

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
 Data File : BF075598.D
 Acq On : 16 Nov 2014 23:57
 Operator : TP / JJ
 Sample : F4738-03
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-3

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-BF111214.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	1.613	43	46	49	rVB	1833266	1924402	100.00%	25.949%
2	1.761	56	59	63	rVB	68790	104380	5.42%	1.407%
3	1.830	63	65	73	rVV	42640	73622	3.83%	0.993%
4	1.967	73	77	93	rVB	436392	734556	38.17%	9.905%
5	5.339	370	372	376	rVB	86932	115258	5.99%	1.554%
6	5.853	414	417	419	rBV	294309	306667	15.94%	4.135%
7	7.099	524	526	528	rBV	250549	305527	15.88%	4.120%
8	7.144	528	530	534	rVV	73814	105808	5.50%	1.427%
9	7.259	538	540	543	rVB	261821	317842	16.52%	4.286%
10	7.556	564	566	568	rBV	147605	153716	7.99%	2.073%
11	7.739	580	582	585	rVB	279366	241520	12.55%	3.257%
12	8.242	624	626	628	rBV	223725	195619	10.17%	2.638%
13	8.996	689	692	696	rBV3	9239	21579	1.12%	0.291%
14	9.133	701	704	706	rBV	239714	210738	10.95%	2.842%
15	10.482	819	822	824	rBV	237862	311955	16.21%	4.206%
16	11.316	892	895	897	rBV	222245	223305	11.60%	3.011%
17	12.299	978	981	983	rBV2	168677	226322	11.76%	3.052%
18	13.019	1042	1044	1047	rVB2	12564	20550	1.07%	0.277%
19	13.168	1054	1057	1059	rBV	179242	236223	12.28%	3.185%
20	13.865	1115	1118	1120	rBV	70203	105466	5.48%	1.422%
21	14.677	1186	1189	1191	rBV	21041	25364	1.32%	0.342%
