

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
 Data File : BF097493.D
 Acq On : 9 Aug 2017 2:47
 Operator : SJ/JU
 Sample : I4652-07 10X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 L-1338-B-COMP

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-BF072517.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	5.028	547	551	563	rBV	41776	94118	12.90%	1.423%
2	6.098	730	733	746	rBV	56322	125421	17.19%	1.896%
3	6.192	746	749	758	rVB	112788	160941	22.06%	2.433%
4	6.404	782	785	798	rBV	620294	586434	80.36%	8.864%
5	6.563	809	812	819	rBV	104233	109355	14.99%	1.653%
6	6.986	882	884	902	rBV	41893	84194	11.54%	1.273%
7	7.686	1000	1003	1016	rBV	724724	729722	100.00%	11.030%
8	8.769	1184	1187	1194	rBV	160527	141593	19.40%	2.140%
9	8.869	1199	1204	1208	rBV2	6589	7605	1.04%	0.115%
10	9.175	1252	1256	1260	rBV2	20345	22415	3.07%	0.339%
11	9.298	1274	1277	1282	rBB	8913	8684	1.19%	0.131%
12	9.392	1288	1293	1296	rBV2	7753	7355	1.01%	0.111%
13	9.433	1296	1300	1304	rVV	718325	632534	86.68%	9.561%
14	9.463	1304	1305	1312	rVB	18369	16267	2.23%	0.246%
15	9.645	1333	1336	1339	rBV	7935	8024	1.10%	0.121%
16	9.886	1375	1377	1381	rVB2	8815	7861	1.08%	0.119%
17	9.980	1391	1393	1401	rVB	12177	13502	1.85%	0.204%
18	10.227	1432	1435	1445	rBV	51503	51623	7.07%	0.780%
19	10.363	1454	1458	1465	rBV2	11504	20367	2.79%	0.308%
20	10.804	1529	1533	1536	rBV2	12591	12429	1.70%	0.188%
