LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.969	143	150	154	rBV	76727	133335	3.37%	0.254%
2	3.016	154	158	166	rVB	97081	159159	4.02%	0.303%
3	3.434	224	229	236	rVB2	56150	99832	2.52%	0.190%
4	3.522	238	244	255	rBV4	62576	118342	2.99%	0.225%
5	3.645	260	265	274	rVV	178997	284194	7.18%	0.541%
6	3.828	289	296	302	rBV3	76991	123370	3.12%	0.235%
7	4.240	360	366	370	rBV2	71710	138891	3.51%	0.264%
8	4.334	376	382	387	rBV2	112224	146822	3.71%	0.280%
9	4.869	467	473	478	rBV	124122	167204	4.22%	0.318%
10	5.016	494	498	500	rBV3	142305	188036	4.75%	0.358%
11	5.363	555	557	559	rVV2	105141	105888	2.68%	0.202%
12	5.387	559	561	568	rVB	987219	971669	24.55%	1.850%
13	5.716	613	617	624	rVB2	108554	140539	3.55%	0.268%
14	5.804	624	632	636	rBV4	84568	118572	3.00%	0.226%
15	5.992	658	664	668	rBV2	108321	163267	4.12%	0.311%
16	6.086	676	680	684	rBV2	97993	94889	2.40%	0.181%
17	6.192	695	698	700	rVV	98373	111283	2.81%	0.212%
18	6.228	700	704	707	rVB	146741	168337	4.25%	0.321%
19	6.269	708	711	717	rBV4	76737	111820	2.83%	0.213%
20	6.363	725	727	730	rBV2	163194	154916	3.91%	0.295%
21	6.398	730	733	734	rVV	499673	423569	10.70%	0.806%
22	6.416	734	736	742	rVV2	608347	806032	20.36%	1.535%
23	6.510	747	752	755	rBV4	88730	126444	3.19%	0.241%
24	6.598	763	767	768	rBV2	93489	112617	2.85%	0.214%
25	6.769	791	796	799	rBV	1085652	979091	24.74%	1.864%
26	6.845	805	809	812	rBV	2339022	1940237	49.02%	3.694%
27	6.928	818	823	825	rBV	3197912	2777406	70.17%	5.288%
28	6.951	825	827	830	rVB	1712323	1198546	30.28%	2.282%
29	7.022	836	839	842	rVB2	328539	272680	6.89%	0.519%
30	7.098	848	852	861	rVB5	269872	441055	11.14%	0.840%
31	7.169	861	864	868	rBV2	115485	124786	3.15%	0.238%
32	7.281	880	883	884	rVV	143707	130551	3.30%	0.249%
33	7.310	884	888	889	rVV3	563420	705584	17.83%	1.343%
34	7.339	889	893	896	rVV	3300333	3153966	79.68%	6.005%
35	7.369	896	898	900	rVV	161906	153487	3.88%	0.292%
36	7.422	904	907	910	rBV4	98836	146912	3.71%	0.280%

LSC Area Percent Report

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Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	7.451	910	912	915	rVB2	123642	107530	2.72%	0.205%
38	7.539	924	927	930	rVB	279416	260600	6.58%	0.496%
39	7.569	930	932	935	rVB	192469	135539	3.42%	0.258%
40	7.622	935	941	942	rBV5	150717	187284	4.73%	0.357%
41	7.710	950	956	957	rBV4	95773	147934	3.74%	0.282%
42	7.792	965	970	974	rVB5	96626	191675	4.84%	0.365%
43	7.833	974	977	979	rBV3	91107	100160	2.53%	0.191%
44	7.998	999	1005	1009	rBV5	250937	478956	12.10%	0.912%
45	8.051	1011	1014	1017	rVV	1300001	1209179	30.55%	2.302%
46	8.198	1033	1039	1042	rVB3	324260	522350	13.20%	0.995%
47	8.233	1042	1045	1047	rBV3	88063	99346	2.51%	0.189%
48	8.298	1051	1056	1057	rBV4	207594	271235	6.85%	0.516%
49	8.363	1063	1067	1072	rVB	186076	219733	5.55%	0.418%
50	8.445	1075	1081	1085	rVV3	529924	792426	20.02%	1.509%
51	8.492	1087	1089	1093	rVV4	142884	216149	5.46%	0.412%
52	8.522	1093	1094	1097	rVV3	122971	132225	3.34%	0.252%
53	8.551	1097	1099	1102	rVB2	158340	167639	4.24%	0.319%
54	8.592	1103	1106	1109	rVB3	327902	344642	8.71%	0.656%
55	8.639	1109	1114	1118	rBV5	451293	812841	20.54%	1.548%
56	8.751	1130	1133	1137	rVB3	361284	445852	11.26%	0.849%
57	8.833	1137	1147	1150	rBV2	659029	1147064	28.98%	2.184%
58	8.863	1150	1152	1154	rVV2	444758	458223	11.58%	0.872%
59	8.910	1157	1160	1163	rVV4	523163	617481	15.60%	1.176%
60	8.945	1163	1166	1168	rVV3	318127	343390	8.68%	0.654%
61	8.986	1169	1173	1176	rVV3	487185	763463	19.29%	1.454%
62	9.022	1176	1179	1183	rVV3	402848	524710	13.26%	0.999%
63	9.063	1183	1186	1190	rVV6	312681	517972	13.09%	0.986%
64	9.098	1190	1192	1194	rVV	214933	195238	4.93%	0.372%
65	9.133	1194	1198	1200	rVV	5002506	3958142	100.00%	7.536%
66	9.157	1200	1202	1205	rVB	342401	315662	7.98%	0.601%
67	9.186	1205	1207	1210	rVB4	164228	157837	3.99%	0.301%
68	9.263	1214	1220	1223	rBV2	743490	1106394	27.95%	2.107%
69	9.298	1223	1226	1229	rBV3	286989	323443	8.17%	0.616%
70	9.380	1237	1240	1244	rBV3	318456	406876	10.28%	0.775%
71	9.439	1247	1250	1254	rBV2	258998	356636	9.01%	0.679%
72	9.498	1254	1260	1266	rVV4	698962	1259134	31.81%	2.397%
73	9.563	1266	1271	1275	rVV6	393254	809978	20.46%	1.542%
74	9.627	1279	1282	1287	rVB3	726498	683374	17.27%	1.301%
75	9.704	1287	1295	1298	rBV8	370722	933082	23.57%	1.777%
76	9.769	1304	1306	1308	rBV2	199912	194882	4.92%	0.371%

LSC Area Percent Report

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Operator : JU/CG
Sample : M2307-03
Misc :
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Instrument : BNA_F
ClientSampleId : MW-05

Integration Parameters: rteint.p
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Smoothing : ON Filtering: 5
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	9.810	1310	1313	1315	rVV	860526	744562	18.81%	1.418%
78	9.874	1321	1324	1326	rVB3	256650	208246	5.26%	0.397%
79	9.904	1326	1329	1331	rBV3	200973	179167	4.53%	0.341%
80	9.933	1332	1334	1337	rVV	239993	254878	6.44%	0.485%
81	9.998	1340	1345	1353	rVB4	592772	1217471	30.76%	2.318%
82	10.063	1353	1356	1357	rBV3	179425	187659	4.74%	0.357%
83	10.080	1357	1359	1362	rVB2	260689	229288	5.79%	0.437%
84	10.116	1362	1365	1369	rBV2	354684	480975	12.15%	0.916%
85	10.198	1377	1379	1383	rVB5	325946	337297	8.52%	0.642%
86	10.245	1383	1387	1388	rBV3	214351	248714	6.28%	0.474%
87	10.327	1398	1401	1403	rBV3	144925	133380	3.37%	0.254%
88	10.357	1403	1406	1409	rVB2	676098	648396	16.38%	1.235%
89	10.404	1412	1414	1418	rVV2	215099	208583	5.27%	0.397%
90	10.439	1418	1420	1423	rBV4	161403	164820	4.16%	0.314%
91	10.521	1431	1434	1436	rBV2	217155	211298	5.34%	0.402%
92	10.569	1440	1442	1444	rVV	235823	205031	5.18%	0.390%
93	10.598	1444	1447	1452	rVB	1748623	1668158	42.14%	3.176%
94	10.780	1475	1478	1479	rBV3	122197	122373	3.09%	0.233%
95	11.292	1562	1565	1569	rVB	932285	759862	19.20%	1.447%
96	11.845	1656	1659	1664	rVB2	509614	544256	13.75%	1.036%
97	12.633	1790	1793	1797	rBV2	286948	283756	7.17%	0.540%
98	12.886	1832	1836	1839	rBV	3544954	2964607	74.90%	5.645%
99	13.939	2012	2015	2018	rVB	684173	629552	15.91%	1.199%
100	15.380	2256	2260	2269	rVB	607621	778367	19.66%	1.482%

