

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
 Data File : BF100139.D
 Acq On : 3 Nov 2017 17:22
 Operator : SJ/JU
 Sample : PB103911BSD
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB103911BSD

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-BF102317.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	2.575	80	83	99	rBV	118788	175681	6.58%	0.221%
2	3.293	201	205	211	rBV2	106292	182320	6.82%	0.229%
3	3.334	211	212	225	rVV	122472	242330	9.07%	0.305%
4	4.957	485	488	491	rBV	49050	43940	1.64%	0.055%
5	4.992	491	494	514	rVB	297020	451962	16.92%	0.568%
6	5.404	561	564	589	rBV	799486	1088585	40.75%	1.369%
7	6.334	720	722	734	rBV	232307	323903	12.12%	0.407%
8	6.422	734	737	739	rBV	1089685	1319828	49.40%	1.660%
9	6.504	748	751	755	rVB	513434	457885	17.14%	0.576%
10	6.545	755	758	774	rVB2	1357044	1839314	68.85%	2.313%
11	6.704	782	785	793	rBV	796170	751492	28.13%	0.945%
12	6.769	793	796	797	rVV	524697	482715	18.07%	0.607%
13	6.787	797	799	813	rVB	759804	721550	27.01%	0.907%
14	6.922	818	822	838	rBV3	1847483	2662130	99.65%	3.348%
15	7.039	838	842	857	rVV	1092740	1323173	49.53%	1.664%
16	7.186	861	867	877	rBV2	1262855	2014820	75.42%	2.534%
17	7.269	877	881	885	rVV	624944	586593	21.96%	0.738%
18	7.345	889	894	896	rVV	934038	1237497	46.32%	1.556%
19	7.363	896	897	908	rVV	489058	312237	11.69%	0.393%
20	7.451	908	912	924	rVB	362057	369020	13.81%	0.464%
