

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
 Data File : BF096742.D
 Acq On : 13 Jul 2017 22:06
 Operator : SJ/JU
 Sample : I4069-05 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(6.5-7.0)

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-BF071317.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	4.799	474	478	489	rBV	185139	237233	19.85%	1.472%
2	5.234	548	552	561	rBV	1318268	1194448	99.95%	7.412%
3	6.169	708	711	714	rBV	16115	15496	1.30%	0.096%
4	6.269	724	728	734	rBV	1234475	1195081	100.00%	7.416%
5	6.398	746	750	754	rBV	1318279	1188357	99.44%	7.374%
6	6.487	763	765	773	rBV6	10060	21146	1.77%	0.131%
7	6.634	786	790	793	rBV	822417	651379	54.51%	4.042%
8	6.669	793	796	798	rVB	59718	53093	4.44%	0.329%
9	6.704	798	802	805	rBV2	16043	21603	1.81%	0.134%
10	6.787	813	816	820	rVV	992306	912639	76.37%	5.663%
11	6.910	834	837	843	rVB3	36276	46430	3.89%	0.288%
12	7.010	848	854	855	rBV3	8860	15723	1.32%	0.098%
13	7.034	855	858	860	rVB2	25795	22126	1.85%	0.137%
14	7.069	860	864	866	rBV4	19117	21429	1.79%	0.133%
15	7.128	870	874	877	rBV4	8918	14209	1.19%	0.088%
16	7.192	881	885	888	rVB	869041	717665	60.05%	4.453%
17	7.292	897	902	907	rBV5	37209	59814	5.01%	0.371%
18	7.340	907	910	912	rBV	18054	19912	1.67%	0.124%
