

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
 Data File : BF085739.D
 Acq On : 25 Mar 2016 3:45
 Operator : UM/SJ
 Sample : H1884-17
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-01(13-15)

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-BF032416.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	5.007	235	238	248	rBV	765589	1130937	28.67%	2.519%
2	5.430	272	275	277	rBV	2820342	3078896	78.06%	6.859%
3	5.830	308	310	316	rVB	104307	102049	2.59%	0.227%
4	6.459	362	365	368	rBV	2100352	3178553	80.59%	7.081%
5	6.596	374	377	379	rBV	3030059	3283509	83.25%	7.315%
6	6.824	395	397	399	rBV	740009	635072	16.10%	1.415%
7	6.984	408	411	413	rBV	2095735	2532865	64.22%	5.643%
8	7.396	444	447	449	rBV	1592617	2156123	54.67%	4.803%
9	8.104	507	509	512	rBV	863583	847907	21.50%	1.889%
10	8.379	531	533	537	rVB3	140226	335067	8.50%	0.746%
11	8.630	553	555	558	rVB	266285	344798	8.74%	0.768%
12	9.190	601	604	605	rBV	3408579	3708127	94.02%	8.261%
13	9.213	605	606	609	rVB2	67431	68186	1.73%	0.152%
14	9.579	636	638	640	rBV	716838	605276	15.35%	1.348%
15	9.796	654	657	659	rBV	99674	87758	2.23%	0.196%
16	9.865	661	663	665	rVB	922748	954809	24.21%	2.127%
17	9.990	671	674	681	rVB4	165608	262161	6.65%	0.584%
18	10.208	692	693	697	rBV2	32309	42731	1.08%	0.095%
19	10.299	697	701	702	rBV	97182	136130	3.45%	0.303%
20	10.516	716	720	723	rBV	43863	74753	1.90%	0.167%
21	10.653	729	732	733	rBV	2404951	2749430	69.71%	6.125%
22	10.688	733	735	737	rVV2	259464	506096	12.83%	1.127%
23	10.768	737	742	744	rVV2	407914	1111873	28.19%	2.477%
