

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
 Data File : BF088802.D
 Acq On : 8 Jul 2016 2:30
 Operator : UM/SJ
 Sample : H3889-10 4X
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-10

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-BF063016.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	1.827	19	21	81	rVB	1763070	4894008	100.00%	33.749%
2	5.324	324	327	329	rBV	114166	133127	2.72%	0.918%
3	6.365	416	418	421	rBV	160214	198163	4.05%	1.367%
4	6.502	428	430	432	rBV	230033	184897	3.78%	1.275%
5	6.742	448	451	453	rBV	558482	478763	9.78%	3.302%
6	6.890	462	464	466	rBV	113366	120307	2.46%	0.830%
7	7.302	497	500	502	rBV	131392	120299	2.46%	0.830%
8	8.022	561	563	566	rVB	575637	568554	11.62%	3.921%
9	8.788	628	630	636	rBV	90527	110592	2.26%	0.763%
10	9.108	655	658	660	rBV	224472	268306	5.48%	1.850%
11	9.496	690	692	695	rBV	214365	233496	4.77%	1.610%
12	9.782	714	717	719	rBV	514549	579637	11.84%	3.997%
13	10.559	783	785	787	rBV	201361	178466	3.65%	1.231%
14	10.754	801	802	804	rBV2	163822	230217	4.70%	1.588%
15	10.891	809	814	817	rBV7	34851	113319	2.32%	0.781%
16	11.039	819	827	828	rBV7	163637	606034	12.38%	4.179%
17	11.096	830	832	835	rBV4	81175	114832	2.35%	0.792%
18	11.142	835	836	838	rBV2	75895	88640	1.81%	0.611%
19	11.211	840	842	843	rBV	165686	242289	4.95%	1.671%
20	11.256	844	846	847	rVB	556920	447343	9.14%	3.085%
21	11.302	847	850	851	rBV2	94893	153406	3.13%	1.058%
22	11.416	857	860	861	rBV3	63271	92939	1.90%	0.641%
23	11.451	861	863	864	rVB2	78868	76761	1.57%	0.529%
24	11.485	864	866	868	rBV2	73491	174172	3.56%	1.201%
