

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
 Data File : BF102670.D
 Acq On : 31 Jan 2018 22:19
 Operator : SJ/JU
 Sample : J1378-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72

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-BF012218.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	3.728	268	279	291	rBV	594423	1298816	4.43%	0.455%
2	4.316	372	379	382	rBV	2946497	4308911	14.69%	1.508%
3	5.339	549	553	562	rVB	1906008	2244267	7.65%	0.785%
4	5.669	605	609	616	rVB	855788	1105909	3.77%	0.387%
5	5.992	652	664	666	rVV	8031721	14668857	50.02%	5.133%
6	6.139	687	689	692	rVB2	1083836	877160	2.99%	0.307%
7	6.263	707	710	713	rBV	979120	985486	3.36%	0.345%
8	6.410	727	735	738	rBV2	6617882	9430818	32.16%	3.300%
9	6.492	747	749	753	rVB	1904971	1766071	6.02%	0.618%
10	6.586	758	765	768	rBV3	976485	1357555	4.63%	0.475%
11	6.651	773	776	780	rBV	2775238	2543265	8.67%	0.890%
12	6.710	783	786	789	rBV2	975261	1205905	4.11%	0.422%
13	6.786	796	799	801	rBV2	955834	1512824	5.16%	0.529%
14	6.810	801	803	804	rVV	1324091	1063874	3.63%	0.372%
15	6.822	804	805	807	rVB	3174187	1646586	5.62%	0.576%
16	6.845	807	809	811	rBV	1631171	1314296	4.48%	0.460%
17	6.863	811	812	815	rVB	1613759	1209133	4.12%	0.423%
18	7.028	834	840	842	rVV4	1082289	1775714	6.06%	0.621%
19	7.045	842	843	848	rVB	1130165	796215	2.72%	0.279%
20	7.110	848	854	859	rBV2	637597	1053360	3.59%	0.369%
21	7.245	870	877	879	rVV3	1613022	2516333	8.58%	0.881%
22	7.281	879	883	889	rVV5	2775787	4033438	13.75%	1.412%
23	7.357	893	896	900	rVB2	1599888	1481629	5.05%	0.519%
24	7.475	910	916	918	rBV3	465383	832313	2.84%	0.291%
25	7.533	922	926	929	rVV	2406815	2463097	8.40%	0.862%
26	7.698	949	954	955	rBV2	1343864	1613780	5.50%	0.565%
27	7.716	955	957	960	rVV5	1066957	1383873	4.72%	0.484%
28	7.804	969	972	974	rBV3	1107080	1356755	4.63%	0.475%
29	7.828	974	976	978	rVV2	1037986	1026524	3.50%	0.359%
30	7.910	978	990	993	rVV3	3080798	7105519	24.23%	2.487%
31	7.939	993	995	998	rVB2	2473665	2792849	9.52%	0.977%
32	7.992	998	1004	1007	rBV3	1356273	2267584	7.73%	0.794%
33	8.039	1007	1012	1013	rVV	5436719	8346599	28.46%	2.921%
34	8.063	1014	1016	1021	rVB2	6401685	5457984	18.61%	1.910%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
 Data File : BF102670.D
 Acq On : 31 Jan 2018 22:19
 Operator : SJ/JU
 Sample : J1378-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72

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-BF012218.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	8.145	1027	1030	1033	rVB2	1931994	1940295	6.62%	0.679%
36	8.180	1033	1036	1041	rVB3	840553	1162682	3.96%	0.407%
37	8.292	1052	1055	1057	rVB	911577	809407	2.76%	0.283%
38	8.392	1065	1072	1074	rBV3	1467152	1767156	6.03%	0.618%
39	8.422	1074	1077	1079	rBV3	586081	878636	3.00%	0.307%
40	8.486	1086	1088	1094	rVB3	2418738	2417937	8.25%	0.846%
41	8.563	1098	1101	1105	rVV2	841951	1266214	4.32%	0.443%
42	8.622	1108	1111	1114	rBV	2976041	2848328	9.71%	0.997%
43	8.739	1128	1131	1133	rVV2	872015	919066	3.13%	0.322%
44	8.775	1133	1137	1146	rVB3	2681391	4522995	15.42%	1.583%
45	8.892	1153	1157	1159	rVV2	1800806	2229805	7.60%	0.780%
46	8.922	1160	1162	1165	rVV2	1063033	1247964	4.26%	0.437%
47	8.980	1168	1172	1174	rVV2	1292422	1839924	6.27%	0.644%
48	9.004	1174	1176	1183	rVV3	1077098	1379227	4.70%	0.483%
49	9.069	1183	1187	1192	rVB	2624039	2544945	8.68%	0.891%
50	9.175	1201	1205	1208	rVV3	1607897	1776761	6.06%	0.622%
51	9.245	1211	1217	1221	rVB	3372352	4726820	16.12%	1.654%
52	9.316	1225	1229	1235	rVB	844817	1109134	3.78%	0.388%
53	9.369	1235	1238	1240	rBV	2274936	2037597	6.95%	0.713%
54	9.427	1244	1248	1254	rVB5	1061221	1642649	5.60%	0.575%
55	9.480	1255	1257	1265	rVB3	665605	939111	3.20%	0.329%
56	9.580	1271	1274	1276	rBV2	971608	928776	3.17%	0.325%
57	9.633	1281	1283	1287	rVV3	1505155	1659942	5.66%	0.581%
58	9.716	1294	1297	1299	rVV2	849607	1021037	3.48%	0.357%
59	9.745	1299	1302	1304	rVV	1072042	1198095	4.09%	0.419%
60	9.857	1317	1321	1323	rBV2	1163561	1064238	3.63%	0.372%
61	9.892	1323	1327	1330	rVV3	591642	824889	2.81%	0.289%
62	10.010	1344	1347	1350	rVV4	945114	1331924	4.54%	0.466%
63	10.045	1350	1353	1354	rVV2	962103	1142382	3.90%	0.400%
64	10.080	1356	1359	1361	rVV	1613999	2114531	7.21%	0.740%
65	10.110	1361	1364	1368	rVV4	457076	858196	2.93%	0.300%
66	10.174	1372	1375	1379	rVV3	1045397	1600658	5.46%	0.560%
67	10.416	1413	1416	1418	rBV	1568534	1248025	4.26%	0.437%
68	10.492	1425	1429	1432	rBV3	1701182	2831962	9.66%	0.991%
69	10.616	1445	1450	1452	rVB3	755671	882363	3.01%	0.309%
70	10.933	1497	1504	1510	rBV4	4104824	7804866	26.62%	2.731%
71	11.063	1524	1526	1529	rBV2	1508787	1280431	4.37%	0.448%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
 Data File : BF102670.D
 Acq On : 31 Jan 2018 22:19
 Operator : SJ/JU
 Sample : J1378-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	11.233	1549	1555	1560	rVV3	1171592	1942518	6.62%	0.680%
73	11.292	1560	1565	1569	rVV	1017106	1758926	6.00%	0.616%
74	11.363	1573	1577	1582	rVV3	876108	1200393	4.09%	0.420%
75	11.763	1640	1645	1647	rBV2	1251145	1810866	6.18%	0.634%
76	11.851	1647	1660	1663	rVB	4359505	15002954	51.16%	5.250%
77	11.921	1669	1672	1675	rBV2	1688129	1897713	6.47%	0.664%
78	11.968	1677	1680	1683	rVV3	776118	962611	3.28%	0.337%
79	12.004	1684	1686	1692	rVB4	963570	871313	2.97%	0.305%
80	12.086	1693	1700	1706	rBV2	4979000	10535447	35.93%	3.687%
81	12.139	1707	1709	1712	rBV3	628890	848267	2.89%	0.297%
82	12.233	1721	1725	1733	rBV5	1205510	2358167	8.04%	0.825%
83	12.316	1733	1739	1741	rBV2	4278512	6025222	20.55%	2.109%
84	12.351	1741	1745	1748	rVV2	3132448	3848575	13.12%	1.347%
85	12.398	1749	1753	1762	rVB4	2169021	2925010	9.97%	1.024%
86	12.474	1763	1766	1768	rBV	1579510	1807841	6.16%	0.633%
87	12.621	1769	1791	1795	rVV5	4277477	29324448	100.00%	10.262%
88	12.668	1795	1799	1801	rVB	2771427	3394642	11.58%	1.188%
89	12.692	1801	1803	1805	rBV	961229	866727	2.96%	0.303%
90	12.815	1819	1824	1826	rBV3	2876512	4143131	14.13%	1.450%
91	12.980	1844	1852	1854	rBV	2829435	6192380	21.12%	2.167%
92	13.039	1857	1862	1868	rVB3	2266508	4391392	14.98%	1.537%
93	13.145	1876	1880	1886	rVB2	2018158	3400109	11.59%	1.190%
94	14.362	2085	2087	2091	rVB	1261743	1219866	4.16%	0.427%
95	14.651	2133	2136	2141	rVB2	1763314	2428499	8.28%	0.850%
96	14.968	2186	2190	2194	rBV	1661830	2207077	7.53%	0.772%
97	15.327	2245	2251	2257	rVB2	2340163	4203750	14.34%	1.471%
98	15.733	2316	2320	2327	rVB	1296505	1908169	6.51%	0.668%
99	15.915	2346	2351	2358	rBV5	1049950	2004303	6.83%	0.701%
100	16.203	2394	2400	2406	rVB2	1839403	3628211	12.37%	1.270%

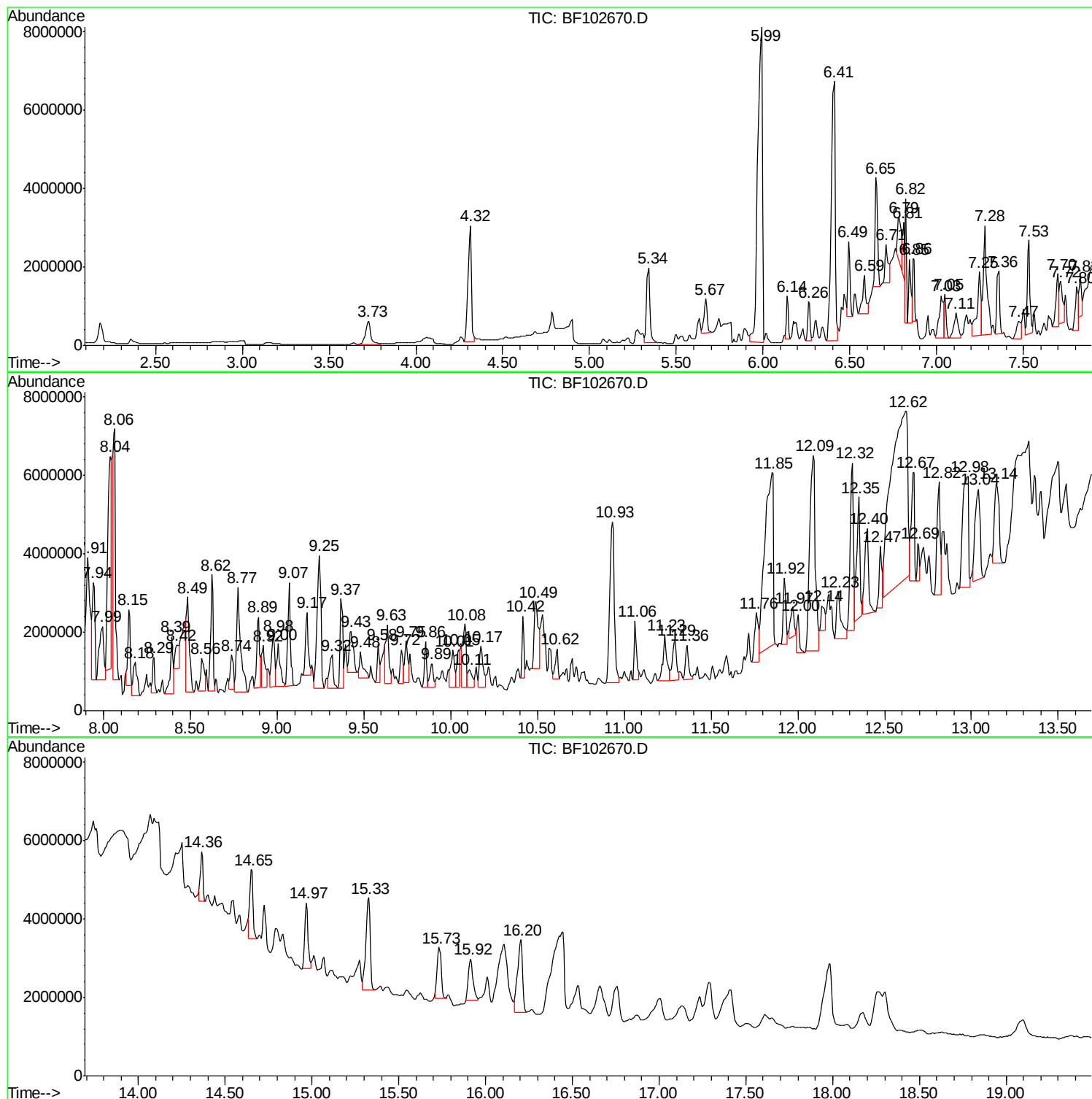
Sum of corrected areas: 285750794

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.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\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

