

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
 Data File : BF086136.D
 Acq On : 7 Apr 2016 18:09
 Operator : UM/SJ
 Sample : PB89612BL
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB89612BL

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	2.155	3	6	7	rBV3	171793	346071	9.67%	0.489%
2	2.293	15	18	22	rBV5	124718	301214	8.42%	0.426%
3	2.430	26	30	34	rVV5	181589	630038	17.61%	0.891%
4	2.498	34	36	39	rVB	120115	210148	5.87%	0.297%
5	2.578	41	43	47	rBV4	192778	390113	10.90%	0.551%
6	3.276	100	104	106	rBV3	157095	411395	11.50%	0.582%
7	3.424	115	117	120	rVB3	104190	254635	7.12%	0.360%
8	3.504	120	124	126	rBV4	262384	626510	17.51%	0.886%
9	4.018	166	169	171	rBV2	195395	419065	11.71%	0.592%
10	4.064	171	173	175	rVB2	269825	332112	9.28%	0.469%
11	4.293	191	193	197	rVB4	178494	457002	12.77%	0.646%
12	4.418	201	204	206	rBV	200599	215729	6.03%	0.305%
13	4.510	209	212	213	rVV2	253355	390415	10.91%	0.552%
14	4.533	213	214	216	rVV2	268383	344482	9.63%	0.487%
15	4.590	216	219	223	rVB2	237125	569818	15.93%	0.805%
16	4.658	223	225	226	rBV	206322	239330	6.69%	0.338%
17	4.704	226	229	232	rVB2	161858	336807	9.41%	0.476%
18	4.761	232	234	237	rVB2	260995	547572	15.31%	0.774%
19	4.830	237	240	241	rBV	233077	360501	10.08%	0.510%
20	4.910	244	247	248	rBV	230043	360427	10.07%	0.509%
21	4.944	248	250	251	rVV	294204	456296	12.75%	0.645%
22	4.979	251	253	256	rVB3	324678	627593	17.54%	0.887%
23	5.299	277	281	282	rBV3	197131	299538	8.37%	0.423%
24	5.333	282	284	292	rVV	2394008	2639899	73.79%	3.732%
25	5.459	292	295	296	rVV2	152495	319844	8.94%	0.452%
26	5.493	296	298	299	rVV2	194654	319641	8.93%	0.452%
27	5.527	299	301	303	rVV2	201405	328611	9.19%	0.465%
28	5.744	318	320	323	rBV2	130874	249966	6.99%	0.353%