24	10.802	744	745	749	rVB3	102733	103845	2.63%	0.231%
25	10.962	757	759	763	rVB2	16429	40370	1.02%	0.090%
26	11.213	779	781	782	rBV	72964	62880	1.59%	0.140%
27	11.339	790	792	795	rBV	986837	1017461	25.80%	2.267%
28	11.568	809	812	813	rBV3	27770	50230	1.27%	0.112%
29	11.602	813	815	817	rBV3	46001	79186	2.01%	0.176%
30	11.739	823	827	829	rBV4	315980	966443	24.50%	2.153%
31	11.876	837	839	843	rVB3	78138	185750	4.71%	0.414%
32	12.059	853	855	856	rVV	64009	68811	1.74%	0.153%
33	12.082	856	857	859	rVB	59568	62069	1.57%	0.138%
34	12.928	928	931	934	rBV	3072884	2998168	76.02%	6.679%

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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 >
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35	12.996	934	937	939	rVB2	76295	88577	2.25%	0.197%
36	13.202	954	955	957	rVB	46761	42007	1.07%	0.094%
37	13.499	978	981	982	rVB2	190936	256460	6.50%	0.571%
38	13.579	986	988	990	rVB3	203883	188238	4.77%	0.419%
39	13.819	1007	1009	1018	rBV	47005	79402	2.01%	0.177%
40	13.979	1020	1023	1025	rBV	639046	740373	18.77%	1.649%
41	14.848	1094	1099	1101	rBV4	239586	636737	16.14%	1.418%
42	14.882	1101	1102	1103	rVB	147470	101216	2.57%	0.225%
43	15.397	1144	1147	1153	rVB	369098	512123	12.98%	1.141%
44	16.368	1229	1232	1234	rBV3	185274	336281	8.53%	0.749%
45	16.825	1268	1272	1274	rBV4	52133	68337	1.73%	0.152%
46	17.465	1326	1328	1329	rBV	356785	349526	8.86%	0.779%
47	17.534	1329	1334	1341	rVV8	1285125	3944030	100.00%	8.786%
48	17.625	1341	1342	1345	rVV	556123	748693	18.98%	1.668%
49	17.728	1348	1351	1353	rVB4	45636	47555	1.21%	0.106%
