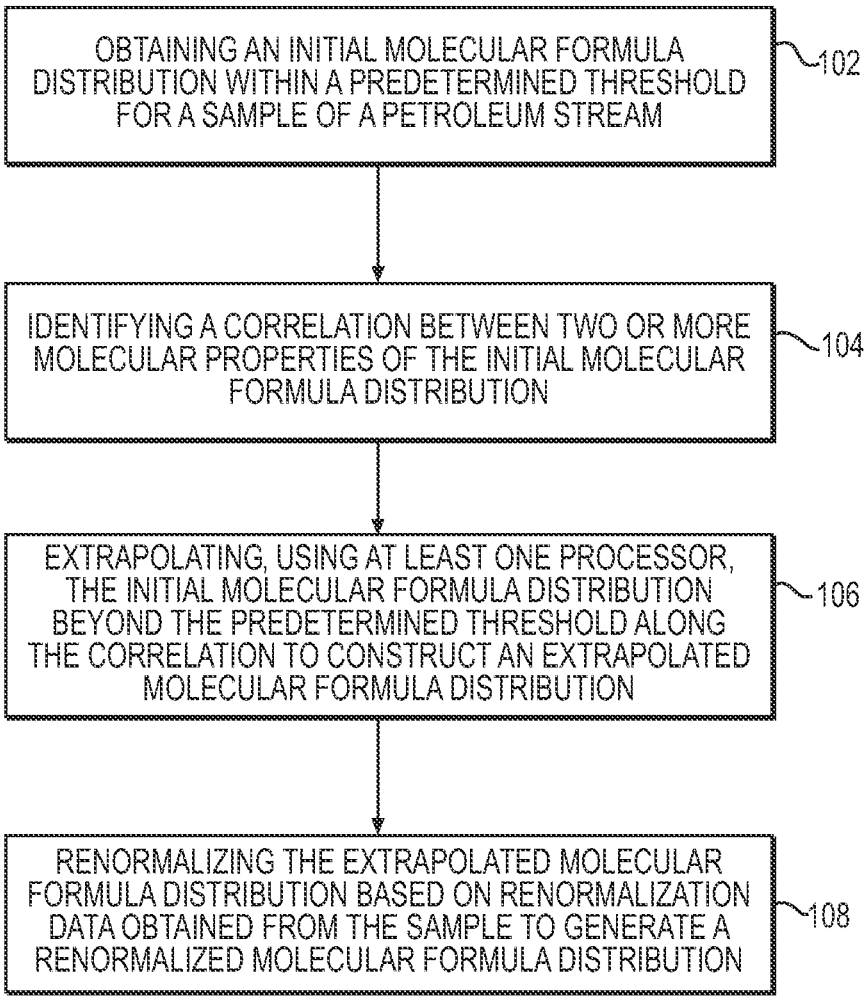
OBTAINING AN INITIAL MOLECULAR FORMULA DISTRIBUTION WITHIN A PREDETERMINED THRESHOLD FOR A SAMPLE OF A PETROLEUM STREAM
102
IDENTIFYING A CORRELATION BETWEEN TWO OR MORE MOLECULAR PROPERTIES OF THE INITIAL MOLECULAR FORMULA DISTRIBUTION
104
EXTRAPOLATING, USING AT LEAST ONE PROCESSOR, THE INITIAL MOLECULAR FORMULA DISTRIBUTION BEYOND THE PREDETERMINED THRESHOLD ALONG THE CORRELATION TO CONSTRUCT AN EXTRAPOLATED MOLECULAR FORMULA DISTRIBUTION
106
RENORMALIZING THE EXTRAPOLATED MOLECULAR FORMULA DISTRIBUTION BASED ON RENORMALIZATION DATA OBTAINED FROM THE SAMPLE TO GENERATE A RENORMALIZED MOLECULAR FORMULA DISTRIBUTION
108

FIG. 1

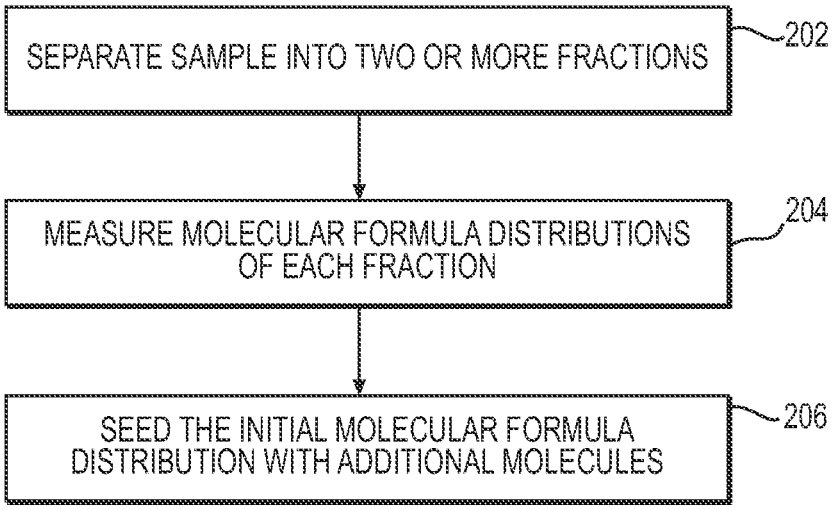
SEPARATE SAMPLE INTO TWO OR MORE FRACTIONS
202
MEASURE MOLECULAR FORMULA DISTRIBUTIONS OF EACH FRACTION
204
SEED THE INITIAL MOLECULAR FORMULA DISTRIBUTION WITH ADDITIONAL MOLECULES
206

