

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100517\
 Data File : BF099122.D
 Acq On : 6 Oct 2017 00:02
 Operator : SJ/JU
 Sample : I5585-15 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G70-2.5-5

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-BF092317.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	2.128	5	7	17	rVB2	64165	103422	10.19%	0.812%
2	5.075	505	508	515	rBV	102537	111526	10.99%	0.876%
3	5.475	572	576	584	rVB	767837	681082	67.12%	5.348%
4	6.480	744	747	754	rBV	744389	700552	69.04%	5.501%
5	6.628	768	772	776	rBV	917764	729372	71.88%	5.727%
6	6.863	808	812	815	rBV	846437	694501	68.44%	5.453%
7	6.916	816	821	825	rBV	14473	14335	1.41%	0.113%
8	7.016	834	838	842	rBV	688118	564822	55.66%	4.435%
9	7.422	903	907	910	rBV	515603	417828	41.18%	3.281%
10	7.757	961	964	967	rBV	41011	32196	3.17%	0.253%
11	8.145	1023	1030	1033	rBV	1158302	970733	95.67%	7.622%
12	8.198	1036	1039	1042	rVB	15286	12312	1.21%	0.097%
13	8.557	1097	1100	1105	rBV	21866	22170	2.18%	0.174%
14	8.727	1126	1129	1132	rBV2	13843	11530	1.14%	0.091%
15	9.216	1207	1212	1215	rBV	1074483	824317	81.24%	6.473%
16	9.292	1220	1225	1228	rBV	17464	16394	1.62%	0.129%
