

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
 Data File : BF085487.D
 Acq On : 17 Mar 2016 3:24
 Operator : UM/SJ
 Sample : H1792-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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	4.024	150	152	154	rVV2	103994	173470	5.40%	0.340%
2	4.207	165	168	170	rVV2	113224	218512	6.80%	0.428%
3	4.310	175	177	179	rVB2	159173	201308	6.27%	0.394%
4	4.390	181	184	187	rVV	114134	176722	5.50%	0.346%
5	4.447	187	189	193	rVV2	80791	219309	6.83%	0.430%
6	4.619	203	204	206	rVV	501262	399825	12.45%	0.783%
7	4.859	222	225	227	rBV3	170399	336637	10.48%	0.660%
8	4.984	234	236	238	rVB	157158	158739	4.94%	0.311%
9	5.041	238	241	244	rBV2	89937	149239	4.65%	0.292%
10	5.144	248	250	252	rVB	102731	144286	4.49%	0.283%
11	5.224	256	257	260	rVB2	138945	181167	5.64%	0.355%
12	5.350	265	268	270	rBV	108702	153643	4.78%	0.301%
13	5.407	272	273	274	rVV	190128	159937	4.98%	0.313%
14	5.441	274	276	279	rVB	142552	243943	7.59%	0.478%
15	5.499	279	281	285	rBV	2618589	3013056	93.79%	5.904%
16	5.864	309	313	315	rBV	112965	286818	8.93%	0.562%
17	5.956	319	321	322	rVV	134515	162219	5.05%	0.318%
18	6.070	327	331	335	rBV2	141744	330145	10.28%	0.647%
19	6.150	335	338	340	rVB	145061	202714	6.31%	0.397%
20	6.219	342	344	348	rBV3	151807	290311	9.04%	0.569%
21	6.333	350	354	355	rVB	83782	177174	5.52%	0.347%
22	6.527	369	371	374	rVV	2648747	2977838	92.70%	5.835%
23	6.664	380	383	385	rBV	2973636	3100639	96.52%	6.076%
24	6.699	385	386	387	rVV	181801	150376	4.68%	0.295%
25	6.859	397	400	401	rVV	79087	167034	5.20%	0.327%
26	6.904	401	404	408	rVV	586396	1044011	32.50%	2.046%
27	6.973	408	410	413	rVV	122551	242367	7.54%	0.475%
28	7.053	415	417	419	rVV	2193638	2403279	74.81%	4.709%