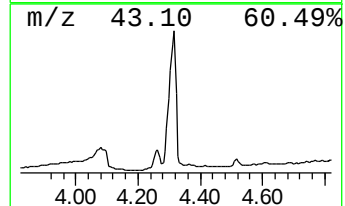
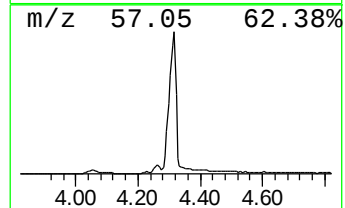
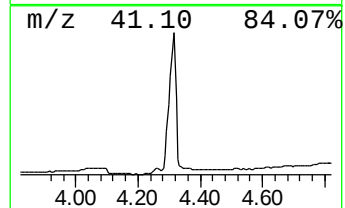
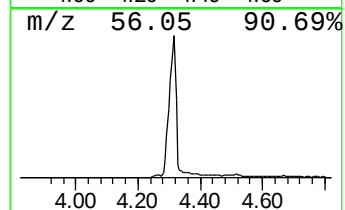
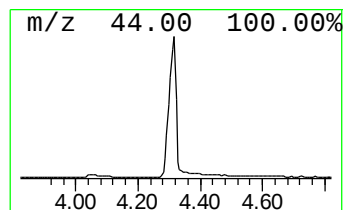
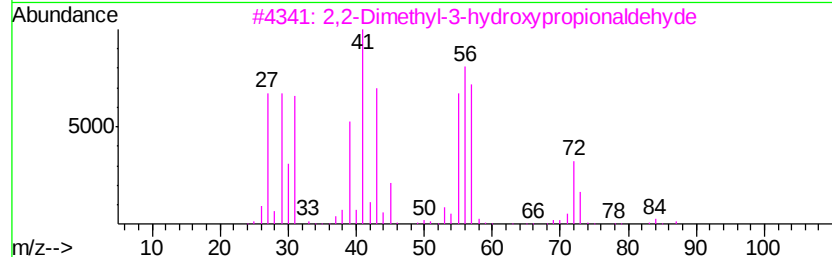
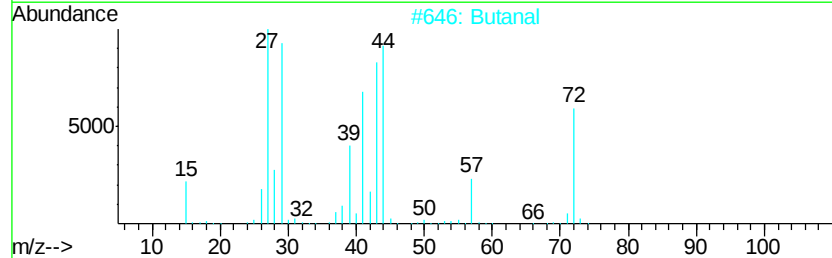
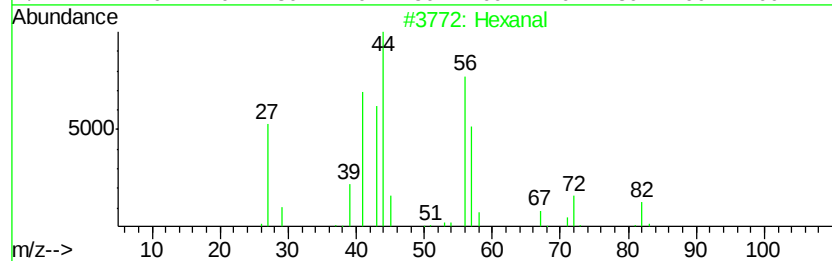
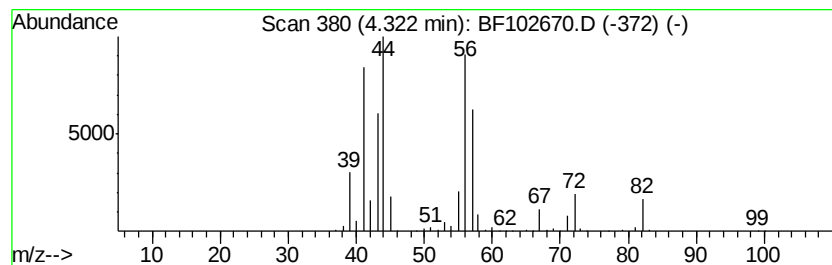
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	71.46 ng	4308910	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	90
2		Butanal	72	C4H8O	000123-72-8	38
3		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
4		Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
5		1-Butanol, 2-methyl-, (S)-	88	C5H12O	001565-80-6	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

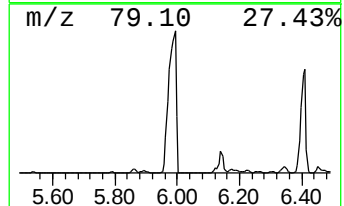
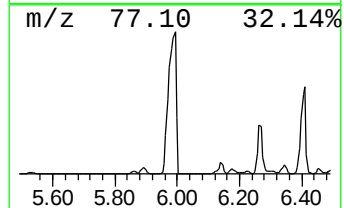
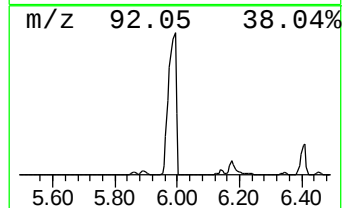
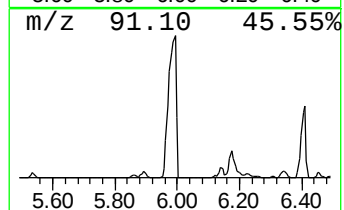
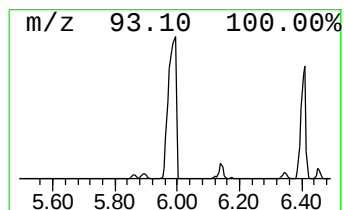
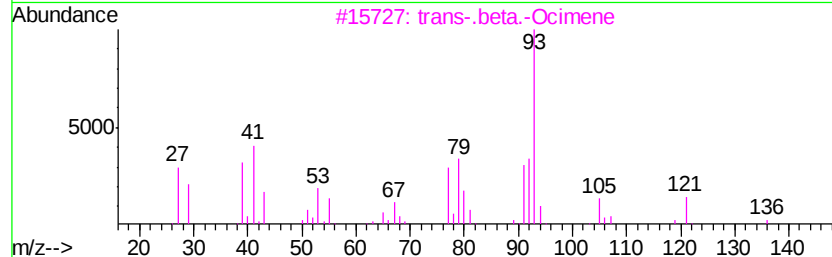
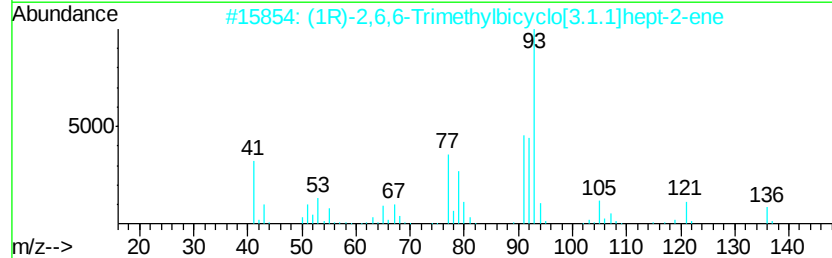
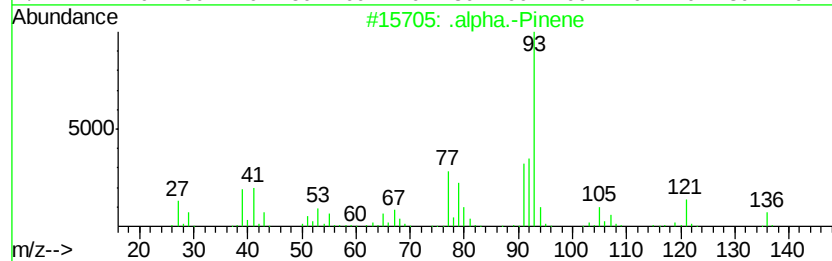
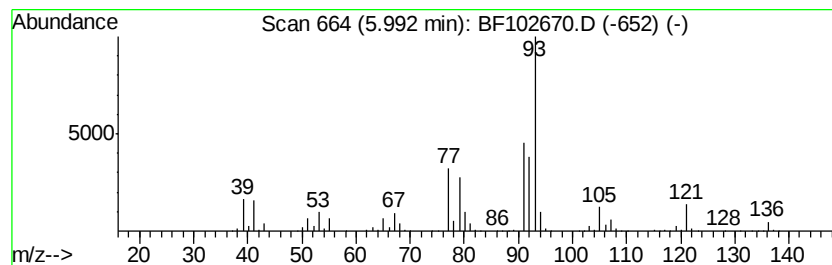
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.99	243.28 ng	14668900	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Pinene	136	C10H16	000080-56-8	95
2		(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
3		trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
4		Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

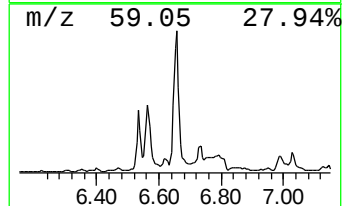
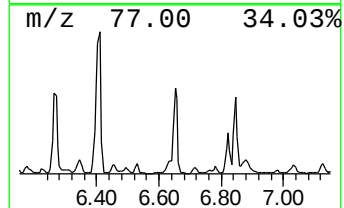
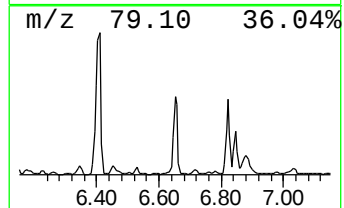
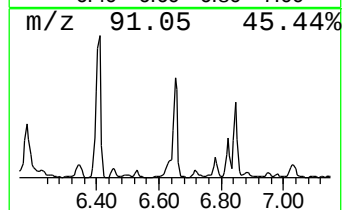
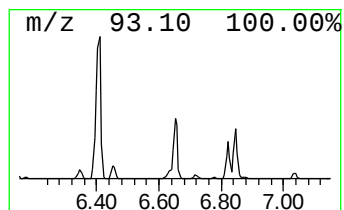
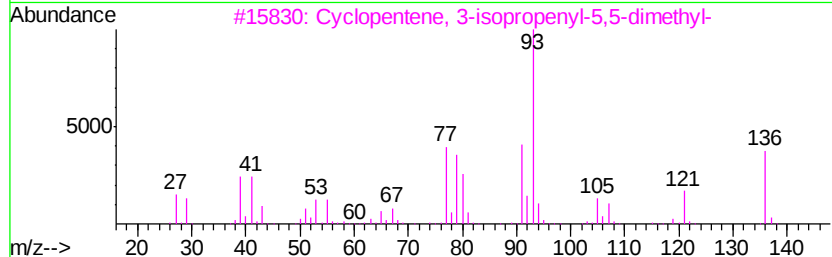
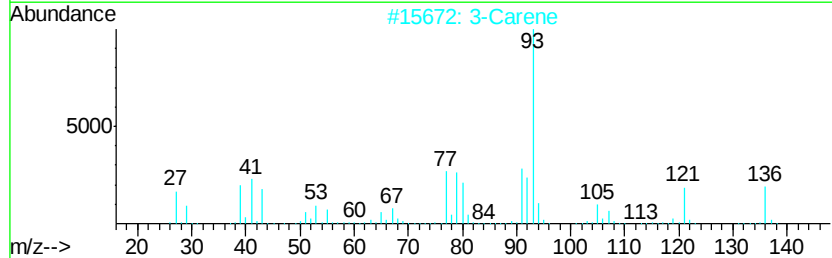
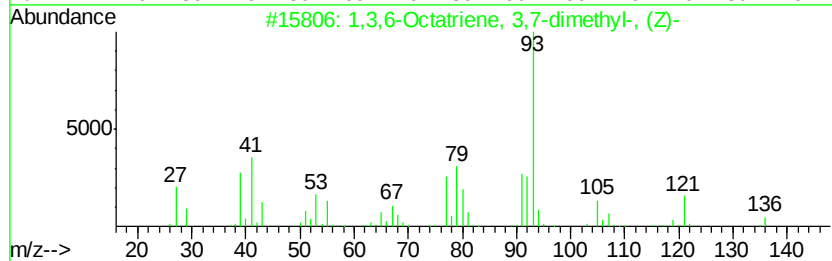
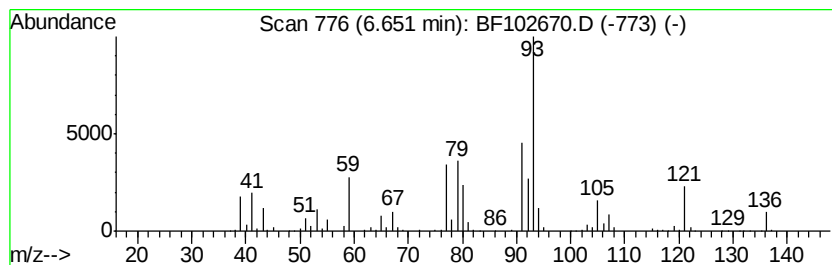
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,3,6-Octatriene, 3,7-dimet... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	42.18 ng	2543270	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	93
2		3-Carene	136	C10H16	013466-78-9	93
3		Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	87
4		4-Carene, (1S,3S,6R)-(-)-	136	C10H16	005208-50-4	83
5		.gamma.-Terpinene	136	C10H16	000099-85-4	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