22	14.745	1192	1195	1198	rBV	29740	50325	2.62%	0.679%
23	14.837	1201	1203	1207	rBV4	16561	38177	1.98%	0.515%
24	14.905	1207	1209	1211	rBV2	11248	19788	1.03%	0.267%
25	14.951	1211	1213	1215	rVB	23750	31325	1.63%	0.422%
26	15.031	1217	1220	1222	rBV	23395	36028	1.87%	0.486%
27	15.157	1229	1231	1233	rBV	353290	353358	18.36%	4.765%
28	15.465	1255	1258	1261	rBV3	24836	47886	2.49%	0.646%
29	15.762	1282	1284	1286	rBV	23001	28414	1.48%	0.383%
30	16.334	1331	1334	1342	rBV3	45143	104990	5.46%	1.416%
31	16.460	1342	1345	1346	rBV	262384	380469	19.77%	5.130%
32	17.580	1441	1443	1445	rBV2	25289	26456	1.37%	0.357%
33	18.197	1494	1497	1504	rVB	181094	291042	15.12%	3.924%
34	19.351	1596	1598	1602	rVB2	23809	47357	2.46%	0.639%

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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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 >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

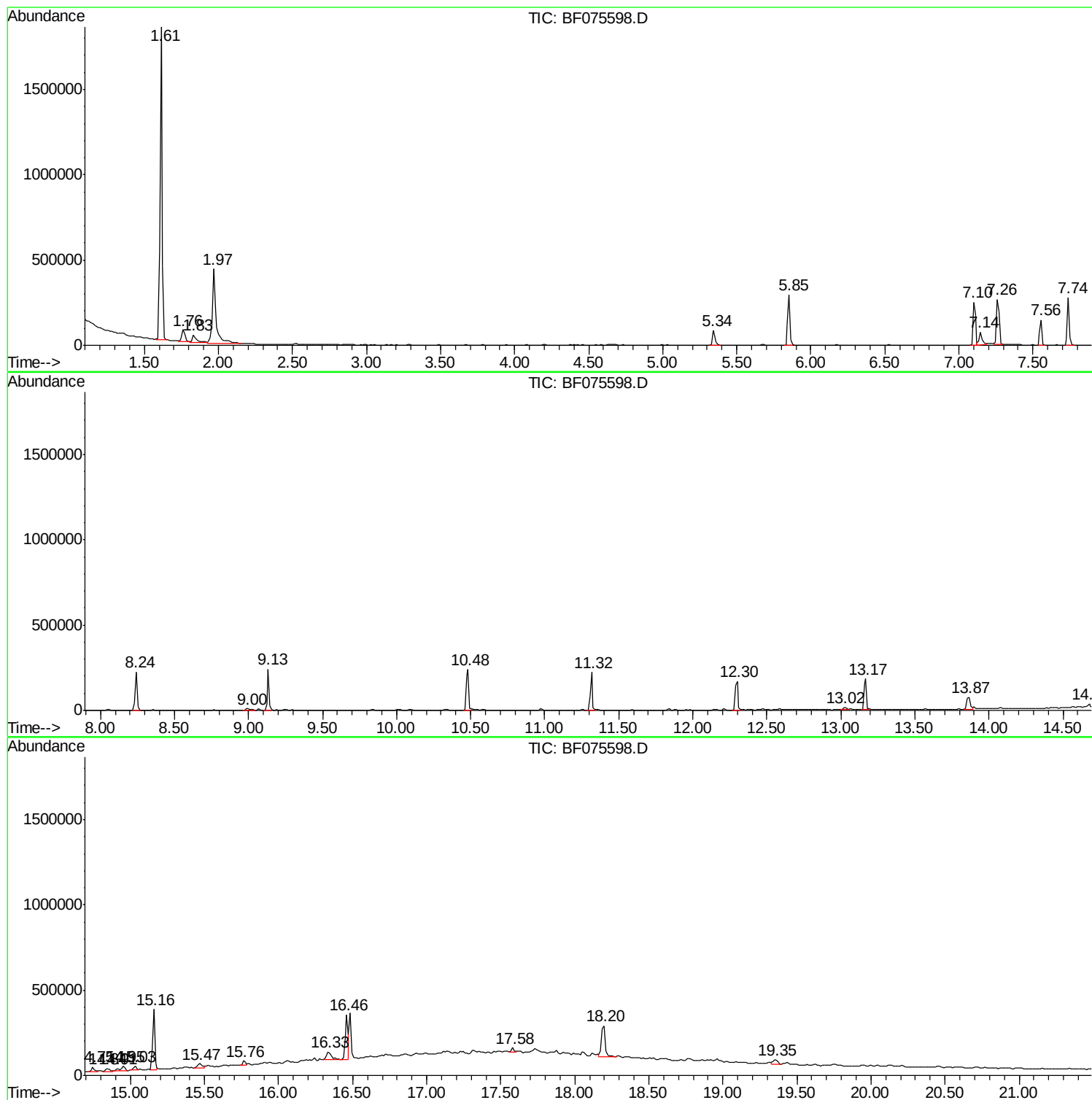
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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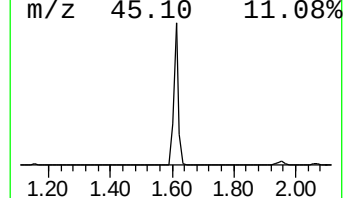
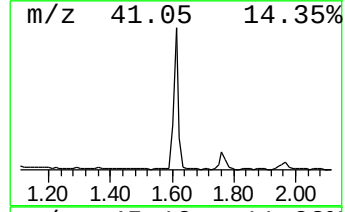
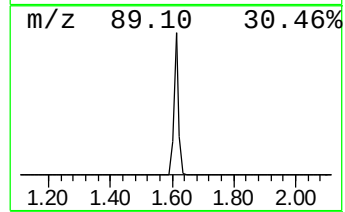
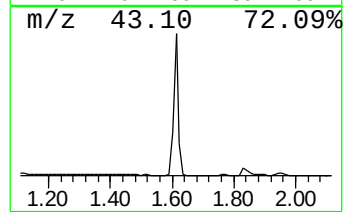
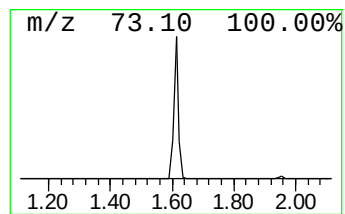
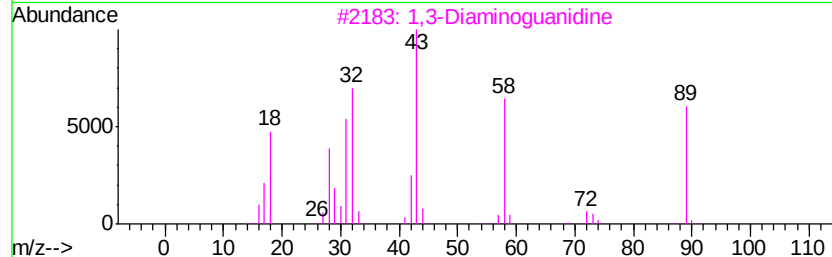
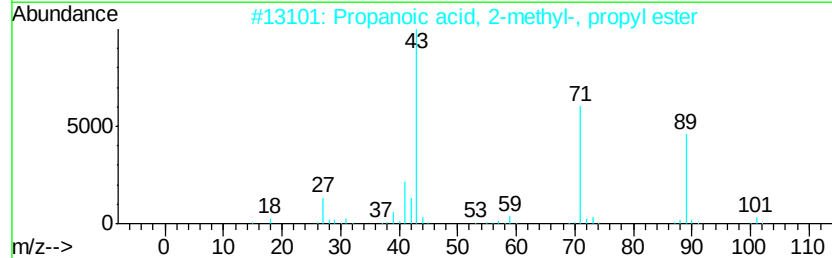
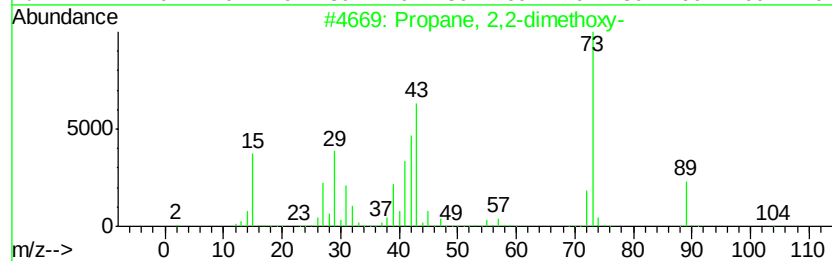