17	9.486	1254	1258	1261	rVB2	13364	11940	1.18%	0.094%
18	9.610	1276	1279	1287	rVB	98804	84184	8.30%	0.661%
19	9.757	1301	1304	1308	rBV	28317	26027	2.56%	0.204%
20	9.821	1310	1315	1319	rVB2	20156	19067	1.88%	0.150%
21	9.898	1323	1328	1332	rBV2	1180013	1014716	100.00%	7.968%
22	10.098	1360	1362	1366	rVB2	12108	11654	1.15%	0.092%
23	10.321	1398	1400	1403	rVB	25181	18147	1.79%	0.142%
24	10.539	1433	1437	1443	rBV4	10816	17245	1.70%	0.135%
25	10.686	1458	1462	1473	rVB	421399	398448	39.27%	3.129%
26	10.792	1477	1480	1481	rBV	30425	24814	2.45%	0.195%
27	11.186	1545	1547	1551	rBV2	10912	12076	1.19%	0.095%
28	11.239	1553	1556	1559	rVV3	25948	23910	2.36%	0.188%
29	11.268	1559	1561	1567	rVB4	9840	13330	1.31%	0.105%
30	11.386	1577	1581	1584	rBV	1150609	966250	95.22%	7.587%
31	11.410	1584	1585	1588	rVV	41065	21803	2.15%	0.171%
32	11.463	1591	1594	1596	rVB	24142	21441	2.11%	0.168%
33	11.668	1626	1629	1632	rVB2	14189	12885	1.27%	0.101%
34	11.886	1663	1666	1668	rBV	14138	14543	1.43%	0.114%

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Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

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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-BF092317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.910	1668	1670	1673	rVB	29353	25892	2.55%	0.203%