25	11.519	868	869	872	rVB3	190704	327557	6.69%	2.259%
26	11.565	872	873	875	rBV	53067	64327	1.31%	0.444%
27	11.622	876	878	881	rBV4	154116	360938	7.38%	2.489%
28	11.668	881	882	883	rBV	101217	75578	1.54%	0.521%
29	11.702	883	885	887	rBV3	81313	162697	3.32%	1.122%
30	11.794	891	893	894	rBV2	110286	187177	3.82%	1.291%
31	11.851	896	898	900	rVB2	156694	245675	5.02%	1.694%
32	11.965	906	908	910	rBV2	140220	199297	4.07%	1.374%
33	12.171	924	926	928	rBV2	223043	461852	9.44%	3.185%
34	12.537	956	958	960	rBV2	155080	296029	6.05%	2.041%

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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-BF063016.M
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35	12.845	984	985	987	rVB	435091	434106	8.87%	2.994%
36	13.897	1075	1077	1078	rVB	608469	520614	10.64%	3.590%
37	15.291	1197	1199	1205	rVB	343442	542799	11.09%	3.743%
38	18.057	1437	1441	1446	rVB2	74611	213795	4.37%	1.474%

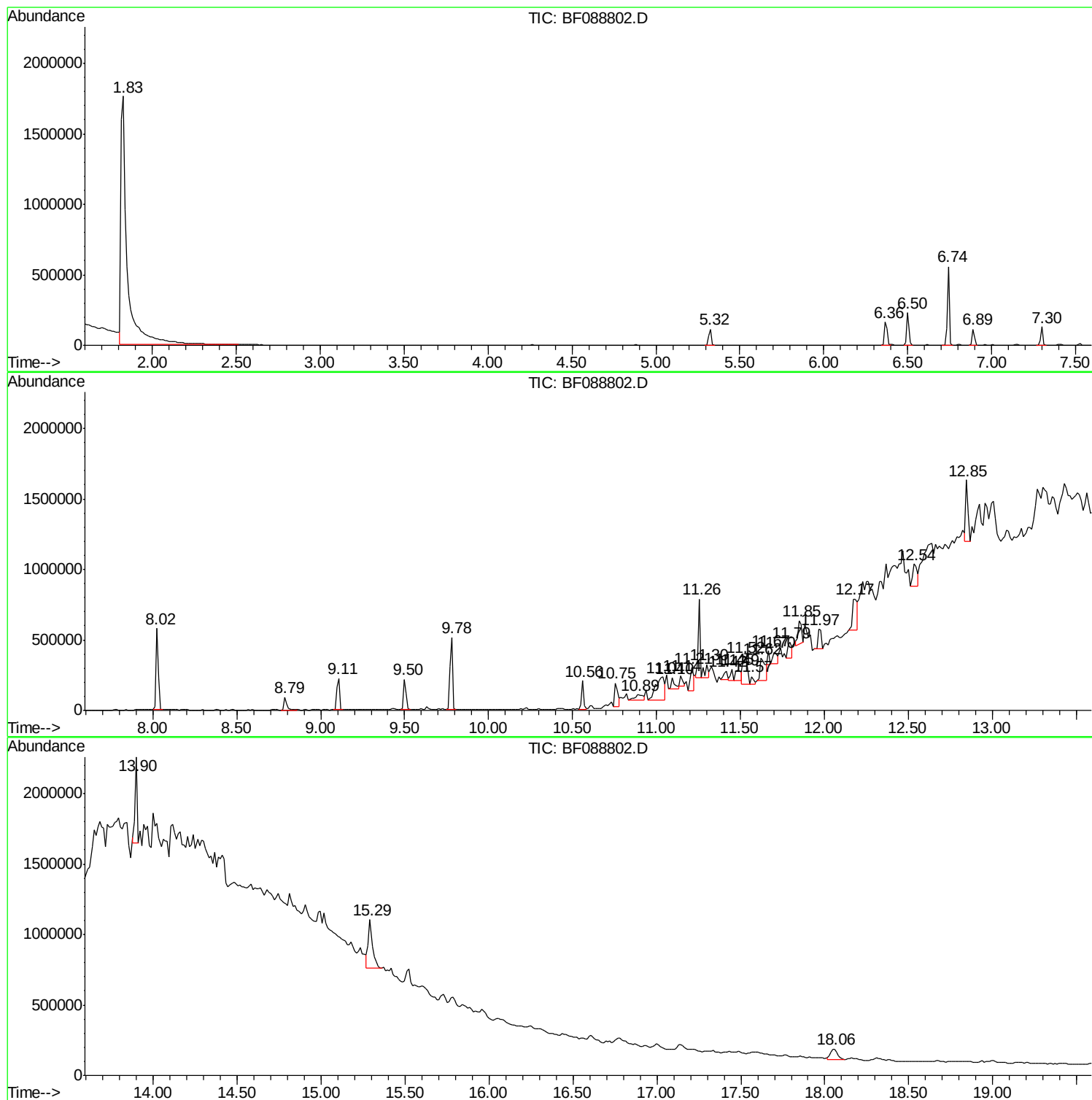
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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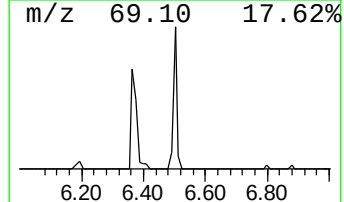
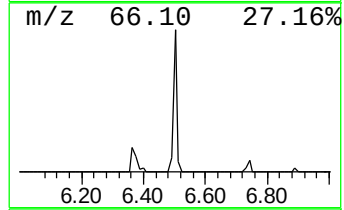
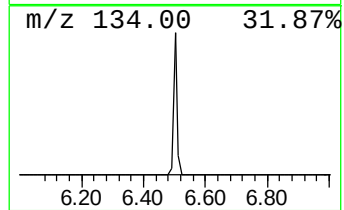
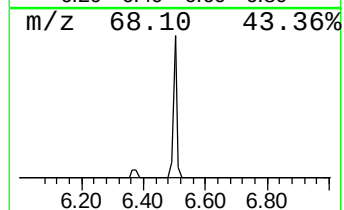
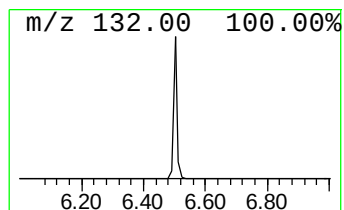
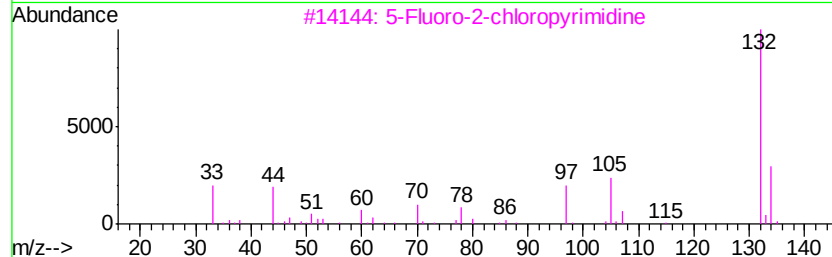
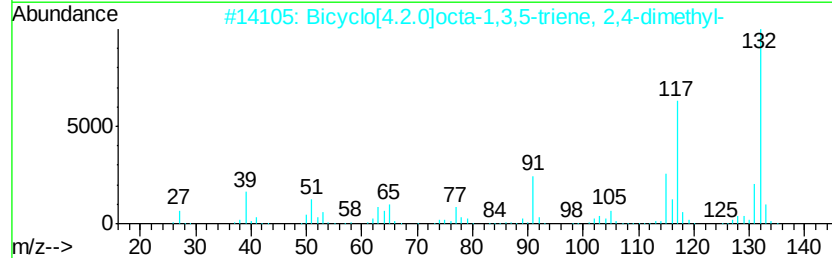
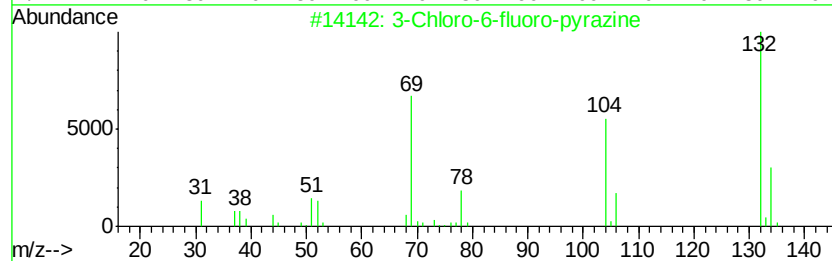
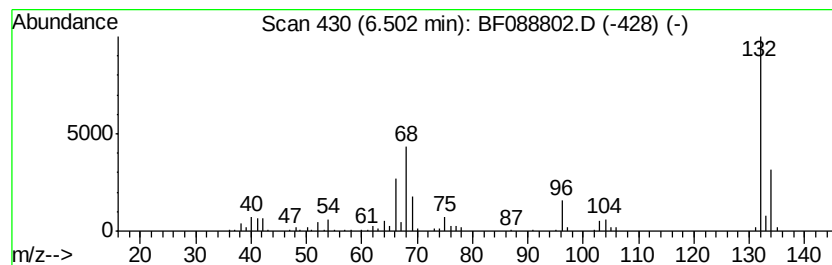
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	7.72 ng	184897	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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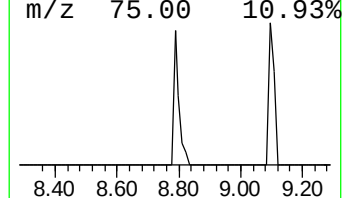