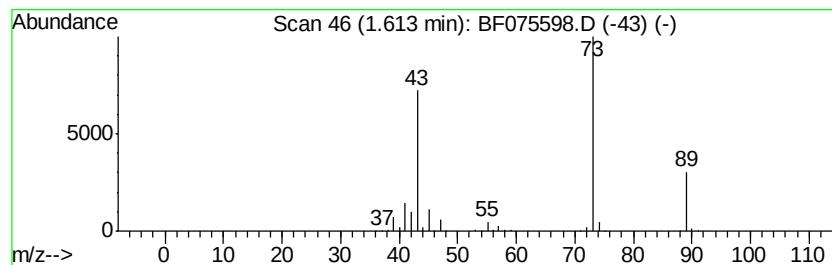
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	250.38 ng	1924400	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	17
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		Methylglyoxal	72	C3H4O2	000078-98-8	9



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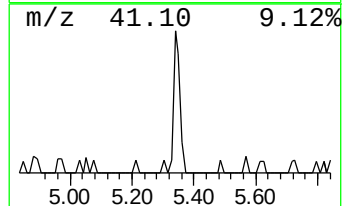
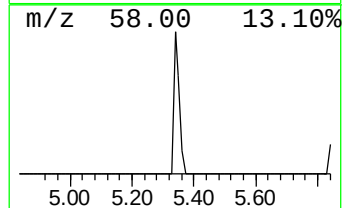
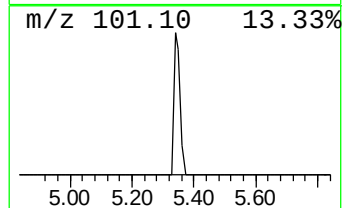
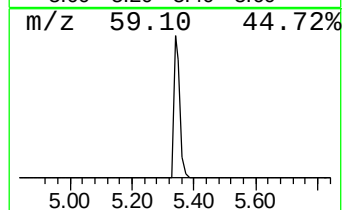
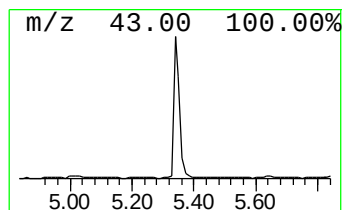
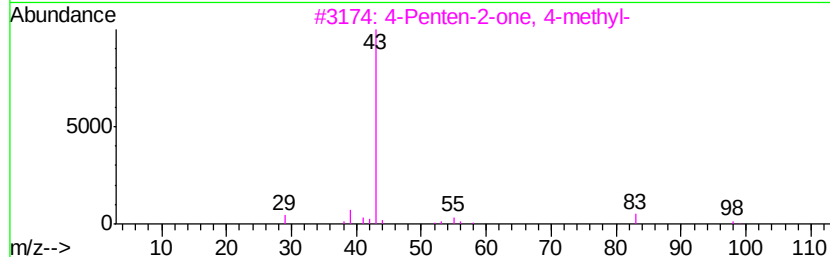
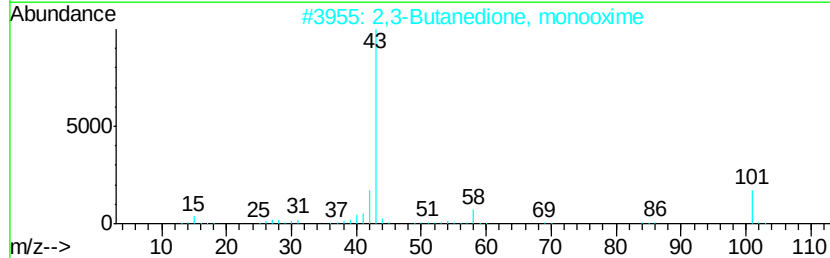
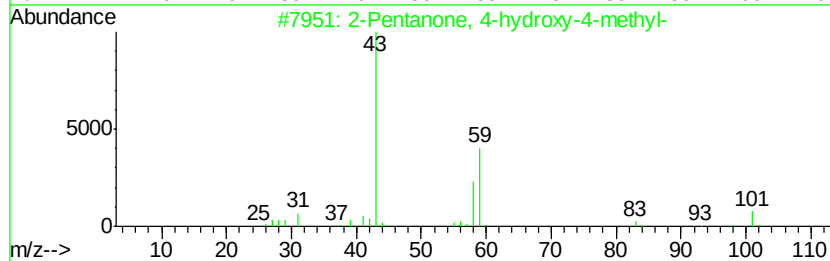
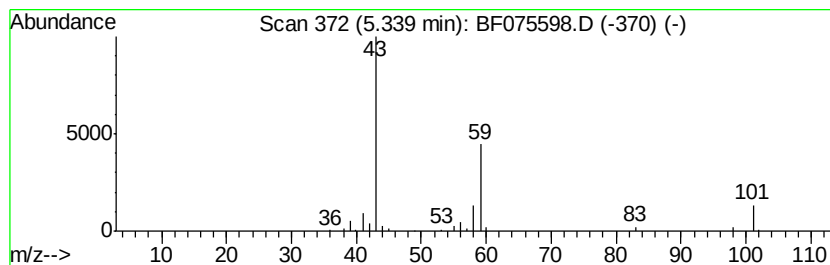
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	15.00 ng	115258	1,4-Dichlorobenzene-d4	7.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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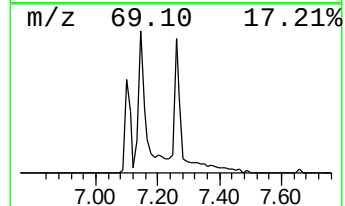
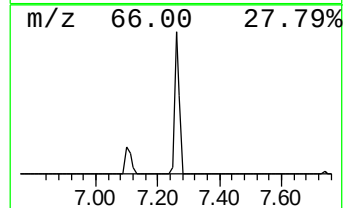
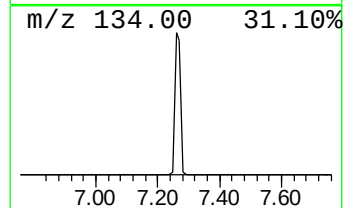
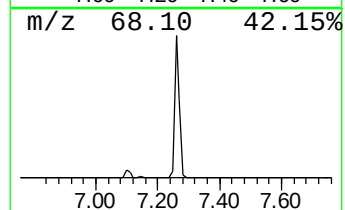
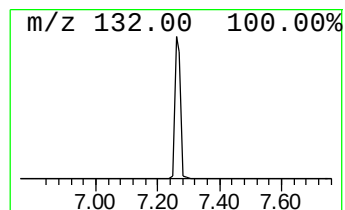
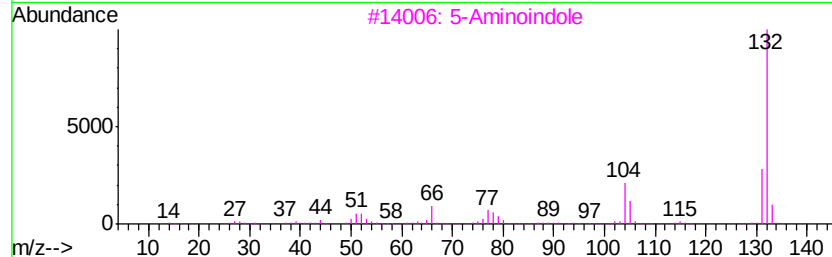
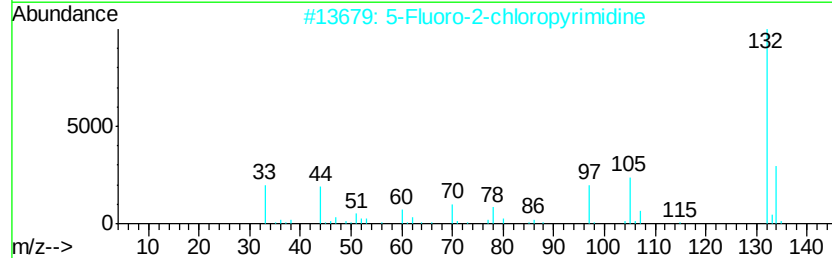
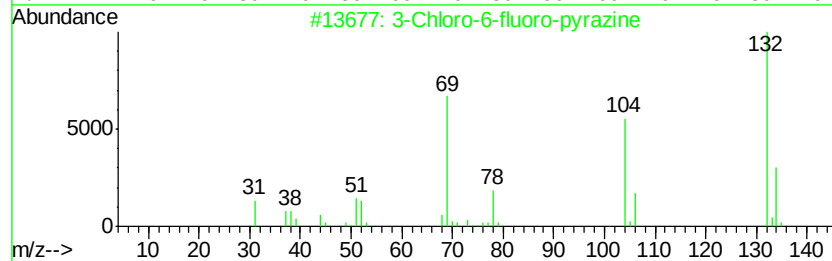
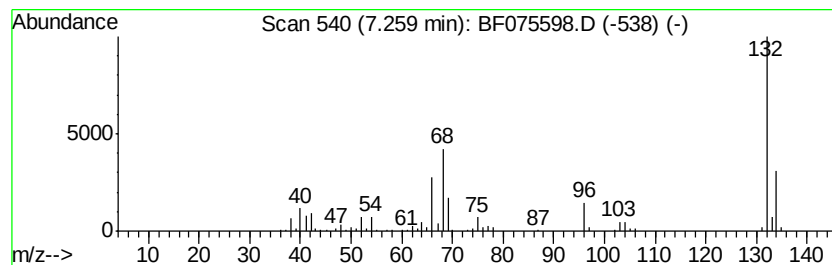
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.26 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	41.35 ng	317842	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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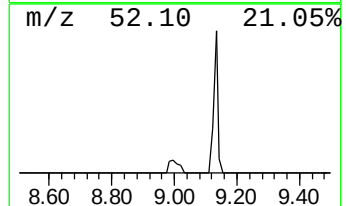