29	7.122	419	423	426	rVV2	267662	318077	9.90%	0.623%
30	7.202	428	430	435	rVB2	187576	371833	11.57%	0.729%
31	7.316	437	440	442	rBV2	167568	263017	8.19%	0.515%
32	7.362	442	444	446	rVB	137724	164800	5.13%	0.323%
33	7.419	446	449	451	rBV2	198188	446383	13.90%	0.875%
34	7.465	451	453	454	rVV	2136480	2167261	67.47%	4.247%

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.487	454	455	457 rVV2	223000	280993	8.75%	0.551%
36	7.727	473	476	480 rVB	246297	534415	16.64%	1.047%
37	7.796	480	482	484 rVB	187805	242982	7.56%	0.476%
38	7.830	484	485	487 rVB	176292	159226	4.96%	0.312%
39	7.865	487	488	490 rBV	227517	190659	5.94%	0.374%
40	7.922	490	493	494 rBV2	228900	272836	8.49%	0.535%
41	8.036	501	503	506 rVB	159009	252110	7.85%	0.494%
42	8.082	506	507	510 rBV	271336	434048	13.51%	0.851%
43	8.139	510	512	514 rBV	185409	211786	6.59%	0.415%
44	8.185	514	516	518 rVB	1146431	940966	29.29%	1.844%
45	8.562	544	549	551 rVV	80305	180904	5.63%	0.354%
46	8.848	573	574	576 rVV	213867	191787	5.97%	0.376%
47	8.962	582	584	585 rBV	253157	180075	5.61%	0.353%
48	9.008	585	588	591 rBV	91196	180585	5.62%	0.354%
49	9.190	602	604	606 rBV	268821	229158	7.13%	0.449%
50	9.259	608	610	613 rVV	2750793	3212410	100.00%	6.295%
51	9.659	643	645	647 rBV	561543	647644	20.16%	1.269%
52	9.876	660	664	666 rBV	114286	213802	6.66%	0.419%
53	9.945	668	670	672 rVV	916090	1059782	32.99%	2.077%
54	10.151	686	688	690 rVV2	172173	172910	5.38%	0.339%
55	10.368	704	707	709 rVV	204473	257187	8.01%	0.504%
56	10.596	721	727	729 rBV	69536	184906	5.76%	0.362%
57	10.733	736	739	741 rVV2	1627079	2112701	65.77%	4.140%
58	10.848	746	749	756 rVB	139220	297663	9.27%	0.583%
59	11.214	778	781	783 rVB2	213091	210888	6.56%	0.413%
