

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093017\
 Data File : BF098968.D
 Acq On : 30 Sep 2017 17:47
 Operator : SJ/JU
 Sample : I5554-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BRICK-FOR-WASTE

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-BF092317.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	2.169	7	14	20	rVB	161229	204429	5.79%	0.697%
2	5.140	515	519	534	rVB	449114	682881	19.35%	2.328%
3	5.540	581	587	590	rBV	3302148	3516045	99.61%	11.989%
4	6.545	748	758	761	rBV	3001550	3529859	100.00%	12.036%
5	6.687	777	782	785	rBV	3413435	3497667	99.09%	11.926%
6	6.916	817	821	825	rBV	1042706	819737	23.22%	2.795%
7	7.075	842	848	851	rBV	3101482	2746031	77.79%	9.363%
8	7.481	912	917	920	rBV	2236493	2123250	60.15%	7.240%
9	8.004	1002	1006	1010	rBV3	39386	64365	1.82%	0.219%
10	8.198	1035	1039	1042	rBV	1250032	988786	28.01%	3.372%
11	8.492	1086	1089	1092	rVB3	69038	75719	2.15%	0.258%
12	8.539	1092	1097	1099	rBV4	39219	74600	2.11%	0.254%
13	8.657	1115	1117	1122	rVB2	106578	110680	3.14%	0.377%
14	8.816	1141	1144	1146	rBV4	80884	106153	3.01%	0.362%
15	8.886	1152	1156	1160	rBV3	131608	176375	5.00%	0.601%
16	8.939	1163	1165	1167	rVV2	123480	90360	2.56%	0.308%
17	8.969	1167	1170	1173	rBV4	78512	107005	3.03%	0.365%
18	9.033	1179	1181	1183	rVB2	86828	65367	1.85%	0.223%
19	9.075	1185	1188	1192	rBV5	148102	228330	6.47%	0.779%
20	9.157	1199	1202	1203	rBV3	123005	123718	3.50%	0.422%
21	9.192	1205	1208	1210	rBV3	303161	287291	8.14%	0.980%
22	9.275	1217	1222	1225	rBV	3445150	3262718	92.43%	11.125%
23	9.351	1231	1235	1238	rBV2	901857	1001632	28.38%	3.415%
24	9.416	1244	1246	1249	rVB3	379775	336846	9.54%	1.149%
25	9.663	1285	1288	1292	rBV	1847110	2017191	57.15%	6.878%
