FIG. 1

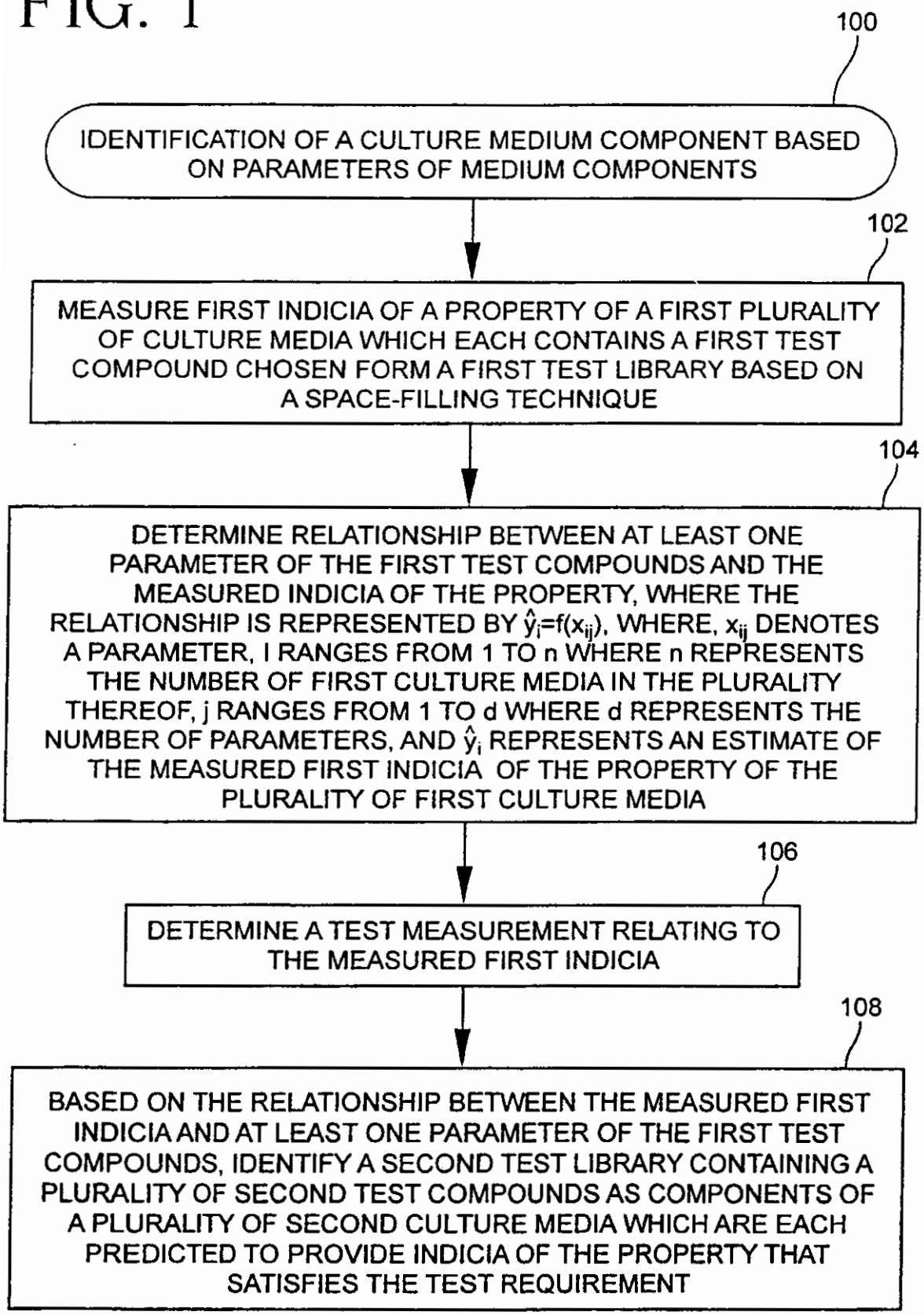

100
IDENTIFICATION OF A CULTURE MEDIUM COMPONENT BASED ON PARAMETERS OF MEDIUM COMPONENTS
102
MEASURE FIRST INDICIA OF A PROPERTY OF A FIRST PLURALITY OF CULTURE MEDIA WHICH EACH CONTAINS A FIRST TEST COMPOUND CHOSEN FORM A FIRST TEST LIBRARY BASED ON A SPACE-FILLING TECHNIQUE
104
DETERMINE RELATIONSHIP BETWEEN AT LEAST ONE PARAMETER OF THE FIRST TEST COMPOUNDS AND THE MEASURED INDICIA OF THE PROPERTY, WHERE THE RELATIONSHIP IS REPRESENTED BY $\hat{y}_i=f(x_{ij})$, WHERE, x_{ij} DENOTES A PARAMETER, I RANGES FROM 1 TO n WHERE n REPRESENTS THE NUMBER OF FIRST CULTURE MEDIA IN THE PLURALITY THEREOF, j RANGES FROM 1 TO d WHERE d REPRESENTS THE NUMBER OF PARAMETERS, AND $\hat{y}_i$ REPRESENTS AN ESTIMATE OF THE MEASURED FIRST INDICIA OF THE PROPERTY OF THE PLURALITY OF FIRST CULTURE MEDIA
106
DETERMINE A TEST MEASUREMENT RELATING TO THE MEASURED FIRST INDICIA
108
BASED ON THE RELATIONSHIP BETWEEN THE MEASURED FIRST INDICIA AND AT LEAST ONE PARAMETER OF THE FIRST TEST COMPOUNDS, IDENTIFY A SECOND TEST LIBRARY CONTAINING A PLURALITY OF SECOND TEST COMPOUNDS AS COMPONENTS OF A PLURALITY OF SECOND CULTURE MEDIA WHICH ARE EACH PREDICTED TO PROVIDE INDICIA OF THE PROPERTY THAT SATISFIES THE TEST REQUIREMENT