60	11.419	797	799	802 rVV2	798033	912028	28.39%	1.787%
61	11.785	830	831	833 rBV2	177793	174191	5.42%	0.341%
62	11.831	833	835	837 rVB3	233370	334717	10.42%	0.656%
63	11.945	844	845	849 rVB2	148450	198666	6.18%	0.389%
64	12.288	869	875	878 rVV3	59510	166670	5.19%	0.327%
65	12.802	918	920	924 rVB3	135825	174831	5.44%	0.343%
66	13.008	936	938	940 rVV	2780282	2499869	77.82%	4.898%
67	13.214	953	956	960 rBV3	82486	193633	6.03%	0.379%
68	13.808	1004	1008	1009 rBV3	139425	233219	7.26%	0.457%
69	13.854	1009	1012	1014 rVV3	392177	729503	22.71%	1.429%
70	13.899	1014	1016	1018 rVV	193254	384575	11.97%	0.754%
71	13.945	1018	1020	1024 rVV4	377837	713234	22.20%	1.398%

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72	14.060	1026	1030	1032	rVV	756534	1208950	37.63%	2.369%
73	14.094	1032	1033	1034	rVV	166641	192404	5.99%	0.377%
74	14.117	1034	1035	1036	rVV	222190	239614	7.46%	0.470%
75	14.151	1036	1038	1039	rVV2	251822	324287	10.09%	0.635%
76	14.174	1039	1040	1041	rVV	214075	251361	7.82%	0.493%
77	14.208	1041	1043	1045	rVV2	318725	469807	14.62%	0.921%
78	14.242	1045	1046	1047	rVV	172112	163145	5.08%	0.320%
79	14.265	1047	1048	1050	rVV2	271244	267234	8.32%	0.524%
80	14.322	1050	1053	1056	rVV5	229672	500160	15.57%	0.980%
81	14.368	1056	1057	1059	rVV2	223573	292193	9.10%	0.573%
82	14.414	1059	1061	1063	rVB2	152486	185008	5.76%	0.363%
83	14.505	1063	1069	1072	rBV6	245364	755425	23.52%	1.480%
84	14.585	1072	1076	1077	rVV2	360150	494958	15.41%	0.970%
85	14.620	1077	1079	1081	rVV3	205523	344480	10.72%	0.675%
86	14.700	1084	1086	1090	rVB4	158967	365043	11.36%	0.715%
87	14.780	1090	1093	1094	rBV3	185635	310872	9.68%	0.609%
88	14.825	1094	1097	1099	rBV4	297413	446607	13.90%	0.875%
89	14.871	1099	1101	1102	rVV2	125037	209026	6.51%	0.410%
