

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053116\
 Data File : BF087594.D
 Acq On : 31 May 2016 22:33
 Operator : UM/SJ
 Sample : H3222-17
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-19

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-BF052316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.918	27	29	33	rVB4	38538	64857	1.27%	0.145%
2	2.158	47	50	54	rBV5	57408	156599	3.06%	0.350%
3	2.238	54	57	59	rVV2	42413	68511	1.34%	0.153%
4	2.318	62	64	70	rVB5	37164	61438	1.20%	0.137%
5	2.970	119	121	125	rVB3	95239	119170	2.33%	0.267%
6	3.038	125	127	131	rBV2	54399	124785	2.44%	0.279%
7	4.524	254	257	262	rVB2	49043	73612	1.44%	0.165%
8	4.741	271	276	280	rBV2	31455	100561	1.96%	0.225%
9	4.821	280	283	288	rVB3	19863	56299	1.10%	0.126%
10	5.187	312	315	319	rBV4	23122	62220	1.21%	0.139%
11	5.359	327	330	342	rBV	741193	1991202	38.86%	4.454%
12	6.456	425	426	427	rBV	45726	57070	1.11%	0.128%
13	6.570	432	436	441	rVV6	55286	183599	3.58%	0.411%
14	7.016	472	475	480	rBV	557640	1229448	23.99%	2.750%
15	7.096	480	482	493	rVV	2556542	4371707	85.32%	9.779%
16	7.302	497	500	506	rVB4	21485	81729	1.60%	0.183%
17	7.450	511	513	522	rBV	435105	834719	16.29%	1.867%
18	7.679	530	533	543	rVB	1967702	3462961	67.58%	7.746%
19	8.090	566	569	571	rVV3	41155	94656	1.85%	0.212%