50	17.785	1353	1356	1358	rBV	32755	60376	1.53%	0.135%
51	17.854	1361	1362	1364	rVB	146426	104896	2.66%	0.234%
52	19.020	1460	1464	1465	rBV3	26784	49325	1.25%	0.110%
53	19.180	1477	1478	1480	rVB2	83249	63428	1.61%	0.141%
54	19.351	1491	1493	1494	rVV2	105702	88335	2.24%	0.197%
55	19.408	1494	1498	1500	rVV4	1028834	2581692	65.46%	5.751%
56	19.443	1500	1501	1504	rVB3	176006	183832	4.66%	0.410%
57	19.534	1508	1509	1510	rBV	35810	48397	1.23%	0.108%

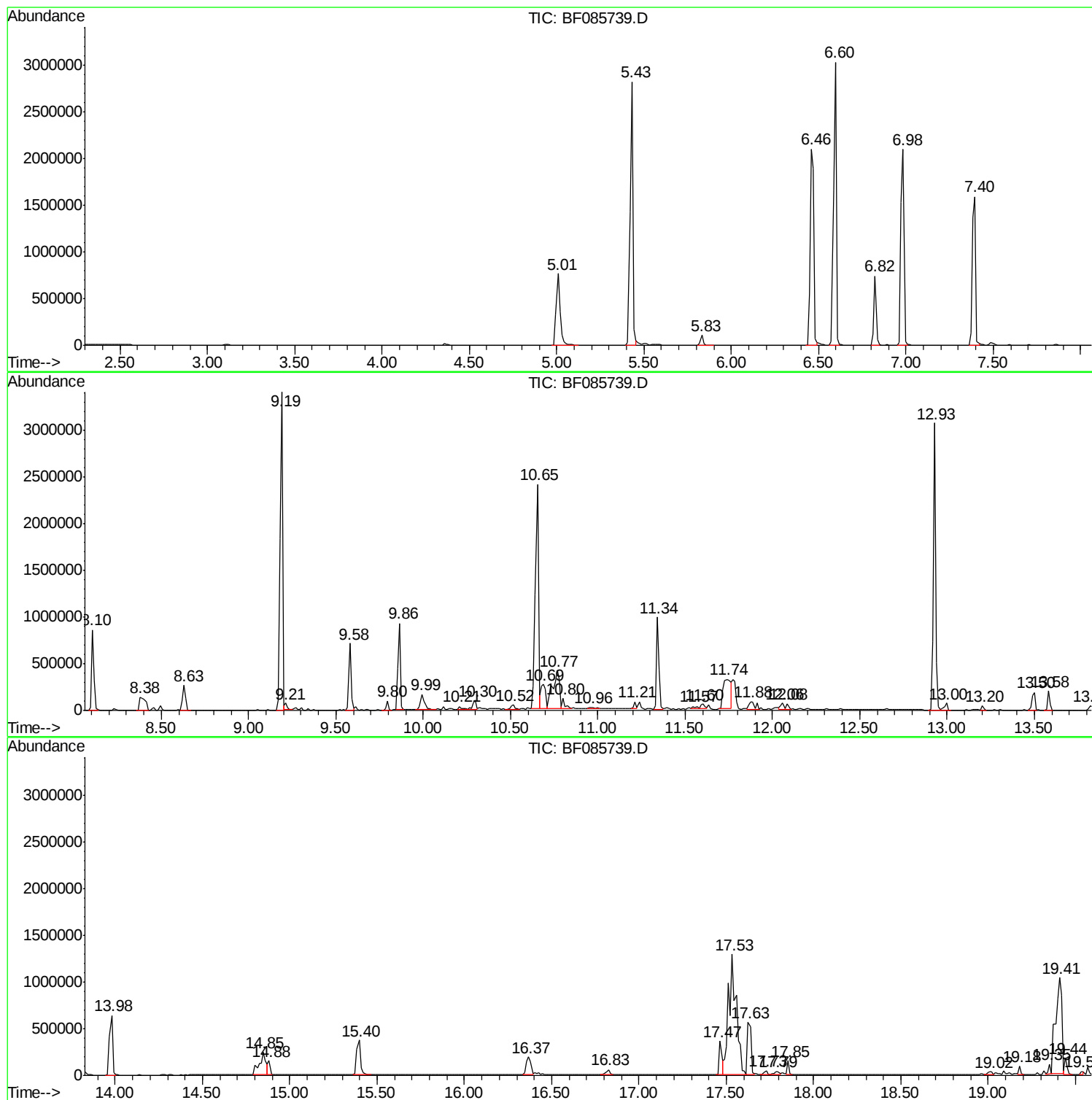
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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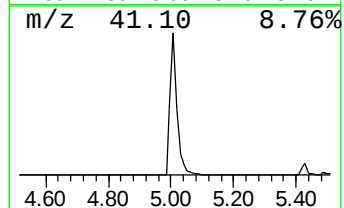
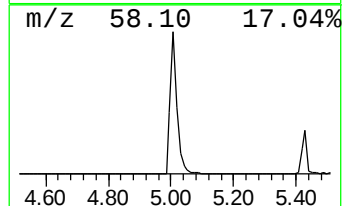
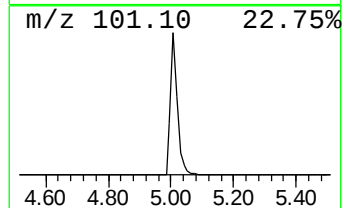
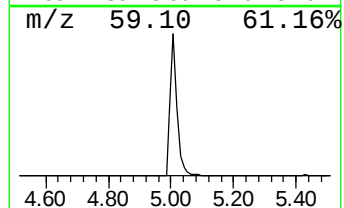
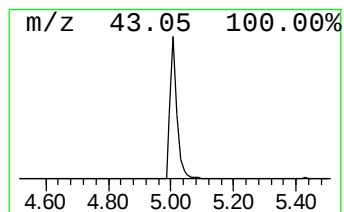
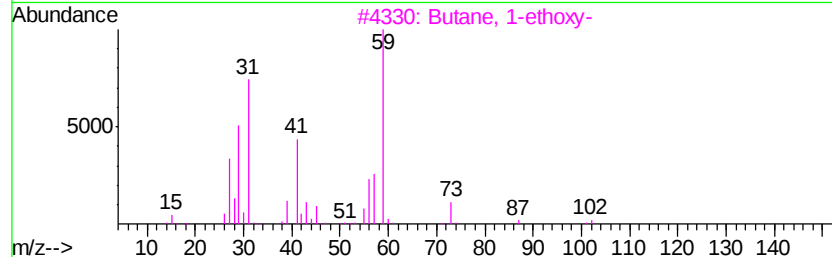
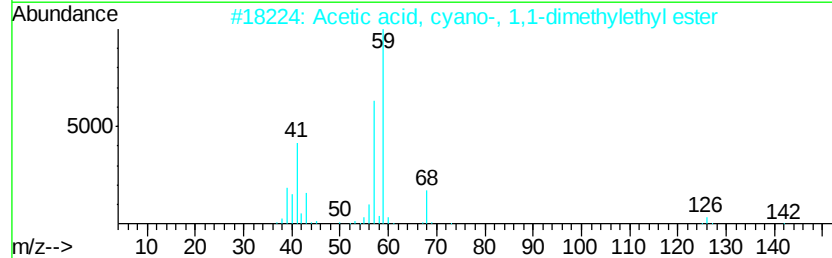
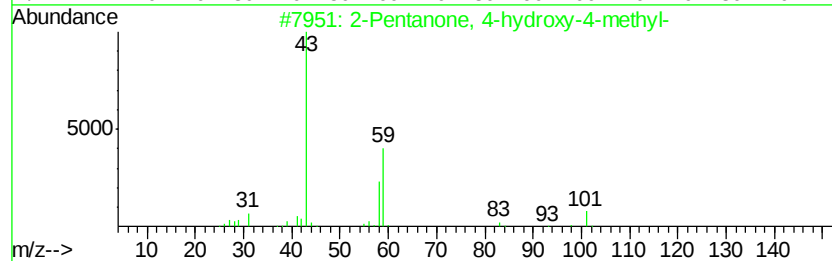
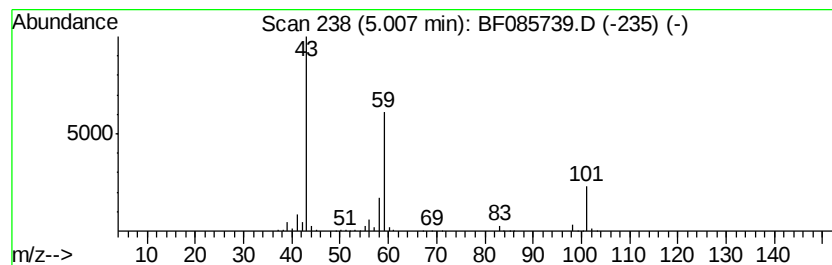
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	35.62 ng	1130940	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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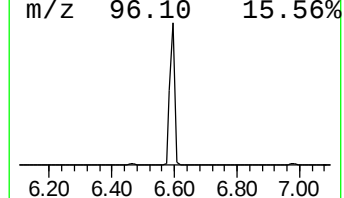
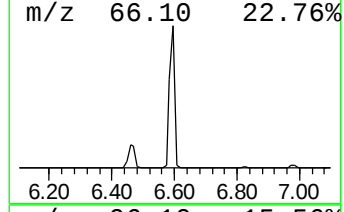
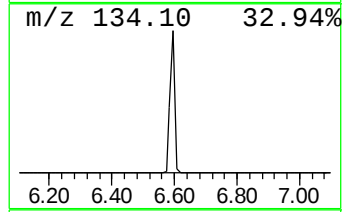
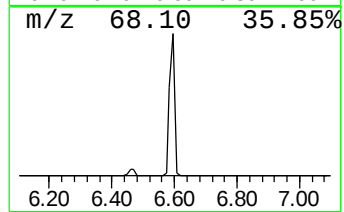
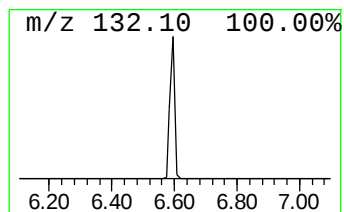
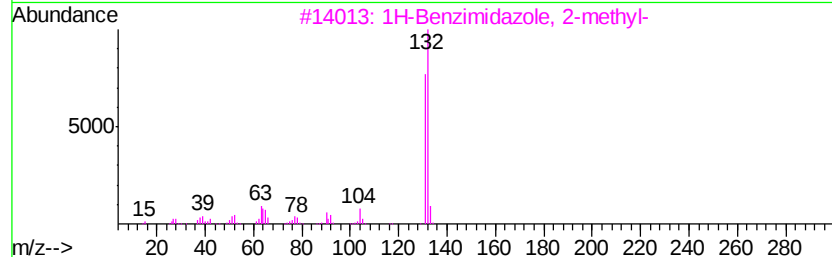
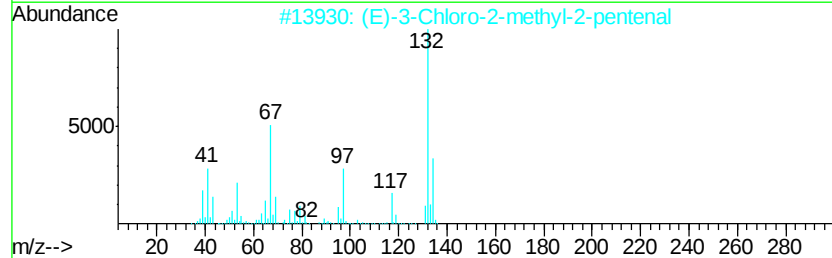
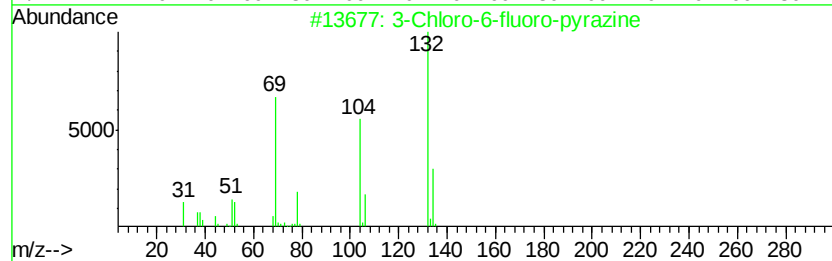
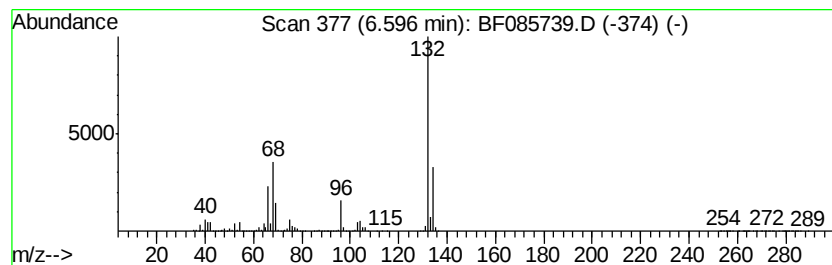