21	7.592	932	936	947	rBV	646679	763632	28.58%	0.960%
22	7.675	947	950	954	rVV	437213	430524	16.12%	0.541%
23	7.716	954	957	967	rVV	1024571	891454	33.37%	1.121%
24	7.798	967	971	976	rVV	633045	610738	22.86%	0.768%
25	7.881	976	985	990	rVV	192523	383554	14.36%	0.482%
26	7.928	990	993	1000	rVV	576621	742505	27.79%	0.934%
27	7.992	1000	1004	1008	rVV	869178	839926	31.44%	1.056%
28	8.051	1009	1014	1015	rVV	698206	703002	26.32%	0.884%
29	8.069	1015	1017	1025	rVB	1075816	1046245	39.16%	1.316%
30	8.139	1025	1029	1031	rBV	277914	295833	11.07%	0.372%
31	8.175	1031	1035	1039	rVB	657778	723200	27.07%	0.910%
32	8.516	1087	1093	1097	rBV	252293	303325	11.35%	0.381%
33	8.557	1097	1100	1110	rVV3	58278	158277	5.92%	0.199%
34	8.633	1110	1113	1121	rVV	737194	747608	27.99%	0.940%

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35	8.716	1121	1127	1131	rVV	528173	638901	23.92%	0.804%
36	8.763	1131	1135	1139	rVV	1327921	1277806	47.83%	1.607%
37	8.822	1140	1145	1147	rVV	177791	221266	8.28%	0.278%
38	8.863	1147	1152	1156	rVV	1428152	1461693	54.72%	1.838%
39	8.904	1156	1159	1161	rVV	280183	280503	10.50%	0.353%
40	8.933	1161	1164	1172	rVB	850495	794763	29.75%	1.000%
41	9.057	1181	1185	1191	rBV2	718848	843981	31.59%	1.061%
42	9.122	1191	1196	1200	rBV	2090092	2671451	100.00%	3.360%
43	9.228	1208	1214	1216	rBV	1474895	1353738	50.67%	1.703%