90	14.894	1102	1103	1106	rVB2	193246	182495	5.68%	0.358%
91	14.940	1106	1107	1109	rBV2	164111	186662	5.81%	0.366%
92	14.985	1109	1111	1112	rVV2	136028	232308	7.23%	0.455%
93	15.054	1116	1117	1119	rVV2	202125	291637	9.08%	0.571%
94	15.100	1119	1121	1122	rVV2	273922	337133	10.49%	0.661%
95	15.145	1122	1125	1129	rVB3	342834	632503	19.69%	1.239%
96	15.500	1153	1156	1159	rBV	490562	644506	20.06%	1.263%
97	15.911	1188	1192	1193	rBV2	107034	177747	5.53%	0.348%
98	17.031	1287	1290	1293	rVB4	98238	189417	5.90%	0.371%
99	18.151	1385	1388	1393	rVV5	73701	224566	6.99%	0.440%
100	18.654	1431	1432	1435	rVB3	122554	150204	4.68%	0.294%

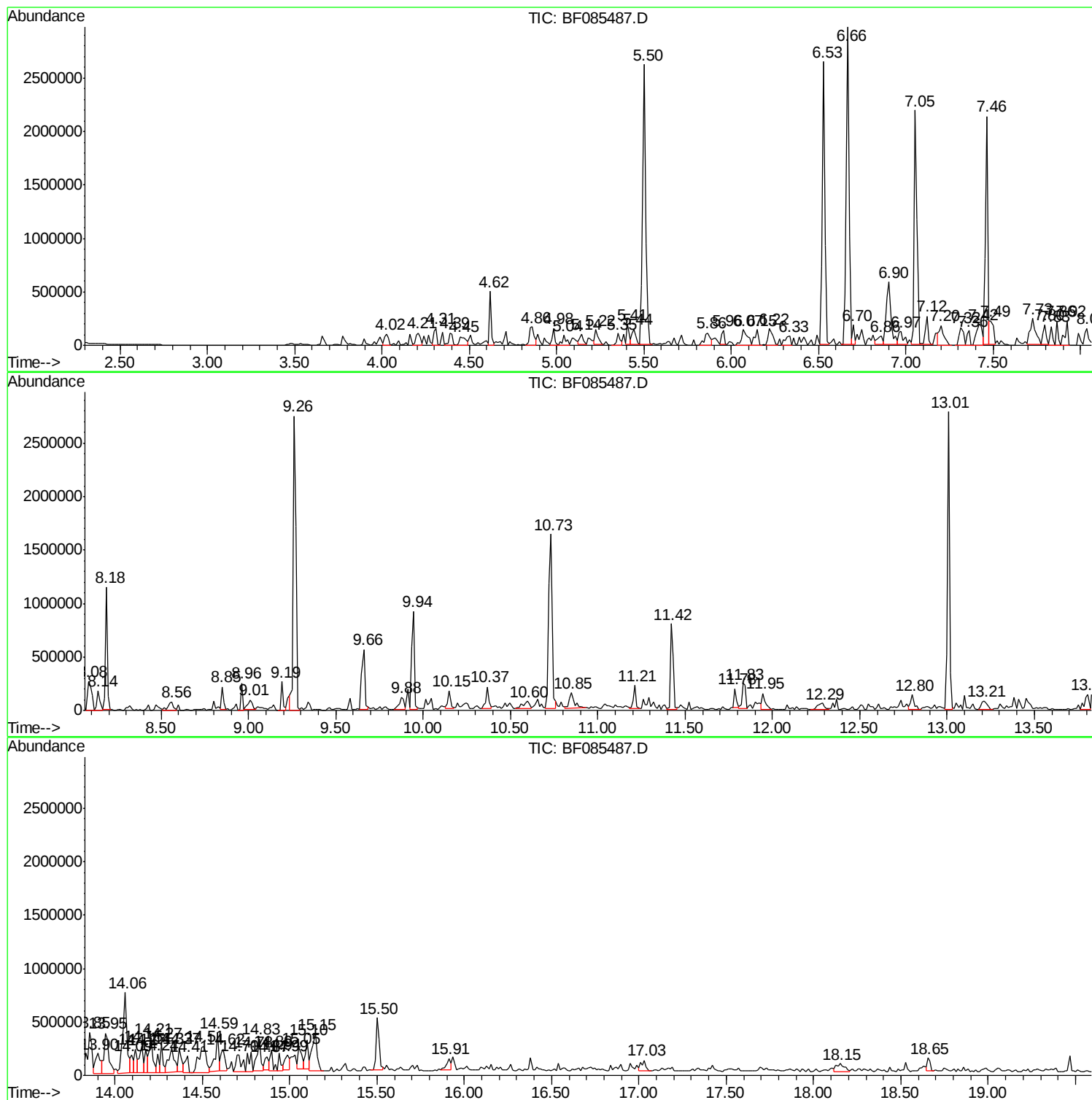
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Instrument :
BNA_F
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SP-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.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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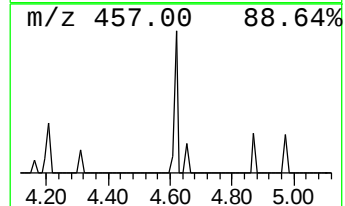
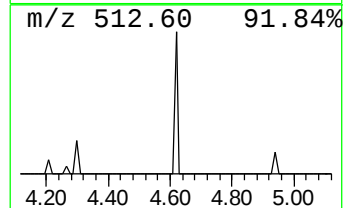
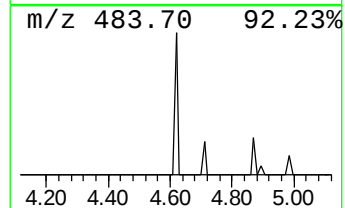
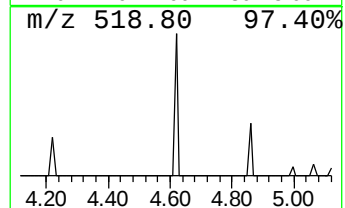
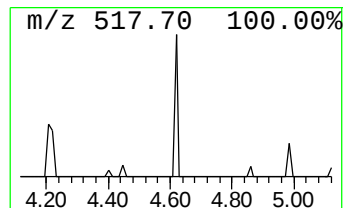
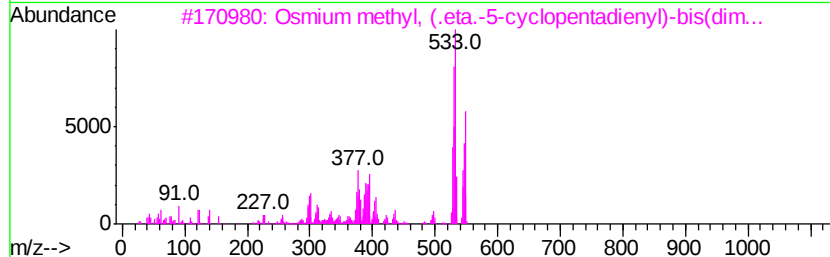
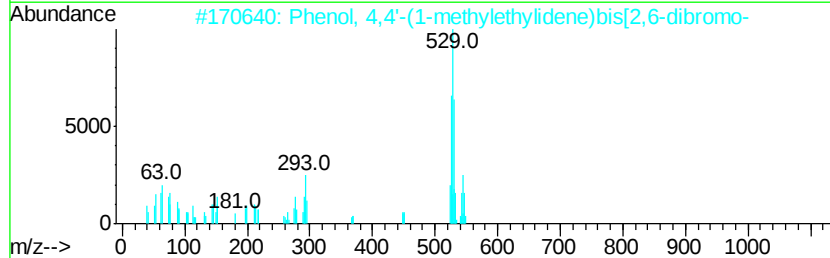
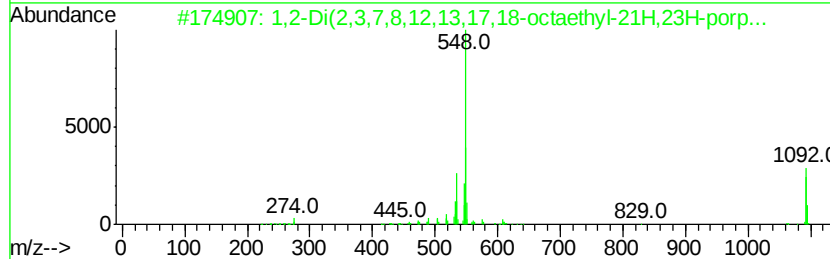
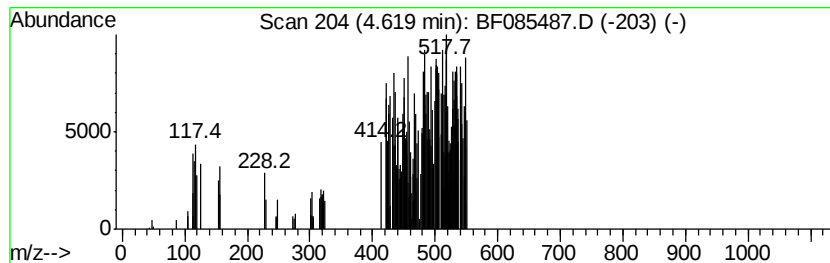
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.62 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	7.66 ng	399825	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Di(2,3,7,8,12,13,17,18-octae...	1093	C74H92N8	106085-73-8	22
2		Phenol, 4,4'-(1-methylethylidene...	540	C15H12Br4O2	000079-94-7	10
3		Osmium methyl, (.eta.-5-cyclopene...	548	C22H30O5P2	1000158-92-4	9
