

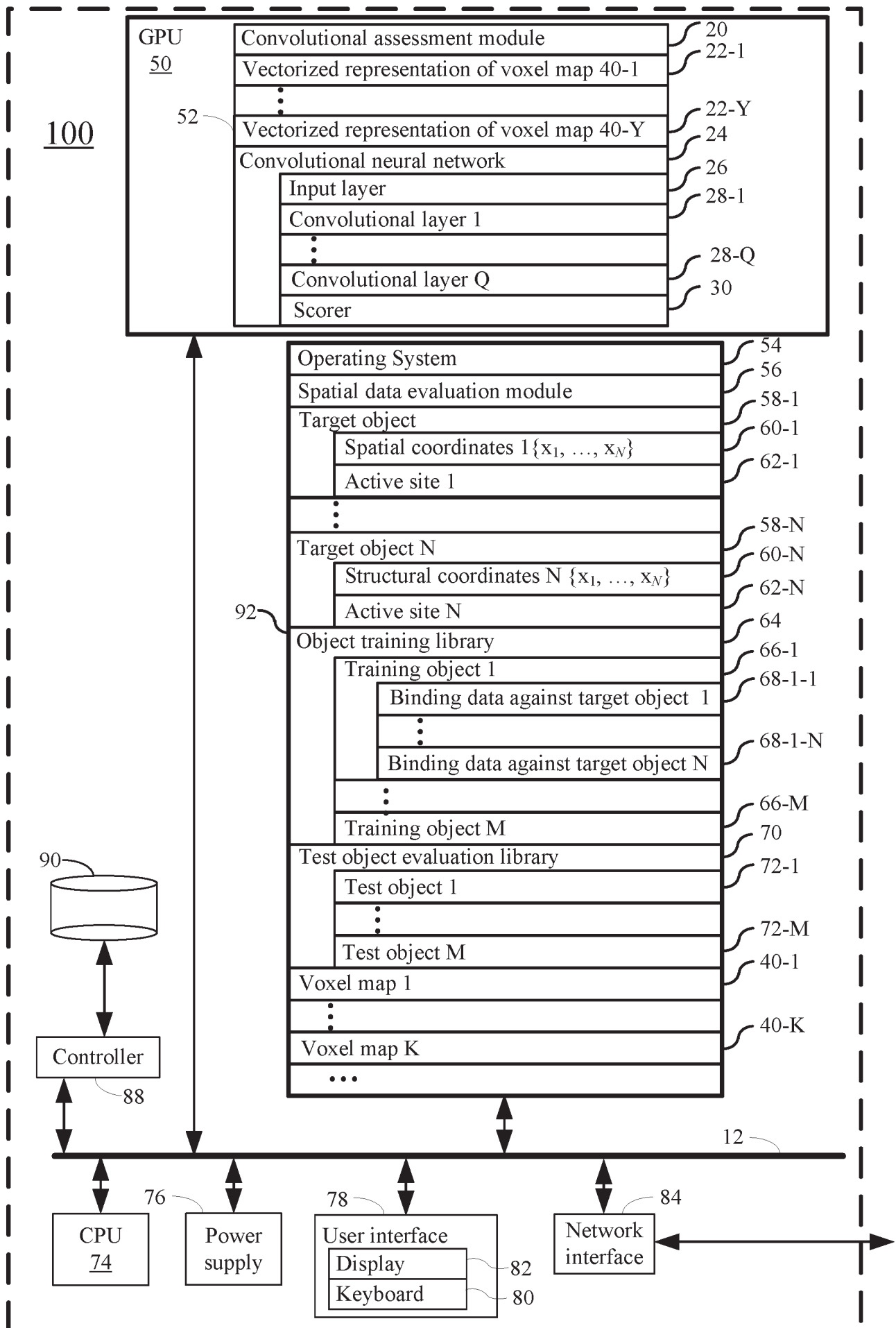


Fig. 1

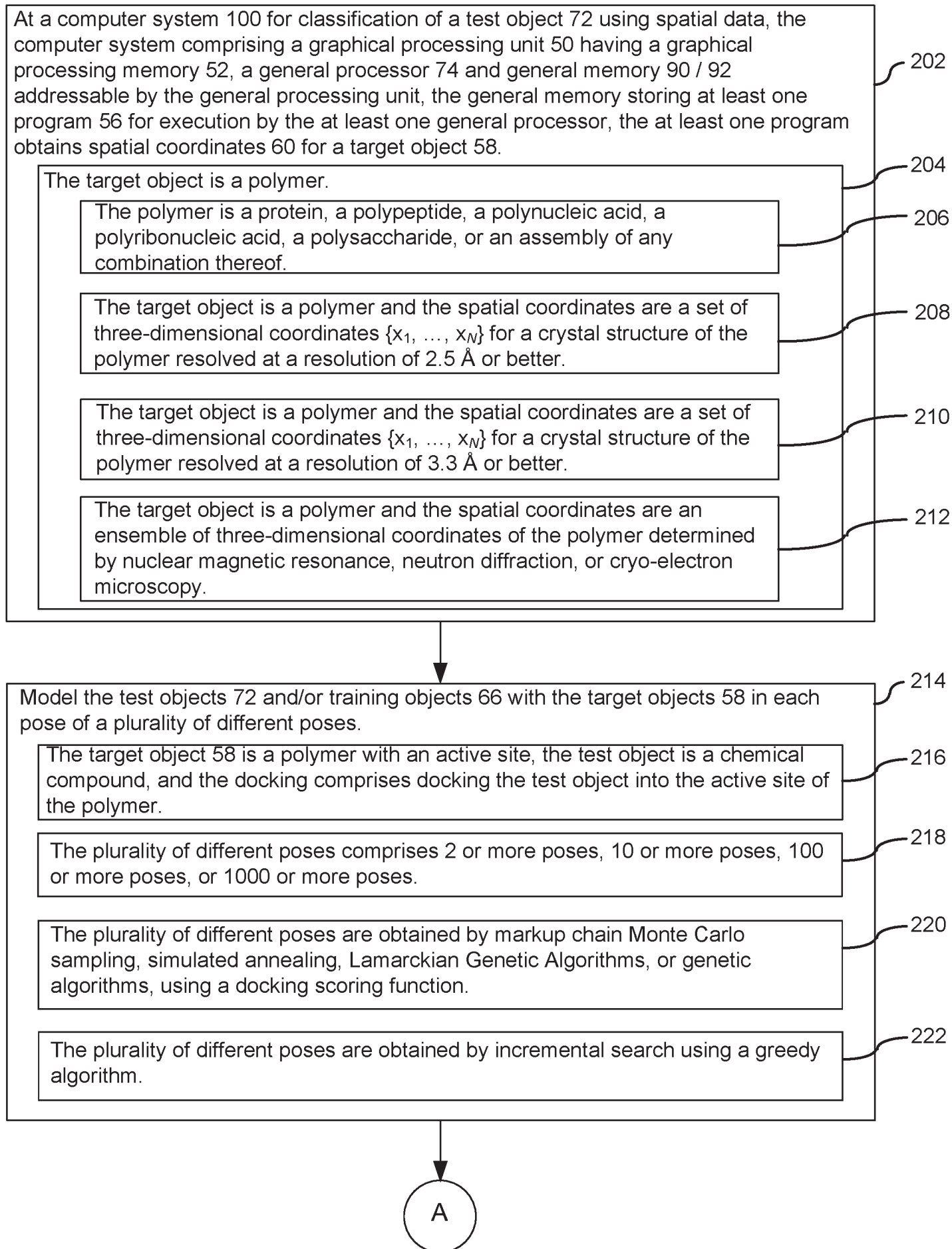


Fig. 2A

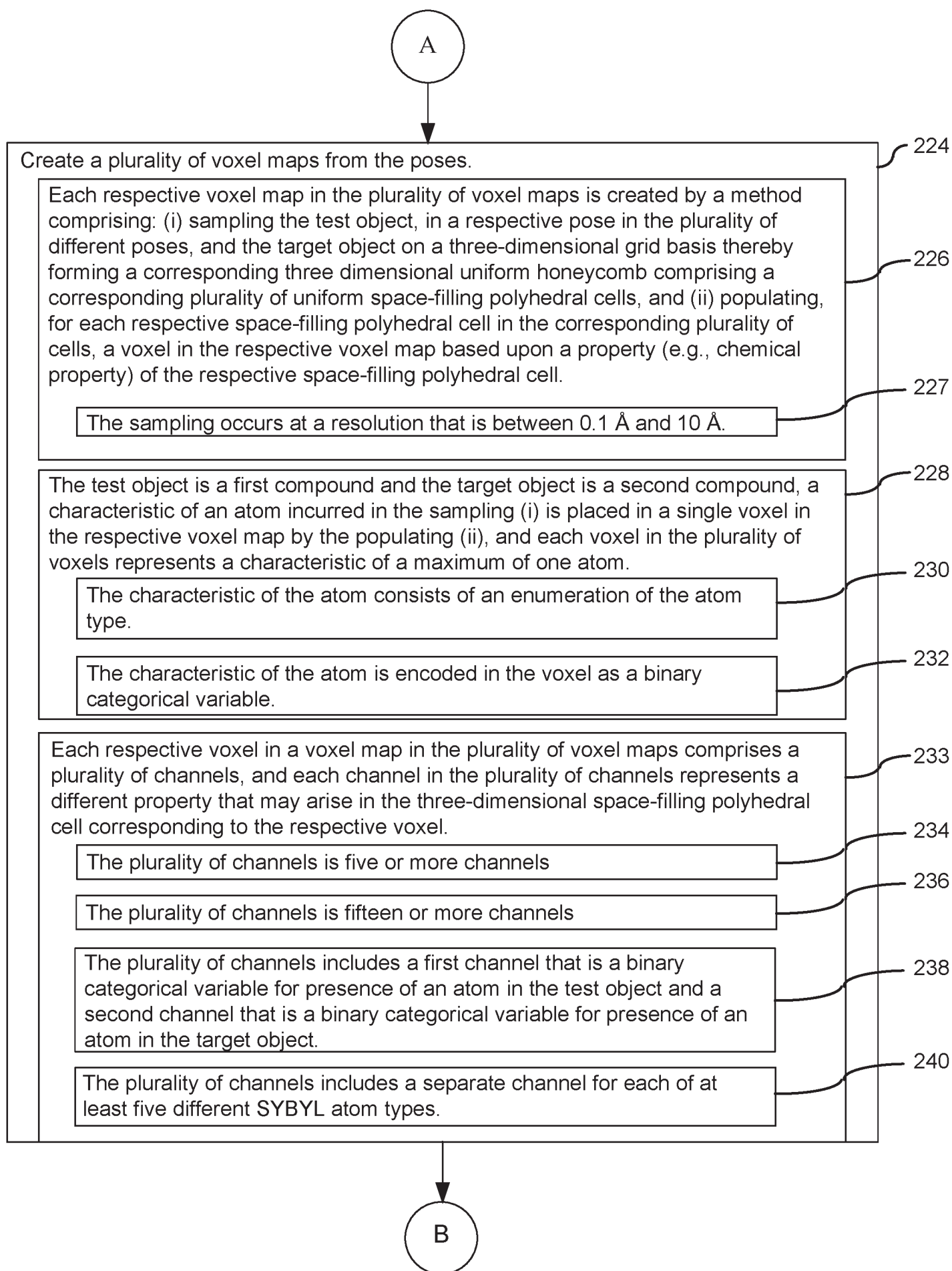


Fig. 2B

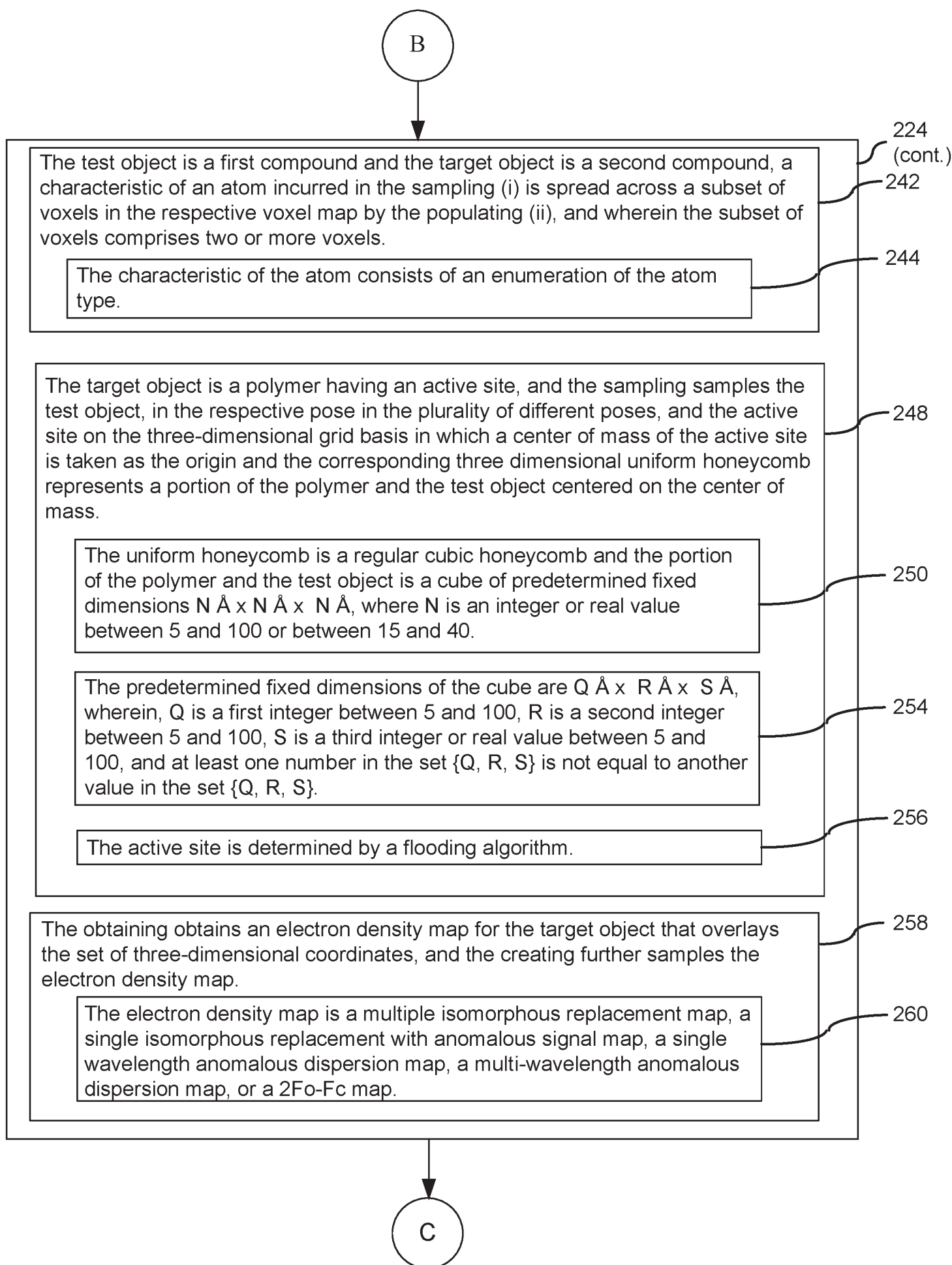


Fig. 2C

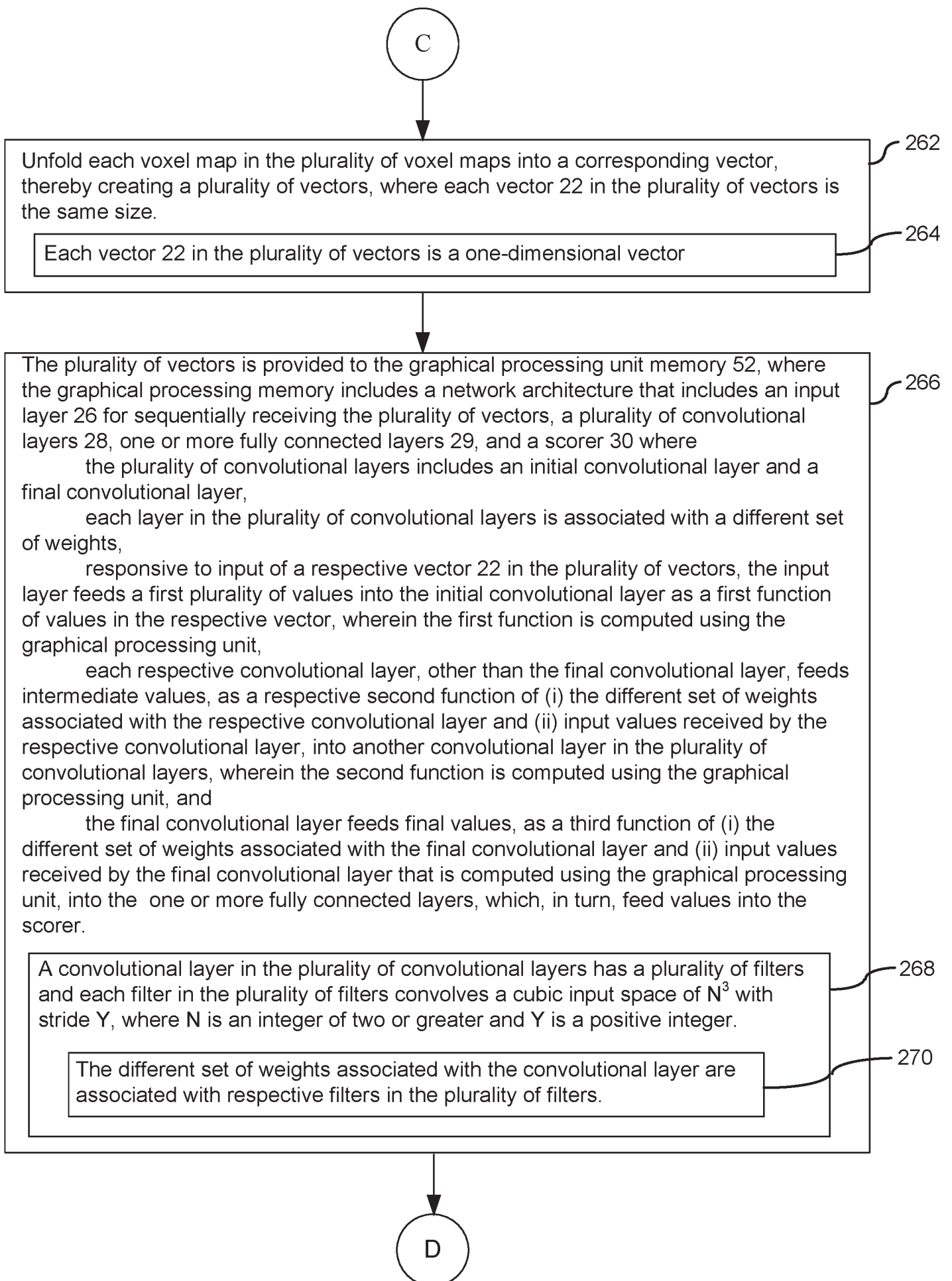


Fig. 2D

D

The scorer comprises a plurality of fully-connected layers and an evaluation layer where a fully-connected layer in the plurality of fully-connected layers feeds into the evaluation layer.

The scorer comprises a decision tree, a multiple additive regression tree, a clustering algorithm, principal component analysis, a nearest neighbor analysis, a linear discriminant analysis, a quadratic discriminant analysis, a support vector machine, an evolutionary method, a projection pursuit, or ensembles thereof

Obtaining a plurality of scores from the scorer, wherein each score in the plurality of scores corresponds to the input of a vector in the plurality of vectors into the input layer.

Use the plurality of scores to characterize the test object.

