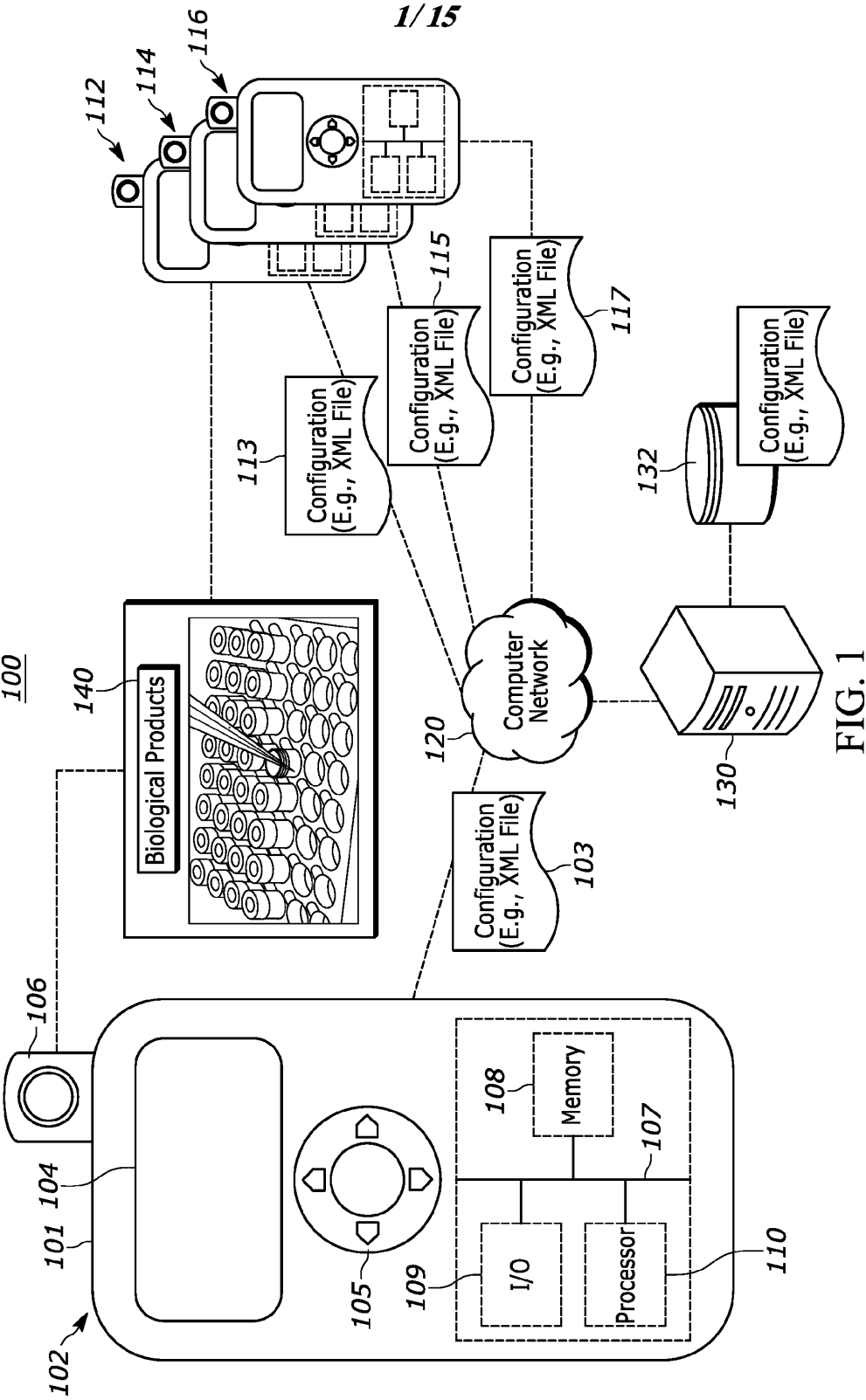




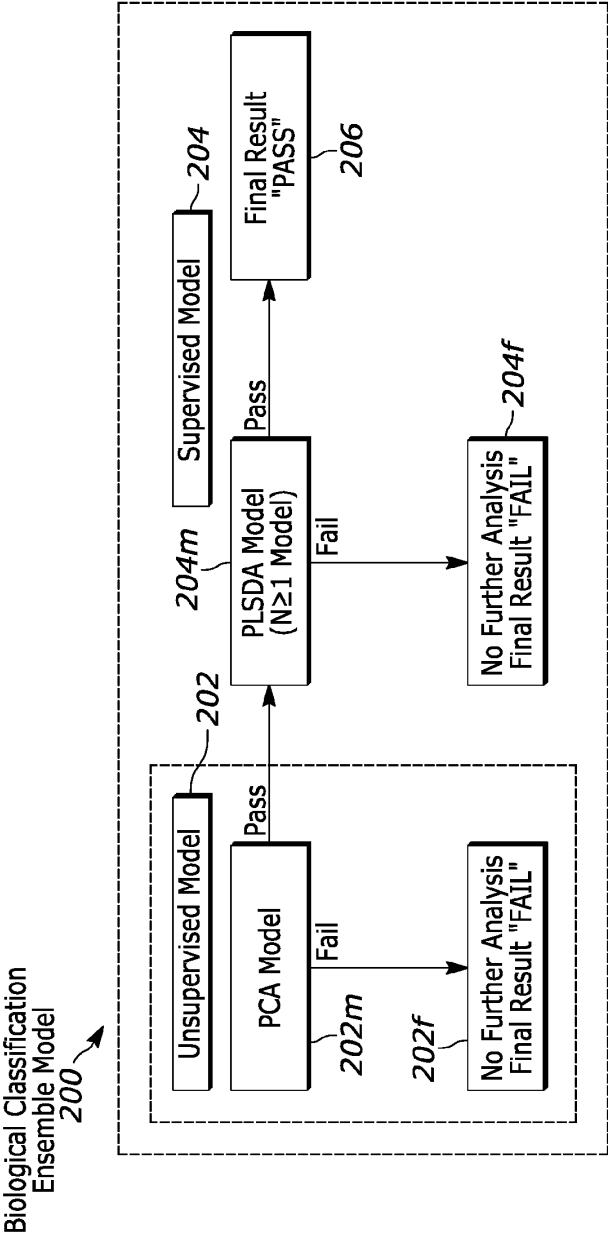