4		Cycloocta[1,2-b:4,3-b':5,6-b'':8...	528	C32H16S4	056598-44-8	9
5		Vanadium, oxo[2,7,12,17-tetraeth...	543	C32H36N4O5V	014055-20-0	9



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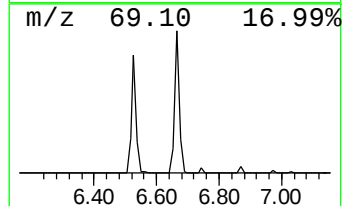
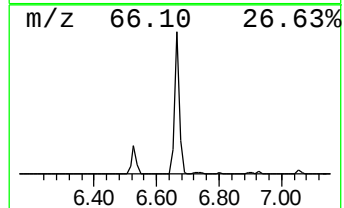
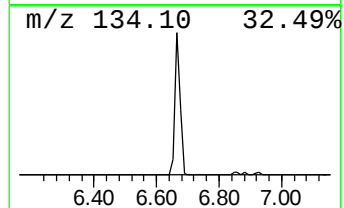
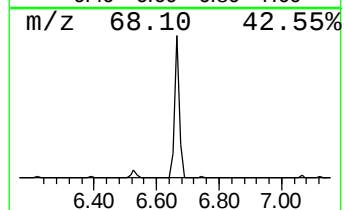
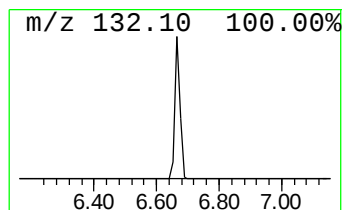
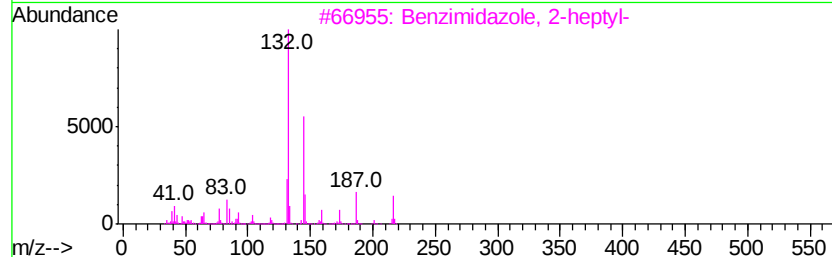
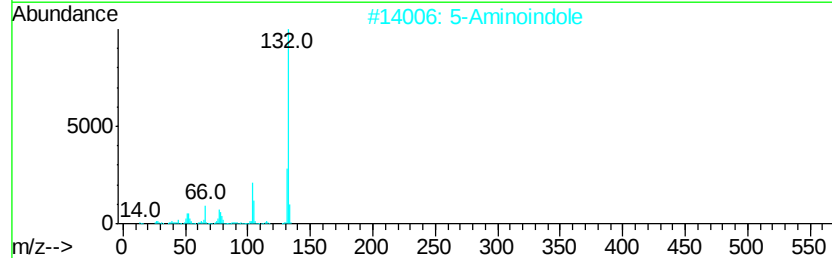
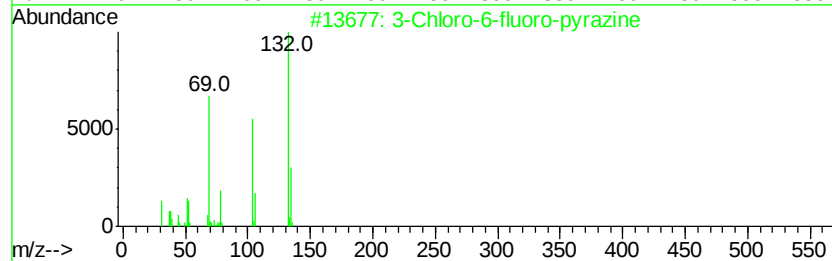
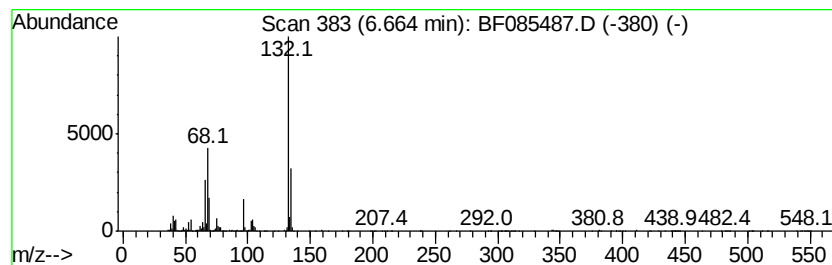
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	59.40 ng	3100640	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	10
3		Benzimidazole, 2-heptyl-	216	C14H20N2	005851-49-0	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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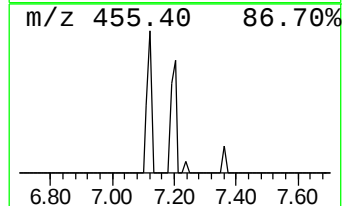
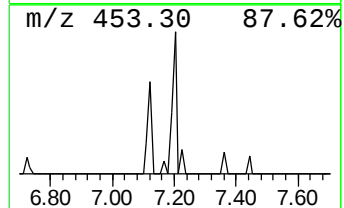
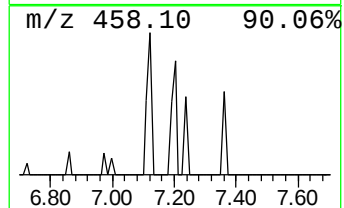
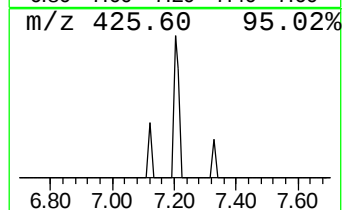
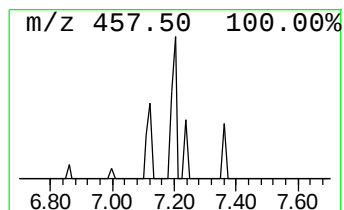
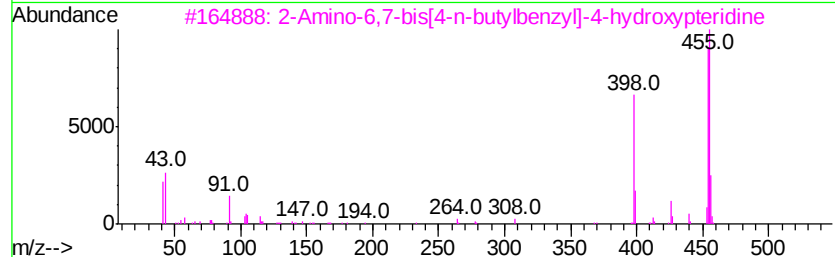
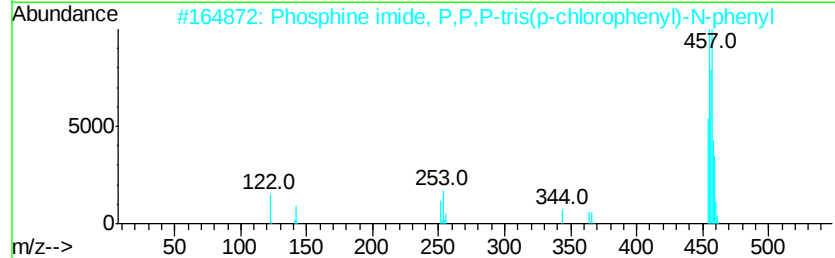
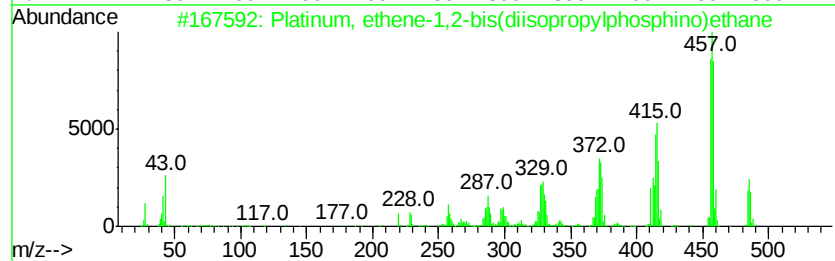
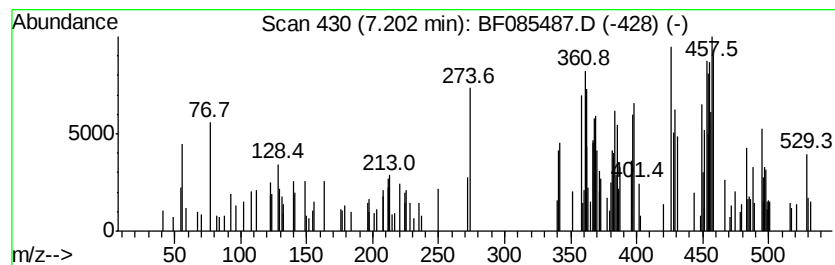
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Peak Number 4 Platinum, ethene-1,2-bis(di... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	7.12 ng	371833	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Platinum, ethene-1,2-bis(diisopr...	485	C16H36P2Pt	1000162-84-9	56
2		Phosphine imide, P,P,P-tris(p-ch...	455	C24H17Cl3NP	014796-92-0	10
3		2-Amino-6,7-bis[4-n-butylbenzyl]...	455	C28H33N5O	049647-34-9	10
4		6,17-Diacetoxv-11,12-epoxv-5,18-...	538	C34H18O7	096722-08-6	10