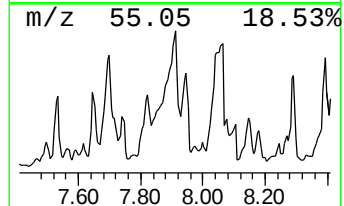
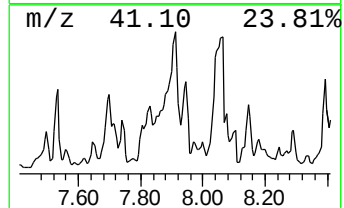
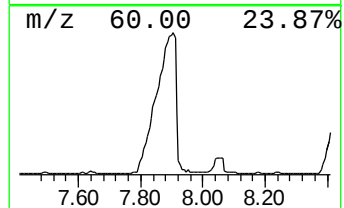
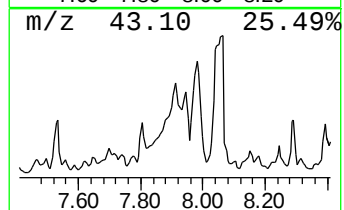
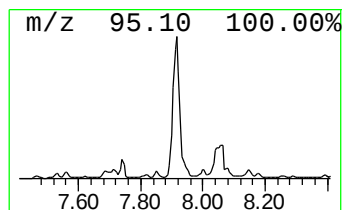
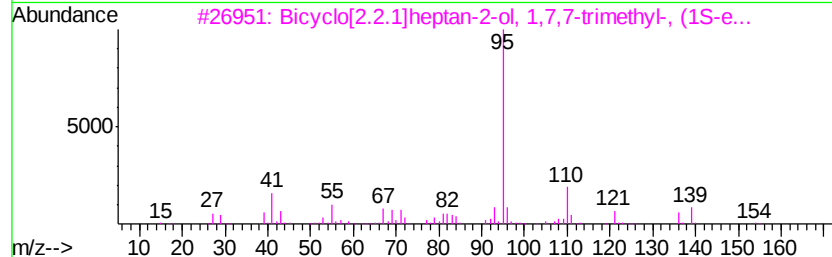
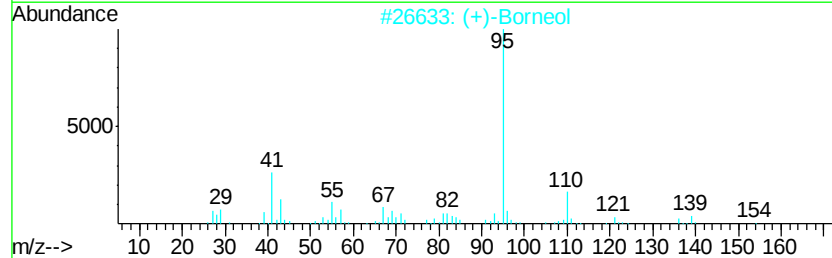
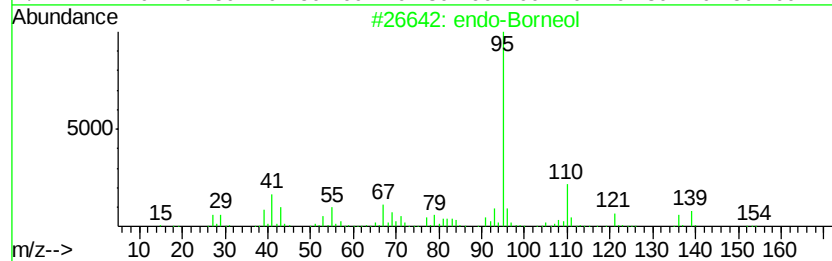
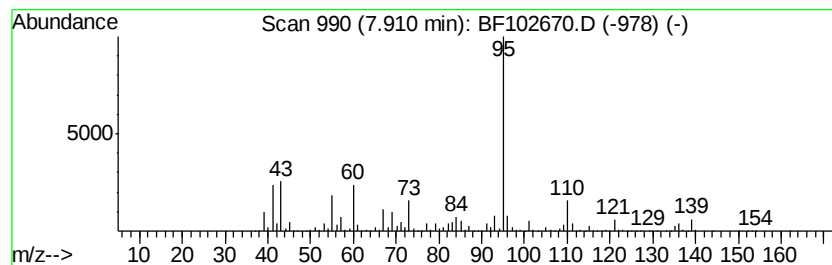
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 endo-Borneol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	62.67 ng	7105520	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	endo-Borneol	154	C10H18O	000507-70-0	76
2		(+)-Borneol	154	C10H18O	1000150-76-3	59
3		Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	53
4		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	52
5		Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

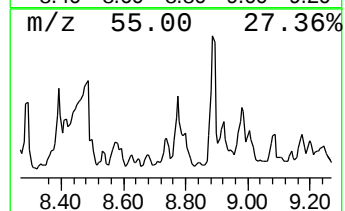
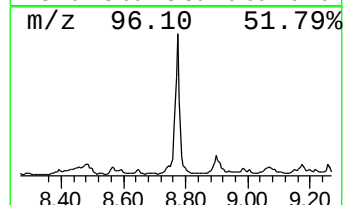
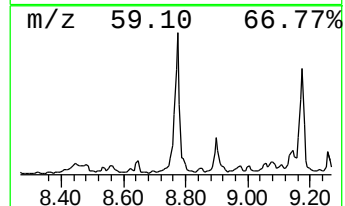
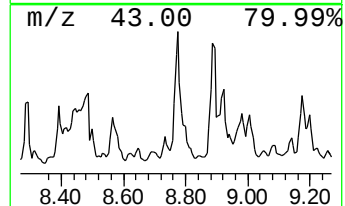
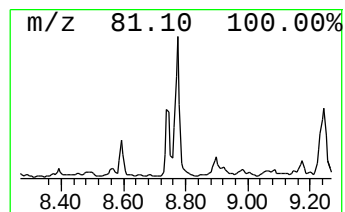
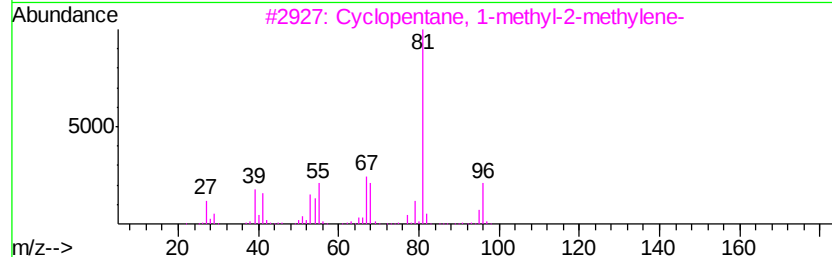
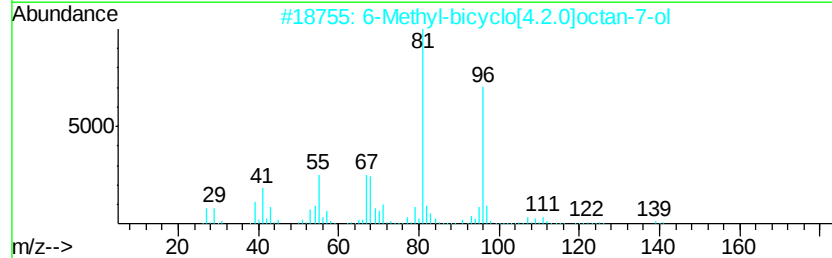
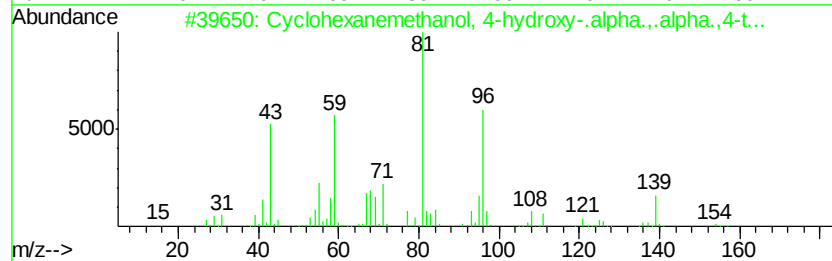
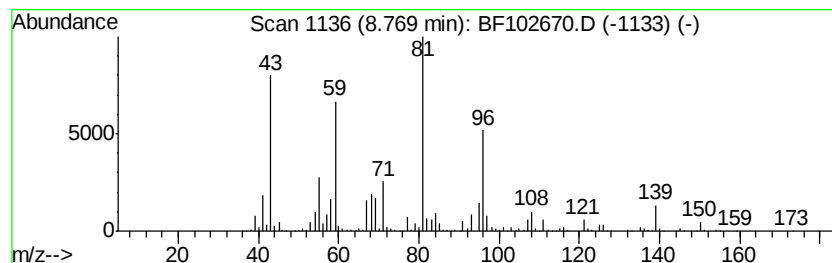
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexanemethanol, 4-hydr... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	39.89 ng	4523000	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanemethanol, 4-hydroxy-....	172	C10H20O2	000080-53-5	91
2		6-Methyl-bicyclo[4.2.0]octan-7-ol	140	C9H16O	1000193-87-3	47
3		Cyclopentane, 1-methyl-2-methylene-	96	C7H12	041158-41-2	47
4		Pentalene, octahydro-2,5-dimethyl-	138	C10H18	028588-55-8	47
5		Formic acid, trans-4-methylcyclo...	142	C8H14O2	1000368-24-5	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

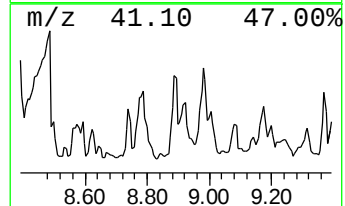
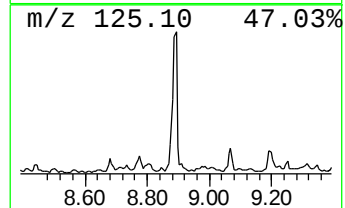
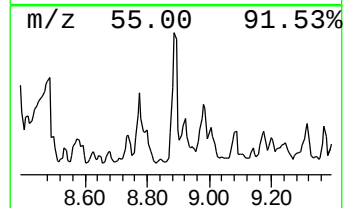
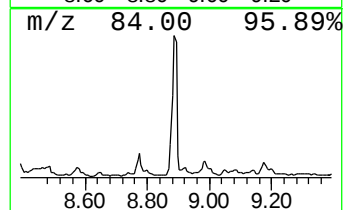
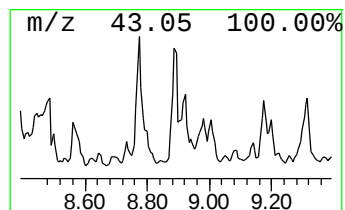
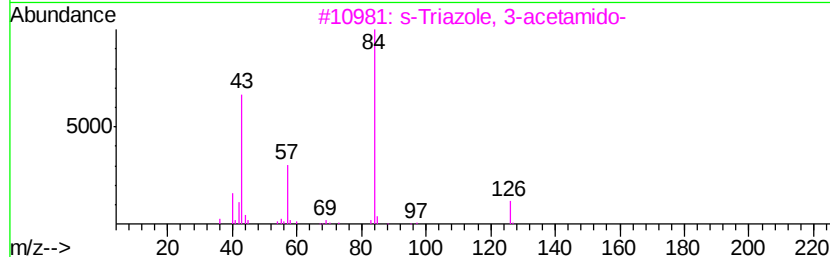
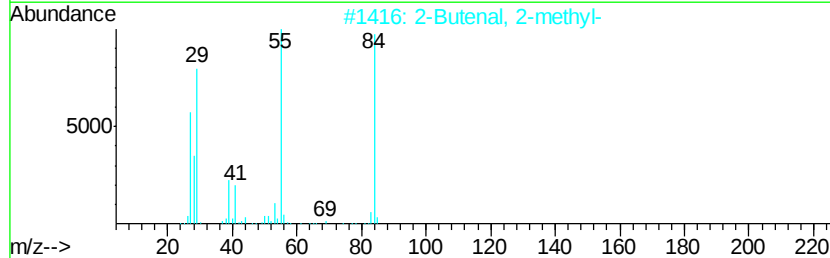
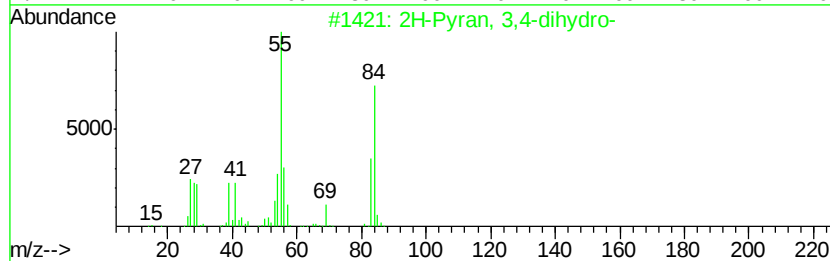
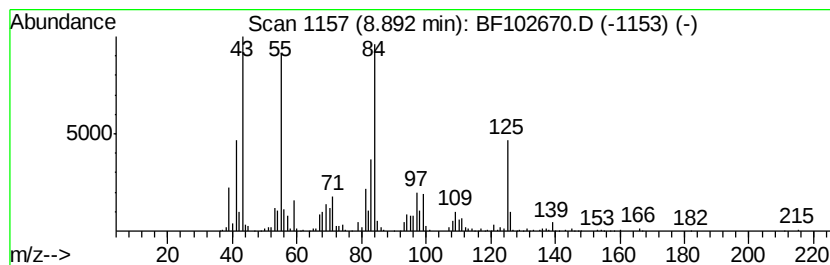
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.89 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	37.22 ng	2229810	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	43
2		2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	35
3		s-Triazole, 3-acetamido-	126	C4H6N4O	005295-23-8	30
4		3-Piperidinone, 1-ethyl-	127	C7H13NO	043152-93-8	27
5		2-Methoxy-4,4,5,5-tetramethyl-2-...	157	C8H15NO2	049680-47-9	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
RO-72