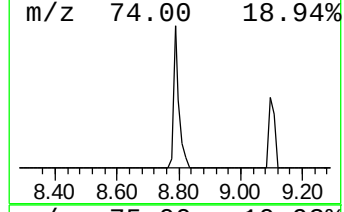
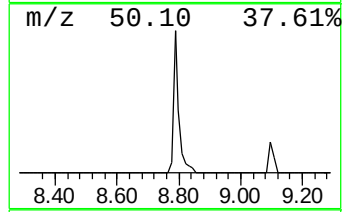
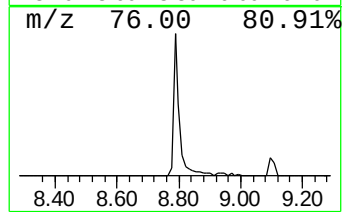
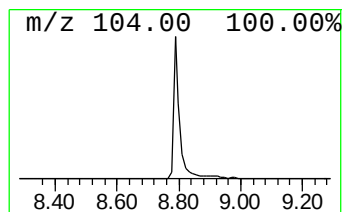
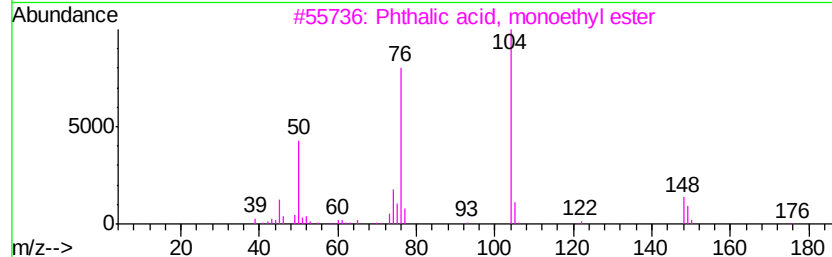
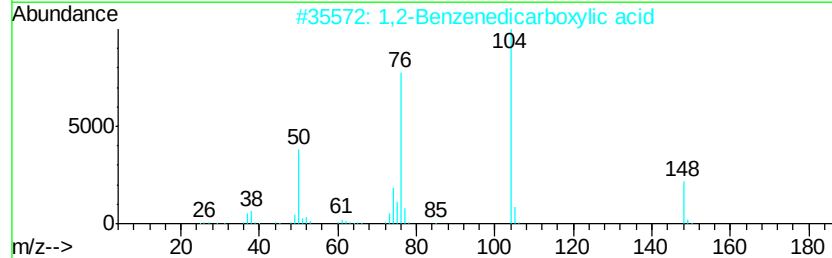
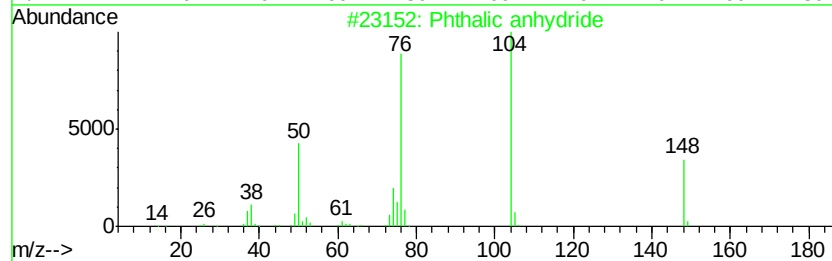
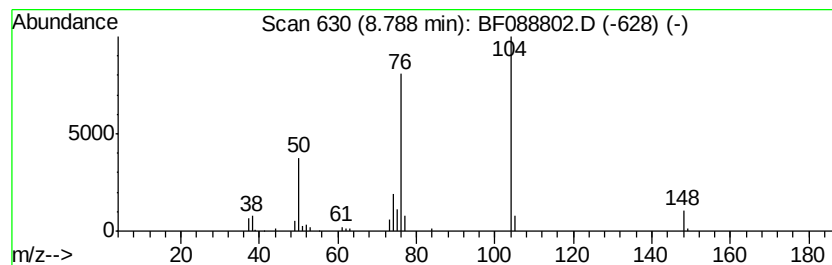
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phthalic anhydride Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	3.89 ng	110592	Naphthalene-d8	8.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phthalic anhydride	148 C8H4O3	000085-44-9	95
2	1,2-Benzenedicarboxylic acid	166 C8H6O4	000088-99-3	83
3	Phthalic acid, monoethyl ester	194 C10H10O4	002306-33-4	83
4	Bicyclo[4.2.0]octa-1,3,5-triene...	132 C8H4O2	006383-11-5	80
5	N-[2-Acetamidoethylthio]phthalimide	264 C12H12N2O3S	025158-14-9	78



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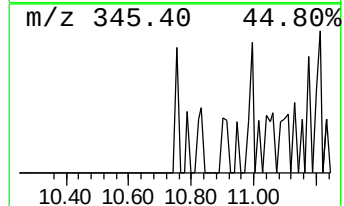
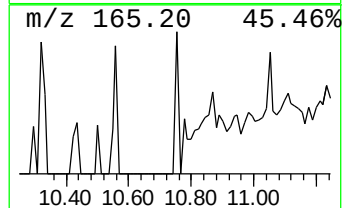
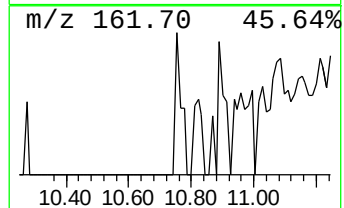
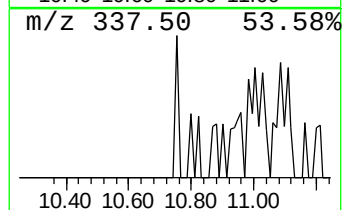
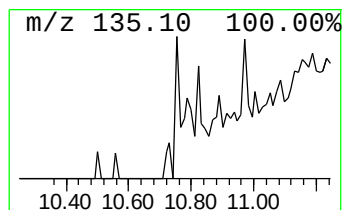
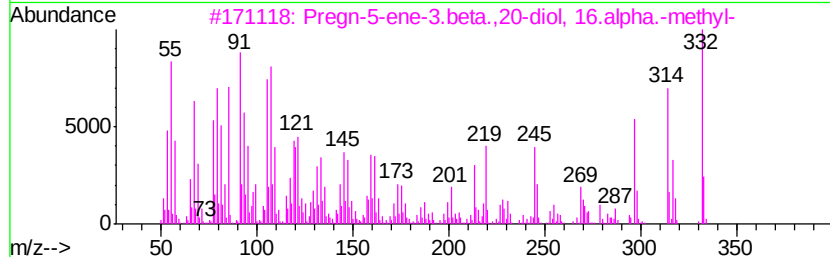
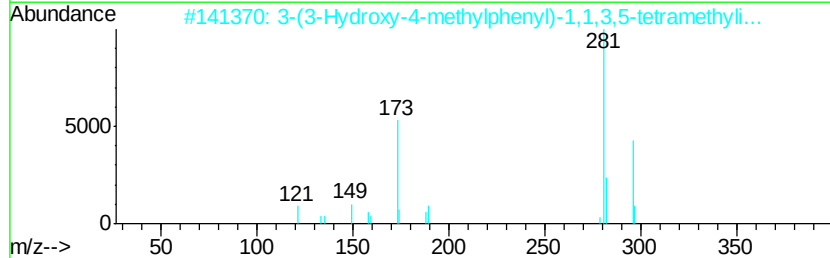
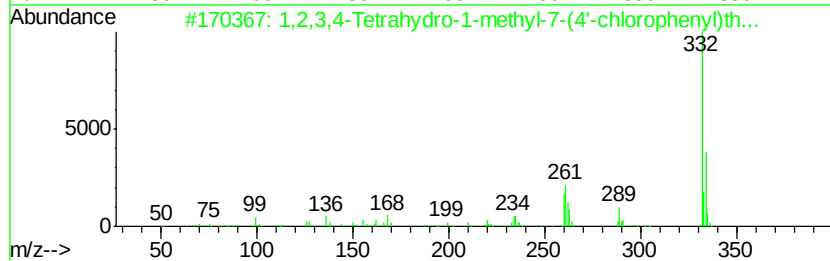
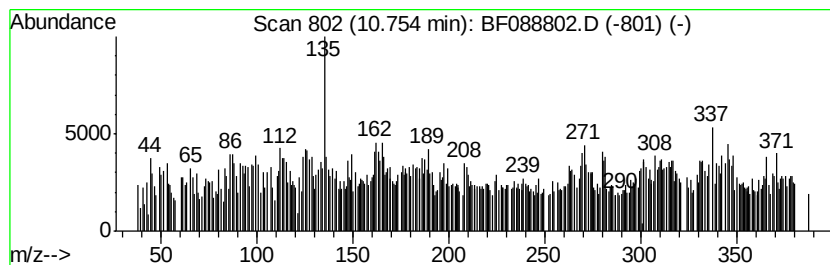
Instrument :
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ClientSampled :
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown10.75 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.75	10.29 ng	230217	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,4-Tetrahydro-1-methyl-7-(4...	332	C14H9ClN4O2S	115872-78-1	15