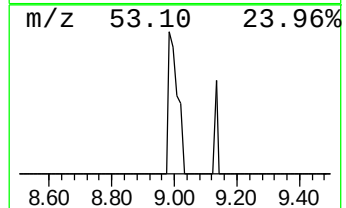
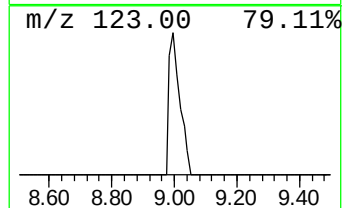
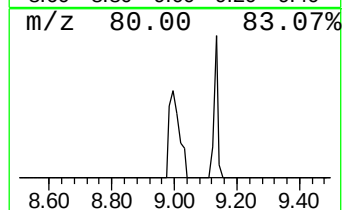
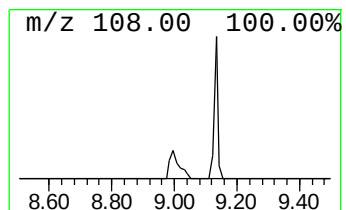
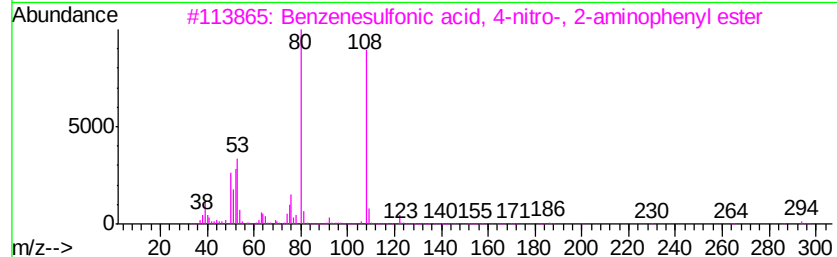
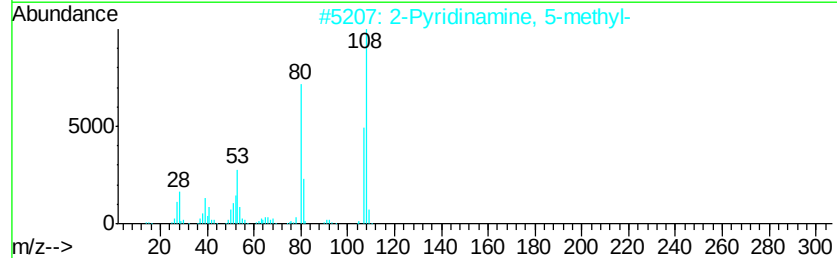
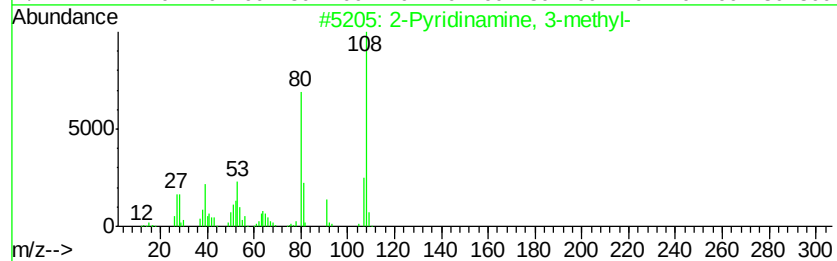
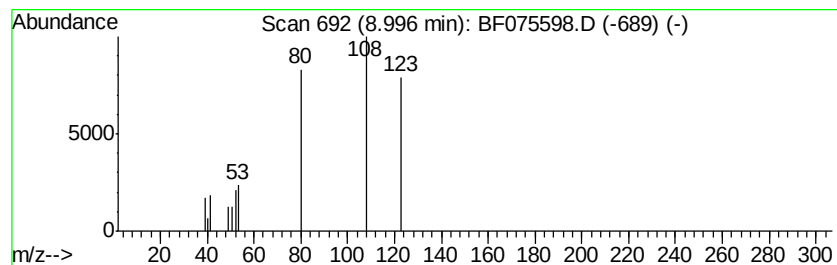
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2-Pyridinamine, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	2.05 ng	21579	Napthalene-d8	9.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pyridinamine, 3-methyl-	108	C6H8N2	001603-40-3	58
2		2-Pyridinamine, 5-methyl-	108	C6H8N2	001603-41-4	53
3		Benzenesulfonic acid, 4-nitro-, ...	294	C12H10N2O5S	018631-75-9	40
4		s-Triazaborane	81	B3H6N3	006569-51-3	36
5		2-Pyridinamine, N-methyl-	108	C6H8N2	004597-87-9	9



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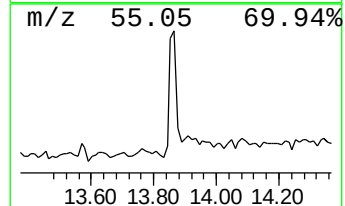
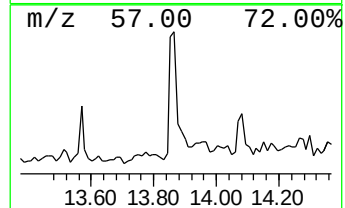
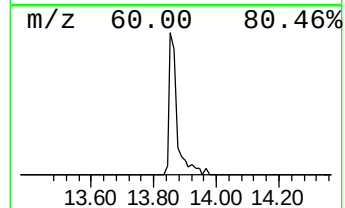
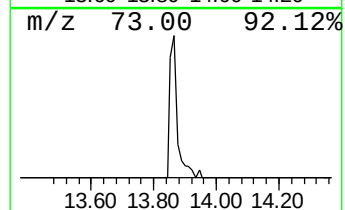
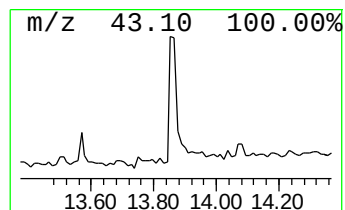
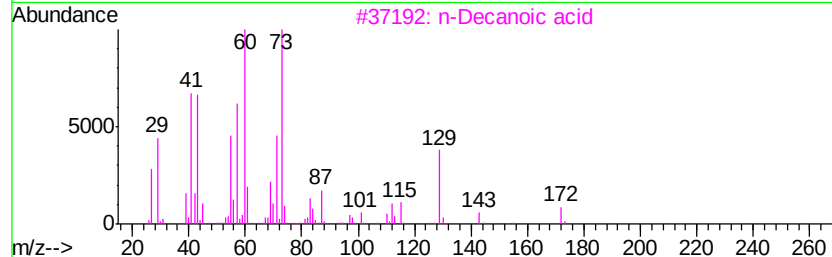
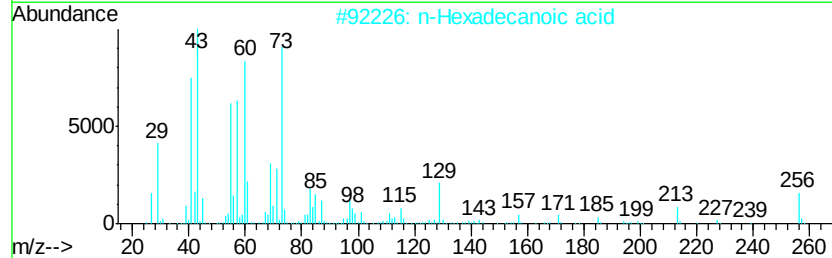
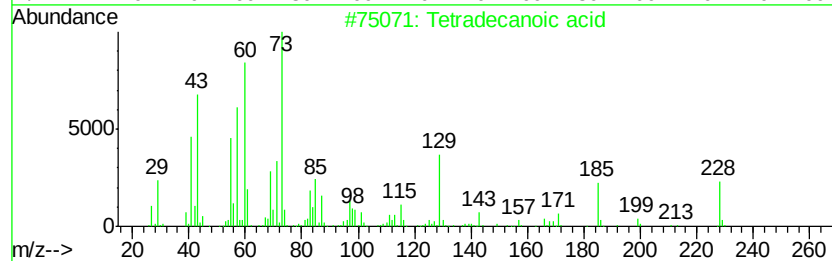
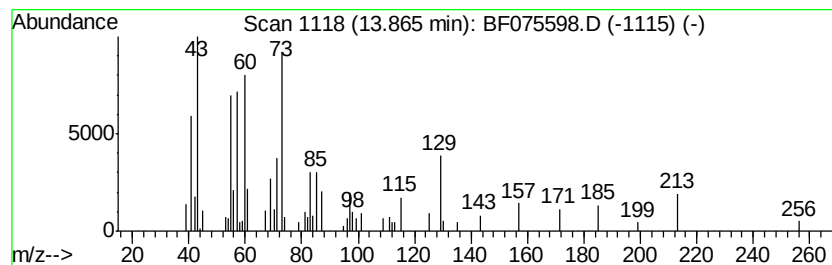