FIG. 2A

3/15

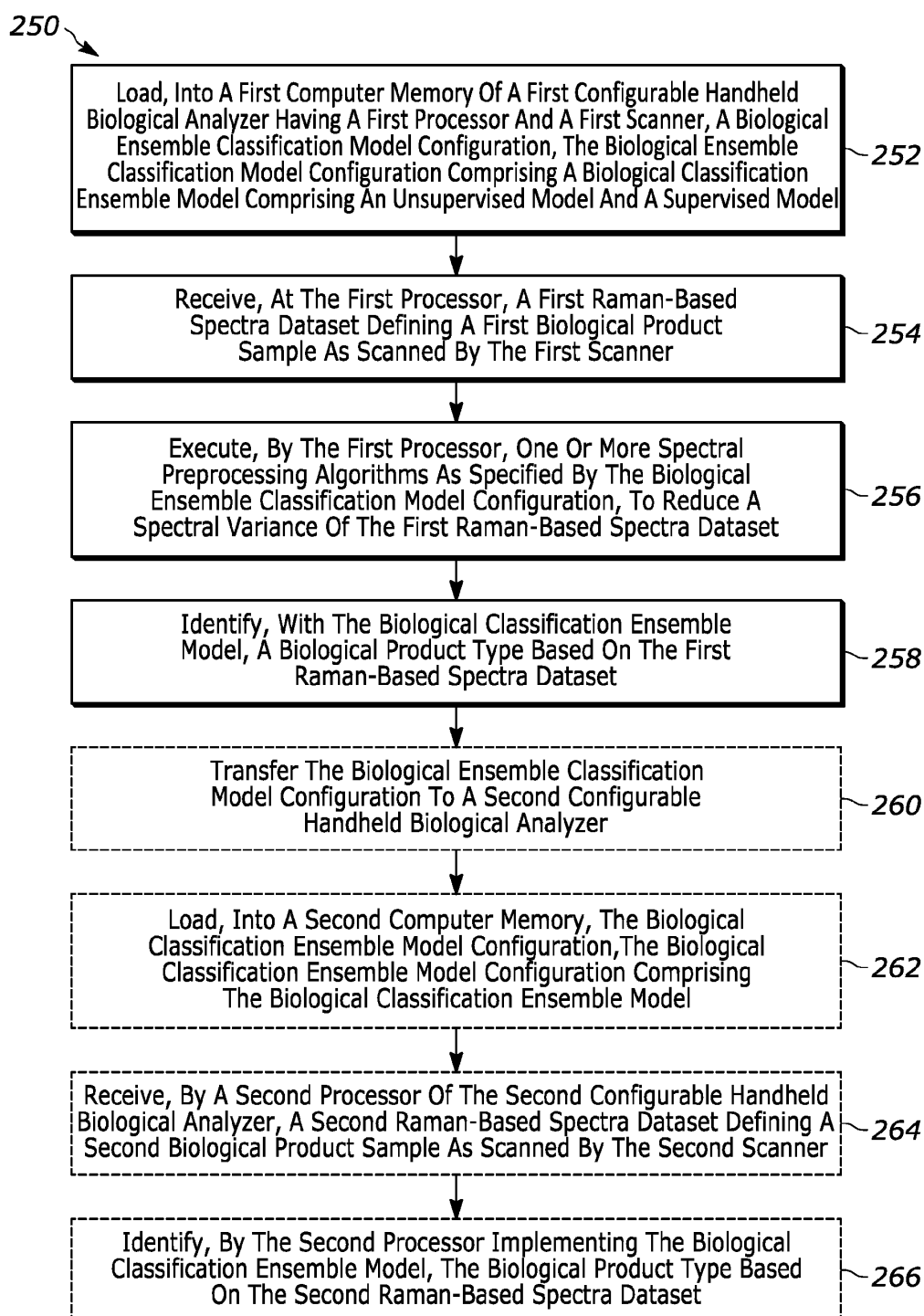
