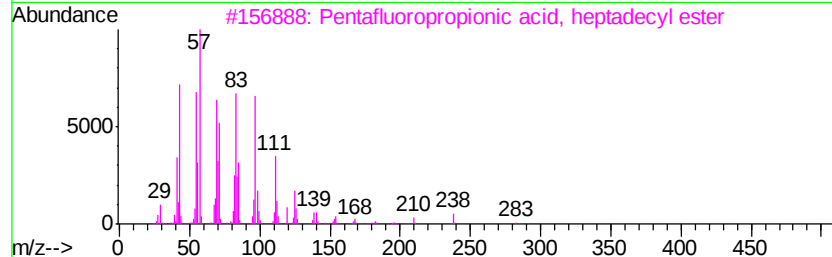
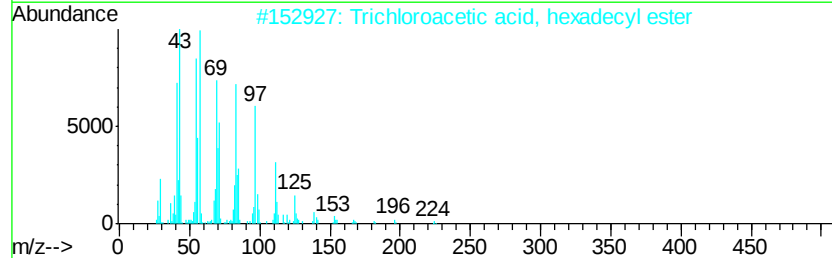
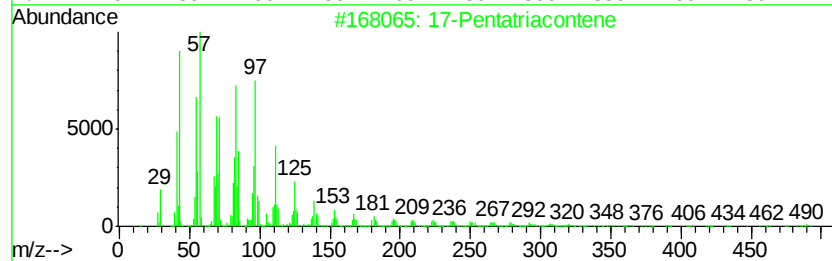
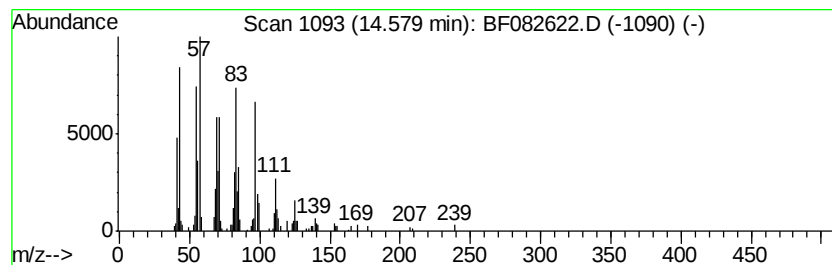
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.58	3.09 ng	245335	Chrysene-d12	14.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
5		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082622.D
Acq On : 31 Oct 2015 15:34
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Sample : G4200-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

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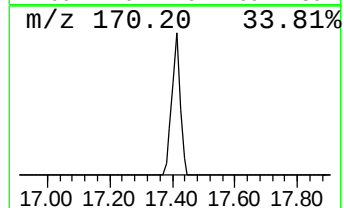
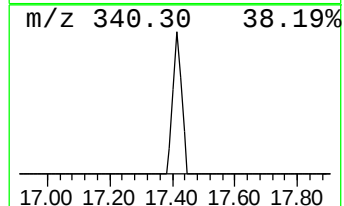
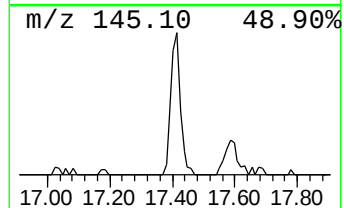
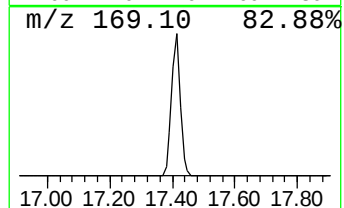
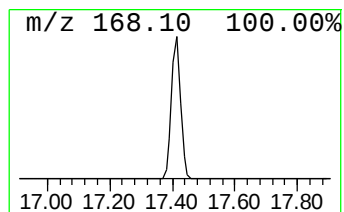
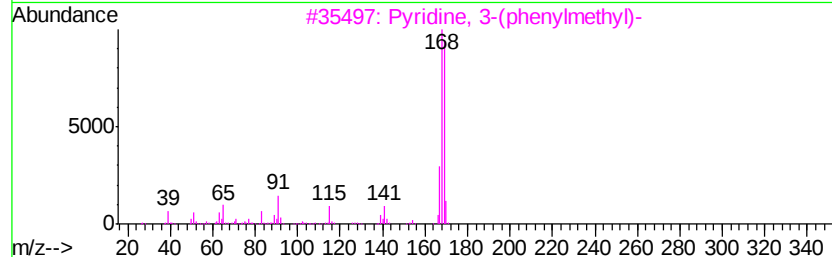
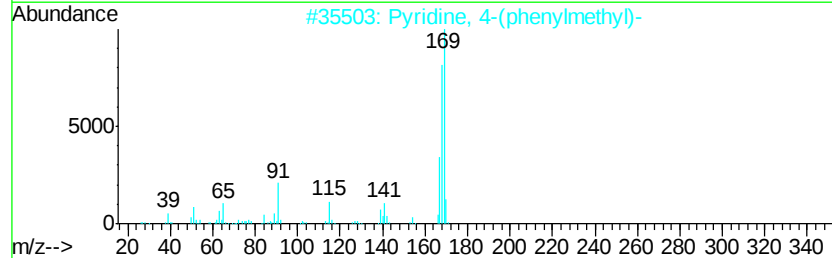
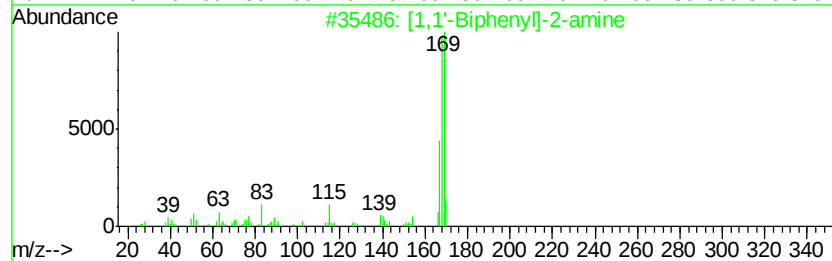
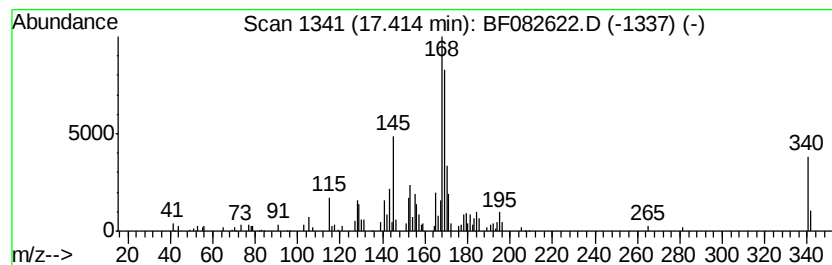
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown17.41 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	4.00 ng	258342	Perylene-d12	15.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	43