36	11.992	1681	1684	1687	rBV2	19436	17273	1.70%	0.136%
37	12.074	1694	1698	1700	rBV2	16961	15640	1.54%	0.123%
38	12.180	1713	1716	1718	rBV2	17225	13128	1.29%	0.103%
39	12.433	1756	1759	1762	rBV	28474	26484	2.61%	0.208%
40	12.462	1762	1764	1767	rVV2	22241	21017	2.07%	0.165%
41	12.521	1771	1774	1778	rBV2	15790	16408	1.62%	0.129%
42	12.598	1783	1787	1791	rVB	122362	102932	10.14%	0.808%
43	12.774	1813	1817	1820	rBV	119428	104088	10.26%	0.817%
44	12.827	1820	1826	1828	rVV	118115	128458	12.66%	1.009%
45	12.845	1828	1829	1833	rVV	68750	58185	5.73%	0.457%
46	12.880	1833	1835	1839	rVB2	17563	16608	1.64%	0.130%
47	12.962	1845	1849	1856	rVB	724825	724422	71.39%	5.688%
48	13.039	1858	1862	1867	rBV5	18451	27558	2.72%	0.216%
49	13.127	1874	1877	1880	rBV3	16182	25482	2.51%	0.200%
50	13.257	1895	1899	1902	rVB3	15723	15900	1.57%	0.125%
51	13.351	1911	1915	1917	rBV	18860	17214	1.70%	0.135%
52	13.439	1927	1930	1937	rBV	56100	58135	5.73%	0.456%
53	13.498	1937	1940	1943	rBV	83542	71413	7.04%	0.561%
54	13.662	1965	1968	1973	rVB	23637	24949	2.46%	0.196%
55	13.774	1981	1987	1990	rBV4	17758	25724	2.54%	0.202%