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	103.41 ng	3283510	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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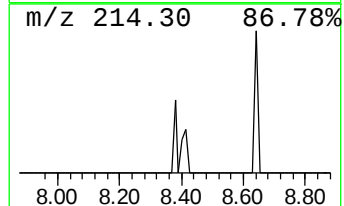
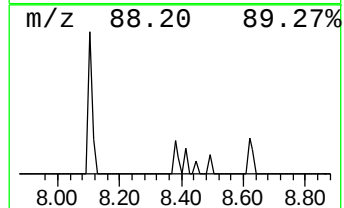
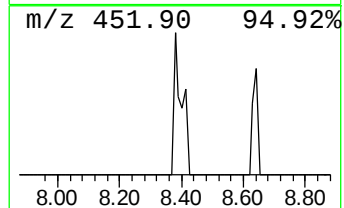
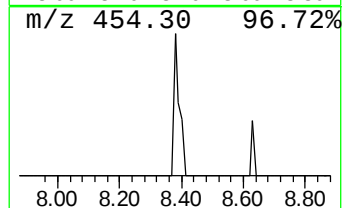
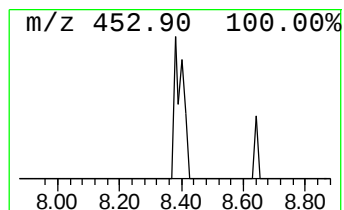
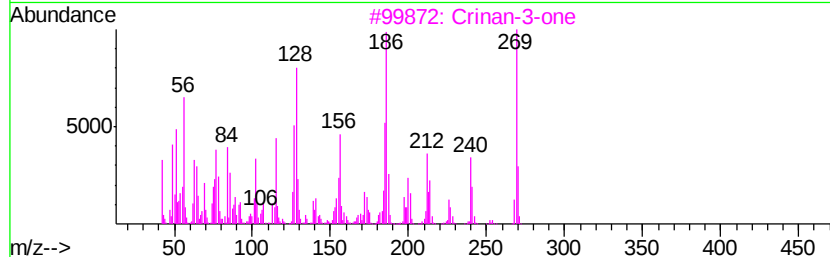
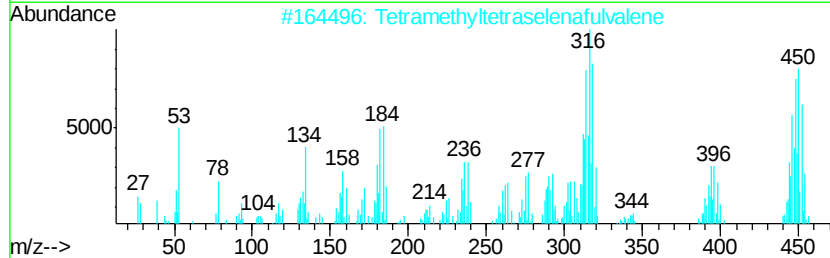
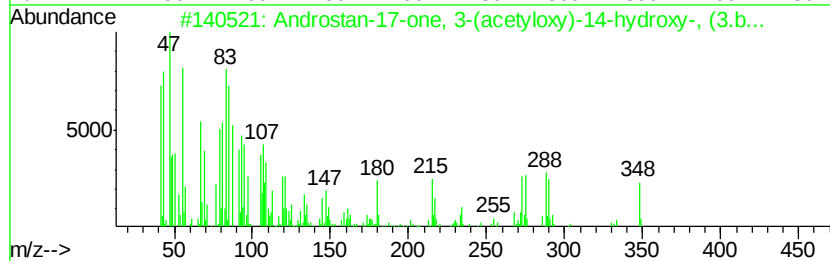
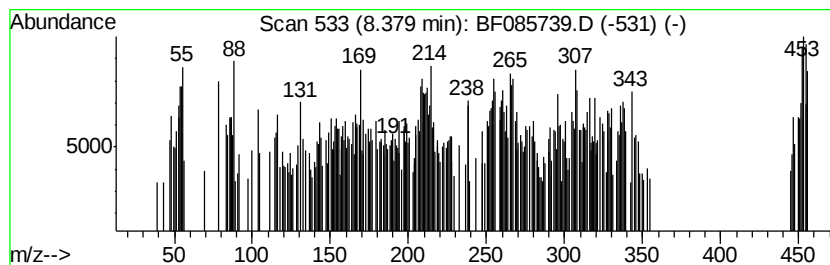
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Androstan-17-one, 3-(acetyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.38	7.90 ng	335067	Napthalene-d8	8.10		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Androstan-17-one, 3-(acetyloxy)-...	348	C21H32O4	001241-30-1	53
2		Tetramethyltetraselenafulvalene	452	C10H12Se4	055259-49-9	44
3		Crinan-3-one	269	C16H15NO3	031106-06-6	11
4		2,20-Cycloaspidospermidine, 6,7-...	306	C21H26N2	056053-37-3	11
5		1,4-Di[7-chloro-4-quinolylamino]...	438	C22H20Cl2N6	023512-27-8	11



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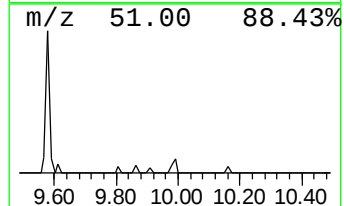
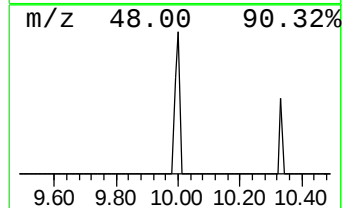
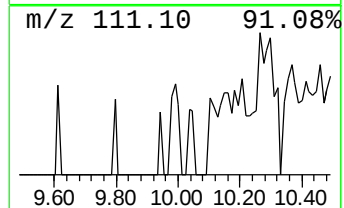
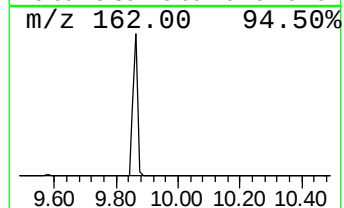
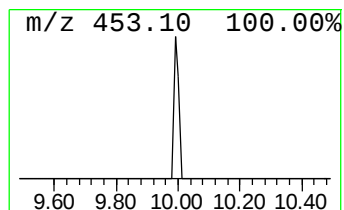
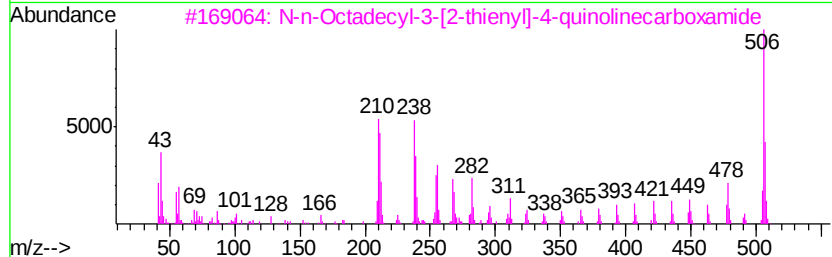
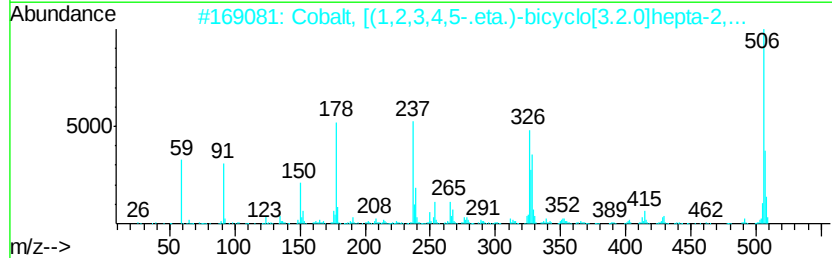
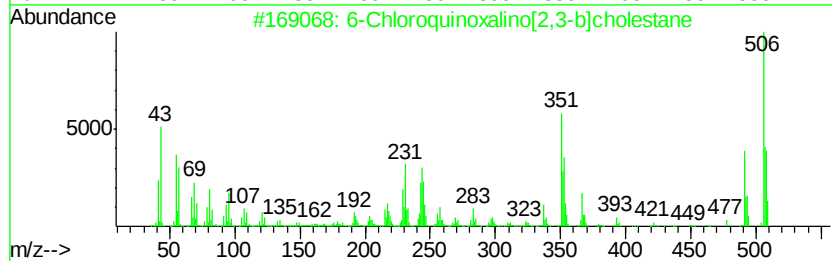
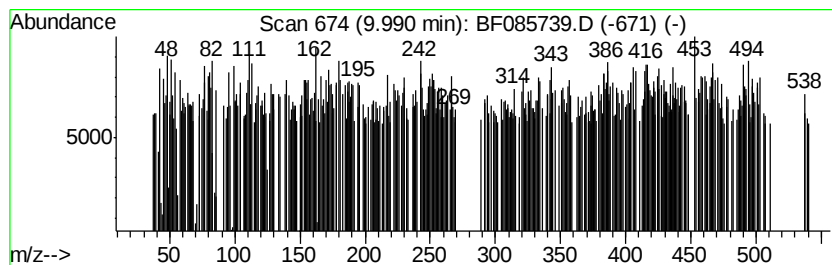