5		Clofazimine	472	C27H22Cl2N4	002030-63-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SP-3

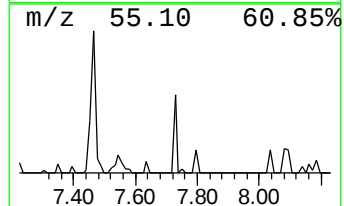
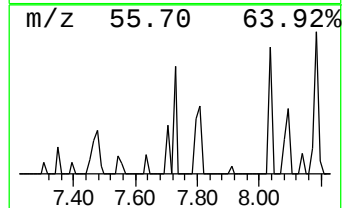
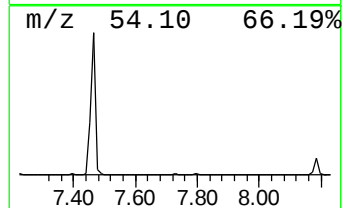
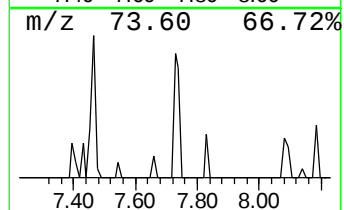
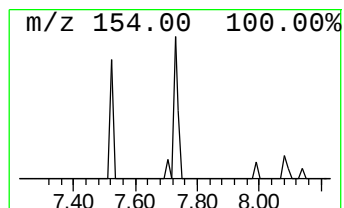
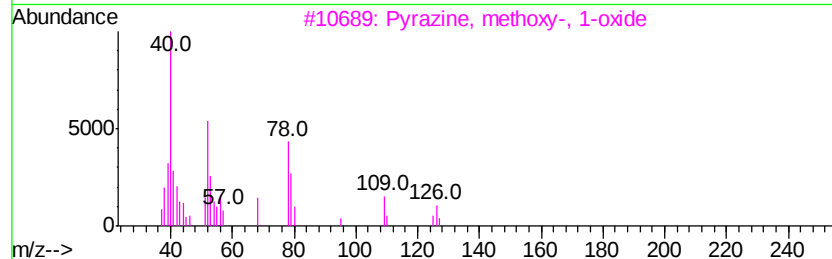
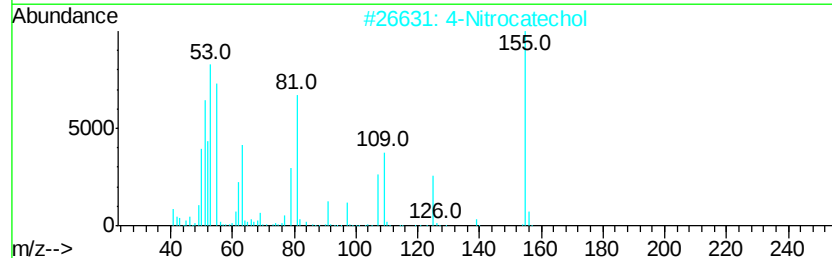
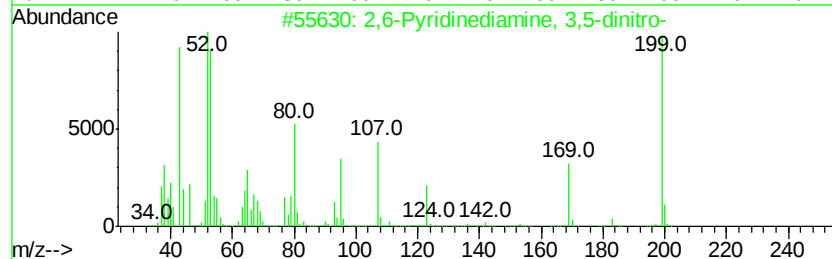
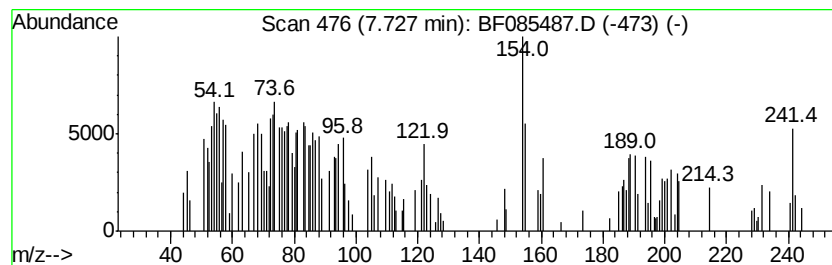
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.73 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	11.36 ng	534415	Napthalene-d8	8.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Pyridinediamine, 3,5-dinitro-	199	C5H5N5O4	034981-11-8	38	
2	4-Nitrocatechol	155	C6H5N04	003316-09-4	38	
3	Pvrazine, methoxy-, 1-oxide	126	C5H6N2O2	032046-05-2	38	
4	Phenol, 4-amino-2-nitro-	154	C6H6N2O3	000119-34-6	37	
5	3-Methyl-2-nitrophenol	153	C7H7N03	004920-77-8	35	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

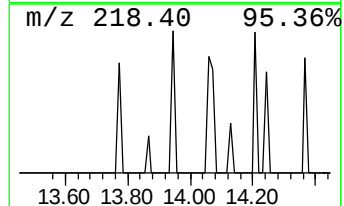
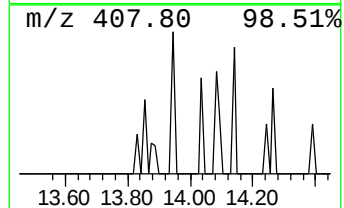
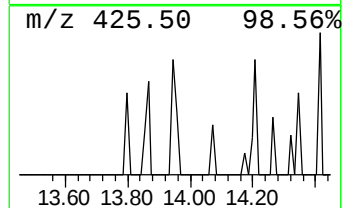
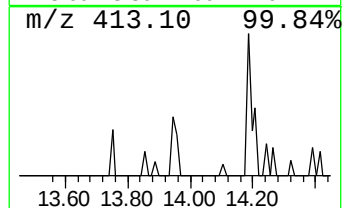
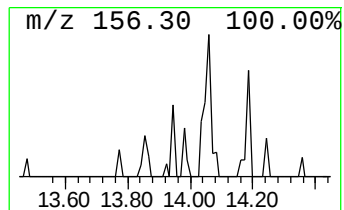
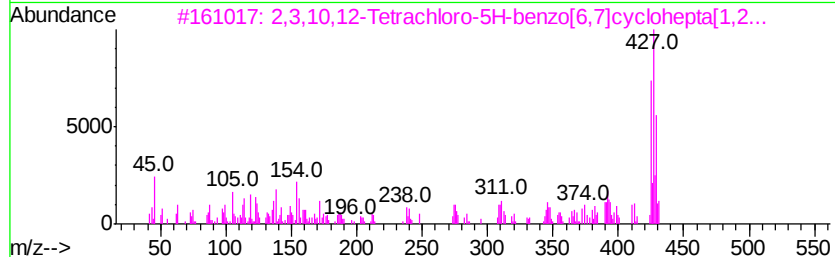
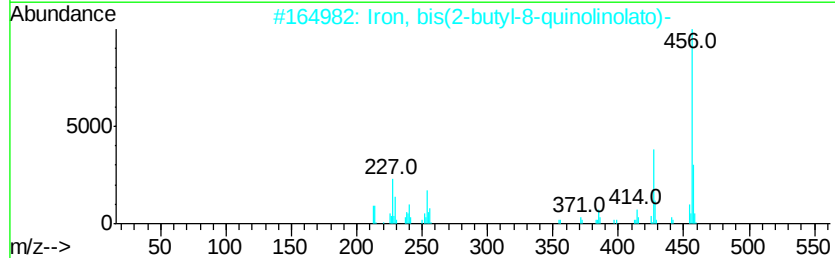
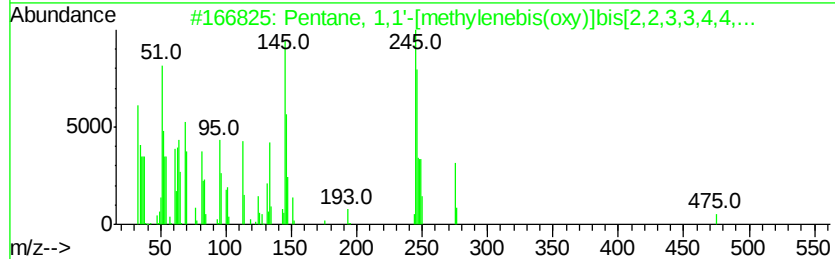
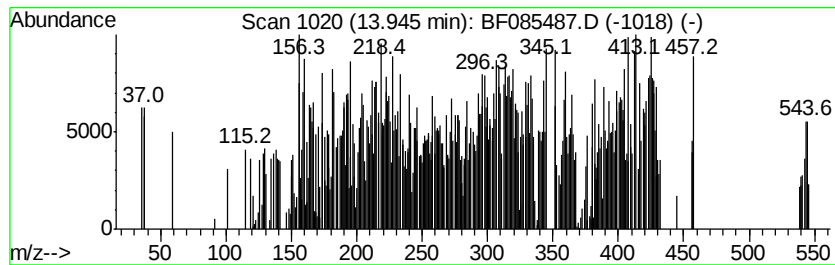
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.95 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	11.80 ng	713234	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 1,1'-[methylenebis(oxv)...	476	C11H8F16O2	084342-23-4	25
2		Iron, bis(2-butyl-8-quinolinolato)-	456	C26H28FeN2O2	030106-81-1	22
3		2,3,10,12-Tetrachloro-5H-benzo[6...	425	C19H11Cl4N02	1000252-22-8	14