FIG. 2

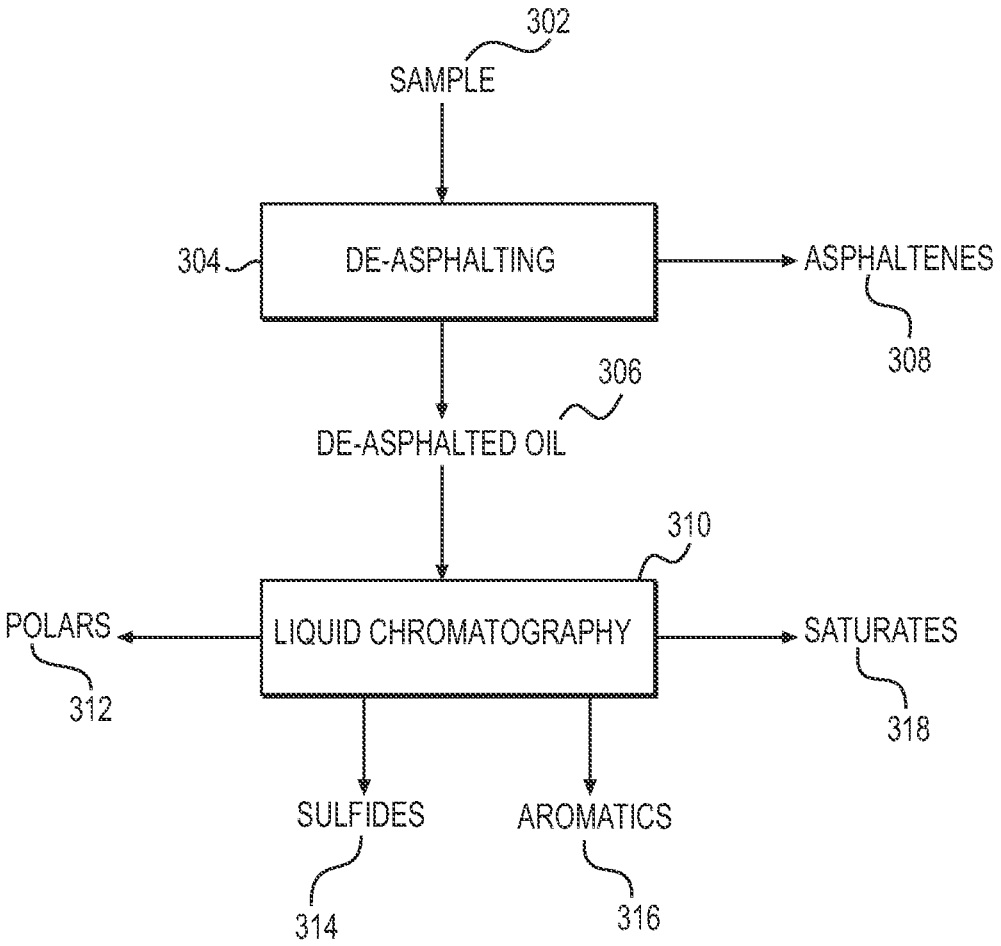
302
SAMPLE
304
DE-ASPHALTING
ASPHALTENES
308
306
DE-ASPHALTED OIL
310
POLARS
LIQUID CHROMATOGRAPHY
SATURATES
312
318
SULFIDES
AROMATICS
314
316

FIG. 3

MOLECULAR ABUNDANCE MAP OF ARAB MEDIUM' VACUUM RESID UN-EXTRAPOLATED FTICR-MS AND FDMS DATA (DAO SATURATES ONLY)