2	3-(3-Hydroxy-4-methylphenyl)-1,1...	296	C20H24O2	1000105-90-6	11
3	Pregn-5-ene-3.beta.,20-diol, 16....	332	C22H36O2	031320-91-9	11
4	Benzothiazole, 2,2'-dithiobis-	332	C14H8N2S4	000120-78-5	10
5	Ethyl 4-((E)-(2-nitrophenyl)met...	298	C16H14N2O4	057707-09-2	10



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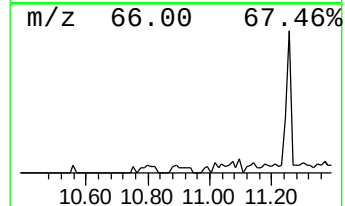
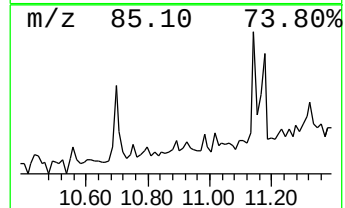
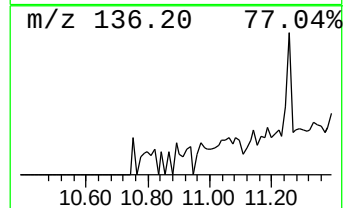
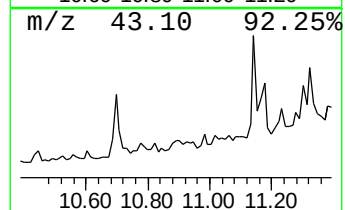
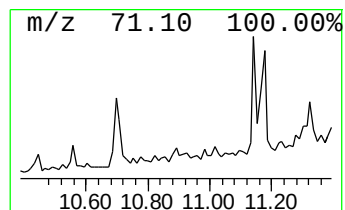
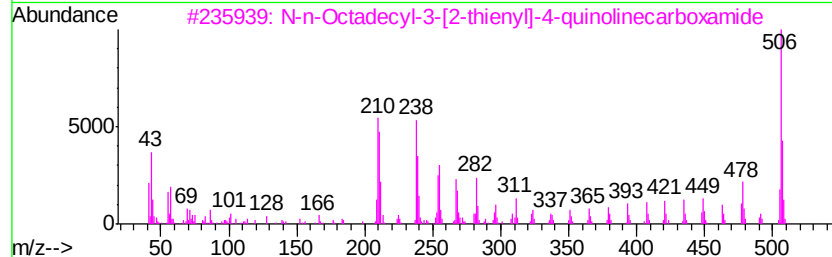
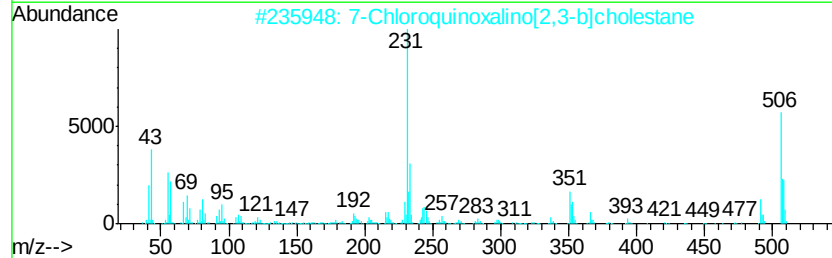
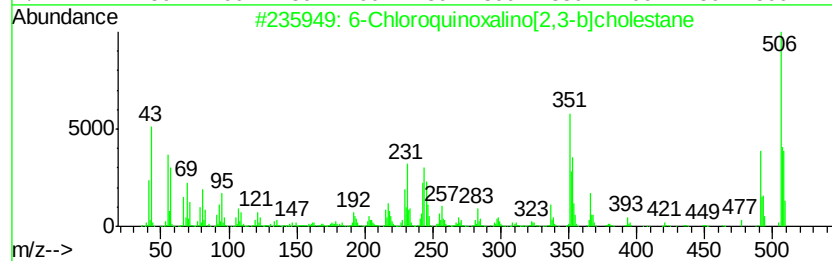
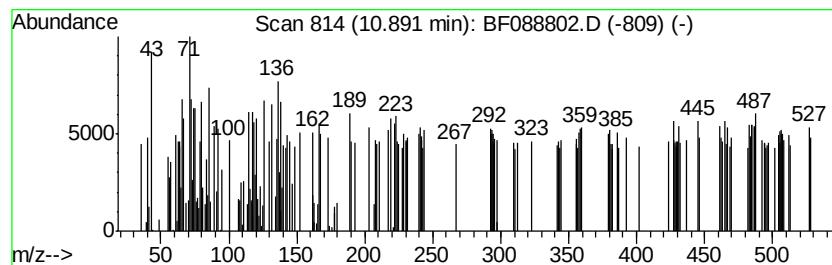
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.89 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.89	5.07 ng	113319	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Chloroquinoxalino[2,3-b]choles...	506	C33H47ClN2	1000210-42-0	14
2	7-Chloroquinoxalino[2,3-b]choles...	506	C33H47ClN2	1000210-42-1	14
3	N-n-Octadecyl-3-[2-thienyl]-4-qu...	506	C32H46N2OS	1000257-06-6	10
4	trans-4-Methoxy-4'-(octadecyloxy...	506	C34H50O3	122207-20-9	9
5	trans-4'-Methoxy-4-(octadecyloxy...	506	C34H50O3	122207-15-2	9



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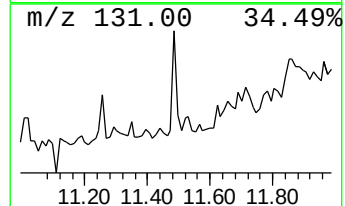
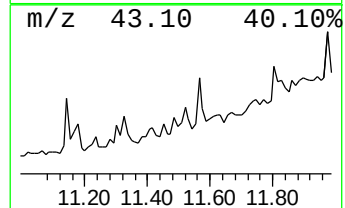
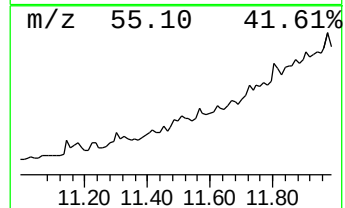
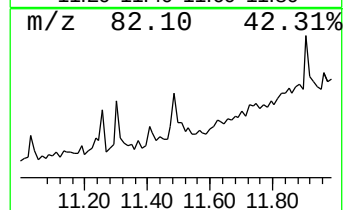
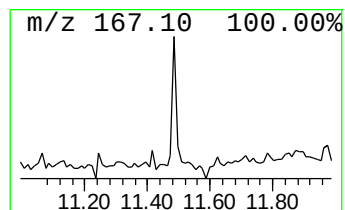
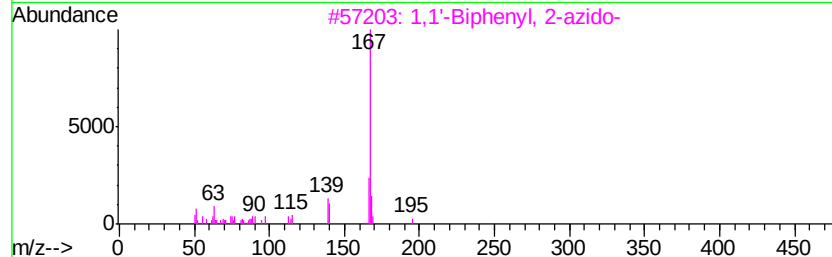