20	8.148	571	574	578	rVV4	47175	159713	3.12%	0.357%
21	8.365	591	593	605	rBV	1975758	3126229	61.01%	6.993%
22	8.970	644	646	648	rBV2	34875	56602	1.10%	0.127%
23	9.199	663	666	670	rVB3	26577	70384	1.37%	0.157%
24	9.370	678	681	685	rBV2	19577	56774	1.11%	0.127%
25	9.485	689	691	696	rBV	460722	1008394	19.68%	2.256%
26	9.679	705	708	711	rVB3	43946	81329	1.59%	0.182%
27	9.931	727	730	732	rVB2	42330	61340	1.20%	0.137%
28	11.245	842	845	848	rBV	3251982	5124062	100.00%	11.462%
29	11.405	857	859	860	rBV2	39653	60352	1.18%	0.135%
30	11.428	860	861	866	rVB2	66785	112055	2.19%	0.251%
31	11.908	901	903	905	rVB2	41921	53789	1.05%	0.120%
32	11.965	905	908	910	rBV3	56553	119869	2.34%	0.268%
33	12.011	910	912	914	rVB2	62789	122766	2.40%	0.275%
34	12.068	914	917	921	rBV5	58026	172087	3.36%	0.385%

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35	12.297	935	937	945	rBV	730470	1213042	23.67%	2.713%
36	12.422	947	948	951	rVB2	69165	73538	1.44%	0.164%
37	13.599	1048	1051	1057	rBV	2199426	3518351	68.66%	7.870%
38	13.691	1057	1059	1061	rVB3	37601	81613	1.59%	0.183%
39	13.851	1070	1073	1074	rBV3	36846	90163	1.76%	0.202%
40	13.885	1074	1076	1083	rVB5	84556	279035	5.45%	0.624%
41	14.080	1091	1093	1095	rBV2	46680	70197	1.37%	0.157%
42	14.114	1095	1096	1098	rVV2	55612	69311	1.35%	0.155%
43	14.160	1098	1100	1101	rVV2	71558	110828	2.16%	0.248%