29	5.870	327	331	334	rVB4	191173	531141	14.85%	0.751%
30	5.984	336	341	344	rBV4	146053	256362	7.17%	0.362%
31	6.064	344	348	351	rVV5	304691	718932	20.10%	1.016%
32	6.144	353	355	360	rBV4	218910	547889	15.32%	0.774%
33	6.259	364	365	367	rBV	289722	429016	11.99%	0.606%
34	6.304	367	369	370	rVV2	334679	563754	15.76%	0.797%

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35	6.384	372	376	378	rVV	2529259	3577463	100.00%	5.057%
36	6.419	378	379	382	rVV2	242038	442018	12.36%	0.625%
37	6.499	384	386	389	rVV	2146069	3330369	93.09%	4.708%
38	6.636	390	398	401	rVV4	431495	938558	26.24%	1.327%
39	6.739	401	407	409	rVV	798152	1828002	51.10%	2.584%
40	6.773	409	410	411	rVV	308720	212003	5.93%	0.300%
41	6.807	411	413	416	rVV2	399820	759201	21.22%	1.073%
42	6.853	416	417	418	rVV	355380	479499	13.40%	0.678%
43	6.887	418	420	424	rVV	2232677	2426167	67.82%	3.429%
44	6.990	428	429	433	rVB2	162789	258879	7.24%	0.366%
45	7.093	436	438	440	rBV2	190646	285236	7.97%	0.403%
46	7.173	443	445	448	rBV2	304462	437870	12.24%	0.619%
47	7.276	450	454	455	rVV3	357752	1044892	29.21%	1.477%
48	7.310	455	457	459	rVV	1326108	1865339	52.14%	2.637%
49	7.379	459	463	465	rVV3	486676	1218481	34.06%	1.722%
50	7.413	465	466	468	rVV2	320791	555666	15.53%	0.785%
51	7.459	468	470	472	rVV3	595949	745079	20.83%	1.053%
52	7.527	472	476	479	rVV4	538789	1494461	41.77%	2.112%
53	7.585	479	481	483	rVV3	505802	974544	27.24%	1.378%
54	7.665	485	488	489	rBV	169630	284201	7.94%	0.402%
55	7.710	491	492	495	rVV	125118	247051	6.91%	0.349%
56	7.813	498	501	506	rVV6	332352	1289724	36.05%	1.823%
57	7.882	506	507	508	rVB6	315530	216454	6.05%	0.306%
58	7.950	511	513	514	rVV	252277	455300	12.73%	0.644%
59	8.019	517	519	522	rVV	1253347	1442698	40.33%	2.039%