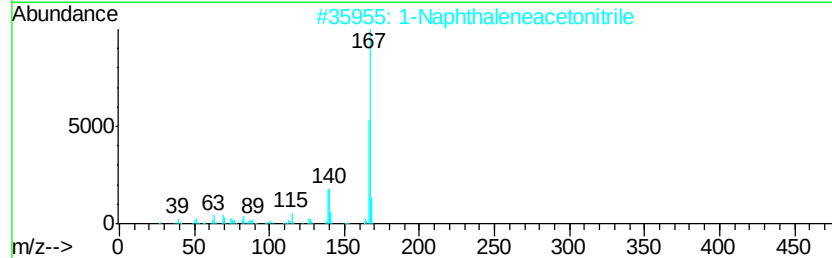
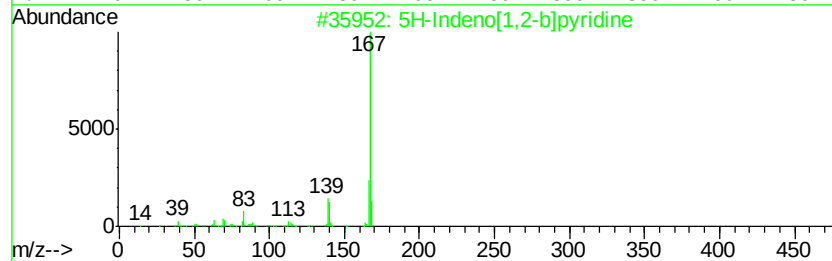
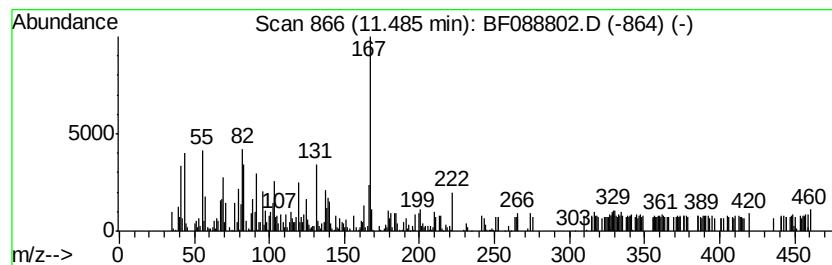
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Peak Number 11 unknown11.49 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.49	7.79 ng	174172	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	46
2	1-Naphthaleneacetonitrile	167	C12H9N	000132-75-2	38
3	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	38
4	Carbazole	167	C12H9N	000086-74-8	38
5	1,3-Benzenedicarbonyl dichloride	202	C8H4Cl2O2	000099-63-8	38



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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10

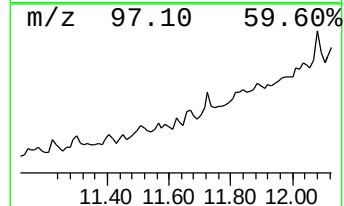
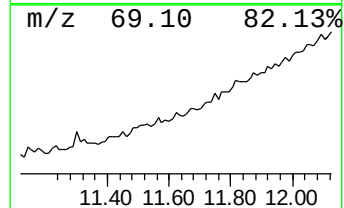
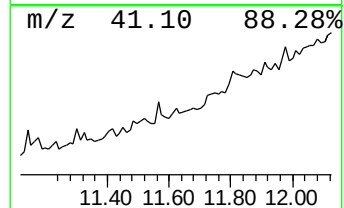
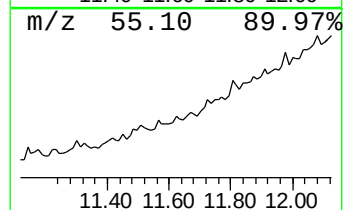
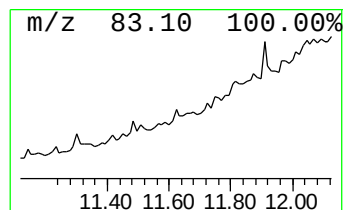
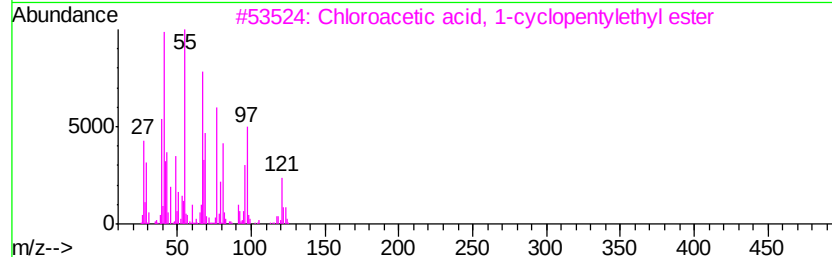
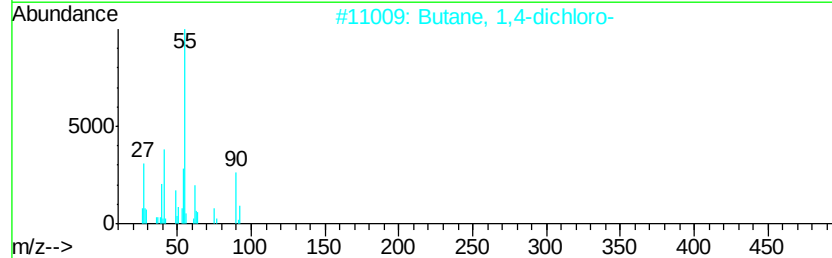
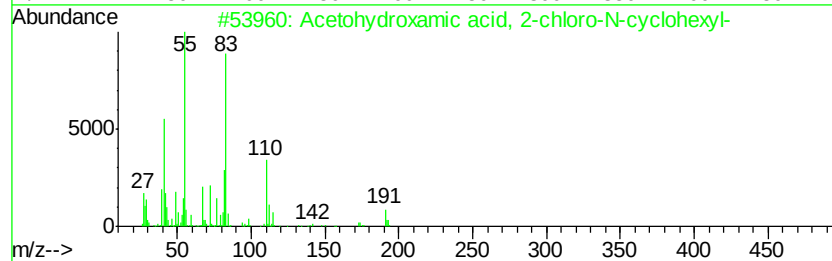
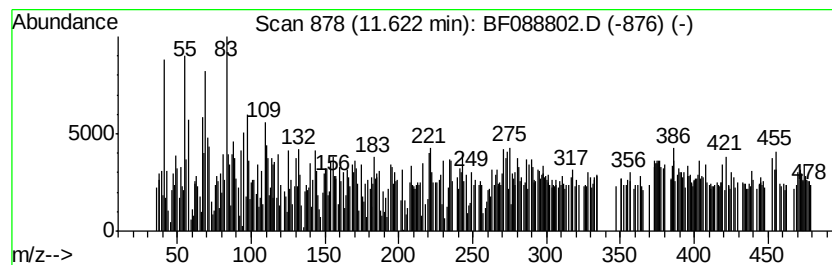
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown11.62 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	16.14 ng	360938	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetohydroxamic acid, 2-chloro-N...	191	C8H14ClNO2	007340-05-8	14
2		Butane, 1,4-dichloro-	126	C4H8Cl2	000110-56-5	10
3		Chloroacetic acid, 1-cyclopentyl...	190	C9H15ClO2	1000279-89-0	10
4		Phosphine, cyclohexyl(1,1-dimeth...	186	C11H23P	074685-81-7	10
5		Chloromethyl 6-chloroundecanoate	268	C12H22Cl2O2	080418-92-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088802.D