44	14.194	1101	1103	1106	rVV4	60400	154978	3.02%	0.347%
45	14.251	1106	1108	1109	rVB	106595	119013	2.32%	0.266%
46	14.297	1109	1112	1113	rBV	156230	270955	5.29%	0.606%
47	14.342	1113	1116	1117	rVV2	47303	90948	1.77%	0.203%
48	14.388	1117	1120	1121	rVB2	46837	75548	1.47%	0.169%
49	14.434	1121	1124	1129	rVB2	161608	363562	7.10%	0.813%
50	14.548	1129	1134	1137	rBV5	68818	266982	5.21%	0.597%
51	14.708	1146	1148	1158	rBV	625850	1343390	26.22%	3.005%
52	15.051	1176	1178	1182	rVB4	47684	111787	2.18%	0.250%
53	15.120	1182	1184	1194	rVB	61811	130662	2.55%	0.292%
54	16.103	1268	1270	1273	rVB3	33815	56657	1.11%	0.127%
55	16.320	1286	1289	1290	rBV	29388	51675	1.01%	0.116%
56	16.343	1290	1291	1294	rVV2	66158	94651	1.85%	0.212%
57	16.423	1294	1298	1301	rVV4	103639	235426	4.59%	0.527%
58	16.468	1301	1302	1305	rVV2	44017	88228	1.72%	0.197%
59	16.525	1305	1307	1308	rVV2	45941	79772	1.56%	0.178%
60	16.594	1311	1313	1316	rVV4	116427	224885	4.39%	0.503%
61	16.686	1318	1321	1324	rVV5	45220	142998	2.79%	0.320%
62	16.743	1324	1326	1328	rVB2	53671	81503	1.59%	0.182%
63	16.800	1328	1331	1337	rBV	132945	271312	5.29%	0.607%
64	17.063	1351	1354	1357	rBV	3969106	4772222	93.13%	10.675%
65	17.863	1419	1424	1428	rBV6	83800	224244	4.38%	0.502%
66	17.920	1428	1429	1432	rVV3	81064	109795	2.14%	0.246%