2			Pyridine, 4-(phenylmethyl)-	169	C12H11N	002116-65-6	38
3			Pyridine, 3-(phenylmethyl)-	169	C12H11N	000620-95-1	38
4			2-Methyl-3-phenylpyridine	169	C12H11N	003256-89-1	38
5			1,2,3,3a,8,9,9a,9b-Octahydrocyclo...	198	C15H18	148145-44-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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Acq On : 31 Oct 2015 15:34
Operator : UM/IZ
Sample : G4200-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

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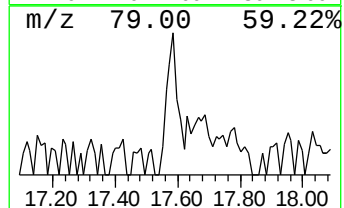
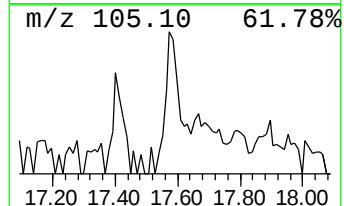
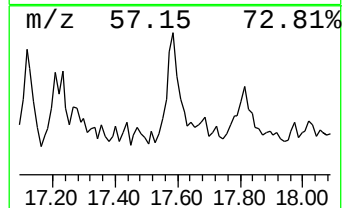
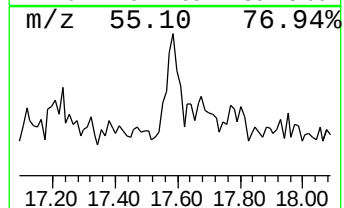
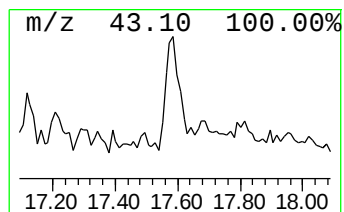
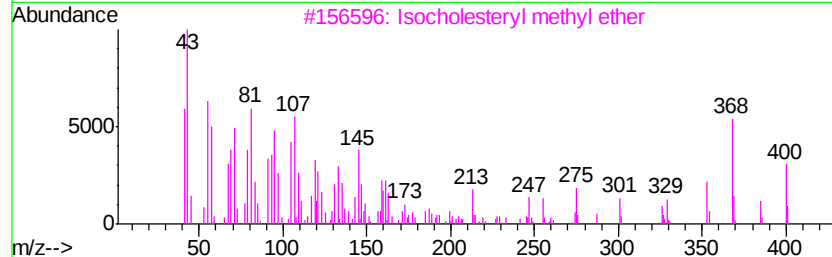
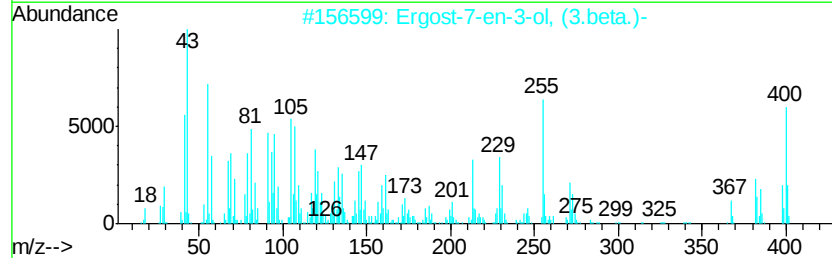
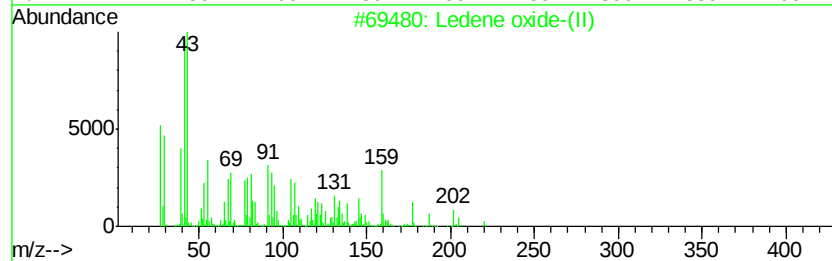
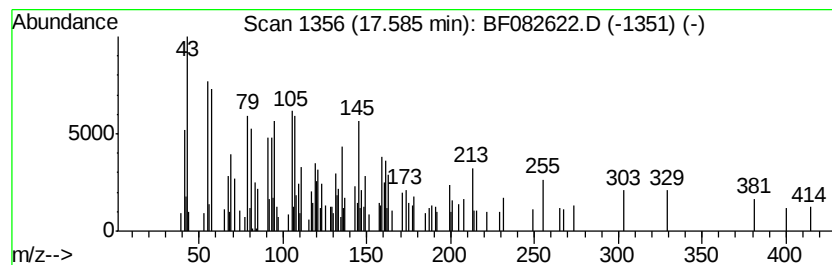
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.59 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	3.56 ng	229747	Perylene-d12	15.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ledene oxide-(II)	220	C15H24O	1000159-36-7	38