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown9.99 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.99	5.49 ng	262161	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Chloroquinoxalino[2,3-b]choles...	506	C33H47ClN2	1000210-42-0	25
2		Cobalt, [(1,2,3,4,5-.eta.)-bicyc...	506	C35H27Co	128632-33-7	25
3		N-n-Octadecyl-3-[2-thienyl]-4-qu...	506	C32H46N2OS	1000257-06-6	11
4		Bis[4-[4-hydroxy]piperidino-3-ni...	506	C22H26N4O8S	024612-36-0	11
5		trans-4'-Methoxy-4-(octadecyloxy...	506	C34H50O3	122207-15-2	10



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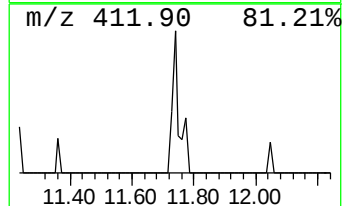
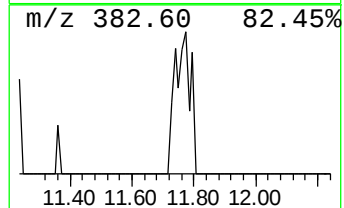
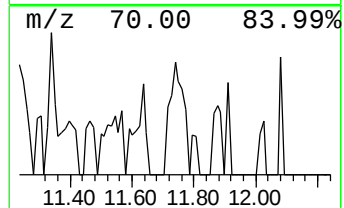
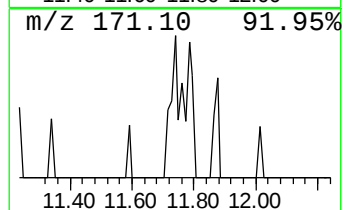
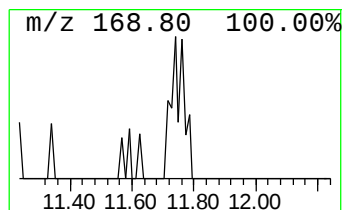
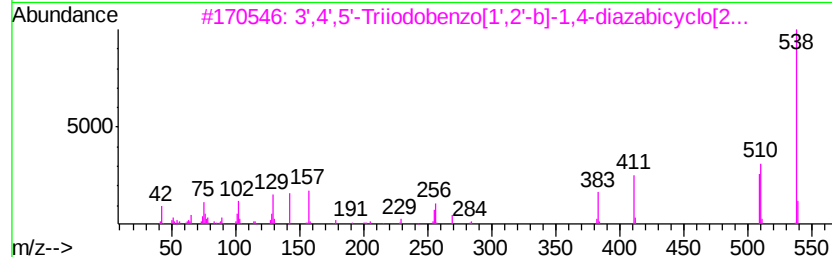
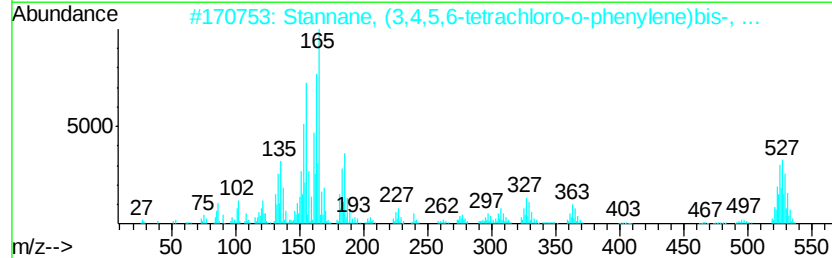
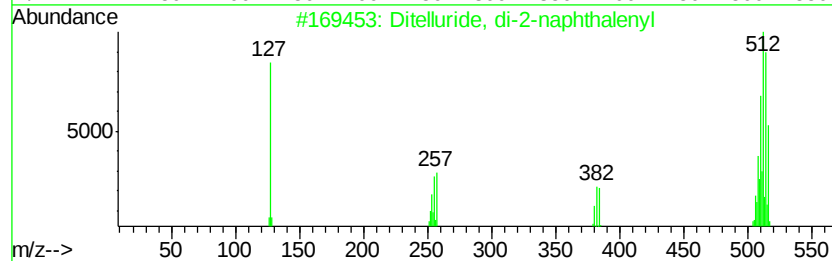
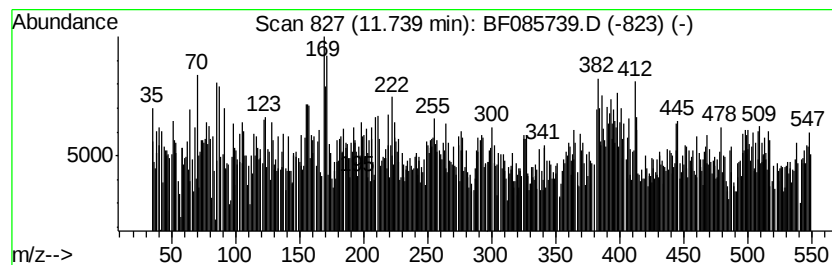
Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.74 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.74	19.00 ng	966443	Phenanthrene-d10		11.34	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ditelluride, di-2-naphthalenyl	514	C20H14Te2	001666-12-2	35
2		Stannane, (3,4,5,6-tetrachloro-o...	542	C12H18Cl4Sn2	015725-05-0	10
3		3',4',5'-Triiodobenzo[1',2'-b]-1...	538	C10H9I3N2	108959-03-1	9
4		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	524	C27H28N2O9	056335-86-5	9
5		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	524	C27H28N2O9	026537-43-9	7



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085739.D
Acq On : 25 Mar 2016 3:45
Operator : UM/SJ
Sample : H1884-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

