

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040616\
 Data File : BF086106.D
 Acq On : 6 Apr 2016 19:06
 Operator : UM/SJ
 Sample : H2254-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-16

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-BF040216.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	2.258	13	15	16	rVB2	79566	86988	2.88%	0.177%
2	4.910	245	247	258	rBV	168286	302923	10.04%	0.615%
3	5.344	282	285	287	rBV	2441329	2955024	97.92%	6.003%
4	6.396	374	377	379	rBV	2477049	3017698	100.00%	6.130%
5	6.510	385	387	390	rBV	2635895	2648831	87.78%	5.381%
6	6.739	405	407	410	rBV	983829	944798	31.31%	1.919%
7	6.899	419	421	423	rBV	2537544	2292287	75.96%	4.656%
8	7.310	454	457	460	rBV	1593908	1805634	59.83%	3.668%
9	7.424	464	467	471	rVB	38914	66315	2.20%	0.135%
10	8.030	517	520	522	rBV	1327545	1232021	40.83%	2.503%
11	8.442	553	556	557	rBV	182539	169404	5.61%	0.344%
12	8.739	578	582	584	rVB3	218245	429731	14.24%	0.873%
13	8.819	587	589	590	rBV2	52573	77502	2.57%	0.157%
14	8.853	590	592	593	rBV	192035	279650	9.27%	0.568%
15	8.910	595	597	602	rVB6	172705	570724	18.91%	1.159%
16	9.036	602	608	611	rVB7	285667	931593	30.87%	1.892%
17	9.105	611	614	617	rBV	2989701	2698873	89.43%	5.482%
18	9.185	619	621	623	rBV3	182485	347423	11.51%	0.706%
19	9.230	623	625	627	rVV3	66449	112205	3.72%	0.228%
20	9.322	632	633	636	rBV2	203651	409648	13.57%	0.832%
21	9.505	645	649	651	rVB	726442	923086	30.59%	1.875%
22	9.596	655	657	663	rVB2	336451	933419	30.93%	1.896%
23	9.722	663	668	670	rBV2	42651	72604	2.41%	0.147%
24	9.779	670	673	675	rBV	1426604	1341273	44.45%	2.725%
25	9.813	675	676	679	rVB2	149806	126450	4.19%	0.257%
26	9.882	679	682	685	rBV5	63924	121502	4.03%	0.247%
27	10.053	691	697	702	rVB8	289329	1329718	44.06%	2.701%