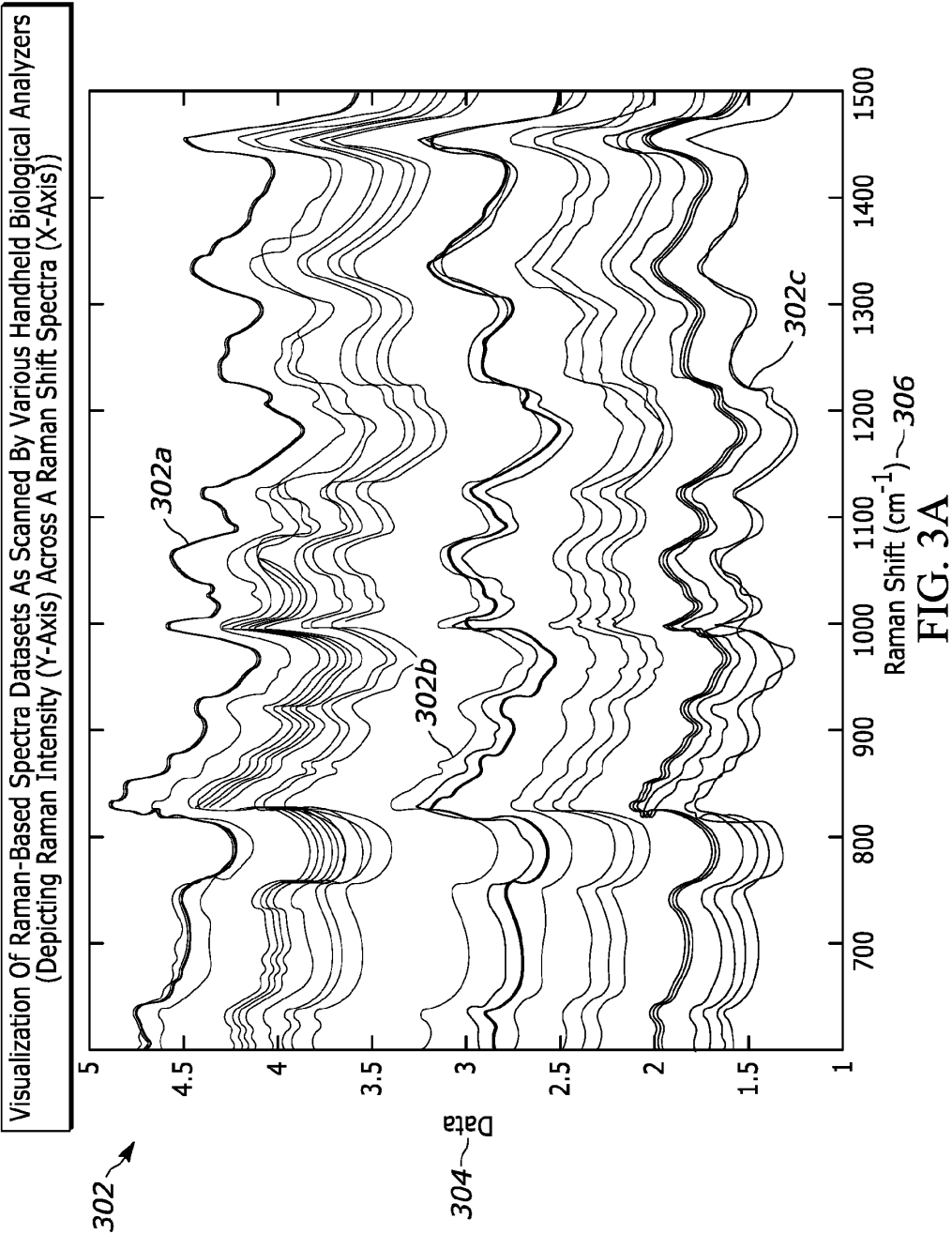