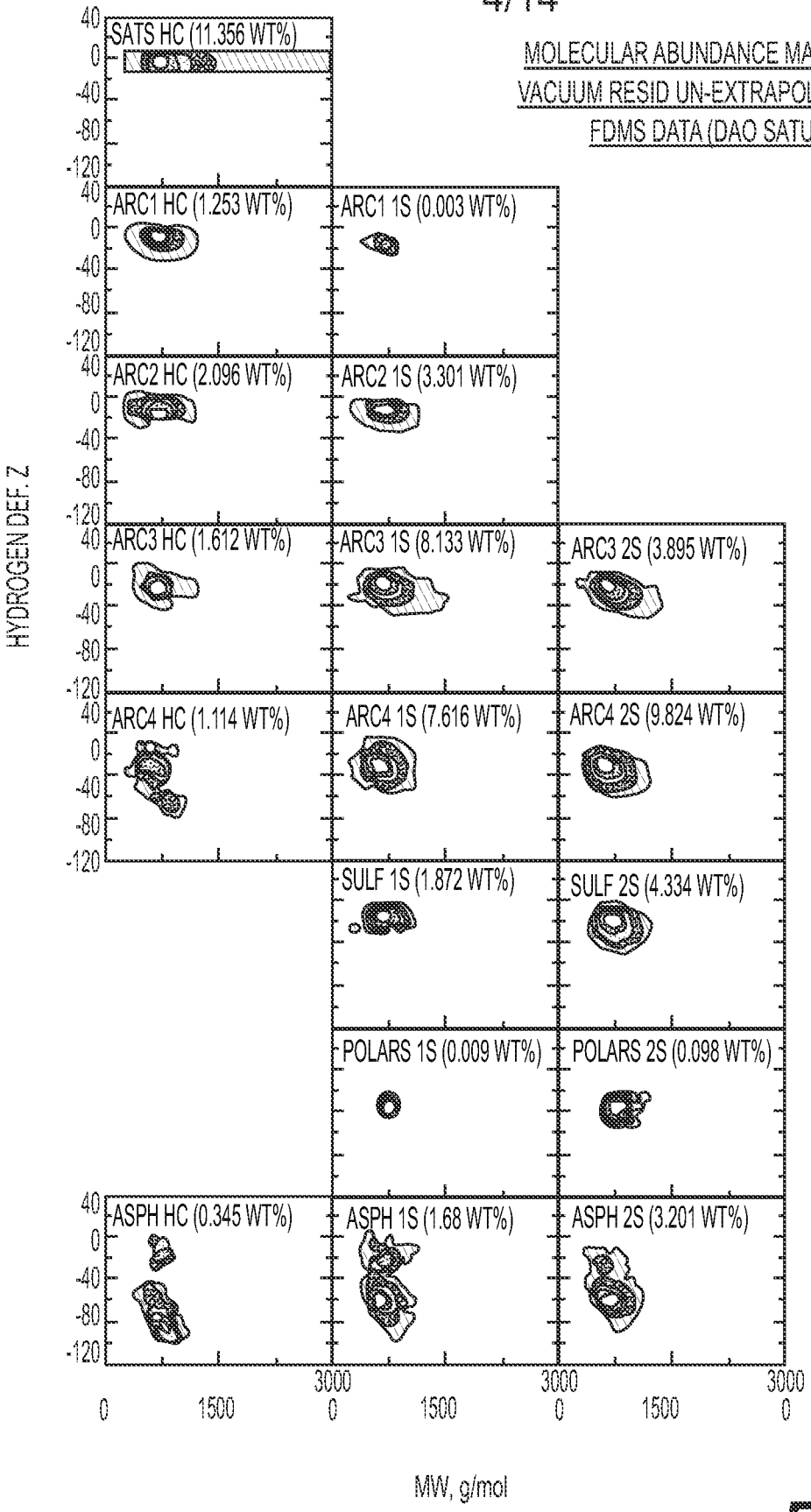

FIG. 4

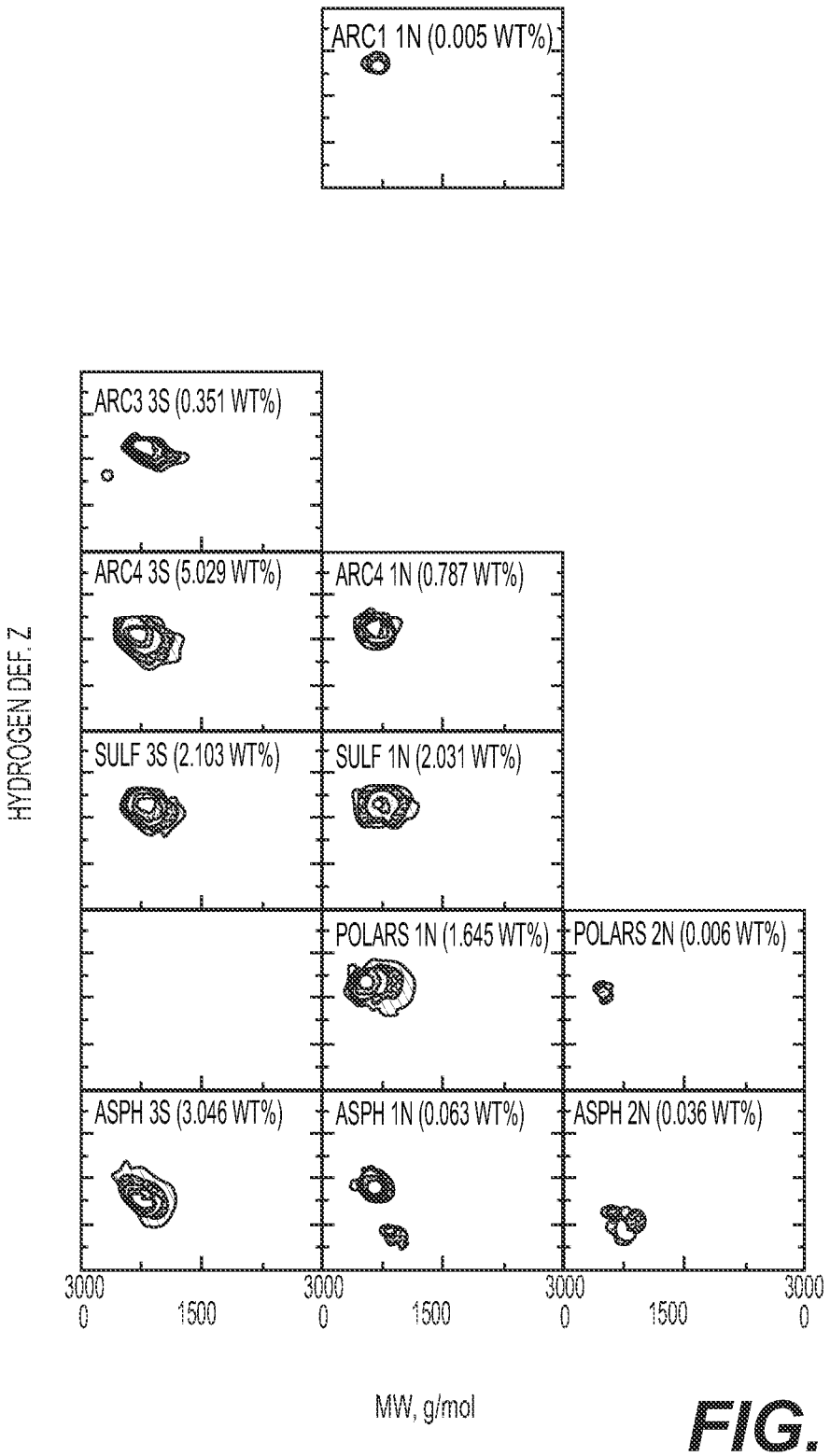

FIG. 4
CONTINUED-1