56	13.827	1993	1996	1999	rVV2	19343	26309	2.59%	0.207%
57	13.868	1999	2003	2007	rVB2	21391	30949	3.05%	0.243%
58	13.956	2012	2018	2021	rBV7	6586	13388	1.32%	0.105%
59	13.992	2021	2024	2025	rVV2	19760	18400	1.81%	0.144%
60	14.021	2025	2029	2032	rVV	766203	763241	75.22%	5.993%
61	14.045	2032	2033	2041	rVB	78985	85600	8.44%	0.672%
62	14.174	2052	2055	2059	rBV4	7992	12335	1.22%	0.097%
63	14.239	2064	2066	2070	rVB3	10028	12824	1.26%	0.101%
64	14.409	2090	2095	2098	rVB	27490	30679	3.02%	0.241%
65	14.445	2098	2101	2104	rBV2	18399	18805	1.85%	0.148%
66	14.474	2104	2106	2108	rBV2	12162	11881	1.17%	0.093%
67	14.533	2113	2116	2118	rBV4	18215	18802	1.85%	0.148%
68	14.821	2163	2165	2169	rVB3	13141	14215	1.40%	0.112%
69	14.903	2174	2179	2181	rVV3	8491	13689	1.35%	0.107%
70	14.968	2186	2190	2195	rVB5	13889	24047	2.37%	0.189%
71	15.062	2201	2206	2209	rBV	157211	217104	21.40%	1.705%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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72	15.174	2222	2225	2228	rVB	23776	26456	2.61%	0.208%
73	15.368	2252	2258	2264	rVB	93308	116711	11.50%	0.916%
74	15.427	2264	2268	2275	rBV	67323	89228	8.79%	0.701%