Acq On : 8 Jul 2016 2:30
Operator : UM/SJ
Sample : H3889-10 4X
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10

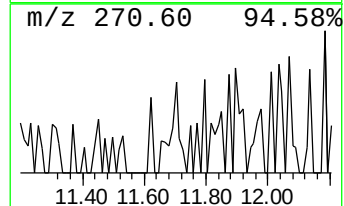
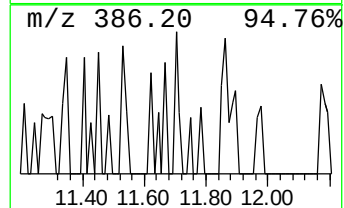
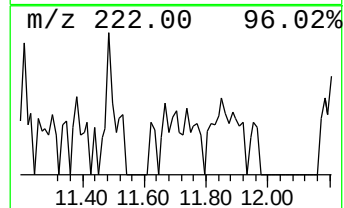
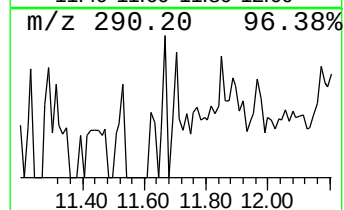
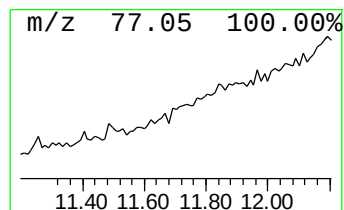
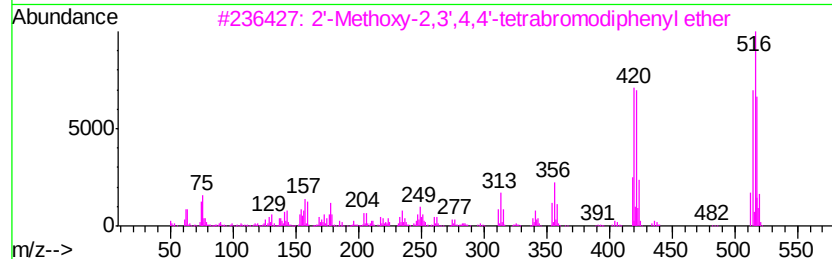
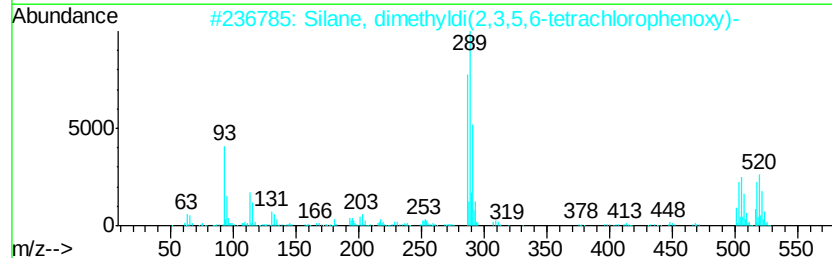
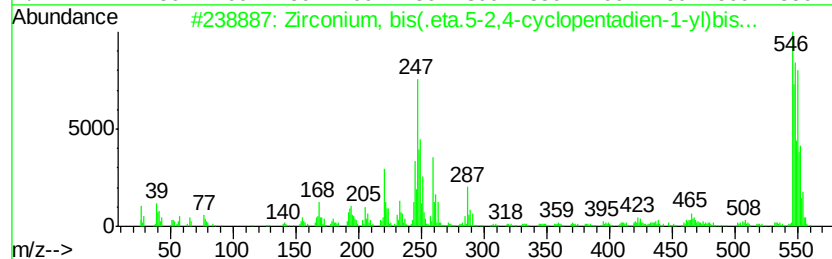
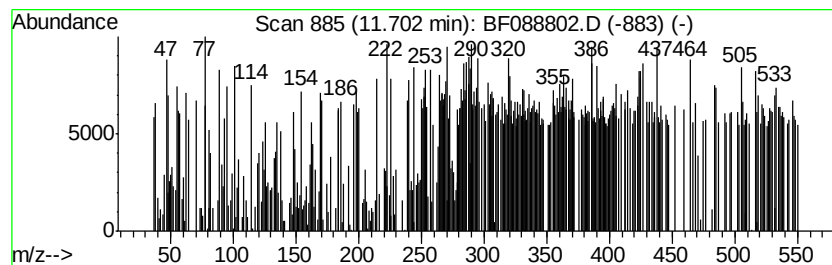
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown11.70 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	7.27 ng	162697	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Zirconium, bis(.eta.5-2,4-cyclop...	546	C28H30Zr2	119144-91-1	15
2		Silane, dimethyldi(2,3,5,6-tetra...	516	C14H8Cl8O2Si	1000347-54-0	12
3		2'-Methoxy-2,3',4,4'-tetrabromod...	512	C13H8Br4O2	1000376-36-8	10
4		Osmium methyl, (.eta.-5-cyclopen...	548	C22H30OsP2	1000158-92-4	9
5		7-Bromo-3-(4-bromo-benzylidene)-...	514	C22H13Br2ClN2O	324526-44-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088802.D
Acq On : 8 Jul 2016 2:30
Operator : UM/SJ
Sample : H3889-10 4X
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10

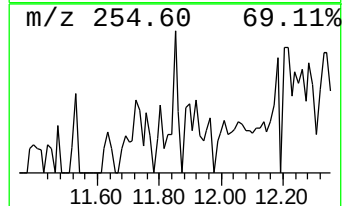
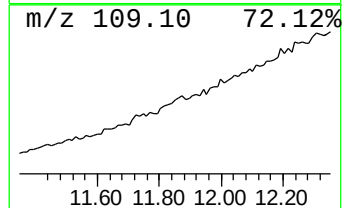
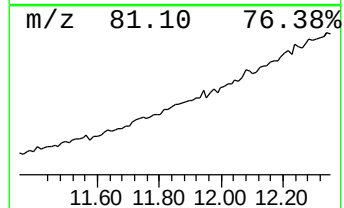
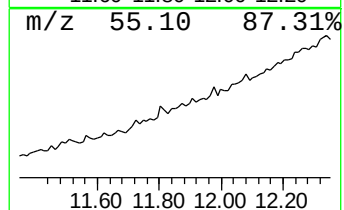
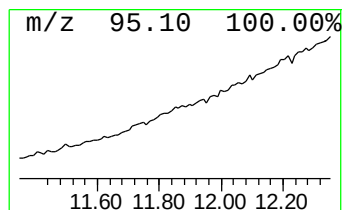
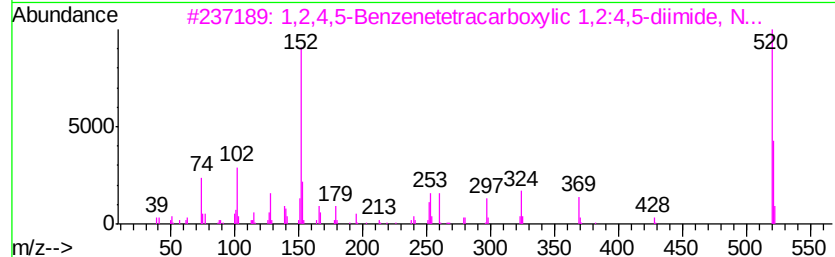
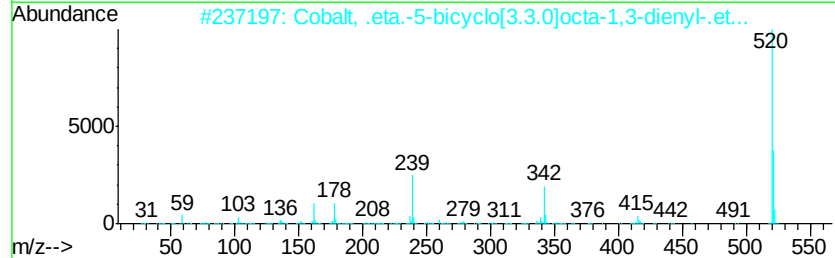
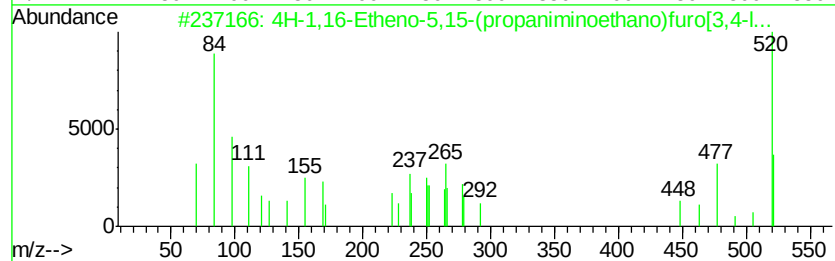
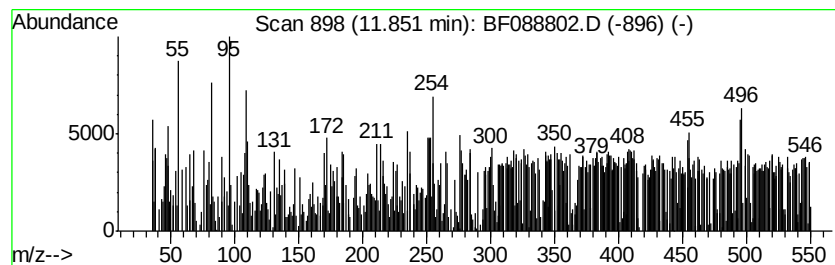