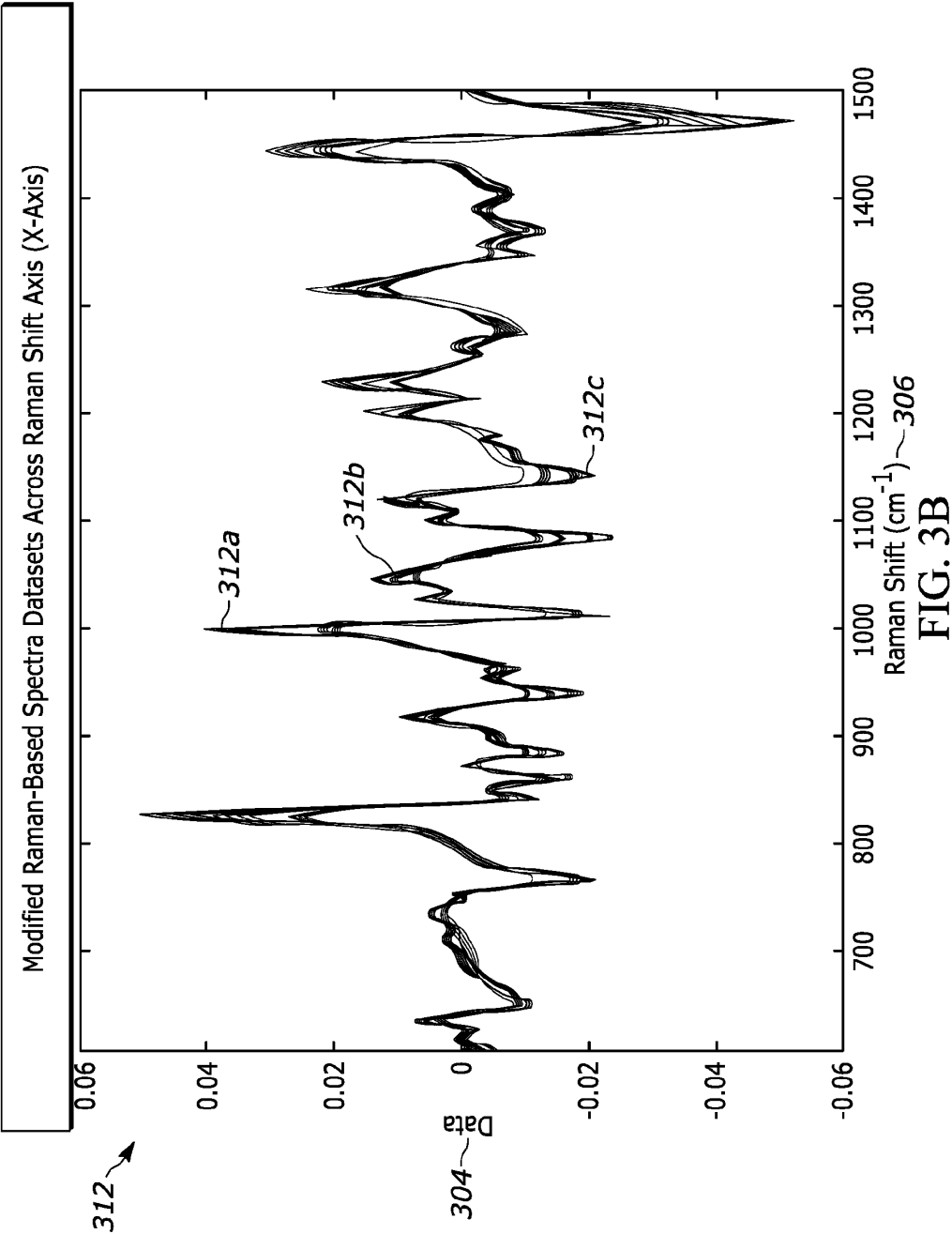
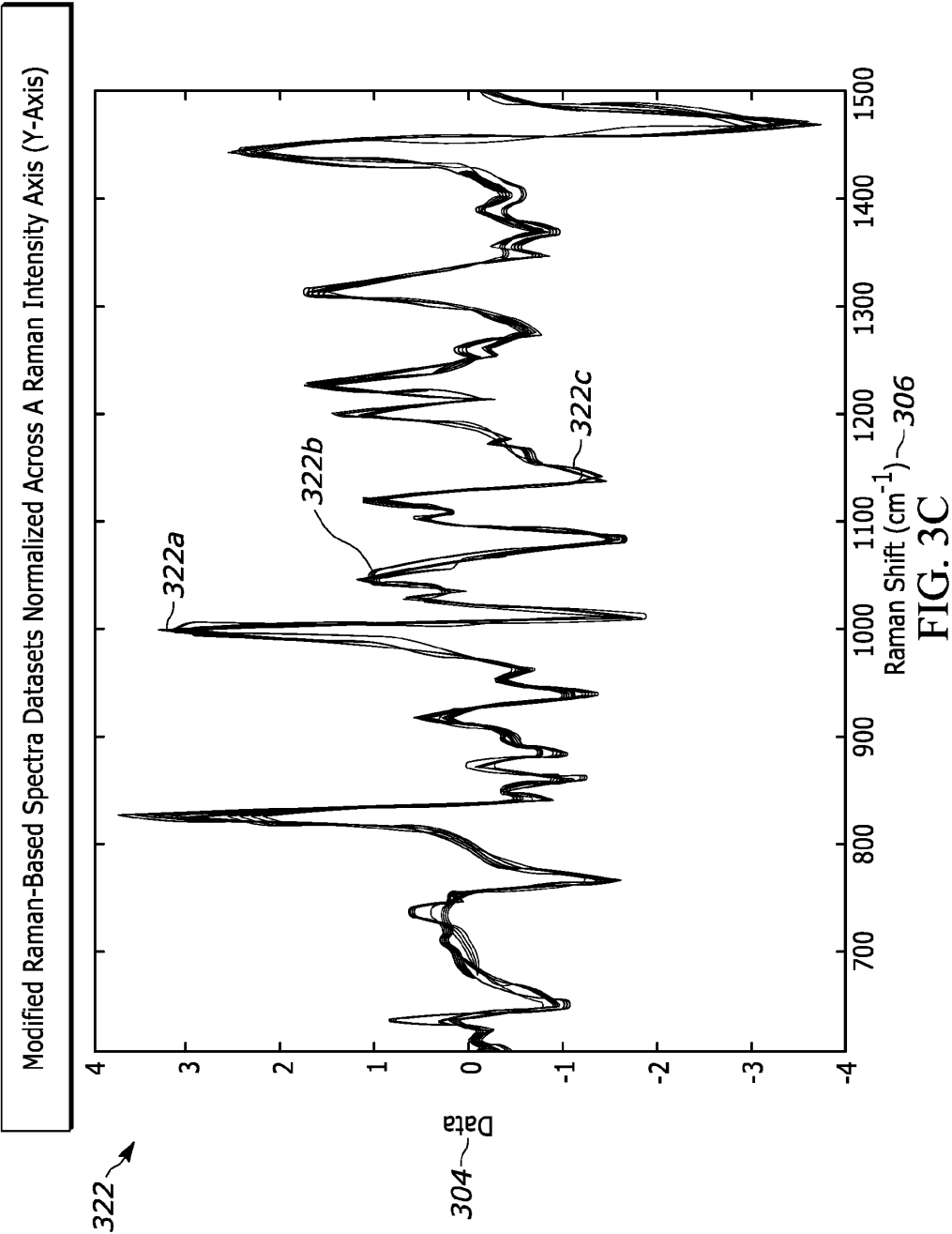