44	9.257	1216	1219	1227	rVB	1222848	1074949	40.24%	1.352%
45	9.369	1235	1238	1247	rBV	642111	559466	20.94%	0.704%
46	9.527	1260	1265	1274	rVB	1149585	1236238	46.28%	1.555%
47	9.610	1274	1279	1284	rBV	947220	965830	36.15%	1.215%
48	9.669	1284	1289	1293	rVV	1469182	1428690	53.48%	1.797%
49	9.733	1296	1300	1303	rBV	81367	62812	2.35%	0.079%
50	9.786	1306	1309	1310	rBV	394401	339422	12.71%	0.427%
51	9.804	1310	1312	1315	rVV	781049	798519	29.89%	1.004%
52	9.839	1315	1318	1322	rVB	1470175	1316528	49.28%	1.656%
53	9.916	1328	1331	1335	rBV	154930	201910	7.56%	0.254%
54	9.957	1335	1338	1344	rVV2	480327	806336	30.18%	1.014%
55	10.016	1344	1348	1359	rVV2	1485975	1797771	67.30%	2.261%
56	10.098	1359	1362	1367	rVV	516926	532852	19.95%	0.670%
57	10.145	1367	1370	1378	rVV	647602	658167	24.64%	0.828%
58	10.227	1378	1384	1387	rVV	1141683	1001329	37.48%	1.259%
59	10.263	1387	1390	1398	rVV	68850	74637	2.79%	0.094%
60	10.345	1398	1404	1405	rVV	1228977	1257789	47.08%	1.582%
61	10.357	1405	1406	1410	rVV	1473452	946897	35.45%	1.191%
62	10.404	1411	1414	1418	rBV	430048	434028	16.25%	0.546%
63	10.439	1418	1420	1422	rVV	227990	242040	9.06%	0.304%
64	10.469	1422	1425	1428	rVV	1411800	1282021	47.99%	1.612%
65	10.510	1428	1432	1435	rVB	963156	908801	34.02%	1.143%
66	10.604	1444	1448	1456	rBV	852105	758396	28.39%	0.954%
67	10.833	1482	1487	1495	rVB	953938	793113	29.69%	0.997%