26	9.722	1296	1298	1301	rVV2	410024	444675	12.60%	1.516%
27	9.822	1312	1315	1317	rBV2	1024235	1179146	33.40%	4.021%
28	9.869	1321	1323	1328	rVB	1200944	1466869	41.56%	5.002%

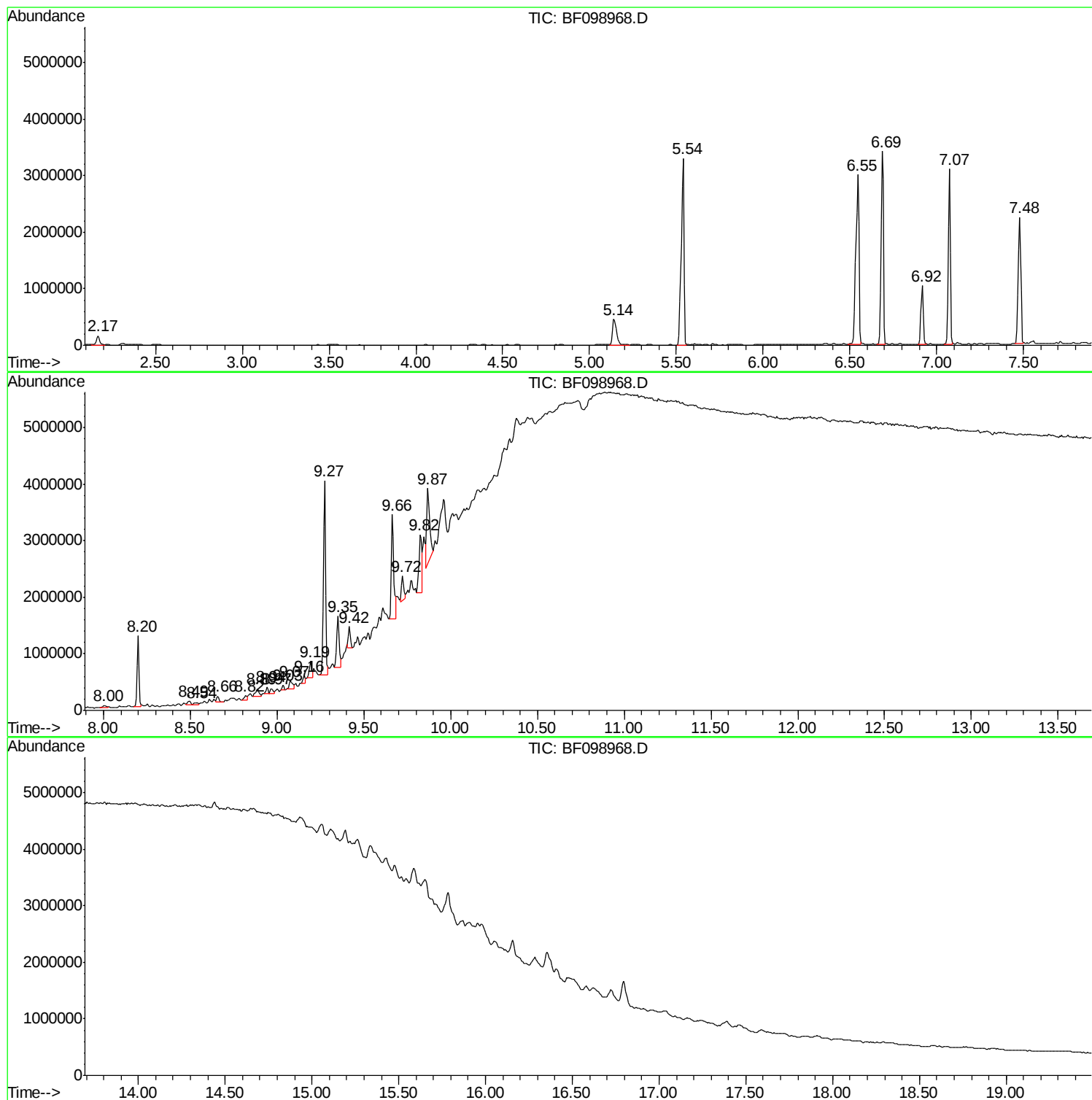
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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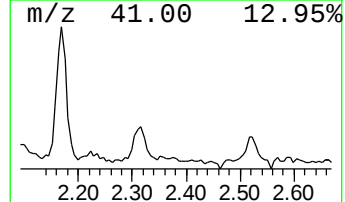
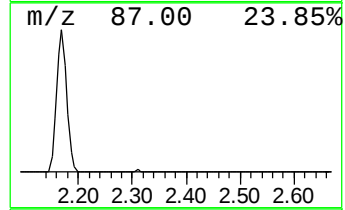
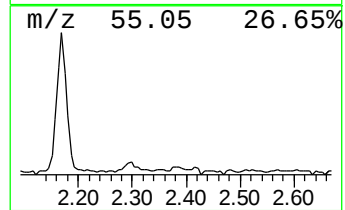
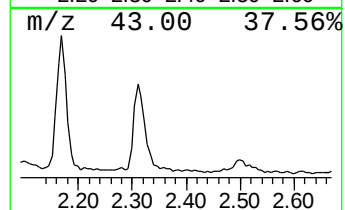
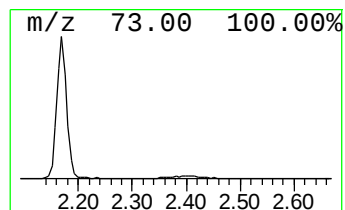
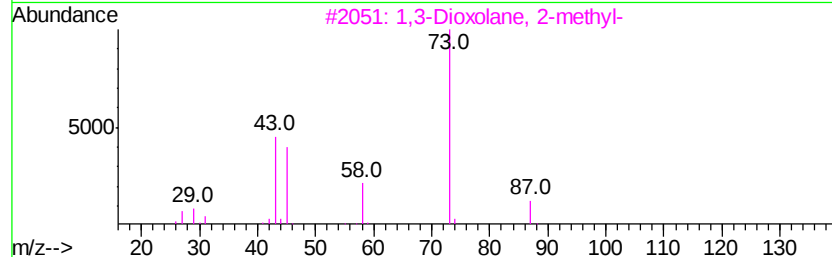
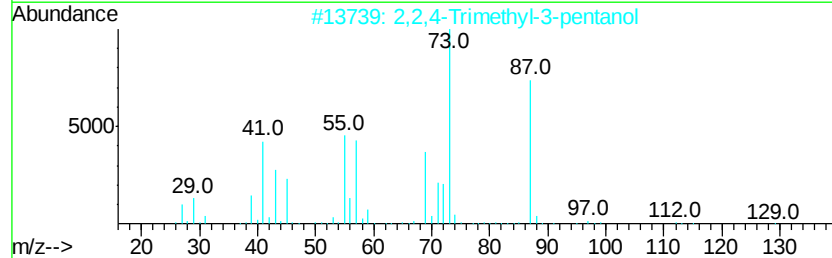
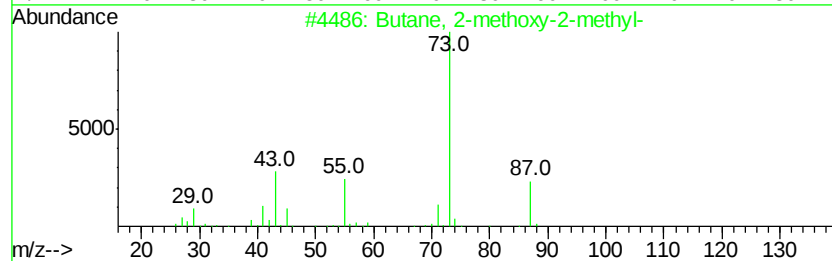
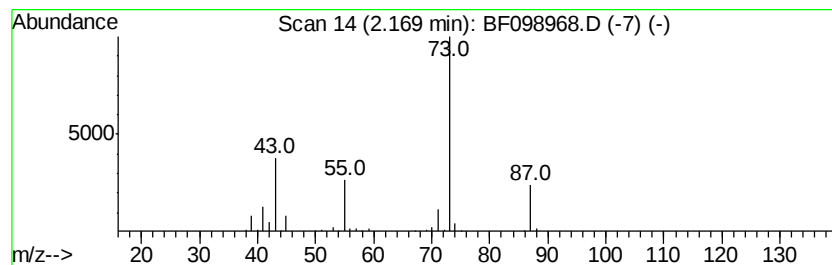
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	4.99 ng	204429	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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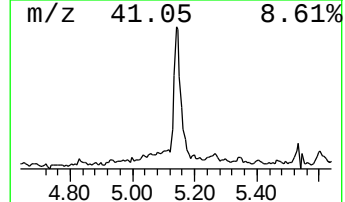
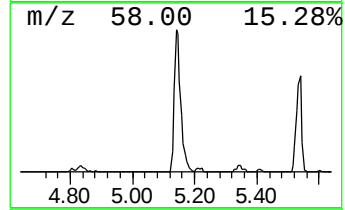
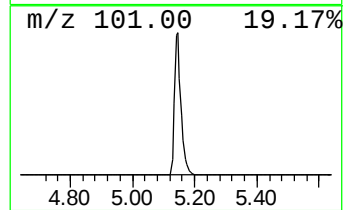
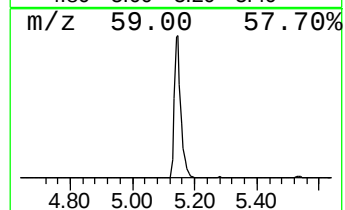
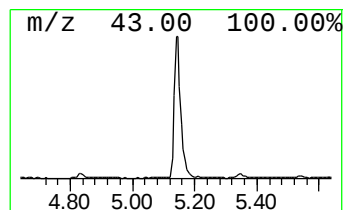
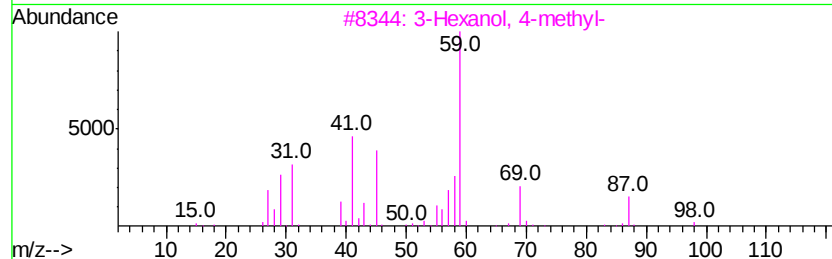
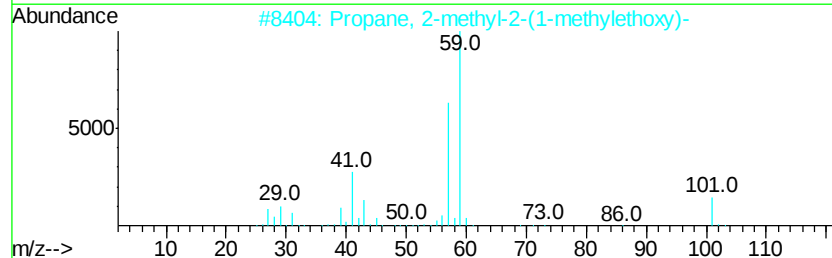
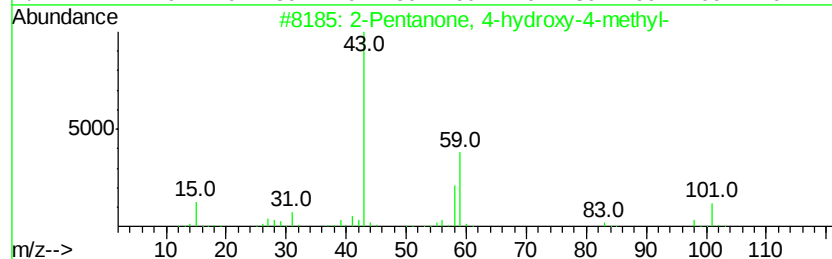
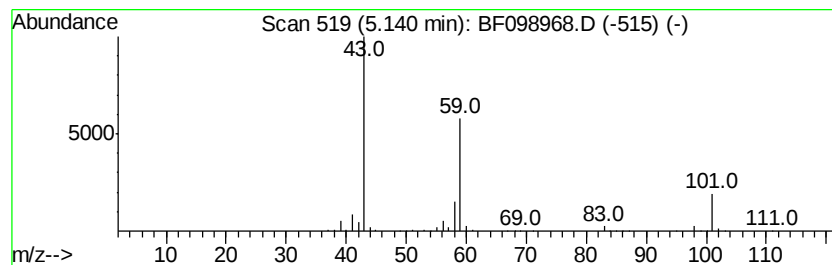
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	16.66 ng	682881	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		1,2-Butanediol	90	C4H10O2	000584-03-2	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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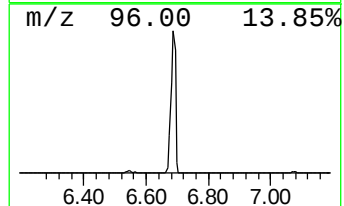
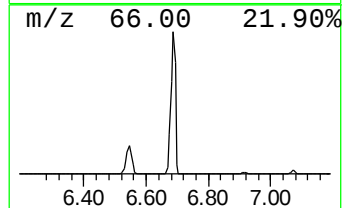
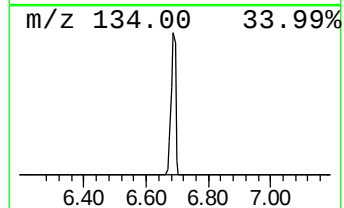
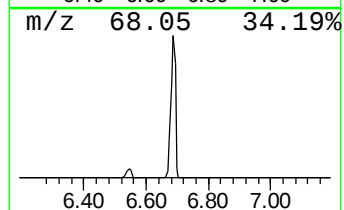
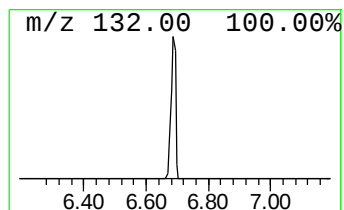
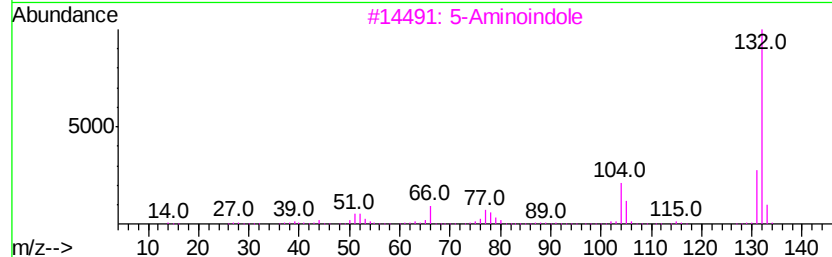