60	8.076	522	524	527	rVB2	349461	548325	15.33%	0.775%
61	8.179	528	533	538	rBV7	307233	1183921	33.09%	1.674%
62	8.247	538	539	543	rVV3	146166	283693	7.93%	0.401%
63	8.339	545	547	548	rVV2	150673	282606	7.90%	0.399%
64	8.465	555	558	560	rVV3	173715	351486	9.83%	0.497%
65	8.545	562	565	568	rVV3	234377	564567	15.78%	0.798%
66	8.613	568	571	572	rVV3	262441	643549	17.99%	0.910%
67	8.647	572	574	575	rVV2	277448	509660	14.25%	0.720%
68	8.670	575	576	580	rVB3	314321	655720	18.33%	0.927%
69	8.739	580	582	583	rBV	308512	429613	12.01%	0.607%
70	8.773	583	585	587	rVV2	320731	594643	16.62%	0.841%
71	8.830	587	590	591	rVV3	222925	368772	10.31%	0.521%

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72	8.865	591	593	596	rVV3	295752	583985	16.32%	0.825%
73	9.013	602	606	611	rVV6	329073	973937	27.22%	1.377%
74	9.093	611	613	615	rVV	2317457	3400024	95.04%	4.806%
75	9.127	615	616	618	rVV2	183688	282467	7.90%	0.399%
76	9.219	622	624	627	rVV3	101090	201874	5.64%	0.285%
77	9.482	644	647	650	rVB3	145657	338269	9.46%	0.478%
78	9.539	650	652	656	rBB3	102001	209478	5.86%	0.296%
79	9.768	669	672	675	rVB	917153	1243538	34.76%	1.758%
80	9.973	686	690	694	rVV7	133741	409771	11.45%	0.579%
81	10.270	711	716	722	rVB6	88617	343671	9.61%	0.486%
82	10.568	739	742	744	rBV	1696773	1998013	55.85%	2.824%
83	11.253	800	802	809	rBV	1229414	1135273	31.73%	1.605%
84	12.842	938	941	943	rBV	3325213	3217724	89.94%	4.548%
85	13.894	1030	1033	1035	rBV	844652	959288	26.81%	1.356%
86	14.054	1044	1047	1050	rBV4	144295	207350	5.80%	0.293%
87	14.659	1098	1100	1102	rVV2	254707	438411	12.25%	0.620%
88	14.900	1118	1121	1125	rBV4	107580	212708	5.95%	0.301%
89	15.060	1131	1135	1136	rVV4	121111	208804	5.84%	0.295%
90	15.140	1136	1142	1145	rVB5	129158	347350	9.71%	0.491%