67	17.966	1432	1433	1436	rVV3	62990	92224	1.80%	0.206%
68	18.057	1436	1441	1444	rVV6	65849	178248	3.48%	0.399%
69	18.126	1444	1447	1448	rVV	105358	163634	3.19%	0.366%
70	18.217	1452	1455	1461	rVB6	101052	259644	5.07%	0.581%
71	18.389	1467	1470	1471	rBV3	41838	92489	1.80%	0.207%

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72	18.434	1471	1474	1489	rVB	545731	1633523	31.88%	3.654%
73	18.846	1508	1510	1512	rBV2	50429	89750	1.75%	0.201%
74	18.914	1514	1516	1519	rVV2	35747	57712	1.13%	0.129%
75	19.063	1524	1529	1530	rBV5	97103	180708	3.53%	0.404%
76	19.109	1530	1533	1534	rBV2	71343	126931	2.48%	0.284%
77	19.326	1550	1552	1553	rBV2	59951	72688	1.42%	0.163%
78	19.360	1553	1555	1557	rVB3	101410	113574	2.22%	0.254%
79	19.417	1557	1560	1564	rBV4	26251	85605	1.67%	0.191%
80	19.600	1575	1576	1580	rBV4	51814	128321	2.50%	0.287%
81	19.657	1580	1581	1584	rVB3	68083	125288	2.45%	0.280%
82	19.703	1584	1585	1588	rBV3	54161	118411	2.31%	0.265%
83	19.954	1605	1607	1608	rBV2	38265	73183	1.43%	0.164%
84	20.012	1610	1612	1614	rVV3	40977	81118	1.58%	0.181%
85	20.069	1614	1617	1619	rVV4	53493	153387	2.99%	0.343%
86	20.114	1619	1621	1628	rVV	415983	1150028	22.44%	2.572%
87	20.206	1628	1629	1636	rVV7	90654	354986	6.93%	0.794%
88	20.297	1636	1637	1638	rVV	75980	56009	1.09%	0.125%