21	10.904	1547	1550	1553	rBV	590741	542119	74.29%	8.194%
22	10.927	1553	1554	1559	rVV	146875	118136	16.19%	1.786%
23	10.986	1561	1564	1568	rVB	28151	26231	3.59%	0.396%
24	11.157	1589	1593	1596	rBV2	9180	10835	1.48%	0.164%
25	11.410	1632	1636	1638	rBV	18496	17070	2.34%	0.258%
26	11.439	1638	1641	1645	rVB	23470	21477	2.94%	0.325%
27	11.486	1645	1649	1652	rBV3	11932	13976	1.92%	0.211%
28	11.516	1652	1654	1657	rVV3	27255	28317	3.88%	0.428%
29	11.539	1657	1658	1662	rVB	10603	9182	1.26%	0.139%
30	11.633	1671	1674	1679	rVB3	7093	8166	1.12%	0.123%
31	11.704	1683	1686	1690	rVB	10668	8395	1.15%	0.127%
32	11.751	1692	1694	1697	rBV3	9789	8136	1.11%	0.123%
33	11.957	1725	1729	1731	rBV	15078	14375	1.97%	0.217%
34	12.021	1737	1740	1741	rBV2	8411	8420	1.15%	0.127%

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35	12.051	1741	1745	1749	rVB3	13611	21086	2.89%	0.319%
36	12.110	1752	1755	1760	rBV	209159	200564	27.48%	3.032%
37	12.163	1760	1764	1765	rBV3	6382	7460	1.02%	0.113%
38	12.263	1777	1781	1783	rBV2	9390	10279	1.41%	0.155%
39	12.333	1788	1793	1797	rBV	184404	205144	28.11%	3.101%
40	12.392	1800	1803	1810	rVB6	17038	27600	3.78%	0.417%
41	12.486	1813	1819	1822	rBV	141137	142046	19.47%	2.147%
42	12.563	1828	1832	1836	rBV6	12723	21692	2.97%	0.328%
43	12.668	1843	1850	1853	rVB	25657	39730	5.44%	0.601%