91	15.288	1152	1155	1161	rBV	535775	824713	23.05%	1.166%
92	15.505	1170	1174	1177	rBV3	213980	538465	15.05%	0.761%
93	15.677	1185	1189	1193	rBV5	192599	465774	13.02%	0.658%
94	15.780	1194	1198	1200	rBV5	280242	647362	18.10%	0.915%
95	15.814	1200	1201	1204	rVV3	205381	348855	9.75%	0.493%
96	15.894	1206	1208	1210	rVB3	170535	245771	6.87%	0.347%
97	16.008	1215	1218	1219	rVV2	253611	594028	16.60%	0.840%
98	16.180	1232	1233	1238	rBV4	127658	280721	7.85%	0.397%
99	16.282	1238	1242	1244	rBV3	195001	382909	10.70%	0.541%
100	16.340	1244	1247	1249	rBV3	168393	446926	12.49%	0.632%

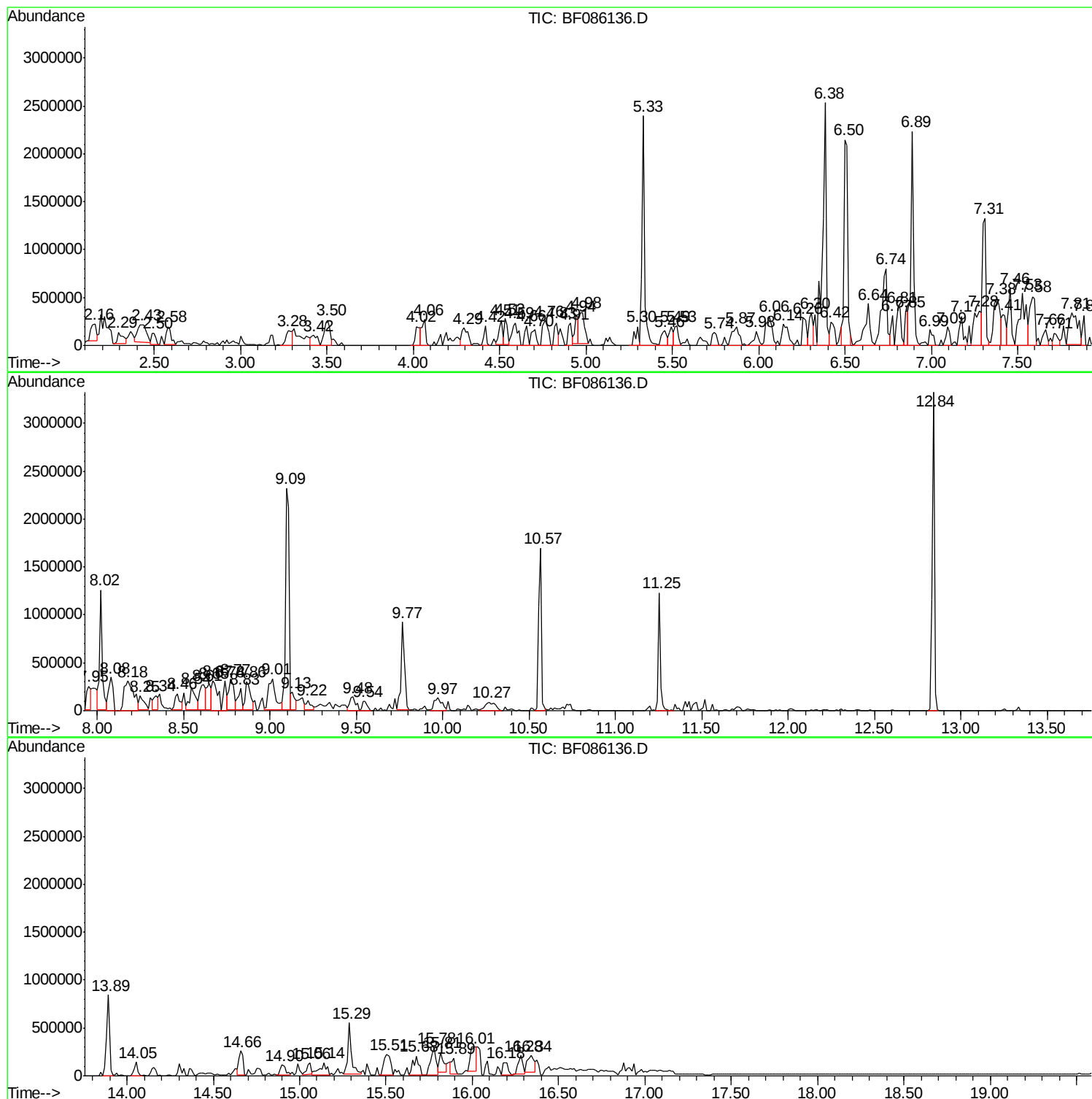
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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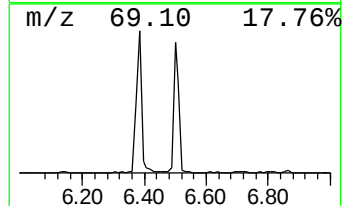
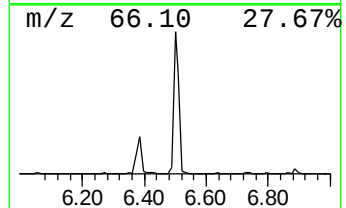
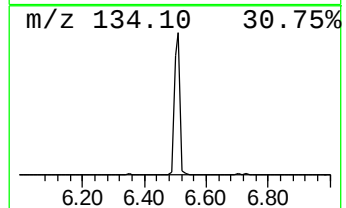
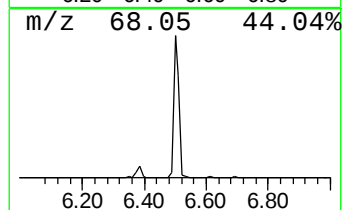
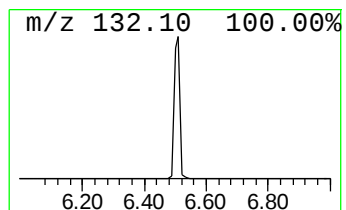
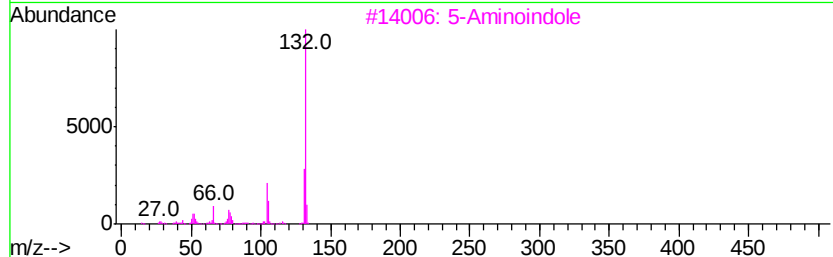
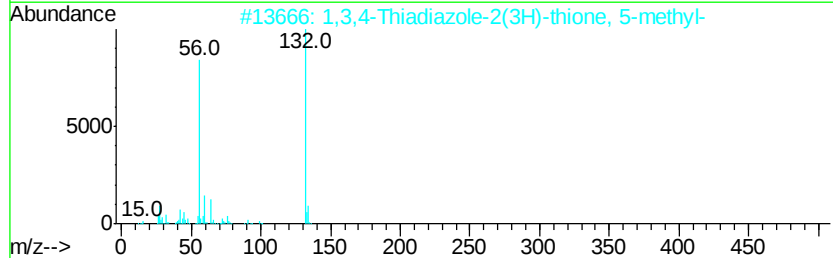
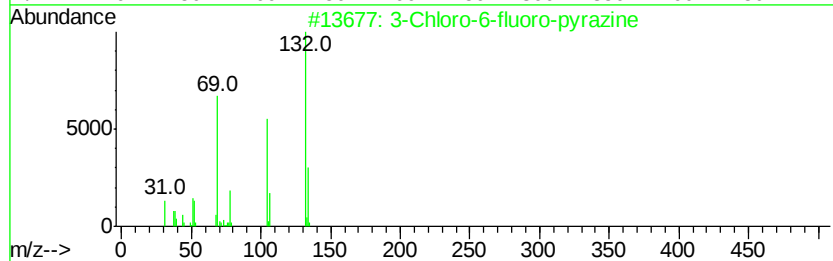
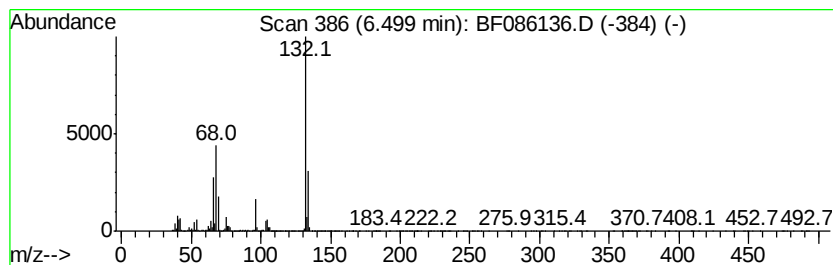
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	36.44 ng	3330370	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	35
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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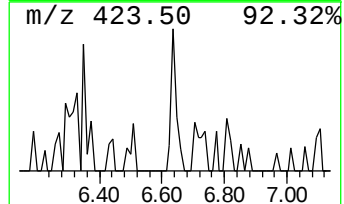
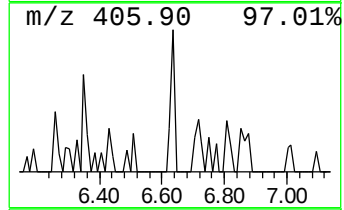
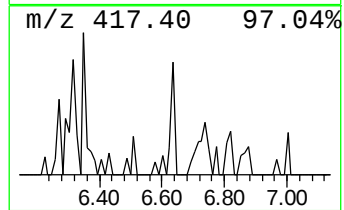
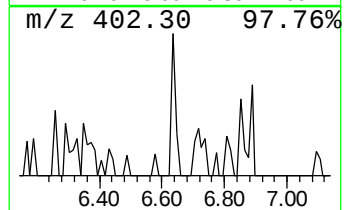
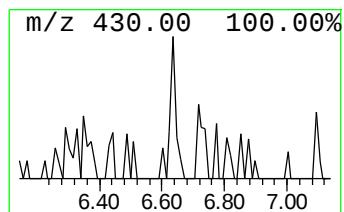
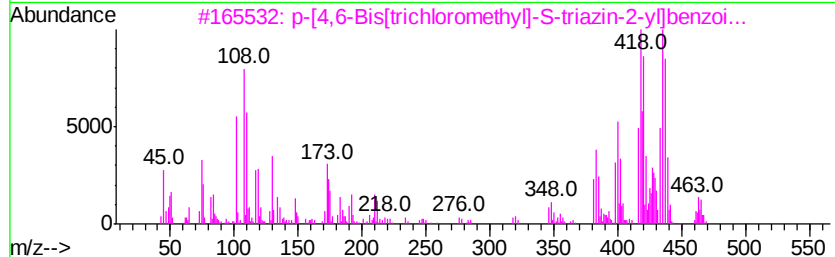
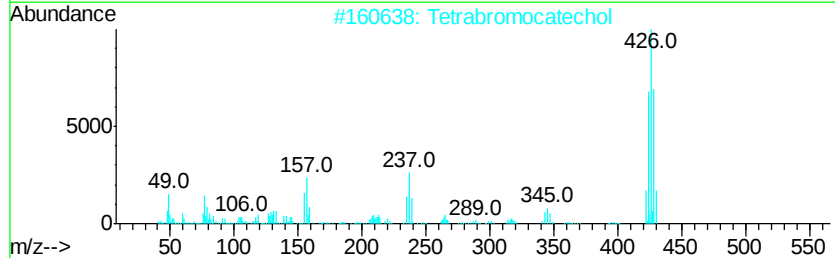
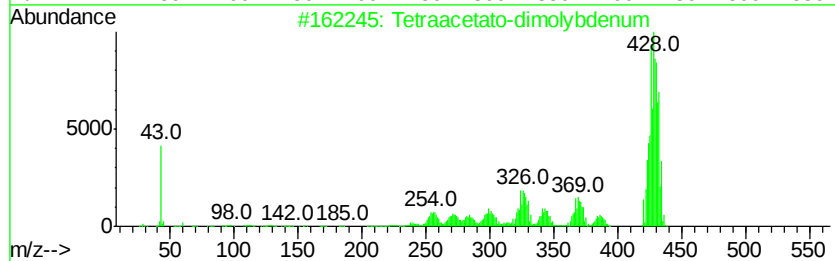
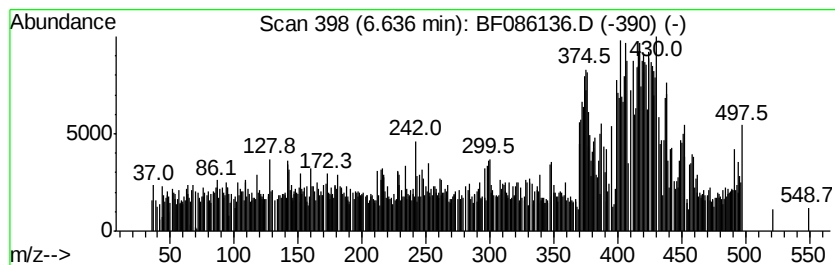