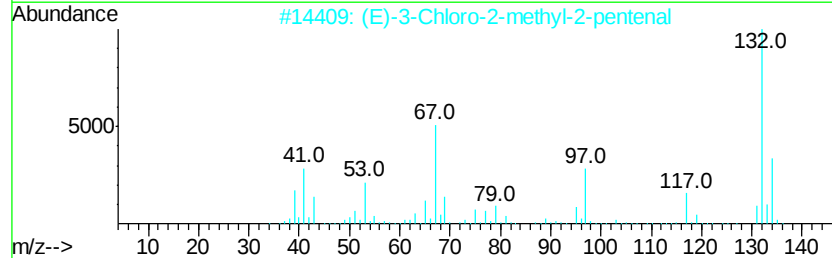
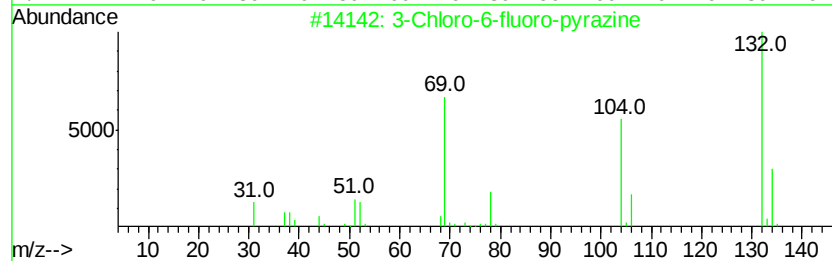
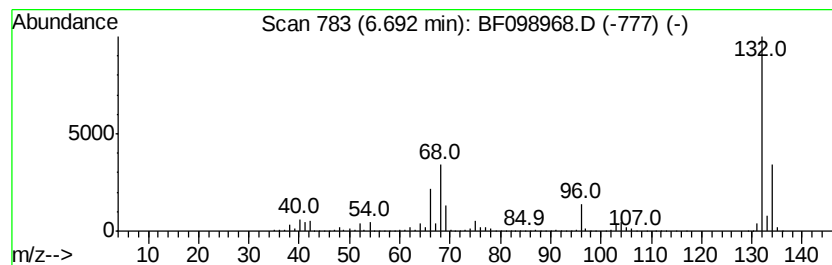
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.34 ng	3497670	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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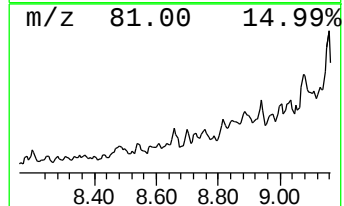
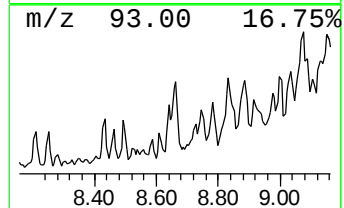
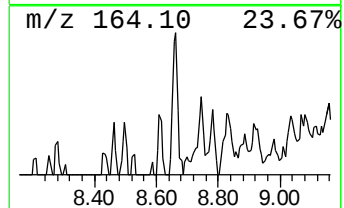
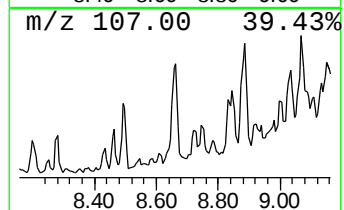
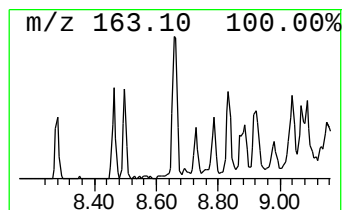
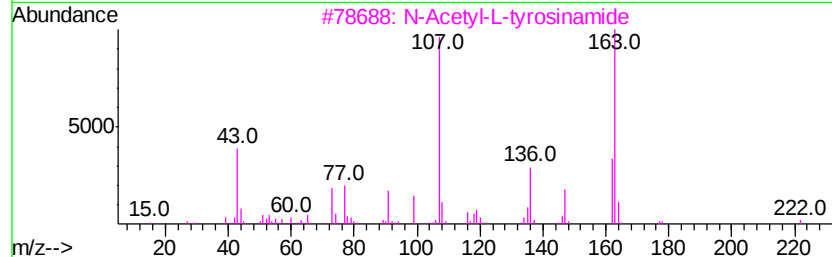
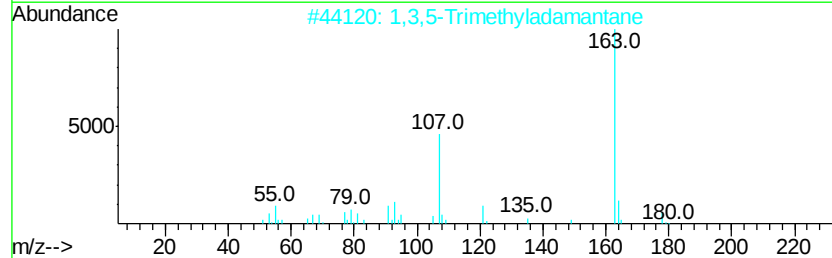
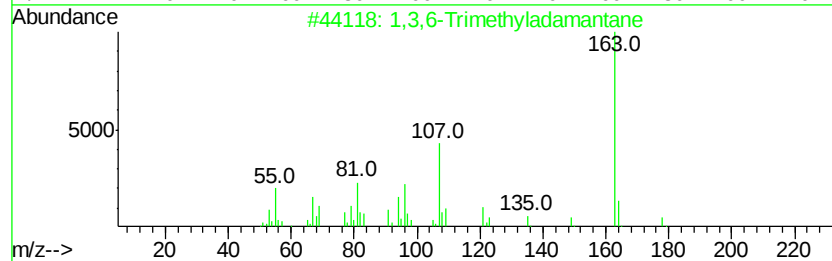
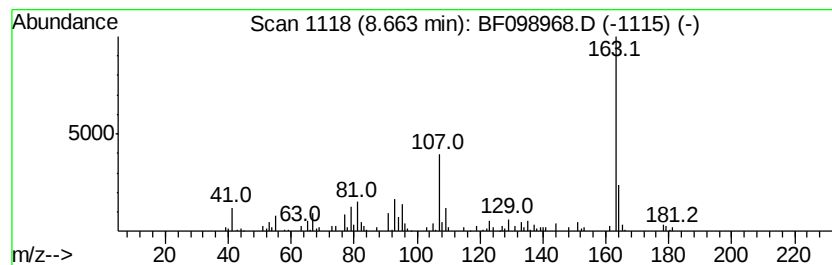
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Peak Number 5 1,3,6-Trimethyladamantane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.24 ng	110680	Naphthalene-d8	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	64
2		1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	64
3		N-Acetyl-L-tyrosinamide	222	C11H14N2O3	001948-71-6	50
4		Ethanone, 1-[4-(1-hydroxy-1-meth...	178	C11H14O2	054549-72-3	49
5		Phosphine oxide, cyclohexyl meth...	300	C17H33O2P	1000195-73-8	47



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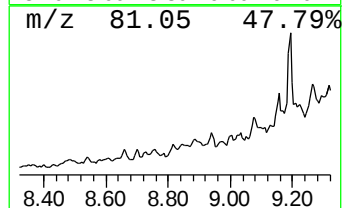
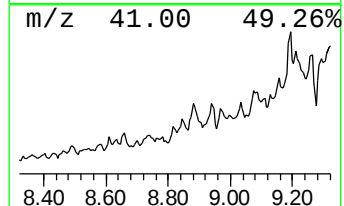
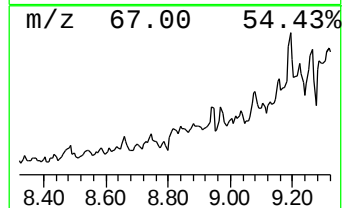
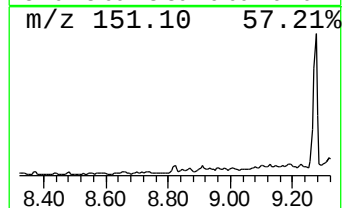
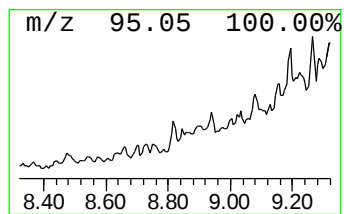
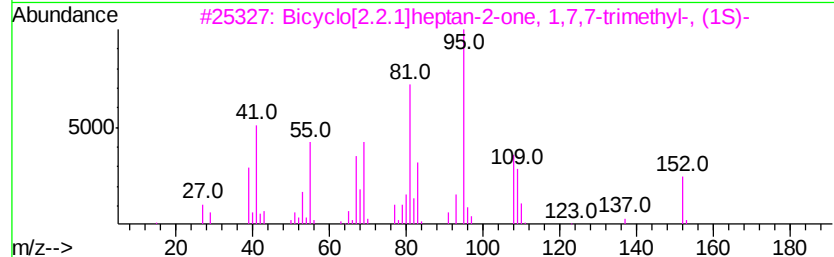
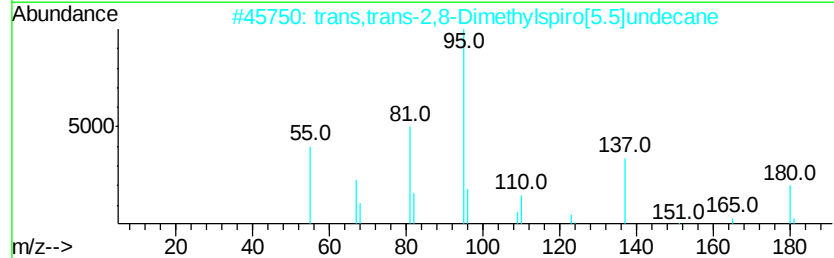
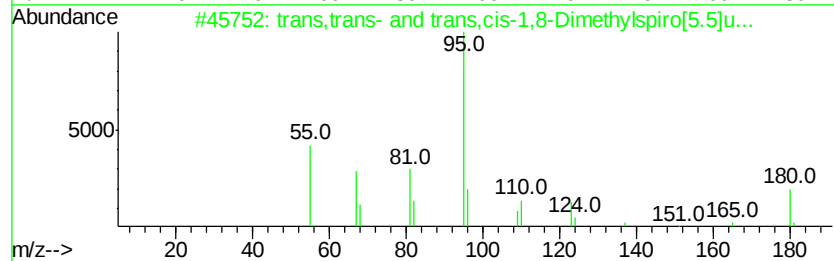
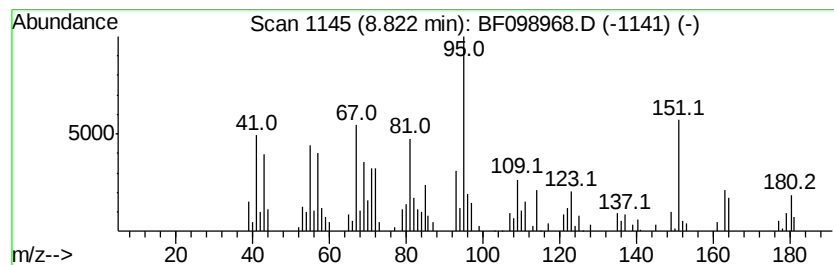