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.93 ng	105466	Phenanthrene-d10	13.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	49



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S-3

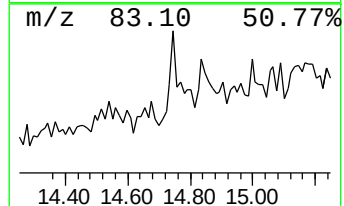
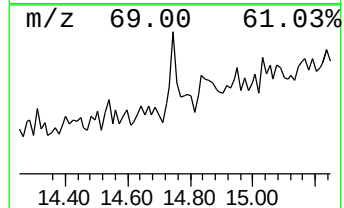
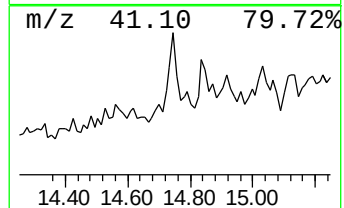
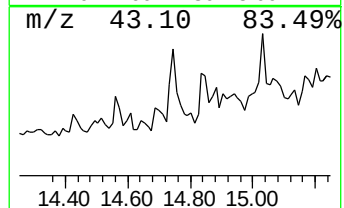
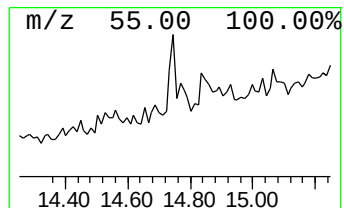
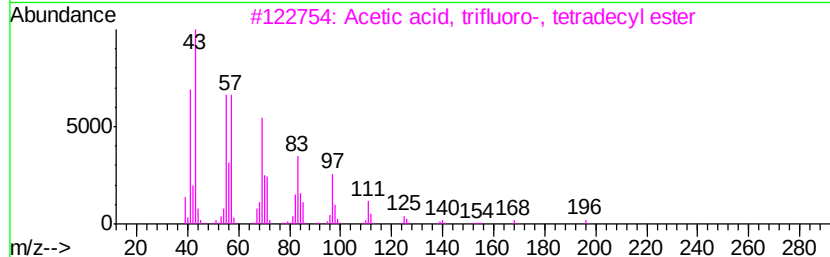
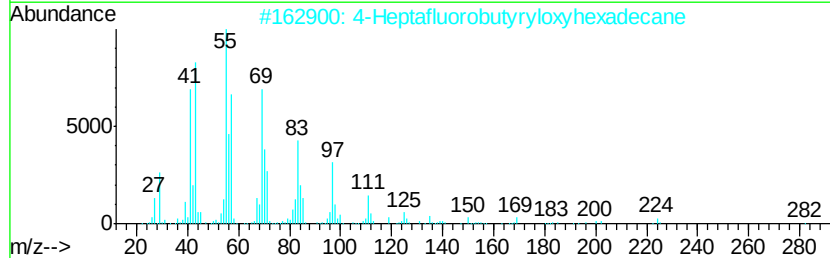
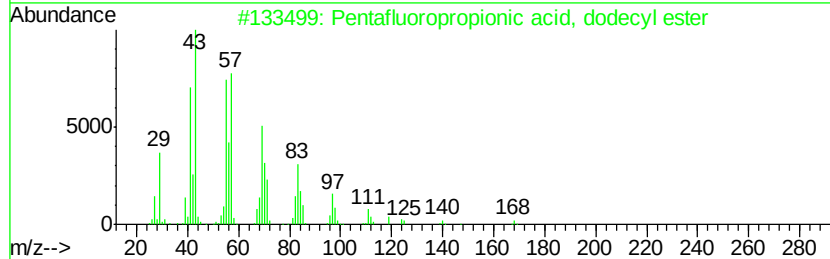
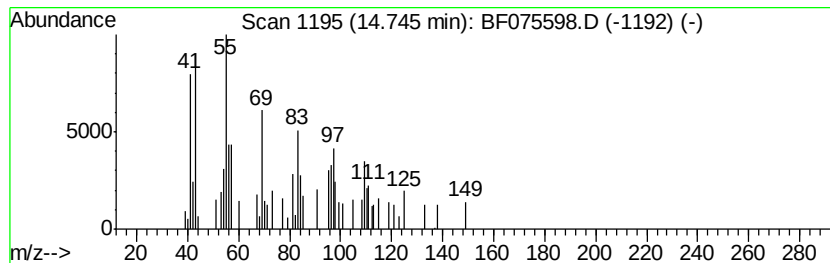
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.75 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	4.26 ng	50325	Phenanthrene-d10	13.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	47
2			4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	43
3			Acetic acid, trifluoro-, tetradec...	310	C16H29F3O2	006222-02-2	38
4			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	38
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075598.D
Acq On : 16 Nov 2014 23:57
Operator : TP / JJ
Sample : F4738-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
S-3

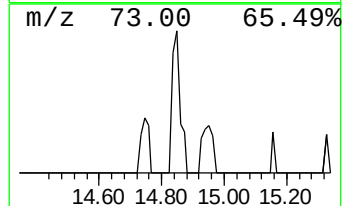
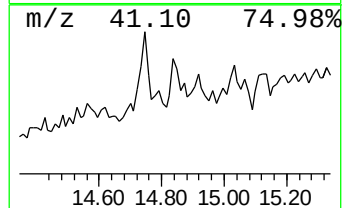
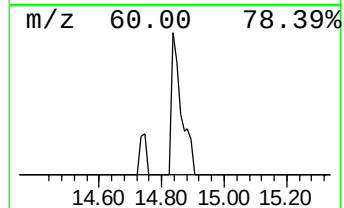
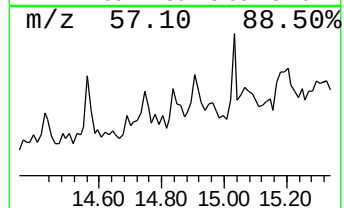
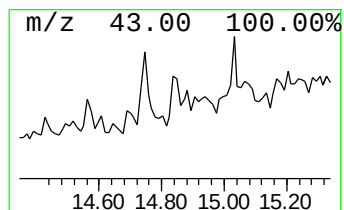
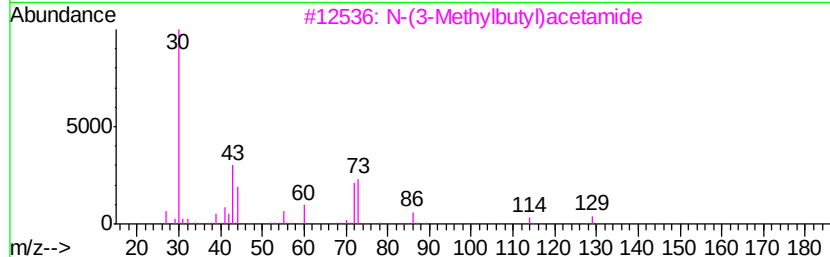
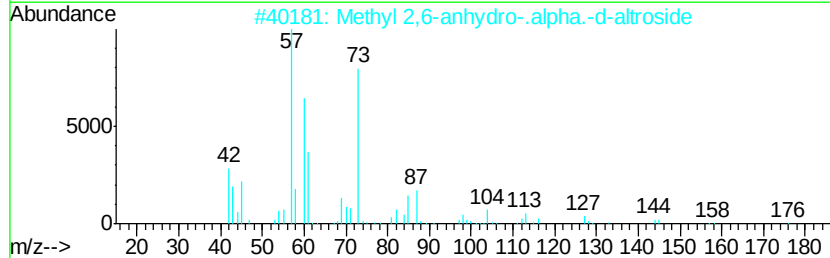
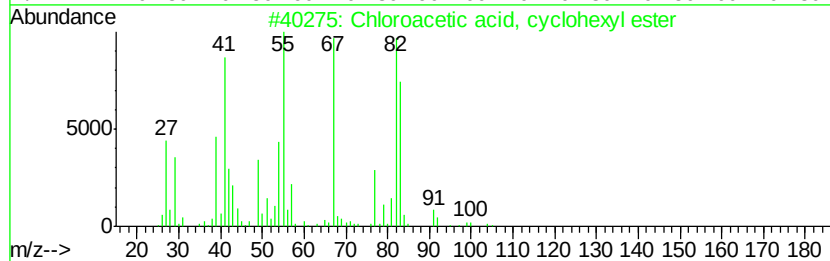