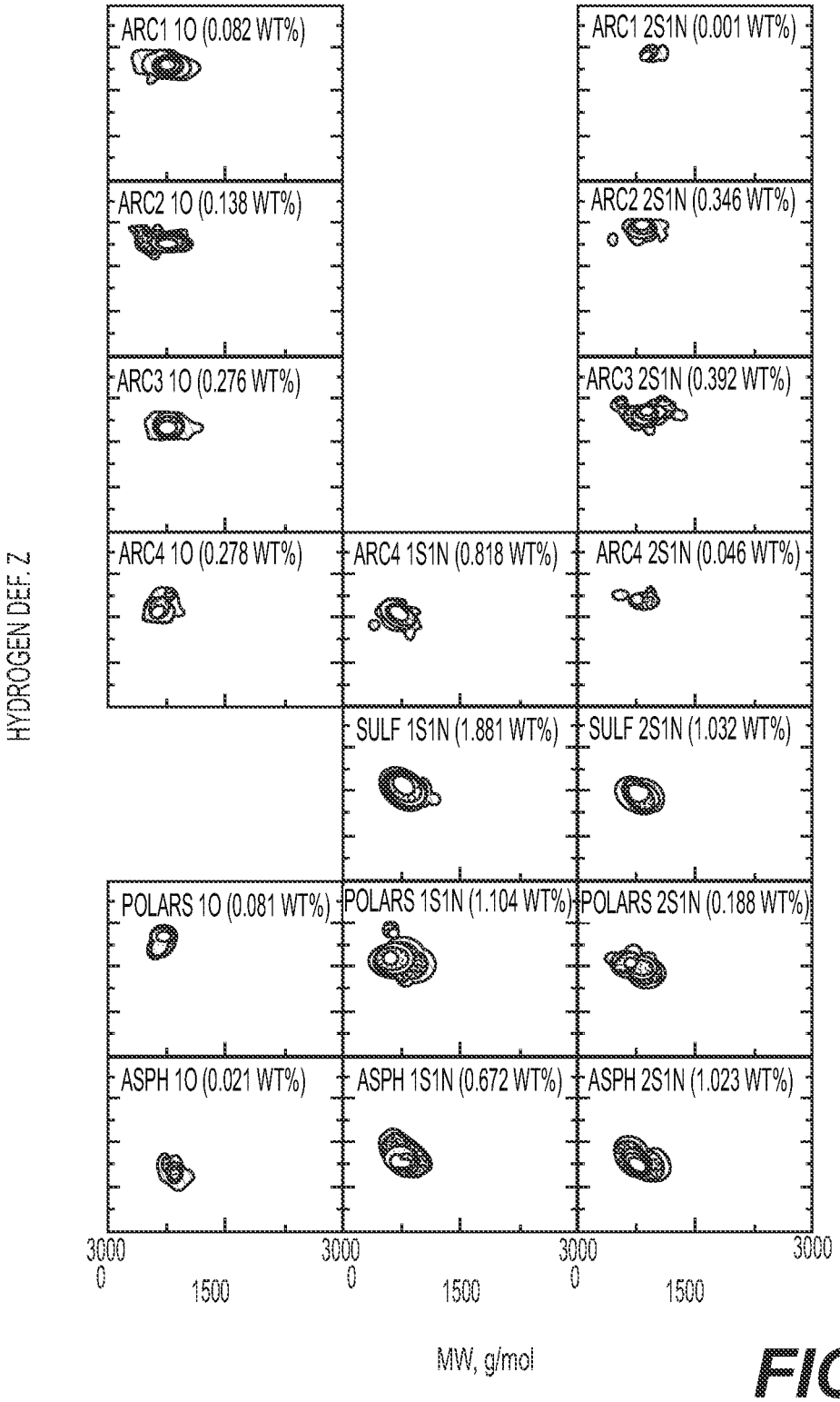

FIG. 4
CONTINUED-2

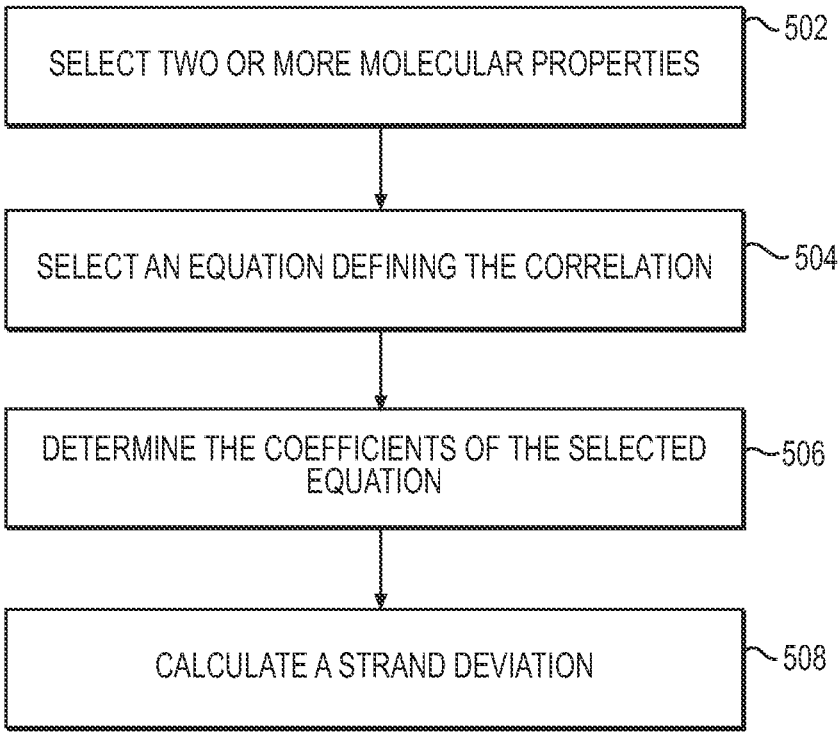
SELECT TWO OR MORE MOLECULAR PROPERTIES
502
SELECT AN EQUATION DEFINING THE CORRELATION
504
DETERMINE THE COEFFICIENTS OF THE SELECTED EQUATION
506
CALCULATE A STRAND DEVIATION
508