68	10.910	1495	1500	1507	rBV	866003	758073	28.38%	0.953%
69	10.998	1507	1515	1518	rBV	974228	820769	30.72%	1.032%
70	11.116	1532	1535	1545	rBV	430502	501148	18.76%	0.630%
71	11.186	1545	1547	1552	rVB2	40428	36655	1.37%	0.046%

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72	11.298	1562	1566	1568	rBV	864012	759484	28.43%	0.955%
73	11.322	1568	1570	1574	rVV	1411788	1306982	48.92%	1.644%
74	11.380	1576	1580	1588	rVB	1426038	1351357	50.59%	1.700%
75	11.539	1603	1607	1621	rBV	1307109	1172882	43.90%	1.475%
76	11.845	1654	1659	1663	rBV	1254958	1106044	41.40%	1.391%
77	12.516	1769	1773	1786	rBV	1454440	1316113	49.27%	1.655%
78	12.639	1791	1794	1799	rVV	365285	408152	15.28%	0.513%
79	12.680	1799	1801	1804	rVV2	56024	51381	1.92%	0.065%
80	12.745	1807	1812	1824	rVB	1366651	1354716	50.71%	1.704%
81	12.880	1830	1835	1838	rBV	2139925	1914101	71.65%	2.407%
82	13.051	1860	1864	1874	rBV	79649	92995	3.48%	0.117%
83	13.345	1910	1914	1918	rBV	1076308	965556	36.14%	1.214%
84	13.404	1918	1924	1927	rVB	1320174	1265000	47.35%	1.591%
85	13.898	2004	2008	2012	rBV	1651603	1451518	54.33%	1.825%
86	13.939	2012	2015	2019	rVV2	1213583	1606759	60.15%	2.021%
87	13.980	2019	2022	2028	rVB	1084890	1052764	39.41%	1.324%
88	14.139	2046	2049	2053	rBV	202023	165181	6.18%	0.208%
89	14.304	2071	2077	2080	rBV4	25462	41936	1.57%	0.053%
90	14.333	2080	2082	2086	rVB2	36345	29207	1.09%	0.037%