89	20.354	1638	1642	1644	rVV5	85562	230920	4.51%	0.517%
90	22.595	1835	1838	1841	rBV5	53566	159529	3.11%	0.357%
91	22.640	1841	1842	1847	rVV4	48403	140431	2.74%	0.314%
92	22.720	1847	1849	1852	rVV3	46442	91660	1.79%	0.205%
93	22.835	1855	1859	1860	rBV3	38332	72420	1.41%	0.162%
94	22.892	1860	1864	1865	rVB4	30448	66670	1.30%	0.149%
95	23.955	1952	1957	1958	rBV4	42664	108920	2.13%	0.244%

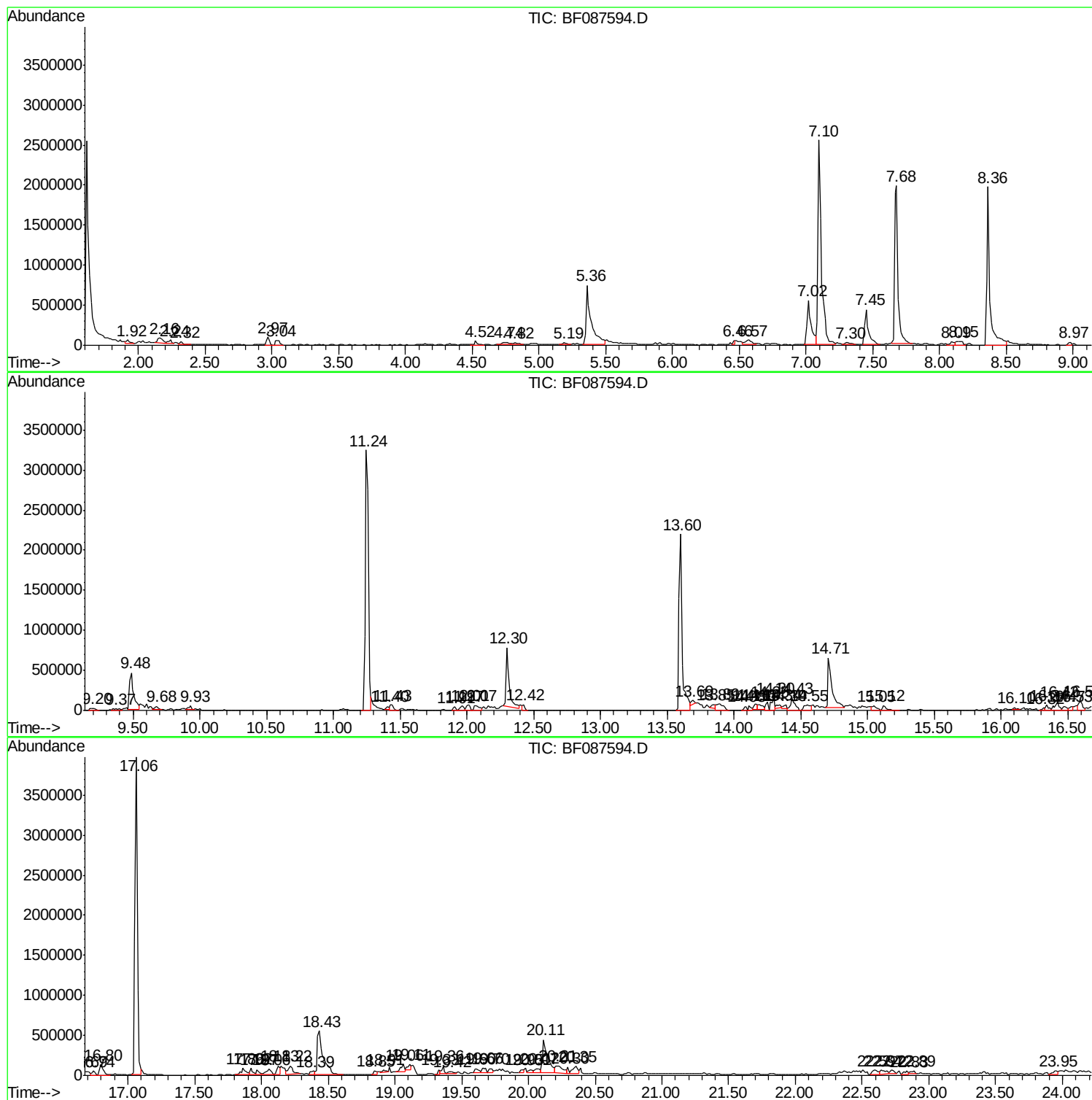
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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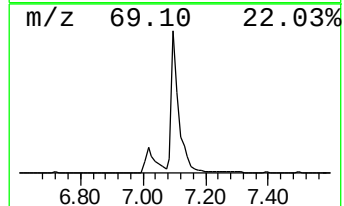
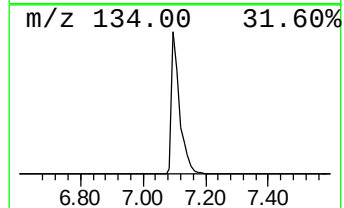
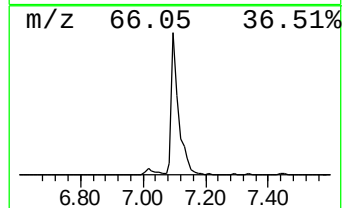
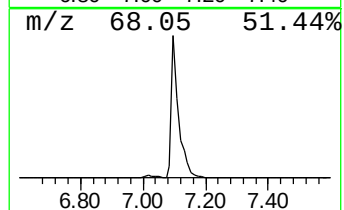
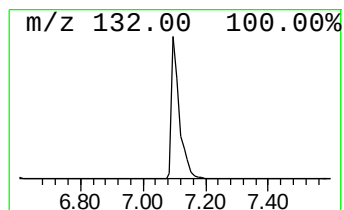
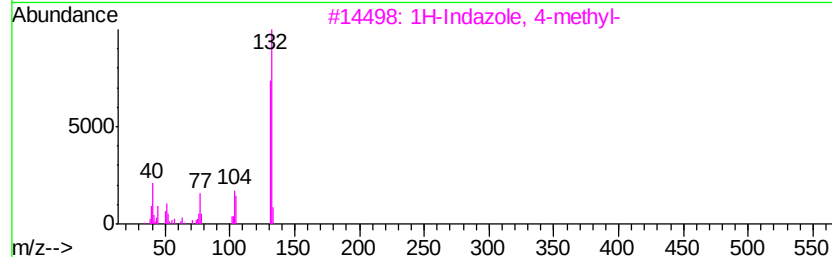
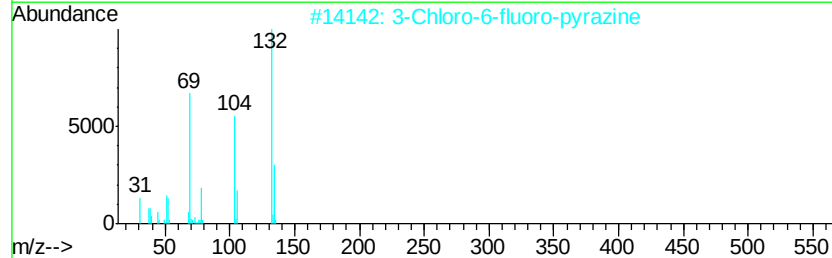
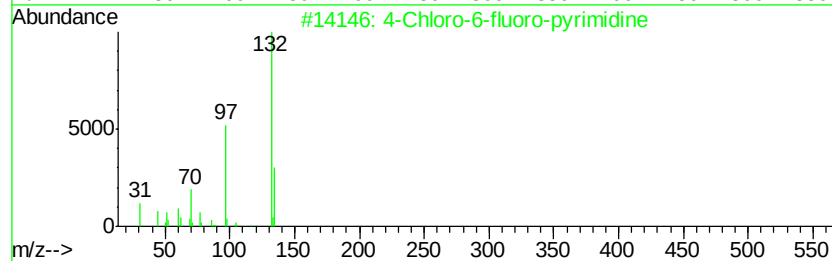
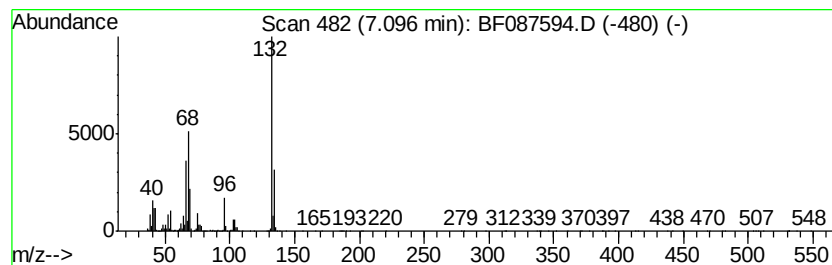
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	104.75 ng	4371710	1,4-Dichlorobenzene-d4	7.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Indazole, 4-methyl-	132	C8H8N2	1000316-00-9	25
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	22



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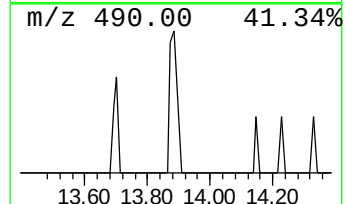
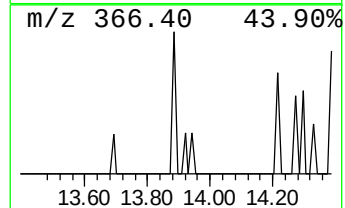
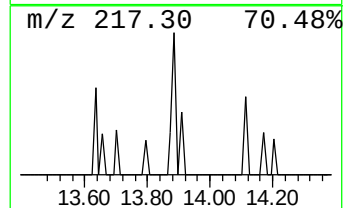