28	10.122	702	703	704	rBV	142072	116861	3.87%	0.237%
29	10.168	704	707	710	rVV4	256147	491443	16.29%	0.998%
30	10.213	710	711	712	rVB	93608	64215	2.13%	0.130%
31	10.259	712	715	716	rBV2	158606	144885	4.80%	0.294%
32	10.350	719	723	727	rVB4	209236	614615	20.37%	1.248%
33	10.430	727	730	733	rBV4	146623	401227	13.30%	0.815%
34	10.522	733	738	740	rVV5	177378	393526	13.04%	0.799%

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35	10.568	740	742	745 rVV	1680559	2022914	67.04%	4.109%
36	10.613	745	746	749 rVV3	274363	541727	17.95%	1.100%
37	10.659	749	750	755 rVV2	206586	445534	14.76%	0.905%
38	10.739	755	757	759 rVV3	161833	347310	11.51%	0.706%
39	10.796	759	762	765 rVB4	329136	658226	21.81%	1.337%
40	11.082	782	787	790 rVB3	230697	601145	19.92%	1.221%
41	11.265	801	803	804 rBV	1135945	1156547	38.33%	2.349%
42	11.356	807	811	814 rVB	55210	108702	3.60%	0.221%
43	11.482	816	822	823 rBV4	141842	305817	10.13%	0.621%
44	11.516	823	825	827 rVB2	234302	258839	8.58%	0.526%
45	11.551	827	828	829 rBV	344216	267606	8.87%	0.544%
46	11.585	829	831	833 rVB3	299326	294123	9.75%	0.597%
47	11.676	833	839	841 rBV6	226956	652287	21.62%	1.325%
48	11.722	841	843	845 rVB3	47233	90361	2.99%	0.184%
49	11.768	845	847	848 rBV	66451	71861	2.38%	0.146%
50	11.791	848	849	851 rBV	185141	229386	7.60%	0.466%
51	11.871	855	856	857 rBV	98932	83785	2.78%	0.170%
52	11.893	857	858	861 rVB	81574	94304	3.13%	0.192%
53	11.973	863	865	869 rVB4	145898	235256	7.80%	0.478%
54	12.053	869	872	874 rBV	45010	88838	2.94%	0.180%
55	12.088	874	875	877 rBV	156462	231187	7.66%	0.470%
56	12.122	877	878	879 rVV	170323	144784	4.80%	0.294%
57	12.145	879	880	882 rVB2	176661	238174	7.89%	0.484%
58	12.191	882	884	887 rVB4	97283	210904	6.99%	0.428%