2			Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	38
3			Isocholesteryl methyl ether	400	C28H48O	029944-53-4	37
4			5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	32
5			Campesterol	400	C28H48O	000474-62-4	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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ALS Vial : 40 Sample Multiplier: 1

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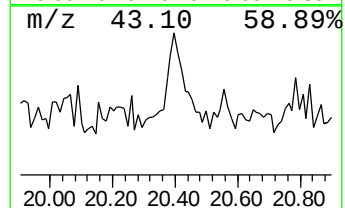
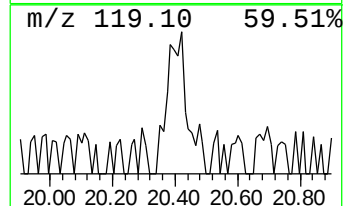
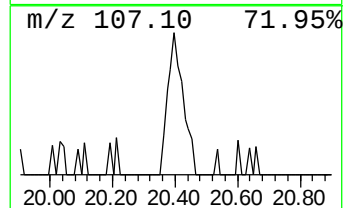
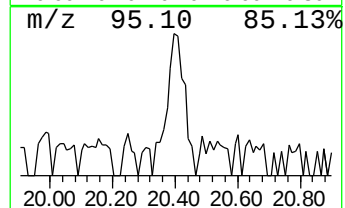
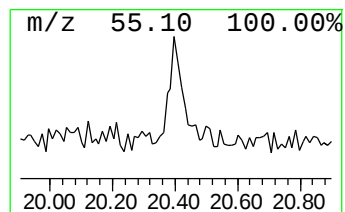
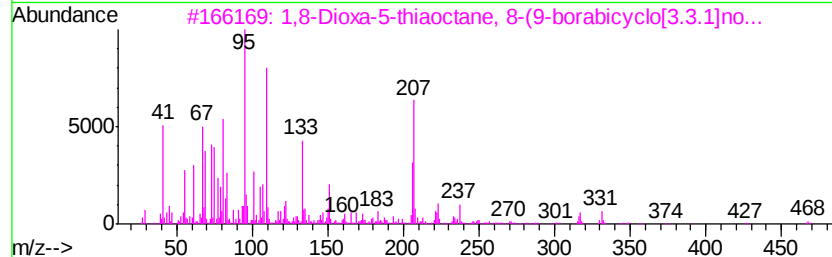
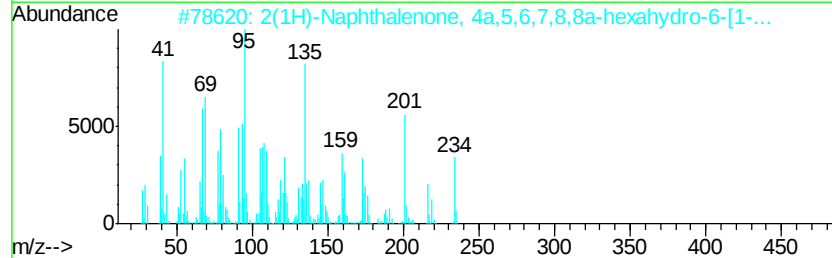
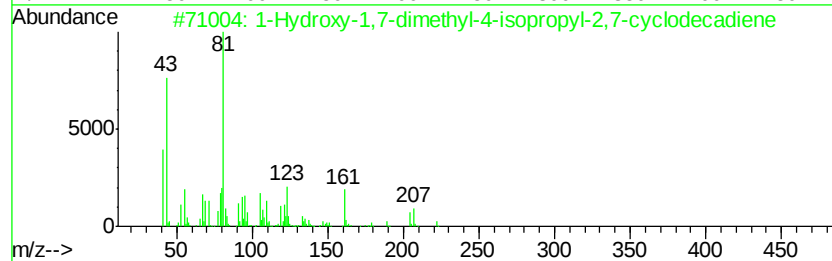
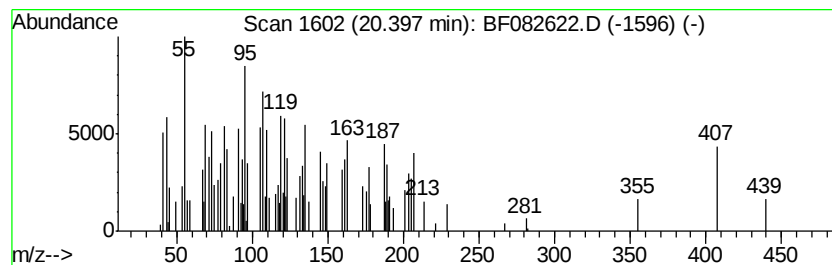
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown20.40 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.40	2.95 ng	190712	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hydroxy-1,7-dimethyl-4-isoprop...	222	C15H26O	072120-50-4	32
2		2(1H)-Naphthalenone, 4a,5,6,7,8,...	234	C15H22O2	109897-57-6	16