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown11.85 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	10.98 ng	245675	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-1,16-Etheno-5,15-(propanimino...	520	C30H40N4O4	1000065-44-3	25
2		Cobalt, .eta.-5-bicyclo[3.3.0]oc...	520	C36H29Co	1000159-35-6	11
3		1,2,4,5-Benzenetetracarboxylic 1...	520	C34H20N2O4	033529-33-8	10
4		Cholest-2-ene, 4,4-dimethyl-3-[(...]	520	C36H56S	069841-47-0	9
5		Tin(IV) chloride	260	Cl4Sn	007646-78-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088802.D
Acq On : 8 Jul 2016 2:30
Operator : UM/SJ
Sample : H3889-10 4X
Misc :
ALS Vial : 32 Sample Multiplier: 1

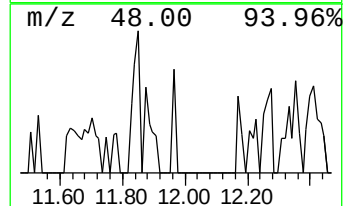
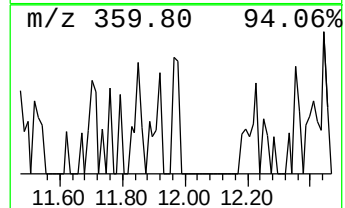
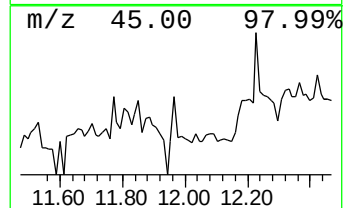
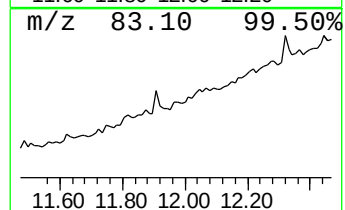
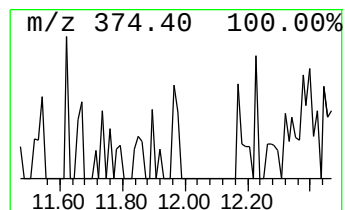
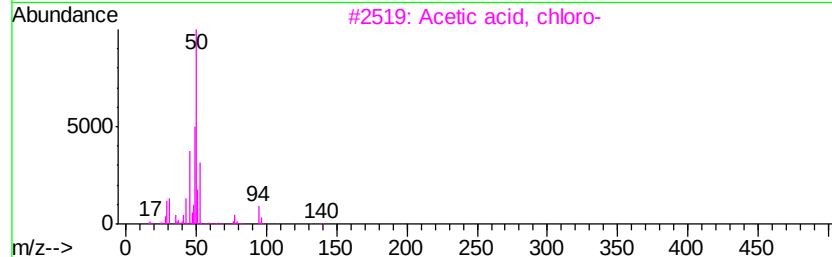
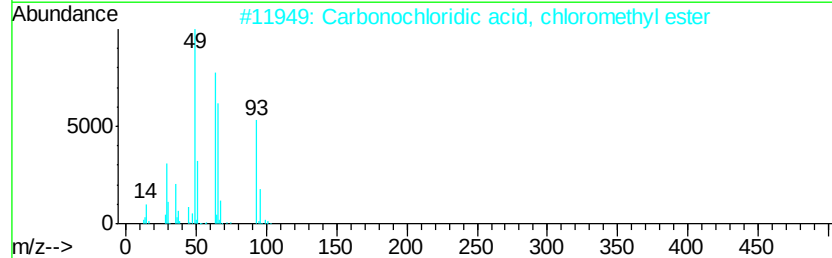
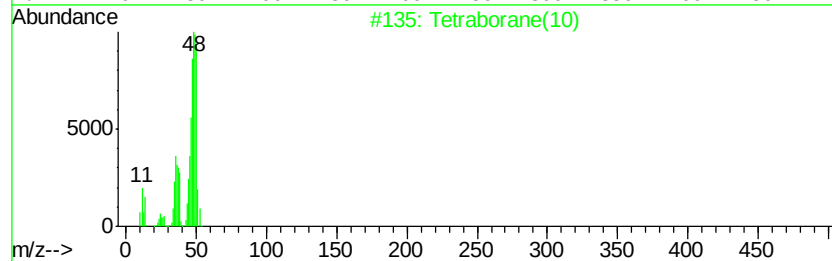
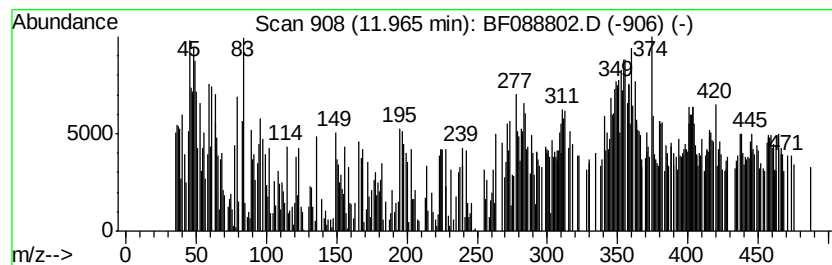
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown11.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.97	8.91 ng	199297	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetraborane(10)	54	B4H10	018283-93-7	27
2	Carbonochloridic acid, chloromet...	128	C2H2Cl2O2	022128-62-7	14
3	Acetic acid, chloro-	94	C2H3ClO2	000079-11-8	14
4	1-Propanol, 3-(methylthio)-	106	C4H10OS	000505-10-2	12
5	1H-1,4-Benzodiazepine-1-propanoi...	414	C20H19BrN2O3	1000142-50-8	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088802.D
Acq On : 8 Jul 2016 2:30
Operator : UM/SJ