FIG. 2

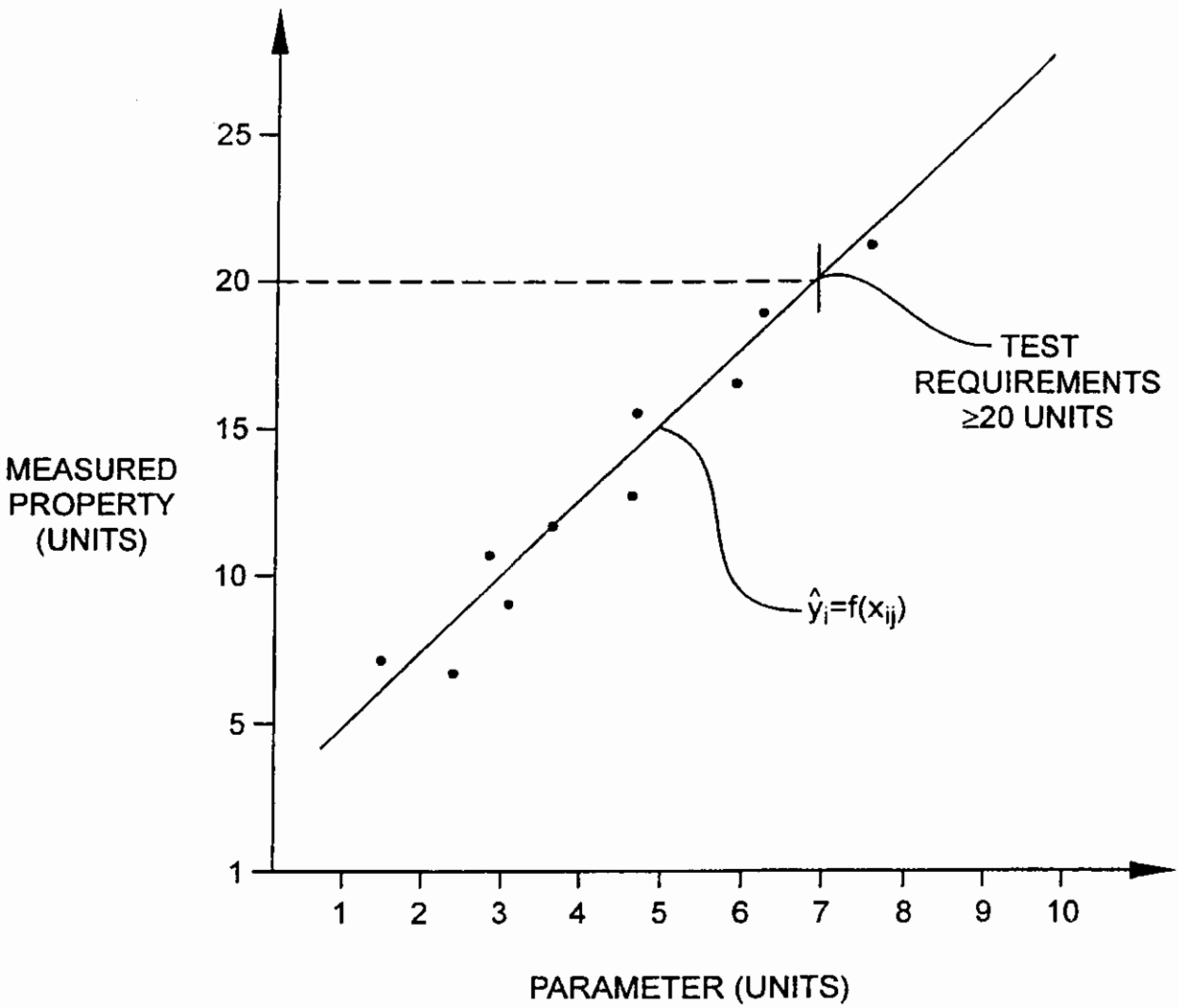

25
20
15
10
5
1
MEASURED PROPERTY (UNITS)
TEST REQUIREMENTS ≥20 UNITS
$\hat{y}_i=f(x_{ij})$
1
2
3
4
5
6
7
8
9
10
PARAMETER (UNITS)