3		1,8-Dioxa-5-thiaoctane, 8-(9-bor...	468	C27H42B2O3S	1000162-66-8	16
4		Tricyclo[5.2.2.0(1,6)]undecan-3-...	220	C15H24O	1000159-37-6	16
5		2,4-Hexadienoanilide	187	C12H13NO	001483-88-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
 Data File : BF082622.D
 Acq On : 31 Oct 2015 15:34
 Operator : UM/IZ
 Sample : G4200-01
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-22L

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...	5.10	37.7	ng	2845960	1	6.90	1511390	20.0
unknown6.67	6.67	67.9	ng	5131670	1	6.90	1511390	20.0
n-Hexadecanoic acid	11.96	4.7	ng	508437	4	11.44	2169670	20.0
9-Eicosene, (E)-	12.49	7.4	ng	806199	4	11.44	2169670	20.0
Tridecanoic acid	12.75	2.4	ng	261430	4	11.44	2169670	20.0
Hexadecanoic acid...	12.85	2.7	ng	211975	5	14.08	1586210	20.0
Phenanthrene, 1-m...	13.16	4.0	ng	317770	5	14.08	1586210	20.0
1-Nonadecene	13.93	5.8	ng	461552	5	14.08	1586210	20.0
17-Pentatriacontene	14.58	3.1	ng	245335	5	14.08	1586210	20.0
unknown17.41	17.41	4.0	ng	258342	6	15.53	1291370	20.0
unknown17.59	17.59	3.6	ng	229747	6	15.53	1291370	20.0
unknown20.40	20.40	3.0	ng	190712	6	15.53	1291370	20.0