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	10.27 ng	938558	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetraacetato-dimolybdenum	432	C8H12Mo2O8	1000161-31-6	27
2		Tetrabromocatechol	422	C6H2Br4O2	000488-47-1	25
3		p-[4,6-Bis[trichloromethyl]-S-triazin-2-yl]benzoic acid	461	C14H9Cl6N3O2	125989-27-7	14
4		7-Bromo-5-(2-chloro-phenyl)-3-furancarboxylic acid	426	C20H12BrClN2O2	1000286-24-0	14
5		Acenaphthylene, octachloro-	424	C12Cl8	007267-16-5	10



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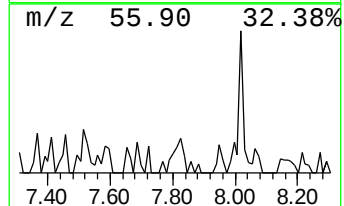
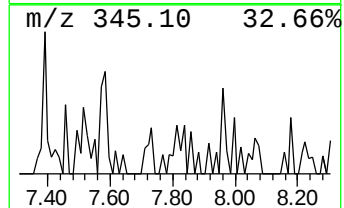
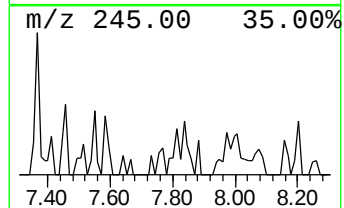
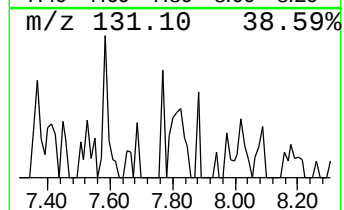
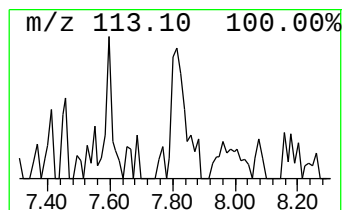
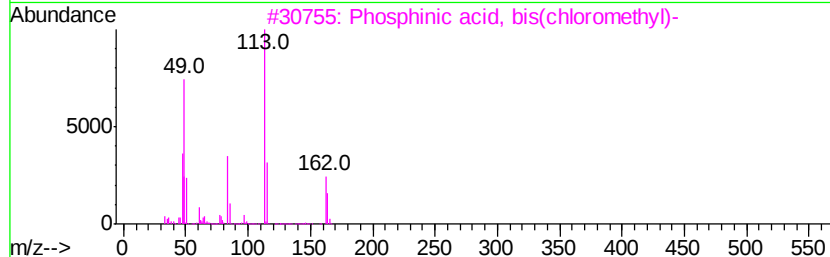
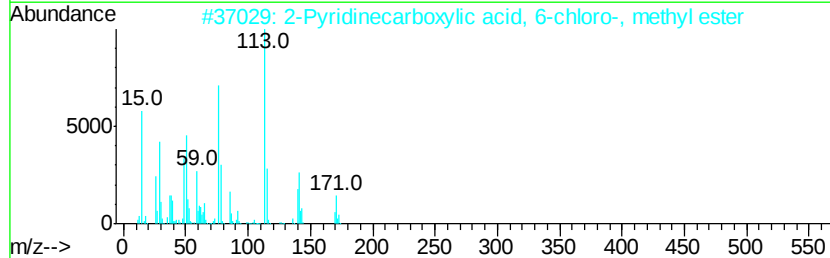
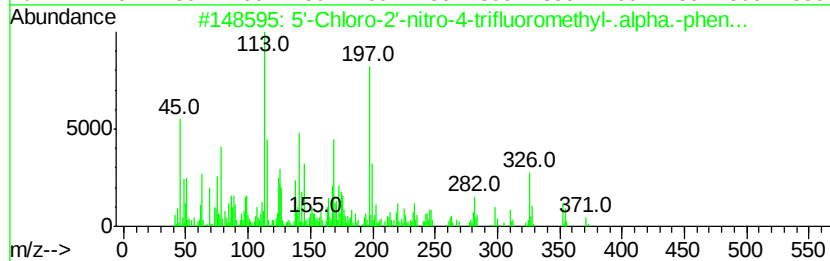
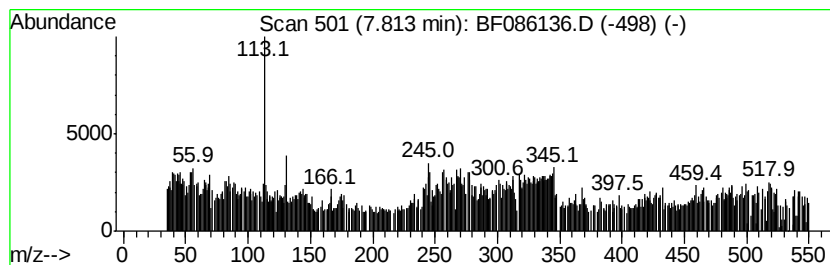
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Peak Number 8 unknown7.81 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	17.88 ng	1289720	Naphthalene-d8	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5'-Chloro-2'-nitro-4-trifluorome...	371	C16H9ClF3NO4	038635-52-8	41
2		2-Pyridinecarboxylic acid, 6-chl...	171	C7H6ClNO2	006636-55-1	22
3		Phosphinic acid, bis(chloromethyl)-	162	C2H5Cl2O2P	013274-83-4	22
4		Ethanol, 2,2-dichloro-	114	C2H4Cl2O	000598-38-9	22
5		Phosphinic acid, bis(chloromethy...	190	C4H9Cl2O2P	013274-84-5	17



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB89612BL

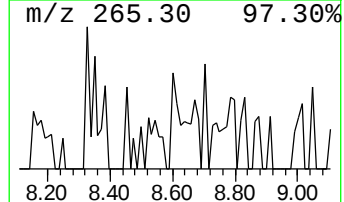
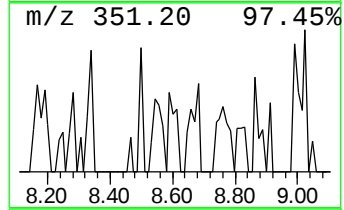
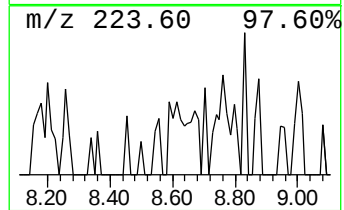
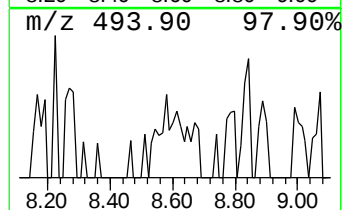
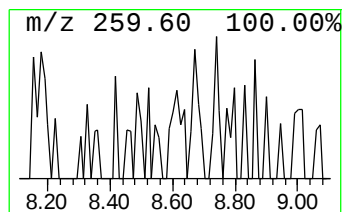
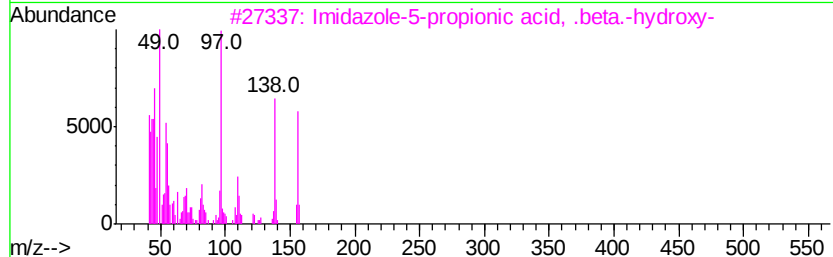