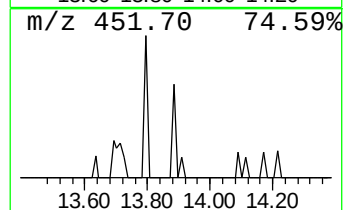
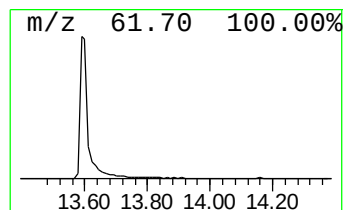
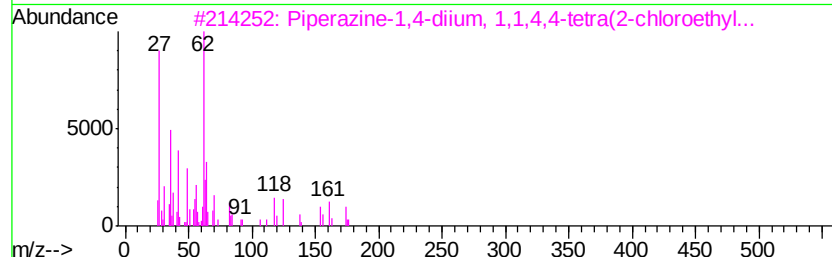
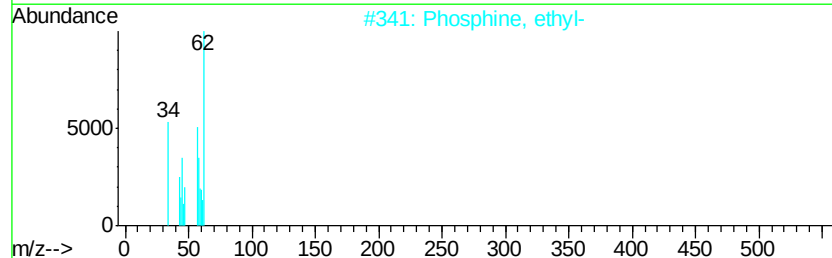
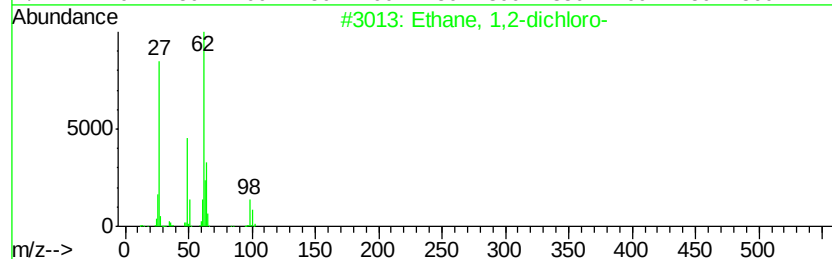
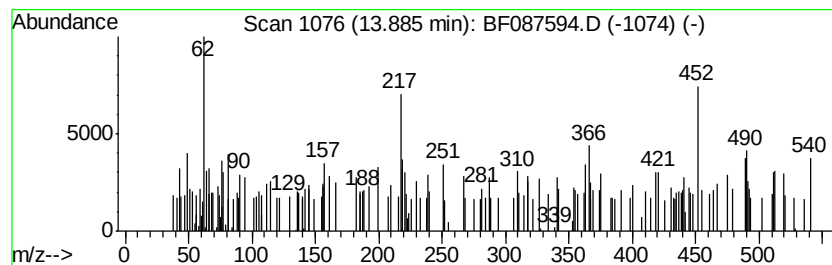
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown13.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	4.15 ng	279035	Phenanthrene-d10	14.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, 1,2-dichloro-	98	C2H4Cl2	000107-06-2	38
2		Phosphine, ethyl-	62	C2H7P	000593-68-0	27
3		Piperazine-1,4-diium, 1,1,4,4-te...	406	C12H24Cl6N2	1000273-25-3	16
4		Iron, .eta.-8-(3,6-dimethylene-1...	308	C16H29FeP	1000161-75-7	16
5		Ethene, chloro-	62	C2H3Cl	000075-01-4	16



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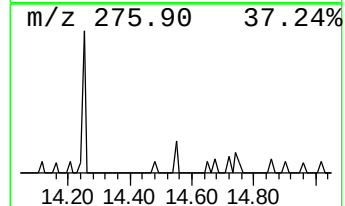
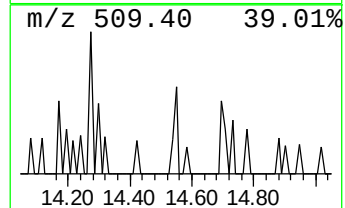
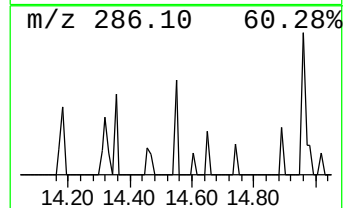
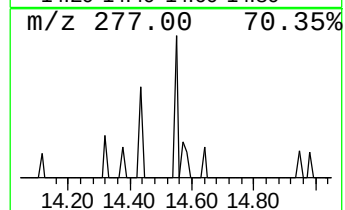
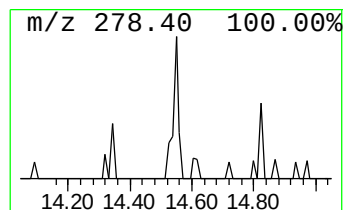
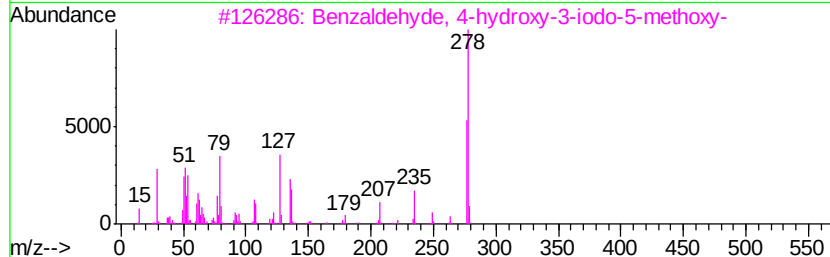
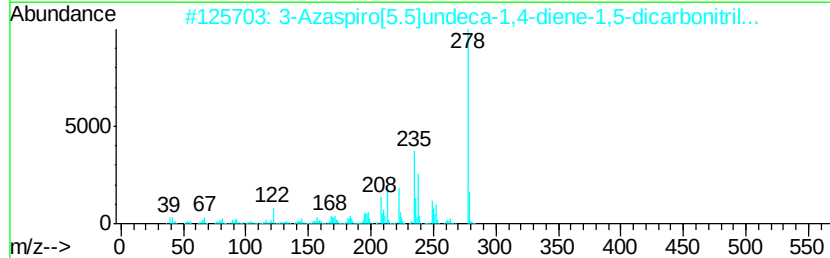
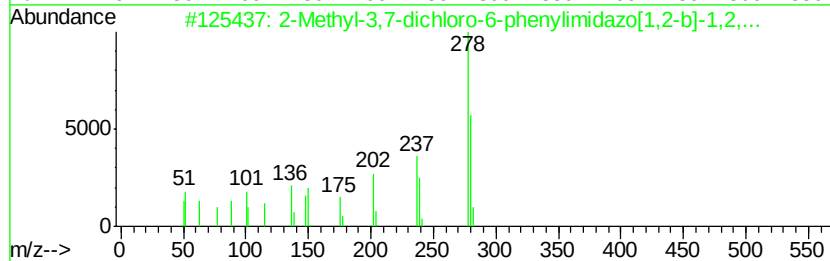
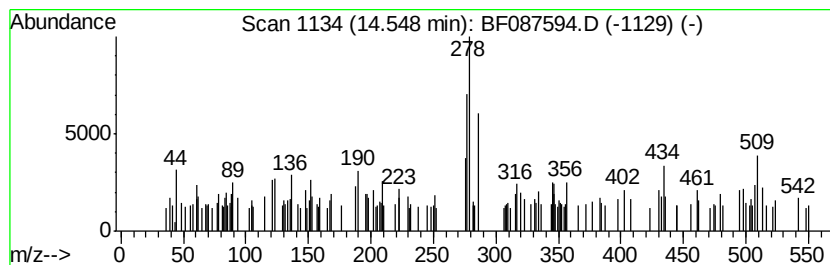
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown14.55 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	3.97 ng	266982	Phenanthrene-d10	14.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Methyl-3,7-dichloro-6-phenylim...	278	C12H8Cl2N4	107805-86-7	25