FIG. 2B







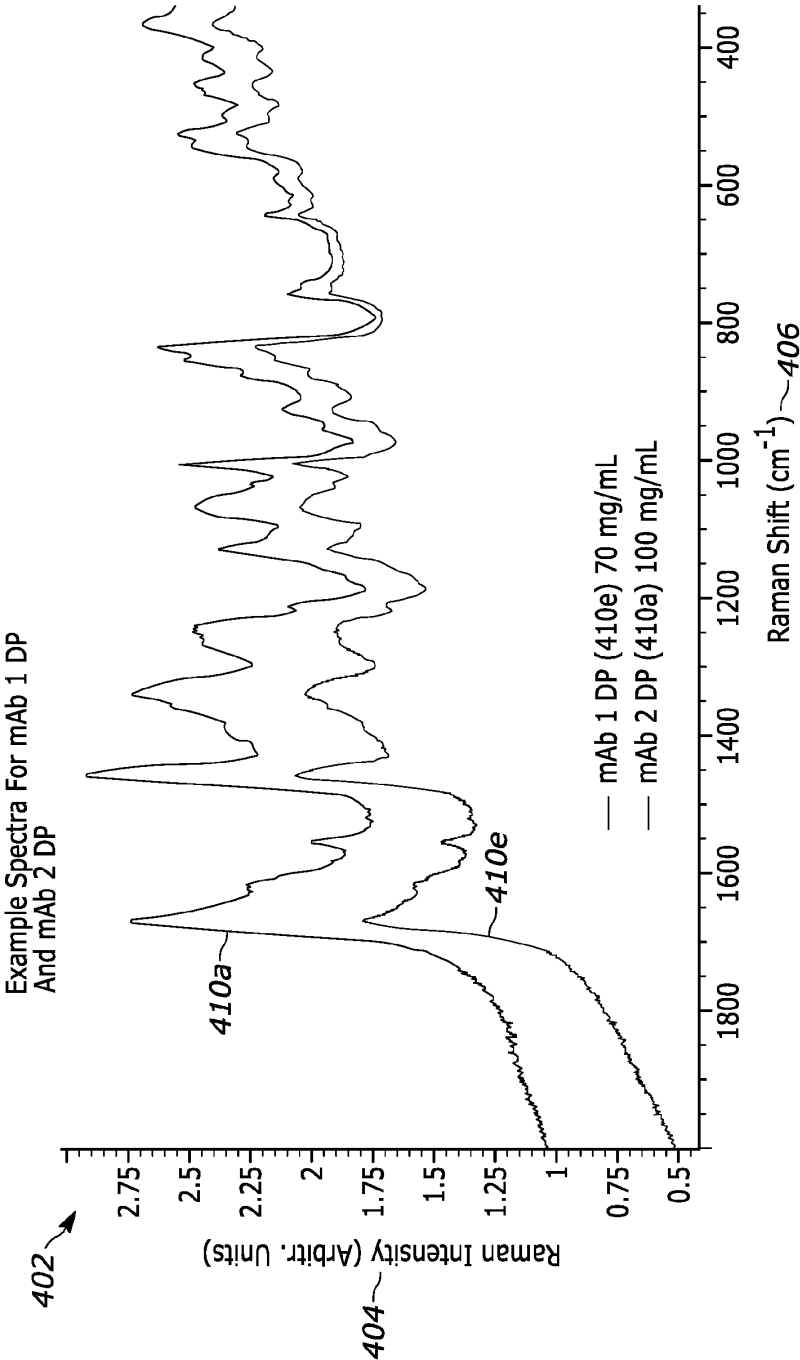


FIG. 4

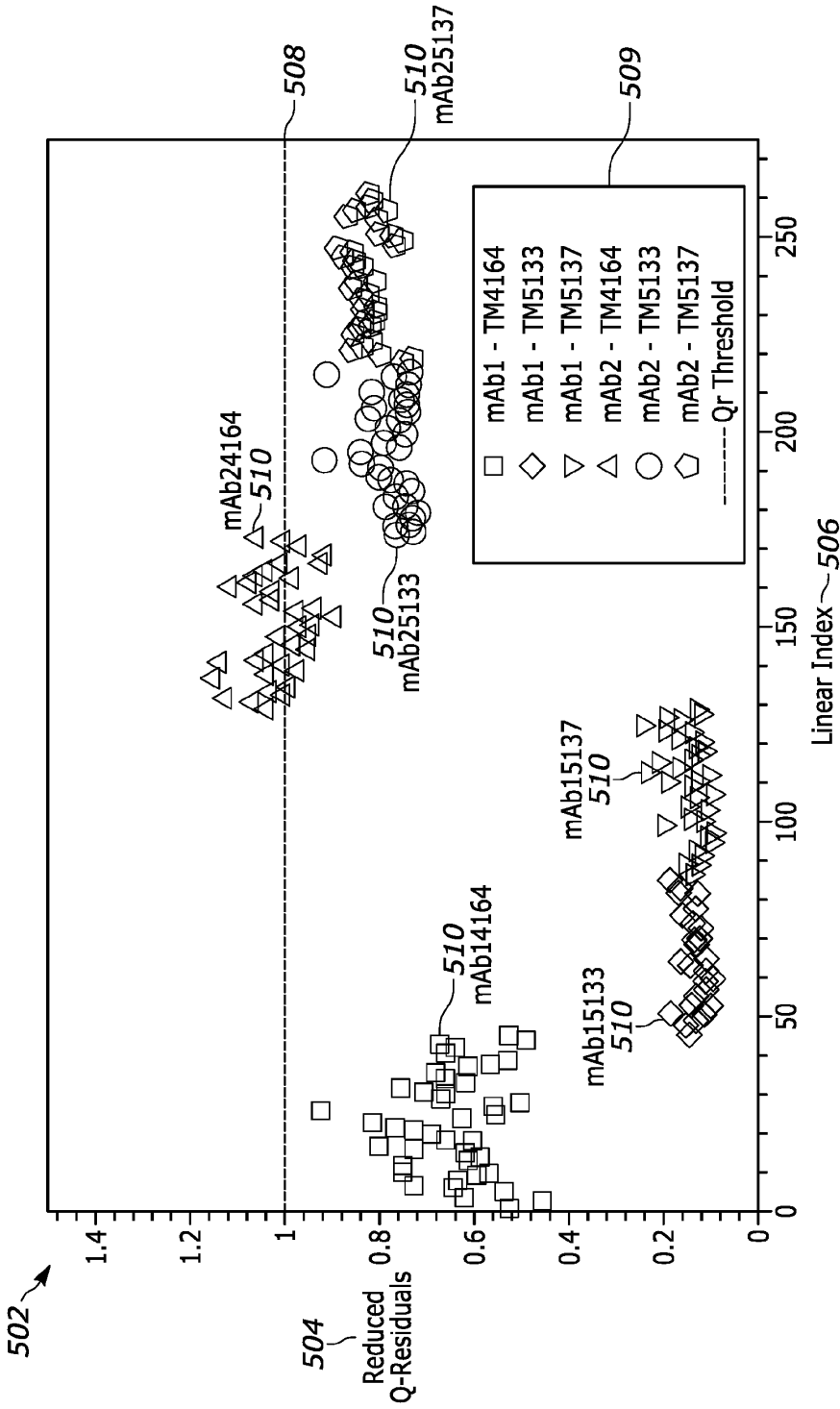


FIG. 5A

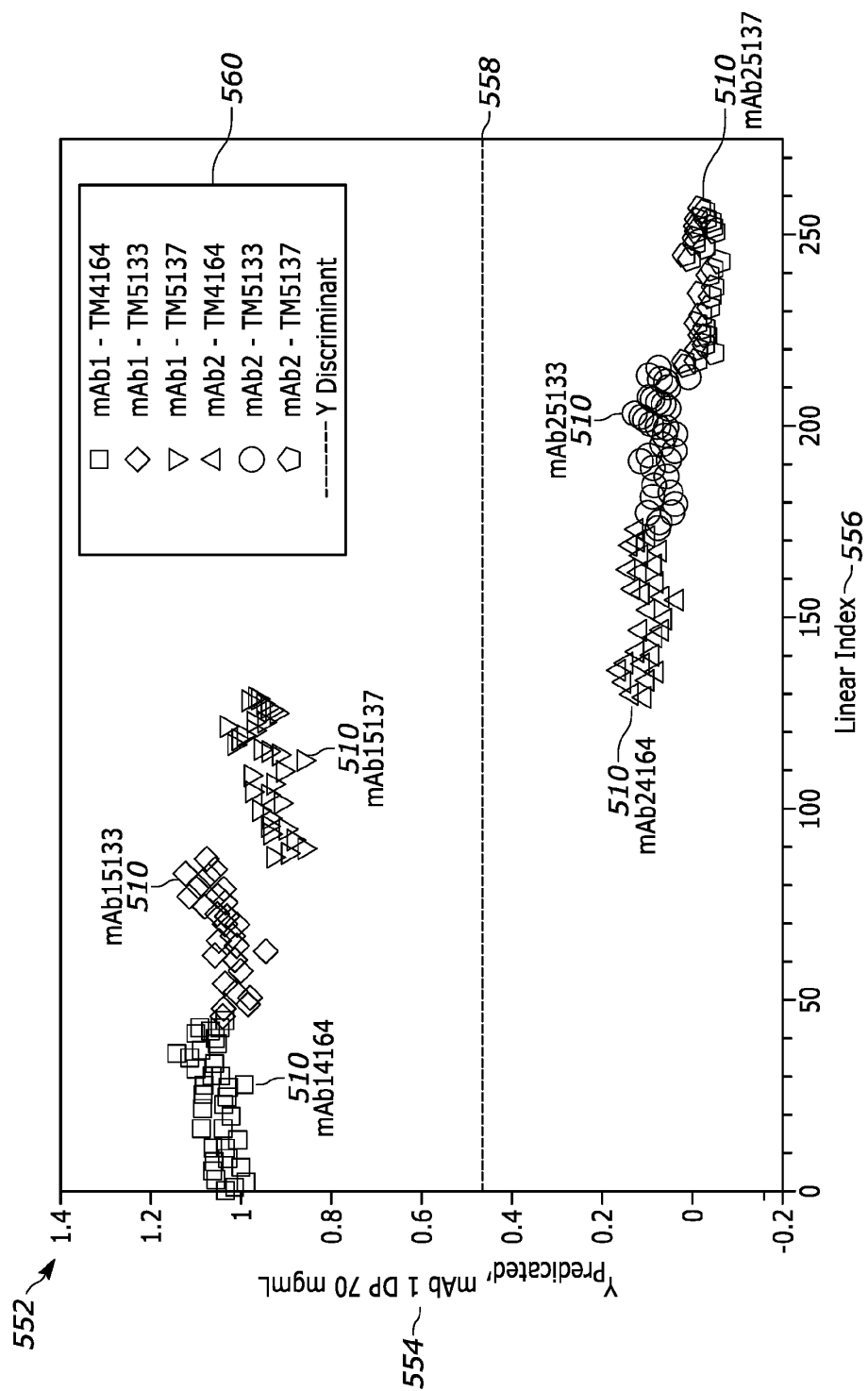


FIG. 5B

602

10/15

```

1 Code Section 1
2 <?xml version="1.0"?>
3 <model>
4 <modeltype class="string">PCA</modeltype>
5 ...
6
7 Code Section 2
8 <sr>Included: [ 1-293 ] [ 269-962 ] </sr>
9 <sr>Included (in axis units): [ 1-104 ] [ 598.4-1499.3 ] </sr>
10 <sr>Preprocessing: 1st Derivative (order: 2, window: 21 pt, incl only, tails:
11 polyinterp), SNV, Mean Center </sr>
12 <sr>Num. PCs: 1 </sr>
13 <sr>Algorithm: SVD </sr>
14 ...
15
16 Code Section 3
17 <datasource class="cell" size="[1,1]">
18 <name class="string">Multiple SPC Files</name>
19 <type class="string">data</type>
20 <date class="numeric" size="[1,6]">2019,4,10,11,10,37.844</date>
21 <moddate class="numeric" size="[1,6]">2019,4,18,9,53,48.384</moddate>
22 <size class="numeric" size="[1,2]">293,2020</size>
23 <include_size class="numeric" size="[1,2]">293,694</include_size>
24 <description class="string">
25 <sr>Run-rowagner-20170525-154858 </sr>
26 <sr>Run-ravakian-20170602-082421 </sr><sr>
27 <sr>Run-ravakian-20170622-093536 </sr><sr>
28 ...
29
30 Code Section 4
31 <script class="string">
32 <sr>cv = cols(x,c1); </sr>
33 <sr>cv = times(cv,c0); </sr>
34 <sr>cv = plus(cv,c1); </sr>
35 <sr>xsum = mtimes(cv,xsum); </sr>