Sample : H3889-10 4X
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SS-10

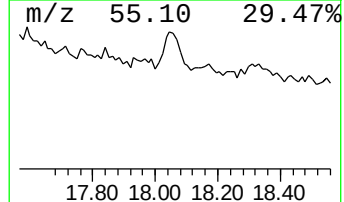
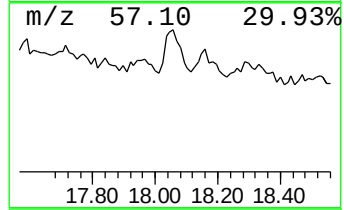
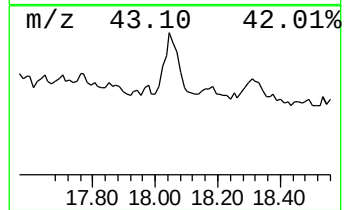
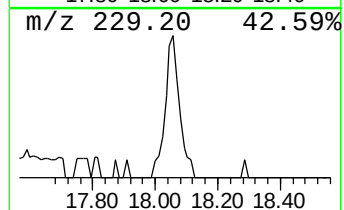
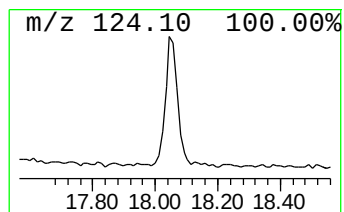
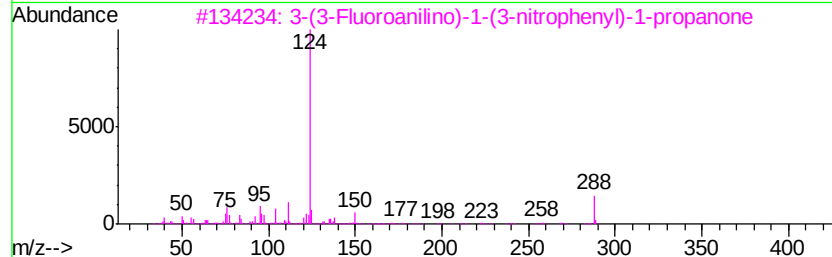
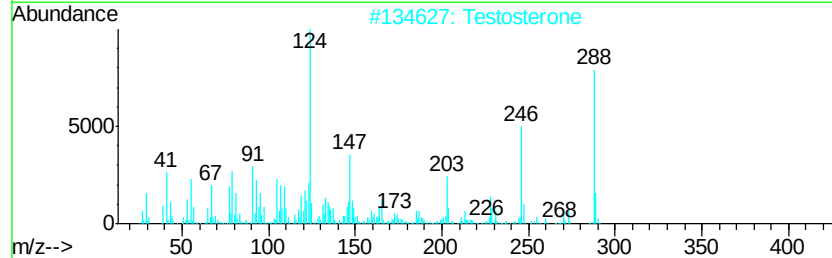
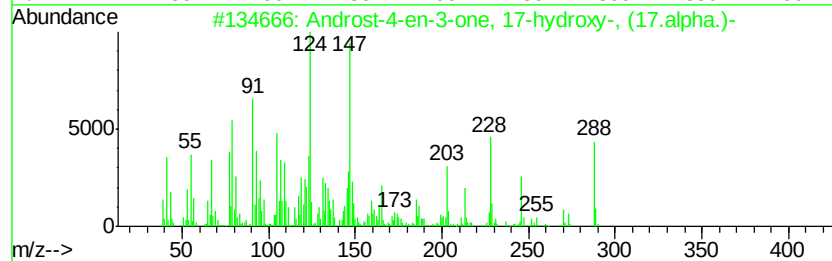
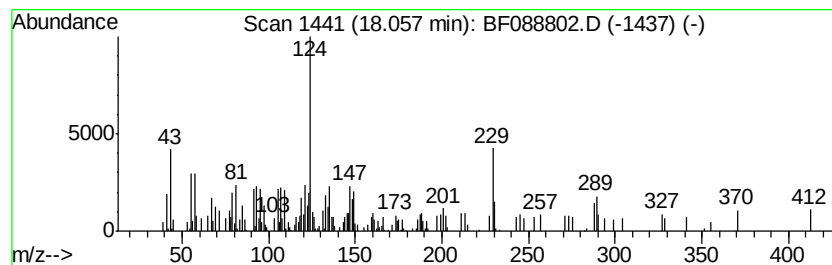
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Androst-4-en-3-one, 17-hydr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	7.88 ng	213795	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	62
2		Testosterone	288	C19H28O2	000058-22-0	50
3		3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	30
4		2,4-Diaminophenol	124	C6H8N2O	000095-86-3	25
5		2-Methyl-4,5-pyrimidinediamine	124	C5H8N4	015579-63-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088802.D
Acq On : 8 Jul 2016 2:30
Operator : UM/SJ
Sample : H3889-10 4X
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
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Phthalic anhydride	8.79	3.9	ng	110592	2	8.02	568554	20.0
unknown10.75	10.75	10.3	ng	230217	4	11.26	447343	20.0
unknown10.89	10.89	5.1	ng	113319	4	11.26	447343	20.0
unknown11.49	11.49	7.8	ng	174172	4	11.26	447343	20.0
unknown11.62	11.62	16.1	ng	360938	4	11.26	447343	20.0
unknown11.70	11.70	7.3	ng	162697	4	11.26	447343	20.0
unknown11.85	11.85	11.0	ng	245675	4	11.26	447343	20.0
unknown11.97	11.97	8.9	ng	199297	4	11.26	447343	20.0
Androst-4-en-3-on...	18.06	7.9	ng	213795	6	15.29	542799	20.0