75	15.498	2275	2280	2284	rBV	548196	682853	67.29%	5.362%
76	15.933	2349	2354	2359	rBV3	15519	25567	2.52%	0.201%
77	16.445	2435	2441	2448	rVB7	14971	31260	3.08%	0.245%
78	16.633	2468	2473	2477	rVB7	8976	14795	1.46%	0.116%
79	16.774	2493	2497	2500	rBV4	9366	14577	1.44%	0.114%
80	16.803	2500	2502	2509	rVB6	11505	18871	1.86%	0.148%
81	16.968	2524	2530	2537	rBV2	47671	90047	8.87%	0.707%
82	17.044	2538	2543	2548	rVB6	11920	25082	2.47%	0.197%
83	17.144	2556	2560	2565	rVB6	6498	11927	1.18%	0.094%
84	17.209	2565	2571	2576	rBV6	9568	20123	1.98%	0.158%
85	17.415	2600	2606	2616	rVB	34189	74382	7.33%	0.584%
86	17.739	2655	2661	2665	rVB7	6328	13093	1.29%	0.103%
87	18.574	2801	2803	2811	rVB8	6175	11824	1.17%	0.093%

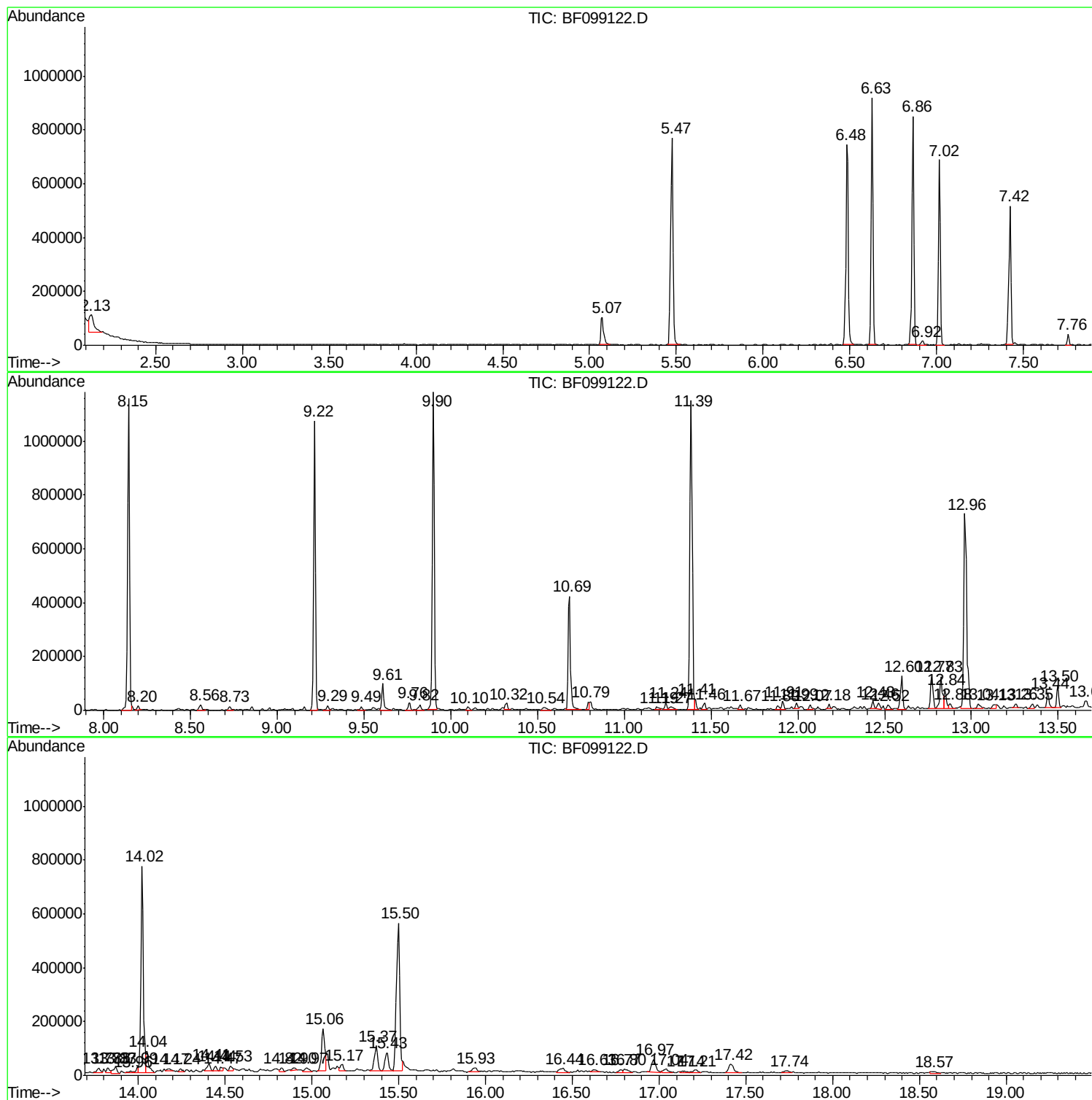
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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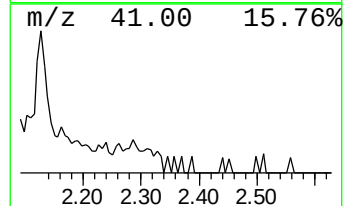
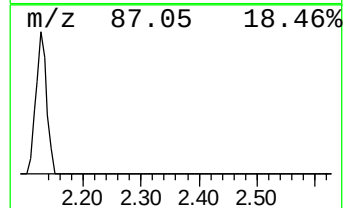
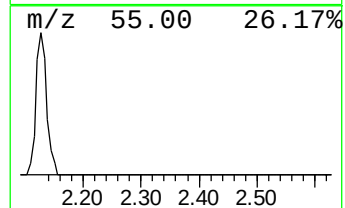
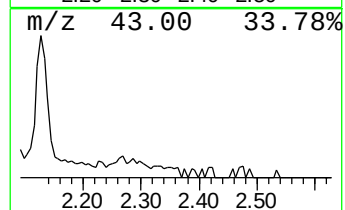
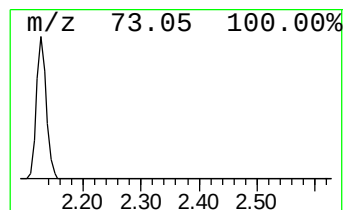
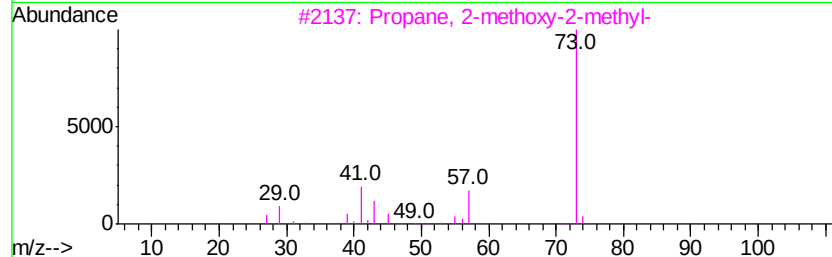
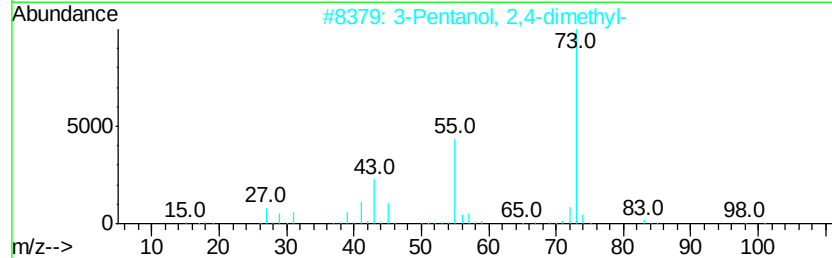
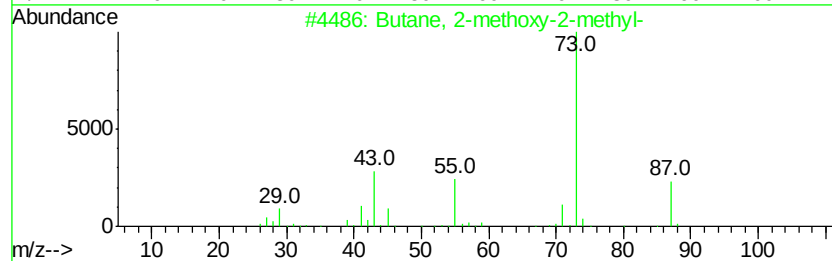