2		3-Azaspiro[5.5]undeca-1,4-diene-...	278	C15H14N6	1000303-13-2	25
3		Benzaldehyde, 4-hydroxy-3-iodo-5...	278	C8H7IO3	005438-36-8	22
4		Benzoic acid, 3,5-dibromo-2-hydr...	294	C7H4Br2O3	003147-55-5	22
5		Naphthalene, 2,6-dimethoxy-1,5-d...	278	C12H10N2O6	025314-97-0	22



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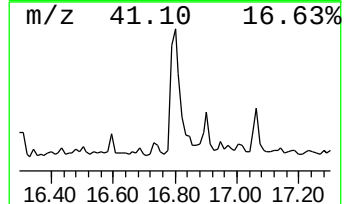
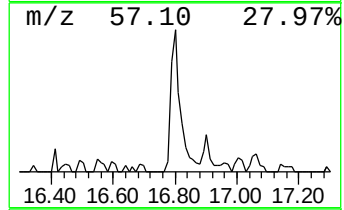
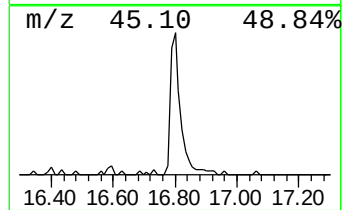
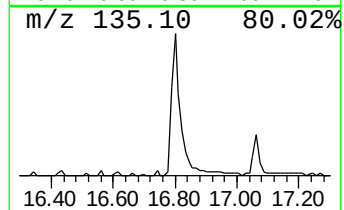
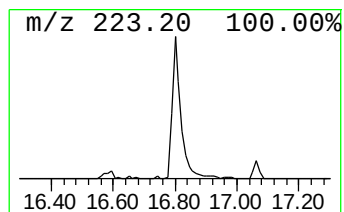
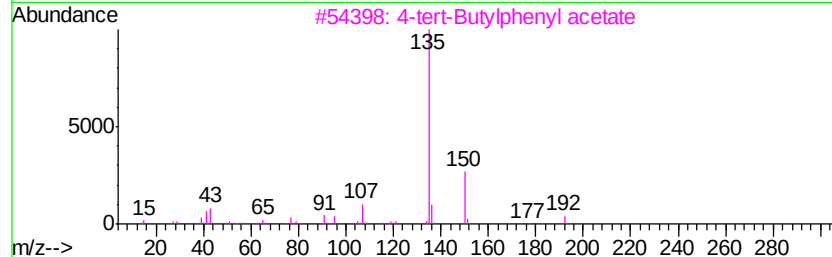
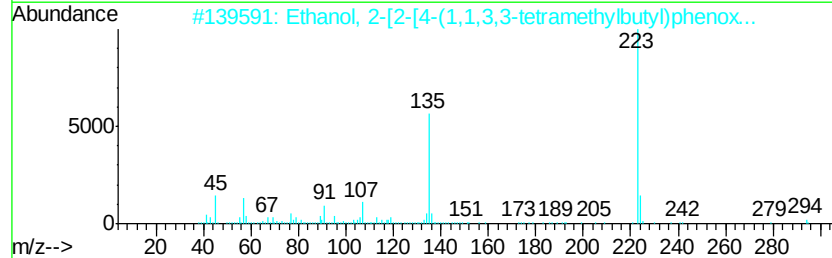
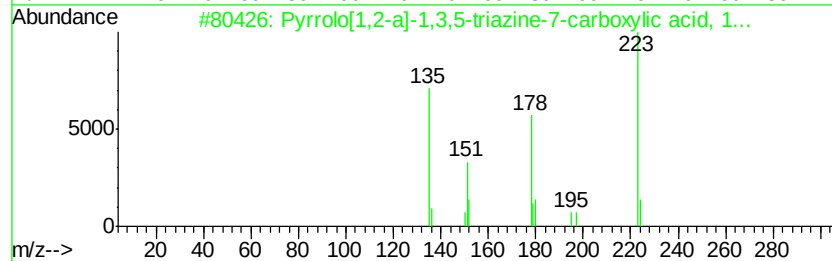
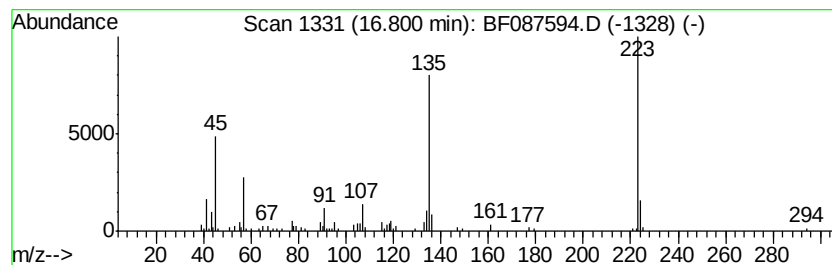
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	3.32 ng	271312	Chrysene-d12	18.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	64
3		4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	27
4		Methanol, (cyclohexyl)(2,3-dimet...	218	C15H22O	349498-47-1	27
5		((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053116\
Data File : BF087594.D
Acq On : 31 May 2016 22:33
Operator : UM/SJ
Sample : H3222-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-19