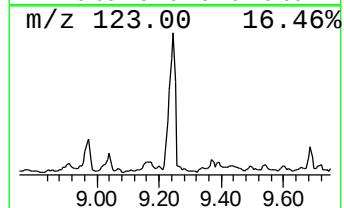
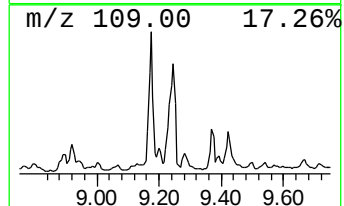
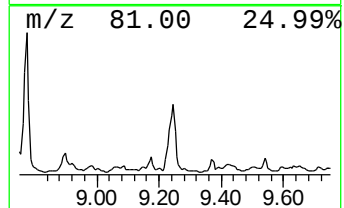
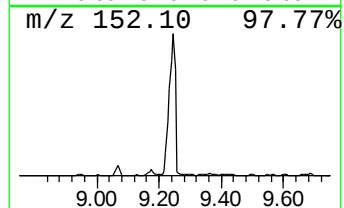
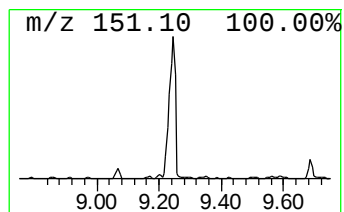
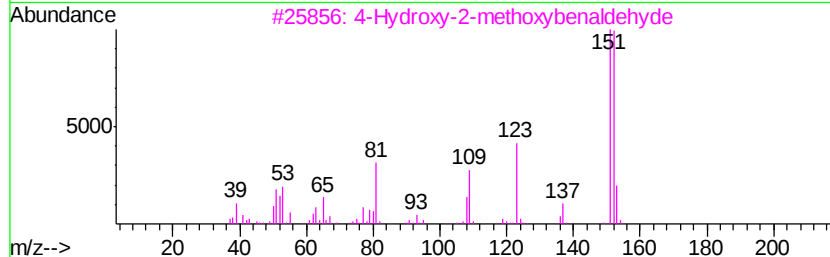
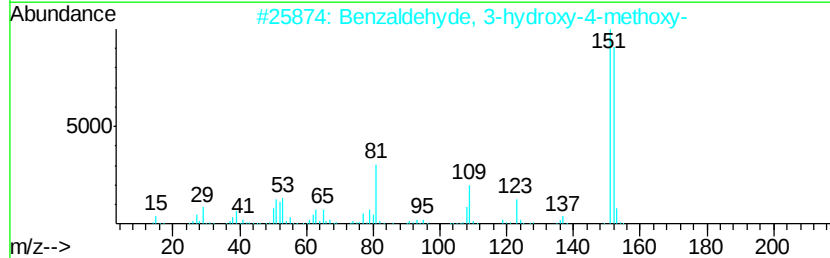
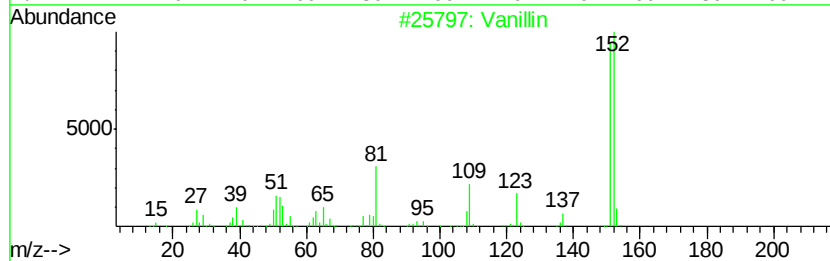
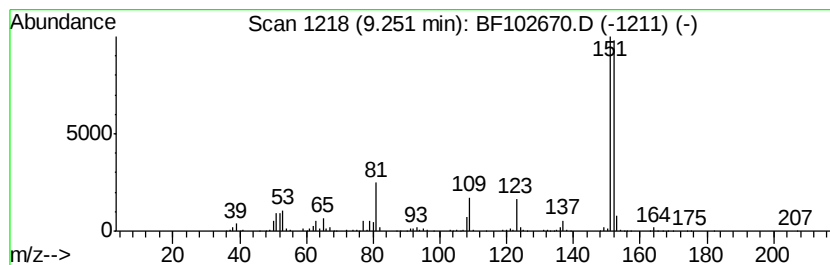
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Vanillin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.25	78.91 ng	4726820	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	97
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3		4-Hydroxy-2-methoxybenzaldehyde	152	C8H8O3	018278-34-7	87
4		Vanillin lactoside	476	C20H28O13	1000129-94-7	72
5		Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

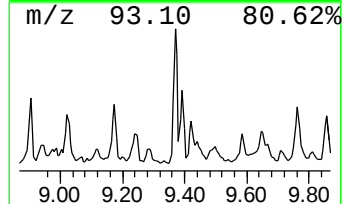
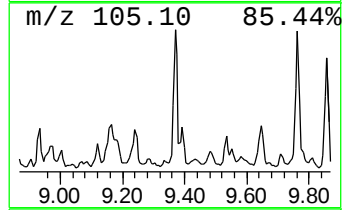
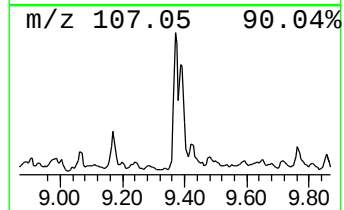
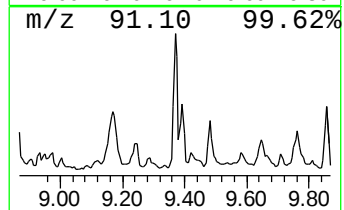
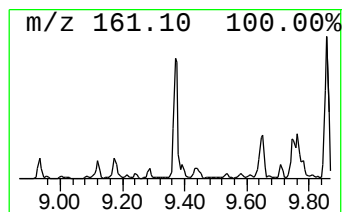
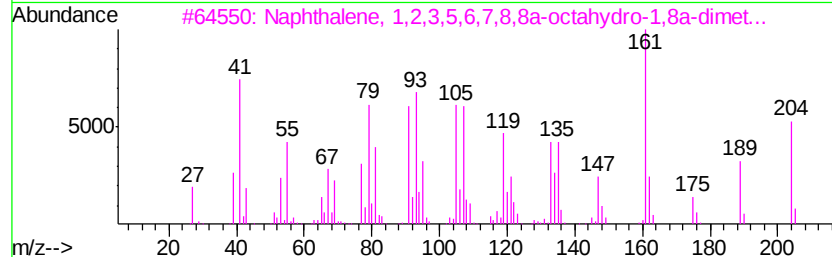
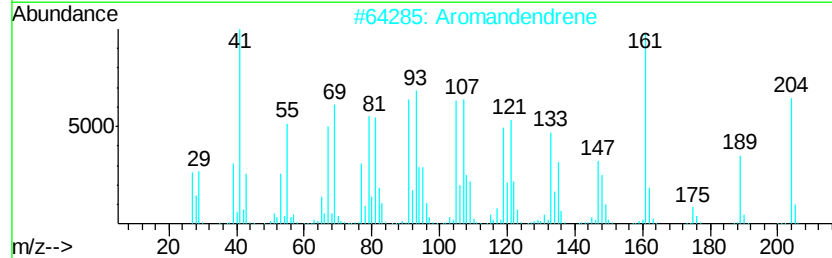
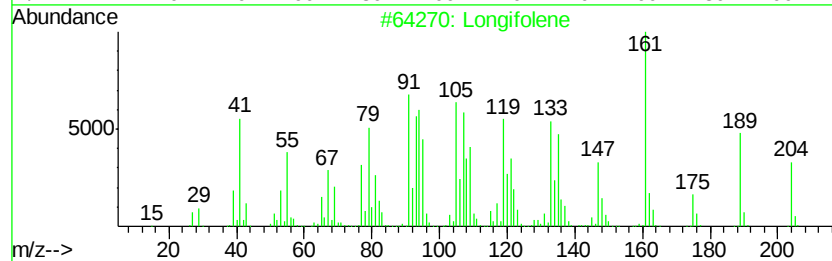
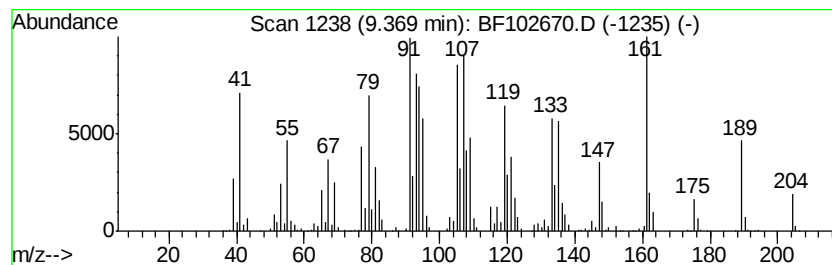
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Longifolene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	34.01 ng	2037600	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Longifolene	204	C15H24	000475-20-7	99
2		Aromandendrene	204	C15H24	000489-39-4	86
3		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	78
4		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	78
5		1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

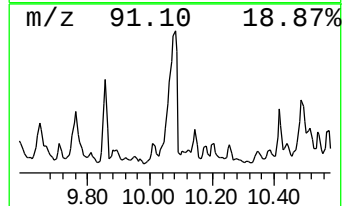
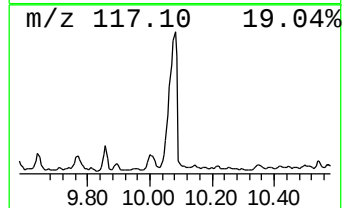
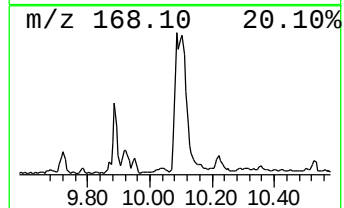
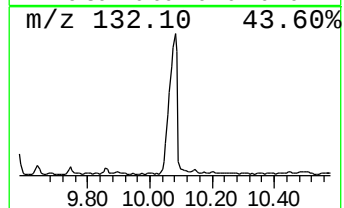
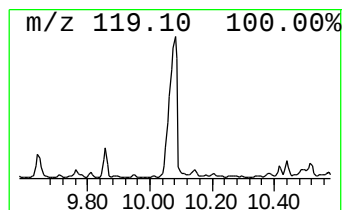
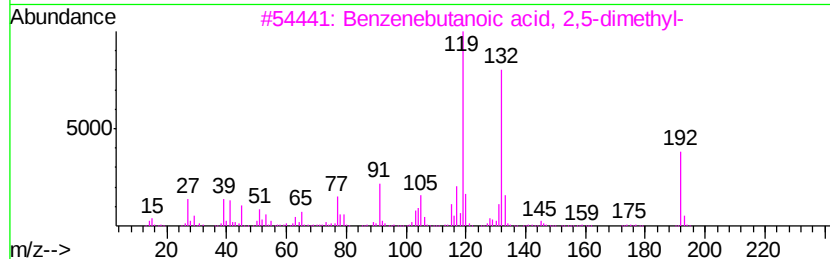
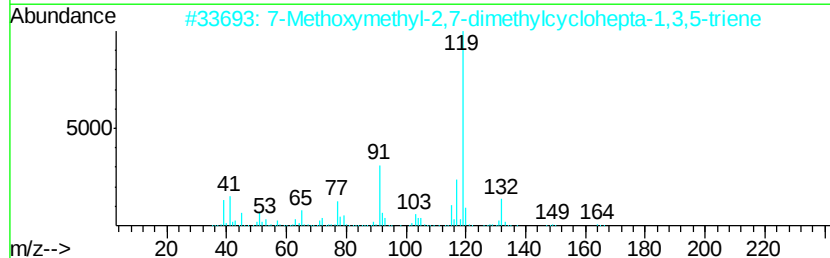
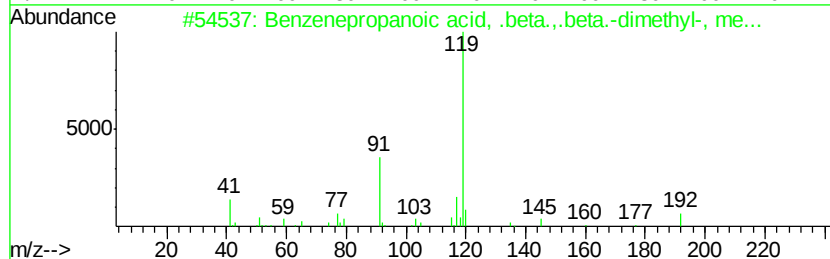
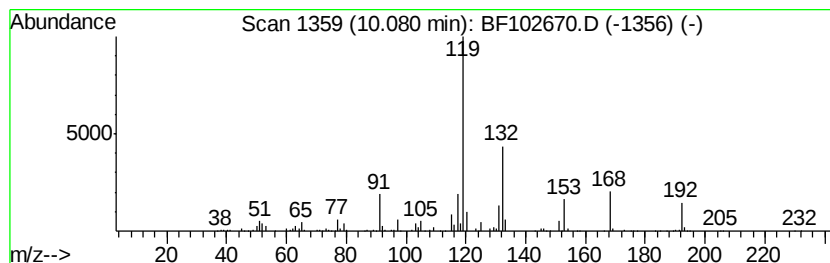
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.08 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.08	35.30 ng	2114530	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanoic acid, .beta.,.b...	192	C12H16O2	025080-84-6	46
2		7-Methoxymethyl-2,7-dimethylcyclo...	164	C11H16O	073992-48-0	45
3		Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	38
4		Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	35
5		Ethyl 1,3-dithiane-2-carboxylate	192	C7H12O2S2	020462-00-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