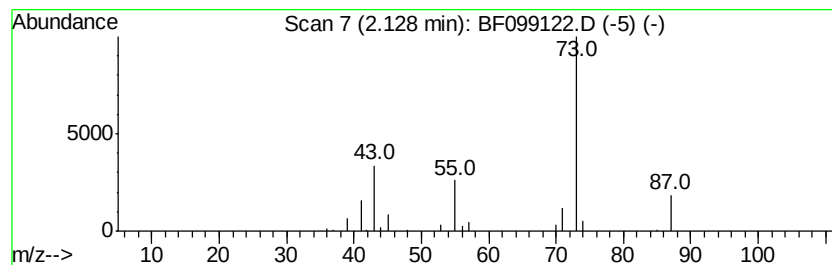
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	2.98 ng	103422	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5			Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9



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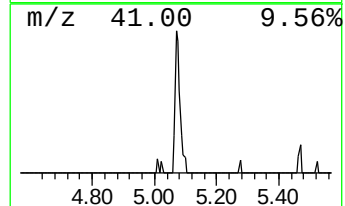
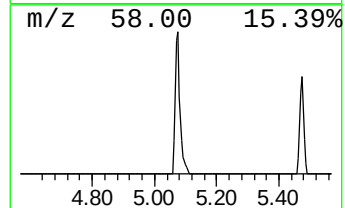
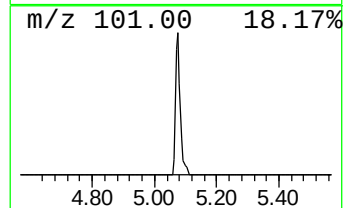
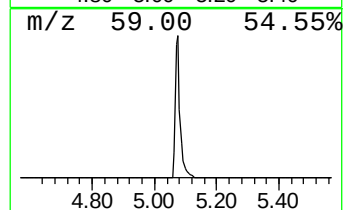
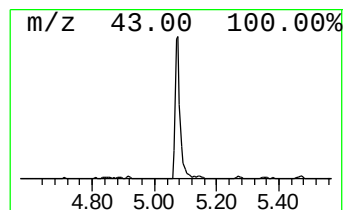
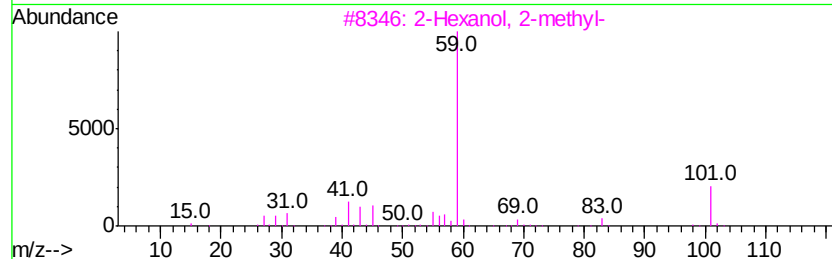
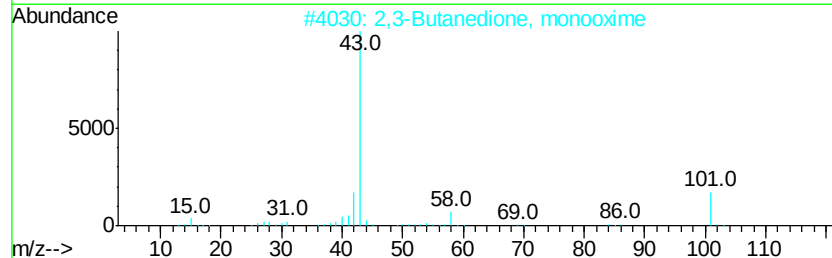
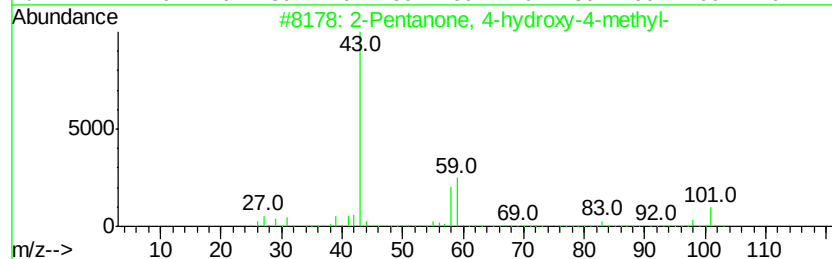
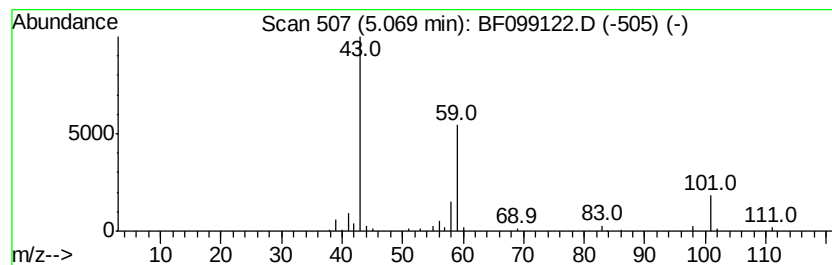
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	3.21 ng	111526	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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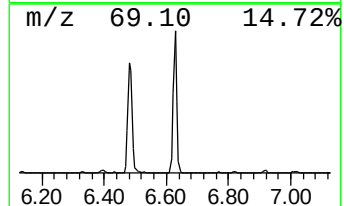
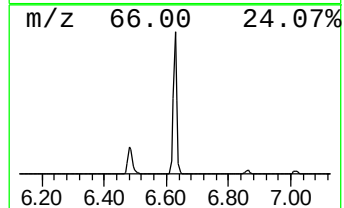
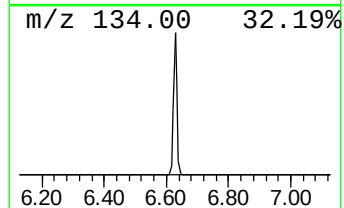
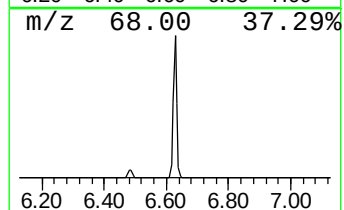
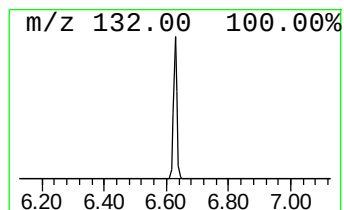
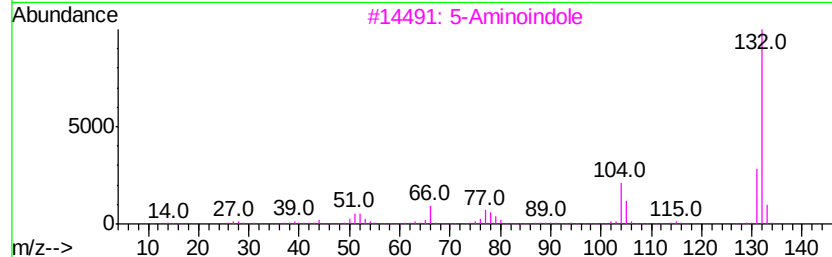
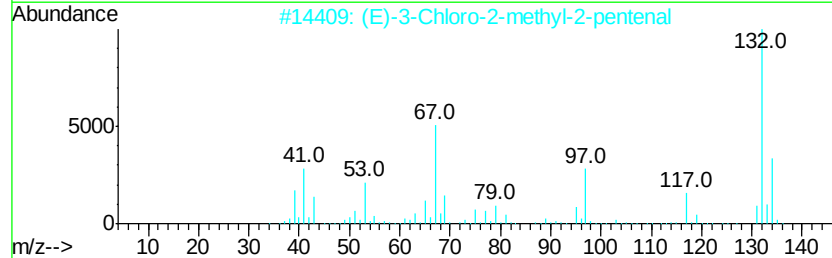
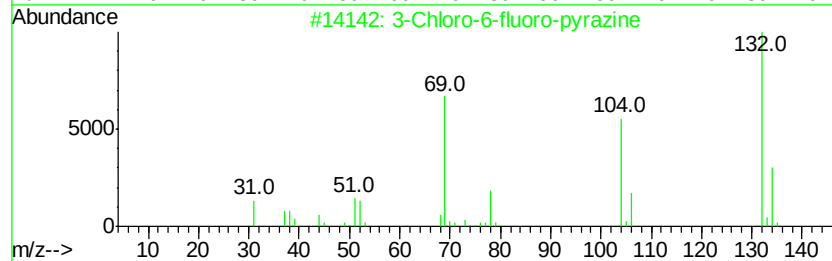
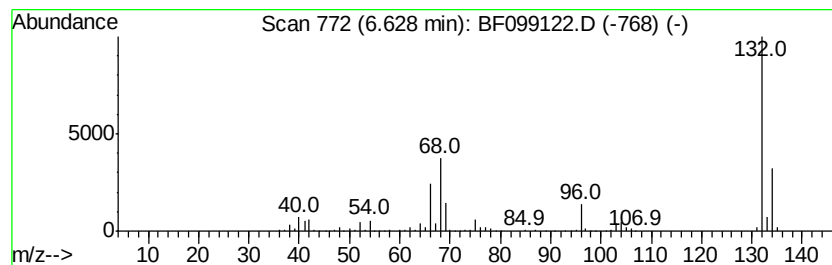