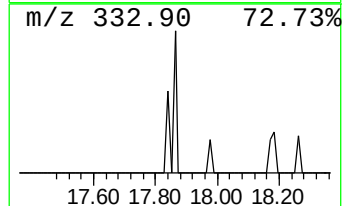
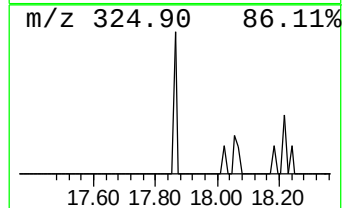
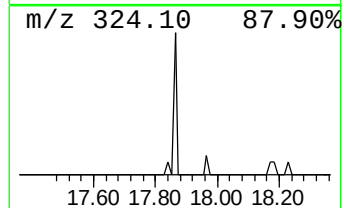
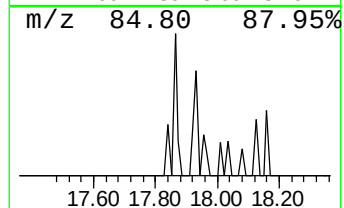
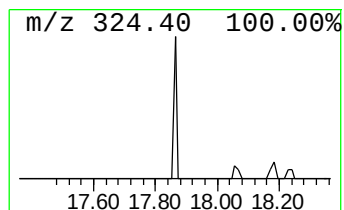
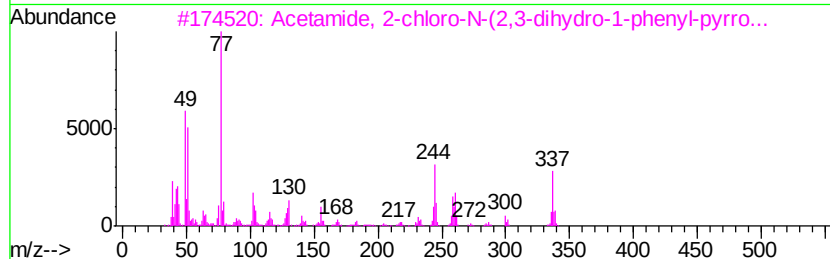
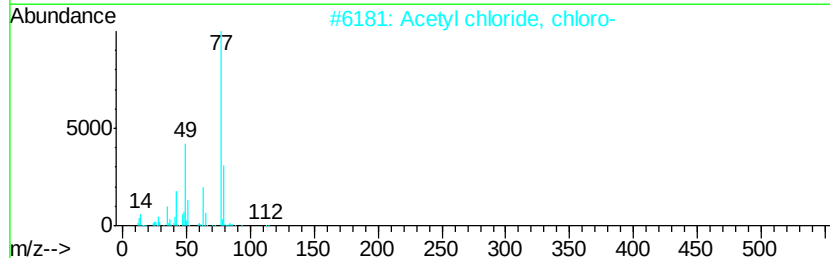
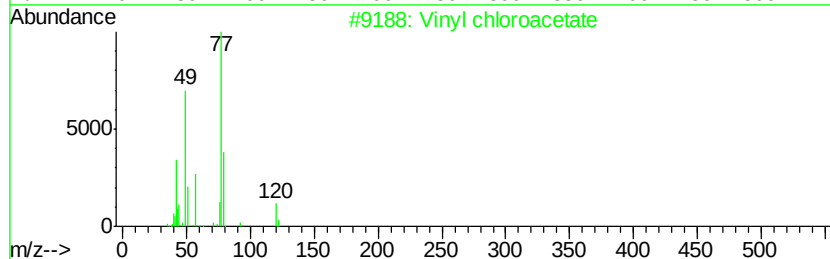
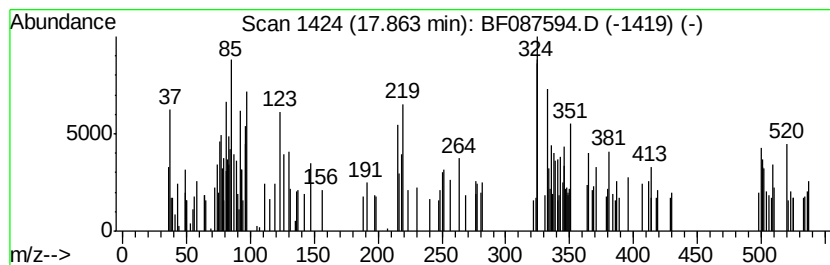
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.86 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	2.75 ng	224244	Chrysene-d12	18.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vinyl chloroacetate	120	C4H5ClO2	002549-51-1	27
2		Acetyl chloride, chloro-	112	C2H2Cl2O	000079-04-9	16
3		Acetamide, 2-chloro-N-(2,3-dihyd...	337	C19H16ClN3O	230308-42-6	16
4		2-Propanone, 1,3-dichloro-	126	C3H4Cl2O	000534-07-6	12
5		Trichloroacetamidoxime	176	C2H3Cl3N2O	002533-67-7	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053116\
Data File : BF087594.D
Acq On : 31 May 2016 22:33
Operator : UM/SJ
Sample : H3222-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.10	7.10	104.8	ng	4371710	1	7.45	834719	20.0
unknown13.89	13.89	4.2	ng	279035	4	14.71	1343390	20.0
unknown14.55	14.55	4.0	ng	266982	4	14.71	1343390	20.0
Pyrrolo[1,2-a]-1,...	16.80	3.3	ng	271312	5	18.43	1633520	20.0
unknown17.86	17.86	2.8	ng	224244	5	18.43	1633520	20.0