Sum of corrected areas: 52520300

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
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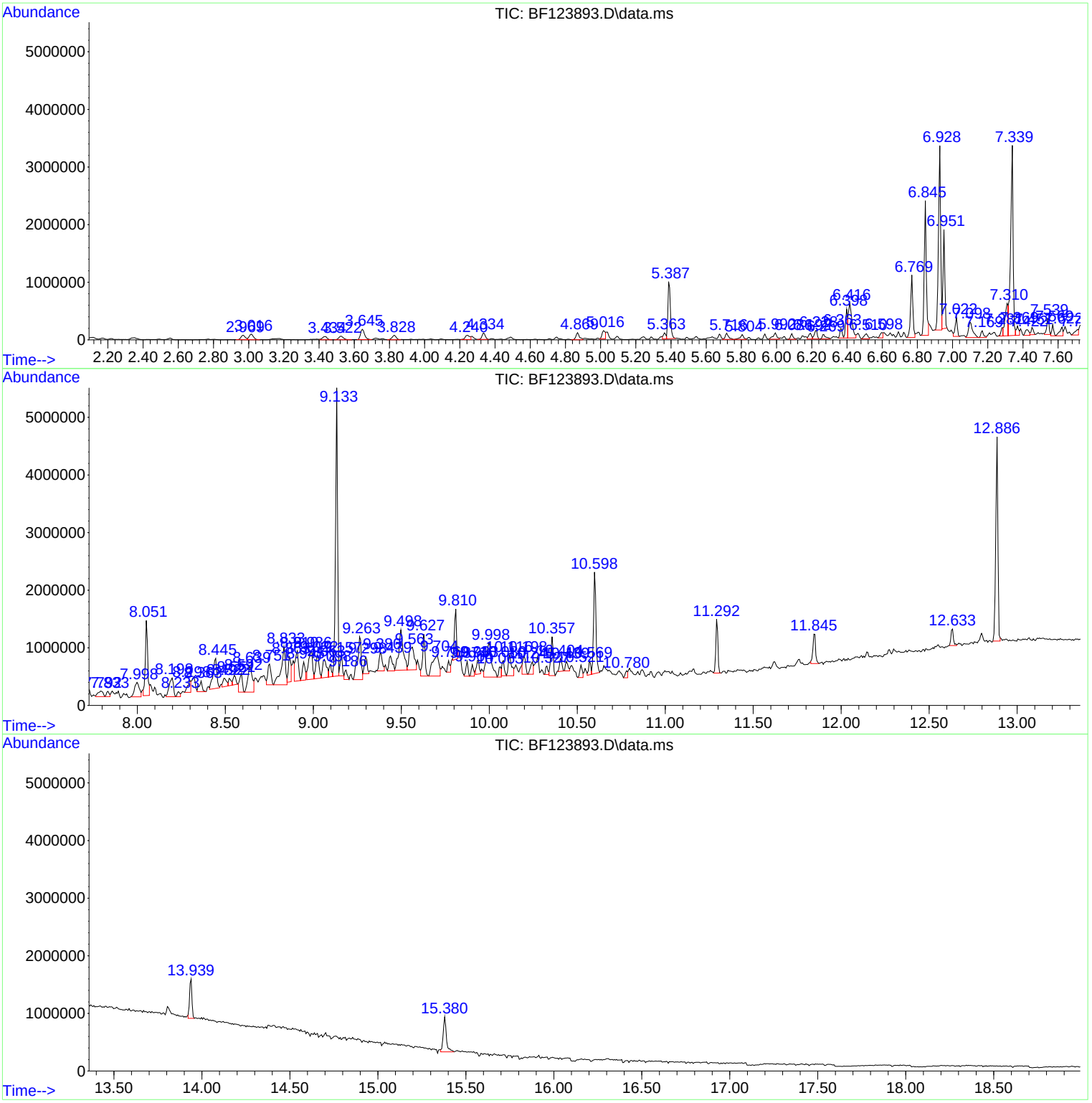
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
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Acq On : 10 May 2021 20:01
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Sample : M2307-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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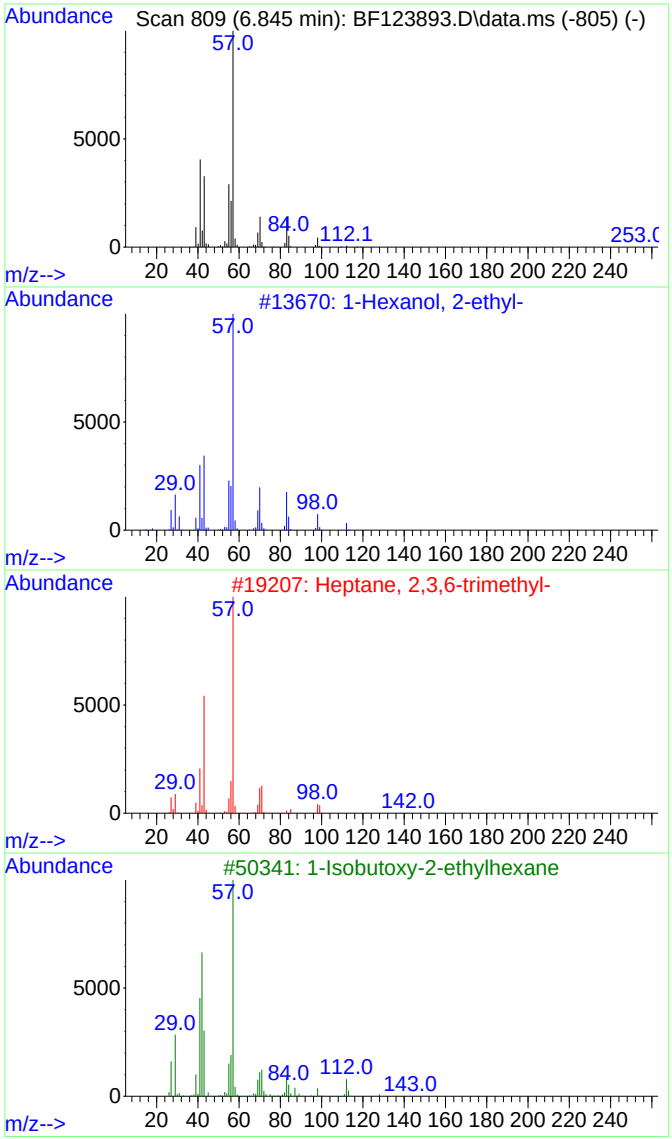
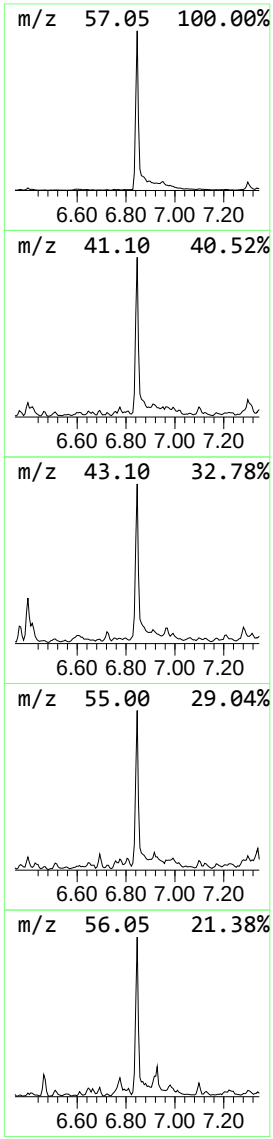
Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	39.63 ng	1940240	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
3	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53





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Data File : BF123893.D
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Sample : M2307-03
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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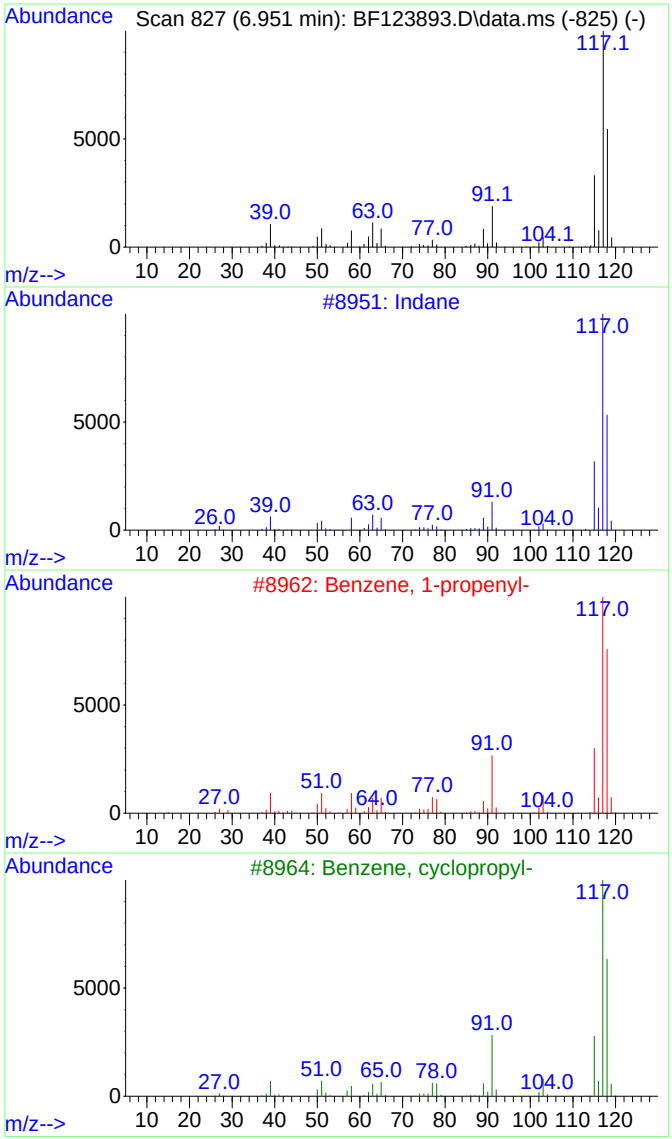
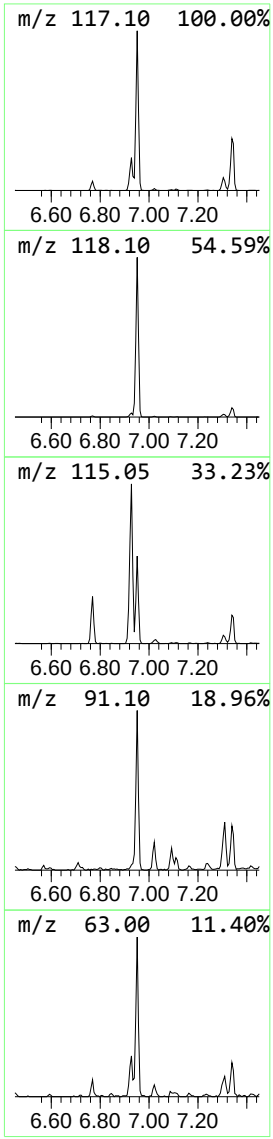
****

Peak Number 3 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.951	24.48 ng	1198550	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	Deltacyclene	118	C9H10	007785-10-6	68
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	53