FIG. 5

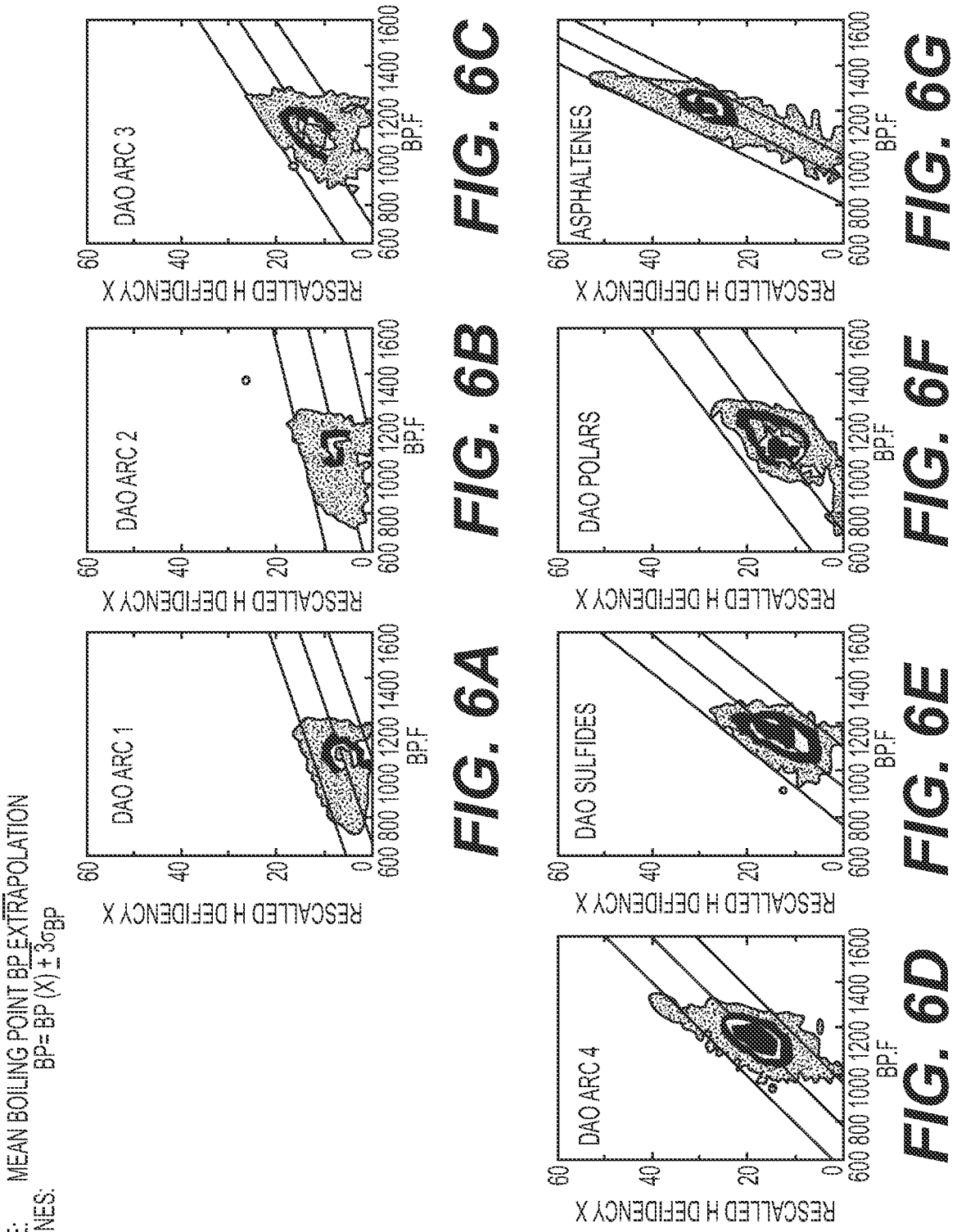

FIG. 6A FIG. 6B FIG. 6C

FIG. 6D FIG. 6E FIG. 6F FIG. 6G

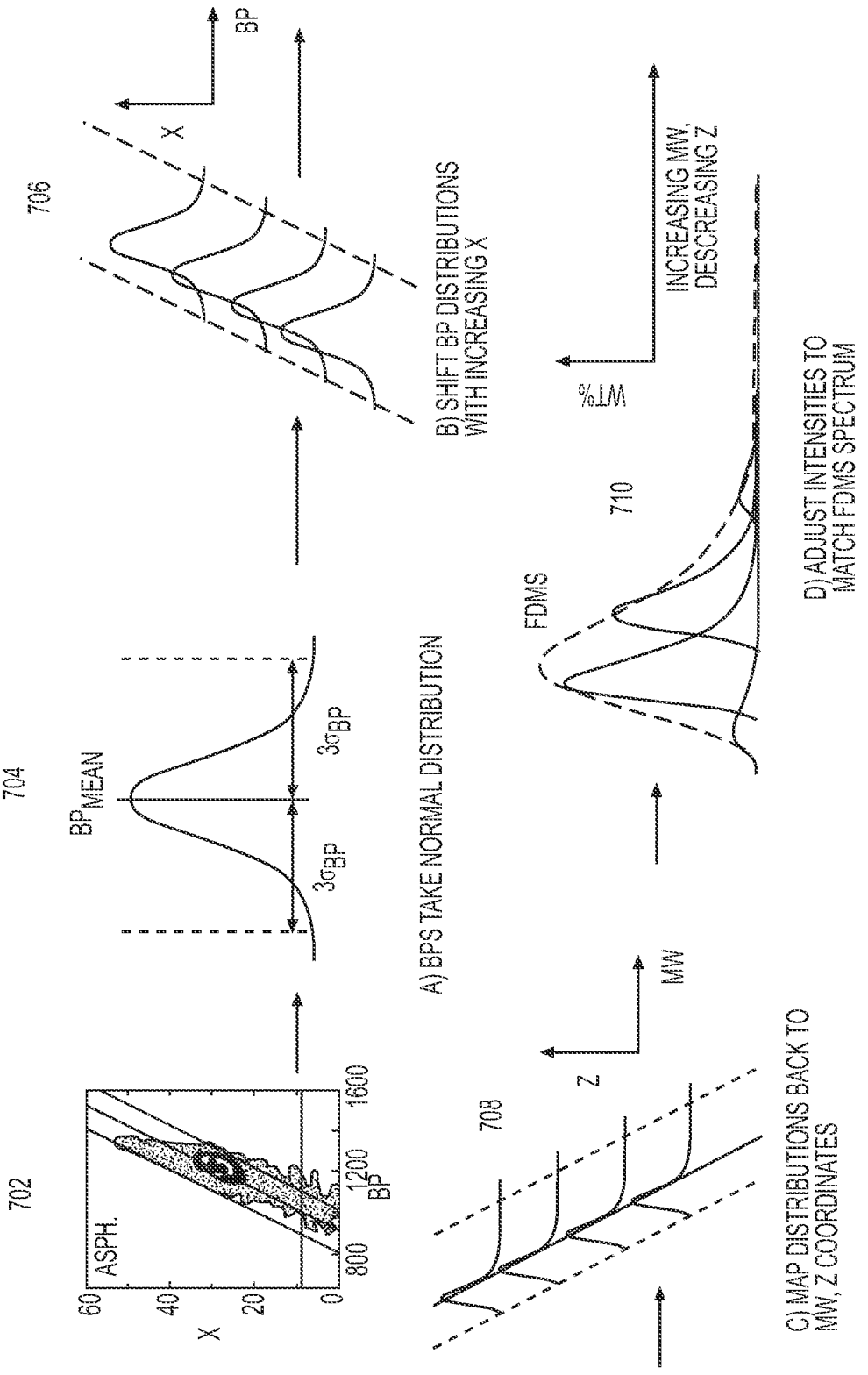
702
ASPH.
60
40
20
0
X
800
1200
1600
BP
704
BP_MEAN
3σ_BP
3σ_BP
A) BPS TAKE NORMAL DISTRIBUTION
706
X
BP
B) SHIFT BP DISTRIBUTIONS WITH INCREASING X
708
Z
MW
C) MAP DISTRIBUTIONS BACK TO MW, Z COORDINATES
FDMS
710
WT%
INCREASING MW, DESCREASING Z
D) ADJUST INTENSITIES TO MATCH FDMS SPECTRUM