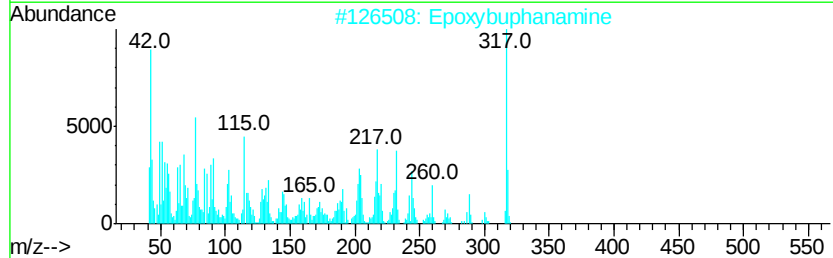
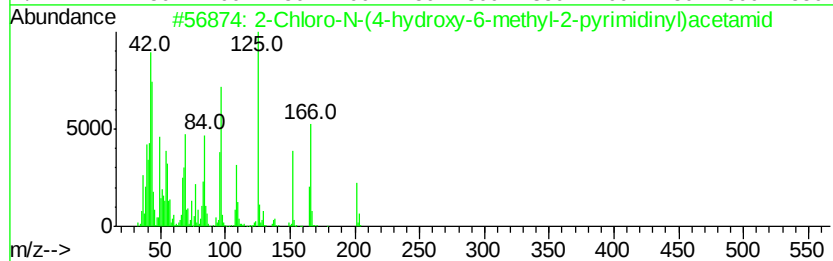
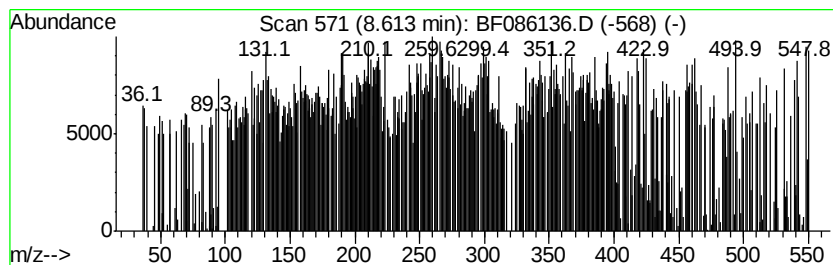
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.61 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	8.92 ng	643549	Napthalene-d8	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Chloro-N-(4-hydroxy-6-methyl-2...	201	C7H8ClN3O2	341010-69-3	20
2		Epoxybuphanamine	317	C17H19N05	1000124-61-7	18
3		Imidazole-5-propionic acid, .bet...	156	C6H8N2O3	1000129-47-8	18
4		Acetamide, 2-chloro-N-(2-ethyl-3...	262	C14H15ClN2O	349498-08-4	14
5		Acetamide, 2-chloro-N-(2-chlorop...	203	C8H7Cl2NO	003289-76-7	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB89612BL

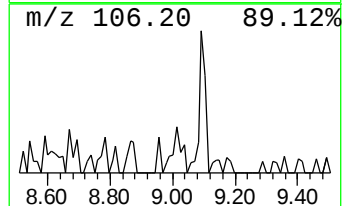
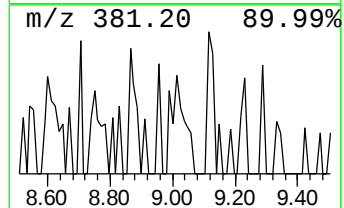
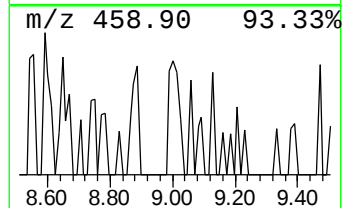
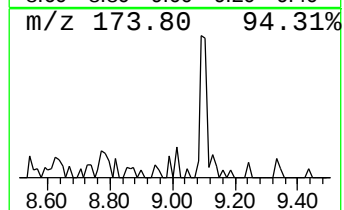
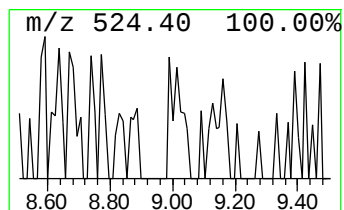
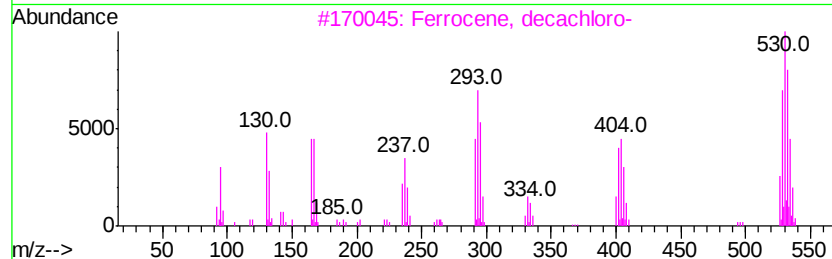
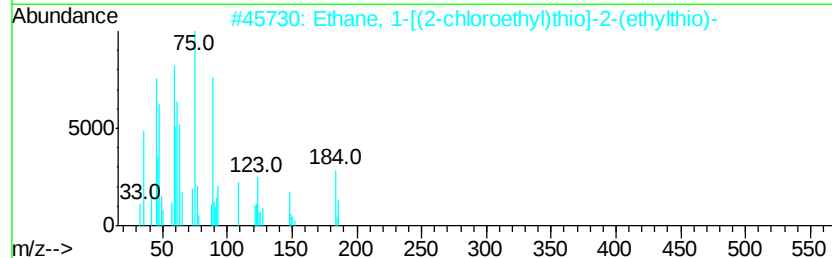
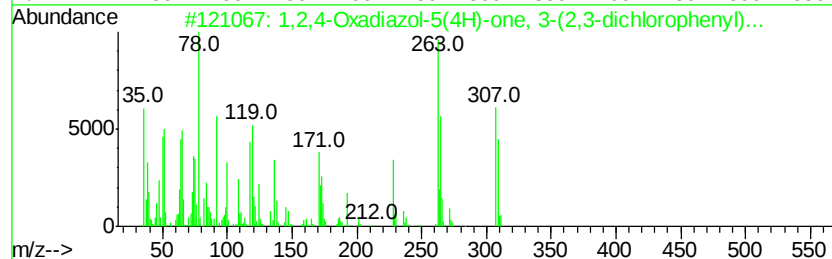
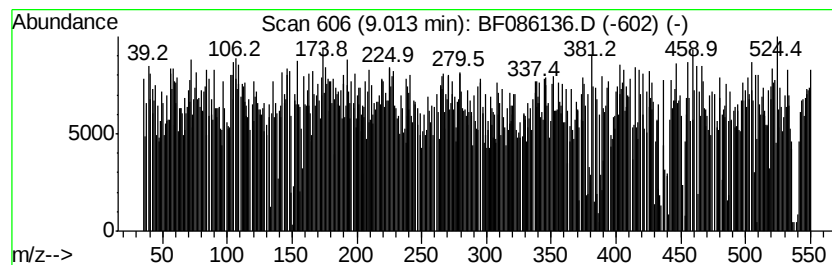
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,2,4-Oxadiazol-5(4H)-one, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	15.66 ng	973937	Acenaphthene-d10	9.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Oxadiazol-5(4H)-one, 3-(2,...	307	C13H7Cl2N3O2	288246-51-5	60
2		Ethane, 1-[(2-chloroethyl)thio]-...	184	C6H13ClS2	092569-22-7	20
3		Ferrocene, decachloro-	526	C10Cl10Fe	011121-63-4	18
4		S-Ethyl methylphosphonothiofluor...	142	C3H8FOPS	000673-98-3	18
5		1,2-Di(2,3,7,8,12,13,17,18-octae...	1093	C74H92N8	106085-73-8	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB89612BL

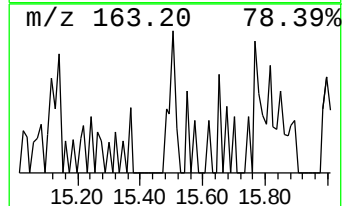
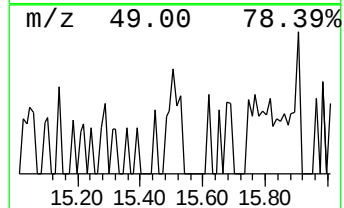