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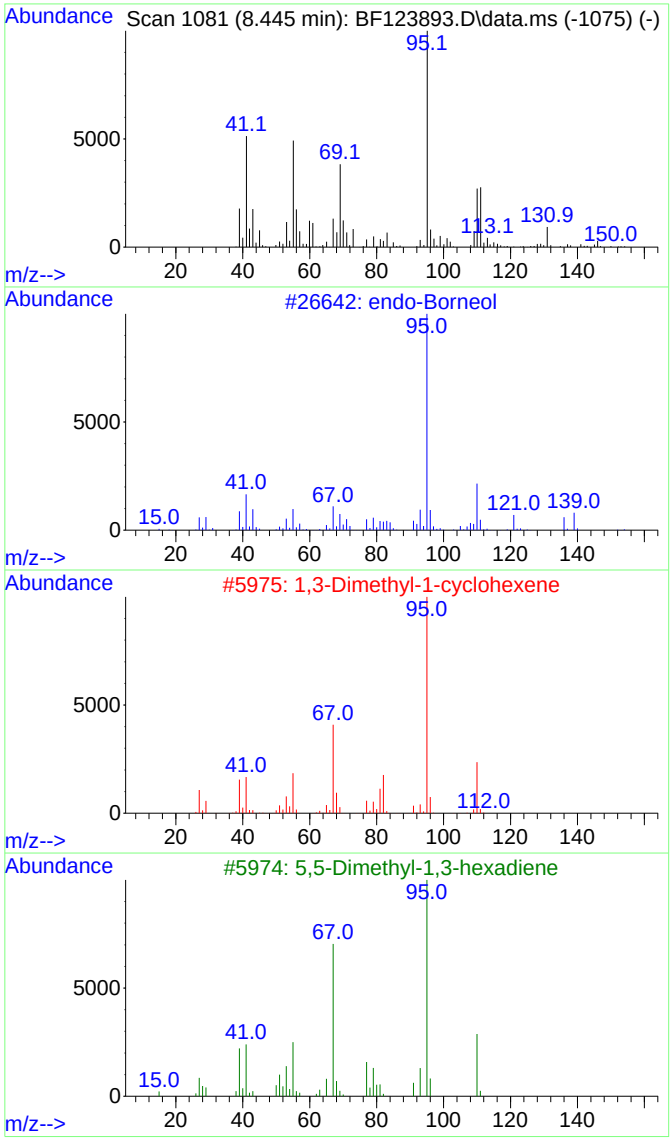
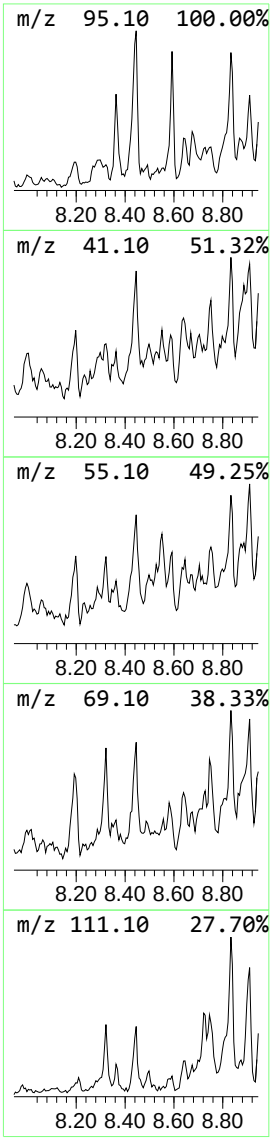
Peak Number 4 endo-Borneol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	13.11 ng	792426	Naphthalene-d8	8.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	endo-Borneol	154	C10H18O	000507-70-0	50
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	47
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	47
4	2-Isopropylimidazole	110	C6H10N2	036947-68-9	38
5	1,3-Dimethyl-5-trifluoroacetoxyc...	224	C10H15F3O2	1000216-63-7	38





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.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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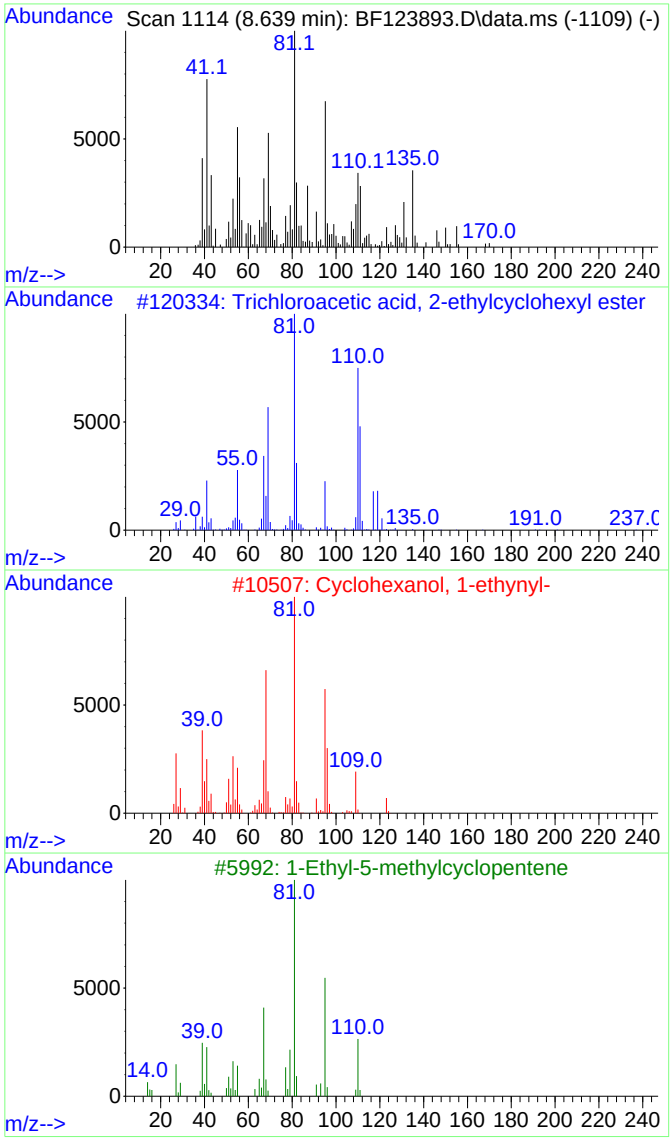
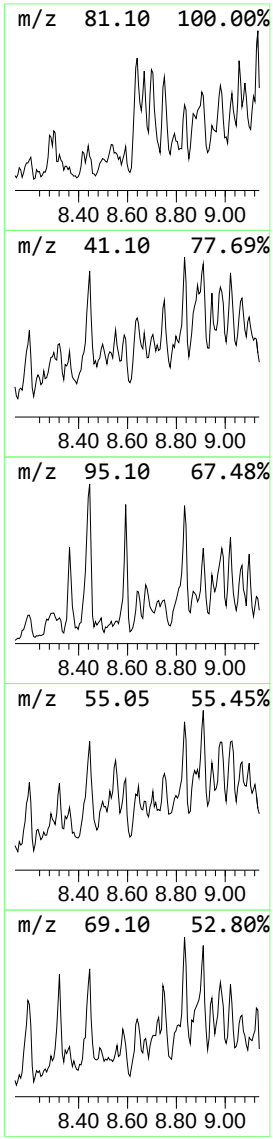
Peak Number 5 unknown8.639 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.639	13.44 ng	812841	Naphthalene-d8	8.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 2-ethylcyc...	272	C10H15Cl3O2	1000282-57-3	46
2	Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	45
3	1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	43
4	2,4-Octadiene	110	C8H14	013643-08-8	38
5	1,4-Hexadiene, 3-ethyl-	110	C8H14	002080-89-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

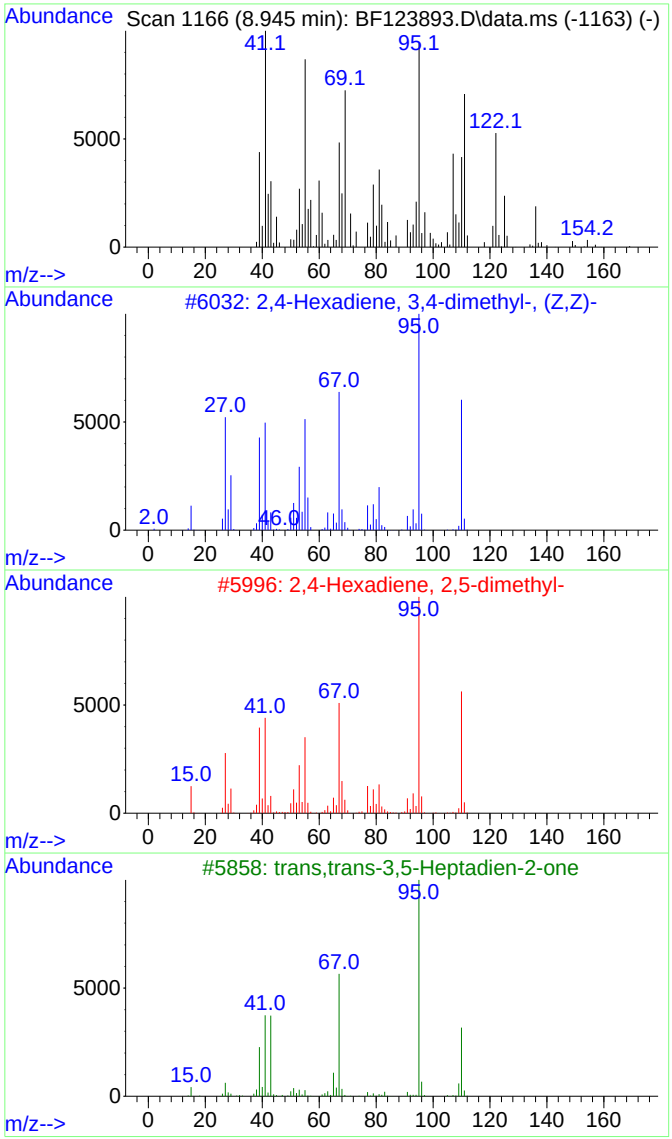
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

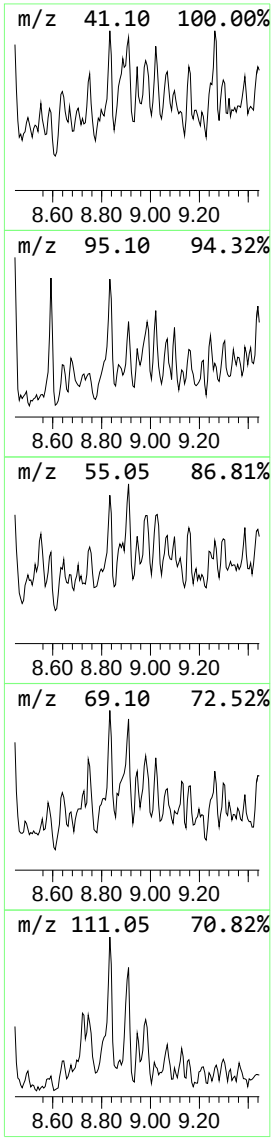
****

Peak Number 6 unknown8.945 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.945	9.22 ng	343390	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	46
2	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	41
3	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	35
4	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	27
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	27





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Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