FIG. 7

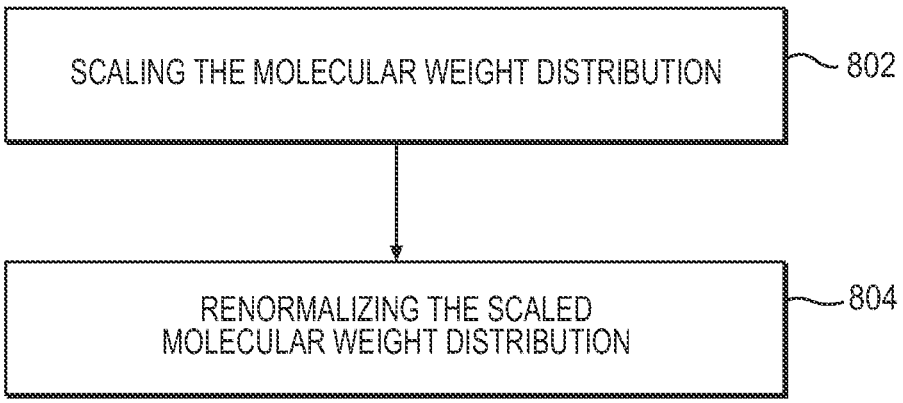
SCALING THE MOLECULAR WEIGHT DISTRIBUTION
802
RENORMALIZING THE SCALED MOLECULAR WEIGHT DISTRIBUTION
804

FIG. 8

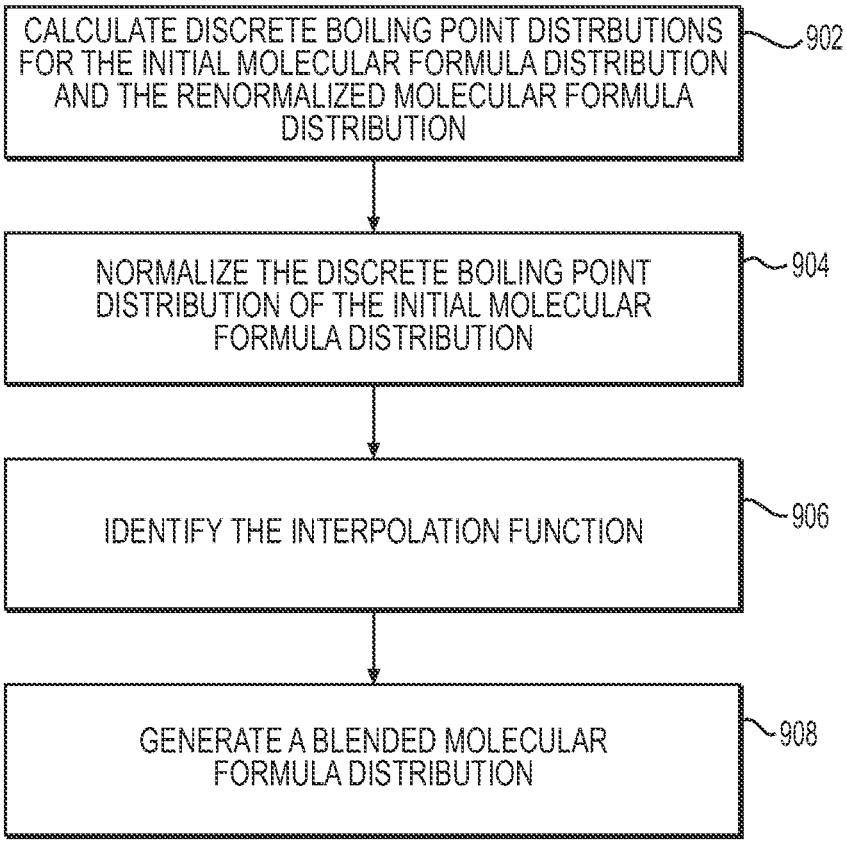
CALCULATE DISCRETE BOILING POINT DISTRBUTIONS FOR THE INITIAL MOLECULAR FORMULA DISTRIBUTION AND THE RENORMALIZED MOLECULAR FORMULA DISTRIBUTION
902
NORMALIZE THE DISCRETE BOILING POINT DISTRIBUTION OF THE INITIAL MOLECULAR FORMULA DISTRIBUTION
904
IDENTIFY THE INTERPOLATION FUNCTION
906
GENERATE A BLENDED MOLECULAR FORMULA DISTRIBUTION
908