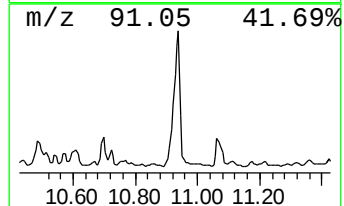
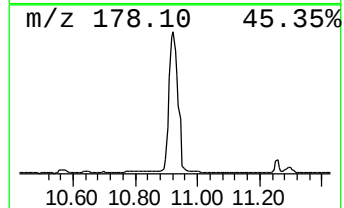
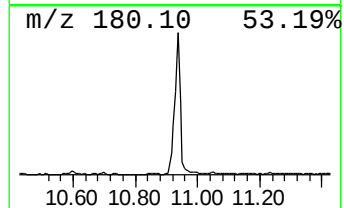
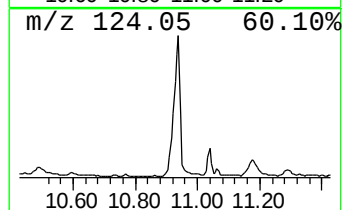
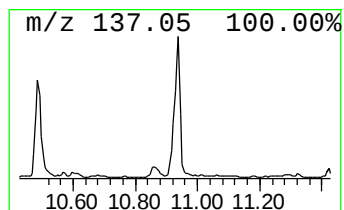
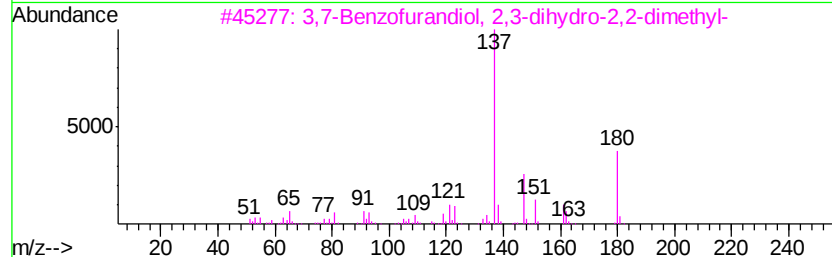
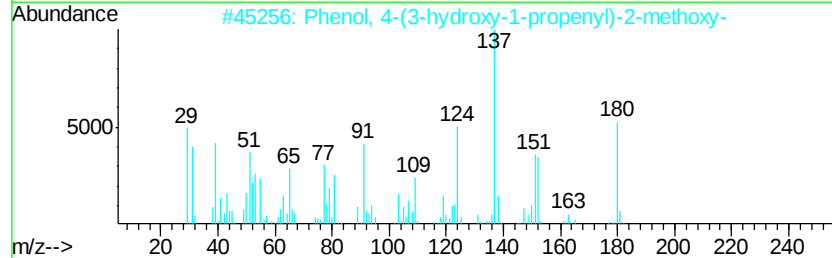
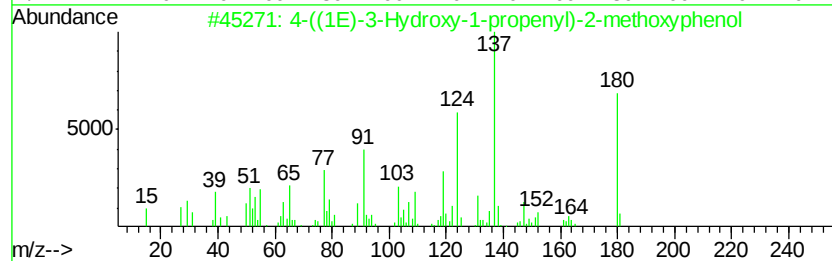
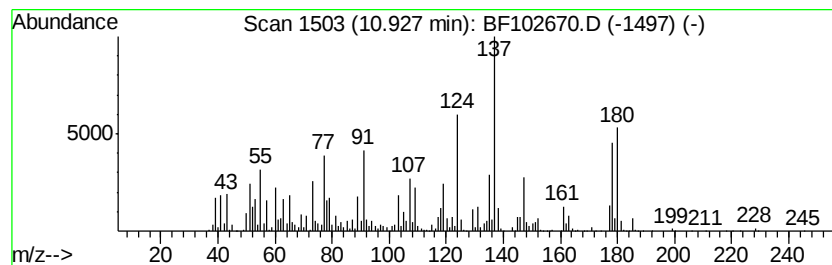
Instrument :
BNA_F
ClientSampleId :
RO-72

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4-((1E)-3-Hydroxy-1-propeny... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.93	80.36 ng	7804870	Phenanthrene-d10	11.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol	180	C10H12O3	1000297-95-5	97	
2	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-	180	C10H12O3	000458-35-5	58	
3	3,7-Benzofurandiol, 2,3-dihydro-	180	C10H12O3	017781-15-6	46	
4	(+)-2-Phenethanamine, 1-methyl-	271	C17H21NO2	1000127-89-8	38	
5	6-Methylnicotinic acid	137	C7H7NO2	003222-47-7	30	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

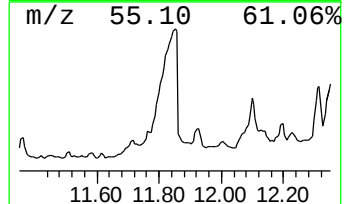
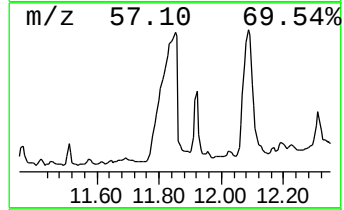
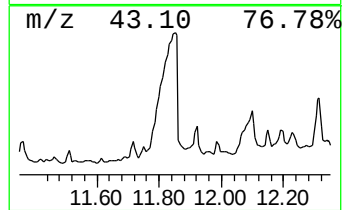
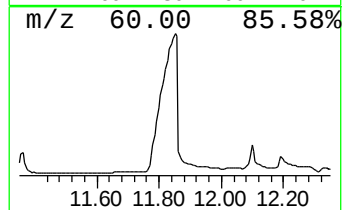
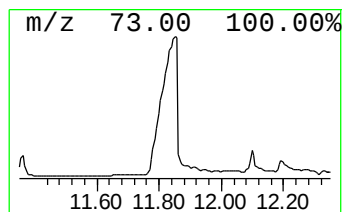
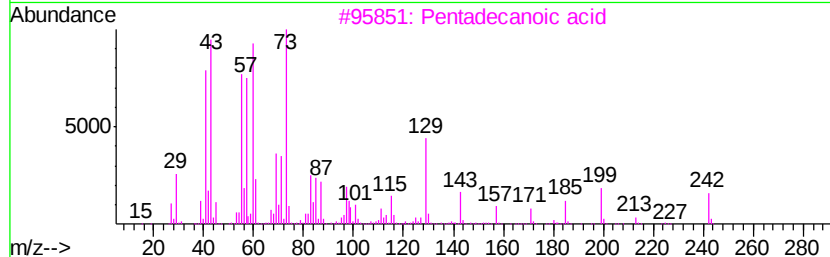
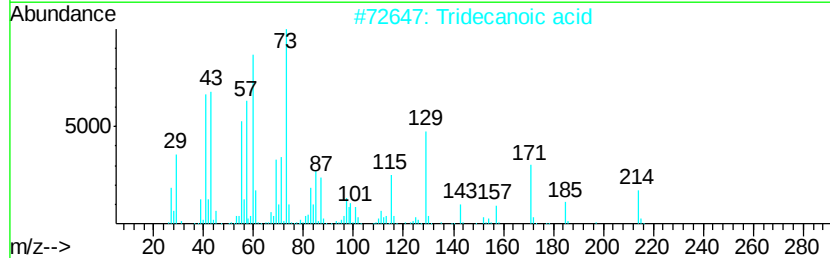
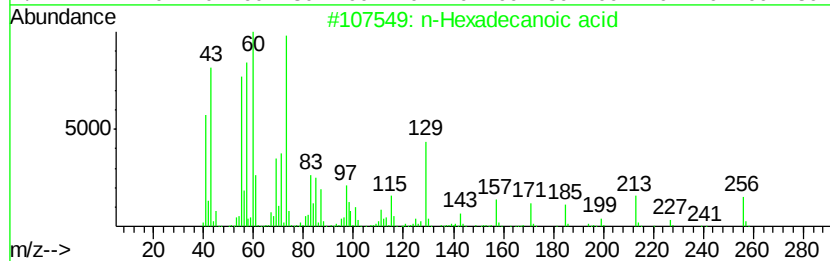
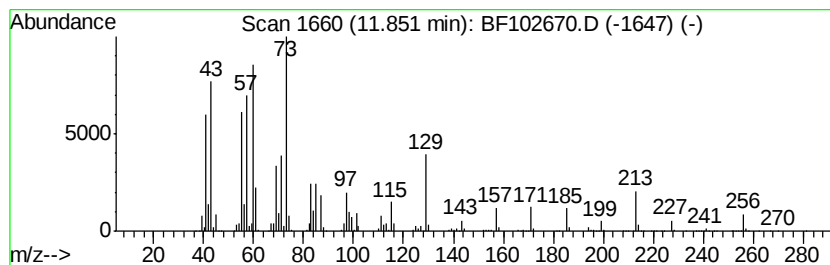
Instrument :
BNA_F
ClientSampleId :
RO-72

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	154.47 ng	15003000	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

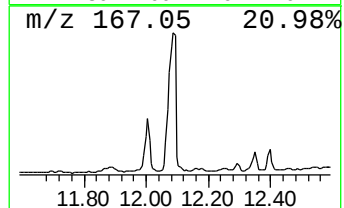
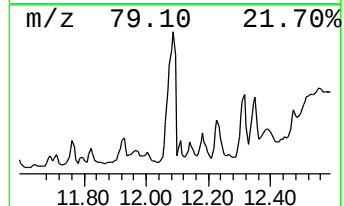
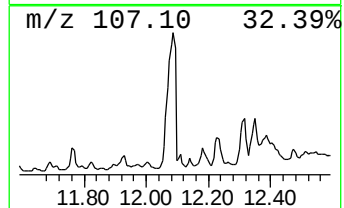
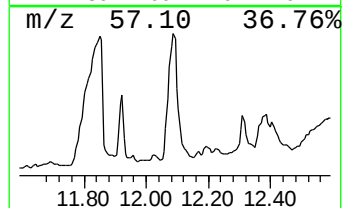
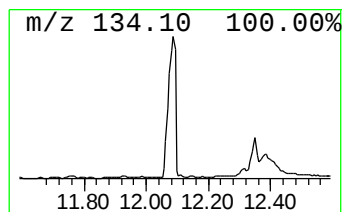
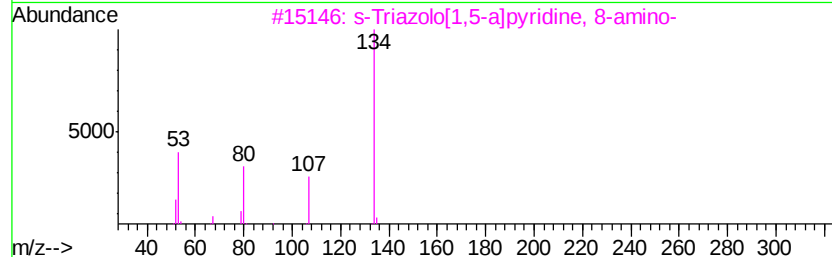
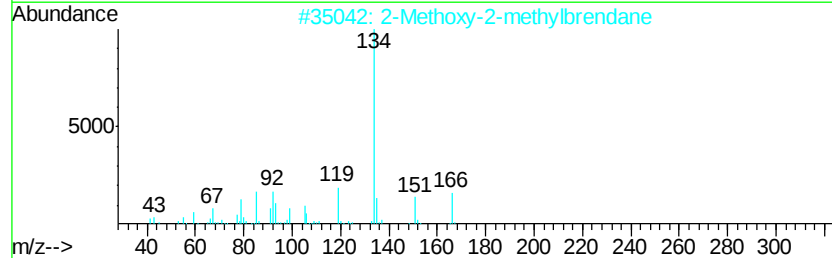
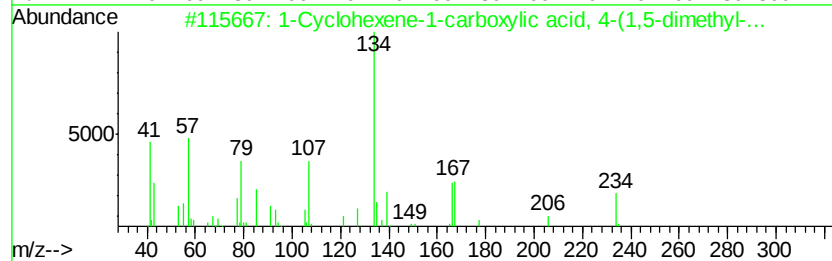
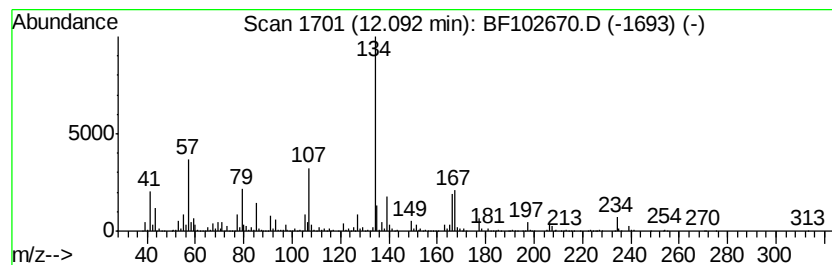
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Cyclohexene-1-carboxylic ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	108.47 ng	10535400	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclohexene-1-carboxylic acid, ...	266	C16H26O3	017904-27-7	64
2		2-Methoxy-2-methylbrendane	166	C11H18O	1000110-53-5	52
3		s-Triazolo[1,5-a]pyridine, 8-amino-	134	C6H6N4	031052-95-6	43
4		5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	43
5		7H-Pyrrolo[2,3-d]pyrimidin-4-amine	134	C6H6N4	001500-85-2	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