44	12.739	1858	1862	1865	rBV2	26560	30709	4.21%	0.464%
45	12.768	1865	1867	1875	rVB3	24779	39657	5.43%	0.599%
46	12.863	1880	1883	1887	rVV3	13086	13827	1.89%	0.209%
47	12.892	1887	1888	1891	rVB3	13250	9124	1.25%	0.138%
48	13.074	1917	1919	1920	rBV2	11259	9802	1.34%	0.148%
49	13.157	1930	1933	1934	rBV3	10635	9931	1.36%	0.150%
50	13.186	1936	1938	1941	rVB	20902	16670	2.28%	0.252%
51	13.286	1950	1955	1956	rBV	20477	22578	3.09%	0.341%
52	13.339	1961	1964	1966	rBV	19782	23180	3.18%	0.350%
53	13.404	1972	1975	1980	rBV4	22527	29962	4.11%	0.453%
54	13.457	1982	1984	1989	rVB5	16446	20686	2.83%	0.313%
55	13.533	1991	1997	2000	rBV2	532347	650952	89.21%	9.839%
56	13.557	2000	2001	2004	rVB	92548	61231	8.39%	0.926%
57	13.633	2011	2014	2019	rBV6	31616	43152	5.91%	0.652%
58	13.698	2022	2025	2027	rBV4	21257	31331	4.29%	0.474%
59	13.927	2061	2064	2066	rBV2	32727	34448	4.72%	0.521%
60	14.039	2082	2083	2085	rBV2	23347	18185	2.49%	0.275%
61	14.180	2105	2107	2110	rVB3	22682	18597	2.55%	0.281%
62	14.451	2150	2153	2156	rBV4	38990	59137	8.10%	0.894%
63	14.527	2163	2166	2169	rBV	98739	122572	16.80%	1.853%
64	14.774	2206	2208	2212	rVB	51798	40354	5.53%	0.610%
65	14.821	2214	2216	2220	rVB	74751	75027	10.28%	1.134%
66	14.874	2221	2225	2229	rBV	321247	376465	51.59%	5.690%
67	16.586	2515	2516	2519	rBV3	22295	18160	2.49%	0.274%
68	16.627	2521	2523	2525	rBV3	27702	31196	4.28%	0.472%