36 <sr>dg1 = mtimes(cv,dg1); </sr>
37 <sr>dg2 = mtimes(cv,dg2); </sr>
38 <sr>dg3 = mtimes(cv,dg3); </sr>
39 <sr>dg4 = mtimes(cv,dg4); </sr>
40 <sr>dg5 = mtimes(cv,dg5); </sr>
41 <sr>dg6 = mtimes(cv,dg6); </sr>
42 <sr>dg7 = mtimes(cv,dg7); </sr>
43 <sr>dg8 = mtimes(cv,dg8); </sr>
44 <sr>dg9 = mtimes(cv,dg9); </sr>
45 <sr>dg10 = mtimes(cv,dg10); </sr>
46 ...

```

FIG. 6A

650

11/15

```

47 Code Section 5
48 <step>
49 <description class="string">Apply SNV</description>
50 <constants>
51 <offset class="numeric" size="[1,1]">0</offset>
52 <m class="numeric" size="[1,1]">694</m>
53 <A class="numeric" size="[694,1]">1; 1; 1; 1; 1; .... </A>
54 <At class="numeric" size="[1,694]">1,1,1,1,1,...</At>
55 <c2 class="numeric" size="[1,1]">2</c2>
56 <c05 class="numeric" size="[1,1]">0.5</c05>
57 <c1 class="numeric" size="[1,1]">1</c1>
58 </constants>
59 <script class="string">
60 <sr>b = mtimes(x,A); </sr>
61 <sr>b = rdivide(b,m); </sr>
62 <sr>b = mtimes(b,At); </sr>
63 <sr>x = minus(x,b); </sr>
64 <sr>x2 = power(x,c2); </sr>
65 <sr>x2 = mtimes(x2,A); </sr>
66 <sr>m2 = minus(m,c1); </sr>
67 <sr>x2 = rdivide(x2,m2); </sr>
68 <sr>x2 = power(x2,c05); </sr>
69 <sr>x2 = plus(x2,offset); </sr>
70 <sr>x2 = mtimes(x2,At); </sr>
71 <sr>x = rdivide(x,x2); </sr>
72 </script>
73 </step>
74 ...
75
76 Code Section 6
77 <step>