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Peak Number 6 trans,trans- and trans,cis-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	2.15 ng	106153	Napthalene-d8	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans,trans- and trans,cis-1,8-D...	180	C13H24	1000111-73-2	55
2		trans,trans-2,8-Dimethylspiro[5....	180	C13H24	095530-76-0	49
3		Bicyclo[2.2.1]heptan-2-one, 1,7....	152	C10H16O	000464-48-2	43
4		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	43
5		E-2-Methyl-5-(furan-3-yl)-pent-1...	164	C10H12O2	1000143-28-6	38



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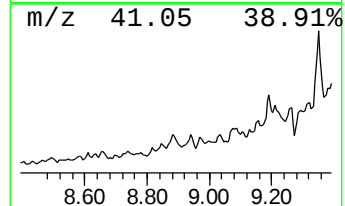
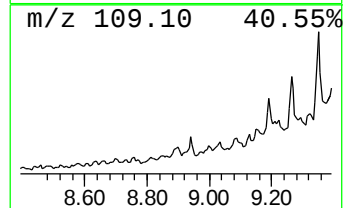
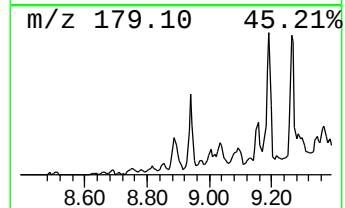
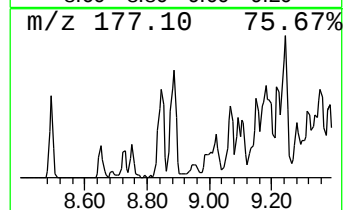
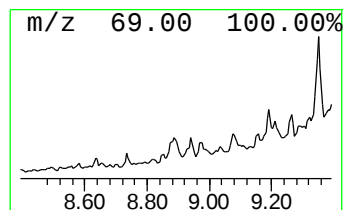
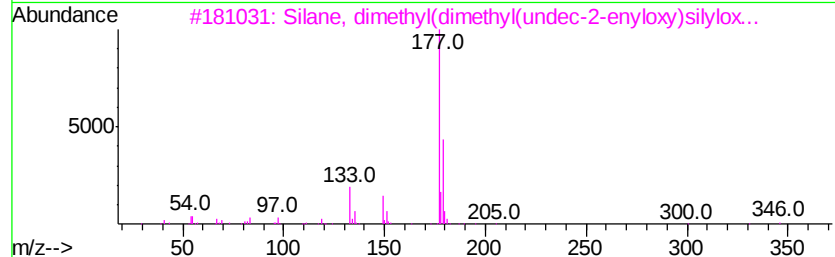
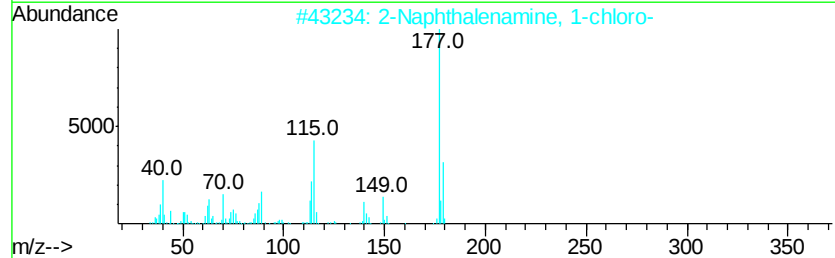
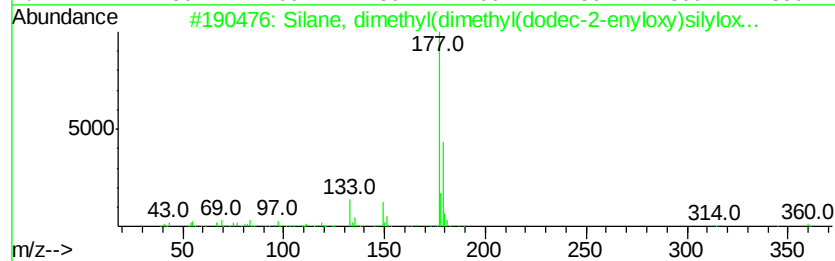
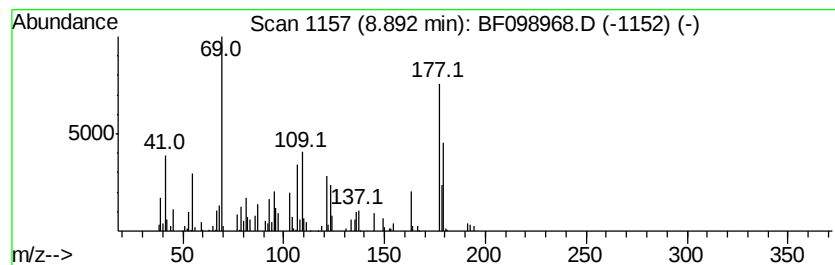
Instrument :
BNA_F
ClientSampleId :
BRICK-FOR-WASTE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown8.89 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	3.57 ng	176375	Naphthalene-d8	8.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Silane, dimethyl(dimethyl(dodec-...	360 C18H40O3Si2	1000348-07-1 25
2		2-Naphthalenamine, 1-chloro-	177 C10H8ClN	016452-11-2 16
3		Silane, dimethyl(dimethyl(undec-...	346 C17H38O3Si2	1000347-94-8 16
4		Cyclandelate	276 C17H24O3	000456-59-7 14
5		1,3,5,6-Tetramethyladamantane	192 C14H24	034694-70-7 12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-FOR-WASTE

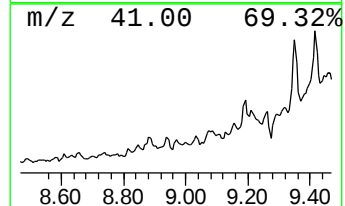
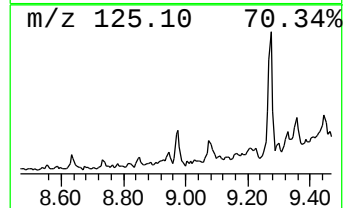
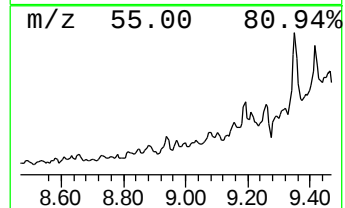
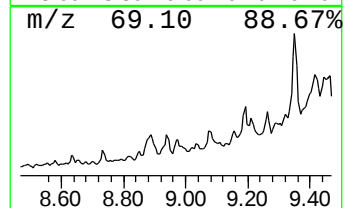
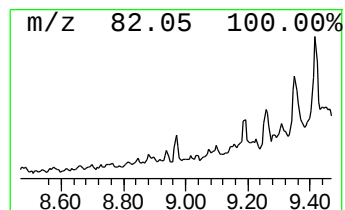
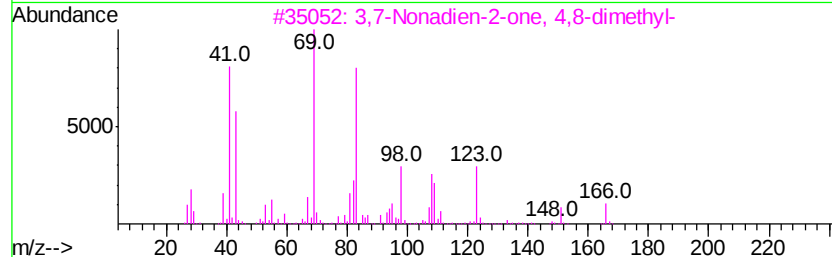
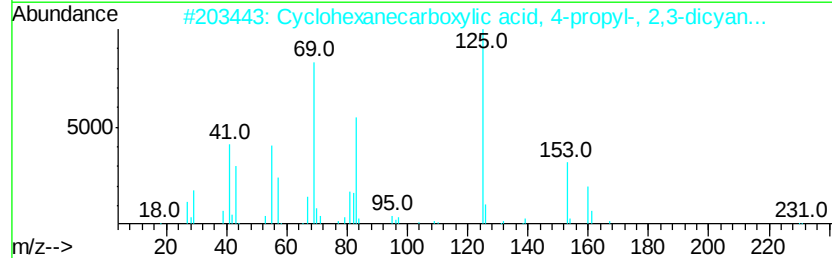