19	7.363	912	914	918	rVV3	30064	31473	2.63%	0.195%
20	7.410	918	922	924	rVV4	13145	20108	1.68%	0.125%
21	7.440	924	927	933	rVB3	46262	72692	6.08%	0.451%
22	7.545	941	945	946	rBV3	21758	24145	2.02%	0.150%
23	7.563	946	948	953	rVB3	55231	53156	4.45%	0.330%
24	7.616	953	957	959	rBV2	23047	31550	2.64%	0.196%
25	7.687	966	969	972	rBV4	18221	19653	1.64%	0.122%
26	7.757	978	981	984	rVB3	22565	23951	2.00%	0.149%
27	7.798	984	988	989	rBV3	13944	17976	1.50%	0.112%
28	7.816	989	991	998	rVB4	24361	39495	3.30%	0.245%
29	7.916	1004	1008	1013	rBV	1058291	884485	74.01%	5.488%
30	7.975	1013	1018	1020	rVV5	17372	28008	2.34%	0.174%
31	7.998	1020	1022	1025	rVV	166257	129974	10.88%	0.807%
32	8.051	1029	1031	1033	rVB2	24076	18690	1.56%	0.116%
33	8.098	1036	1039	1041	rBV2	29968	27107	2.27%	0.168%
34	8.134	1042	1045	1048	rVB	68408	54018	4.52%	0.335%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
 Data File : BF096742.D
 Acq On : 13 Jul 2017 22:06
 Operator : SJ/JU
 Sample : I4069-05 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(6.5-7.0)

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-BF071317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	8.216	1055	1059	1061	rVB4	34548	40051	3.35%	0.249%
36	8.245	1061	1064	1067	rVB3	19202	20316	1.70%	0.126%