FIG. 3

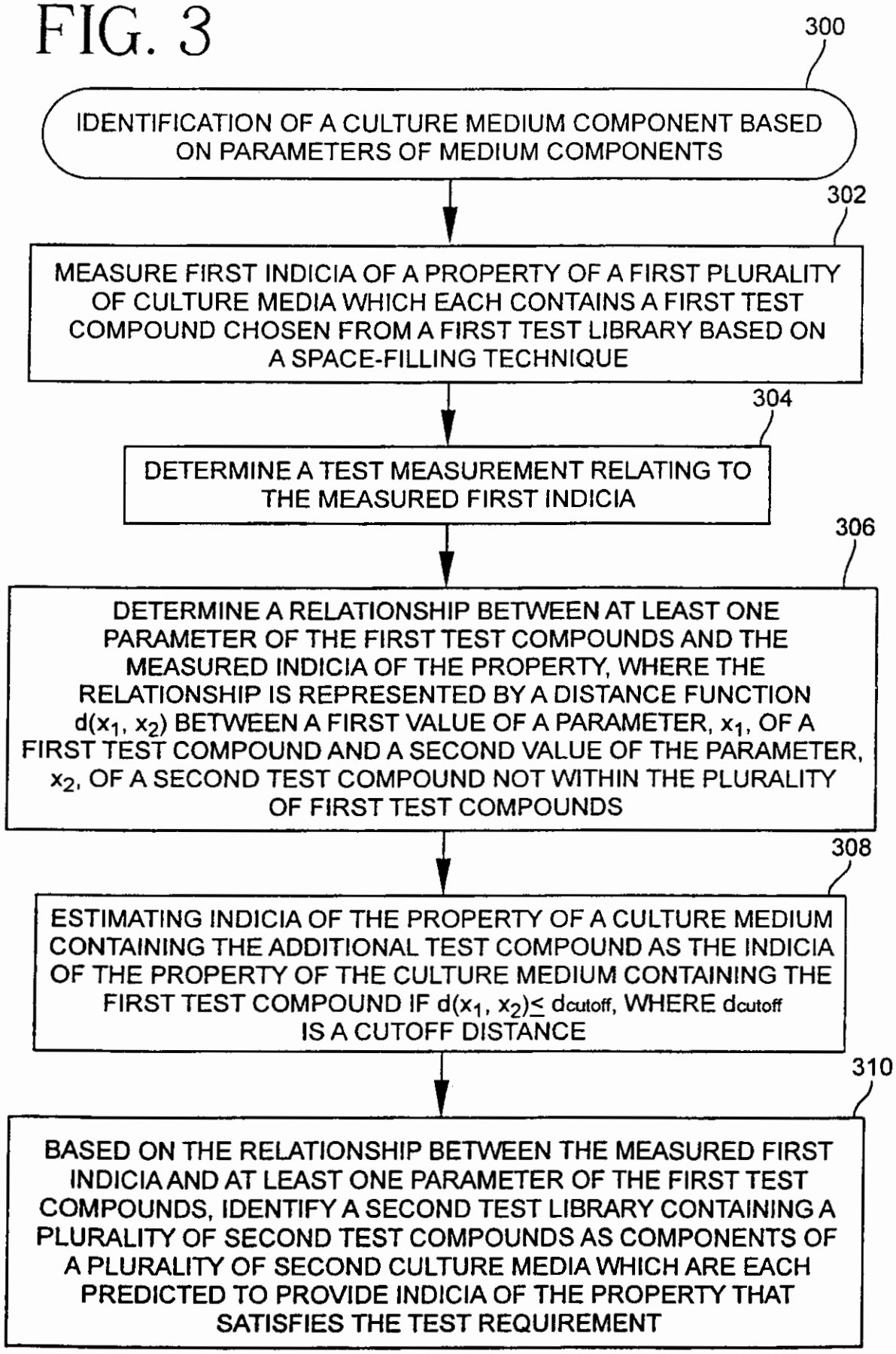

300
IDENTIFICATION OF A CULTURE MEDIUM COMPONENT BASED ON PARAMETERS OF MEDIUM COMPONENTS
302
MEASURE FIRST INDICIA OF A PROPERTY OF A FIRST PLURALITY OF CULTURE MEDIA WHICH EACH CONTAINS A FIRST TEST COMPOUND CHOSEN FROM A FIRST TEST LIBRARY BASED ON A SPACE-FILLING TECHNIQUE
304
DETERMINE A TEST MEASUREMENT RELATING TO THE MEASURED FIRST INDICIA
306
DETERMINE A RELATIONSHIP BETWEEN AT LEAST ONE PARAMETER OF THE FIRST TEST COMPOUNDS AND THE MEASURED INDICIA OF THE PROPERTY, WHERE THE RELATIONSHIP IS REPRESENTED BY A DISTANCE FUNCTION $d(x_1, x_2)$ BETWEEN A FIRST VALUE OF A PARAMETER, x_1, OF A FIRST TEST COMPOUND AND A SECOND VALUE OF THE PARAMETER, x_2, OF A SECOND TEST COMPOUND NOT WITHIN THE PLURALITY OF FIRST TEST COMPOUNDS
308
ESTIMATING INDICIA OF THE PROPERTY OF A CULTURE MEDIUM CONTAINING THE ADDITIONAL TEST COMPOUND AS THE INDICIA OF THE PROPERTY OF THE CULTURE MEDIUM CONTAINING THE FIRST TEST COMPOUND IF $d(x_1, x_2) \leq d_{cutoff}$, WHERE d_{cutoff} IS A CUTOFF DISTANCE
310
BASED ON THE RELATIONSHIP BETWEEN THE MEASURED FIRST INDICIA AND AT LEAST ONE PARAMETER OF THE FIRST TEST COMPOUNDS, IDENTIFY A SECOND TEST LIBRARY CONTAINING A PLURALITY OF SECOND TEST COMPOUNDS AS COMPONENTS OF A PLURALITY OF SECOND CULTURE MEDIA WHICH ARE EACH PREDICTED TO PROVIDE INDICIA OF THE PROPERTY THAT SATISFIES THE TEST REQUIREMENT