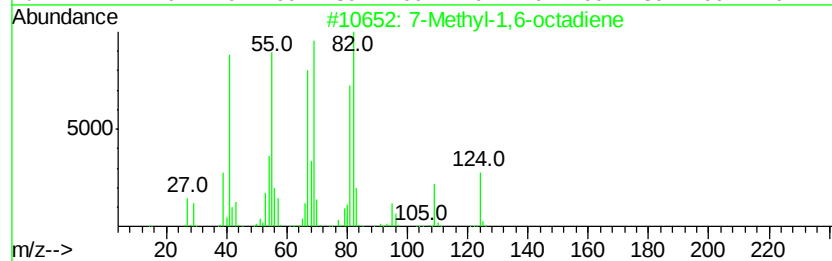
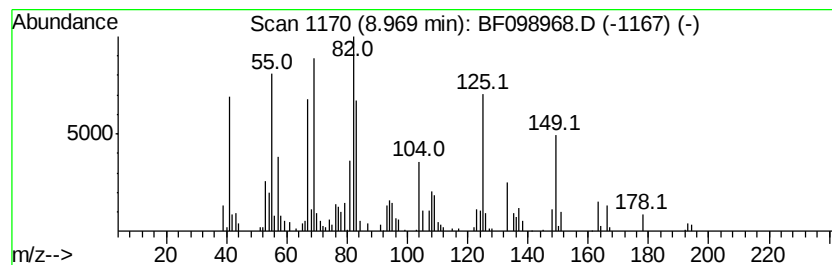
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown8.97 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	2.16 ng	107005	Napthalene-d8	8.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl-1,6-octadiene			124	C9H16	042152-47-6	43
2	Cyclohexanecarboxylic acid, 4-propyl-, 2,3-dicyano-			382	C23H30N2O3	075941-50-3	35
3	3,7-Nonadien-2-one, 4,8-dimethyl-			166	C11H18O	000817-88-9	30
4	1,1'-Bicyclohexyl			166	C12H22	000092-51-3	27
5	Cyclohexane, 2,4-diethyl-1-methyl-			154	C11H22	061142-70-9	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-FOR-WASTE

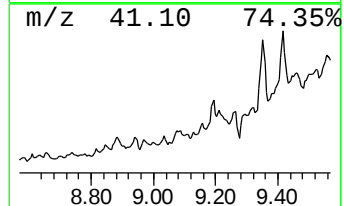
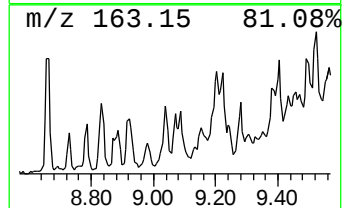
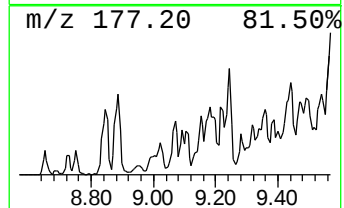
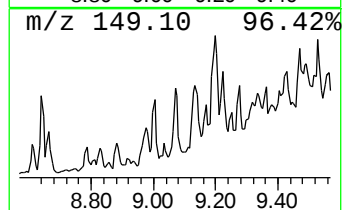
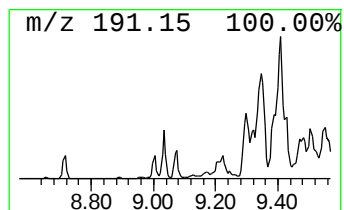
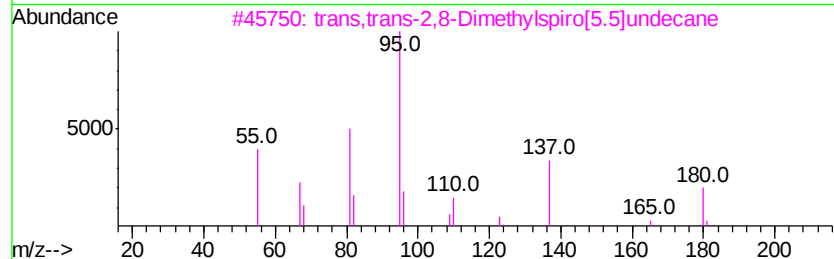
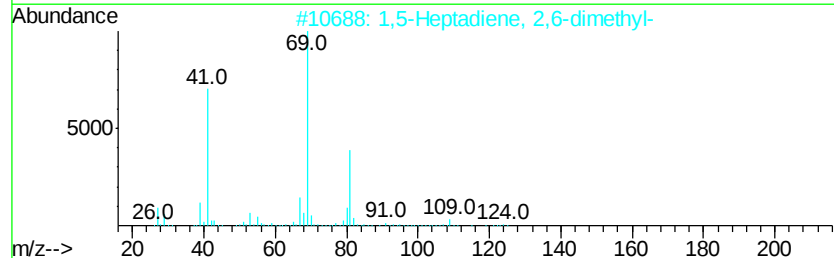
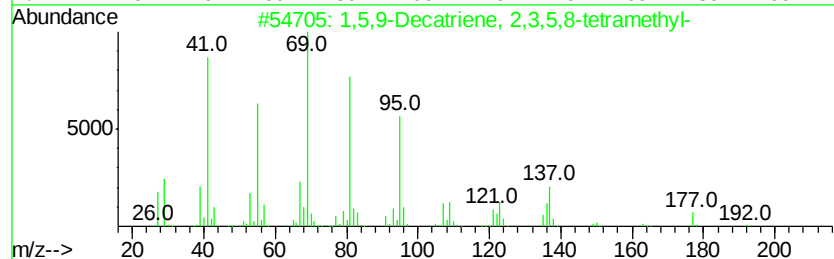
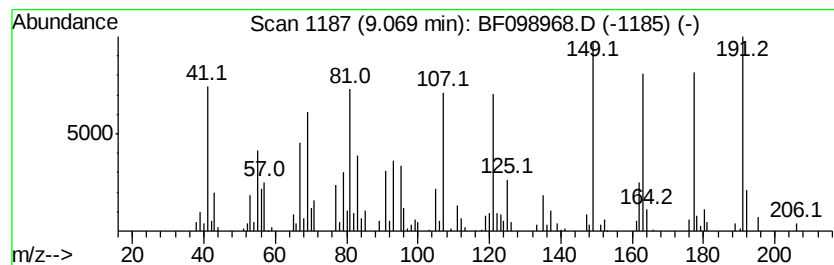
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown9.07 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	4.62 ng	228330	Naphthalene-d8	8.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	38
2			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	27
3			trans,trans-2,8-Dimethylspiro[5....	180	C13H24	095530-76-0	22
4			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	14
5			photocitral B	152	C10H16O	006040-45-5	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-FOR-WASTE

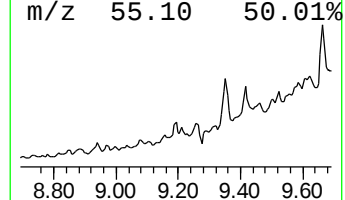
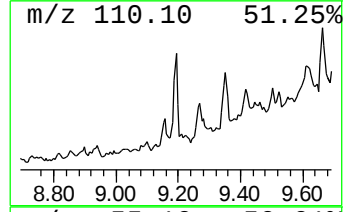
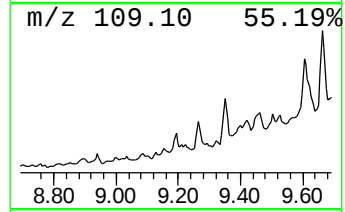
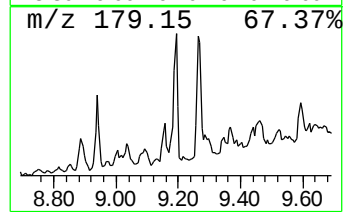
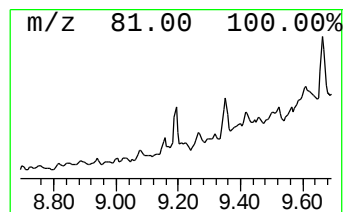