37	8.281	1067	1070	1073	rBV4	28142	39242	3.28%	0.244%
38	8.357	1080	1083	1092	rVB	195390	241161	20.18%	1.496%
39	8.428	1092	1095	1098	rBV	28581	27315	2.29%	0.169%
40	8.469	1098	1102	1109	rBV3	73794	84190	7.04%	0.522%
41	8.528	1109	1112	1115	rBV4	28170	37953	3.18%	0.236%
42	8.569	1117	1119	1121	rVV3	21198	27111	2.27%	0.168%
43	8.622	1125	1128	1133	rVB3	49706	64000	5.36%	0.397%
44	8.669	1133	1136	1138	rBV3	27728	30096	2.52%	0.187%
45	8.810	1157	1160	1162	rBV4	28187	26419	2.21%	0.164%
46	8.910	1175	1177	1179	rBV2	27084	19571	1.64%	0.121%
47	8.957	1179	1185	1187	rBV	179408	144189	12.07%	0.895%
48	8.992	1187	1191	1194	rVV	1353442	1047757	87.67%	6.501%
49	9.075	1202	1205	1211	rBV7	73108	119296	9.98%	0.740%
50	9.139	1213	1216	1219	rVV5	16656	21779	1.82%	0.135%
51	9.304	1241	1244	1246	rBV4	15914	14539	1.22%	0.090%
52	9.386	1254	1258	1260	rBV2	167951	157864	13.21%	0.980%
53	9.410	1260	1262	1265	rVB	133626	98385	8.23%	0.610%
54	9.492	1274	1276	1278	rVB2	26922	17508	1.47%	0.109%
55	9.586	1289	1292	1295	rVB	60176	62608	5.24%	0.388%
56	9.616	1295	1297	1300	rBV3	28838	24707	2.07%	0.153%
57	9.663	1300	1305	1309	rBV	842473	807391	67.56%	5.010%
58	9.939	1349	1352	1356	rBV5	22556	22026	1.84%	0.137%
59	10.004	1359	1363	1366	rVB5	20376	25493	2.13%	0.158%