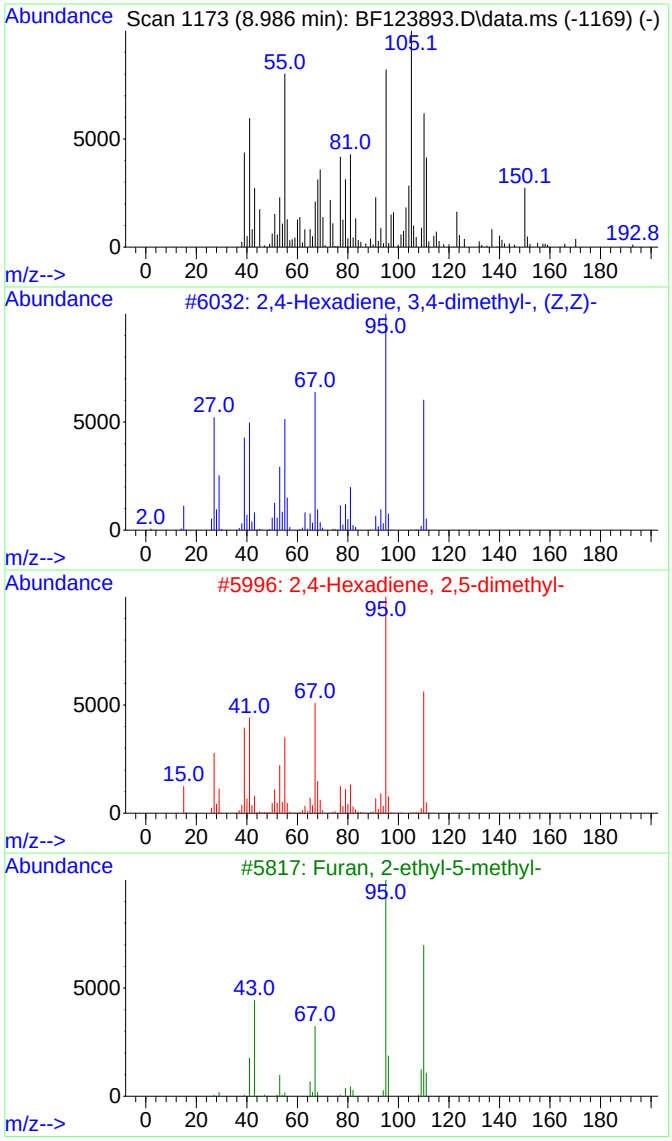
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

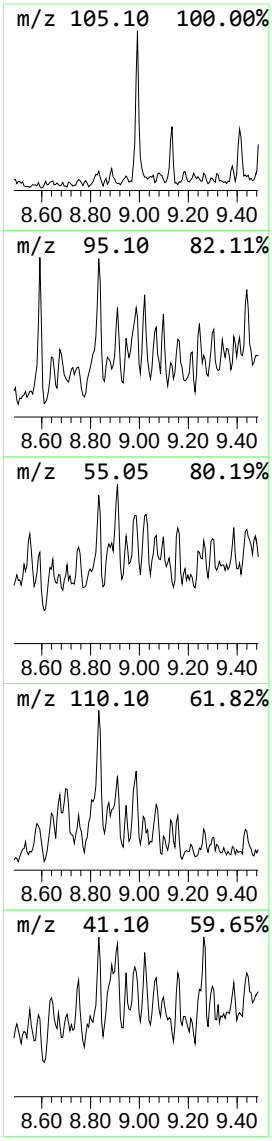
****

Peak Number 7 unknown8.986 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.986	20.51 ng	763463	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	41
2	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38
3	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	38
4	Hexanoic acid, 3,5-dimethylcyclo...	226	C14H26O2	1000279-28-3	38
5	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	35





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Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

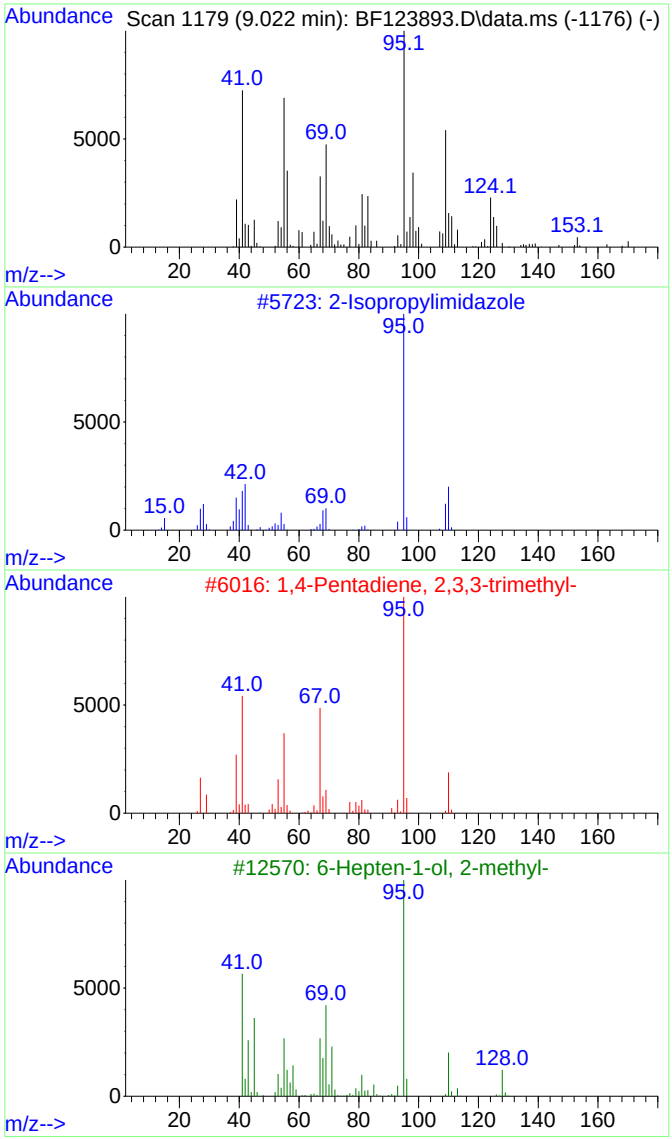
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

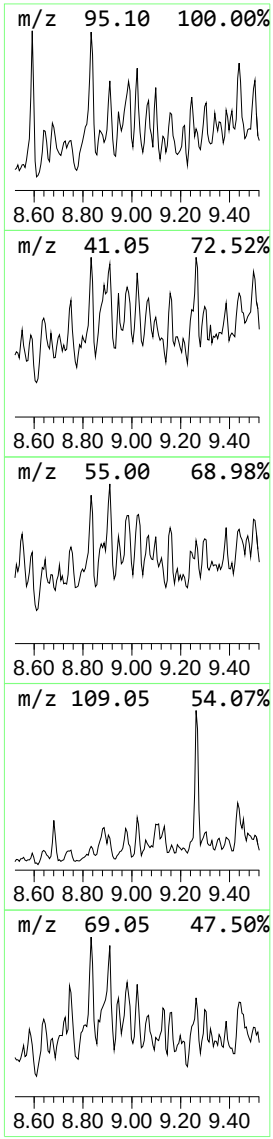
****

Peak Number 8 unknown9.022 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.022	14.09 ng	524710	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropylimidazole	110	C6H10N2	036947-68-9	35
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	30
3	6-Hepten-1-ol, 2-methyl-	128	C8H16O	1000132-12-0	27
4	2-Norbornyl bromide	174	C7H11Br	029342-65-2	22
5	Cyclohexene, 1-methyl-3-(1-methy...	138	C10H18	013828-31-4	22





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Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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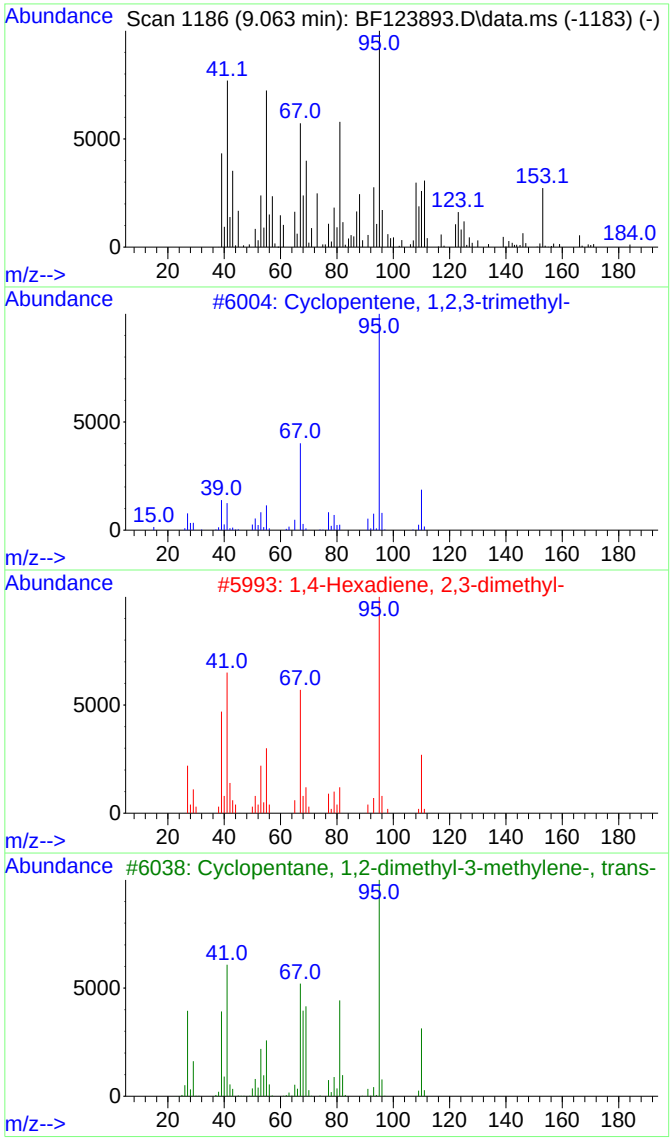
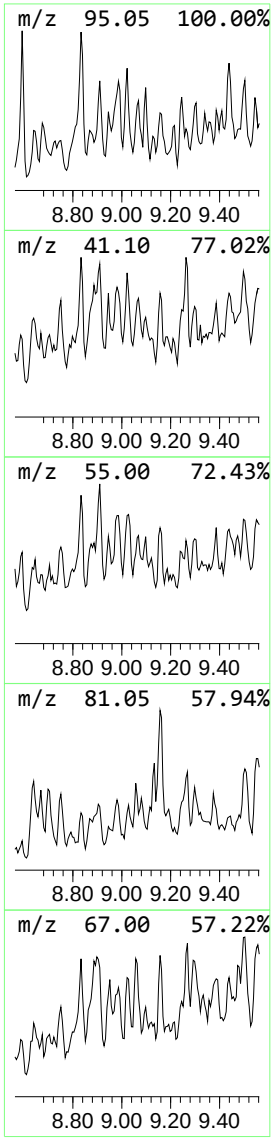
Peak Number 9 unknown9.063 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.063	13.91 ng	517972	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	46
2	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	46
3	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	46
4	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	46
5	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	43





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Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