69	16.768	2545	2547	2550	rBV4	24782	23177	3.18%	0.350%
70	16.839	2556	2559	2560	rBV3	22794	26250	3.60%	0.397%
71	16.927	2573	2574	2581	rVB6	26025	44126	6.05%	0.667%

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72	17.251	2625	2629	2632	rBV6	22878	32832	4.50%	0.496%
73	17.292	2634	2636	2638	rVB3	22703	19631	2.69%	0.297%
74	17.498	2669	2671	2672	rBV2	21158	17173	2.35%	0.260%
75	17.562	2679	2682	2684	rBV4	29229	46640	6.39%	0.705%
76	17.792	2719	2721	2723	rBV3	21137	20799	2.85%	0.314%
77	17.845	2728	2730	2734	rBV4	27356	44968	6.16%	0.680%
78	17.927	2742	2744	2747	rBV3	24195	16551	2.27%	0.250%
79	18.086	2768	2771	2776	rBV7	26172	47782	6.55%	0.722%
80	18.256	2798	2800	2801	rBV2	23914	20039	2.75%	0.303%
81	18.645	2863	2866	2868	rBV4	22021	34022	4.66%	0.514%
82	18.821	2895	2896	2897	rBV	19358	13042	1.79%	0.197%
83	18.909	2908	2911	2912	rBV2	23941	28484	3.90%	0.431%
84	19.162	2953	2954	2956	rBV2	23478	22578	3.09%	0.341%

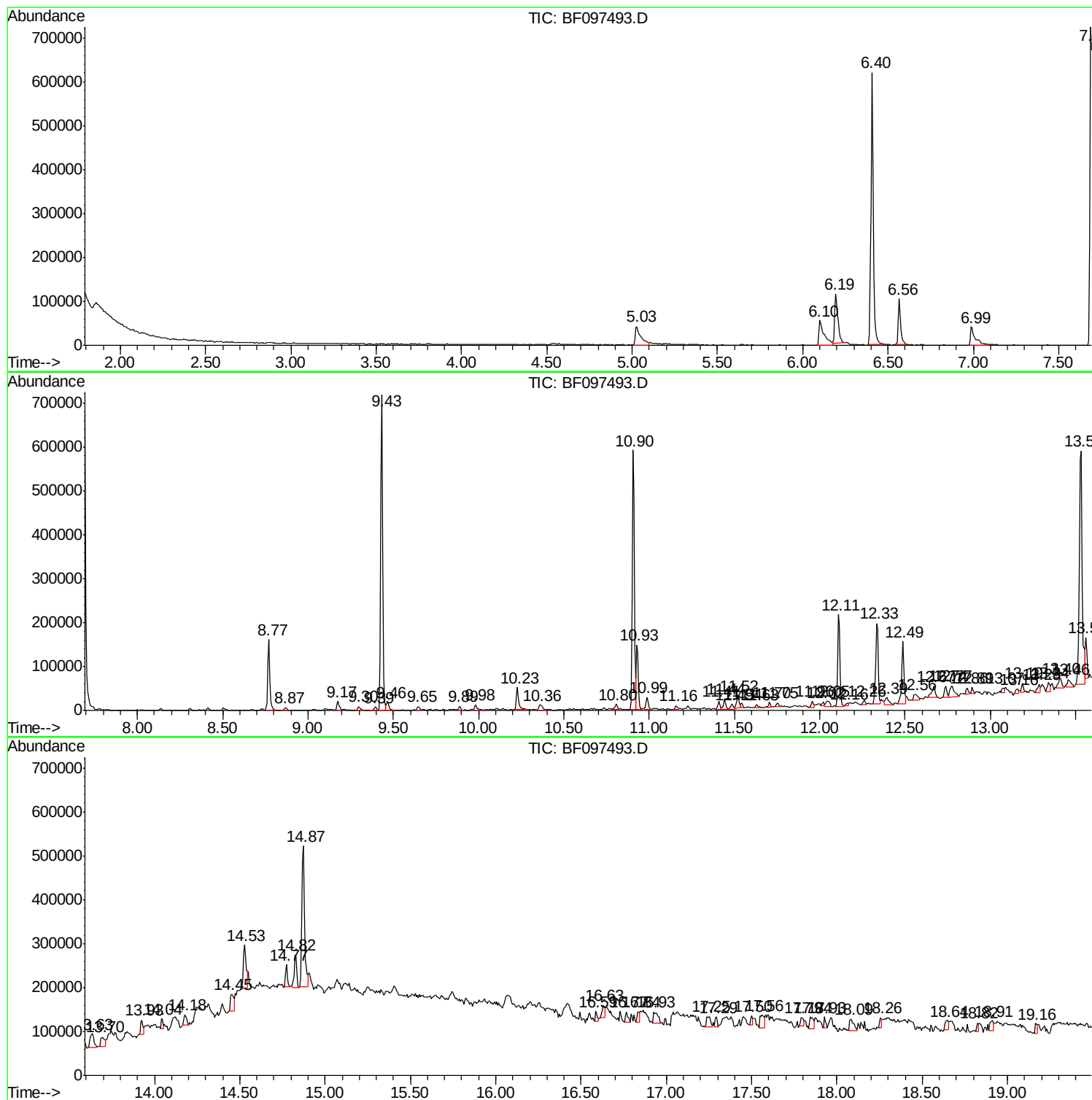
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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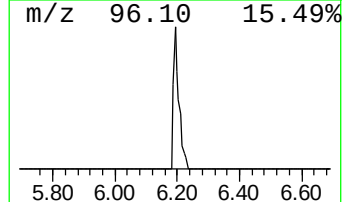
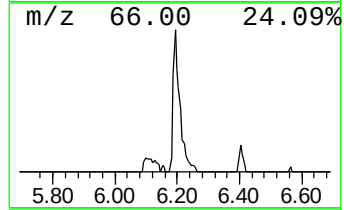
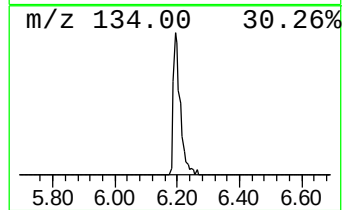
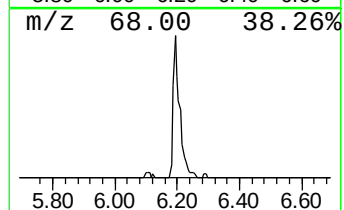
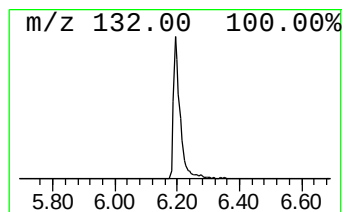
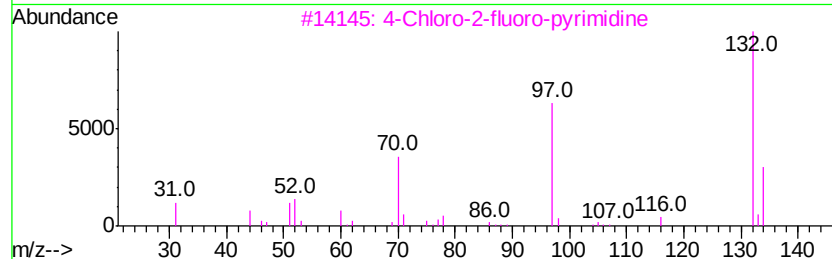
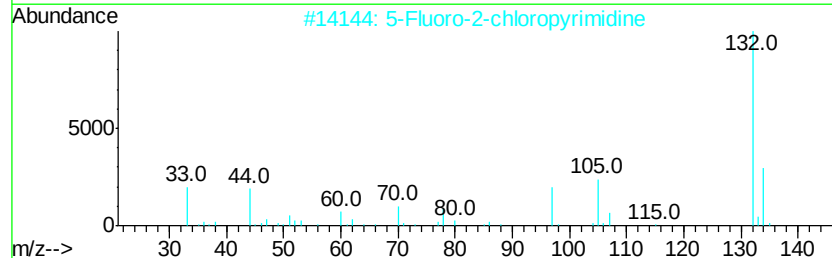