60	10.075	1372	1375	1378	rVB4	16308	19682	1.65%	0.122%
61	10.116	1379	1382	1386	rBV2	26477	29650	2.48%	0.184%
62	10.210	1396	1398	1400	rVB2	25688	19644	1.64%	0.122%
63	10.333	1416	1419	1422	rVB	39991	41613	3.48%	0.258%
64	10.445	1435	1438	1445	rVB	574560	492366	41.20%	3.055%
65	10.598	1458	1464	1469	rVB	54483	88086	7.37%	0.547%
66	11.033	1535	1538	1541	rVV2	16468	17422	1.46%	0.108%
67	11.063	1541	1543	1548	rVB2	19116	17021	1.42%	0.106%
68	11.139	1551	1556	1559	rBV	665211	622953	52.13%	3.866%
69	11.163	1559	1560	1564	rVV	236920	155479	13.01%	0.965%
70	11.216	1565	1569	1572	rVB	54863	46711	3.91%	0.290%
71	11.369	1592	1595	1599	rBV	15021	15062	1.26%	0.093%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	11.469	1605	1612	1616	rVB7	10957	29445	2.46%	0.183%
73	11.645	1638	1642	1644	rBV	30482	30539	2.56%	0.189%
74	11.669	1644	1646	1651	rVB2	44232	50536	4.23%	0.314%
75	11.751	1657	1660	1663	rBV	51498	49415	4.13%	0.307%
76	11.775	1663	1664	1668	rVB	29345	20591	1.72%	0.128%
77	11.939	1689	1692	1694	rBV	23437	19452	1.63%	0.121%
78	11.957	1694	1695	1699	rVB3	23042	16715	1.40%	0.104%
79	12.092	1712	1718	1720	rBV4	21057	23608	1.98%	0.146%
80	12.192	1732	1735	1738	rBV3	19494	21012	1.76%	0.130%
81	12.275	1747	1749	1754	rVB4	24929	25660	2.15%	0.159%