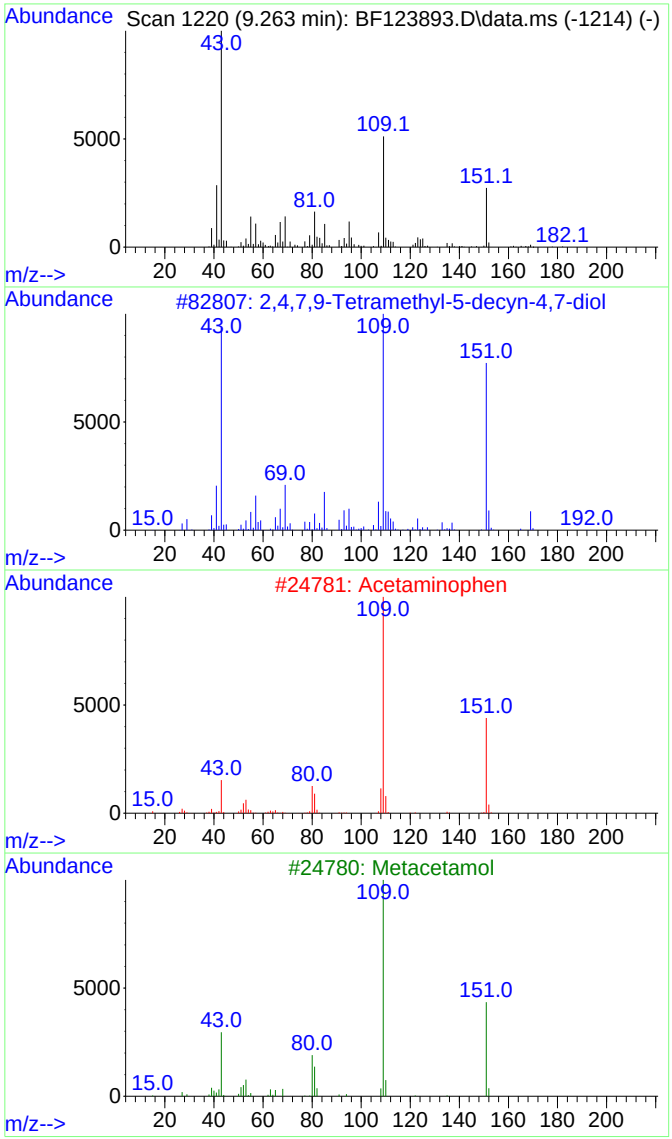
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

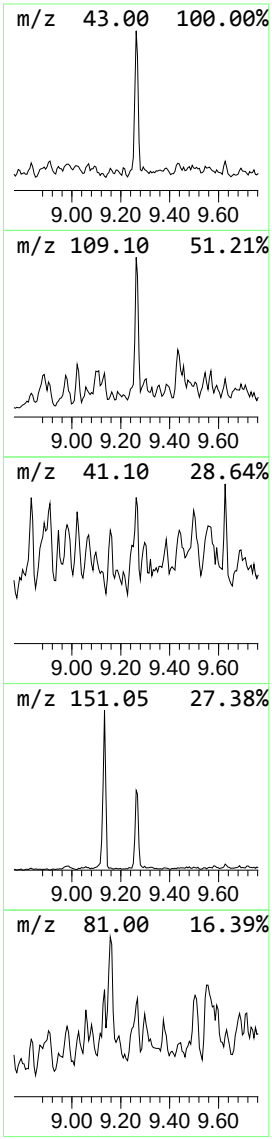
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	29.72 ng	1106390	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	50
2	Acetaminophen	151	C8H9NO2	000103-90-2	49
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	47
5	2,3-Dimethyl-8-oxo-non-2-enal	182	C11H18O2	1000186-82-6	40





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Acq On : 10 May 2021 20:01
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Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

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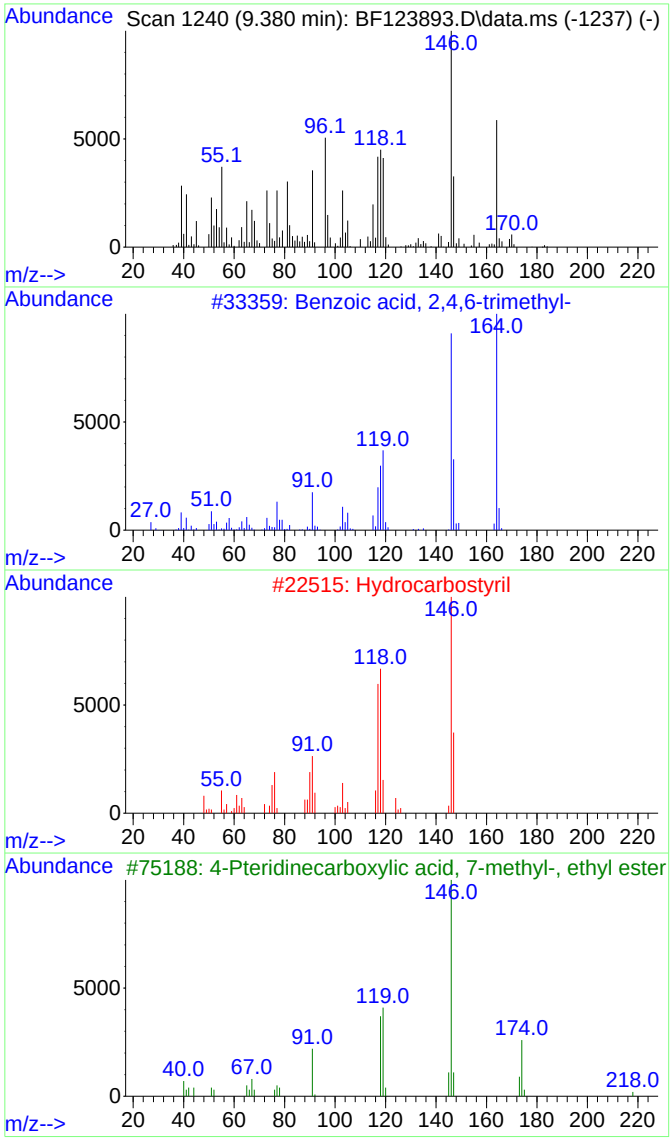
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

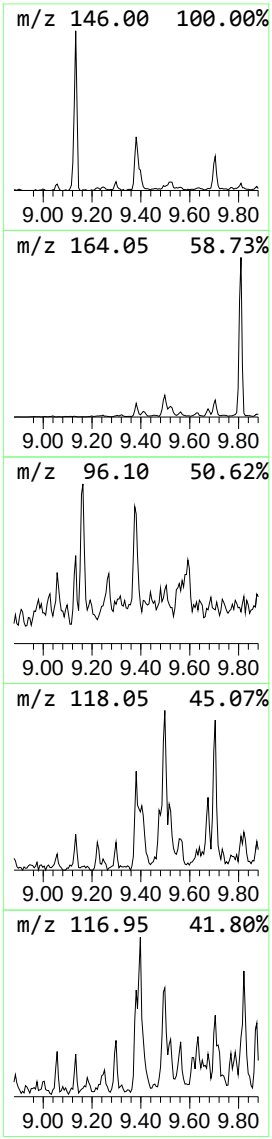
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	10.93 ng	406876	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	60
2	Hydrocarbostyril	147	C9H9NO	000553-03-7	46
3	4-Pteridinecarboxylic acid, 7-me...	218	C10H10N4O2	016008-52-9	38
4	7-Quinazolinol	146	C8H6N2O	007556-97-0	27
5	Pteridine, 7-methyl-	146	C7H6N4	000936-40-3	22





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Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

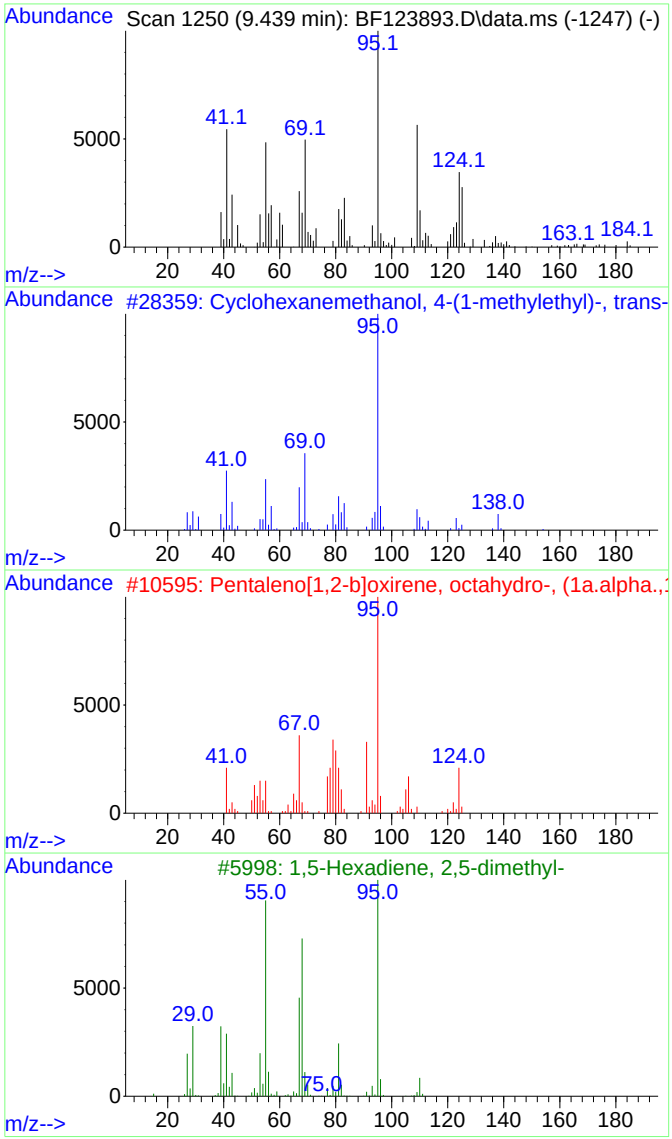
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

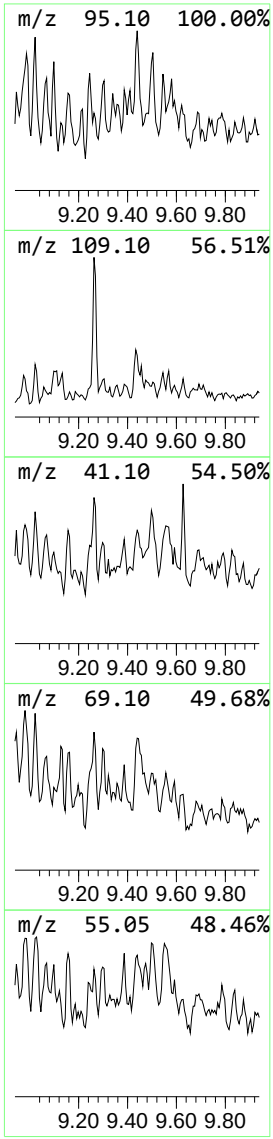
****

Peak Number 12 unknown9.439 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.439	9.58 ng	356636	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-(1-methyl...	156	C10H20O	013674-19-6	43
2	Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-71-3	38
3	1,5-Hexadiene, 2,5-dimethyl-	110	C8H14	000627-58-7	35
4	Ketone, 1,5-dimethylbicyclo[2.1....	138	C9H14O	024081-57-0	35
5	Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	30