91	14.451	2099	2102	2105	rBV	37551	29887	1.12%	0.038%
92	14.510	2108	2112	2116	rVV	1201430	1020746	38.21%	1.284%
93	14.986	2189	2193	2195	rBV	748713	774280	28.98%	0.974%
94	15.015	2195	2198	2208	rVB	692179	801268	29.99%	1.008%
95	15.351	2251	2255	2261	rBV	602716	743017	27.81%	0.934%
96	15.409	2261	2265	2280	rVB	249030	372830	13.96%	0.469%
97	16.874	2507	2514	2530	rBV2	617355	1304038	48.81%	1.640%
98	17.321	2584	2590	2606	rBV	290074	689906	25.83%	0.868%

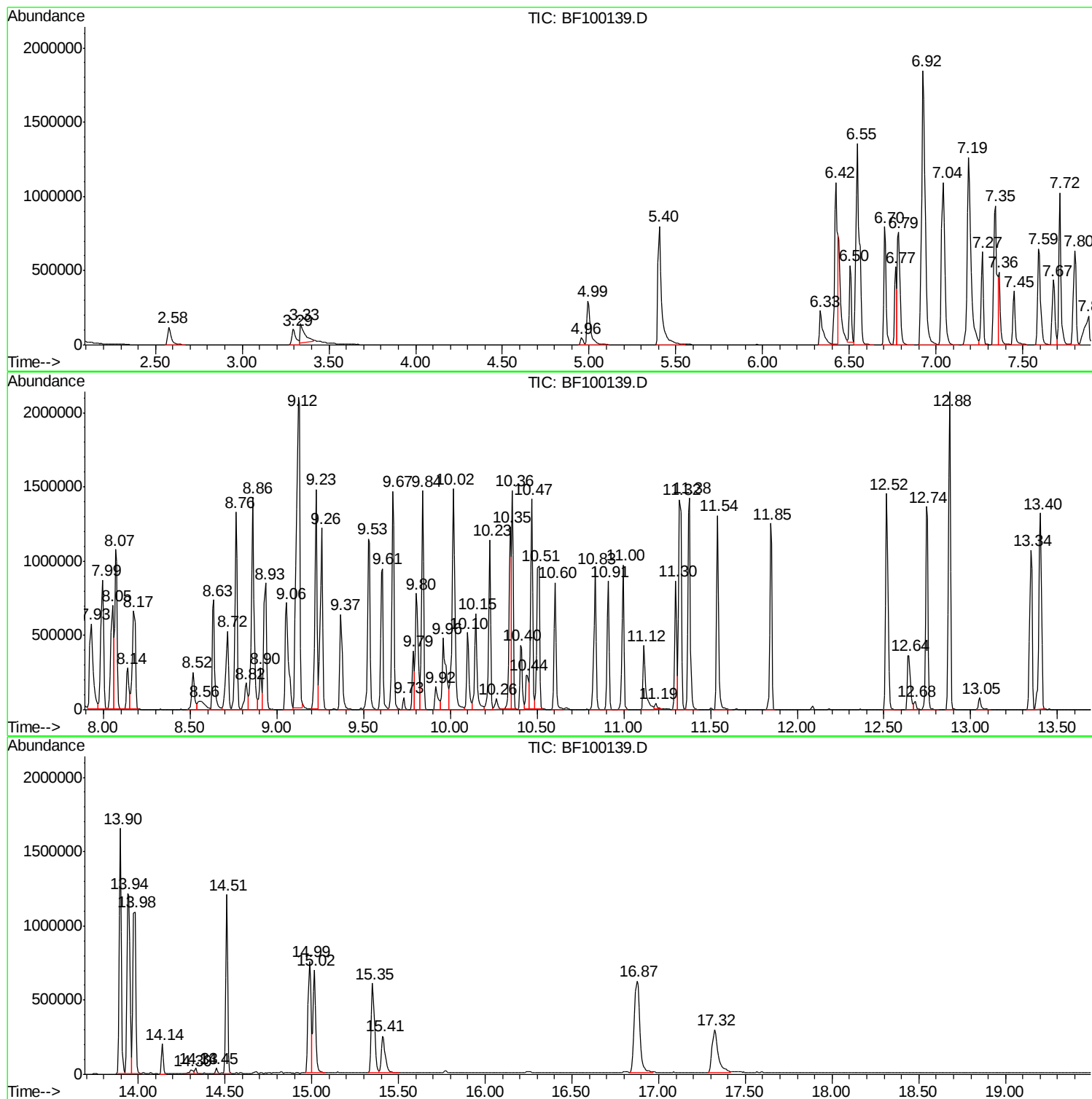
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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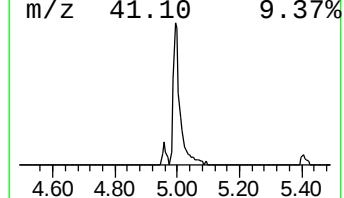
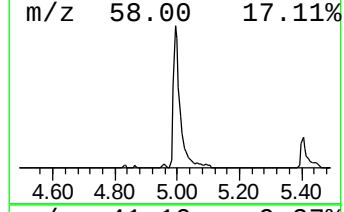
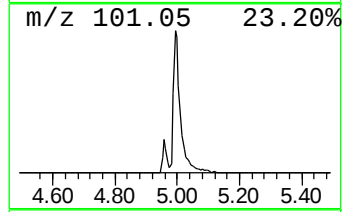
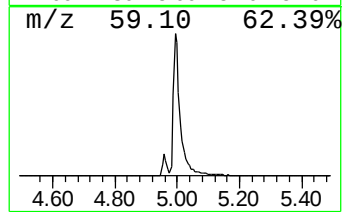
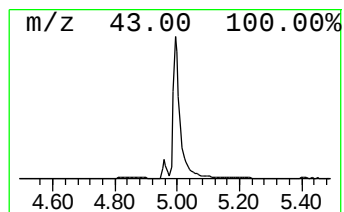
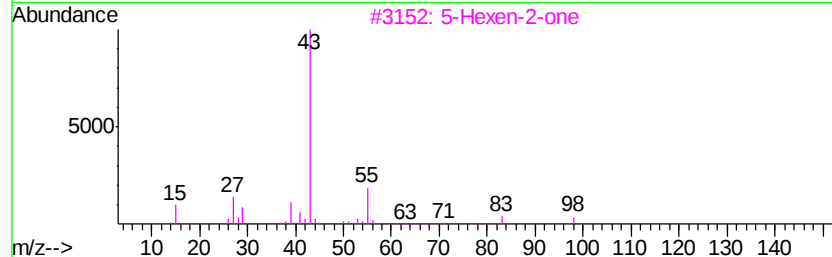
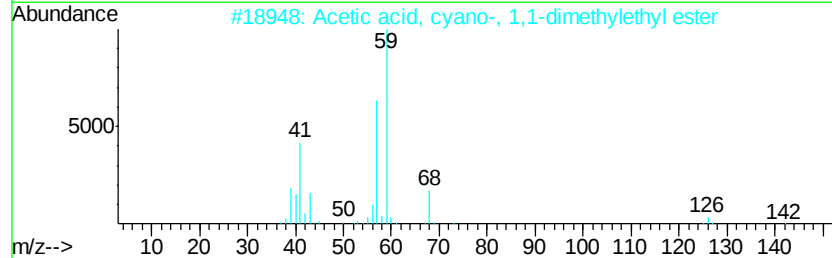
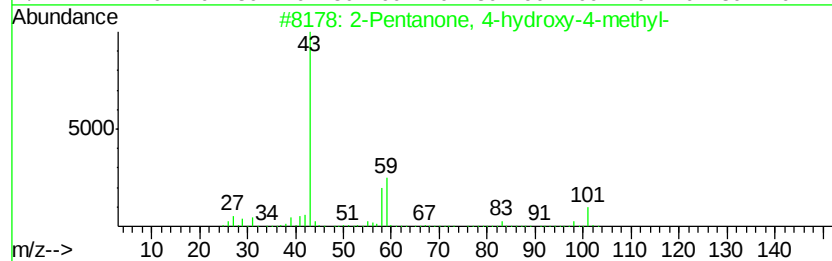
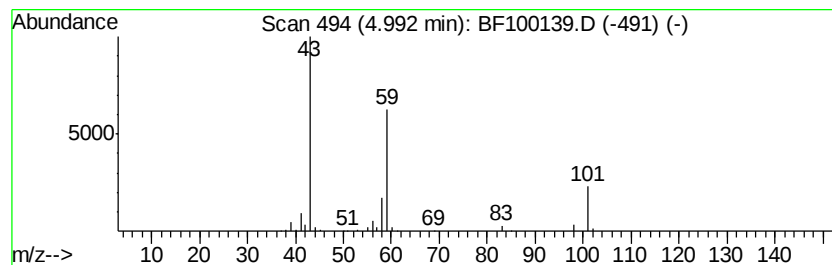
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	18.73 ng	451962	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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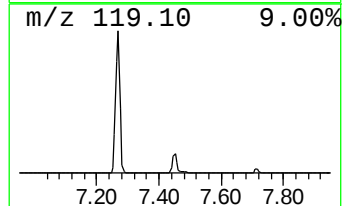
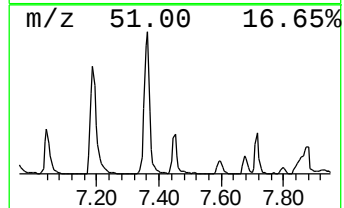
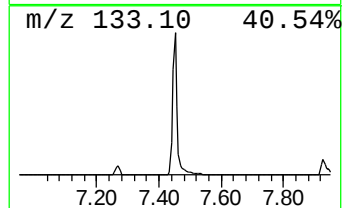
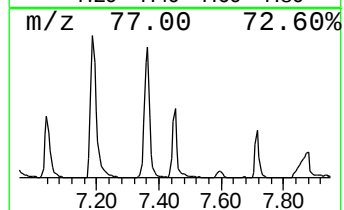
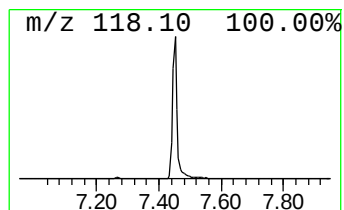