82	12.351	1758	1762	1765	rVB	308789	292117	24.44%	1.813%
83	12.398	1767	1770	1773	rBV4	18002	24334	2.04%	0.151%
84	12.574	1795	1800	1803	rBV	335973	326870	27.35%	2.028%
85	12.698	1818	1821	1822	rBV	25276	21115	1.77%	0.131%
86	12.727	1822	1826	1830	rVB	758596	691892	57.89%	4.293%
87	12.798	1836	1838	1841	rVB2	20570	20398	1.71%	0.127%
88	12.863	1845	1849	1850	rBV4	21131	25807	2.16%	0.160%
89	12.904	1854	1856	1859	rVB	44101	38355	3.21%	0.238%
90	12.969	1865	1867	1870	rBV3	19465	17268	1.44%	0.107%
91	13.010	1870	1874	1878	rBV	35116	42996	3.60%	0.267%
92	13.127	1892	1894	1896	rBV3	22612	19080	1.60%	0.118%
93	13.410	1940	1942	1944	rBV	22212	15064	1.26%	0.093%
94	13.516	1958	1960	1964	rBV2	30305	38045	3.18%	0.236%
95	13.639	1979	1981	1988	rVB5	44496	55497	4.64%	0.344%
96	13.769	1998	2003	2006	rBV2	666219	756346	63.29%	4.693%
97	13.792	2006	2007	2010	rVB	115958	93664	7.84%	0.581%
98	14.774	2171	2174	2182	rVB2	117036	233083	19.50%	1.446%
99	15.045	2217	2220	2225	rVB2	108810	126768	10.61%	0.787%
100	15.157	2236	2239	2242	rBV	319003	319039	26.70%	1.980%

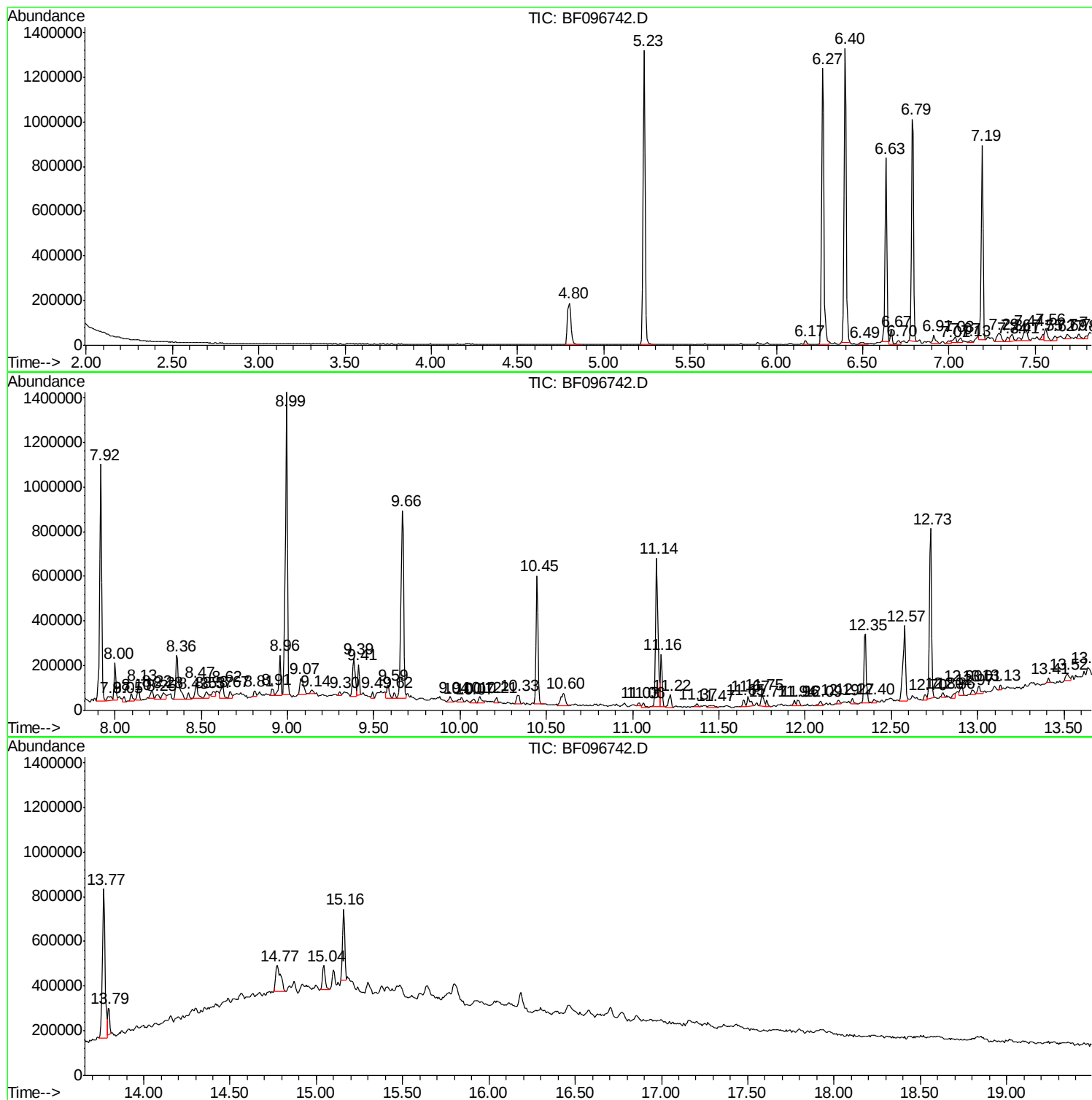
Sum of corrected areas: 16115631

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

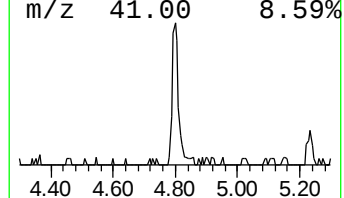