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Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

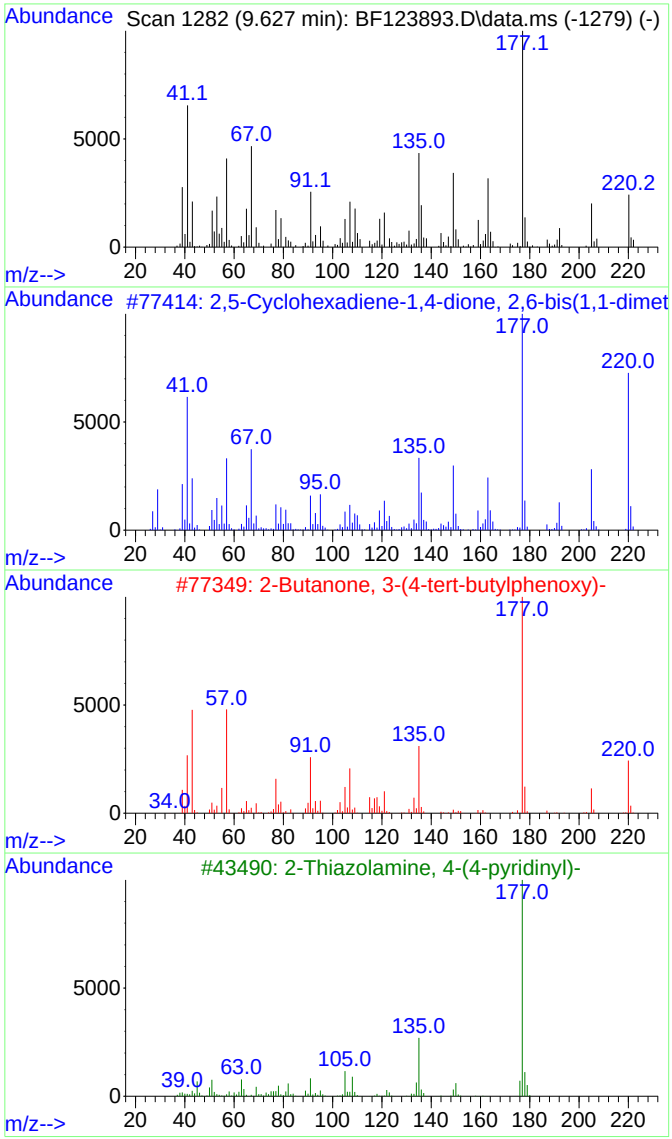
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

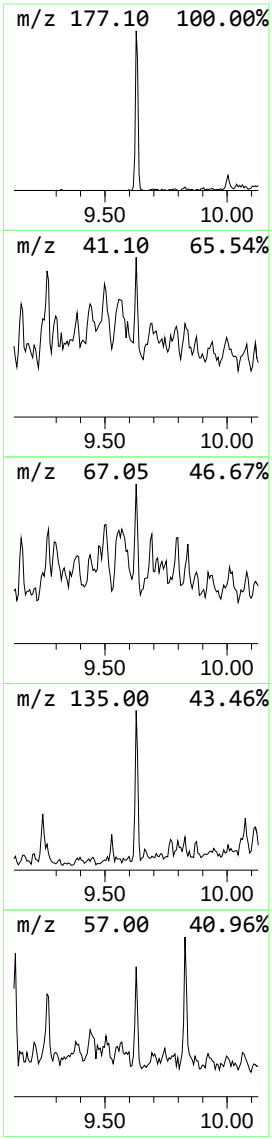
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.627	18.36 ng	683374	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	64
3	2-Thiazolamine, 4-(4-pyridinyl)-	177	C8H7N3S	1000351-69-3	35
4	trans-.beta.-Ionone	192	C13H20O	000079-77-6	30
5	N-Cyclohexylidene-2-carbamylcycl...	220	C13H20N2O	007149-51-1	25





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Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.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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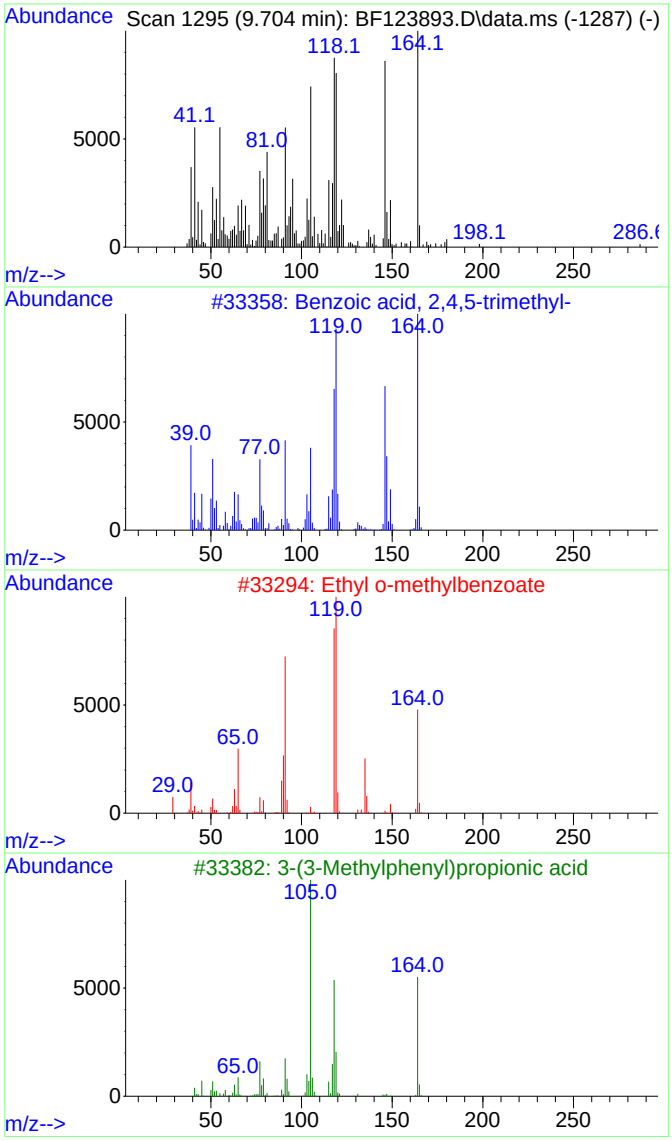
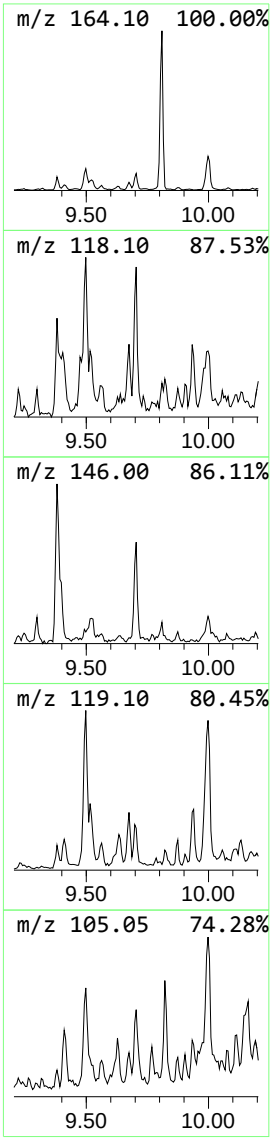
Peak Number 14 unknown9.704 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	25.06 ng	933082	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	49
2	Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	46
3	3-(3-Methylphenyl)propionic acid	164	C10H12O2	003751-48-2	45
4	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	41
5	2-Propenoic acid, 3-(2-hydroxyph...	164	C9H8O3	000614-60-8	30





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Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.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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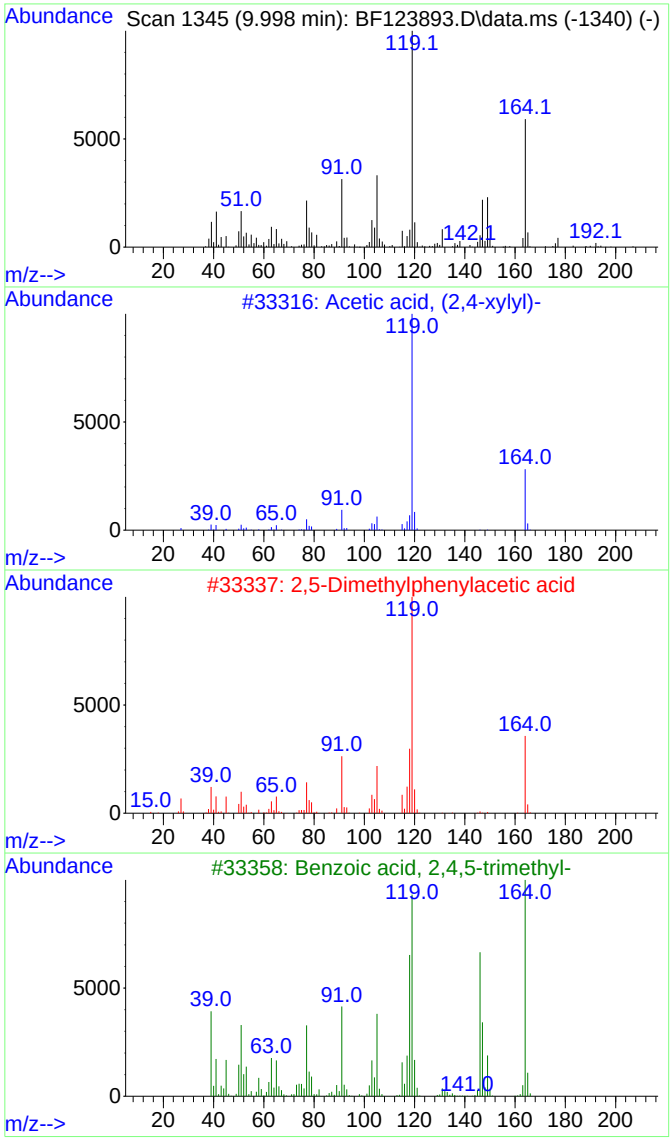
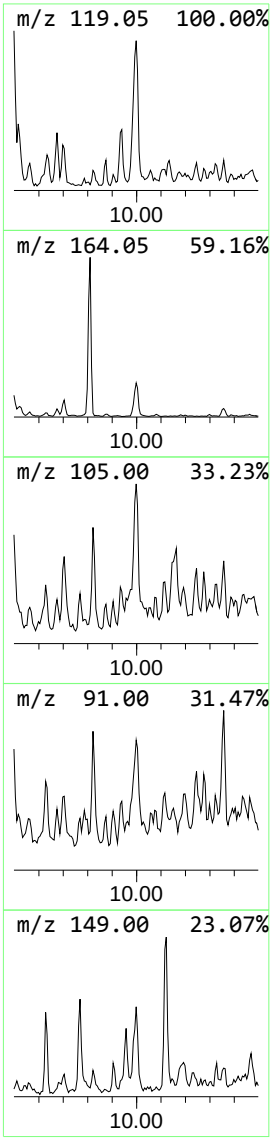
Peak Number 15 Acetic acid, (2,4-xylyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	32.70 ng	1217470	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	76
2	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	74
3	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	58
4	.alpha.-Bromomesitylene	198	C9H11Br	027129-86-8	55
5	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	52