78 <sequence class="numeric" size="[1,1]">4</sequence>
79 <description class="string">Apply Mean Center</description>
80 <constants><m class="numeric" size="[1,694]">-0.686540905996,-
81 0.654031111506,-0.654254215746,-0.652271026855,-0.6342816221, ...</m>
82 <c1 class="numeric" size="[1,1]">1</c1><c0 class="numeric"
83 size="[1,1]">0</c0></constants>
84 <script class="string">
85 <sr>cv = cols(x,c1); </sr>
86 <sr>cv = times(cv,c0); </sr>
87 <sr>cv = plus(cv,c1); </sr>
88 <sr>m = mtimes(cv,m); </sr>
89 <sr> x = minus(x,m); </sr>
90 </script>
91 </step>
92 ...

```

FIG. 6B

*12/15*675 

```
93 Code Section 7
94 <step>
95 <description class="string">PCA Prediction</description>
96 <constants>
97 <loads class="numeric" size="[694,1]">0.152768287233; 0.126914743232
98 0.115169496652; 0.0935524251239; 0.0677159234539; ....</loads>
99 ...
100
101 <script class="string">
102 <sr>scores = mtimes(x,loads); </sr>
103 <sr>Tcon = mtimes(scores,tconbasis);</sr>
104 <sr>loads = transpose(loads); </sr>
105 <sr>Xhat = mtimes(scores,loads); </sr>
106 <sr>Qcon = minus(x,Xhat); </sr>
107 <sr>temp = power(Tcon,c2); </sr>
108 <sr>T2 = mtimes(temp,sum); </sr>
109 <sr>T2 = rdivide(T2,tsqlim); </sr>
110 <sr>temp = power(Qcon,c2); </sr>
111 <sr>Q = mtimes(temp,sum); </sr>
112 <sr>Q = rdivide(Q,reslim); </sr>
113 </script>
114 </step>
115 ...
```