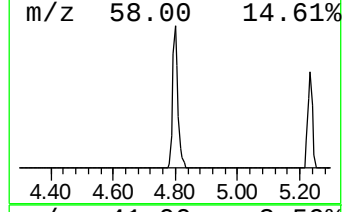
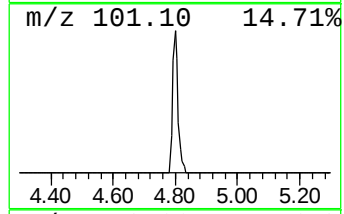
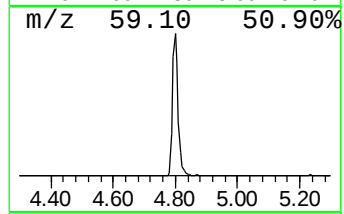
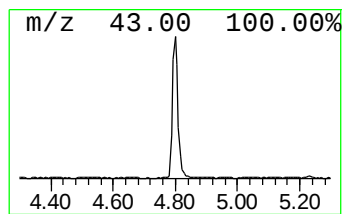
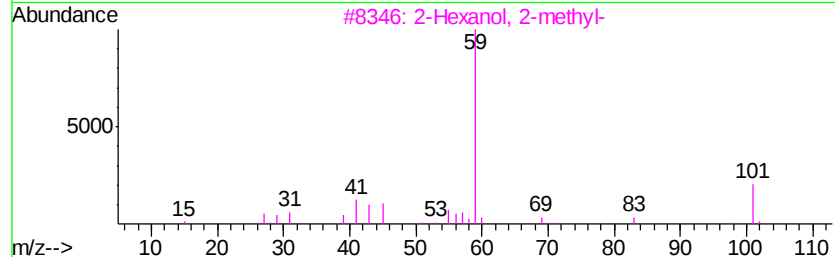
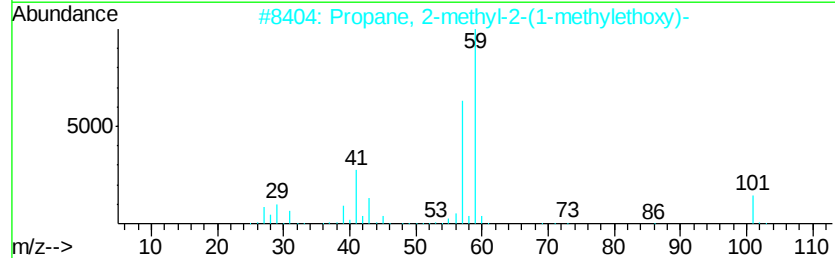
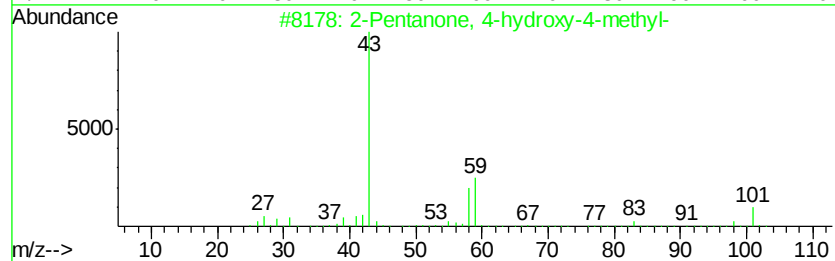
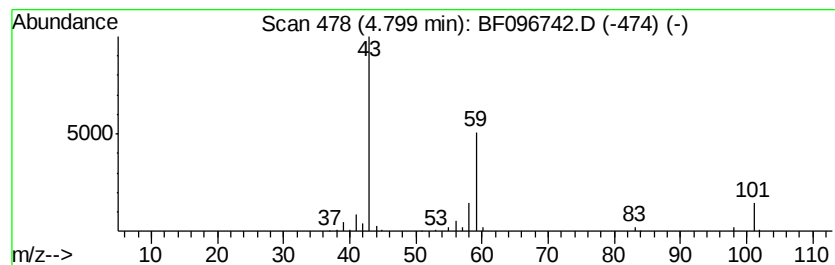
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.28 ng	237233	1,4-Dichlorobenzene-d4	6.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

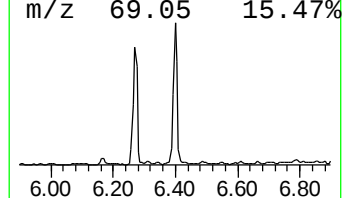
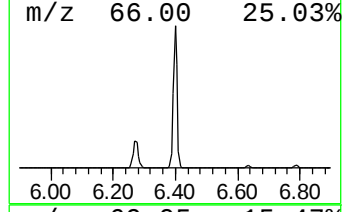
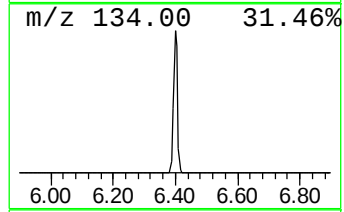
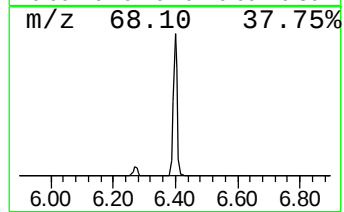
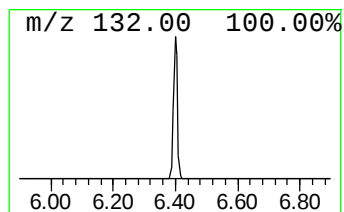
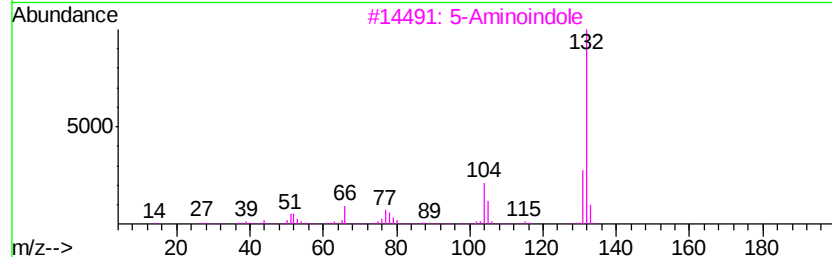
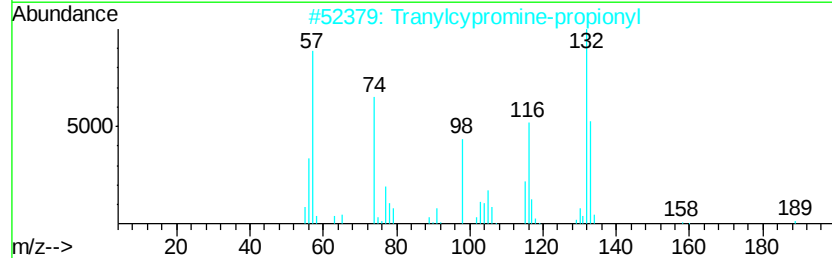
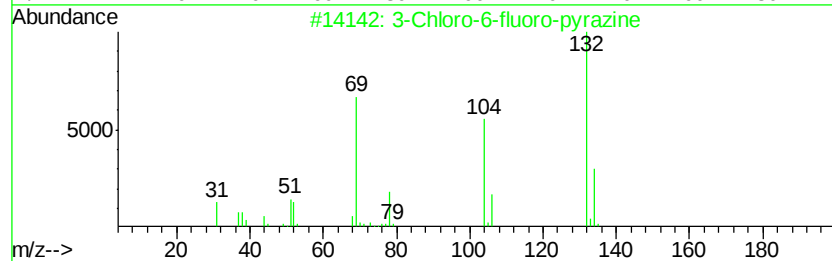
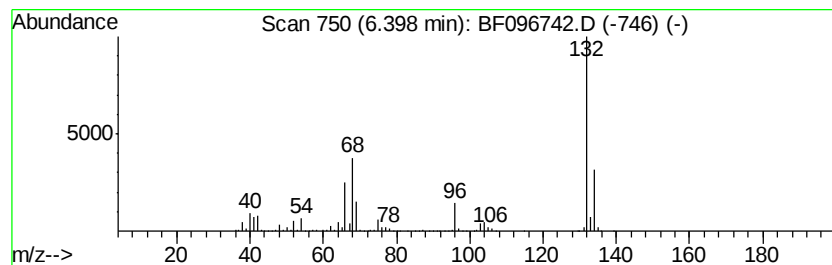
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	36.49 ng	1188360	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

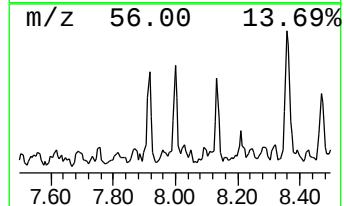
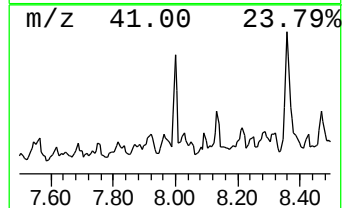
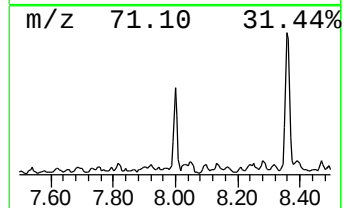
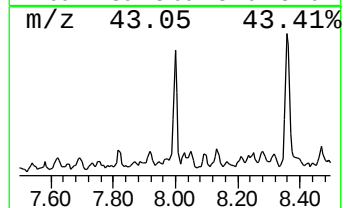
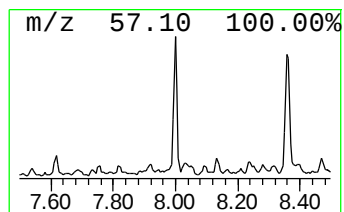
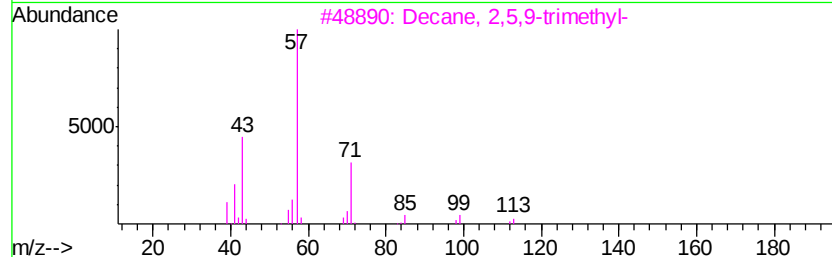
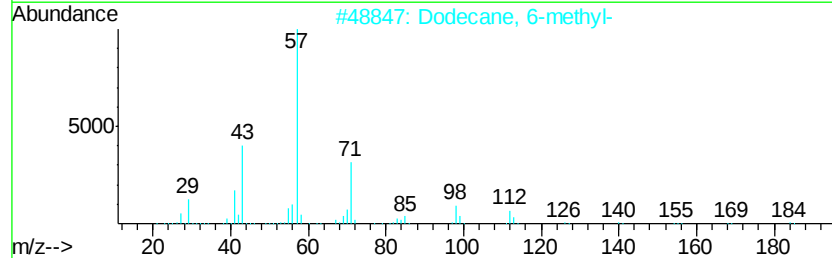