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Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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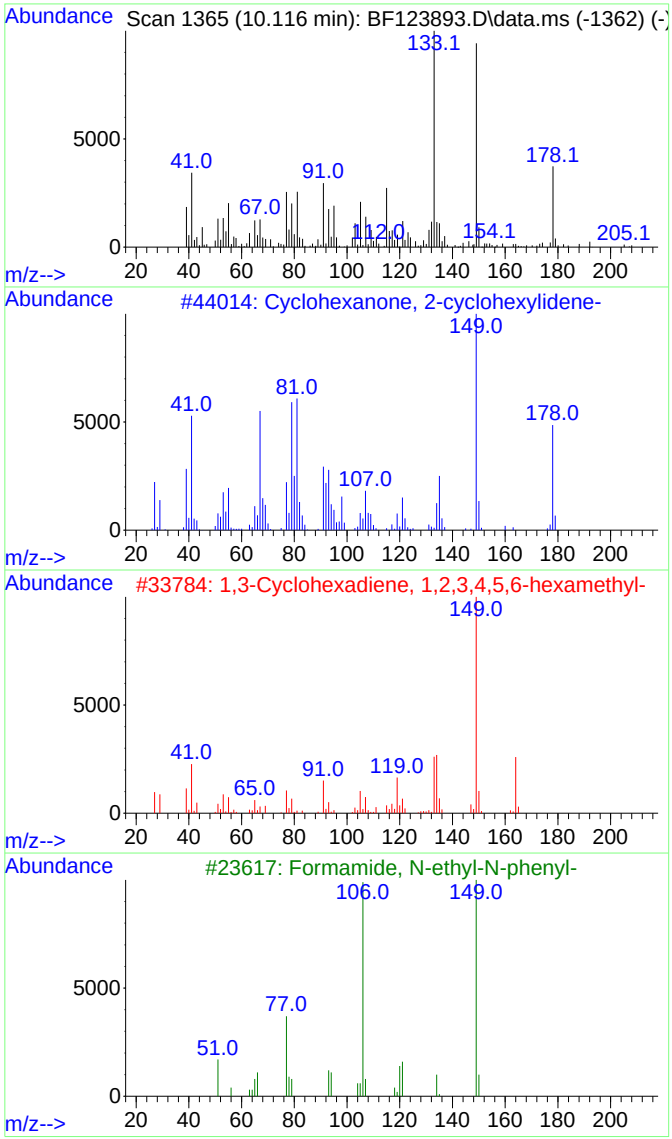
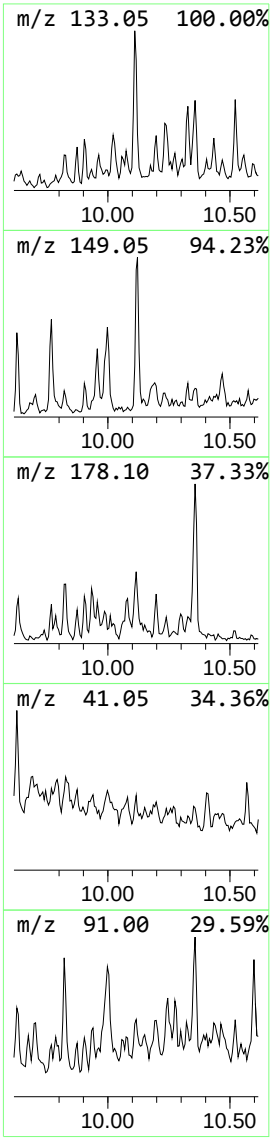
Peak Number 16 unknown10.116 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.116	12.92 ng	480975	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-cyclohexylidene-	178	C12H18O	001011-12-7	38
2	1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164	C12H20	1000152-09-6	38
3	Formamide, N-ethyl-N-phenyl-	149	C9H11NO	005461-49-4	30
4	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	27
5	5-Aminoindazole	133	C7H7N3	019335-11-6	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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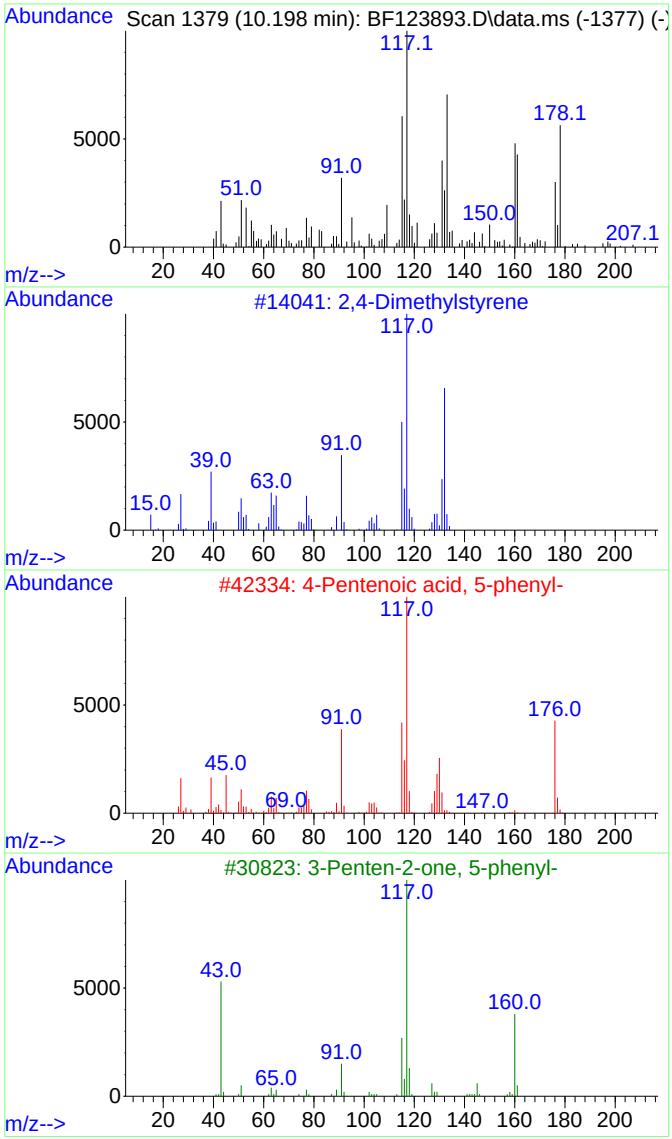
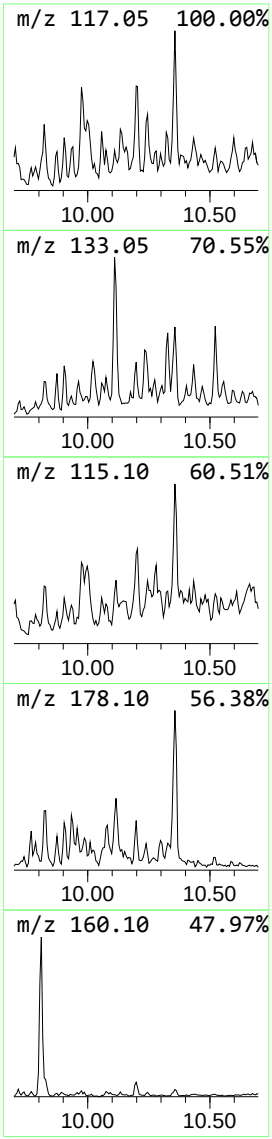
Peak Number 17 unknown10.198 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	9.06 ng	337297	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	46
2	4-Pentenoic acid, 5-phenyl-	176	C11H12O2	028525-69-1	38
3	3-Penten-2-one, 5-phenyl-	160	C11H12O	010521-97-8	30
4	(5-Methylenebicyclo[2.2.1]hept-2...	176	C11H12O2	1000211-09-6	30
5	Bicyclo[4.2.1]nona-2,4,7-triene,...	160	C11H12O	1000141-51-6	25





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Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

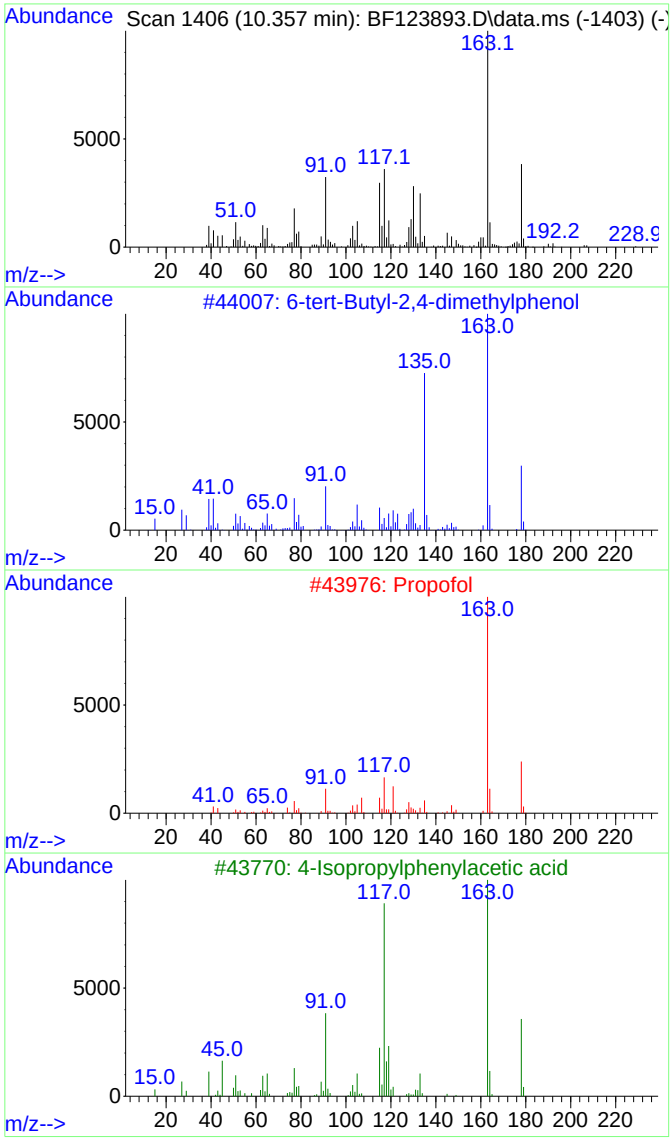
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