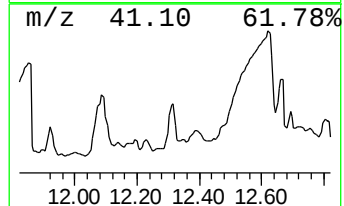
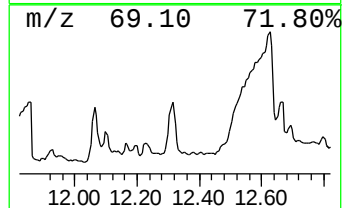
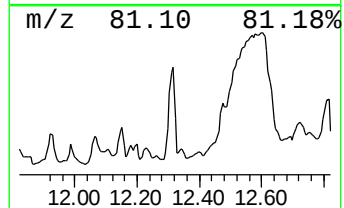
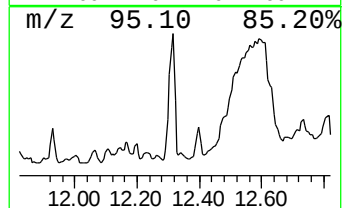
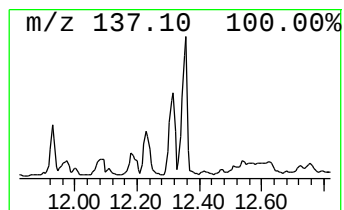
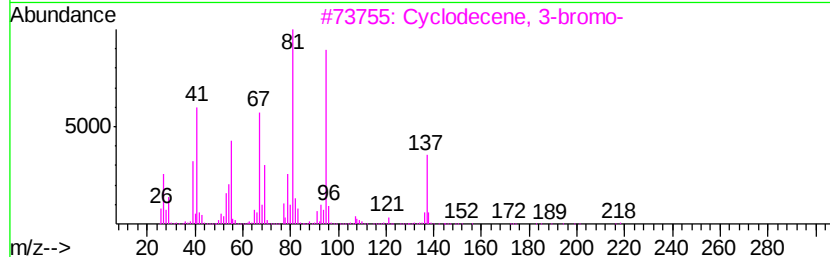
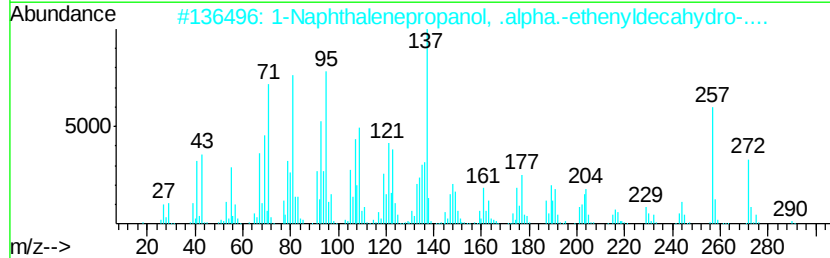
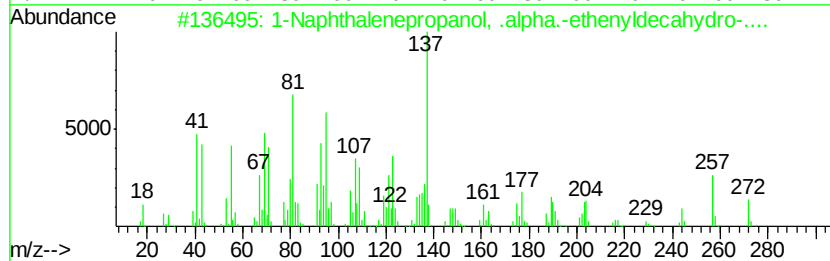
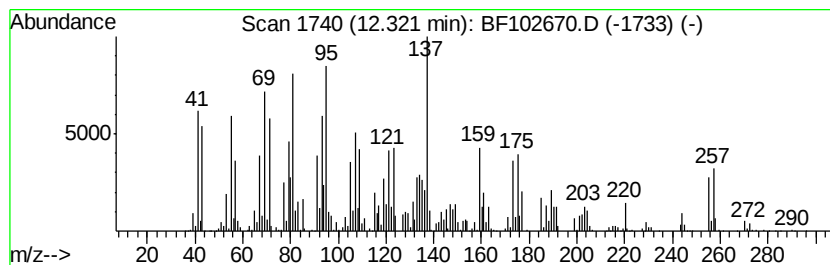
Instrument :
BNA_F
ClientSampleId :
RO-72

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Naphthalenepropanol, .alp... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	62.04 ng	6025220	Phenanthrene-d10	11.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Naphthalenepropanol, .alpha.-e...	290 C20H34O	001438-62-6 76
2		1-Naphthalenepropanol, .alpha.-e...	290 C20H34O	000596-85-0 74
3		Cyclodecene, 3-bromo-	216 C10H17Br	056325-56-5 49
4		Bicyclo[6.1.0]nonane, 9-bromo-9-...	216 C10H17Br	059474-03-2 49
5		Isoaromadendrene epoxide	220 C15H24O	1000159-36-6 44



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

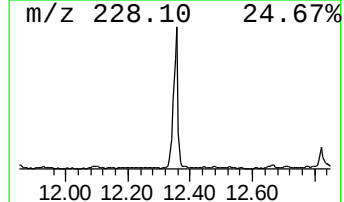
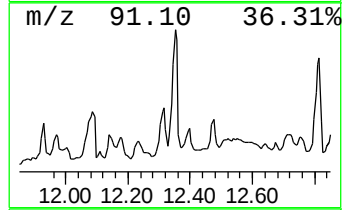
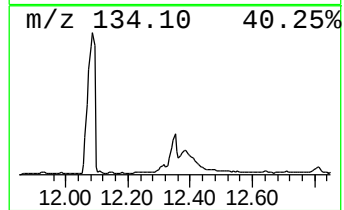
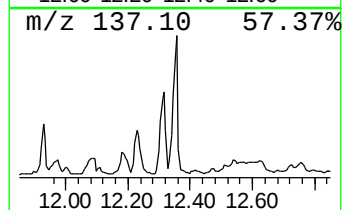
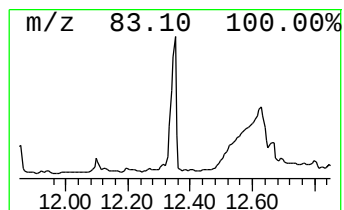
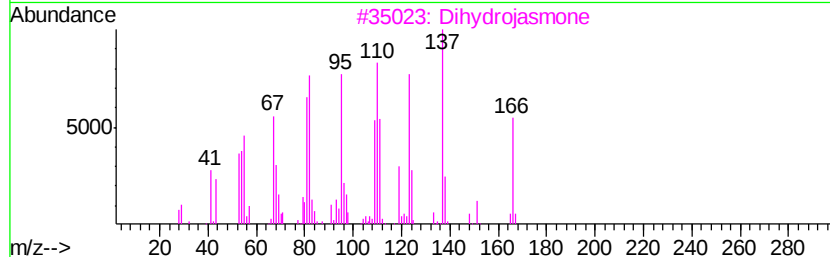
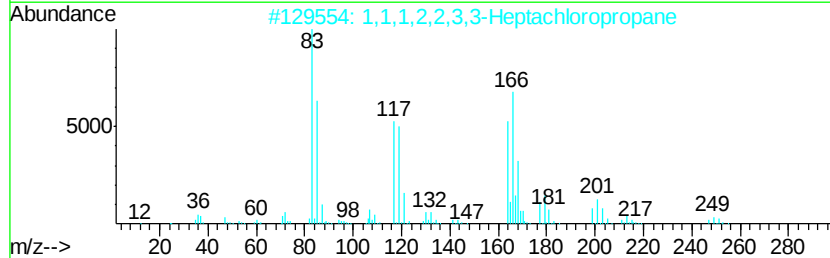
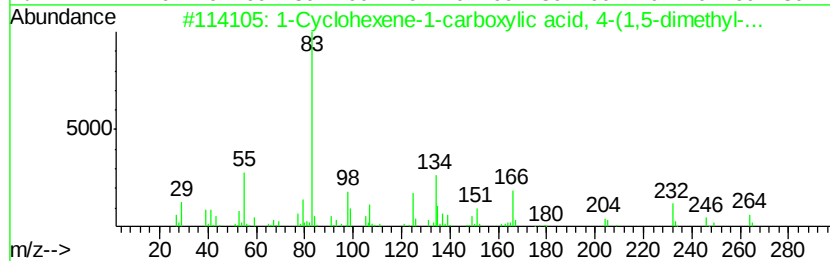
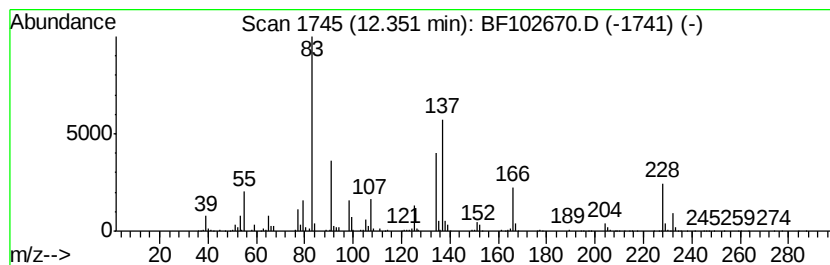
Instrument :
BNA_F
ClientSampleId :
RO-72

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown12.35 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.35	39.62 ng	3848580	Phenanthrene-d10	11.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Cyclohexene-1-carboxylic acid,...	264	C16H24O3	016060-78-9	22
2		1,1,1,2,2,3,3-Heptachloropropane	282	C3HCl7	000594-89-8	16
3		Dihydrojasmane	166	C11H18O	001128-08-1	11
4		Ethyl Vanillin	166	C9H10O3	000121-32-4	10
5		3-Aminopyrazole	83	C3H5N3	001820-80-0	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

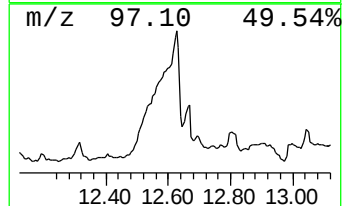
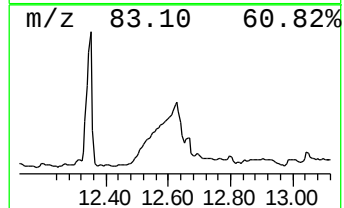
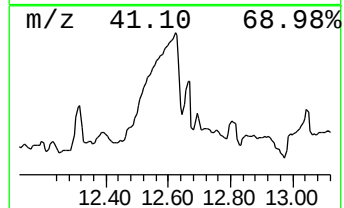
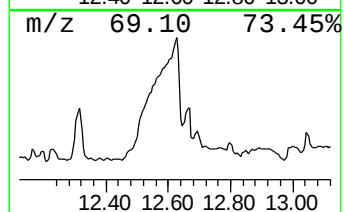
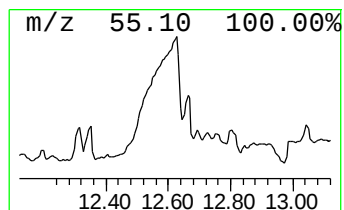
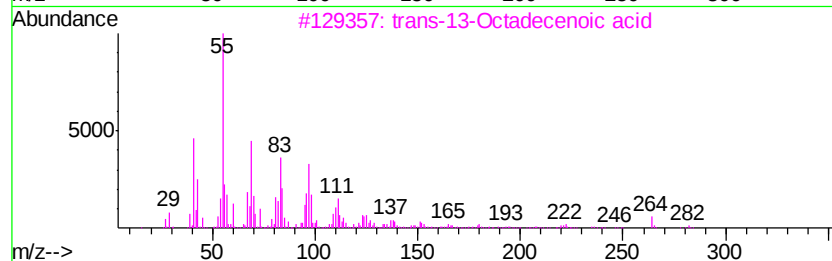
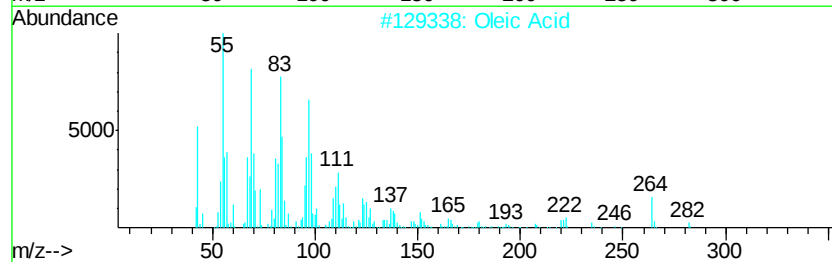
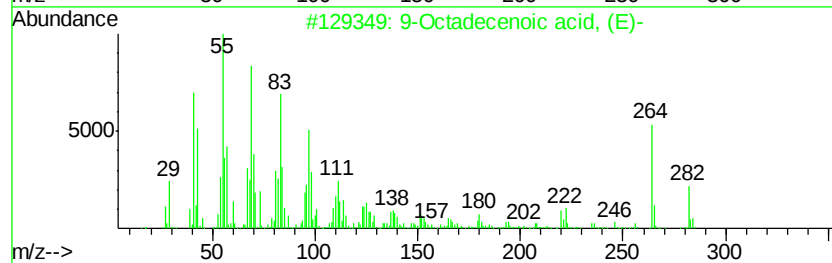
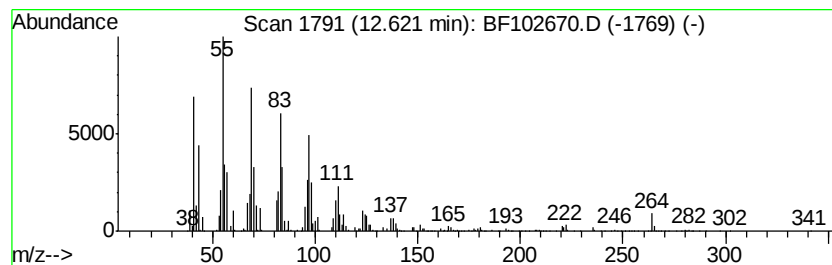
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 9-Octadecenoic acid, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	480.78 ng	29324400	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	97
2		Oleic Acid	282	C18H34O2	000112-80-1	70
3		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	64
4		11-Dodecen-1-ol, 2,4,6-trimethyl...	226	C15H30O	027829-54-5	53
5		cis-Vaccenic acid	282	C18H34O2	000506-17-2	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