59	12.259	887	890	891 rBV2	93402	151183	5.01%	0.307%
60	12.316	891	895	896 rVB2	113190	200909	6.66%	0.408%
61	12.351	896	898	899 rBV	143525	163474	5.42%	0.332%
62	12.408	899	903	904 rVB	88599	125836	4.17%	0.256%
63	12.476	904	909	911 rBV	321389	518455	17.18%	1.053%
64	12.579	916	918	920 rBV2	139106	211138	7.00%	0.429%
65	12.694	926	928	931 rBV	362203	515482	17.08%	1.047%
66	12.762	931	934	935 rVB3	43007	76832	2.55%	0.156%
67	12.842	939	941	944 rBV	1896051	2012475	66.69%	4.088%
68	12.922	944	948	951 rVB2	37619	79060	2.62%	0.161%
69	13.025	953	957	960 rVB2	72574	174226	5.77%	0.354%
70	13.128	965	966	968 rBV	54328	79297	2.63%	0.161%
71	13.219	972	974	976 rBV	52161	85076	2.82%	0.173%

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72	13.414	987	991	994	rBV4	94576	174067	5.77%	0.354%
73	13.471	994	996	1000	rBV5	31134	65839	2.18%	0.134%
74	13.539	1000	1002	1006	rVB	69185	91355	3.03%	0.186%
75	13.654	1009	1012	1013	rBV	51501	95665	3.17%	0.194%
76	13.699	1014	1016	1018	rVV	130087	156579	5.19%	0.318%
77	13.756	1018	1021	1025	rVB2	171697	345983	11.47%	0.703%
78	13.894	1030	1033	1038	rBV2	940819	1399138	46.36%	2.842%
79	14.282	1065	1067	1069	rBV	51879	86455	2.86%	0.176%
80	14.454	1079	1082	1084	rVB3	116606	253959	8.42%	0.516%
81	14.911	1119	1122	1125	rBV	190618	341383	11.31%	0.693%
82	15.185	1144	1146	1148	rBV	176046	201461	6.68%	0.409%
83	15.242	1148	1151	1154	rVV	179271	290030	9.61%	0.589%
84	15.299	1154	1156	1163	rVB	780774	1056011	34.99%	2.145%
85	15.540	1174	1177	1179	rBV4	210712	380045	12.59%	0.772%
86	15.585	1179	1181	1184	rVB3	206111	348127	11.54%	0.707%
87	16.157	1228	1231	1232	rBV3	45945	70852	2.35%	0.144%
88	16.648	1271	1274	1283	rVB2	75408	200273	6.64%	0.407%
89	16.945	1298	1300	1303	rVB3	121332	168725	5.59%	0.343%