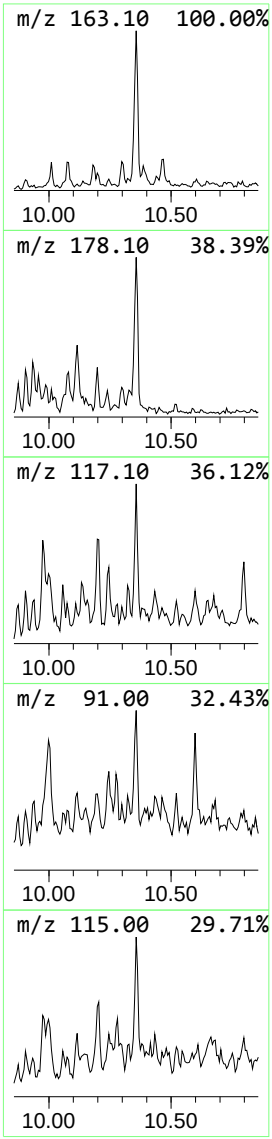
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 6-tert-Butyl-2,4-dimethylph... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.357	17.42 ng	648396	Acenaphthene-d10	9.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
2	Propofol	178	C12H18O	002078-54-8	58
3	4-Isopropylphenylacetic acid	178	C11H14O2	004476-28-2	49
4	Ethanone, 1-(2,3-dihydro-1,4-ben...	178	C10H10O3	002879-20-1	46
5	7-Nitroindazole	163	C7H5N3O2	002942-42-9	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.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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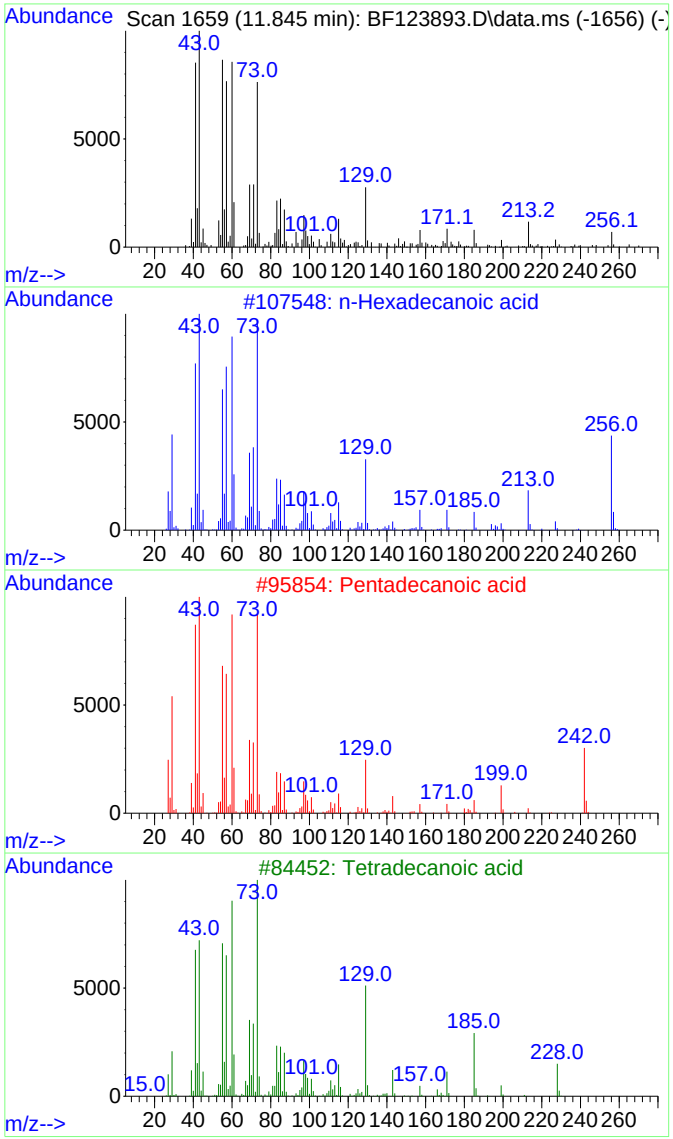
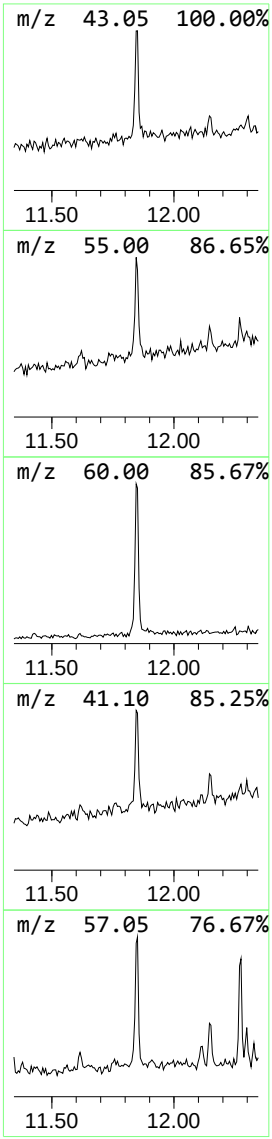
Peak Number 19 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	14.33 ng	544256	Phenanthrene-d10	11.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.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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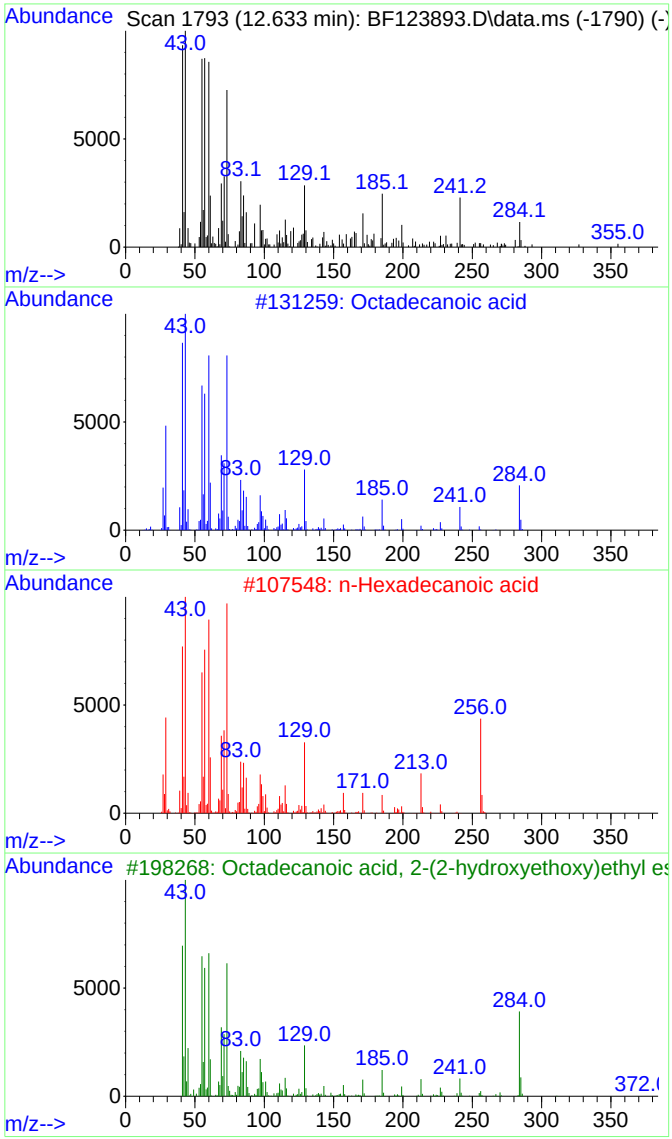
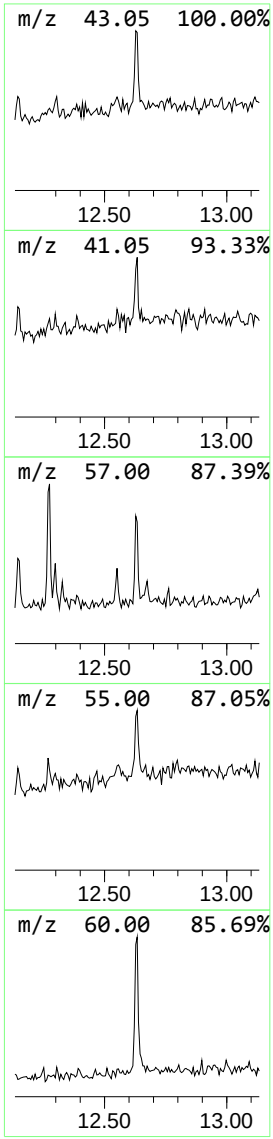
Peak Number 20 Octadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	9.01 ng	283756	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051021\
Data File : BF123893.D
Acq On : 10 May 2021 20:01
Operator : JU/CG
Sample : M2307-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	6.845	39.6	ng	1940240	1	6.769	979091	20.0
Indane	6.951	24.5	ng	1198550	1	6.769	979091	20.0
endo-Borneol	8.445	13.1	ng	792426	2	8.051	1209180	20.0
unknown8.639	8.639	13.4	ng	812841	2	8.051	1209180	20.0
unknown8.945	8.945	9.2	ng	343390	3	9.810	744562	20.0
unknown8.986	8.986	20.5	ng	763463	3	9.810	744562	20.0
unknown9.022	9.022	14.1	ng	524710	3	9.810	744562	20.0
unknown9.063	9.063	13.9	ng	517972	3	9.810	744562	20.0
2,4,7,9-Tetrame...	9.263	29.7	ng	1106390	3	9.810	744562	20.0
Benzoic acid, 2...	9.380	10.9	ng	406876	3	9.810	744562	20.0
unknown9.439	9.439	9.6	ng	356636	3	9.810	744562	20.0
2,5-Cyclohexadi...	9.627	18.4	ng	683374	3	9.810	744562	20.0
unknown9.704	9.704	25.1	ng	933082	3	9.810	744562	20.0
Acetic acid, (2...	9.998	32.7	ng	1217470	3	9.810	744562	20.0
unknown10.116	10.116	12.9	ng	480975	3	9.810	744562	20.0
unknown10.198	10.198	9.1	ng	337297	3	9.810	744562	20.0
6-tert-Butyl-2,...	10.357	17.4	ng	648396	3	9.810	744562	20.0
n-Hexadecanoic ...	11.845	14.3	ng	544256	4	11.292	759862	20.0
Octadecanoic acid	12.633	9.0	ng	283756	5	13.939	629552	20.0