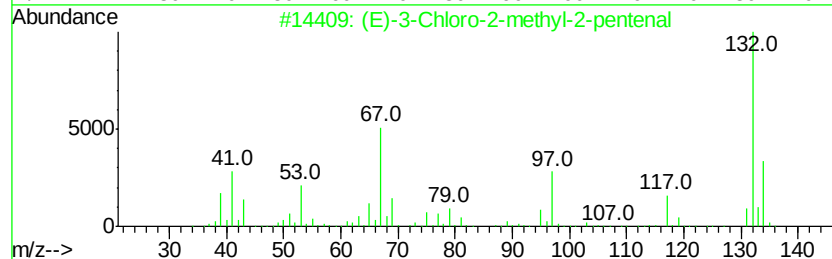
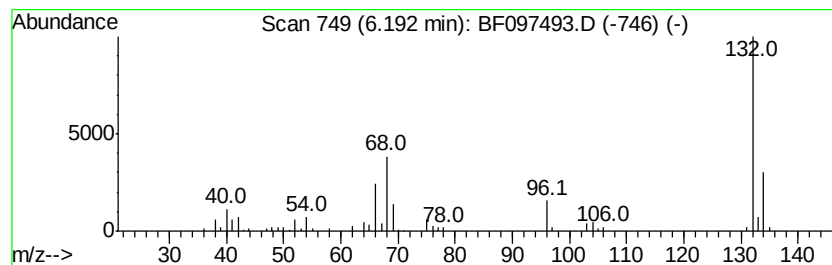
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	5.49 ng	160941	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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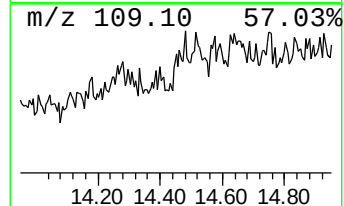
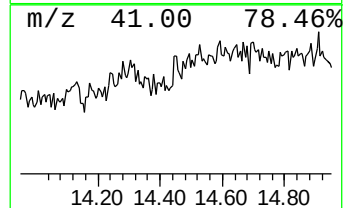
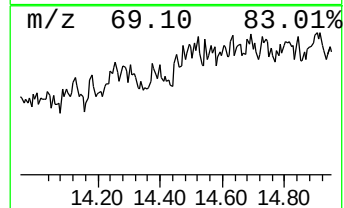
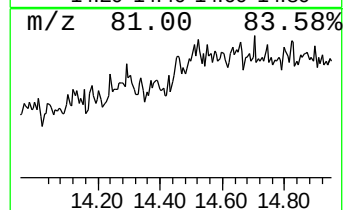
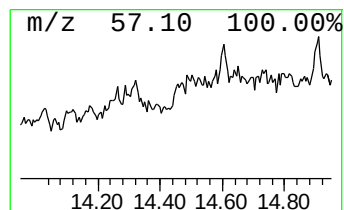
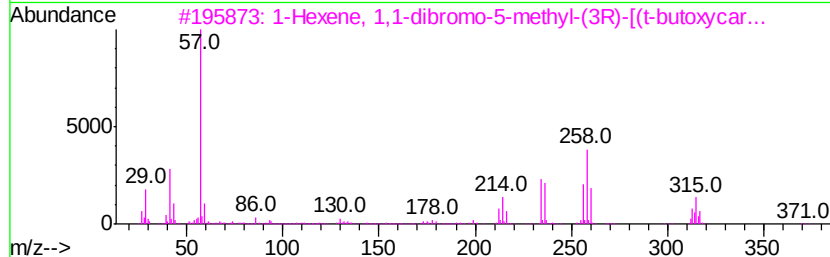
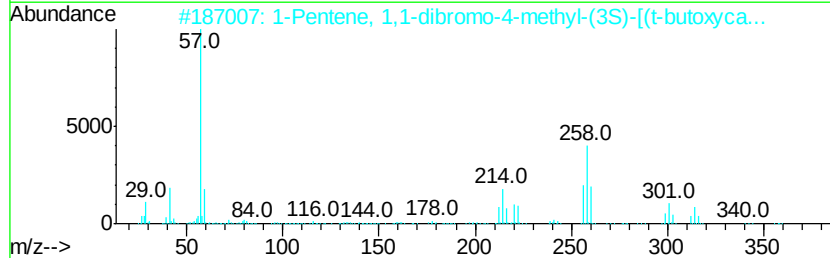
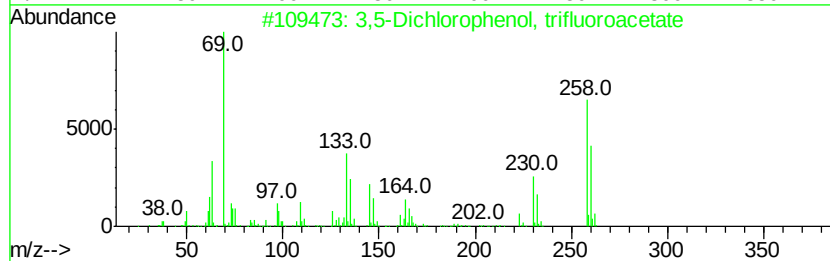
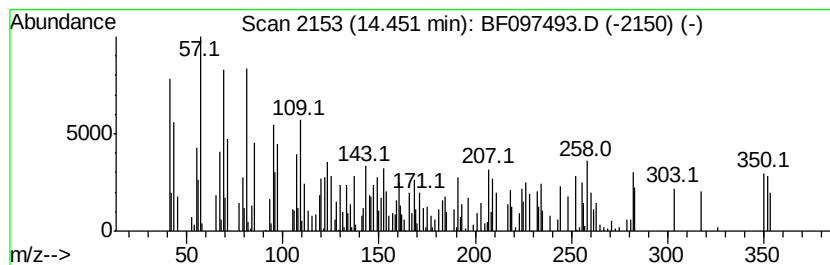
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.45 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.14 ng	59137	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Dichlorophenol, trifluoroace...	258	C8H3Cl2F3O2	1000365-28-0	10
2		1-Pentene, 1,1-dibromo-4-methyl-...	355	C11H19Br2NO2	176962-19-9	9
3		1-Hexene, 1,1-dibromo-5-methyl-(...	369	C12H21Br2NO2	1000162-35-9	7
4		1-Butene, 1,1-dibromo-4-phenyl-(...	403	C15H19Br2NO2	176962-18-8	4
5		Oxadiazon	344	C15H18Cl2N2O3	019666-30-9	2



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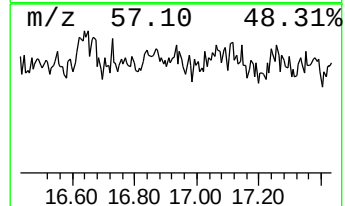
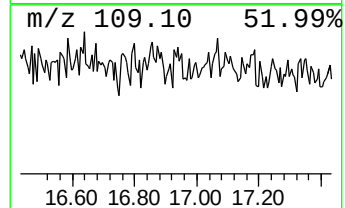
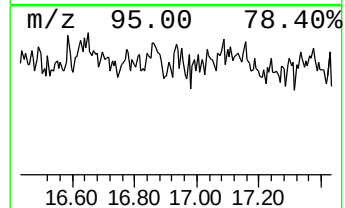
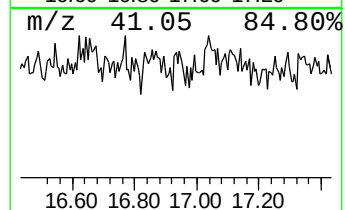