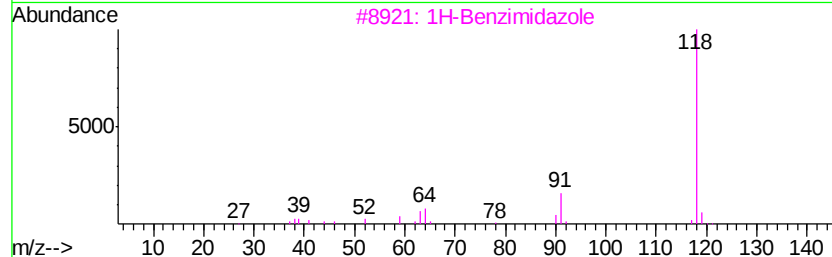
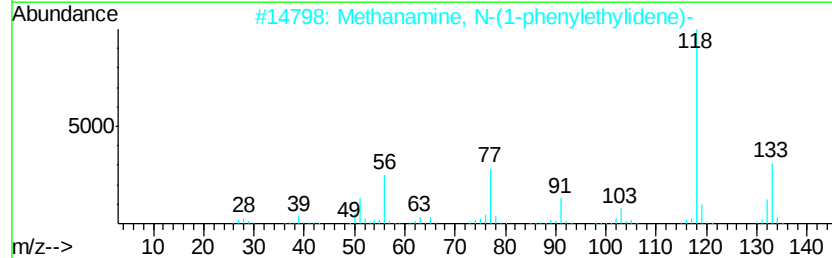
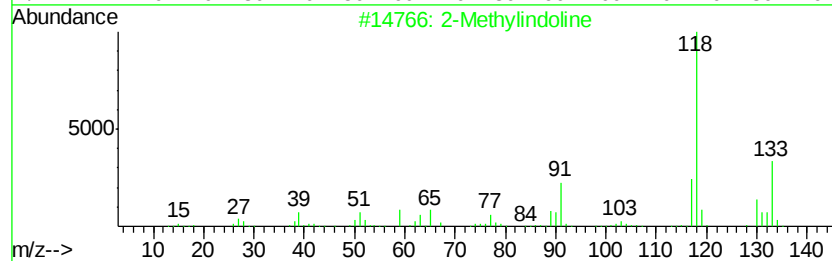
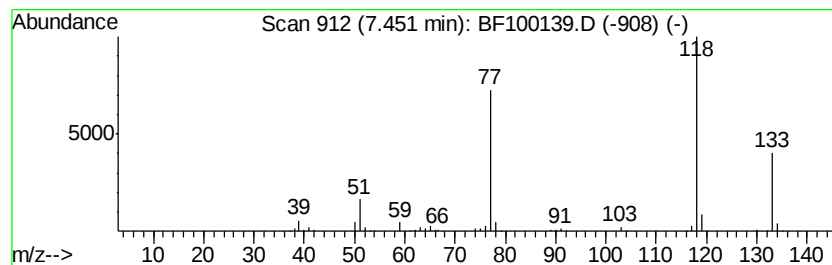
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Methylindoline Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	10.50 ng	369020	Naphthalene-d8	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindoline	133	C9H11N	006872-06-6	53
2			Methanamine, N-(1-phenylethylidene-...	133	C9H11N	006907-71-7	50
3			1H-Benzimidazole	118	C7H6N2	000051-17-2	38
4			Benzenecarboximidoyl bromide, N-...	197	C8H8BrN	041182-85-8	33
5			Benzeneacetic acid, phenyl ester	212	C14H12O2	000722-01-0	17



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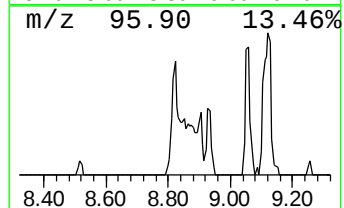
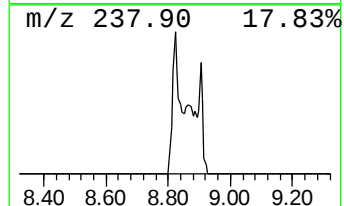
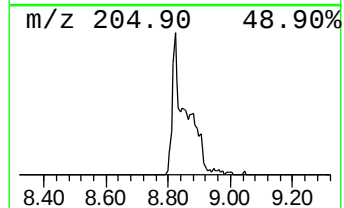
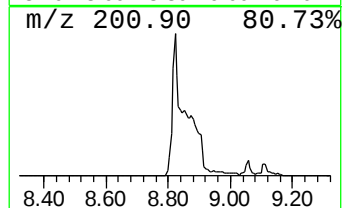
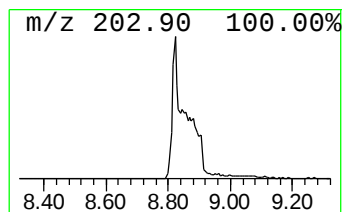
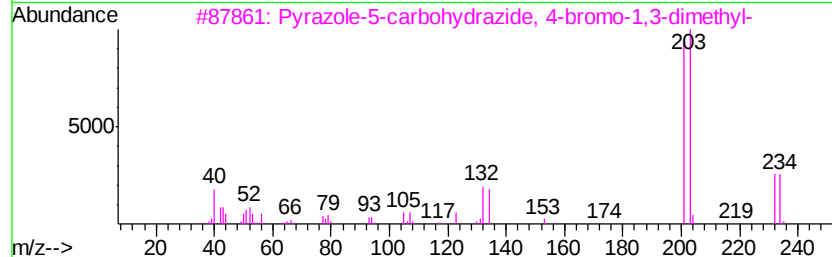
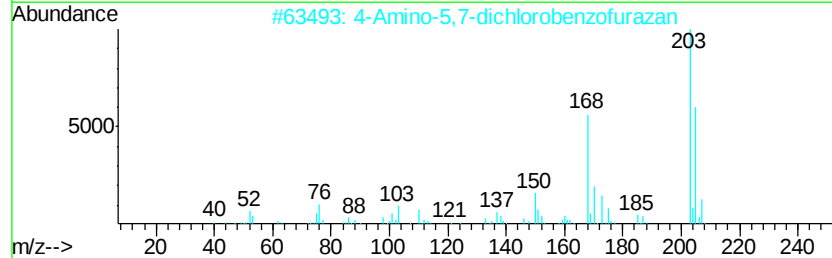
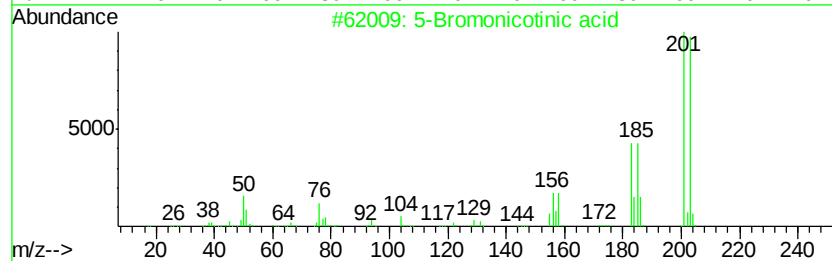
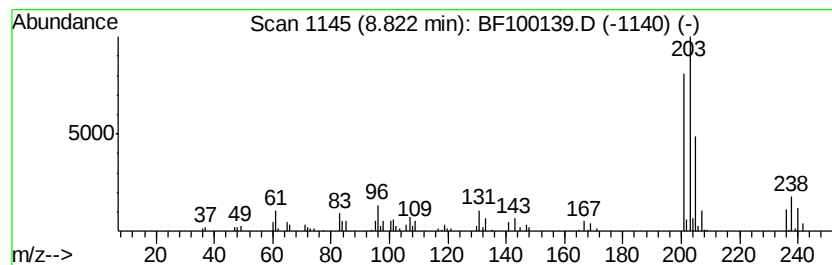
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Peak Number 3 5-Bromonicotinic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.82	6.29 ng	221266	Napthalene-d8	8.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromonicotinic acid	201	C6H4BrNO2	020826-04-4	47