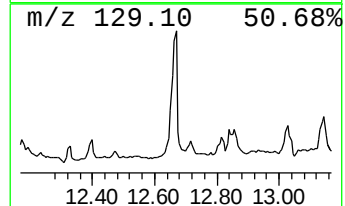
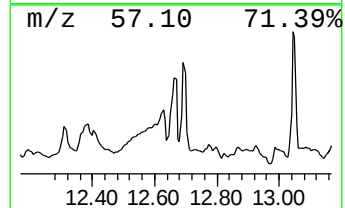
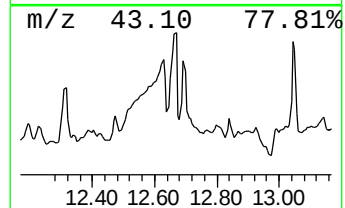
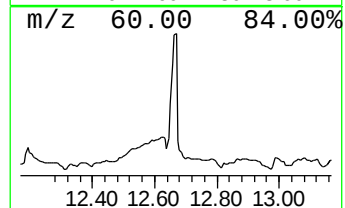
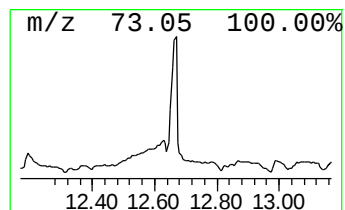
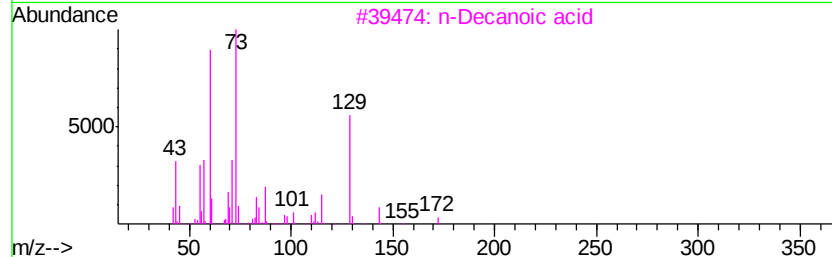
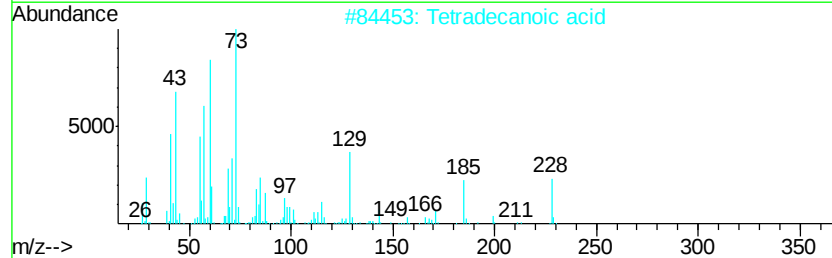
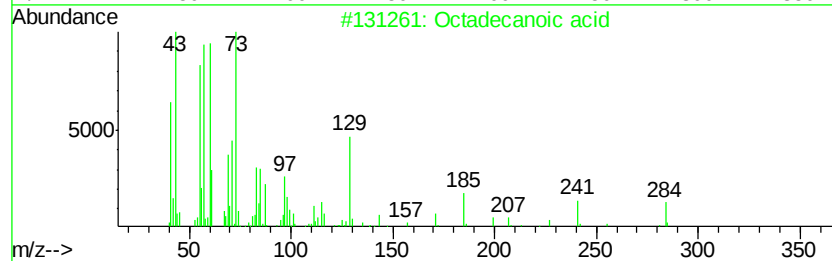
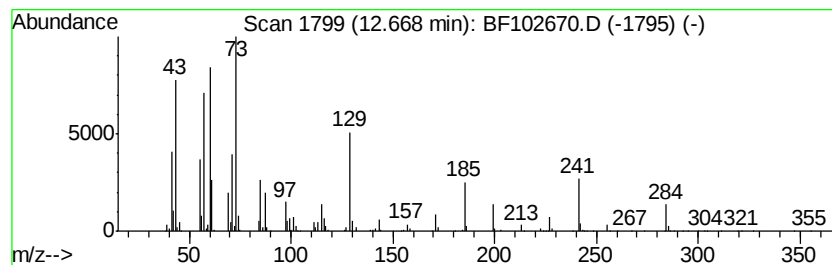
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	55.66 ng	3394640	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	86
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		n-Decanoic acid	172	C10H20O2	000334-48-5	70
4		Undecanoic acid	186	C11H22O2	000112-37-8	53
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

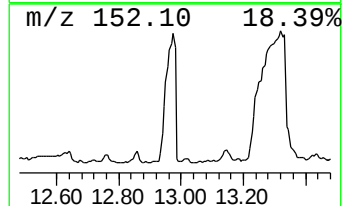
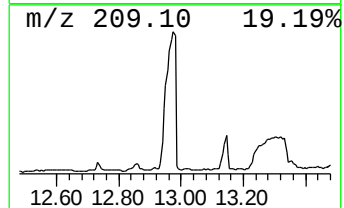
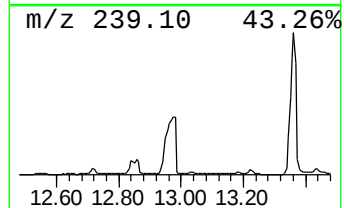
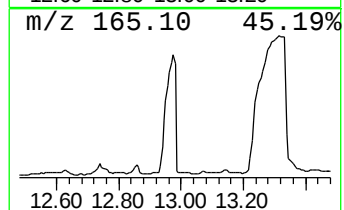
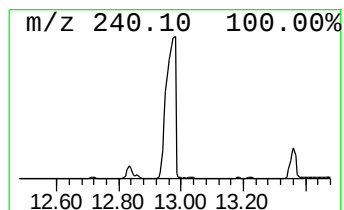
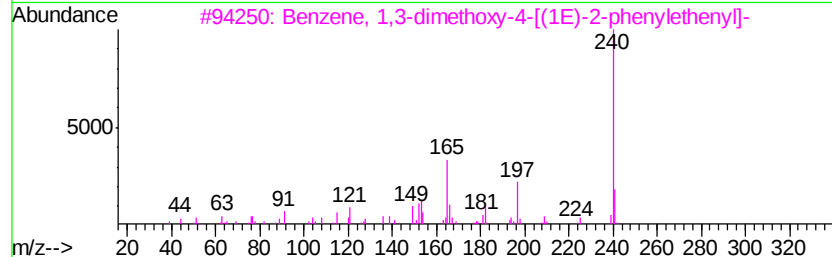
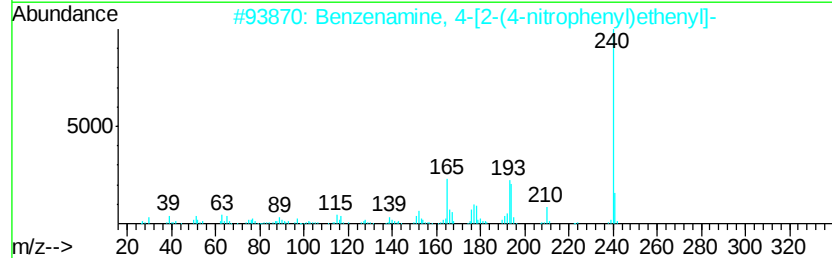
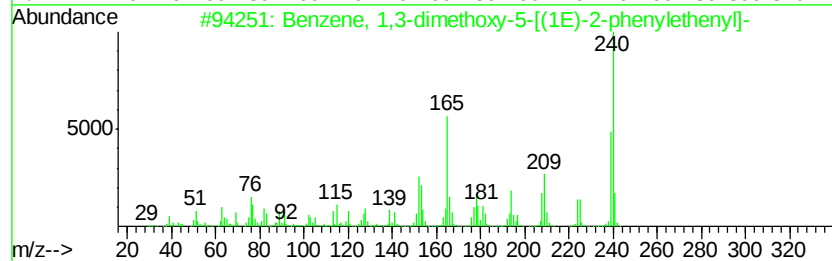
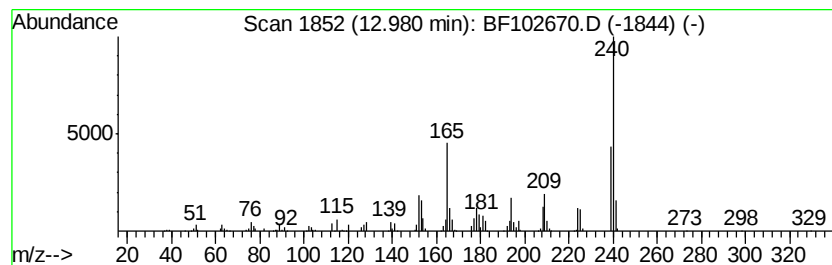
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzene, 1,3-dimethoxy-5-[...] Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	101.53 ng	6192380	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-dimethoxy-5-[(1E)-2-phenylethenyl]-	240	C16H16O2	021956-56-9	99
2		Benzenamine, 4-[2-(4-nitrophenyl)ethenyl]-	240	C14H12N2O2	004629-58-7	53
3		Benzene, 1,3-dimethoxy-4-[(1E)-2-phenylethenyl]-	240	C16H16O2	1000368-46-0	50
4		4-Methyl-5-(1-naphthyl)-2-thiazolecarboxamide	240	C14H12N2S	092149-93-4	47
5		4-[2-(4-Hydroxy-phenyl)-vinyl]-benzyl alcohol	240	C15H12O3	152027-61-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

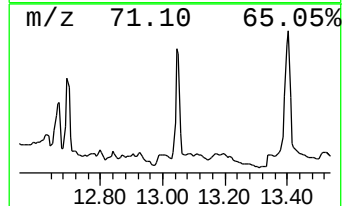
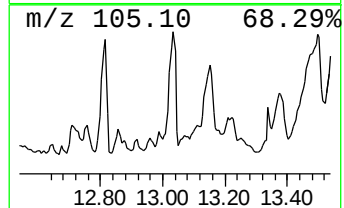
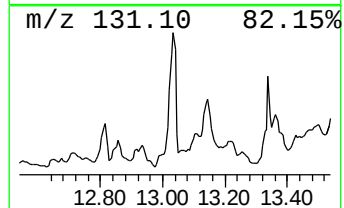
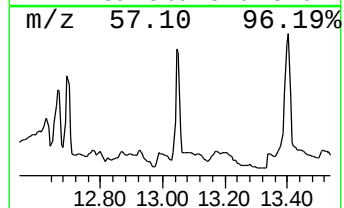
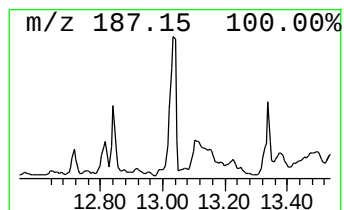
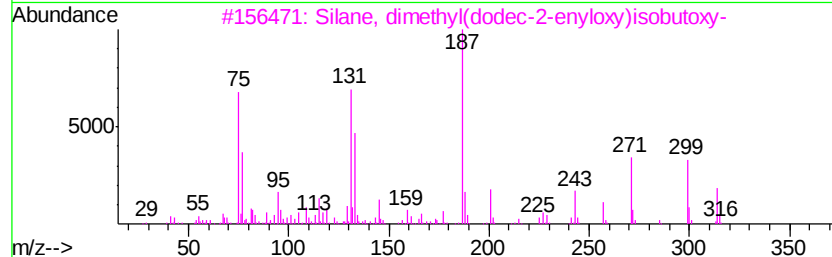
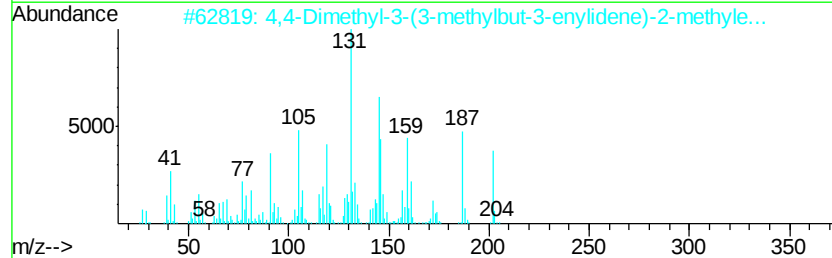
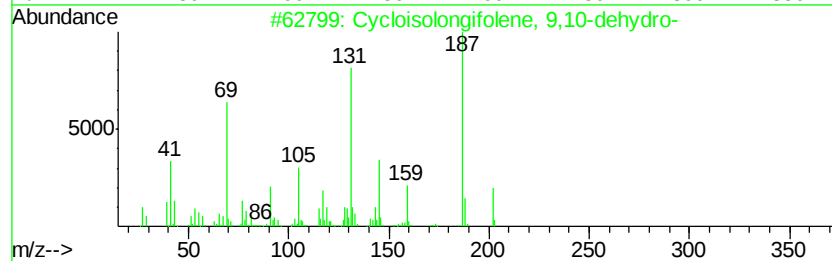
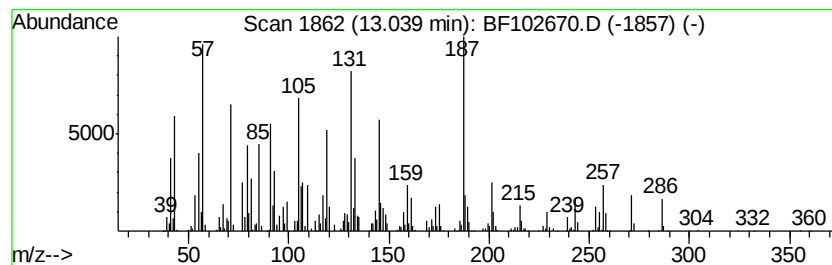
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown13.04 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.04	72.00 ng	4391390	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloisolongifolene, 9,10-dehydro-	202	C15H22	1000156-81-6	49
2		4,4-Dimethyl-3-(3-methylbut-3-en...	202	C15H22	079718-83-5	38
3		Silane, dimethyl(dodec-2-enyloxy...	314	C18H38O2Si	1000348-06-6	27
4		1H-Benzimidazole, 1-isobutyl-2-...	280	C18H20N2O	1000303-90-0	25
5		1,3-Cyclopentadiene, 5-(trans-2-...	146	C11H14	079209-36-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