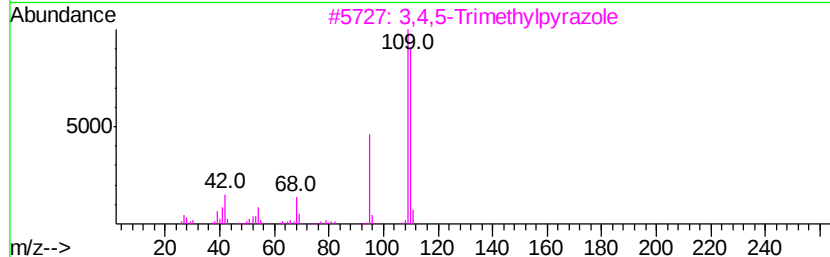
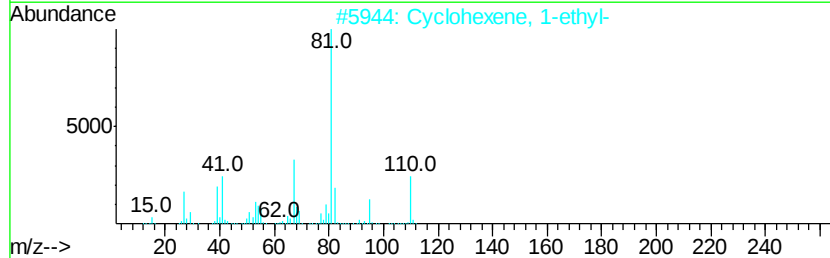
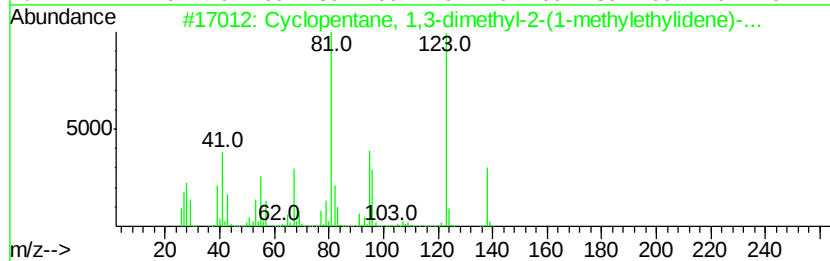
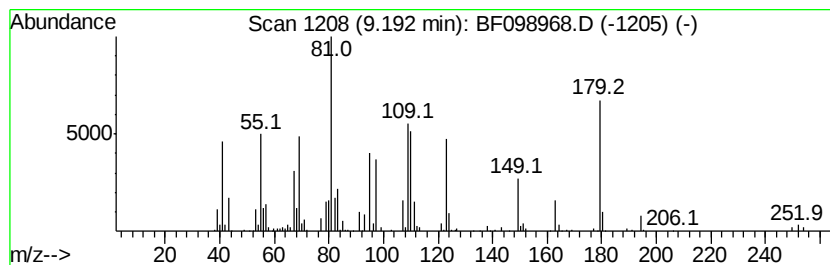
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown9.19 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	3.92 ng	287291	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-30-1	35
2		Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	27
3		3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	22
4		1-Methoxy-1,3-cyclohexadiene	110	C7H10O	002161-90-2	22
5		Cyclohexene, 3-ethyl-	110	C8H14	002808-71-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BRICK-FOR-WASTE

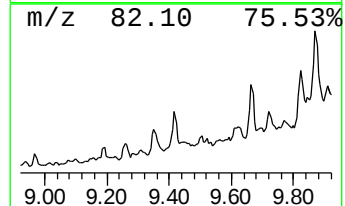
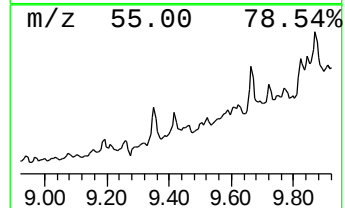
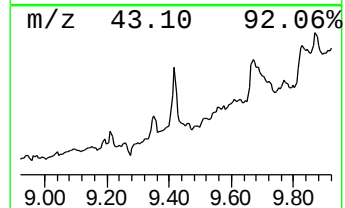
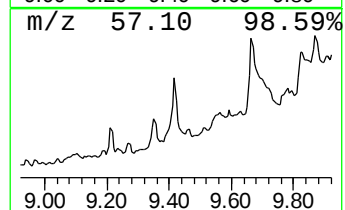
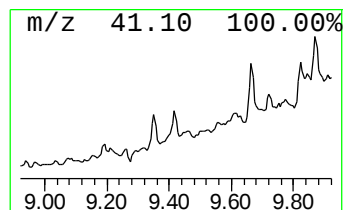
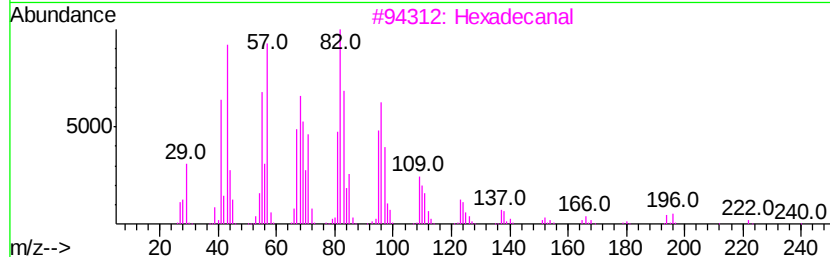
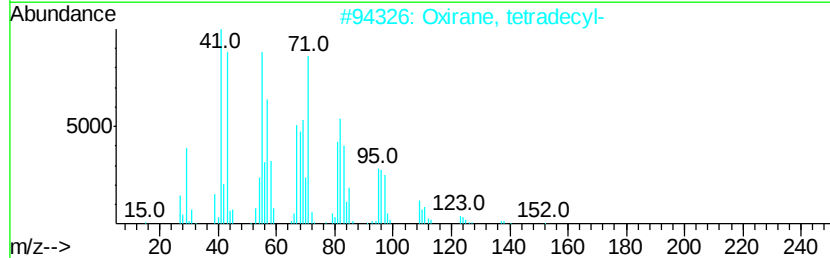
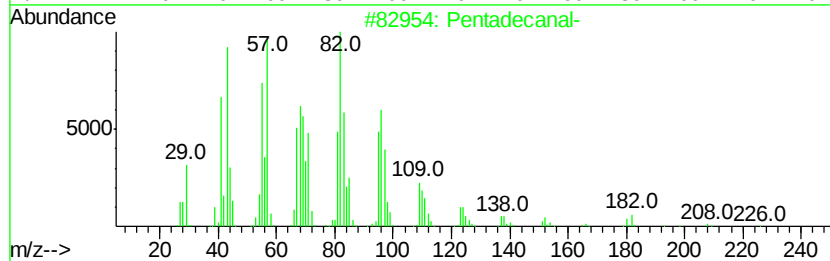
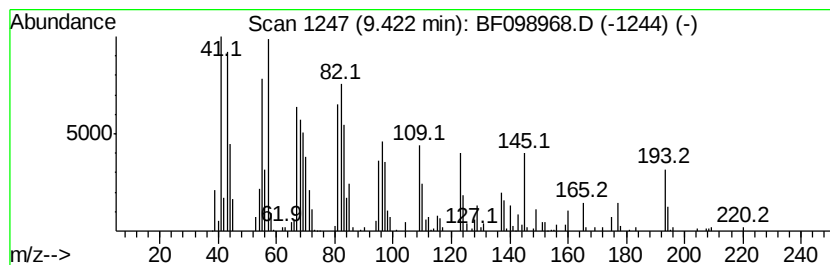
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Pentadecanal- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	4.59 ng	336846	Acenaphthene-d10	9.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanal-	226	C15H30O	002765-11-9	87
2			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	83
3			Hexadecanal	240	C16H32O	000629-80-1	81
4			Tetradecanal	212	C14H28O	000124-25-4	81
5			Tridecanal	198	C13H26O	010486-19-8	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BRICK-FOR-WASTE

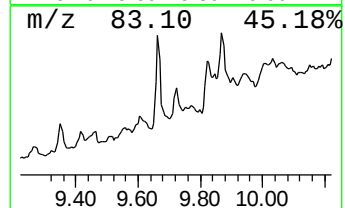
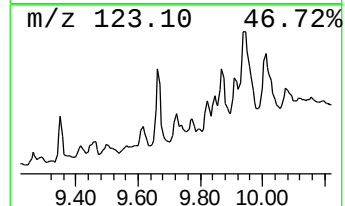
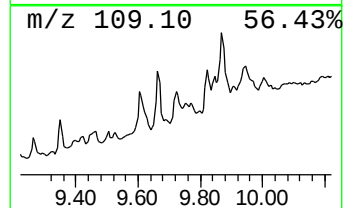
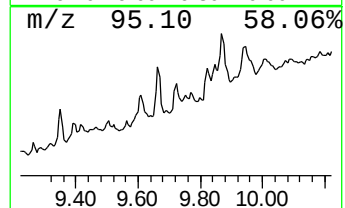
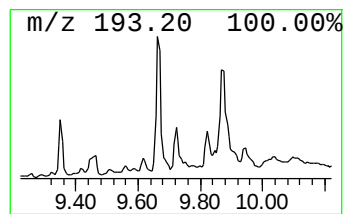