90	17.060	1306	1310	1315	rVB	84601	218573	7.24%	0.444%
91	17.311	1330	1332	1335	rVB4	65466	113715	3.77%	0.231%
92	17.631	1357	1360	1361	rBV3	36448	69023	2.29%	0.140%
93	17.700	1364	1366	1368	rVV3	59477	103947	3.44%	0.211%
94	17.745	1368	1370	1372	rVV2	76846	110278	3.65%	0.224%
95	18.180	1406	1408	1412	rVB4	95836	200754	6.65%	0.408%
96	18.271	1415	1416	1420	rBV3	55735	143817	4.77%	0.292%
97	18.443	1428	1431	1433	rBV4	50190	85781	2.84%	0.174%
98	18.660	1448	1450	1452	rVB2	60853	67898	2.25%	0.138%
99	18.774	1458	1460	1462	rVV3	58591	82869	2.75%	0.168%
100	19.517	1522	1525	1527	rBV4	33672	79053	2.62%	0.161%

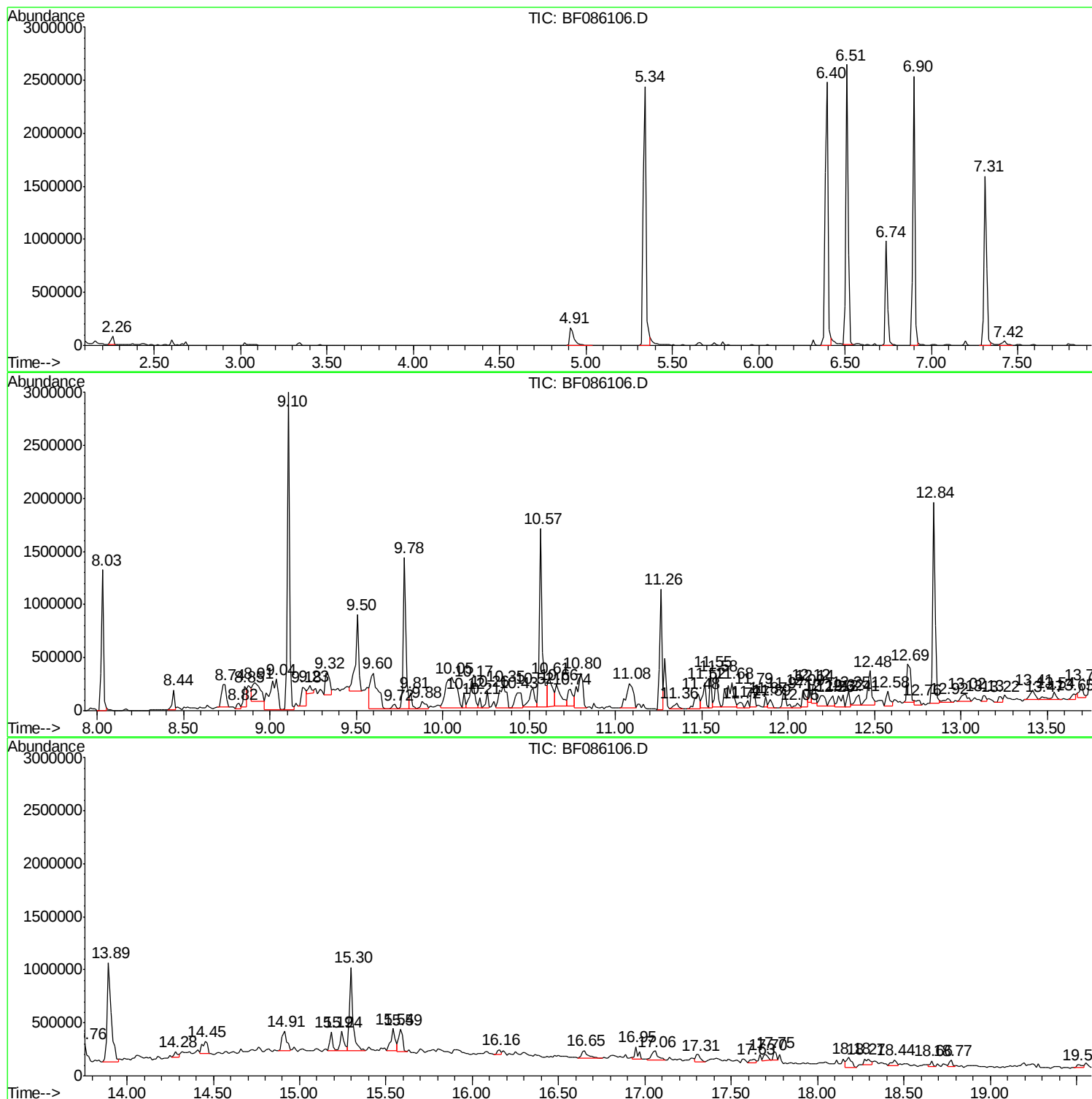
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
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TIC Library : C:\DATABASE\NIST02.L
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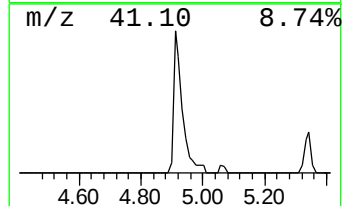
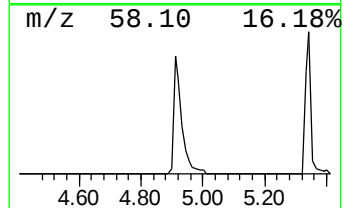
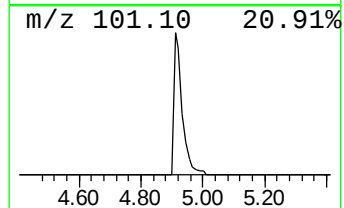
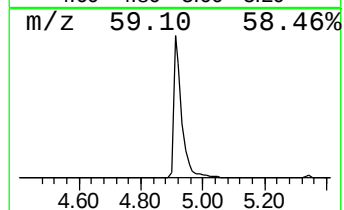
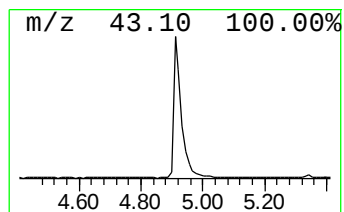
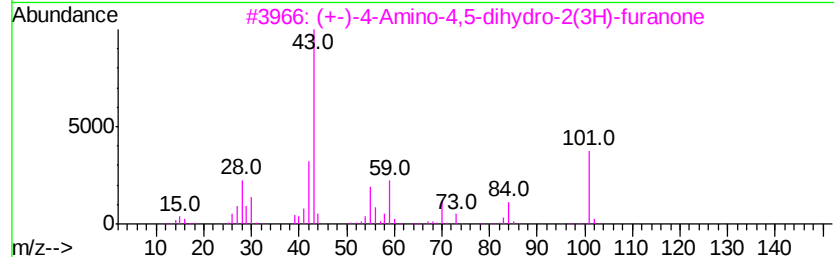
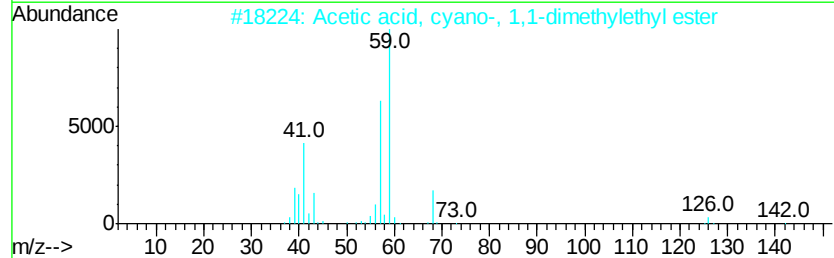
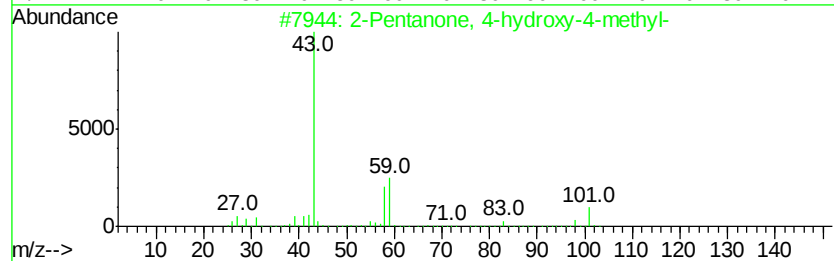
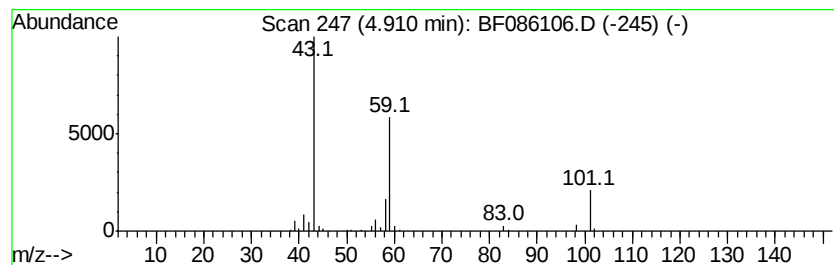
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	6.41 ng	302923	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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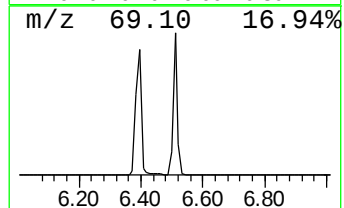
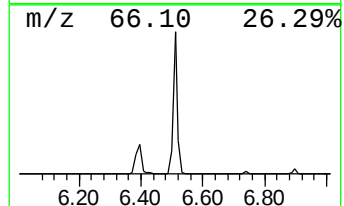
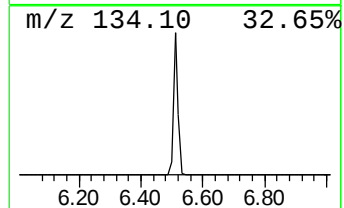
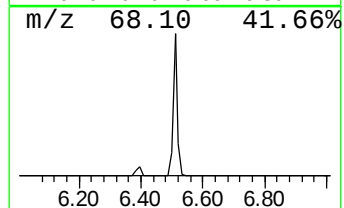
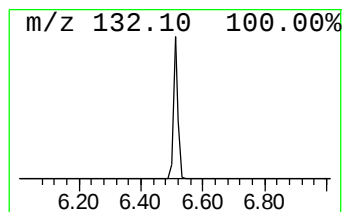
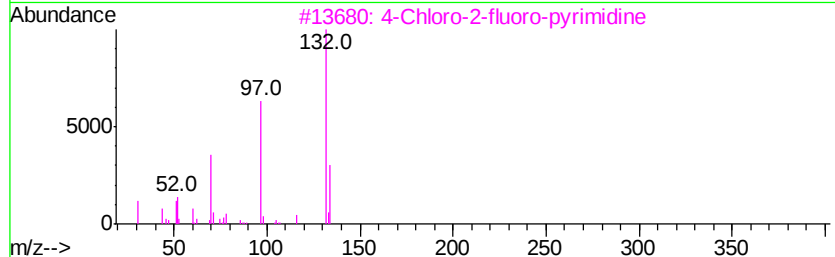
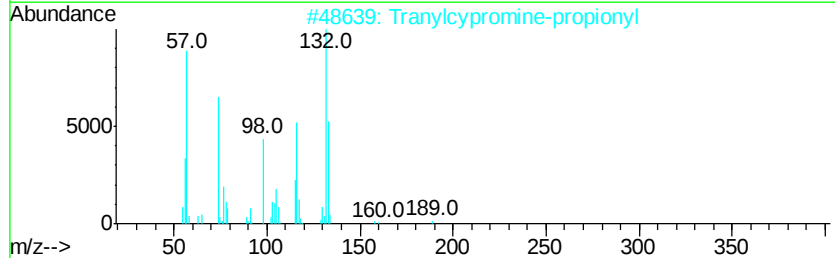
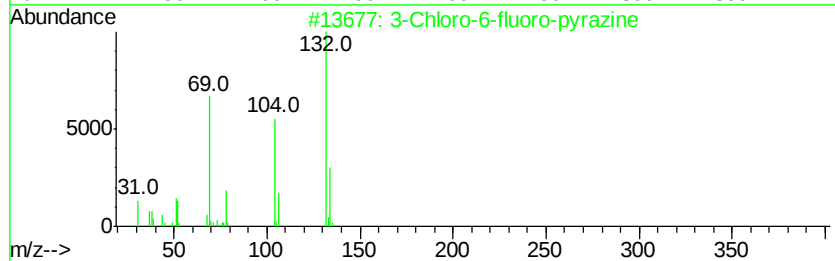
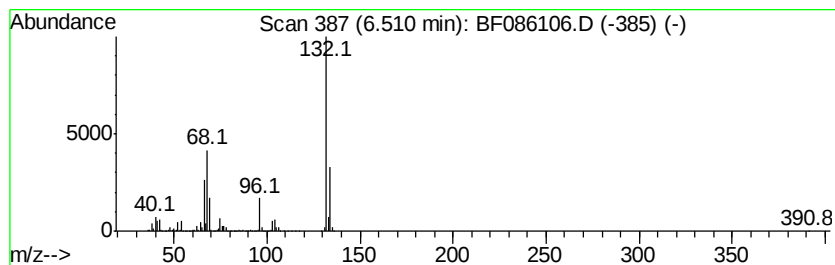