FIG. 4A

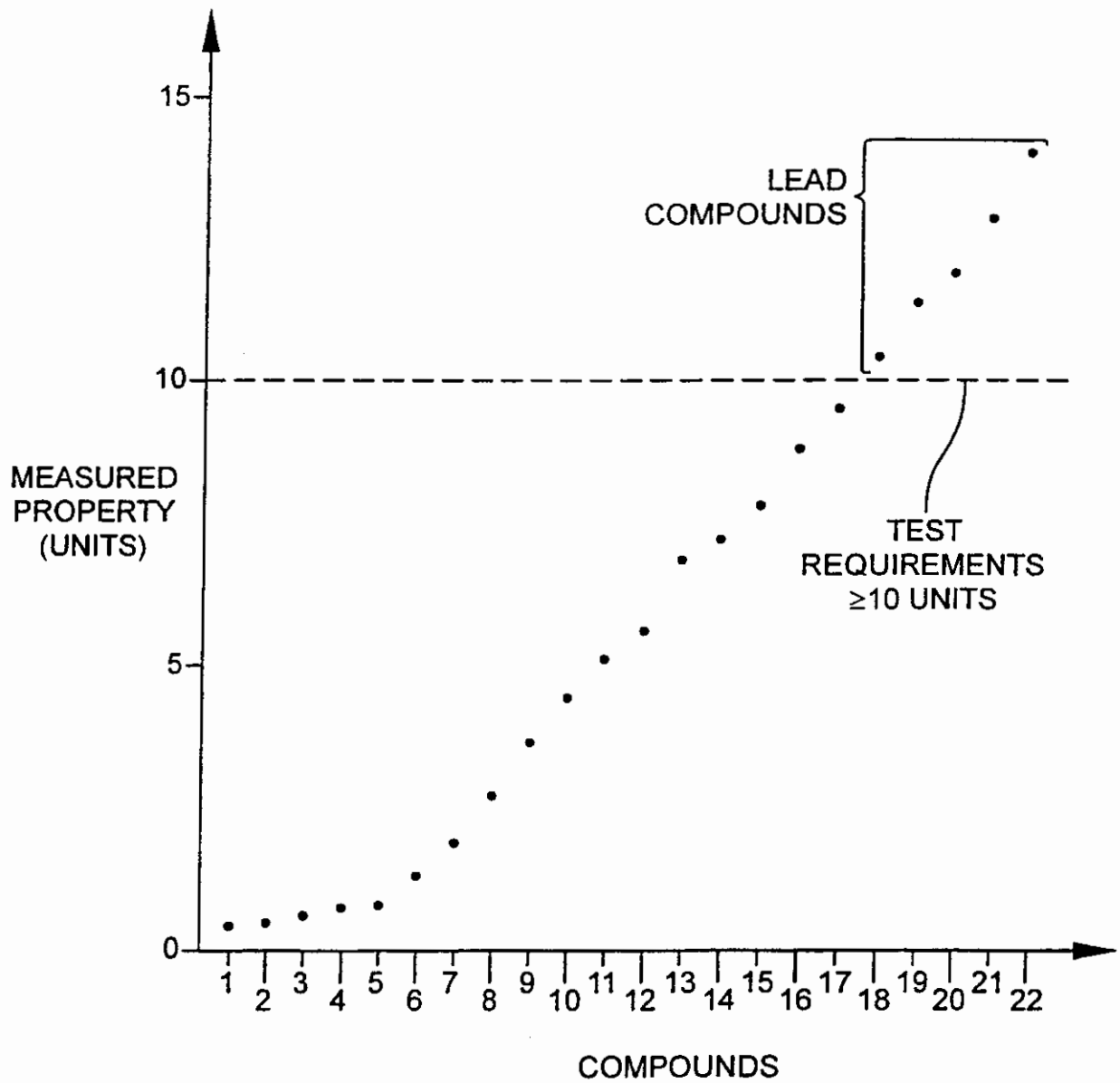

15
10
5
0
MEASURED PROPERTY (UNITS)
LEAD COMPOUNDS
TEST REQUIREMENTS ≥10 UNITS
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
COMPOUNDS