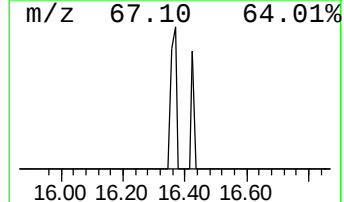
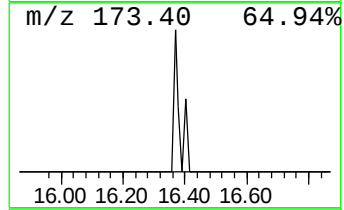
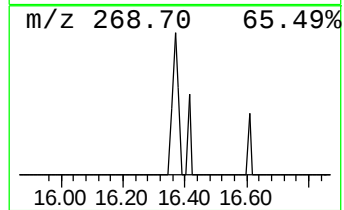
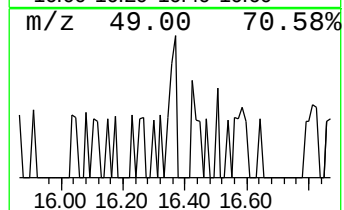
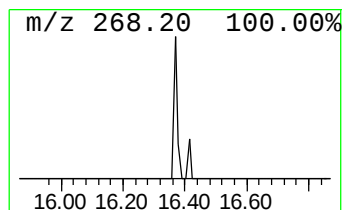
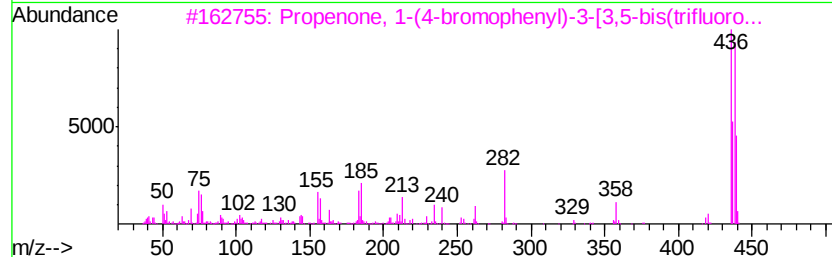
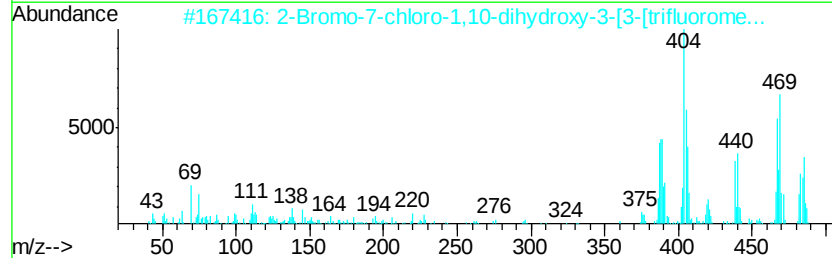
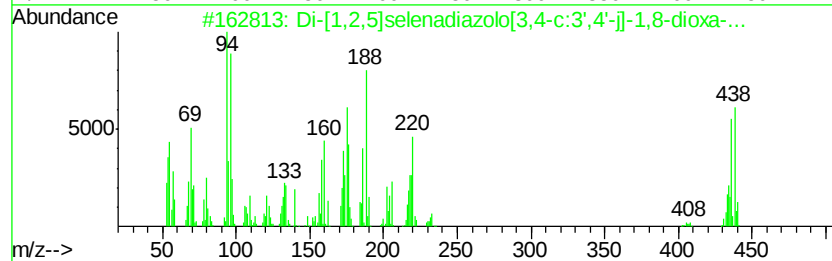
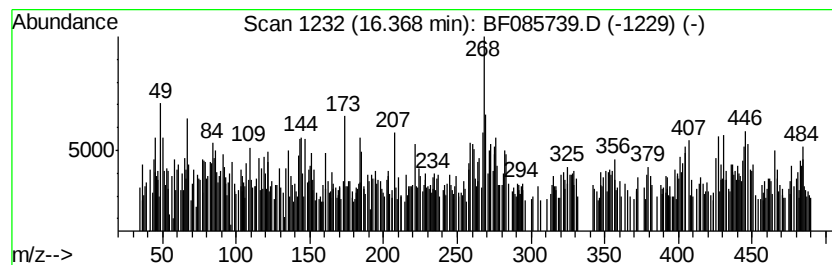
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.37 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	13.13 ng	336281	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Di-[1,2,5]selenadiazolo[3,4-c:3'...	438	C10H10N6O4Se2	185116-18-1	46
2		2-Bromo-7-chloro-1,10-dihydroxy-...	483	C20H10BrClF3N03	1000213-18-8	14
3		Propenone, 1-(4-bromophenyl)-3-[...	437	C17H10BrF6N0	277326-01-9	11
4		2,2',4',5,5',6-Hexachloro-3-meth...	436	C13H6Cl6O2S	149949-88-2	10
5		Benzo[1,2-c:4,5-c']dipyrrole-1,3...	436	C22H10Cl2N2O4	006626-73-9	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085739.D
Acq On : 25 Mar 2016 3:45
Operator : UM/SJ
Sample : H1884-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

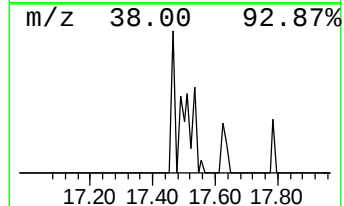
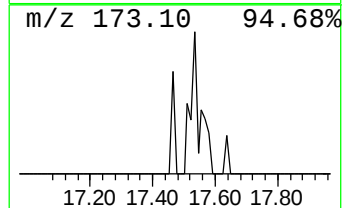
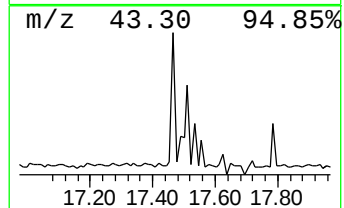
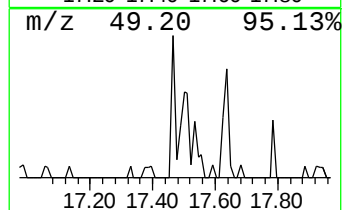
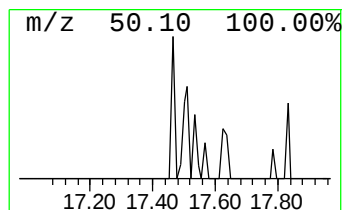
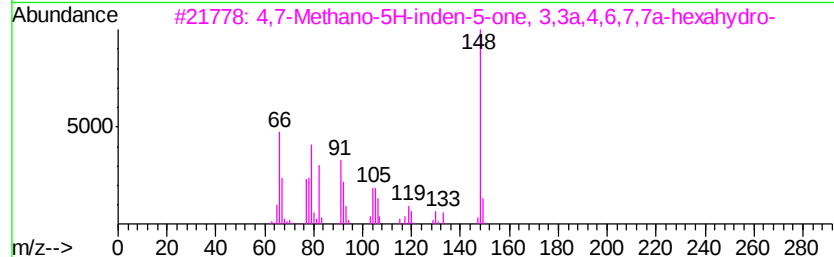
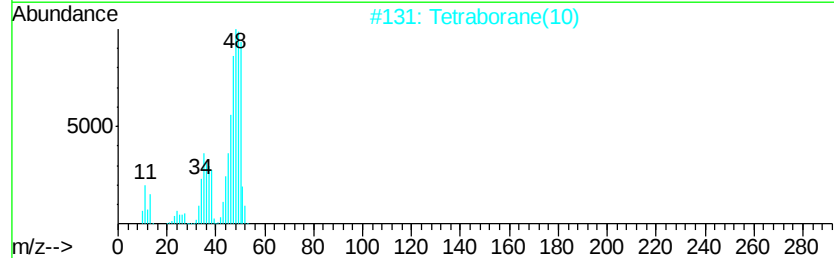
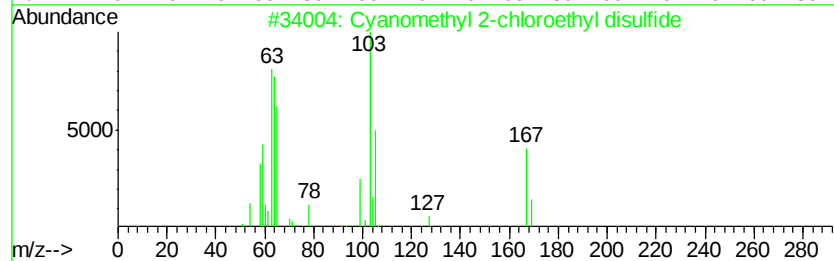
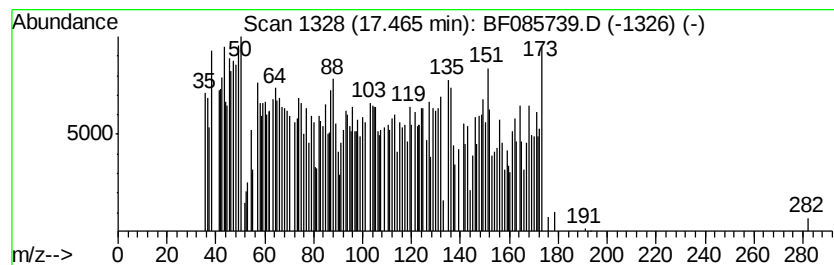