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	56.07 ng	2648830	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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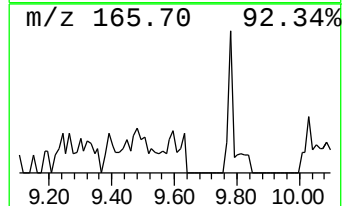
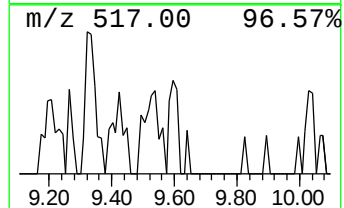
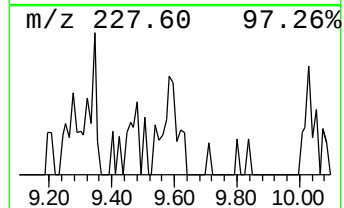
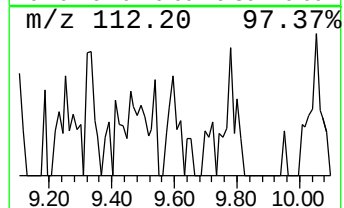
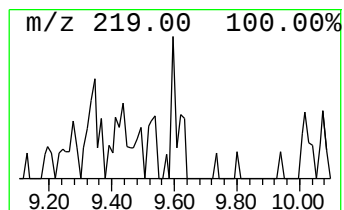
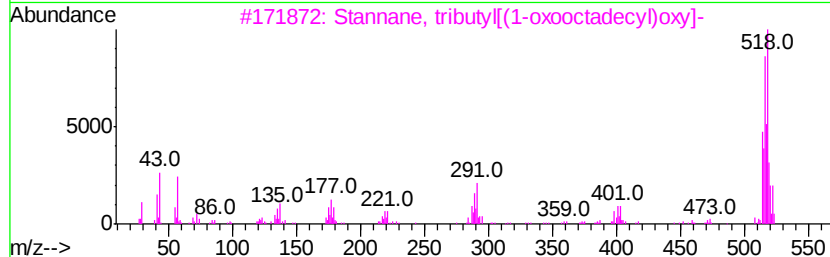
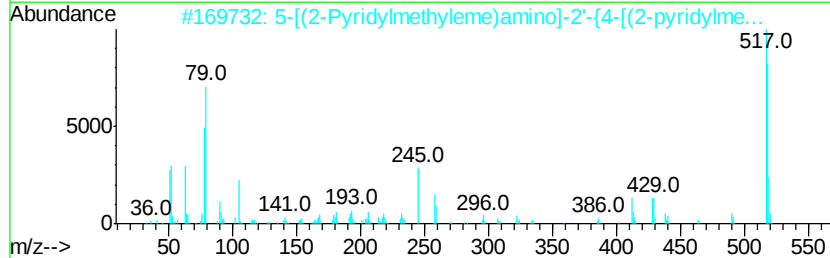
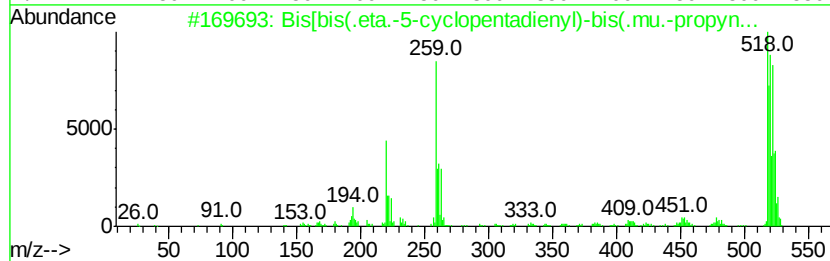
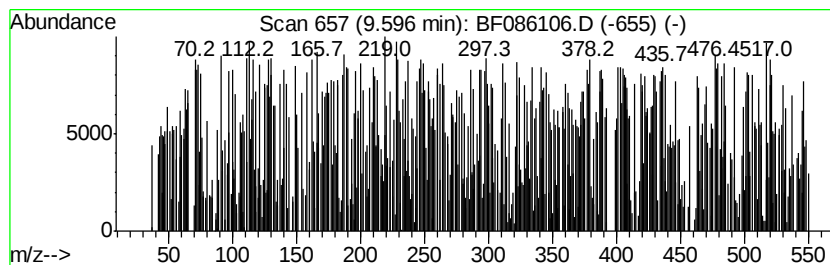
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Peak Number 8 unknown9.60 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	13.92 ng	933419	Acenaphthene-d10	9.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bis[bis(.eta.-5-cyclopentadienyl)...	518 C26H26Zr2	1000159-84-6 20
2		5-[(2-Pyridylmethyleme)amino]-2'...	518 C32H22N8	294651-18-6 9
3		Stannane, tributyl[(1-oxooctadec...	574 C30H62O2Sn	004027-13-8 9
4		1,3,5,7,9,11,13-Heptaethyl-5,9,1...	546 C14H38O9Si7	080177-43-1 9
5		Iron, (.eta.5-2,4-cyclopentadien...	520 C31H30FeP2	051509-20-7 7



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086106.D
Acq On : 6 Apr 2016 19:06
Operator : UM/SJ
Sample : H2254-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

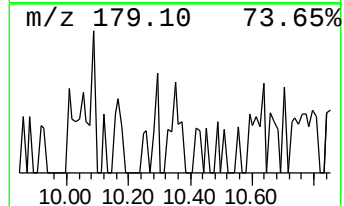
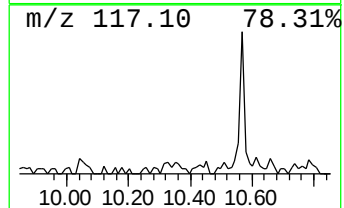
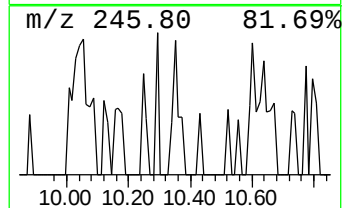
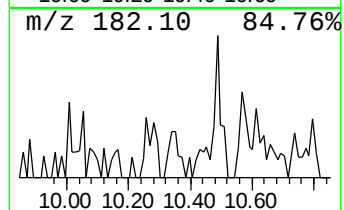
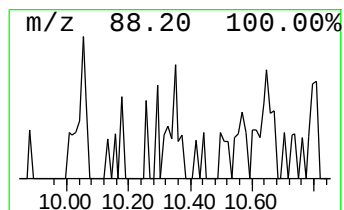
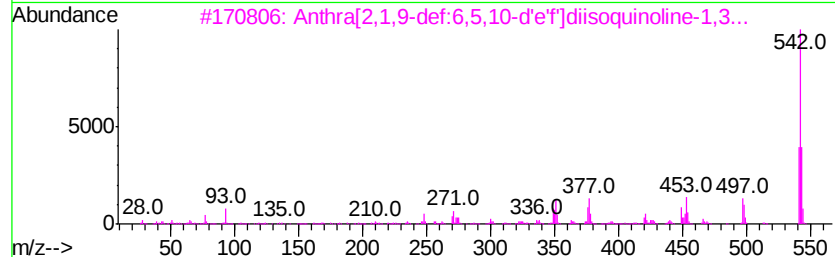
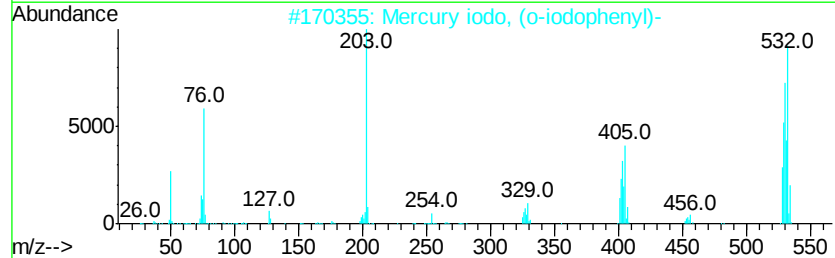
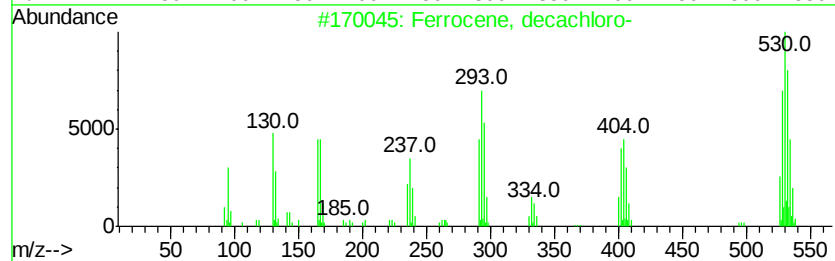
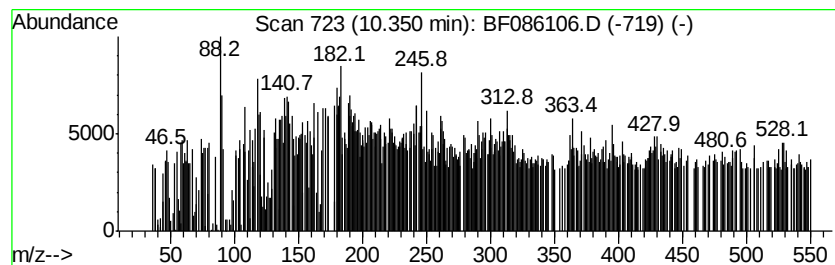
Instrument :
BNA_F
ClientSampleId :
SP-16