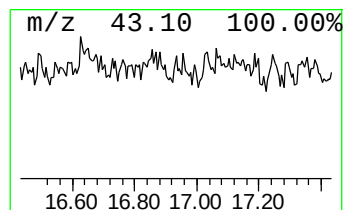
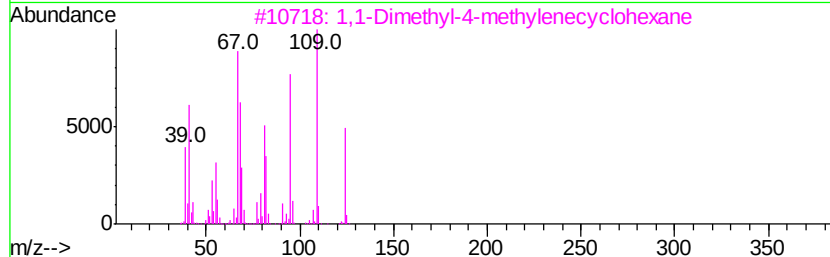
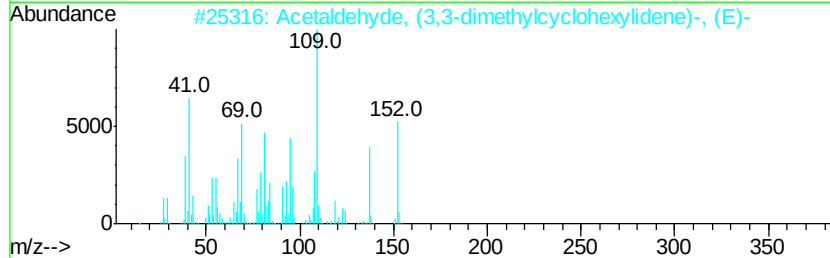
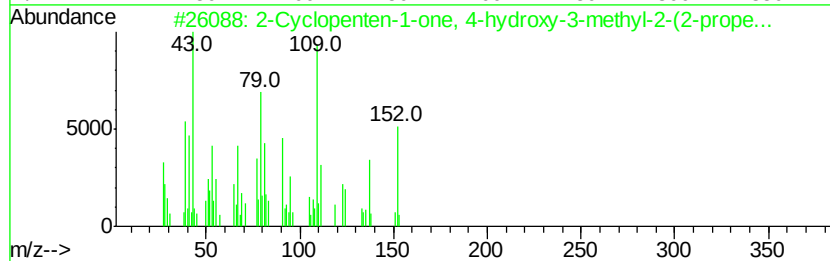
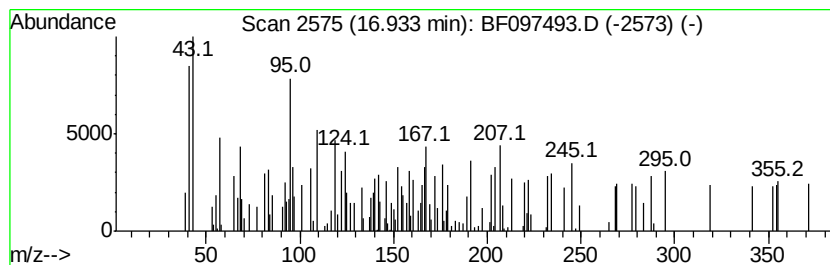
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.93 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	2.34 ng	44126	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclopenten-1-one, 4-hydroxy-3...	152	C9H12O2	000551-45-1	25
2		Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	25
3		1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	15
4		Aspidofractinine, 1-acetyl-17-me...	352	C22H28N2O2	055724-53-3	14
5		3-Buten-2-ol, 3-methyl-4-(2,6,6-...	208	C14H24O	070172-00-8	11



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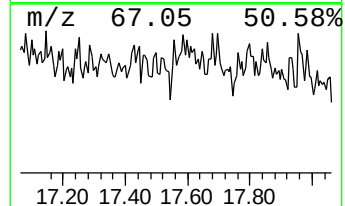
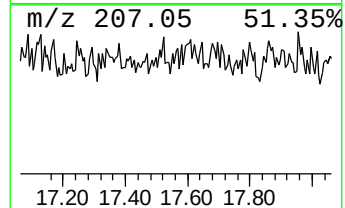
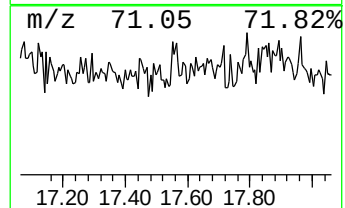
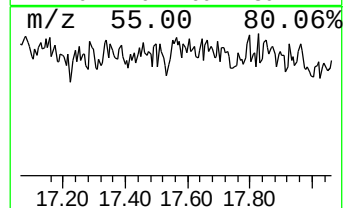
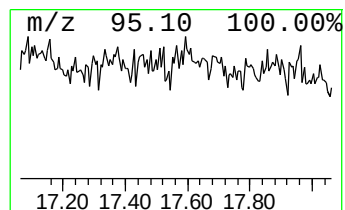
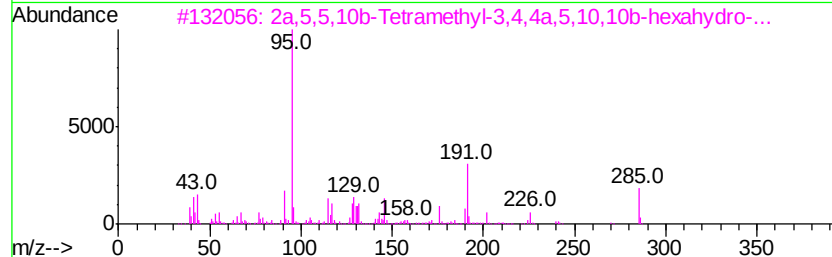
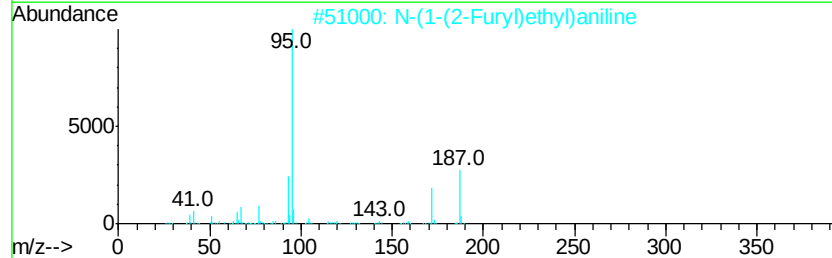
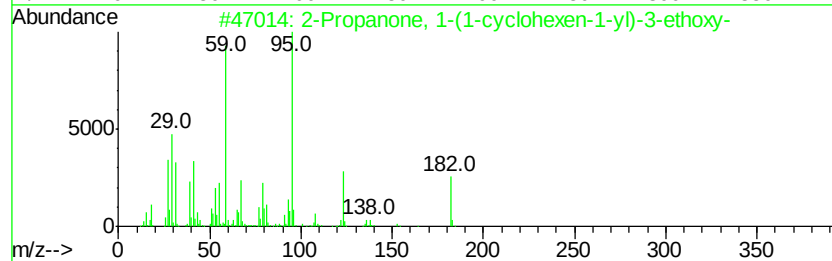
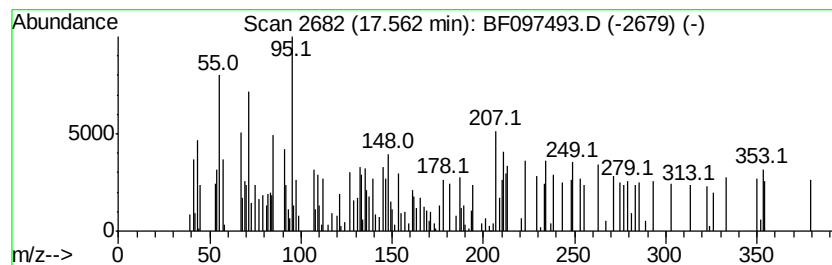
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.56 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	2.48 ng	46640	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanone, 1-(1-cyclohexen-1-yl)-3-ethoxy-	182	C11H18O2	051149-72-5	20