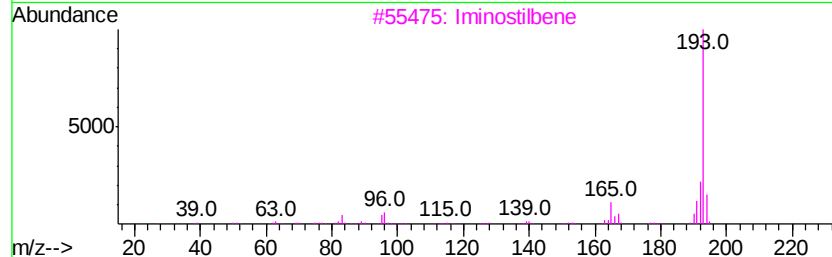
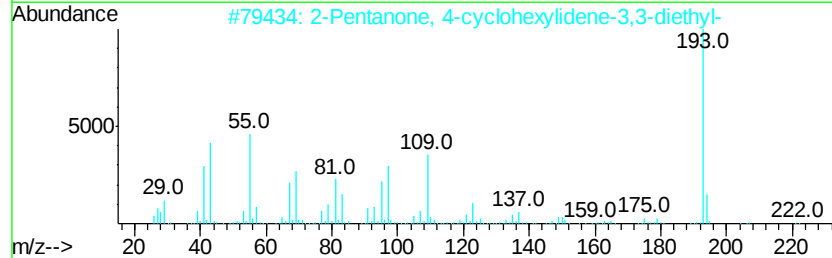
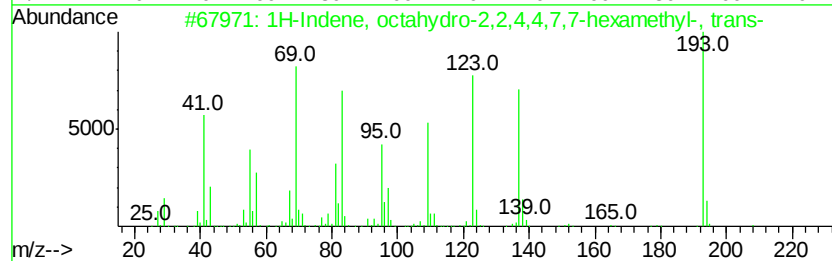
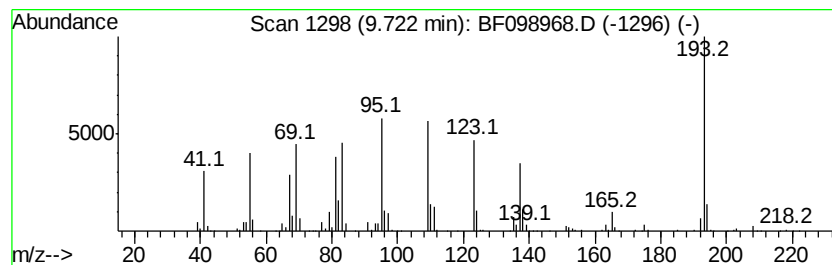
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1H-Indene, octahydro-2,2,4,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	6.06 ng	444675	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
2		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3		Iminostilbene	193	C14H11N	000256-96-2	38
4		Pyrrolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35
5		6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF093017\
Data File : BF098968.D
Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BRICK-FOR-WASTE

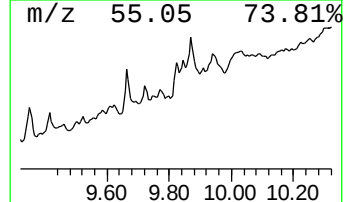
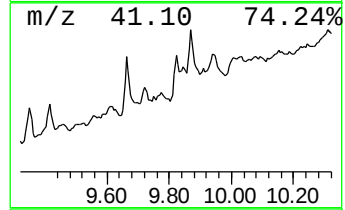
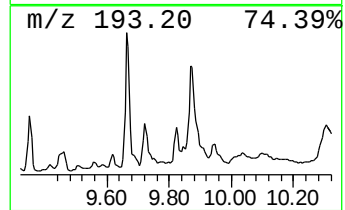
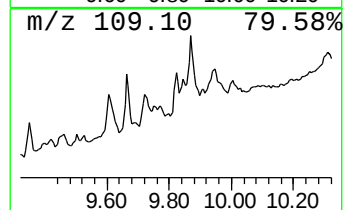
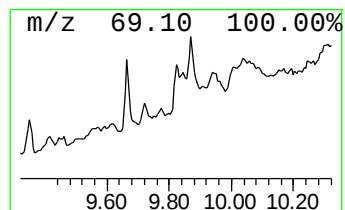
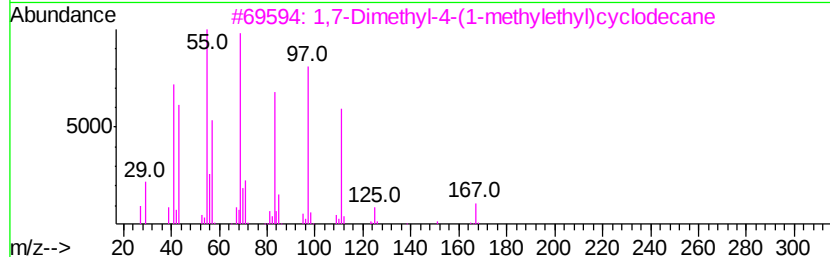
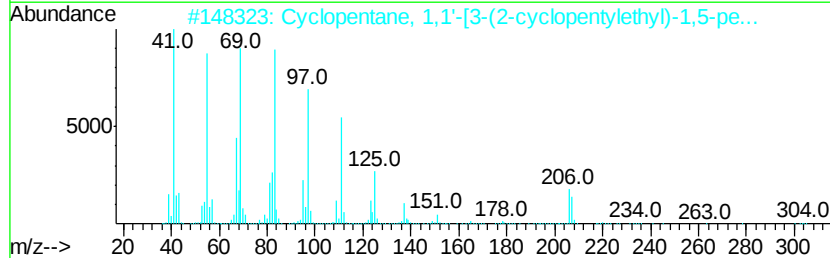
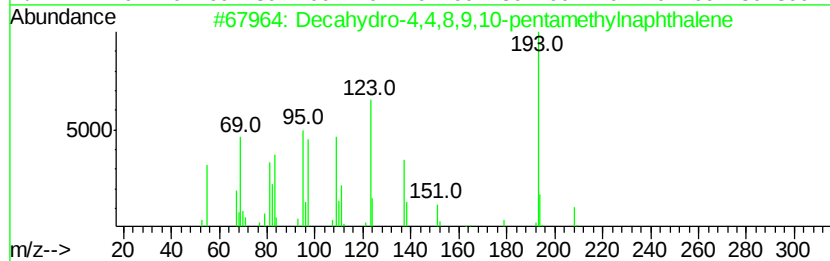
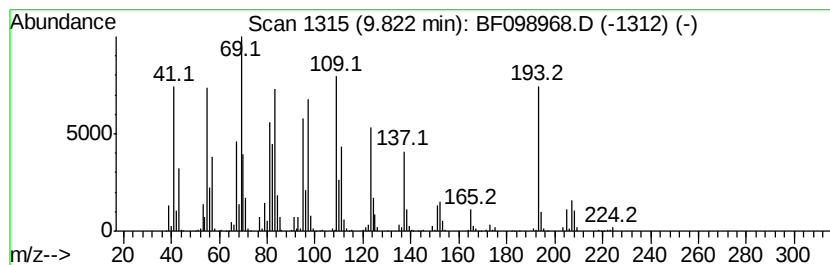
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Decahydro-4,4,8,9,10-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	16.08 ng	1179150	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	92
2		Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	43
3		1,7-Dimethyl-4-(1-methylethyl)cv...	210	C15H30	000645-10-3	38
4		Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	35
5		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	25



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Acq On : 30 Sep 2017 17:47
Operator : SJ/JU
Sample : I5554-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-FOR-WASTE