2		4-Amino-5,7-dichlorobenzofurazan	203	C6H3Cl2N3O	330982-41-7	35
3		Pyrazole-5-carbohydrazide, 4-bro...	232	C6H9BrN4O	1000273-85-6	28
4		Methyl 3,5-dichloro-4-methoxyben...	234	C9H8Cl2O3	024295-27-0	25
5		Pyridine, 2,4-dichloro-3,5,6-tri...	201	C5Cl2F3N	054889-43-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100139.D
Acq On : 3 Nov 2017 17:22
Operator : SJ/JU
Sample : PB103911BSD
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB103911BSD

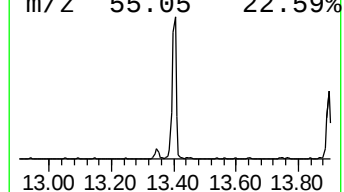
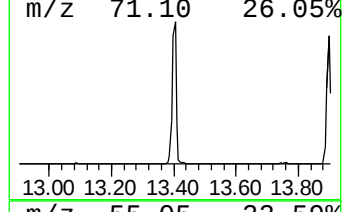
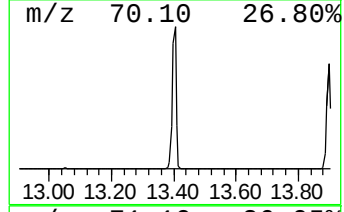
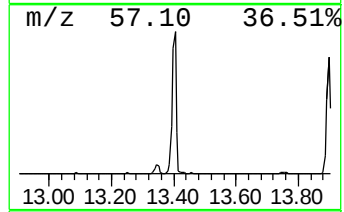
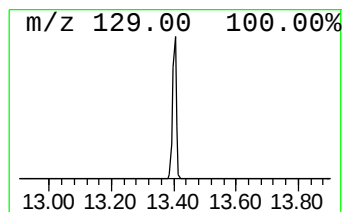
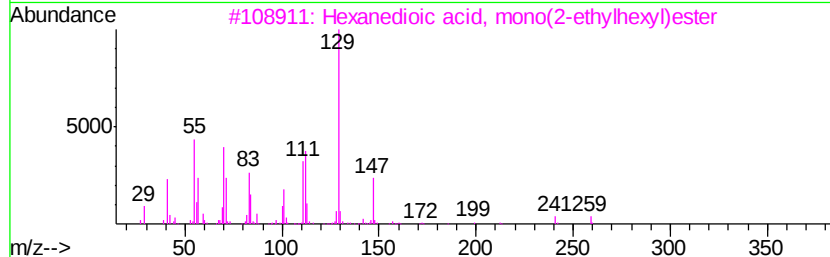
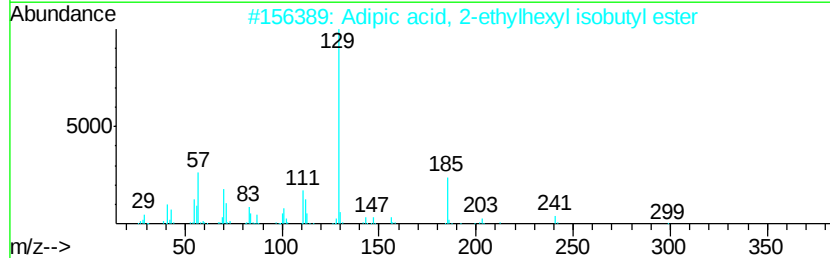
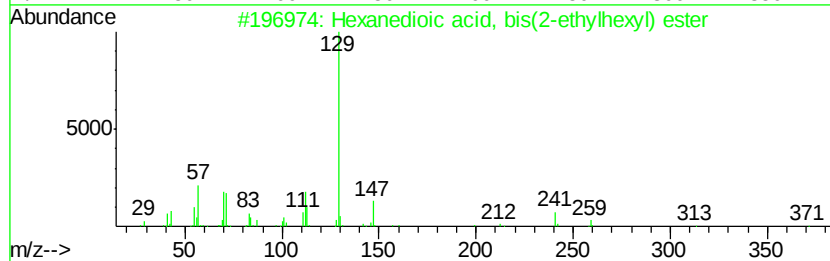
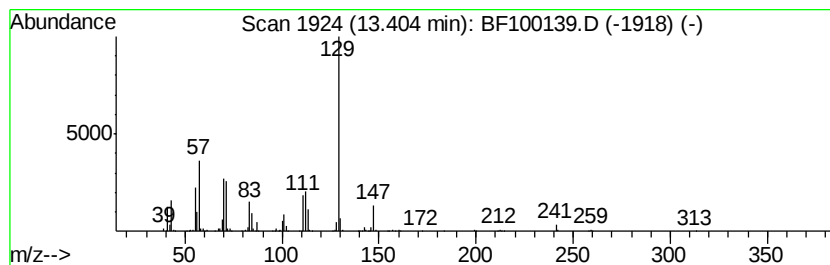
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	15.75 ng	1265000	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2		Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	64
3		Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	62
4		Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58
5		Adipic acid, 2-pentyl octyl ester	328	C19H36O4	1000324-16-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100139.D
Acq On : 3 Nov 2017 17:22
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Sample : PB103911BSD