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.35 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	9.16 ng	614615	Acenaphthene-d10	9.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ferrocene, decachloro-	526 C10Cl10Fe	011121-63-4 41
2		Mercury iodo, (o-iodophenyl)-	532 C6H4HgI2	089487-89-8 12
3		Anthra[2,1,9-def:6,5,10-d'e'f']d...	542 C36H18N2O4	000128-65-4 9
4		Benzenepropanoic acid, 3,5-bis(1...	530 C35H62O3	002082-79-3 9
5		N,5-Bis[3,4-dichlorophenyl]-3,5-...	540 C27H20Cl4N4	333399-40-9 9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040616\
Data File : BF086106.D
Acq On : 6 Apr 2016 19:06
Operator : UM/SJ
Sample : H2254-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-16

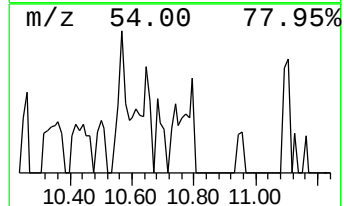
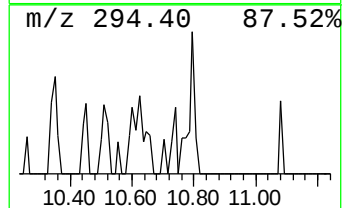
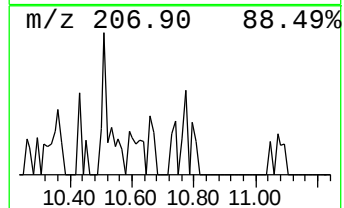
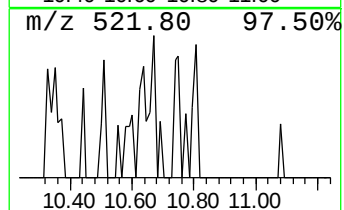
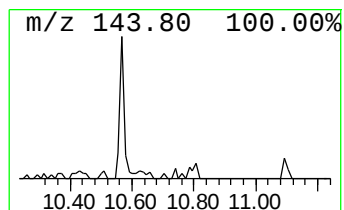
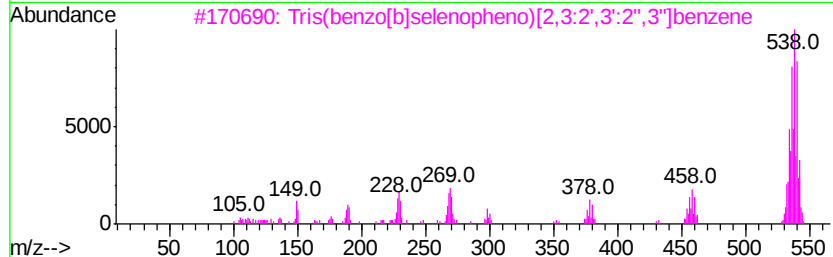
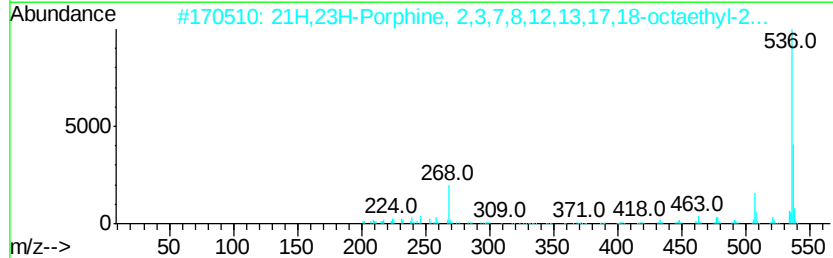
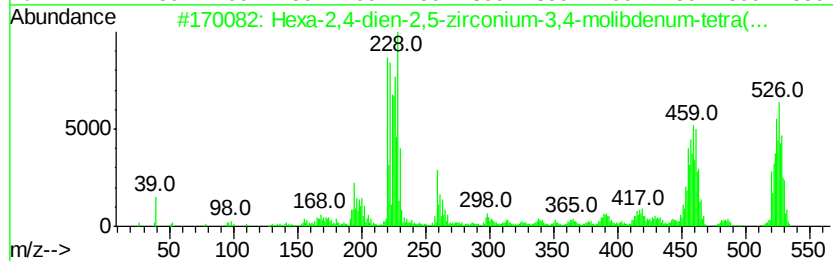
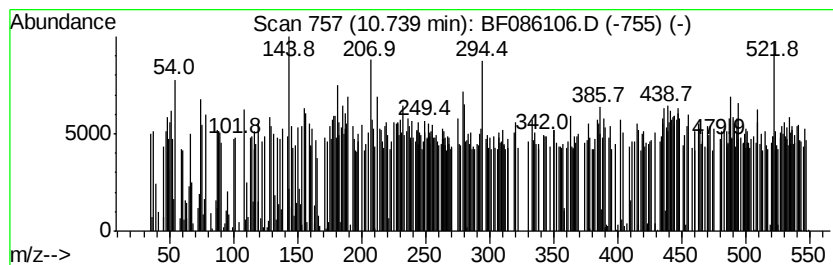
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexa-2,4-dien-2,5-zirconium... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	6.01 ng	347310	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexa-2,4-dien-2,5-zirconium-3,4-...	526	C26H26MoZr	1000154-45-6	55
2		21H,23H-Porphine, 2,3,7,8,12,13,...	536	C36H48N4	000991-74-2	12
3		Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	10
4		Ferrocene, [(16-bromohexadecylox...	532	C27H41BrFeO2	1000115-80-9	10
5		Osmium hydride, (.eta.-5-cyclope...	534	C21H28OsP2	1000158-66-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086106.D
Acq On : 6 Apr 2016 19:06
Operator : UM/SJ
Sample : H2254-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-16