4		Formosan-16-carboxylic acid,10...	428	C23H28N2O6	1000149-12-9	10
5		Germanium tetrachloride	214	Cl4Ge	010038-98-9	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

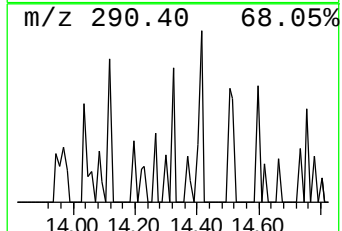
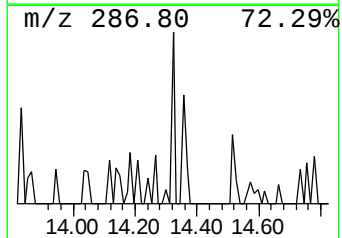
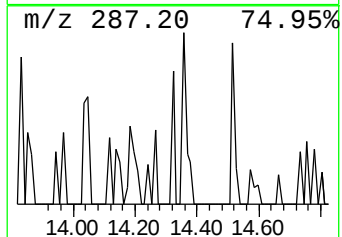
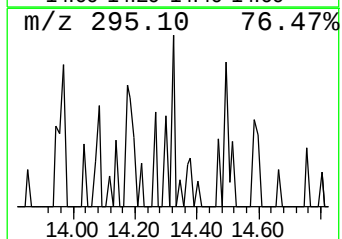
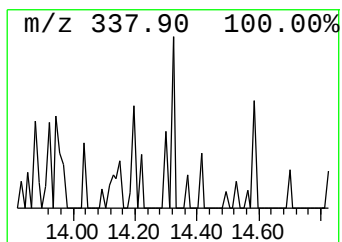
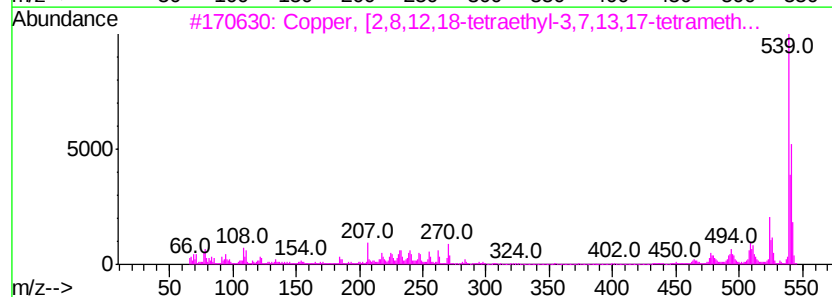
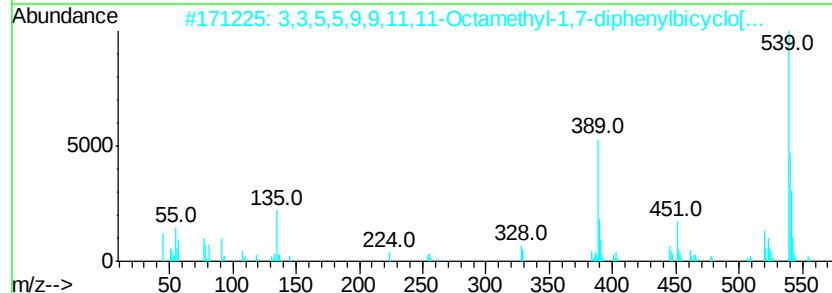
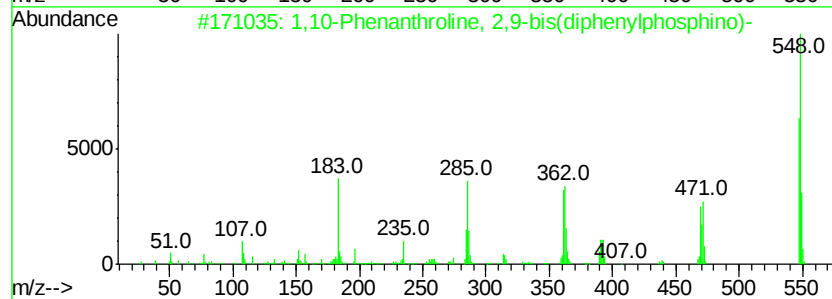
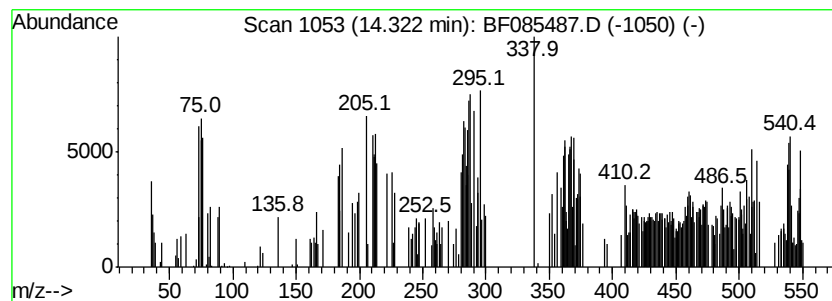
Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.32 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	8.27 ng	500160	Chrysene-d12	14.06
Hit# of	3	Tentative ID	MW MolForm	CAS# Qual
1	1,10-Phenanthroline, 2,9-bis(dip...	548 C36H26N2P2	122768-46-1	45
2	3,3,5,5,9,9,11,11-Octamethyl-1,7...	554 C20H34O7Si6	049538-51-4	10
3	Copper, [2,8,12,18-tetraethyl-3,...	539 C32H36CuN4	014055-18-6	7



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

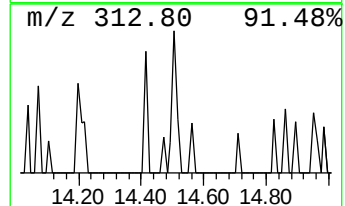
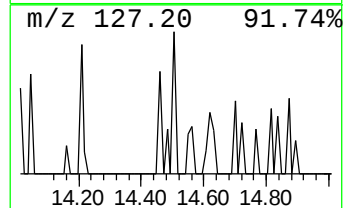
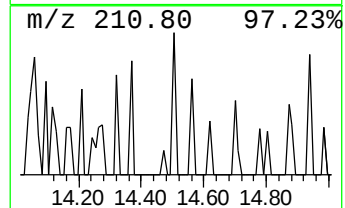
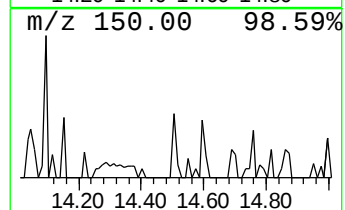
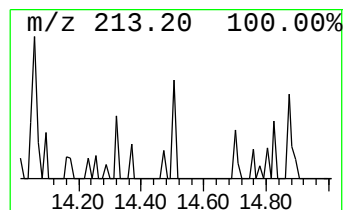
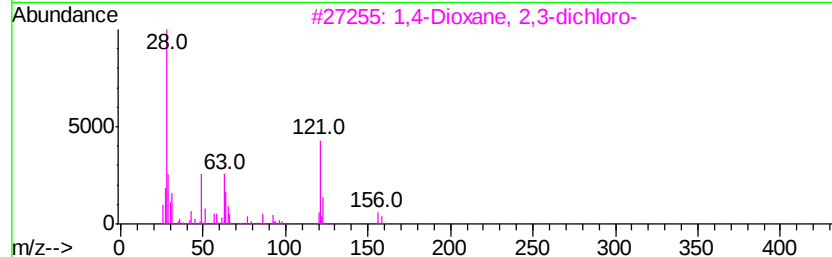
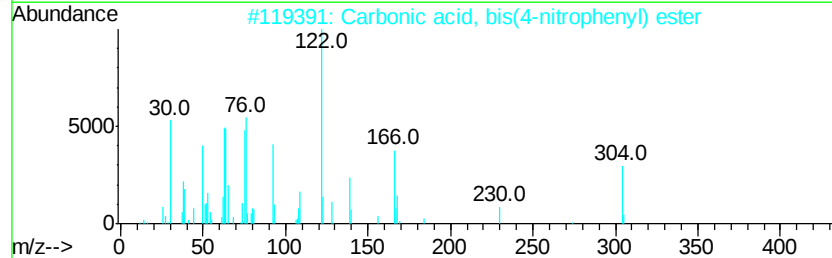
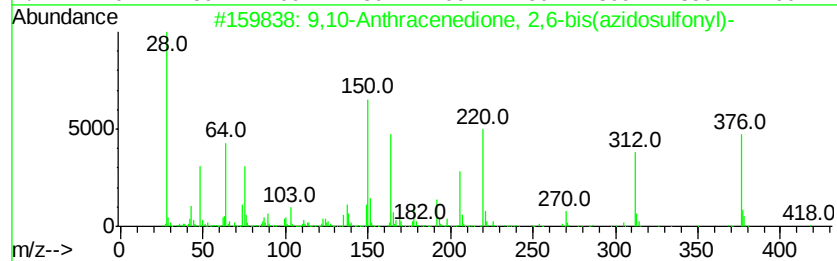
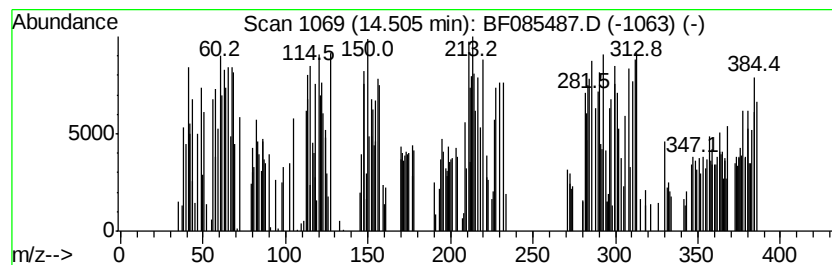
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.51 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	12.50 ng	755425	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione, 2,6-bis(az...	418	C14H6N6O6S2	1000221-52-7	27		
2	Carbonic acid, bis(4-nitrophenyl...	304	C13H8N2O7	005070-13-3	25		
3	1,4-Dioxane, 2,3-dichloro-	156	C4H6Cl2O2	000095-59-0	23		