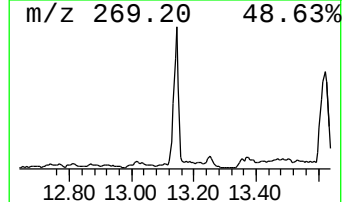
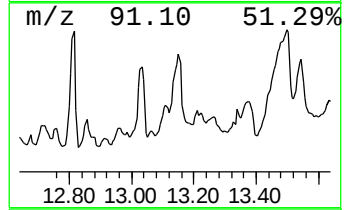
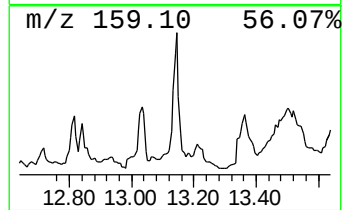
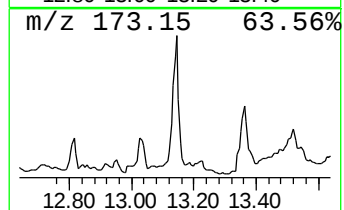
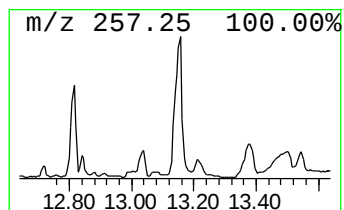
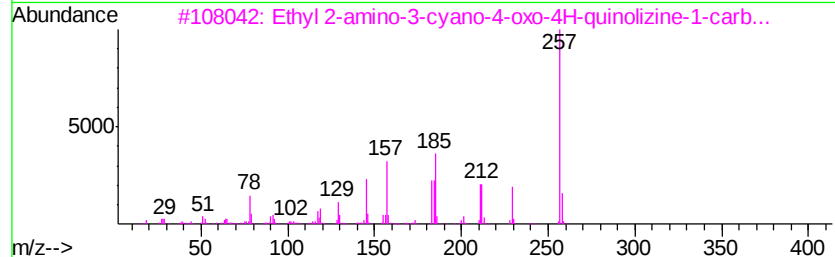
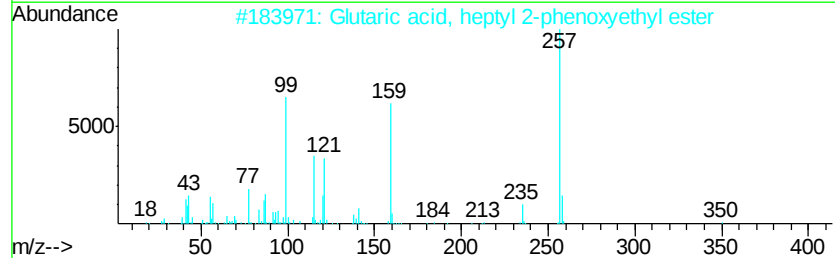
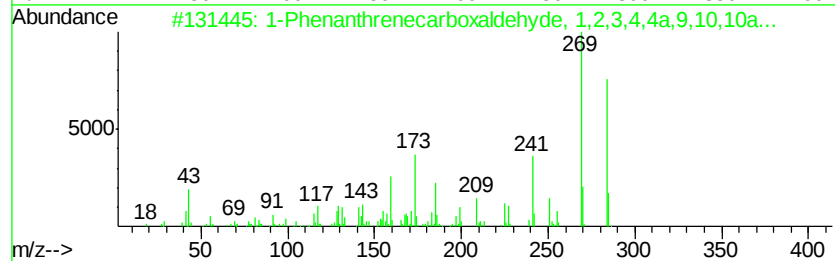
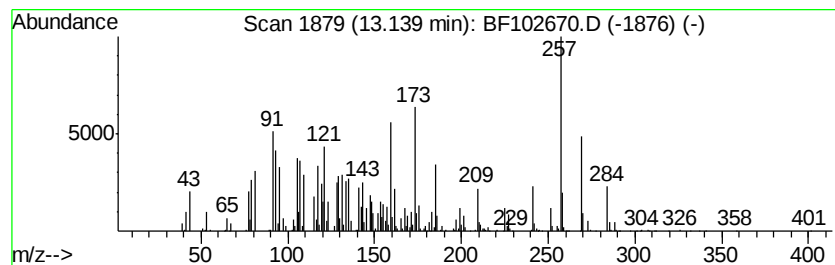
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1-Phenanthrenecarboxaldehyd... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	55.75 ng	3400110	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenanthrenecarboxaldehyd...	284	C20H28O	013601-88-2	99
2		Glutaric acid, heptyl 2-phenoxye...	350	C20H30O5	1000376-91-9	35
3		Ethyl 2-amino-3-cyano-4-oxo-4H-q...	257	C13H11N3O3	022353-70-4	30
4		Octanoic acid, triisopropylsilyl...	300	C17H36O2Si	1000279-49-2	22
5		Propenone, 3-(2-methoxyphenyl)-1...	288	C20H16O2	052601-56-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102670.D
Acq On : 31 Jan 2018 22:19
Operator : SJ/JU
Sample : J1378-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72

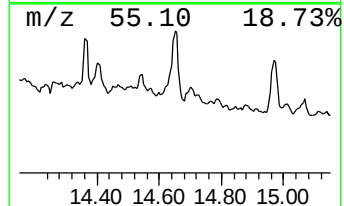
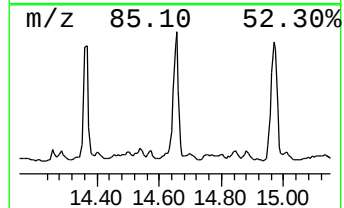
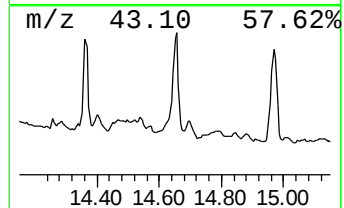
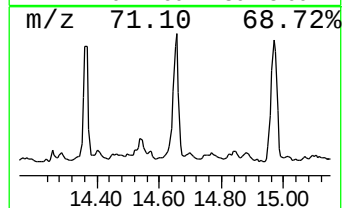
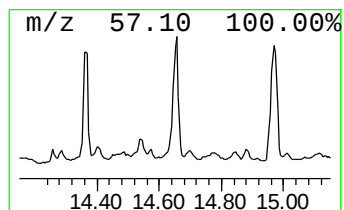
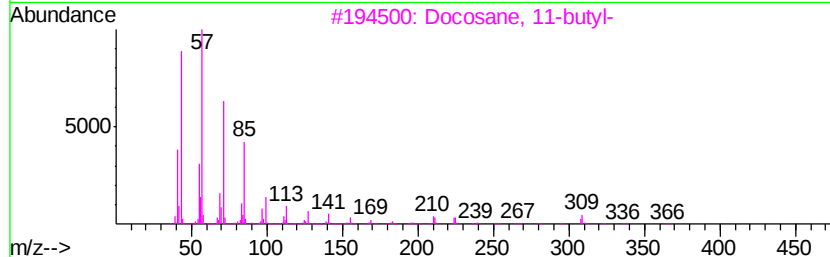
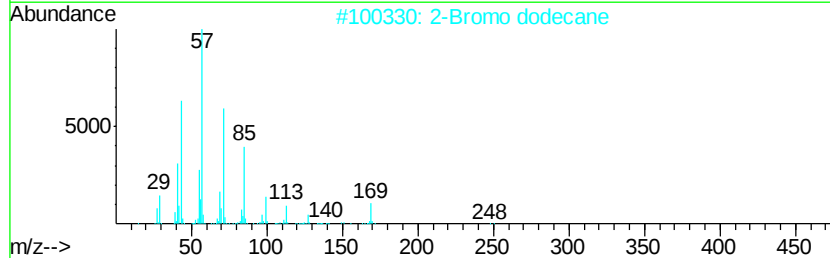
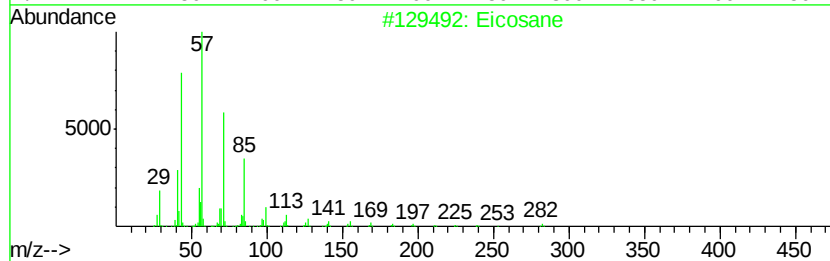
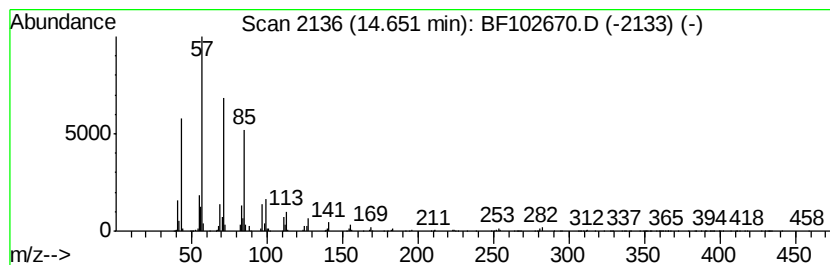
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Eicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	39.82 ng	2428500	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4		Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
 Data File : BF102670.D
 Acq On : 31 Jan 2018 22:19
 Operator : SJ/JU
 Sample : J1378-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
Hexanal	4.32	71.5	ng	4308910	1	6.71	1205910	20.0
.alpha.-Pinene	5.99	243.3	ng	14668900	1	6.71	1205910	20.0
1,3,6-Octatriene,...	6.65	42.2	ng	2543270	1	6.71	1205910	20.0
endo-Borneol	7.91	62.7	ng	7105520	2	7.99	2267580	20.0
Cyclohexanemethan...	8.77	39.9	ng	4523000	2	7.99	2267580	20.0
unknown8.89	8.89	37.2	ng	2229810	3	9.75	1198100	20.0
Vanillin	9.25	78.9	ng	4726820	3	9.75	1198100	20.0
Longifolene	9.37	34.0	ng	2037600	3	9.75	1198100	20.0
unknown10.08	10.08	35.3	ng	2114530	3	9.75	1198100	20.0
4-((1E)-3-Hydroxy...	10.93	80.4	ng	7804870	4	11.23	1942520	20.0
n-Hexadecanoic acid	11.85	154.5	ng	15003000	4	11.23	1942520	20.0
1-Cyclohexene-1-c...	12.09	108.5	ng	10535400	4	11.23	1942520	20.0
1-Naphthaleneprop...	12.32	62.0	ng	6025220	4	11.23	1942520	20.0
unknown12.35	12.35	39.6	ng	3848580	4	11.23	1942520	20.0
9-Octadecenoic ac...	12.62	480.8	ng	29324400	5	13.93	1219870	20.0
Octadecanoic acid	12.67	55.7	ng	3394640	5	13.93	1219870	20.0
Benzene, 1,3-dime...	12.98	101.5	ng	6192380	5	13.93	1219870	20.0
unknown13.04	13.04	72.0	ng	4391390	5	13.93	1219870	20.0
1-Phenanthrenecar...	13.14	55.8	ng	3400110	5	13.93	1219870	20.0
Eicosane	14.65	39.8	ng	2428500	5	13.93	1219870	20.0