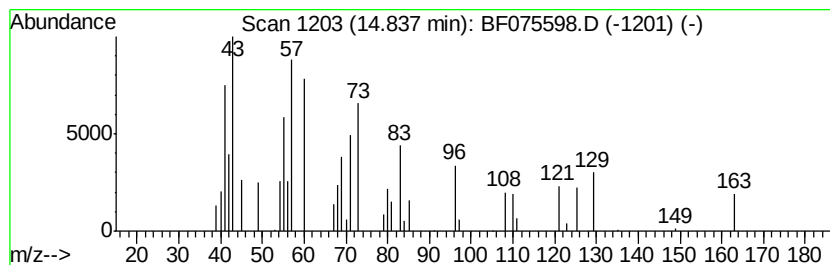
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.84 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.01 ng	38177	Chrysene-d12	16.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, cyclohexyl ester	176	C8H13ClO2	006975-91-3	12
2		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	10
3		N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	10
4		1,3,4-Thiadiazol-2-amine, 5-ethyl-	129	C4H7N3S	014068-53-2	9
5		2-Deoxy-D-glucose	164	C6H12O5	000154-17-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075598.D
Acq On : 16 Nov 2014 23:57
Operator : TP / JJ
Sample : F4738-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3

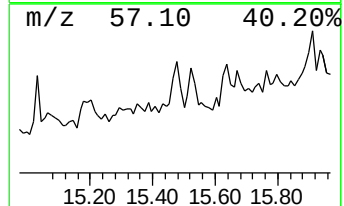
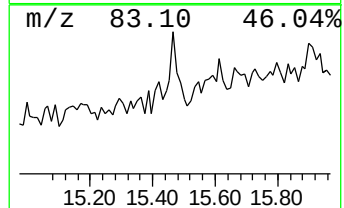
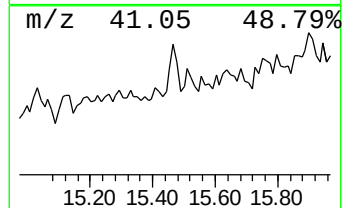
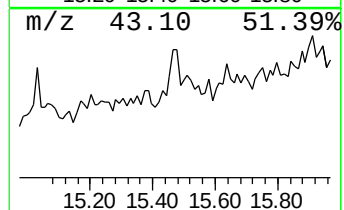
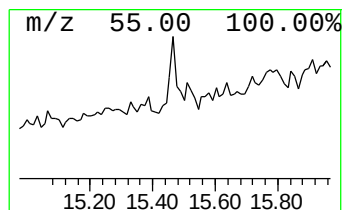
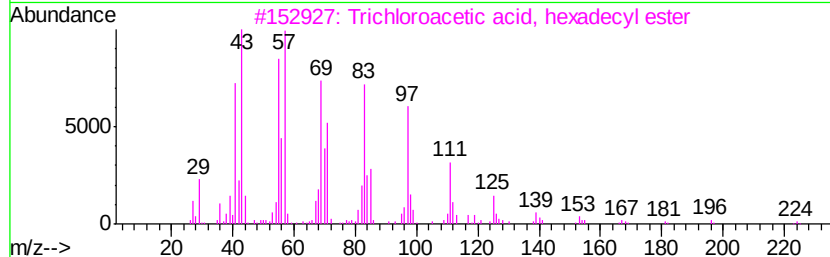
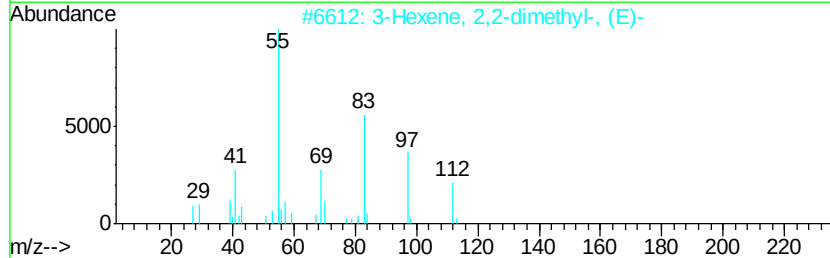
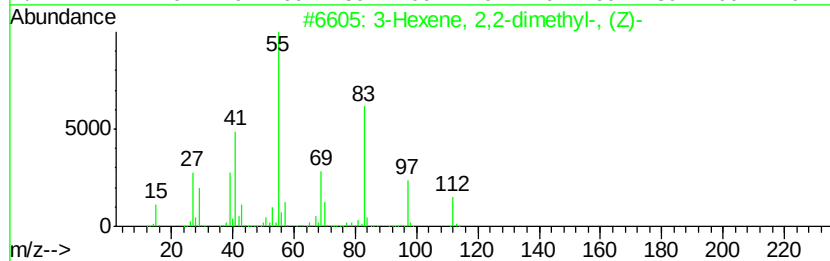
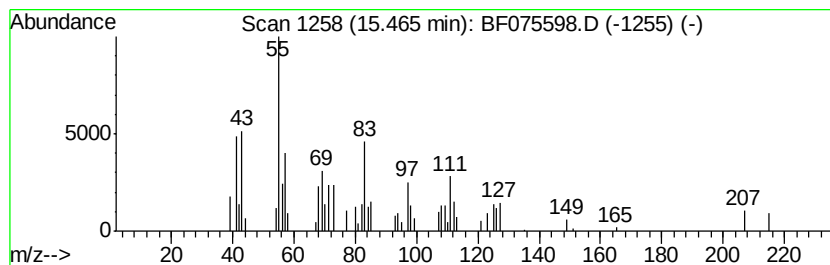
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.47 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	2.52 ng	47886	Chrysene-d12	16.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexene, 2,2-dimethyl-, (Z)-	112	C8H16	000690-92-6	25
2			3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	25
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	22