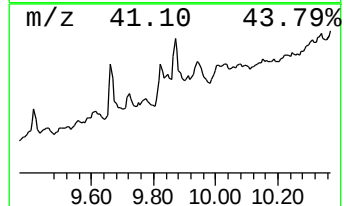
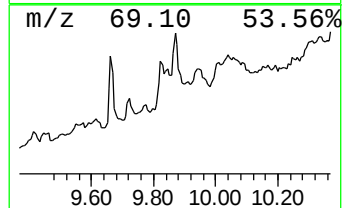
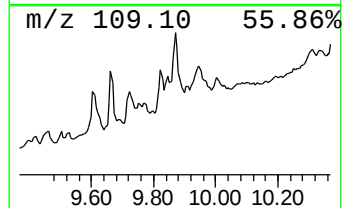
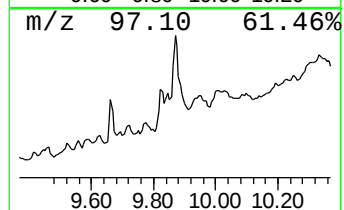
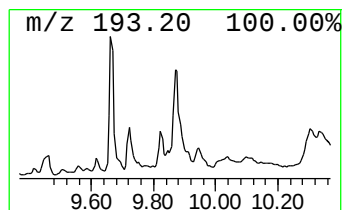
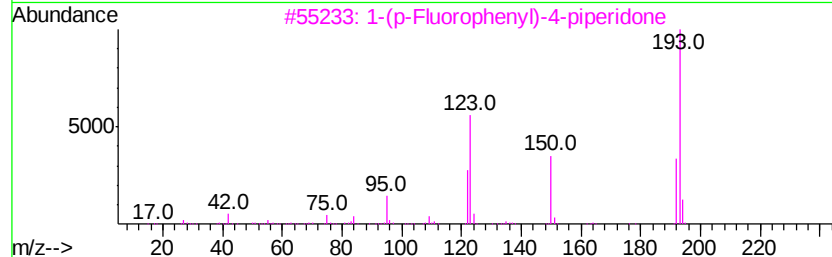
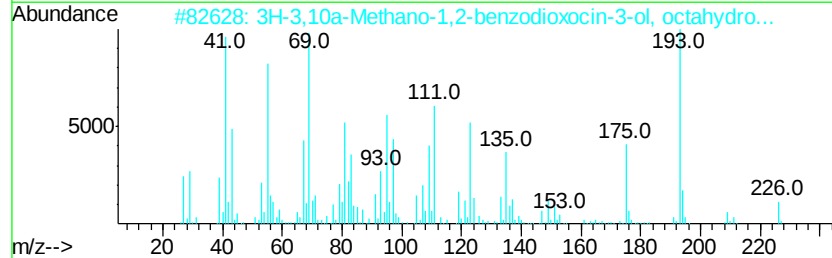
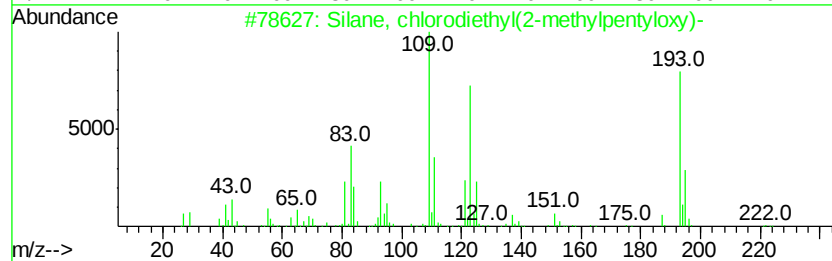
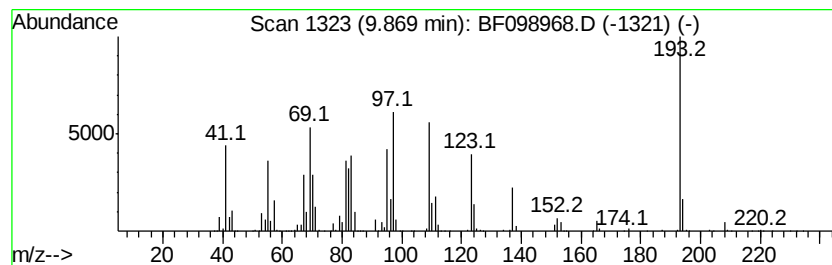
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown9.87 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	20.00 ng	1466870	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	40
2		3H-3,10a-Methano-1,2-benzodioxoc...	226	C13H22O3	095906-83-5	37
3		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4		Cyclopentanol, 1-(methylenecyclo...	138	C9H14O	086951-58-8	14
5		Citronellol	156	C10H20O	000106-22-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093017\
 Data File : BF098968.D
 Acq On : 30 Sep 2017 17:47
 Operator : SJ/JU
 Sample : I5554-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BRICK-FOR-WASTE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	5.0	ng	204429	1	6.92	819737	20.0
2-Pentanone, 4-hy...	5.14	16.7	ng	682881	1	6.92	819737	20.0
unknown6.69	6.69	85.3	ng	3497670	1	6.92	819737	20.0
1,3,6-Trimethylad...	8.66	2.2	ng	110680	2	8.20	988786	20.0
trans,trans- and ...	8.82	2.1	ng	106153	2	8.20	988786	20.0
unknown8.89	8.89	3.6	ng	176375	2	8.20	988786	20.0
unknown8.97	8.97	2.2	ng	107005	2	8.20	988786	20.0
unknown9.07	9.07	4.6	ng	228330	2	8.20	988786	20.0
unknown9.19	9.19	3.9	ng	287291	3	9.96	1466870	20.0
Pentadecanal-	9.42	4.6	ng	336846	3	9.96	1466870	20.0
1H-Indene, octahy...	9.72	6.1	ng	444675	3	9.96	1466870	20.0
Decahydro-4,4,8,9...	9.82	16.1	ng	1179150	3	9.96	1466870	20.0
unknown9.87	9.87	20.0	ng	1466870	3	9.96	1466870	20.0