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	21.00 ng	729372	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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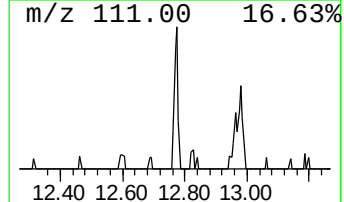
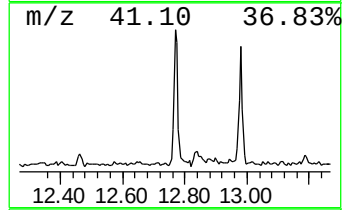
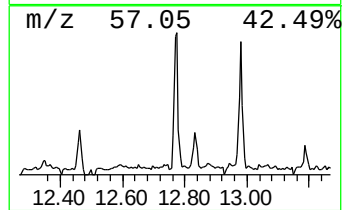
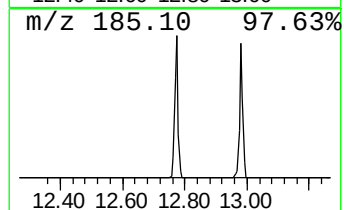
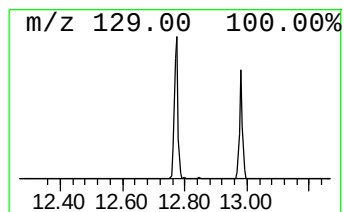
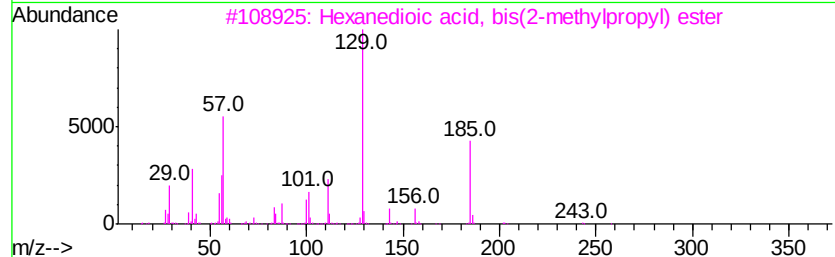
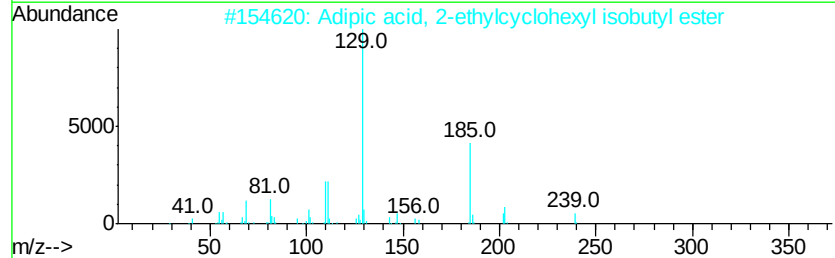
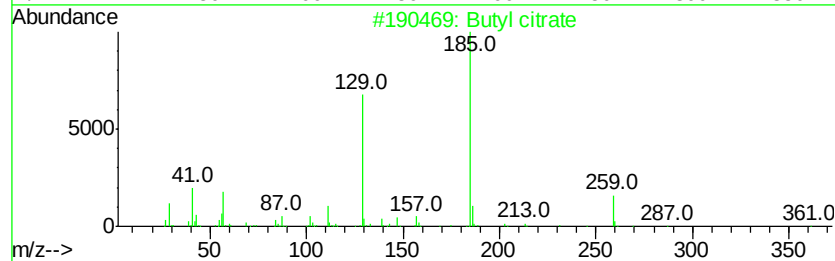
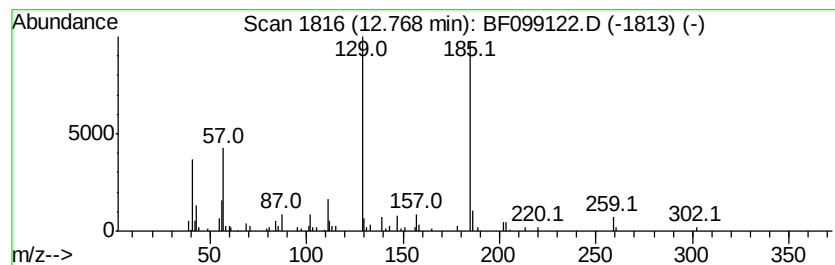
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BNA_F
ClientSampleId :
G70-2.5-5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.73 ng	104088	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 91
2		Adipic acid, 2-ethylcyclohexyl i...	312 C18H32O4	1000324-22-5 78
3		Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8 72
4		Adipic acid, butyl 3-pentyl ester	272 C15H28O4	1000324-60-5 64
5		Adipic acid, butyl 3-heptyl ester	300 C17H32O4	1000353-64-9 47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100517\
Data File : BF099122.D
Acq On : 6 Oct 2017 00:02
Operator : SJ/JU
Sample : I5585-15 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G70-2.5-5