FIG. 4B

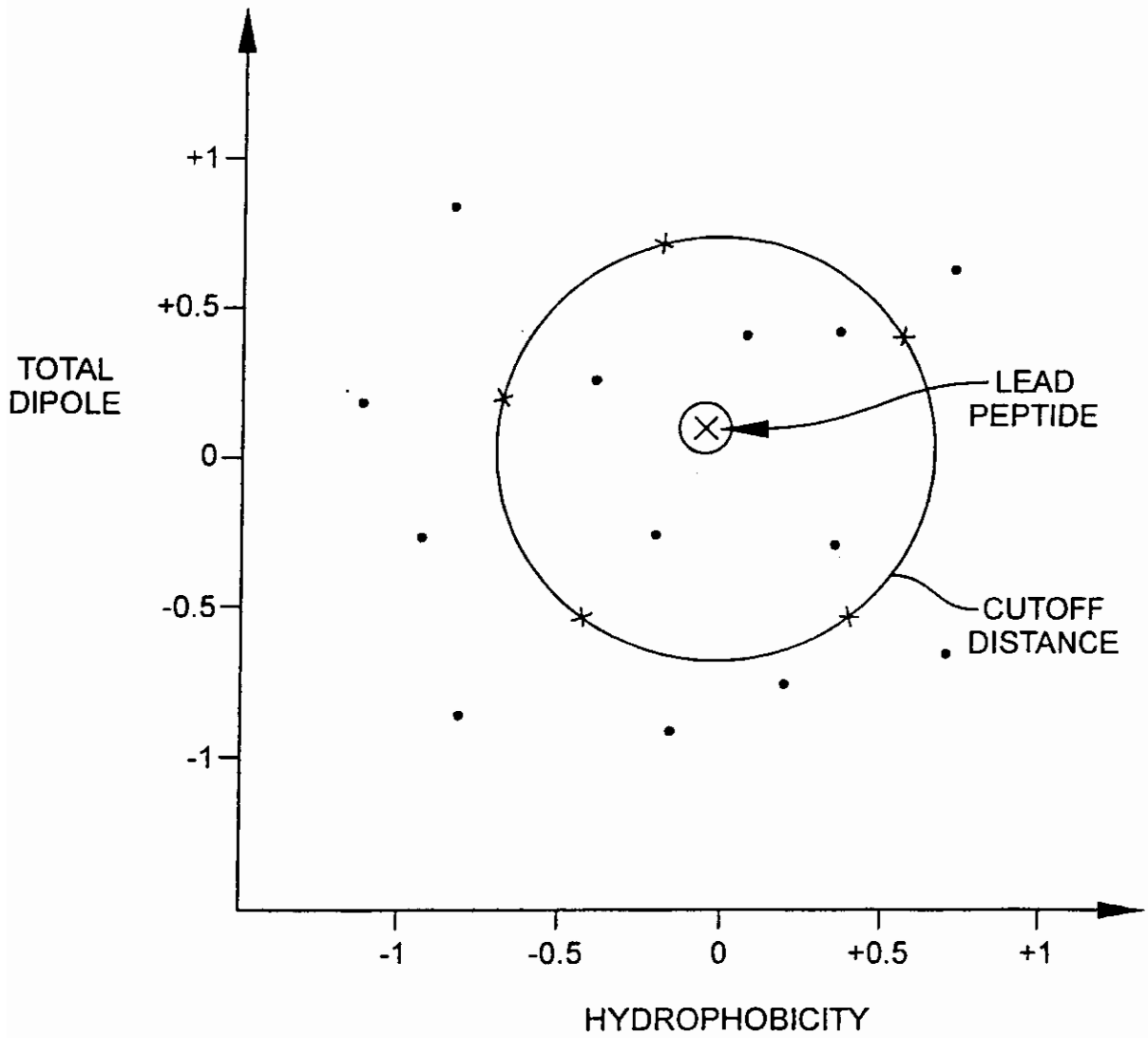

TOTAL DIPOLE
+1
+0.5
0
-0.5
-1
-1
-0.5
0
+0.5
+1
HYDROPHOBICITY
LEAD PEPTIDE
CUTOFF DISTANCE

FIG. 5

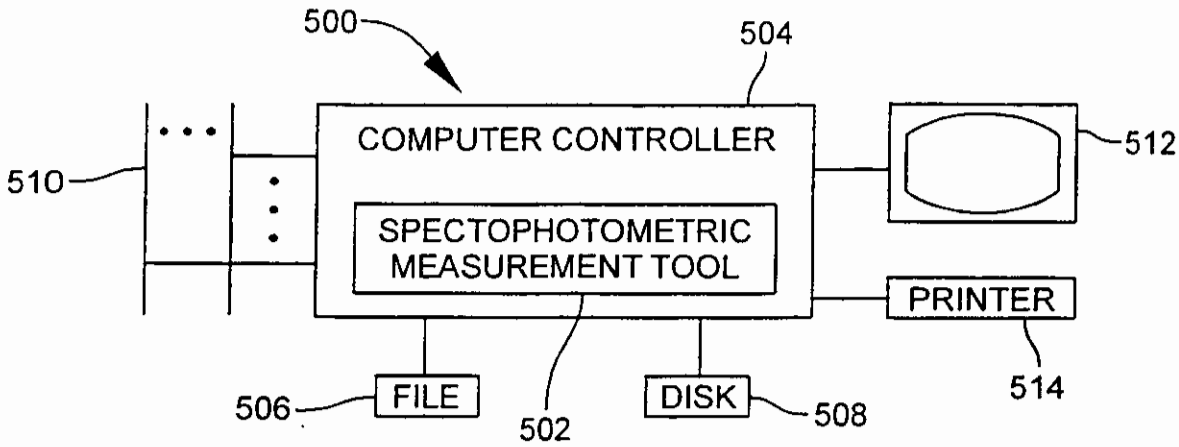

500
504
COMPUTER CONTROLLER
SPECTOPHOTOMETRIC MEASUREMENT TOOL
510
512
PRINTER
514
506
FILE
502
DISK
508

FIG. 6

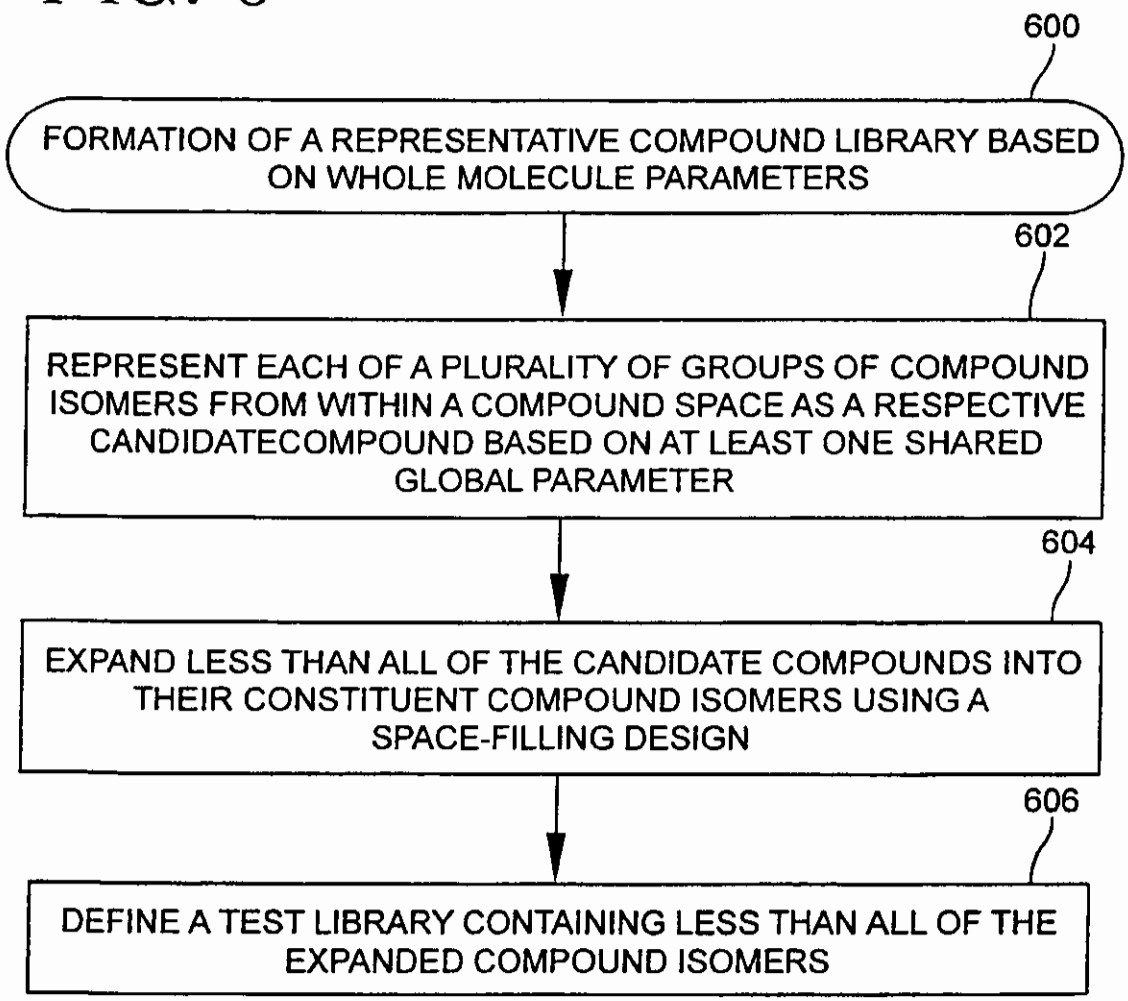

600
FORMATION OF A REPRESENTATIVE COMPOUND LIBRARY BASED ON WHOLE MOLECULE PARAMETERS
602
REPRESENT EACH OF A PLURALITY OF GROUPS OF COMPOUND ISOMERS FROM WITHIN A COMPOUND SPACE AS A RESPECTIVE CANDIDATECOMPOUND BASED ON AT LEAST ONE SHARED GLOBAL PARAMETER
604
EXPAND LESS THAN ALL OF THE CANDIDATE COMPOUNDS INTO THEIR CONSTITUENT COMPOUND ISOMERS USING A SPACE-FILLING DESIGN
606
DEFINE A TEST LIBRARY CONTAINING LESS THAN ALL OF THE EXPANDED COMPOUND ISOMERS