2		N-(1-(2-Furyl)ethyl)aniline	187	C12H13NO	014497-49-5	14
3		2a,5,5,10b-Tetramethyl-3,4,4a,5,10,10b-hexahydro-1,2,8-trimethyl-1H-pyrene	285	C18H23NO2	1000274-52-8	14
4		Pyridine, 2-ethoxy-3-(5-furan-2-yl)-	271	C14H13N3O3	1000316-98-8	14
5		Methyl aciphyllate	248	C16H24O2	057110-50-6	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097493.D
Acq On : 9 Aug 2017 2:47
Operator : SJ/JU
Sample : I4652-07 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L-1338-B-COMP

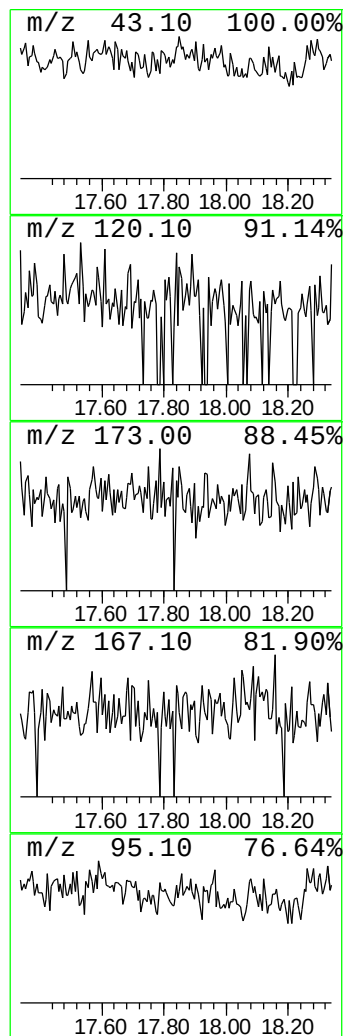
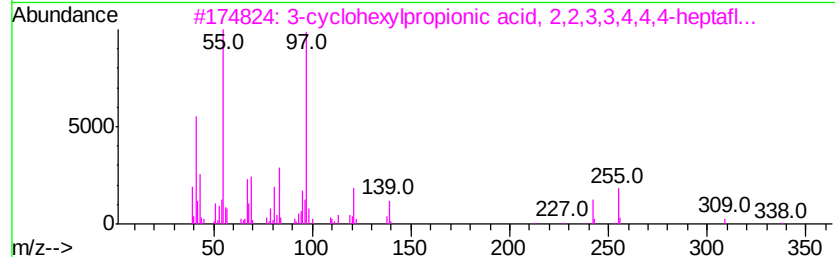
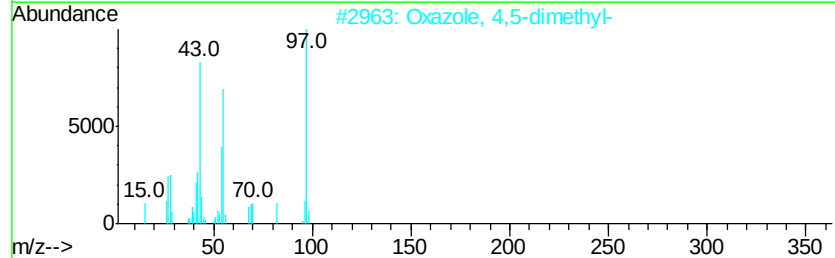
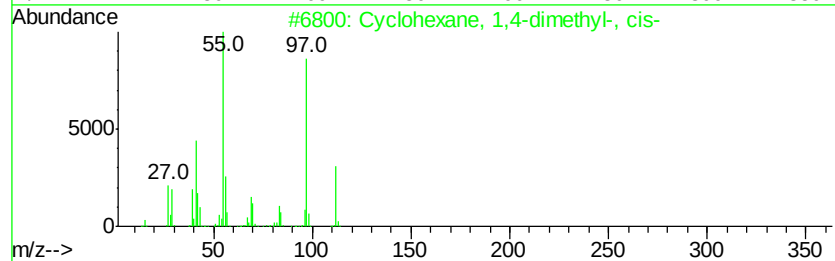
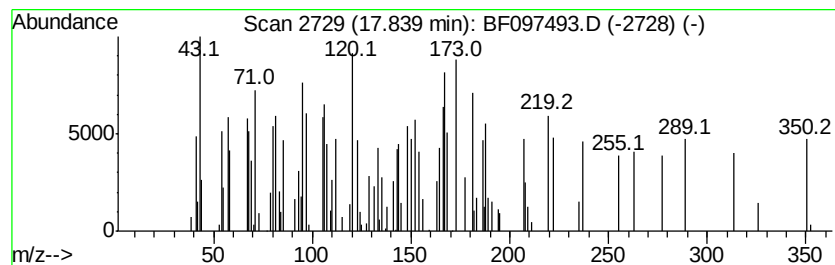
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.84 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	2.39 ng	44968	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	14
2		Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	14
3		3-cyclohexylpropionic acid, 2,2,...	338	C13H17F7O2	1000376-61-3	14
4		Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	14
5		2,3,4,6-Tetra-O-acetyl-D-glucopy...	348	C14H20O10	010343-06-3	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097493.D
Acq On : 9 Aug 2017 2:47
Operator : SJ/JU
Sample : I4652-07 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L-1338-B-COMP

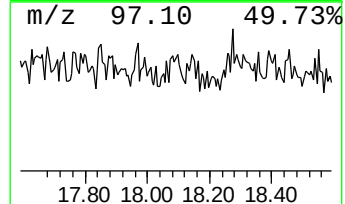
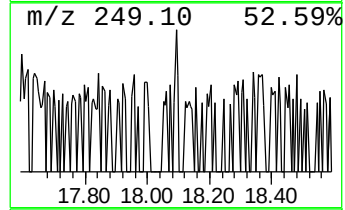