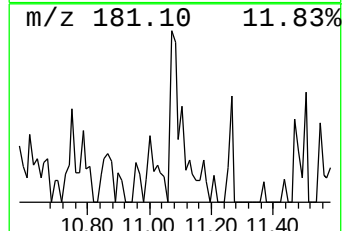
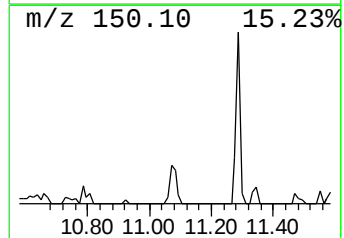
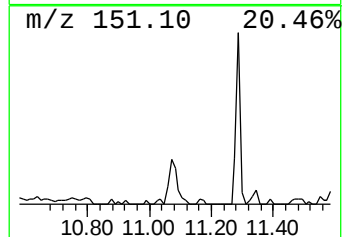
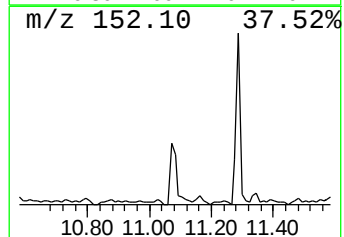
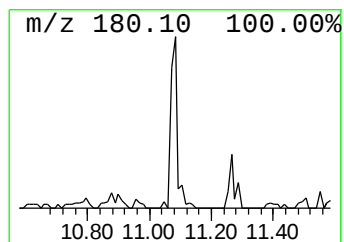
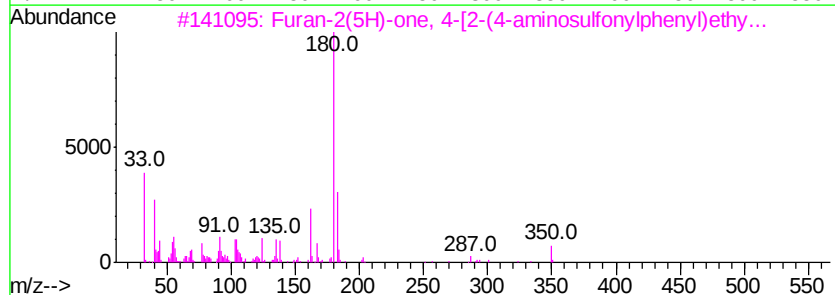
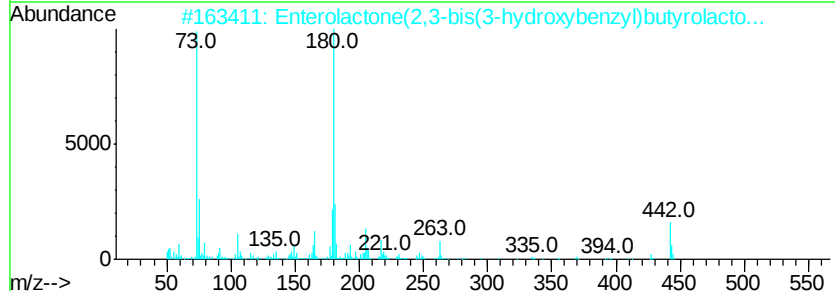
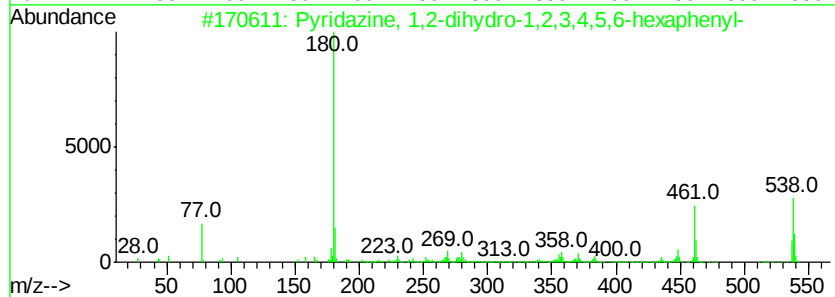
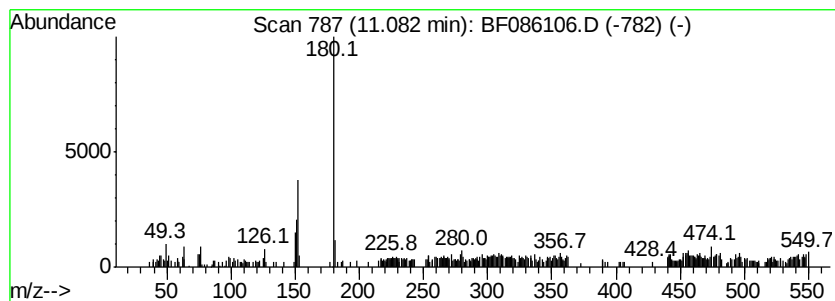
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Pyridazine, 1,2-dihydro-1,2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	10.40 ng	601145	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Pyridazine, 1,2-dihydro-1,2,3,4,...	538	C40H30N2	074810-58-5	52
2		Enterolactone(2,3-bis(3-hydroxyb...	442	C24H34O4Si2	077545-19-8	5
3		Furan-2(5H)-one, 4-[2-(4-aminosu...	350	C17H22N2O4S	1000269-69-6	4



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086106.D
Acq On : 6 Apr 2016 19:06
Operator : UM/SJ
Sample : H2254-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-16

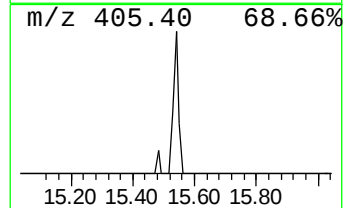
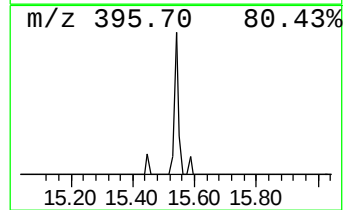
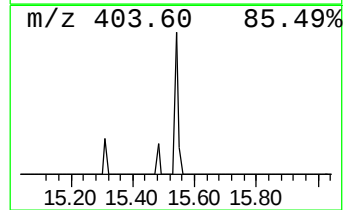
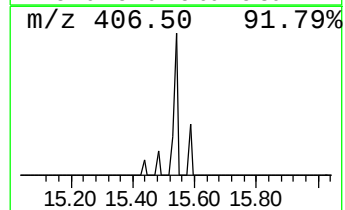
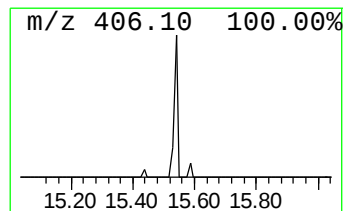
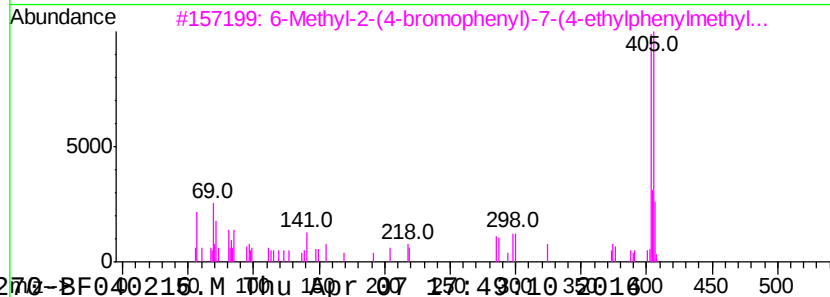
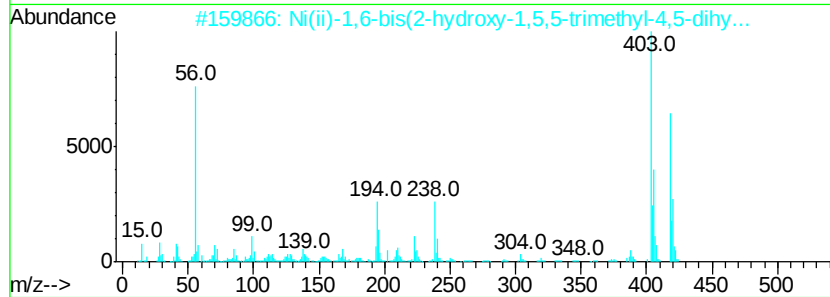
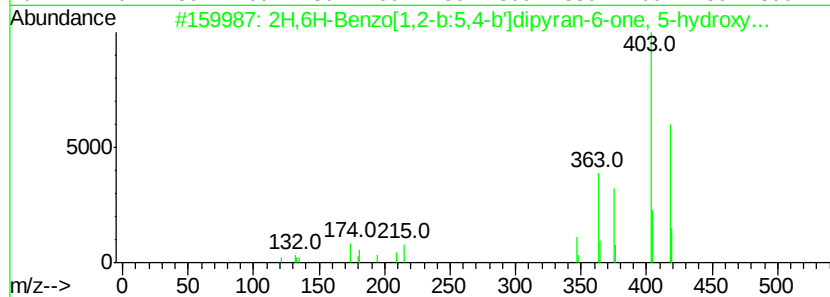
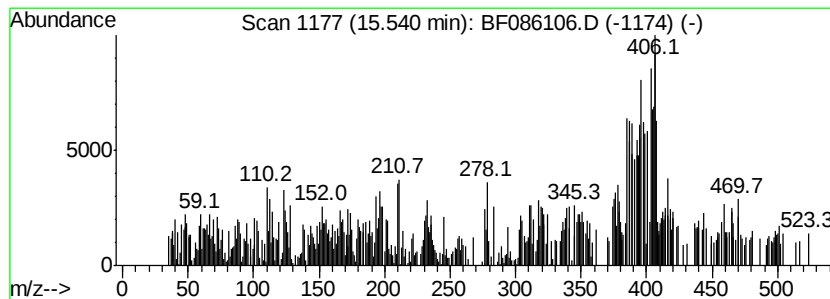
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown15.54 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	7.20 ng	380045	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4	2H,6H-Benzo[1,2-b:5,4-b']dipyran...	418	C26H26O5	004225-28-9	25
2		Ni(ii)-1,6-bis(2-hydroxy-1,5,5-t...	418	C18H24N4NiO4	1000287-36-1	11
3		6-Methyl-2-(4-bromophenyl)-7-(4-...	403	C24H22BrN	078394-91-9	6
4		4H,8H-Benzo[1,2-b:3,4-b']dipyran...	418	C26H26O5	005233-97-6	2