4	4-Nitro-benzenesulfonic acid 2-c...	313	C12H8ClN05S	147991-82-0	15		
5	1H-Pyrrole-2,5-dione, 1-[4-(2-be...	290	C17H10N2O3	016707-41-8	12		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-3

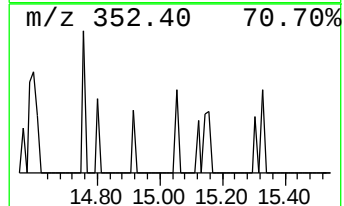
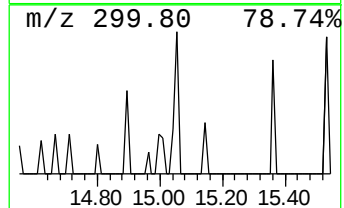
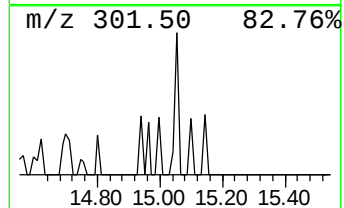
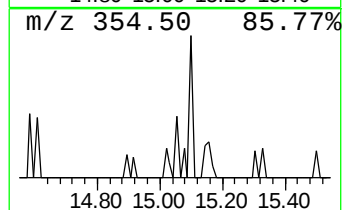
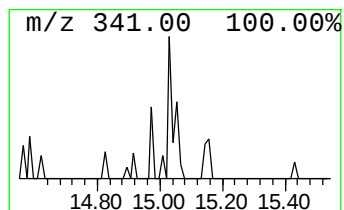
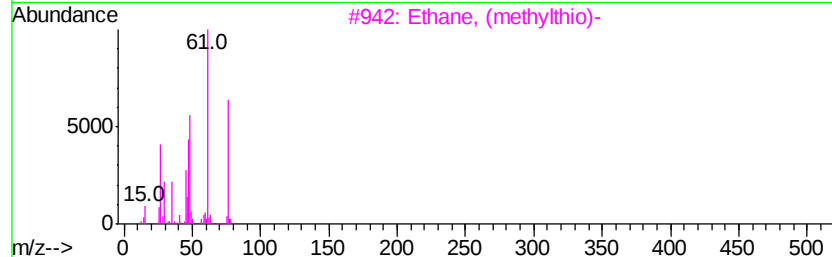
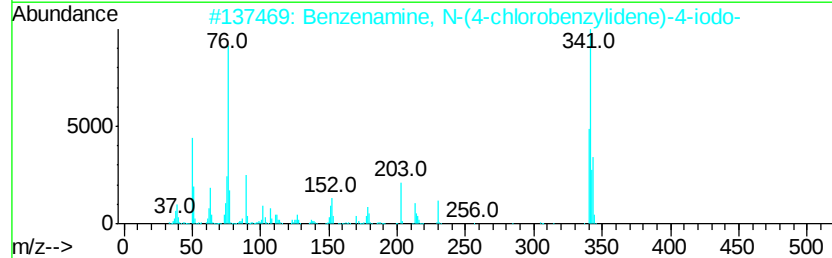
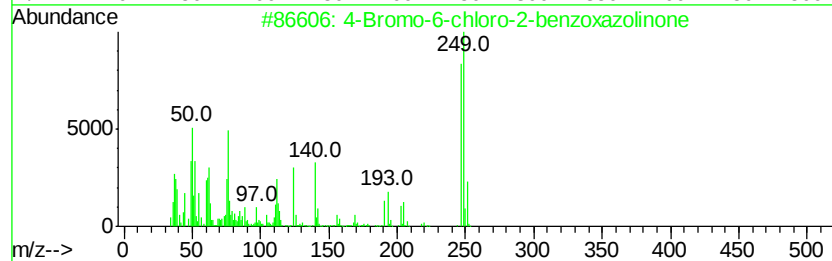
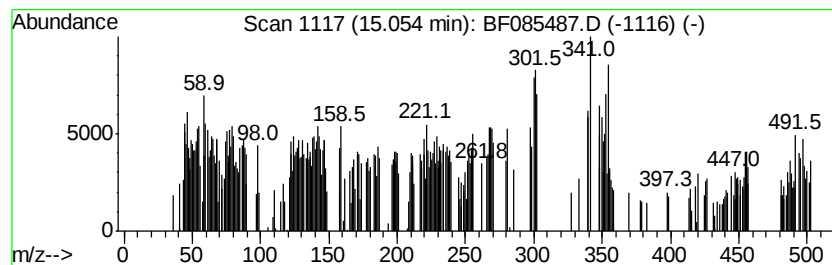
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown15.05 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	9.05 ng	291637	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Bromo-6-chloro-2-benzoxazolinone	247	C7H3BrClN02	313503-21-8	38
2			Benzenamine, N-(4-chlorobenzylidene)-4-iodo-	341	C13H9ClIN	071511-62-1	30
3			Ethane, (methylthio)-	76	C3H8S	000624-89-5	27
4			Dipalladium(0), tris[μ-bis(di...]	620	C15H42P6Pd2	1000159-26-8	16
5			1,3,4-Oxadiazole, 2-(3,4-dichlor...	350	C14H8Cl2N4O3	1000266-30-9	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085487.D
Acq On : 17 Mar 2016 3:24
Operator : UM/SJ
Sample : H1792-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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unknown6.66	6.66	59.4	ng	3100640	1	6.90	1044010	20.0
Platinum, ethene-...	7.20	7.1	ng	371833	1	6.90	1044010	20.0
unknown7.73	7.73	11.4	ng	534415	2	8.18	940966	20.0
unknown13.95	13.95	11.8	ng	713234	5	14.06	1208950	20.0
unknown14.32	14.32	8.3	ng	500160	5	14.06	1208950	20.0
unknown14.51	14.51	12.5	ng	755425	5	14.06	1208950	20.0
unknown15.05	15.05	9.1	ng	291637	6	15.50	644506	20.0