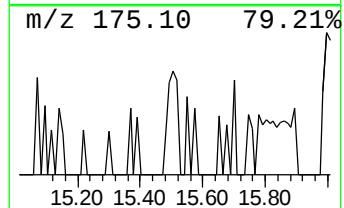
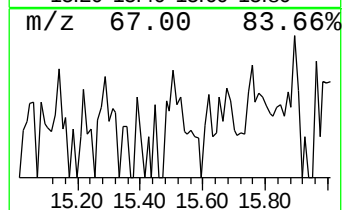
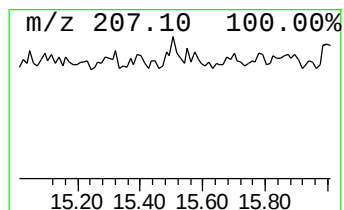
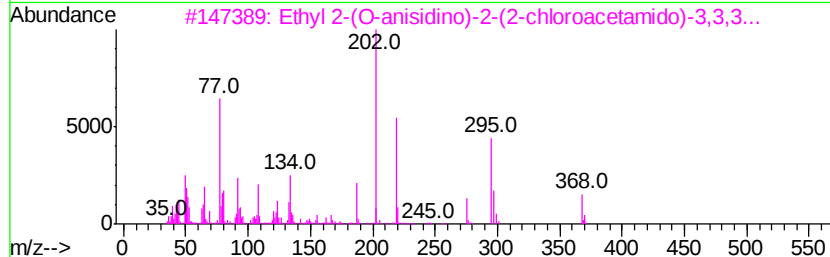
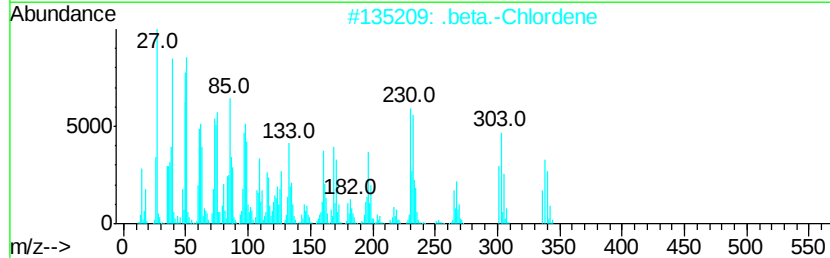
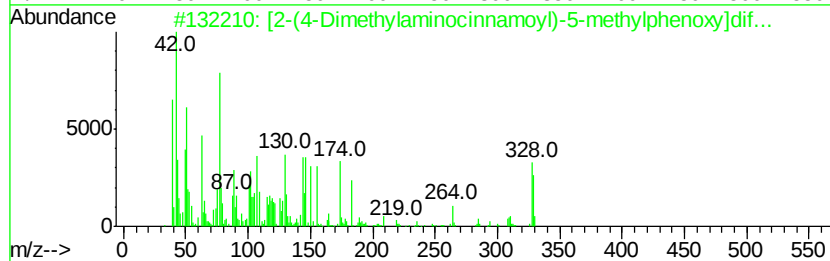
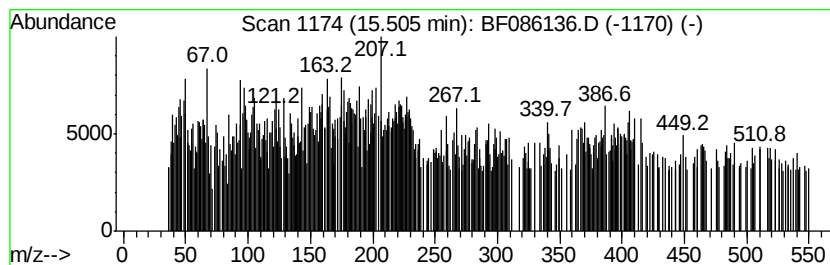
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 [2-(4-Dimethylaminocinnamoyl)-5-methylphenoxy]dif... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	13.06 ng	538465	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	[2-(4-Dimethylaminocinnamoyl)-5-...	329	C18H18BF2N02	1000223-62-3	59
2		.beta.-Chlordene	336	C10H6Cl6	056534-03-3	46
3		Ethyl 2-(O-anisidino)-2-(2-chlor...	368	C14H16ClF3N2O4	339352-61-3	46
4		2-Chloroacetyl-1-phenyl-1,2,3,4-...	324	C19H17ClN2O	114896-46-7	41
5		1,5-Hexadiene, 2,3,3,4,4,5-hexac...	286	C6H4Cl6	108562-66-9	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

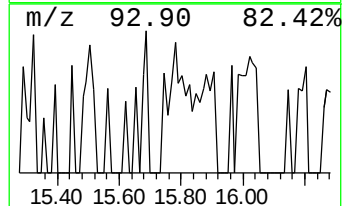
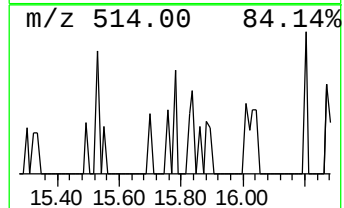
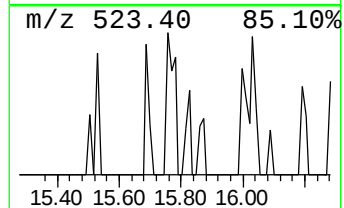
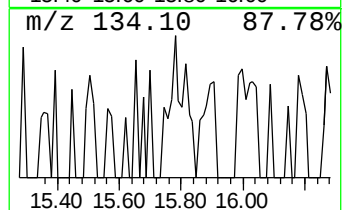
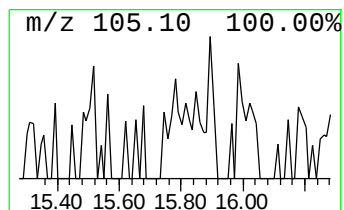
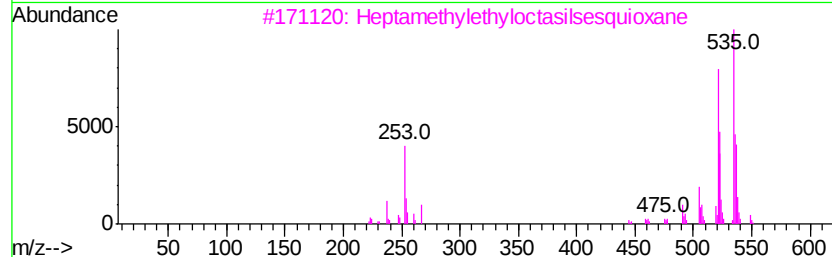
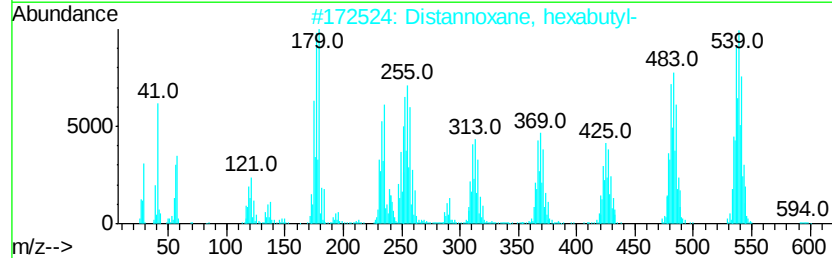
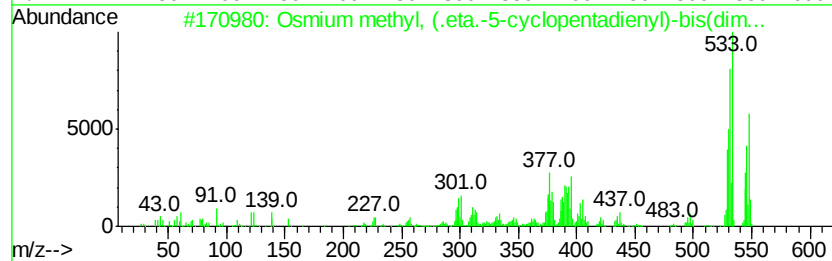
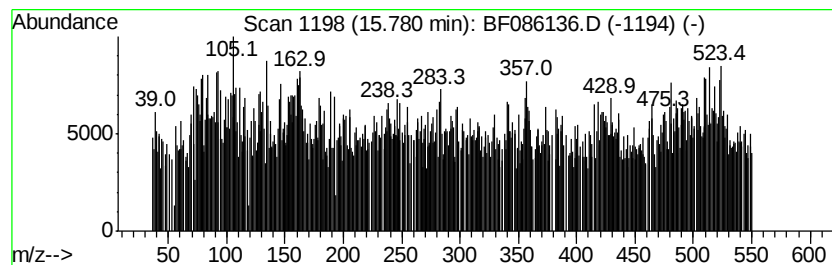
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.78	15.70 ng	647362	Perylene-d12	15.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Osmium methyl, (.eta.-5-cvclopen...	548	C22H300sP2	1000158-92-4	25	
2	Distannoxane, hexabutyl-	598	C24H540Sn2	000056-35-9	14	
3	Heptamethylethyloctasilsesquioxane	550	C9H26012Si8	077626-17-6	14	
4	1,3,5-Triazine, 2,4-bis(2,2,2-tr...	522	C15H7F13N4O2	302602-73-9	10	