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.47 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	13.65 ng	349526	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyanomethyl 2-chloroethyl disulfide	167	C4H6ClNS2	1000226-70-1	35
2		Tetraborane(10)	54	B4H10	018283-93-7	35
3		4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	25
4		2,4-Dicyanopyrrole	117	C6H3N3	074023-87-3	25
5		1H-Pyrrole-2,5-dicarbonitrile	117	C6H3N3	059215-66-6	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085739.D
Acq On : 25 Mar 2016 3:45
Operator : UM/SJ
Sample : H1884-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

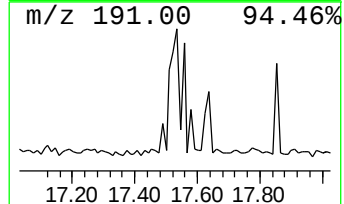
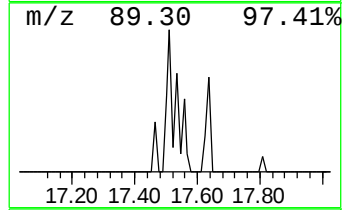
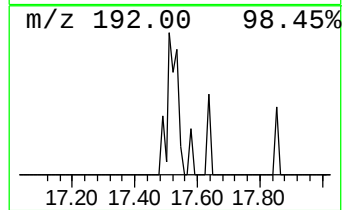
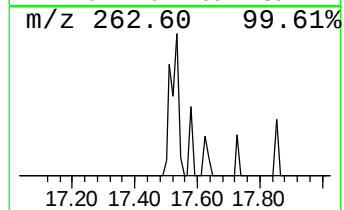
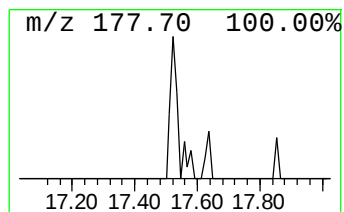
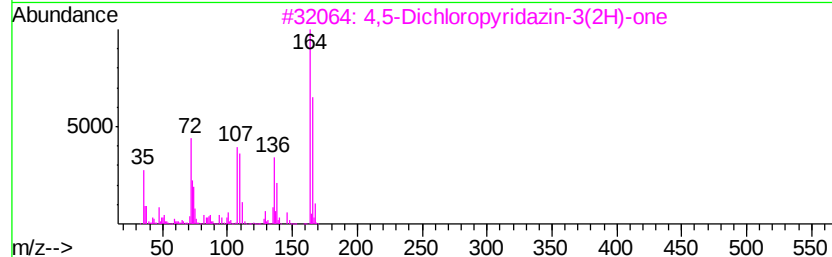
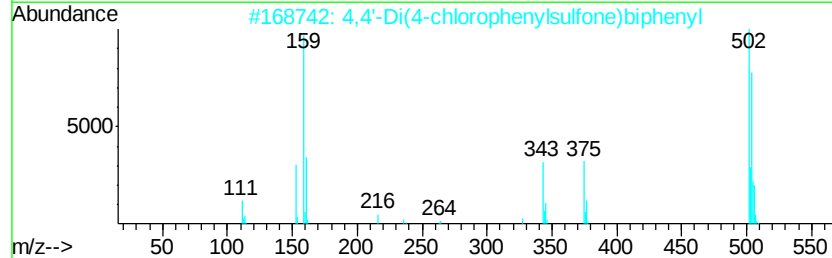
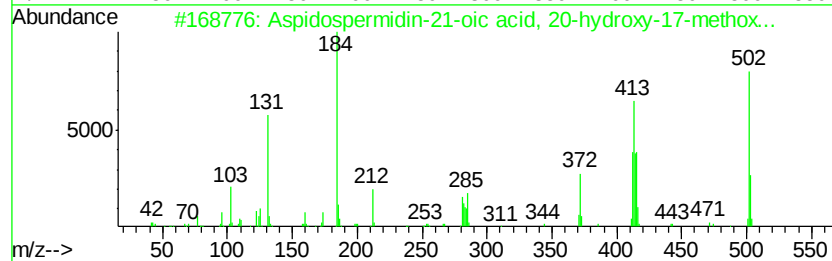
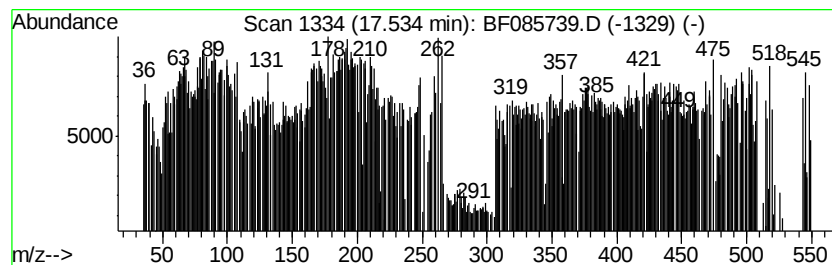
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.53	154.03 ng	3944030	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Aspidospermidin-21-oic acid, 20-...	502	C30H34N2O5	056143-43-2	25
2		4,4'-Di(4-chlorophenylsulfone)bi...	502	C24H16Cl2O4S2	022287-56-5	15
3		4,5-Dichloropyridazin-3(2H)-one	164	C4H2Cl2N2O	000932-22-9	15
4		1H-Benzotriazole, 4,5,6,7-tetrac...	255	C6HCl4N3	002338-10-5	15
5		Guanosine, 2'-O-methyl-	297	C11H15N5O5	002140-71-8	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085739.D
Acq On : 25 Mar 2016 3:45
Operator : UM/SJ
Sample : H1884-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

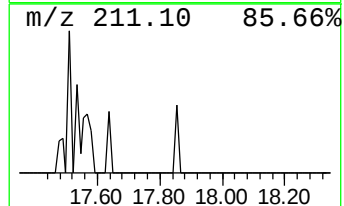