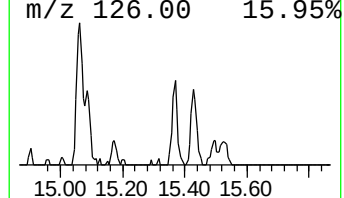
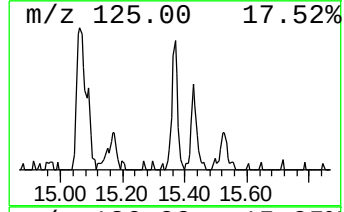
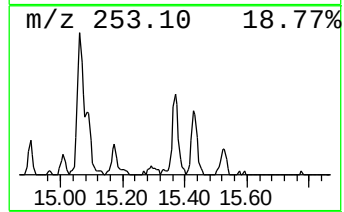
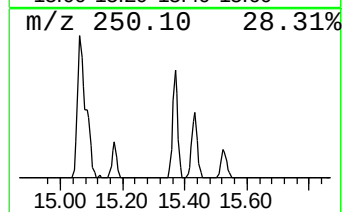
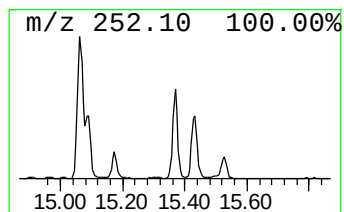
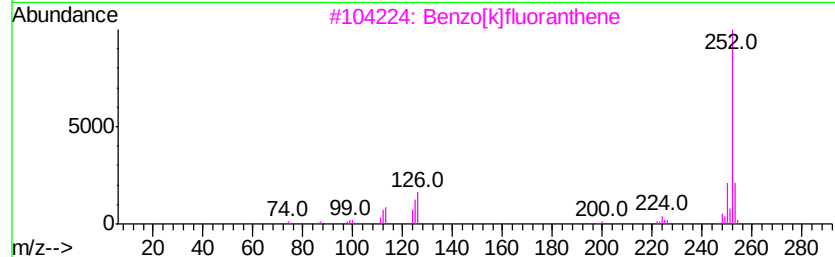
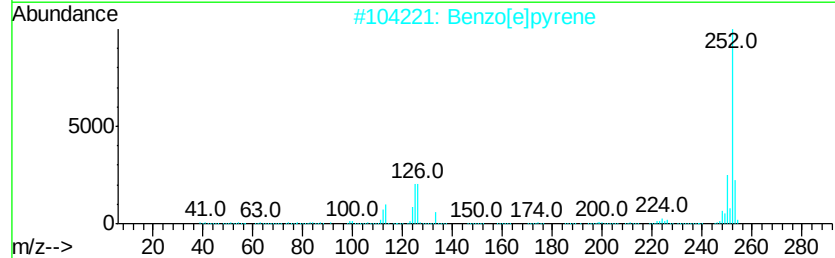
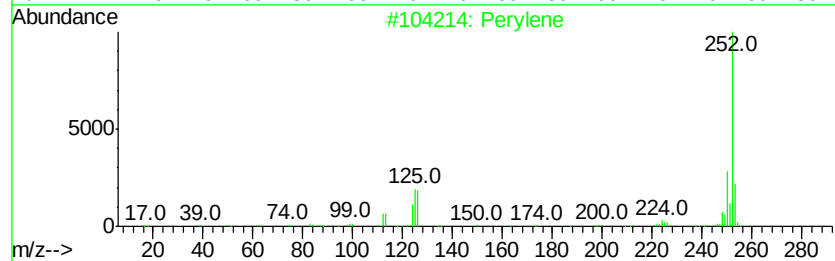
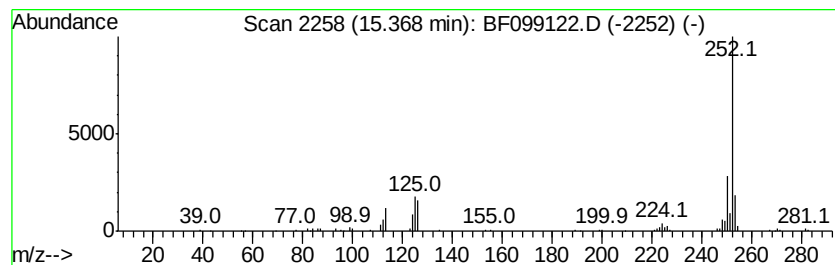
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	3.42 ng	116711	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	99
2		Benzo[e]pyrene	252	C20H12	000192-97-2	98
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	97
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	97



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100517\
Data File : BF099122.D
Acq On : 6 Oct 2017 00:02
Operator : SJ/JU
Sample : I5585-15 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G70-2.5-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.13	3.0	ng	103422	1	6.86	694501	20.0
2-Pentanone, 4-hy...	5.07	3.2	ng	111526	1	6.86	694501	20.0
unknown6.63	6.63	21.0	ng	729372	1	6.86	694501	20.0
Butyl citrate	12.77	2.7	ng	104088	5	14.02	763241	20.0
Perylene	15.37	3.4	ng	116711	6	15.50	682853	20.0