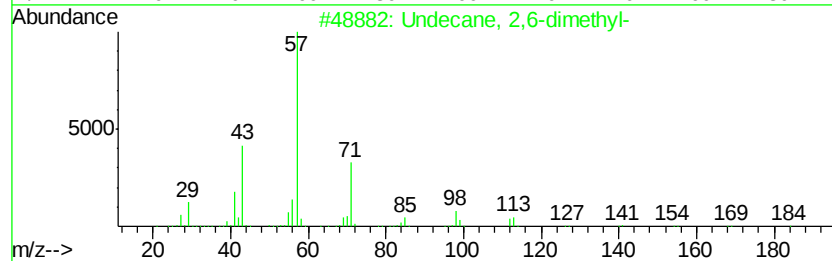
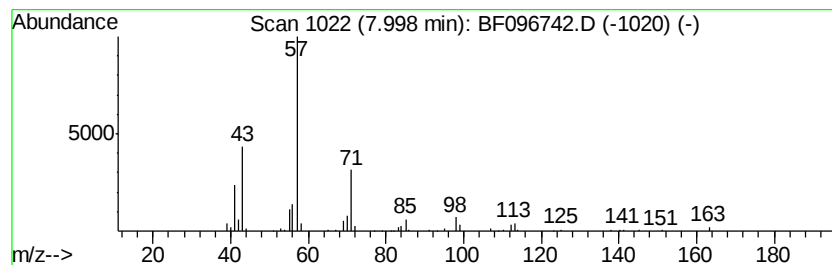
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Undecane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.00	2.94 ng	129974	Napthalene-d8	7.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	86	
2	Dodecane, 6-methyl-	184	C13H28	006044-71-9	80	
3	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	72	
4	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	72	
5	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	64	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

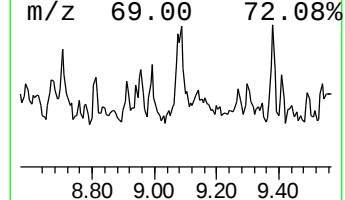
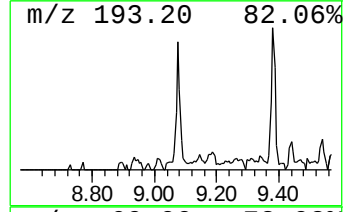
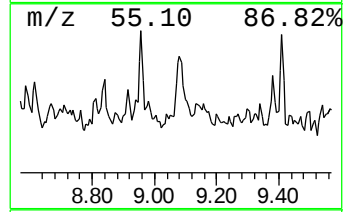
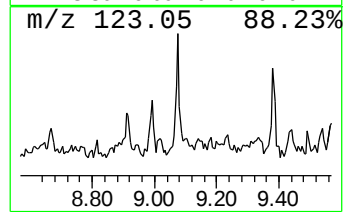
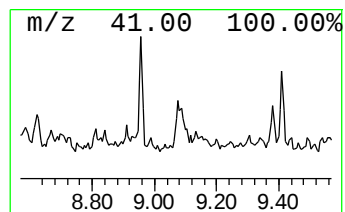
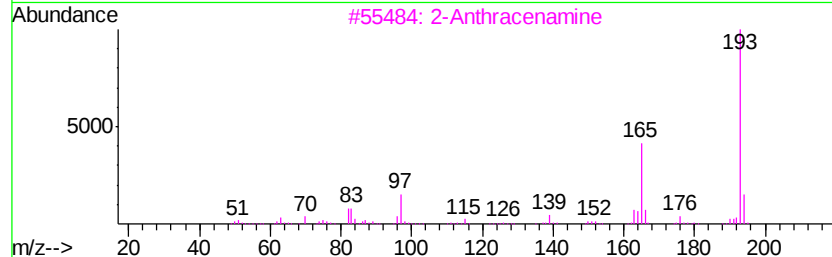
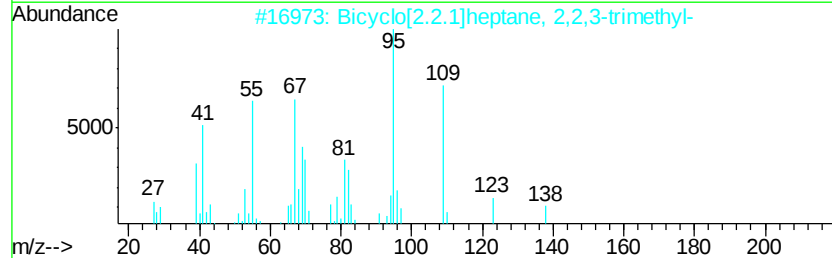
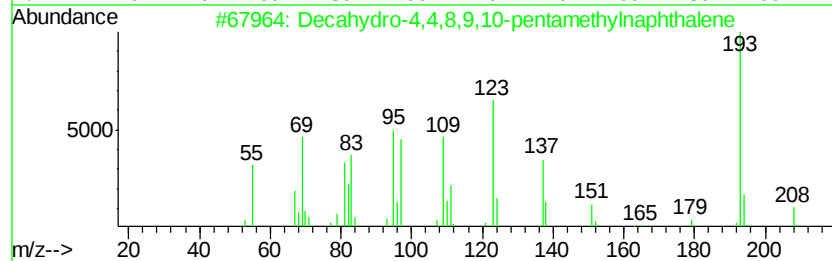
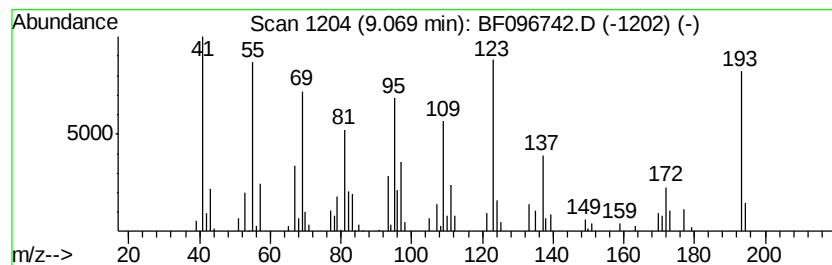
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.07 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	2.96 ng	119296	Acenaphthene-d10	9.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	45
2		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	22
3		2-Anthracenamine	193	C14H11N	000613-13-8	18