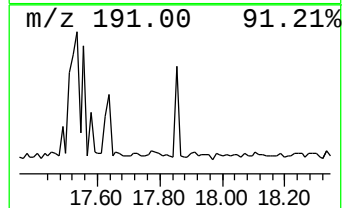
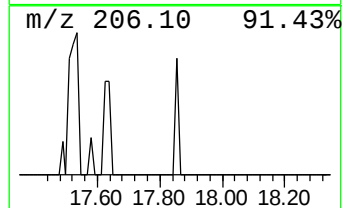
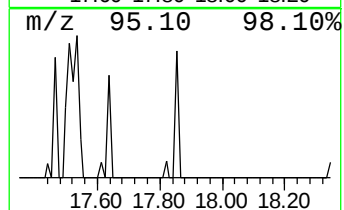
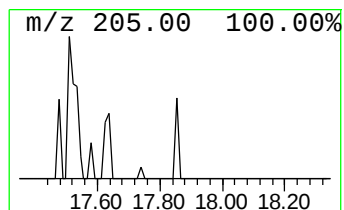
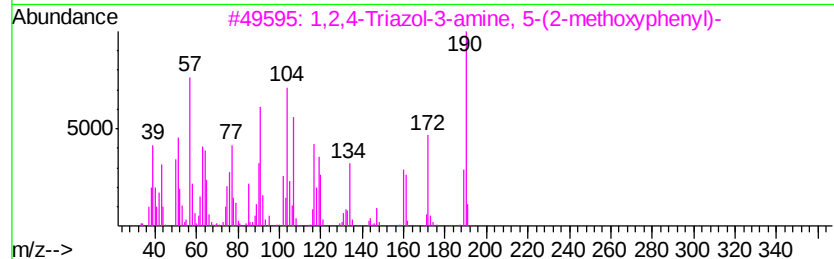
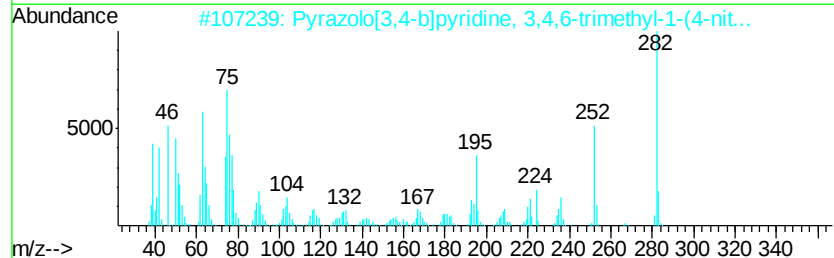
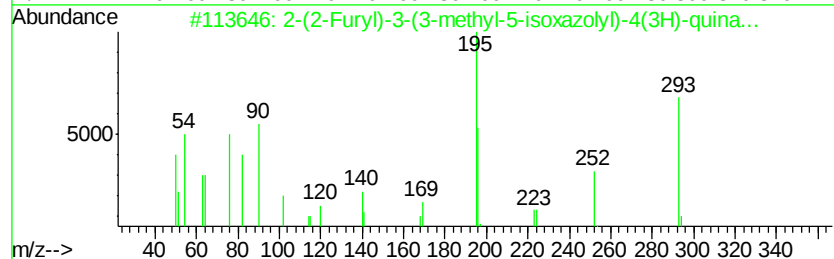
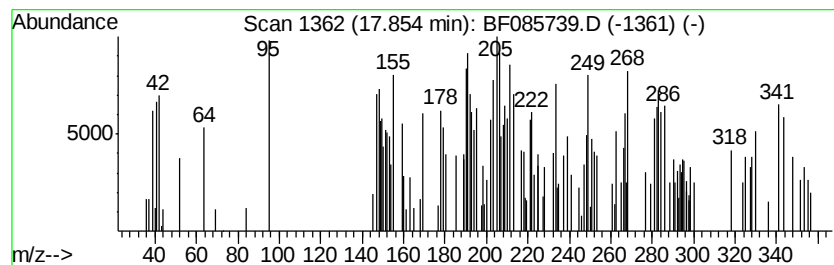
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.85 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	4.10 ng	104896	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2-Furyl)-3-(3-methyl-5-isoxaz...	293	C16H11N3O3	090059-44-2	25
2			Pyrazolo[3,4-b]pyridine, 3,4,6-t...	282	C15H14N4O2	116835-04-2	25
3			1,2,4-Triazol-3-amine, 5-(2-meth...	190	C9H10N4O	303192-36-1	15
4			1,2,3,4-Tetrahydroisoquinolin-1-...	249	C13H15N04	021148-88-9	15
5			Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085739.D
Acq On : 25 Mar 2016 3:45
Operator : UM/SJ
Sample : H1884-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-01(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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...	5.01	35.6	ng	1130940	1	6.82	635072	20.0
unknown6.60	6.60	103.4	ng	3283510	1	6.82	635072	20.0
Androstan-17-one, ...	8.38	7.9	ng	335067	2	8.10	847907	20.0
unknown9.99	9.99	5.5	ng	262161	3	9.86	954809	20.0
unknown11.74	11.74	19.0	ng	966443	4	11.34	1017460	20.0
unknown16.37	16.37	13.1	ng	336281	6	15.40	512123	20.0
unknown17.47	17.47	13.7	ng	349526	6	15.40	512123	20.0
unknown17.53	17.53	154.0	ng	3944030	6	15.40	512123	20.0
unknown17.85	17.85	4.1	ng	104896	6	15.40	512123	20.0