5	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	9	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB89612BL

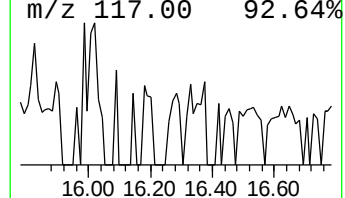
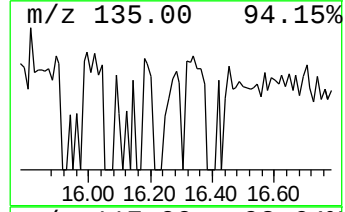
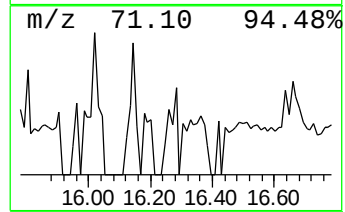
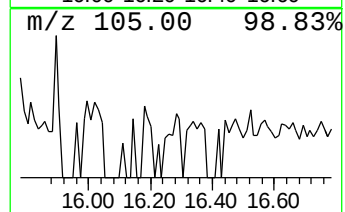
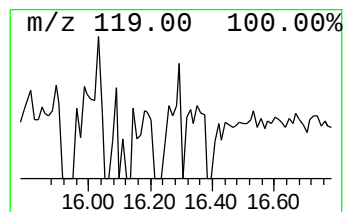
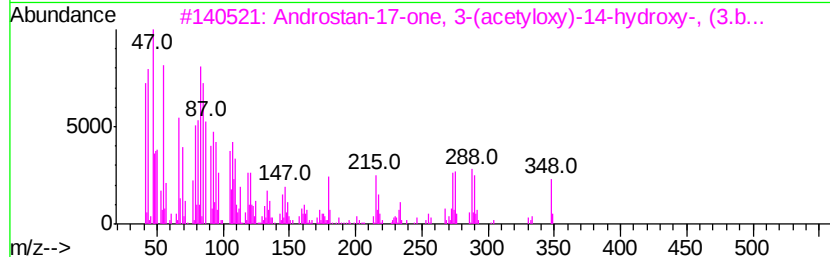
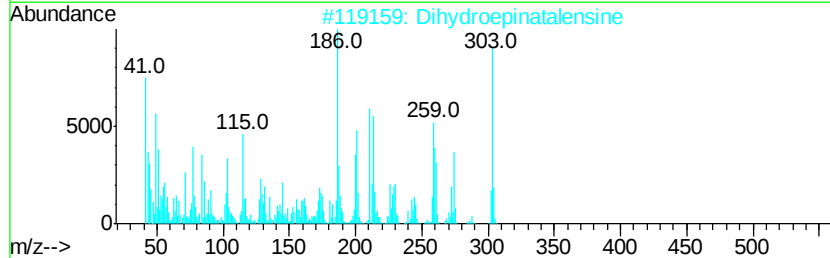
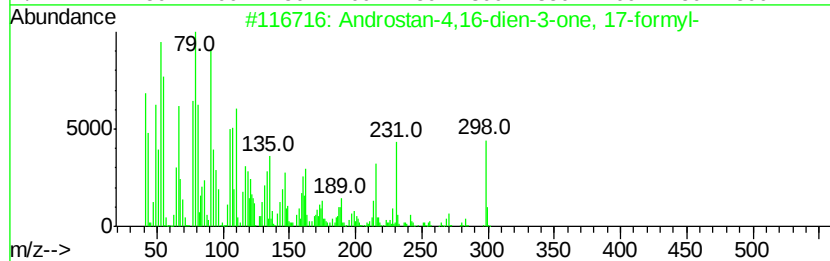
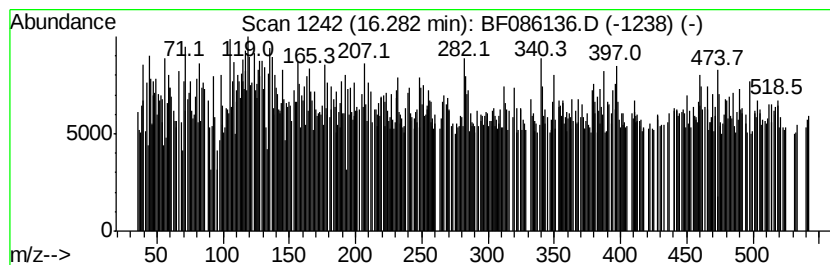
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Androstan-4,16-dien-3-one, ... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	9.29 ng	382909	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Androstan-4,16-dien-3-one, 17-formyl-	298	C20H26O2	114724-34-4	51
2		Dihydroepinatalensine	303	C17H21NO4	098843-28-8	38
3		Androstan-17-one, 3-(acetyloxy)-	348	C21H32O4	001241-30-1	38
4		Acetanilide, 2-chloro-4'-nitro-	214	C8H7ClN2O3	017329-87-2	38
5		Ethylene, 1-[2,3,4-methoxyphenyl]-	239	C11H13NO5	1000129-08-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040716\
Data File : BF086136.D
Acq On : 7 Apr 2016 18:09
Operator : UM/SJ
Sample : PB89612BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB89612BL

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
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unknown6.64	6.64	10.3	ng	938558	1	6.74	1828000	20.0
unknown7.81	7.81	17.9	ng	1289720	2	8.02	1442700	20.0
unknown8.61	8.61	8.9	ng	643549	2	8.02	1442700	20.0
1,2,4-Oxadiazol-5...	9.01	15.7	ng	973937	3	9.77	1243540	20.0
unknown14.66	14.66	10.6	ng	438411	6	15.29	824713	20.0
[2-(4-Dimethylami...	15.51	13.1	ng	538465	6	15.29	824713	20.0
unknown15.78	15.78	15.7	ng	647362	6	15.29	824713	20.0
Androstan-4,16-di...	16.28	9.3	ng	382909	6	15.29	824713	20.0