FIG. 9

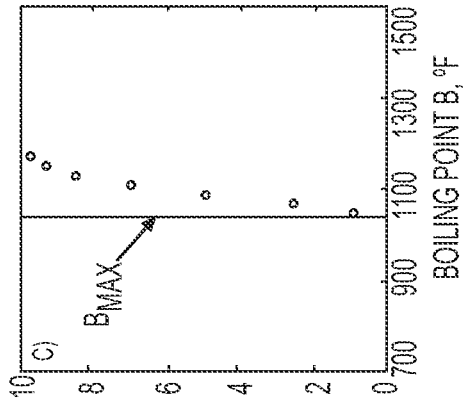

FIG. 10C

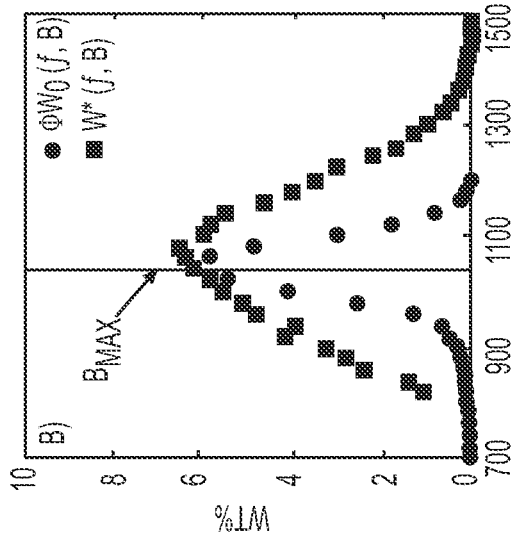

FIG. 10B

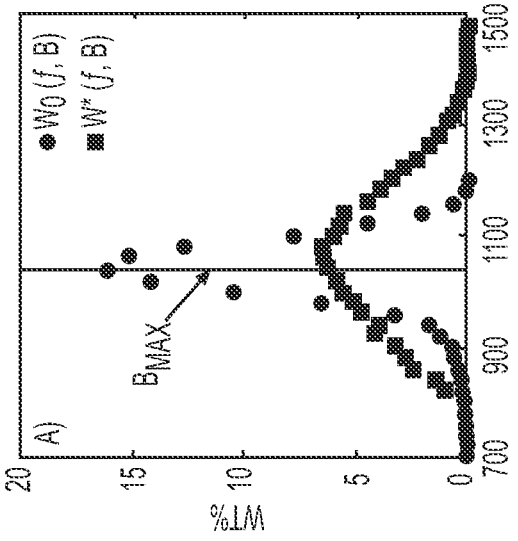

FIG. 10A

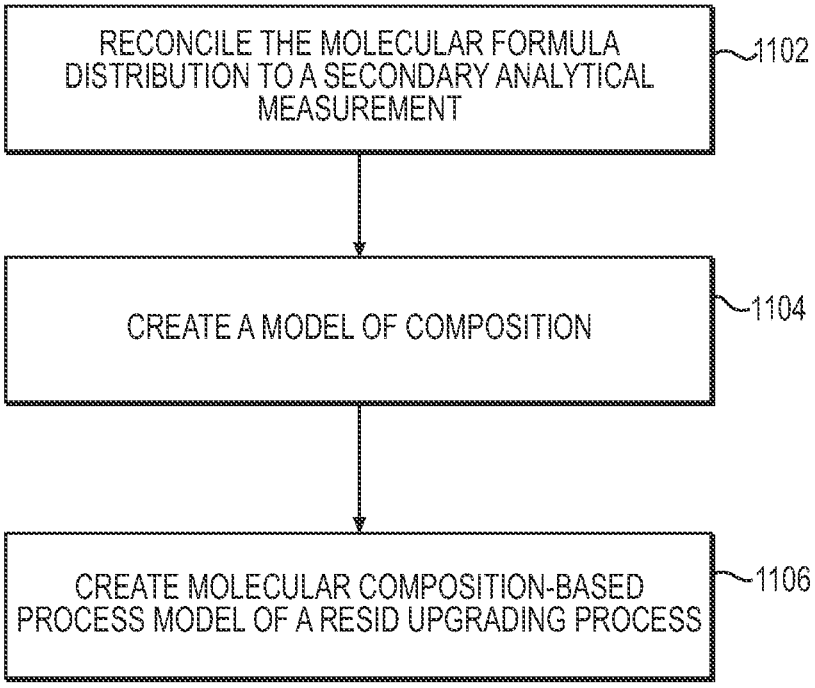
RECONCILE THE MOLECULAR FORMULA DISTRIBUTION TO A SECONDARY ANALYTICAL MEASUREMENT
1102
CREATE A MODEL OF COMPOSITION
1104
CREATE MOLECULAR COMPOSITION-BASED PROCESS MODEL OF A RESID UPGRADING PROCESS
1106

FIG. 11

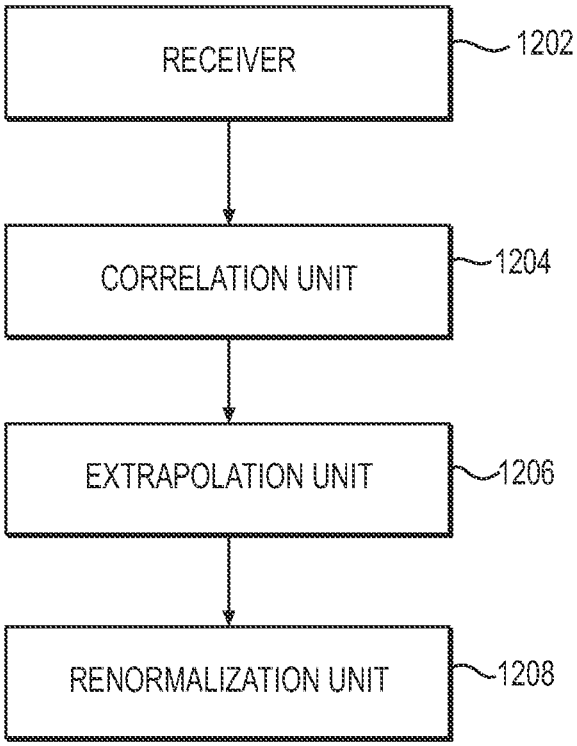
RECEIVER
1202
CORRELATION UNIT
1204
EXTRAPOLATION UNIT
1206
RENORMALIZATION UNIT
1208

FIG. 12