4			1-Docosene	308	C22H44	001599-67-3	22
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075598.D
Acq On : 16 Nov 2014 23:57
Operator : TP / JJ
Sample : F4738-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

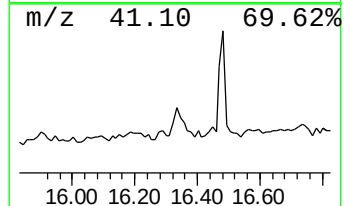
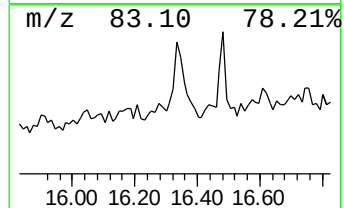
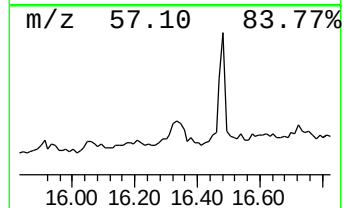
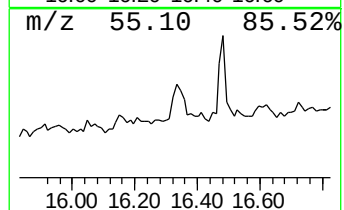
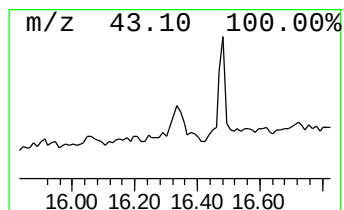
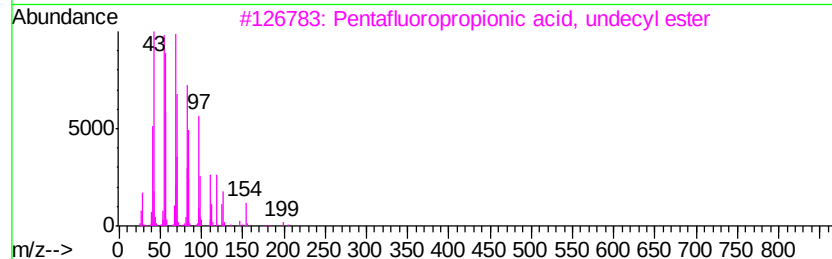
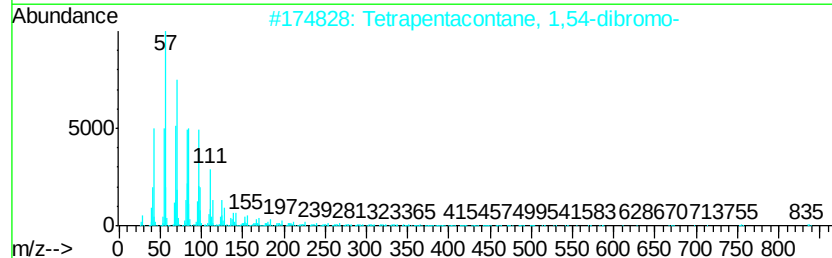
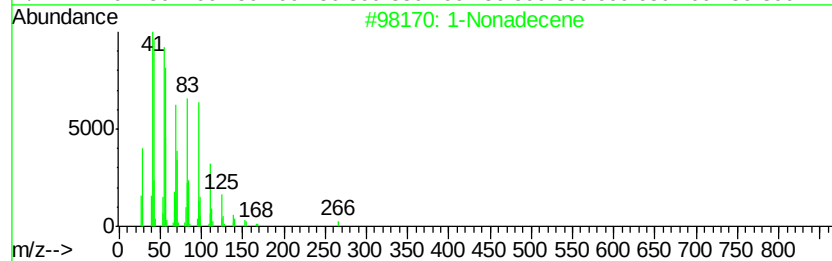
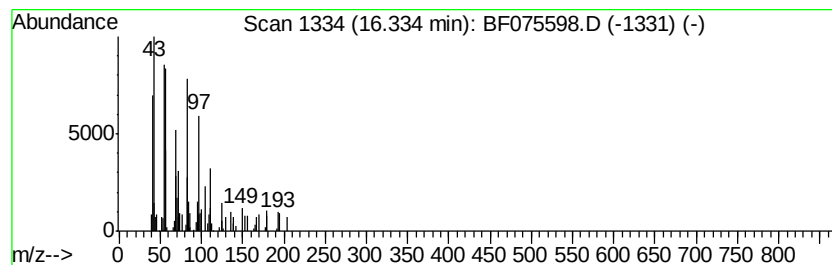
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	5.52 ng	104990	Chrysene-d12	16.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene		266 C19H38	018435-45-5 64
2	Tetrapentacontane, 1,54-dibromo-		915 C54H108Br2	1000156-09-4 53
3	Pentafluoropropionic acid, undec...		318 C14H23F5O2	1000283-04-0 49
4	Dodecane, 5-cyclohexyl-		252 C18H36	013151-85-4 47
5	17-Pentatriacontene		491 C35H70	006971-40-0 43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075598.D
Acq On : 16 Nov 2014 23:57
Operator : TP / JJ
Sample : F4738-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3

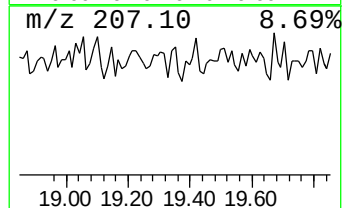
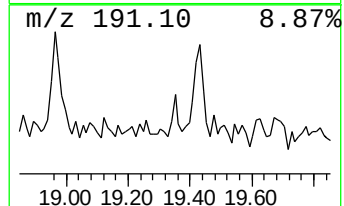
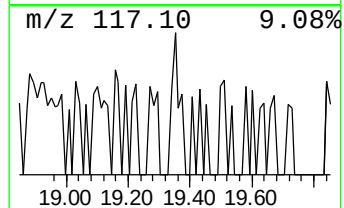
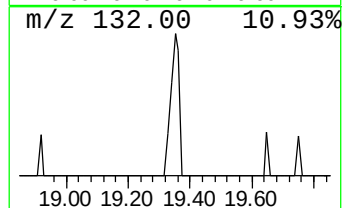
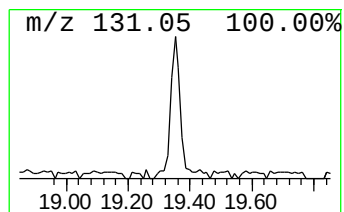
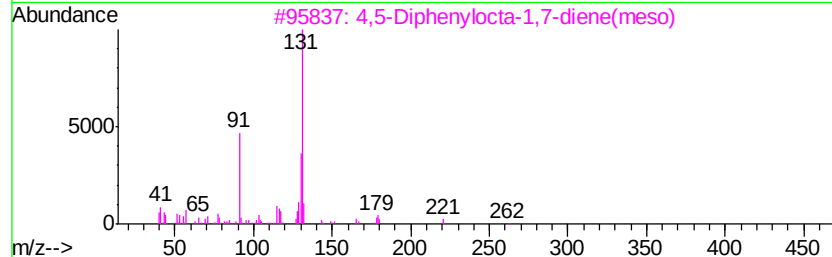