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040616\
Data File : BF086106.D
Acq On : 6 Apr 2016 19:06
Operator : UM/SJ
Sample : H2254-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

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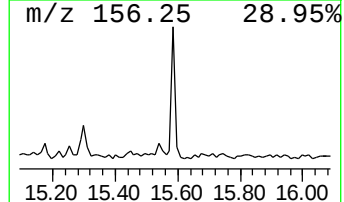
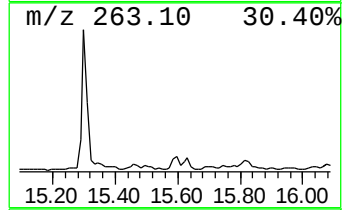
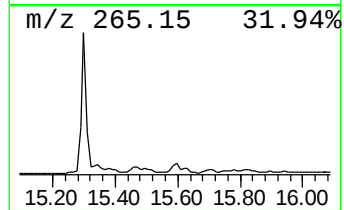
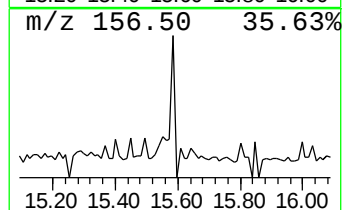
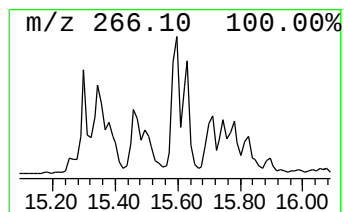
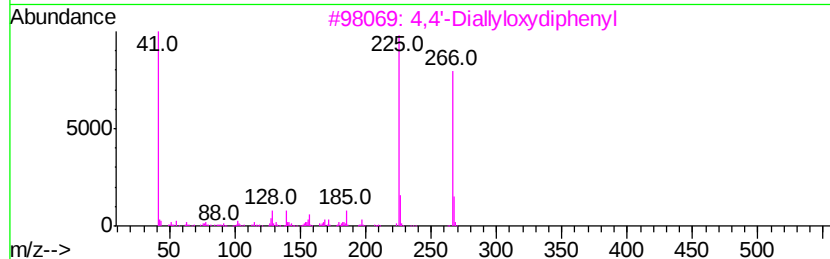
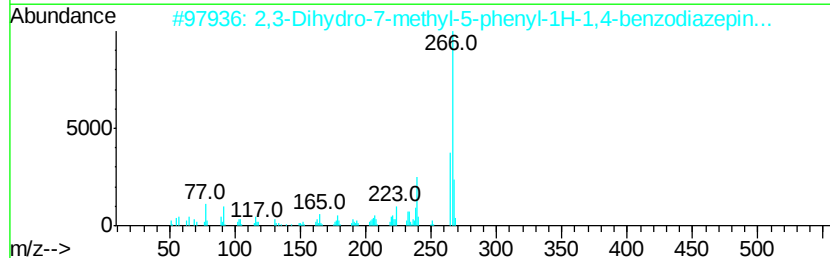
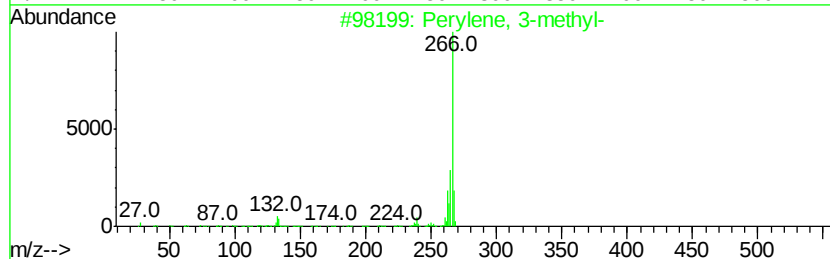
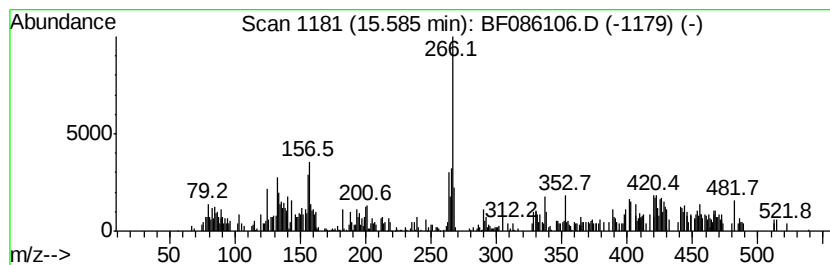
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown15.59 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	6.59 ng	348127	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene, 3-methyl-	266	C21H14	024471-47-4	38
2			2,3-Dihydro-7-methyl-5-phenyl-1H...	266	C16H14N2S	002888-60-0	30
3			4,4'-Diallvloxydiphenyl	266	C18H18O2	041481-62-3	30
4			Equilenin	266	C18H18O2	000517-09-9	30
5			trans-4'-Amino-4-(dimethylamino)...	266	C17H18N2O	1000234-51-4	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040616\
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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...	4.91	6.4	ng	302923	1	6.74	944798	20.0
unknown6.51	6.51	56.1	ng	2648830	1	6.74	944798	20.0
unknown9.60	9.60	13.9	ng	933419	3	9.78	1341270	20.0
unknown10.35	10.35	9.2	ng	614615	3	9.78	1341270	20.0
Hexa-2,4-dien-2,5...	10.74	6.0	ng	347310	4	11.26	1156550	20.0
Pyridazine, 1,2-d...	11.08	10.4	ng	601145	4	11.26	1156550	20.0
unknown11.68	11.68	11.3	ng	652287	4	11.26	1156550	20.0
unknown15.54	15.54	7.2	ng	380045	6	15.30	1056010	20.0
unknown15.59	15.59	6.6	ng	348127	6	15.30	1056010	20.0