FIG. 7

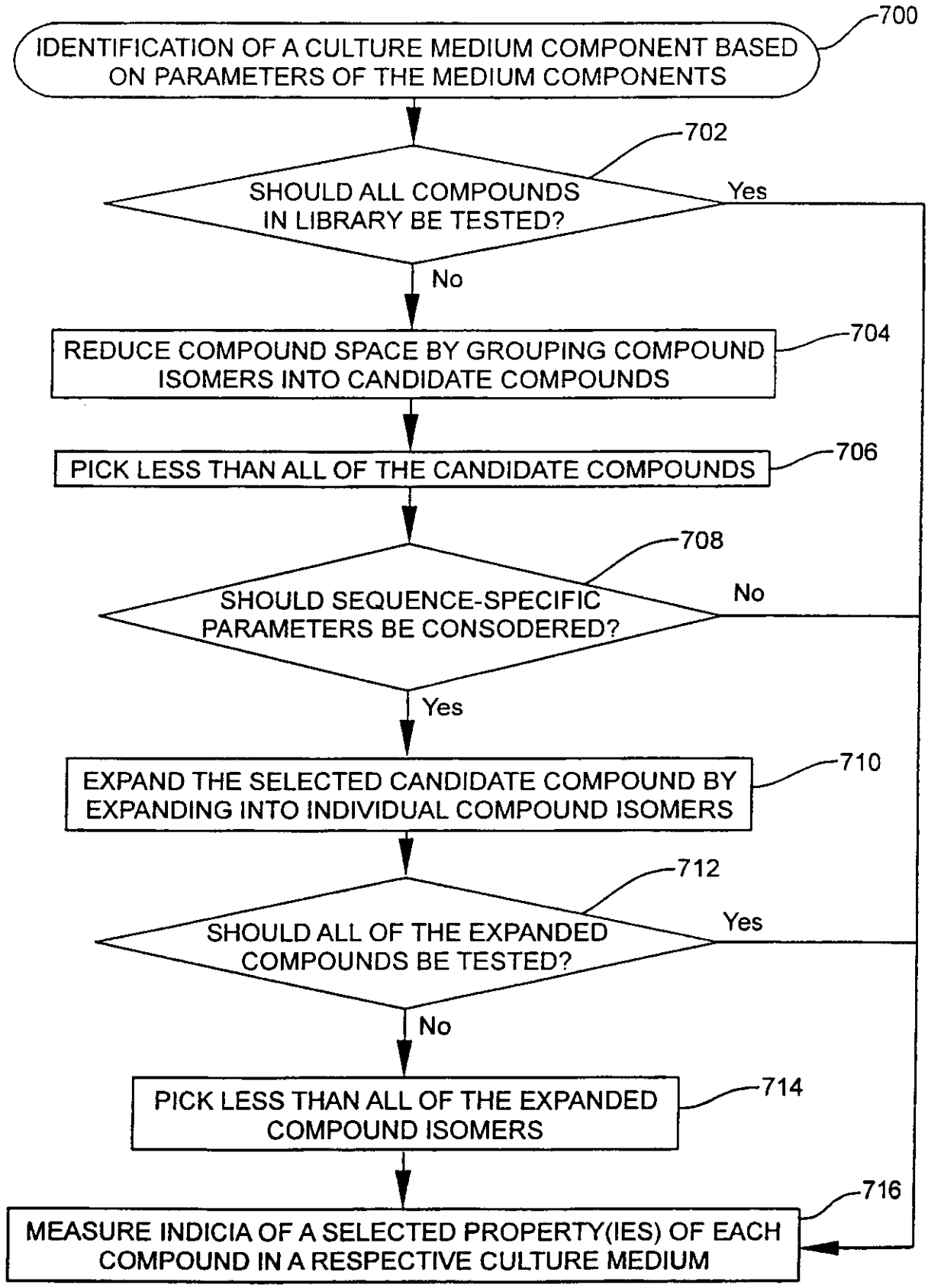
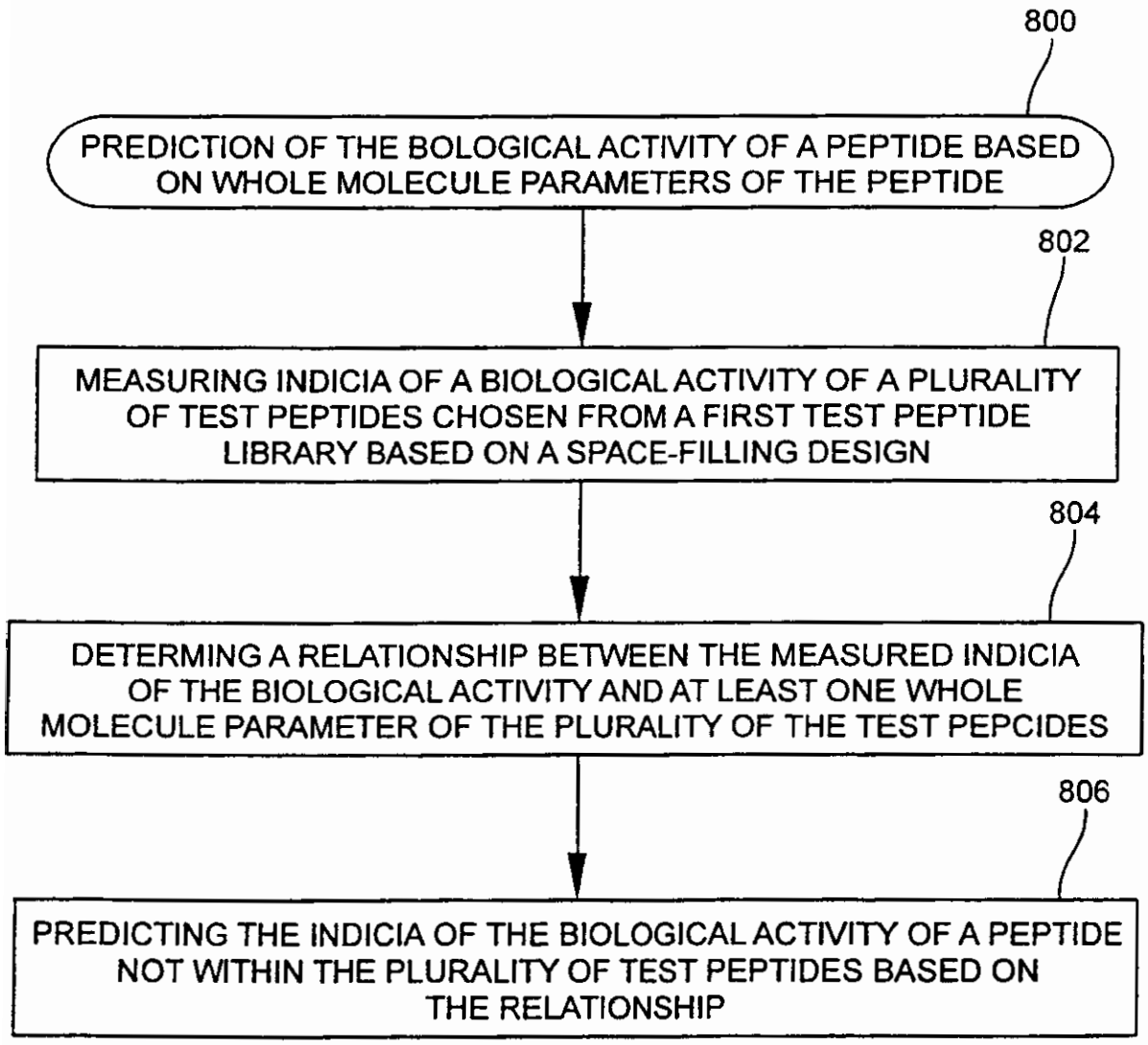