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB103911BSD

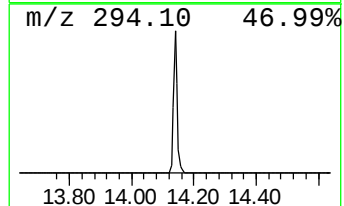
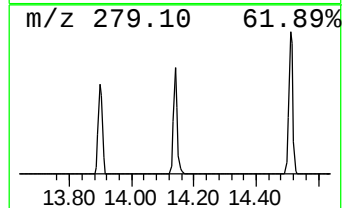
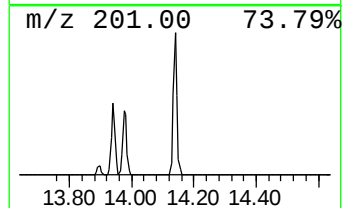
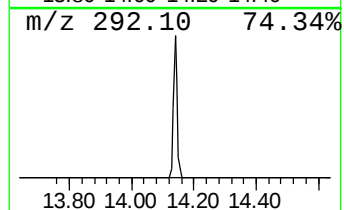
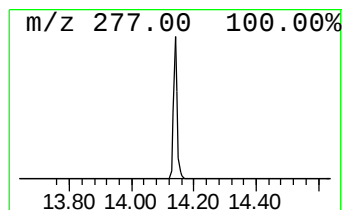
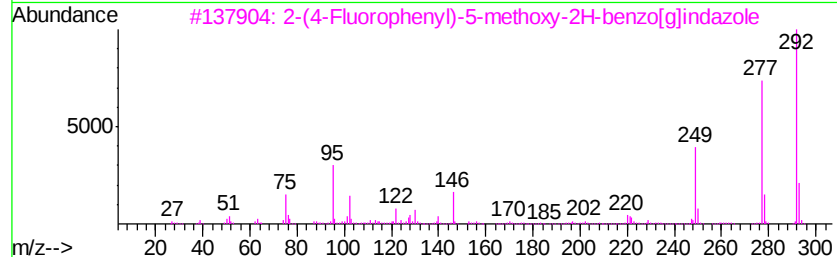
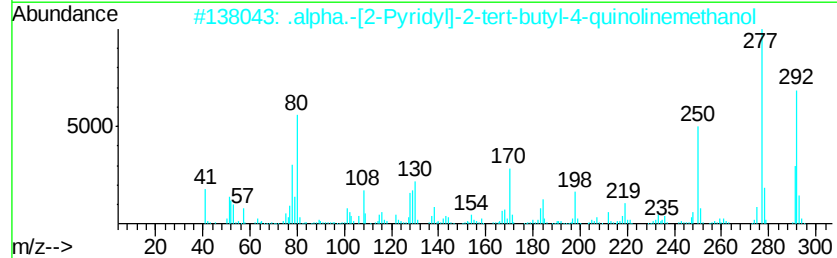
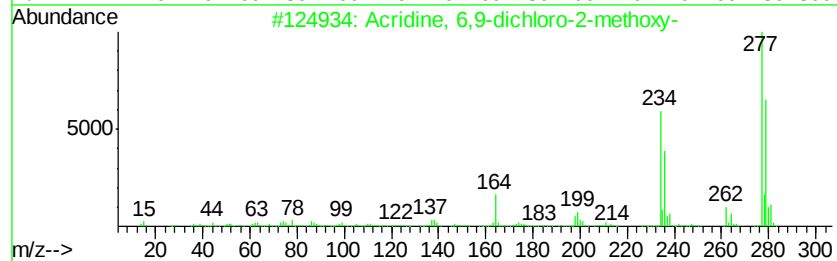
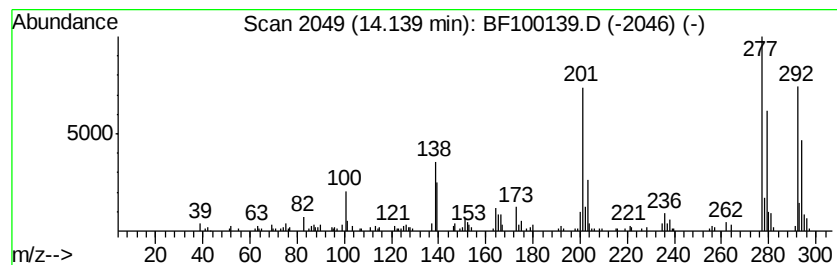
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Acridine, 6,9-dichloro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.06 ng	165181	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acridine, 6,9-dichloro-2-methoxy-	277	C14H9Cl2NO	000086-38-4	42
2		.alpha.-[2-Pyridyl]-2-tert-butyl...	292	C19H20N2O	027302-63-2	38
3		2-(4-Fluorophenyl)-5-methoxy-2H-...	292	C18H13FN2O	1000194-51-1	27
4		3,5-Dibromobenzo(b)thiophene	290	C8H4Br2S	001423-62-7	22
5		9H-Xanthen-9-one, 4-chloro-1,3,6...	292	C14H9ClO5	065658-58-4	18



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB103911BSD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
2-Pentanone, 4-hy...	4.99	18.7	ng	451962	1	6.77	482715	20.0
2-Methylindoline	7.45	10.5	ng	369020	2	8.05	703002	20.0
5-Bromonicotinic ...	8.82	6.3	ng	221266	2	8.05	703002	20.0
Hexanedioic acid,...	13.40	15.7	ng	1265000	5	13.95	1606760	20.0
Acridine, 6,9-dic...	14.14	2.1	ng	165181	5	13.95	1606760	20.0