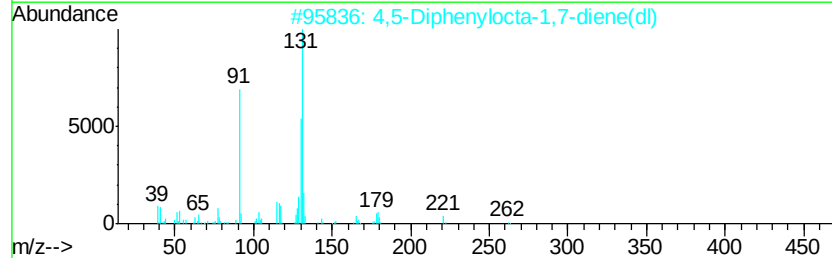
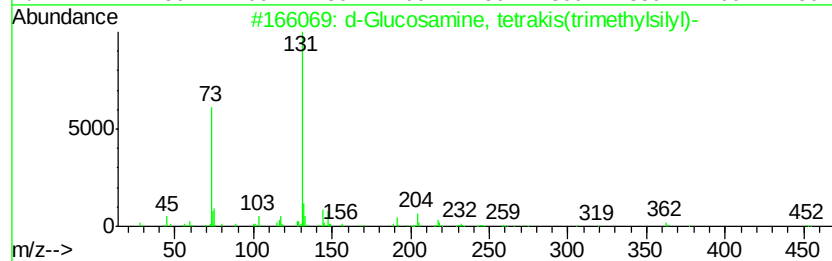
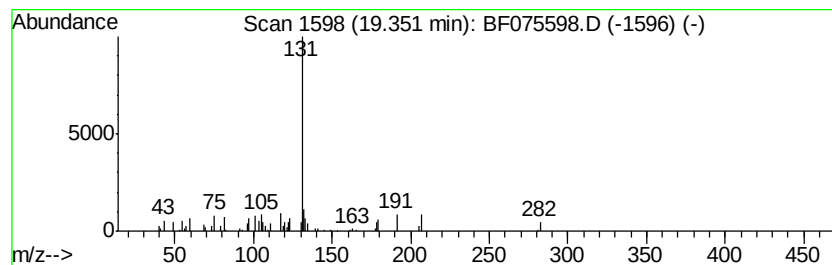
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 d-Glucosamine, tetrakis(tri... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.25 ng	47357	Perylene-d12	18.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	d-Glucosamine, tetrakis(trimethy...	467	C18H45N05Si4	1000079-26-2	59
2		4,5-Diphenylocta-1,7-diene(dl)	262	C20H22	1000215-92-8	50
3		4,5-Diphenylocta-1,7-diene(meso)	262	C20H22	1000215-92-7	50
4		4-Methyltetrahydro-1,3-oxazine-2...	131	C5H9NOS	014760-60-2	50
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
Data File : BF075598.D
Acq On : 16 Nov 2014 23:57
Operator : TP / JJ
Sample : F4738-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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
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2-Pentanone, 4-hy...	5.34	15.0	ng	115258	1	7.56	153716	20.0
unknown7.26	7.26	41.4	ng	317842	1	7.56	153716	20.0
2-Pyridinamine, 3...	9.00	2.0	ng	21579	2	9.13	210738	20.0
Tetradecanoic acid	13.87	8.9	ng	105466	4	13.17	236223	20.0
unknown14.75	14.75	4.3	ng	50325	4	13.17	236223	20.0
unknown14.84	14.84	2.0	ng	38177	5	16.46	380469	20.0
unknown15.47	15.47	2.5	ng	47886	5	16.46	380469	20.0
1-Nonadecene	16.33	5.5	ng	104990	5	16.46	380469	20.0
d-Glucosamine, te...	19.35	3.3	ng	47357	6	18.20	291042	20.0