700
IDENTIFICATION OF A CULTURE MEDIUM COMPONENT BASED ON PARAMETERS OF THE MEDIUM COMPONENTS
702
SHOULD ALL COMPOUNDS IN LIBRARY BE TESTED?
Yes
No
704
REDUCE COMPOUND SPACE BY GROUPING COMPOUND ISOMERS INTO CANDIDATE COMPOUNDS
706
PICK LESS THAN ALL OF THE CANDIDATE COMPOUNDS
708
SHOULD SEQUENCE-SPECIFIC PARAMETERS BE CONSODERED?
No
Yes
710
EXPAND THE SELECTED CANDIDATE COMPOUND BY EXPANDING INTO INDIVIDUAL COMPOUND ISOMERS
712
SHOULD ALL OF THE EXPANDED COMPOUNDS BE TESTED?
Yes
No
714
PICK LESS THAN ALL OF THE EXPANDED COMPOUND ISOMERS
716
MEASURE INDICIA OF A SELECTED PROPERTY(IES) OF EACH COMPOUND IN A RESPECTIVE CULTURE MEDIUM

FIG. 8


800
PREDICTION OF THE BOLOGICAL ACTIVITY OF A PEPTIDE BASED ON WHOLE MOLECULE PARAMETERS OF THE PEPTIDE
802
MEASURING INDICIA OF A BIOLOGICAL ACTIVITY OF A PLURALITY OF TEST PEPTIDES CHOSEN FROM A FIRST TEST PEPTIDE LIBRARY BASED ON A SPACE-FILLING DESIGN
804
DETERMING A RELATIONSHIP BETWEEN THE MEASURED INDICIA OF THE BIOLOGICAL ACTIVITY AND AT LEAST ONE WHOLE MOLECULE PARAMETER OF THE PLURALITY OF THE TEST PEPCIDES
806
PREDICTING THE INDICIA OF THE BIOLOGICAL ACTIVITY OF A PEPTIDE NOT WITHIN THE PLURALITY OF TEST PEPTIDES BASED ON THE RELATIONSHIP