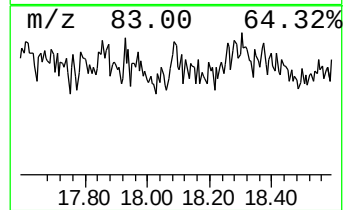
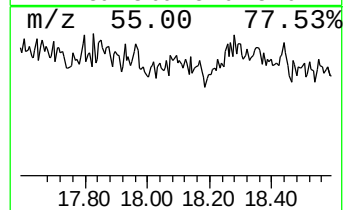
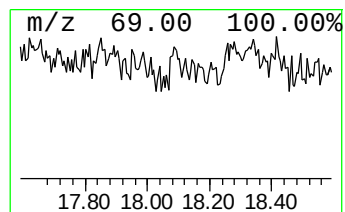
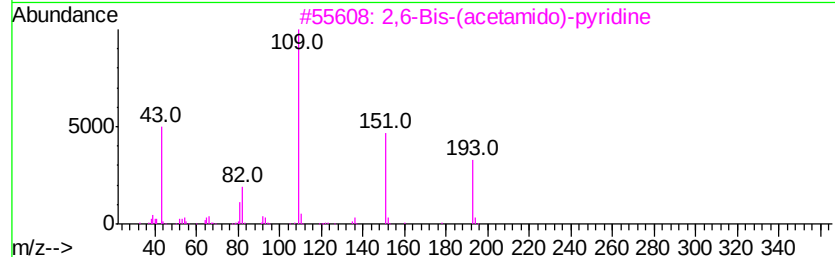
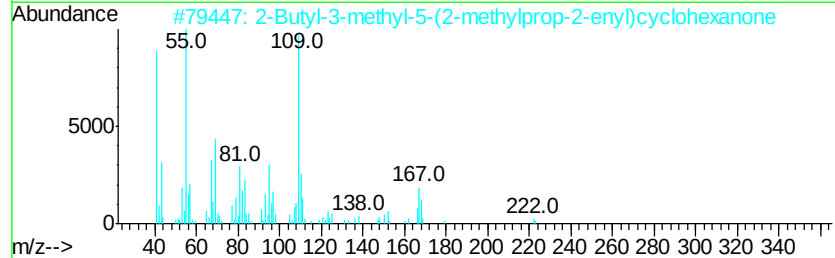
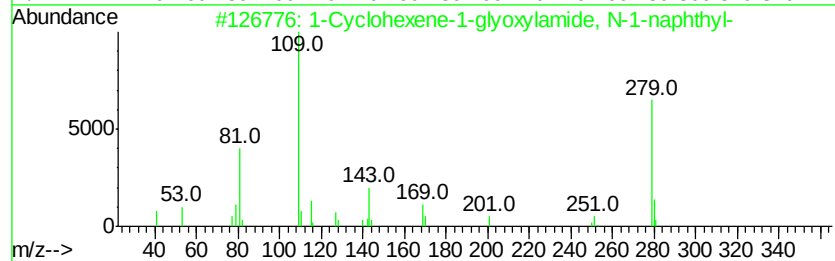
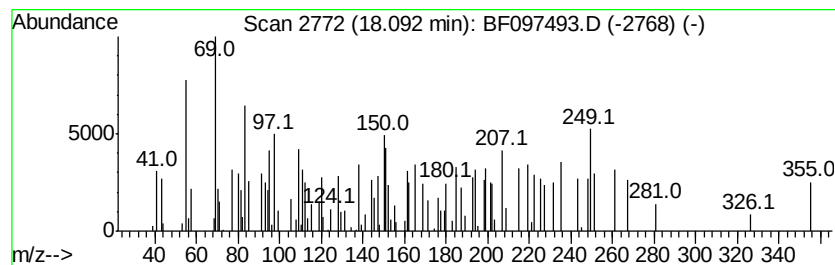
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.09 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	2.54 ng	47782	Perylene-d12	14.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Cyclohexene-1-ylvoxyamide, N-...	279	C18H17NO2	022914-94-9	16
2		2-Butyl-3-methyl-5-(2-methylprop...	222	C15H26O	1000281-10-7	14
3		2,6-Bis-(acetamido)-pyridine	193	C9H11N3O2	005441-02-1	14
4		3,5-Dimethyl-1-octylpyrazole	208	C13H24N2	001138-46-1	14
5		1,3-Cyclopentanedicarboxylic aci...	228	C12H20O4	007282-27-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097493.D
Acq On : 9 Aug 2017 2:47
Operator : SJ/JU
Sample : I4652-07 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L-1338-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
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unknown14.45	14.45	3.1	ng	59137	6	14.87	376465	20.0
unknown16.93	16.93	2.3	ng	44126	6	14.87	376465	20.0
unknown17.56	17.56	2.5	ng	46640	6	14.87	376465	20.0
unknown17.84	17.84	2.4	ng	44968	6	14.87	376465	20.0
unknown18.09	18.09	2.5	ng	47782	6	14.87	376465	20.0