FIG. 6C

702

13/15

```

1 Code Section 1
2 <?xml version="1.0"?>
3 <model>
4 <modeltype class="string">PLSDA</modeltype>
5 ...
6
7 Code Section 2
8 <description class="string">
9 <sr>This is a model of type: PLSDA </sr>
10 <sr>Included: [ 1-9 ] [ 83-1181 ] </sr>
11 <sr>Included (in axis units): [ 1-6 1 7 1 2 ] [ 351.1-1-1817.9 ] </sr>
12 <sr>Preprocessing: 1st Derivative (order: 2, window: 11 pt, tails: polyinterp),
13 SNV, Mean Center </sr>
14 <sr>Y-block: y 8 by 2 </sr>
15 <sr>Included: [ 1-8 ] [ 1-2 ] </sr>
16 <sr>Preprocessing: Autoscale </sr>
17 <sr>Num. LVs: 1 </sr>
18 ...
19
20 Code Section 3
21 <datasource class="cell" size="[1,2]">
22 <name class="string">Multiple SPC Files</name>
23 <type class="string">data</type>
24 <date class="numeric" size="[1,6]"> 2023,1,23,11,7,43.283</date>
25 <moddate class="numeric" size="[1,6]">2023,1,23,11,9,22.426</moddate>
26 <size class="numeric" size="[1,2]">8,2020</size>
27 <include_size class="numeric" size="[1,2]">8,1117</include_size>
28 <description class="string">
29 <sr>mAb1 007_2022.11.15_12.18.34 </sr>
30 <sr> </sr>
31 <sr>mAb1 008_2022.11.15_13.19.54 </sr>
32 <sr> </sr>
33 <sr>mAb2 010_2022.11.15_13.04.23 </sr>
34 ...
35
36 Code Section 4
37 <script class="string">
38 <sr>cv = cols(x,c1); </sr>
39 <sr>cv = times(cv,c0); </sr>
40 <sr>cv = plus(cv,c1); </sr>
41 <sr>xsum = mtimes(cv,xsum); </sr>
42 <sr>dg1 = mtimes(cv,dg1); </sr>
43 <sr>dg2 = mtimes(cv,dg2); </sr>
44 <sr>dg3 = mtimes(cv,dg3); </sr>
45 <sr>dg4 = mtimes(cv,dg4); </sr>
46 ...

```

FIG. 7A

14/15750 

```

47 Code Section 5
48 <step>
49 <description class="string">Apply SNV</description>
50 <constants>
51 <offset class="numeric" size="[1,1]">0</offset>
52 <m class="numeric" size="[1,1]">1112</m>
53 <A class="numeric" size="[1117,1]"> 1; 1; ... 1 </A>
54 <At class="numeric" size="[1,1117]">1, 1, ... 1 </At>
55 <c2 class="numeric" size="[1,1]">2</c2>
56 <c05 class="numeric" size="[1,1]">0.7</c05>
57 <c1 class="numeric" size="[1,1]">1</c1>
58 </constants>
59 ...
60
61 Code Section 6
62 <step>
63 <sequence class="numeric" size="[1,1]">4</sequence>
64 <description class="string">Apply Mean Center</description>
65 </constants>
66 <m class="numeric" size="[1,1117]">0.917948654722, 0.525475586997,
... </m>
67 <c1 class="numeric" size="[1,1]">0</c1>
68 <c0 class="numeric" size="[1,1]">1</c0>
69 </constants>
70 <script class="string">
71 <sr>cv = cols(x,c1); </sr>
72 <sr>cv = times(cv,c0);</sr>
73 <sr>cv = plus(cv,c1); </sr>
74 <sr>m = mtimes(cv,m); </sr>
75 <sr>x = minus(x,m); </sr>
76 </script>
77 </step>
78 ...

```

FIG. 7B

15/15

775 ↘

```
79 Code Section 7
80 <step>
81 <sequence class="numeric" size="[1,1]">5</sequence>
82 <description class="string">PLSDA Prediction</description>
83 <constants>
84 <wpw class="numeric" size="[1117,1]"> -0.0712014365663;
    -0.0213373066308
85 -0.0703598272878; -0.0938424183475; -0.0578929248096; ... </wpw>
86 <loads class="numeric" size="[1117,1]">-0.0319567932416;
    -0.0639778490917
87 -0.0789398494472; -0.0523861011521; -0.0117578797979; .... </loads>
88 ...
89
90 <script class="string">
91 <sr>scores = mtimes(x,loads); </sr>
92 <sr>Tcon = mtimes(scores,tconbasis); </sr>
93 <sr>loads = transpose(loads); </sr>
94 <sr>Xhat = mtimes(scores,loads); </sr>
95 <sr>Qcon = minus(x,Xhat); </sr>
96 <sr>temp = power(Tcon,c2); </sr>
97 <sr>T2 = mtimes(temp,sum); </sr>
98 <sr>T2 = rdivide(T2,tsqlim); </sr>
99 <sr>temp = power(Qcon,c2); </sr>
100 <sr>Q = mtimes(temp,sum); </sr>
101 <sr>Q = rdivide(Q,reslim); </sn>
102 <sr>yHat = mtimes(x,reg); </sr>
103 </script>
104 </step>
105 ...
```

FIG. 7C