4		Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	14
5		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

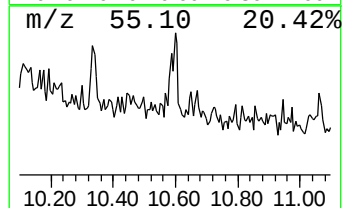
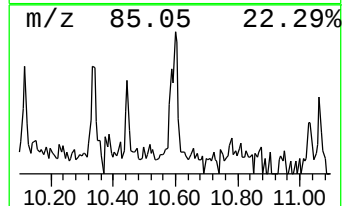
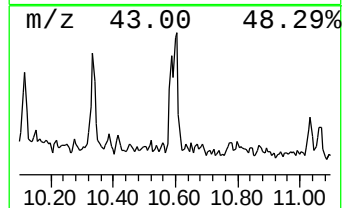
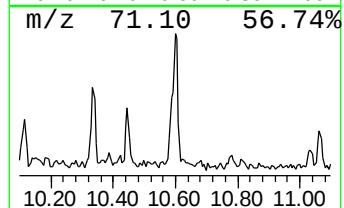
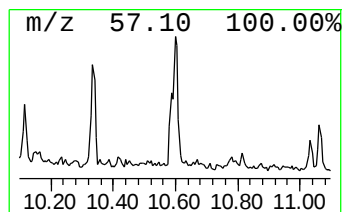
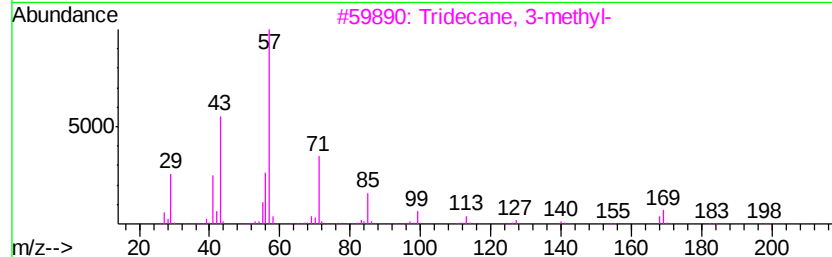
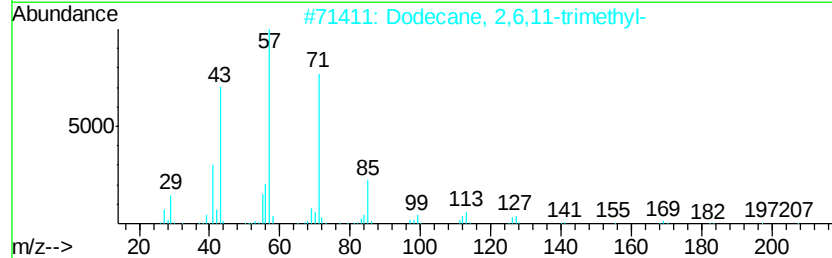
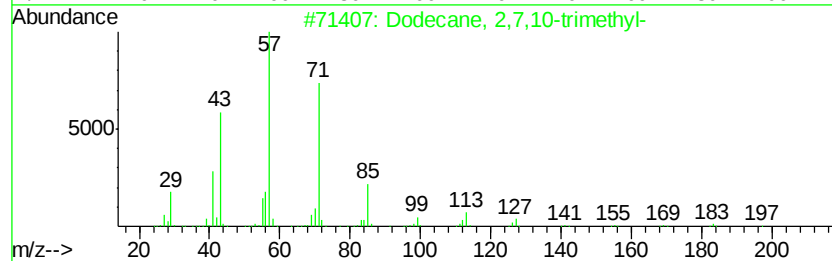
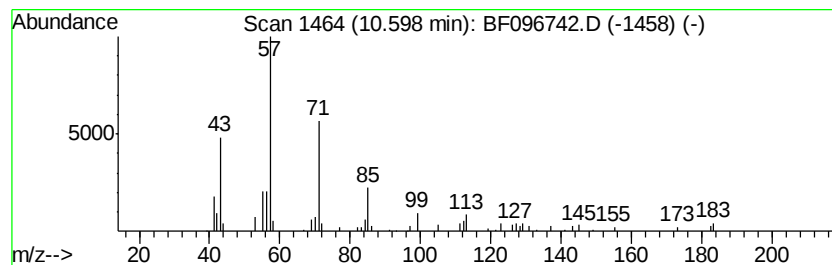
Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2,7,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.60	2.83 ng	88086	Phenanthrene-d10	11.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
4	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
5	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071317\
Data File : BF096742.D
Acq On : 13 Jul 2017 22:06
Operator : SJ/JU
Sample : I4069-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6.5-7.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.80	7.3	ng	237233	1	6.63	651379	20.0
unknown6.40	6.40	36.5	ng	1188360	1	6.63	651379	20.0
Undecane, 2,6-dim...	8.00	2.9	ng	129974	2	7.92	884485	20.0
unknown9.07	9.07	3.0	ng	119296	3	9.66	807391	20.0
Dodecane, 2,7,10-...	10.60	2.8	ng	88086	4	11.14	622953	20.0