The test object is a chemical compound and using the plurality of scores to characterize the test object comprises taking a measure of central tendency of the plurality of scores. When the measure of central tendency satisfies a predetermined threshold value or predetermined threshold value range, the test object is deemed to have a first classification. When the measure of central tendency fails to satisfy the predetermined threshold value or predetermined threshold value range, the test object is deemed to have a second classification.

The using the plurality of scores to characterize the test object comprises taking a weighted average of the plurality of scores. When the weighted average satisfies a predetermined threshold value or predetermined threshold value range, the test object is deemed to have a first classification. When the measure of central tendency fails to satisfy the predetermined threshold value or predetermined threshold value range, the test object is deemed to have a second classification.

The weighted average is a Boltzman average of the plurality of scores.

The first classification is an IC50, EC50, Kd or KI for the test object with respect to the target object that is above a first binding value (e.g., one micromolar, ten micromolar, and the second classification is an IC50, EC50, or KI for the test object with respect to the target object that is below the first binding value.

E

Fig. 2E

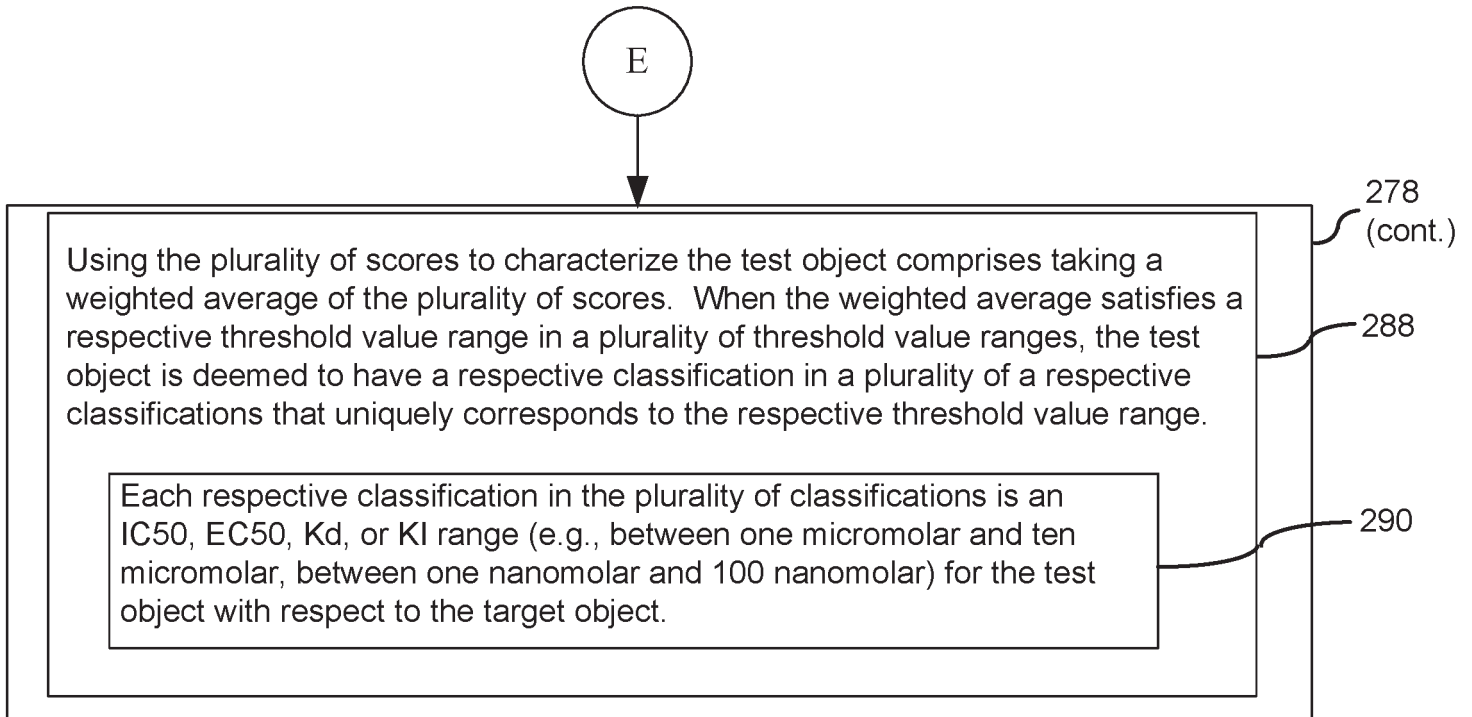


Fig. 2F

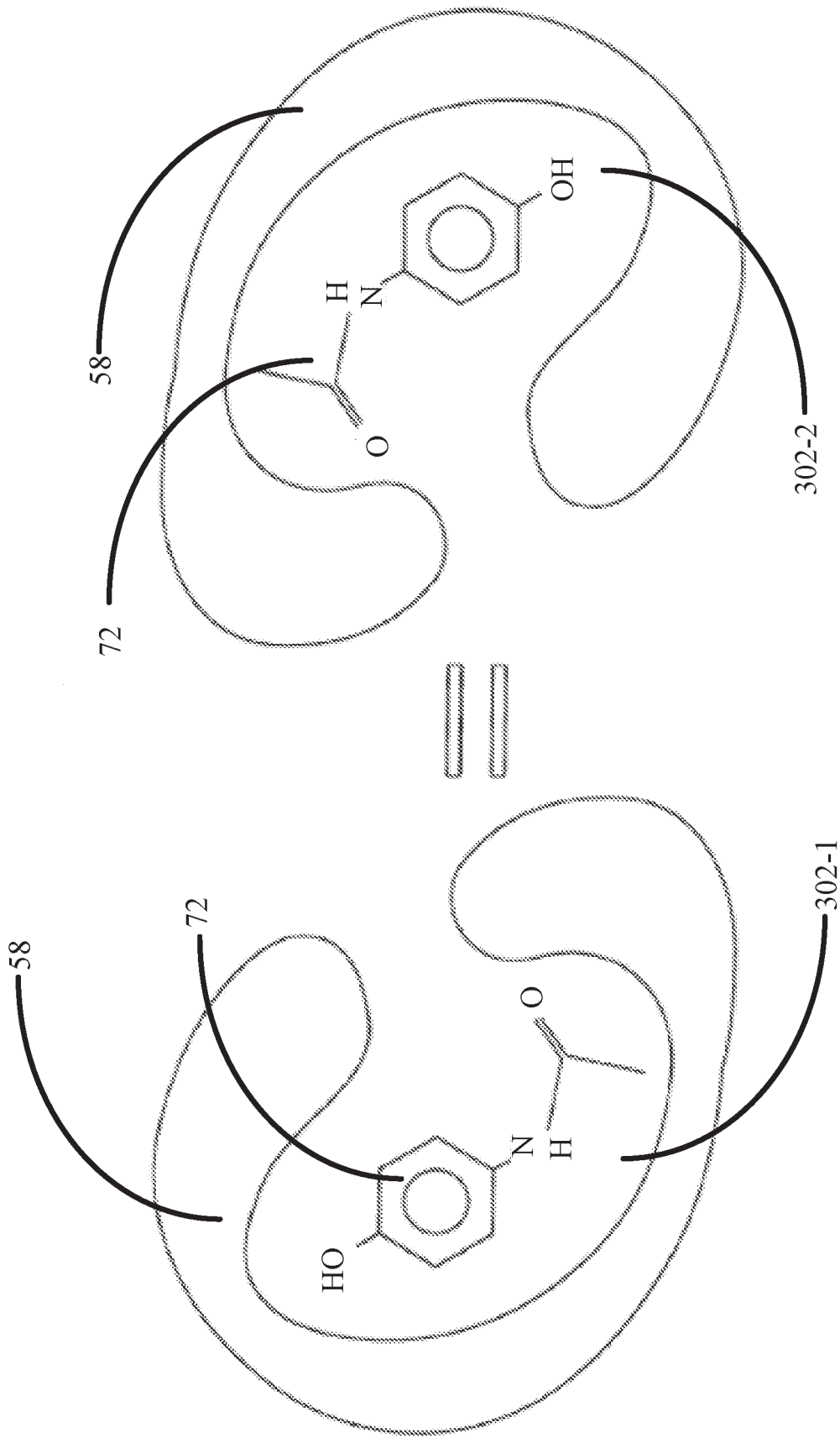


Fig. 3

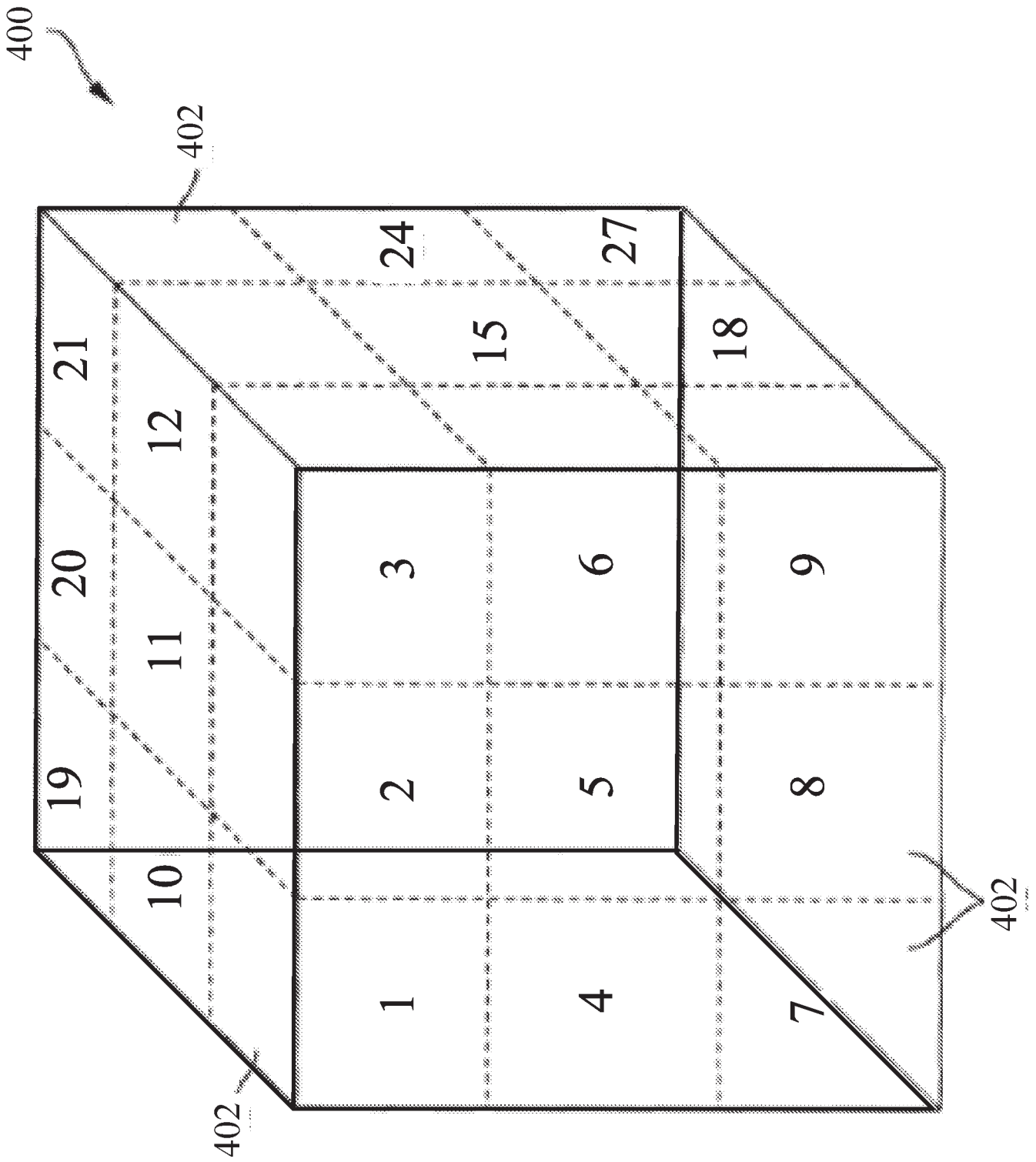


Fig. 4

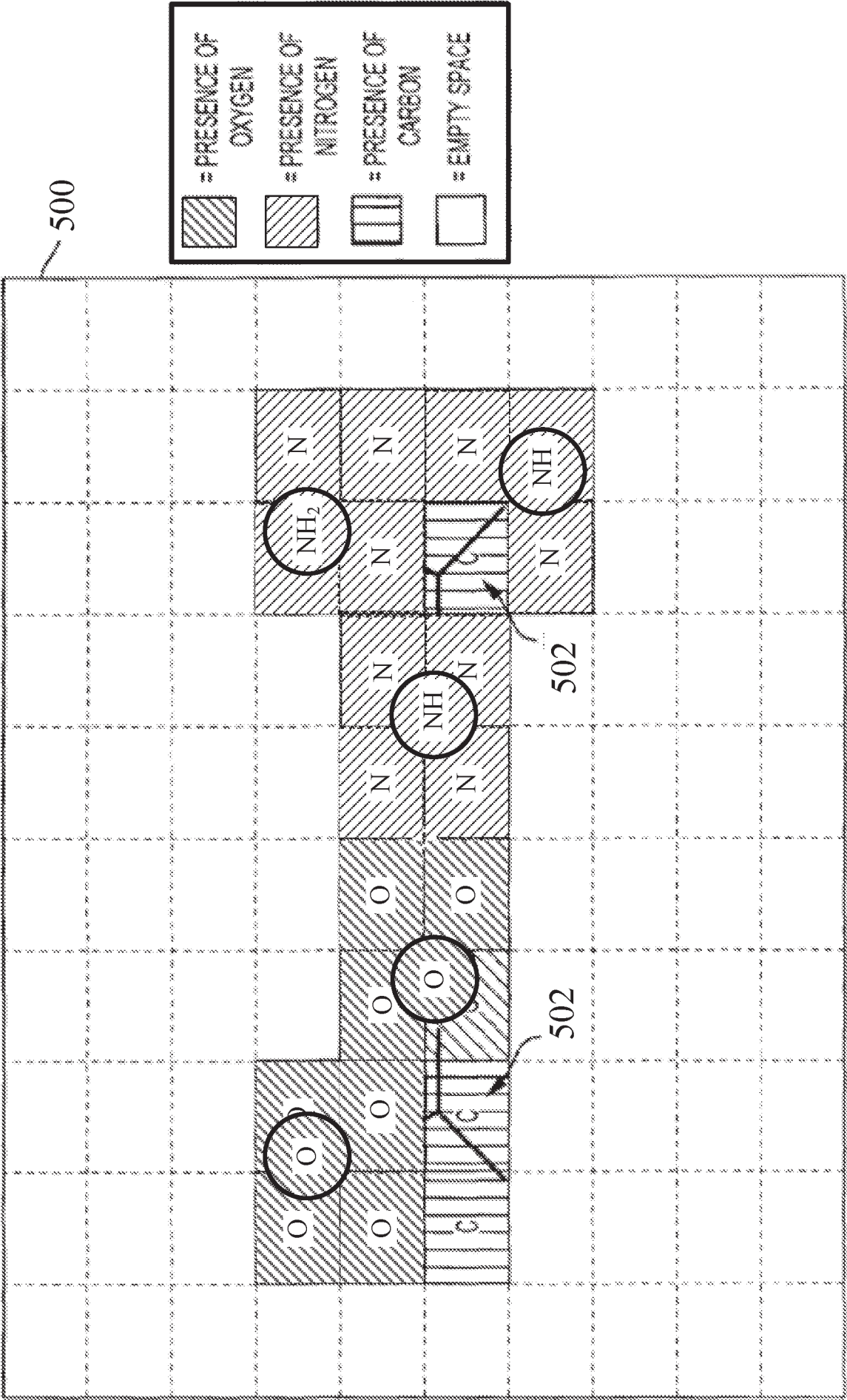


Fig. 5

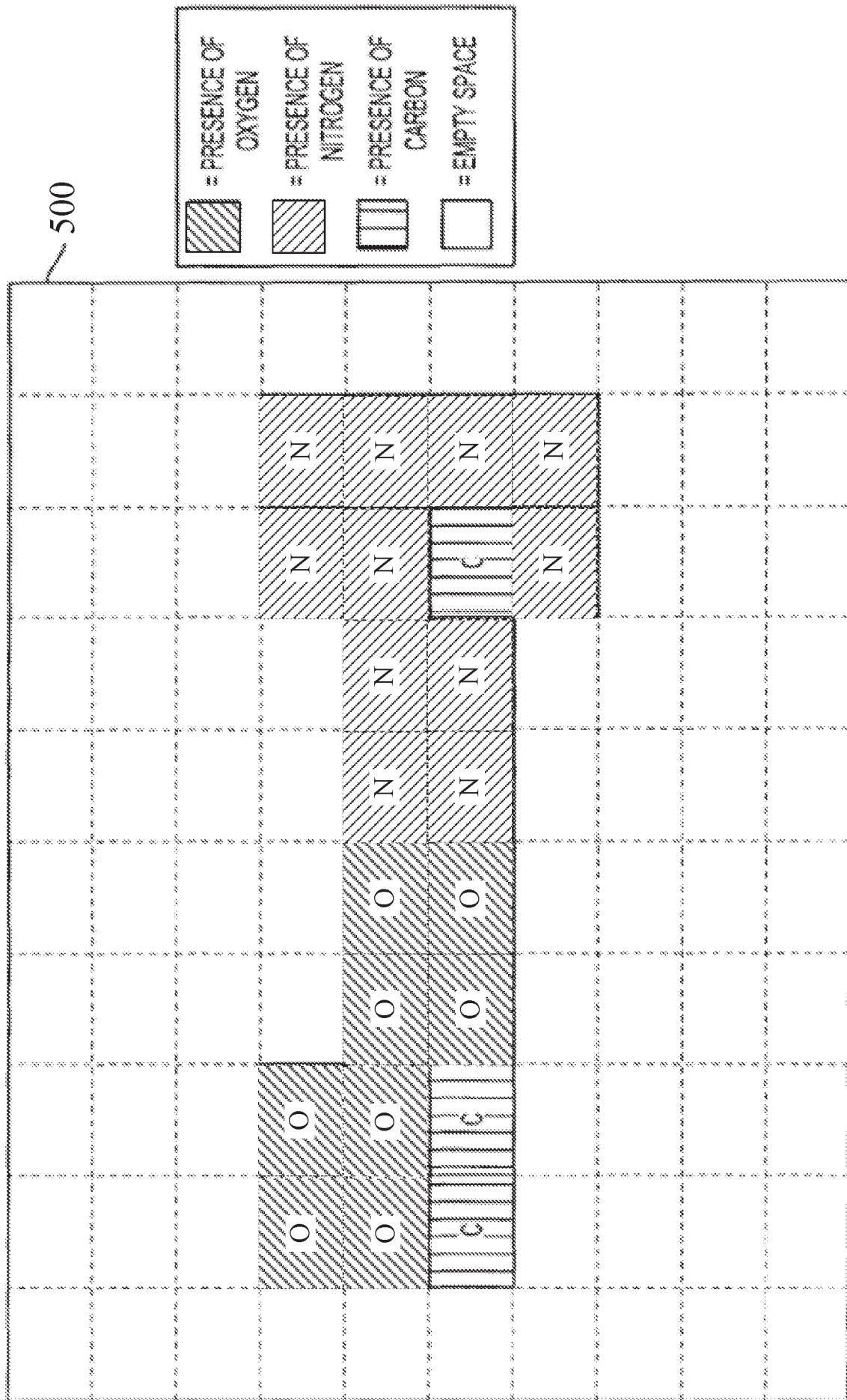


Fig. 6

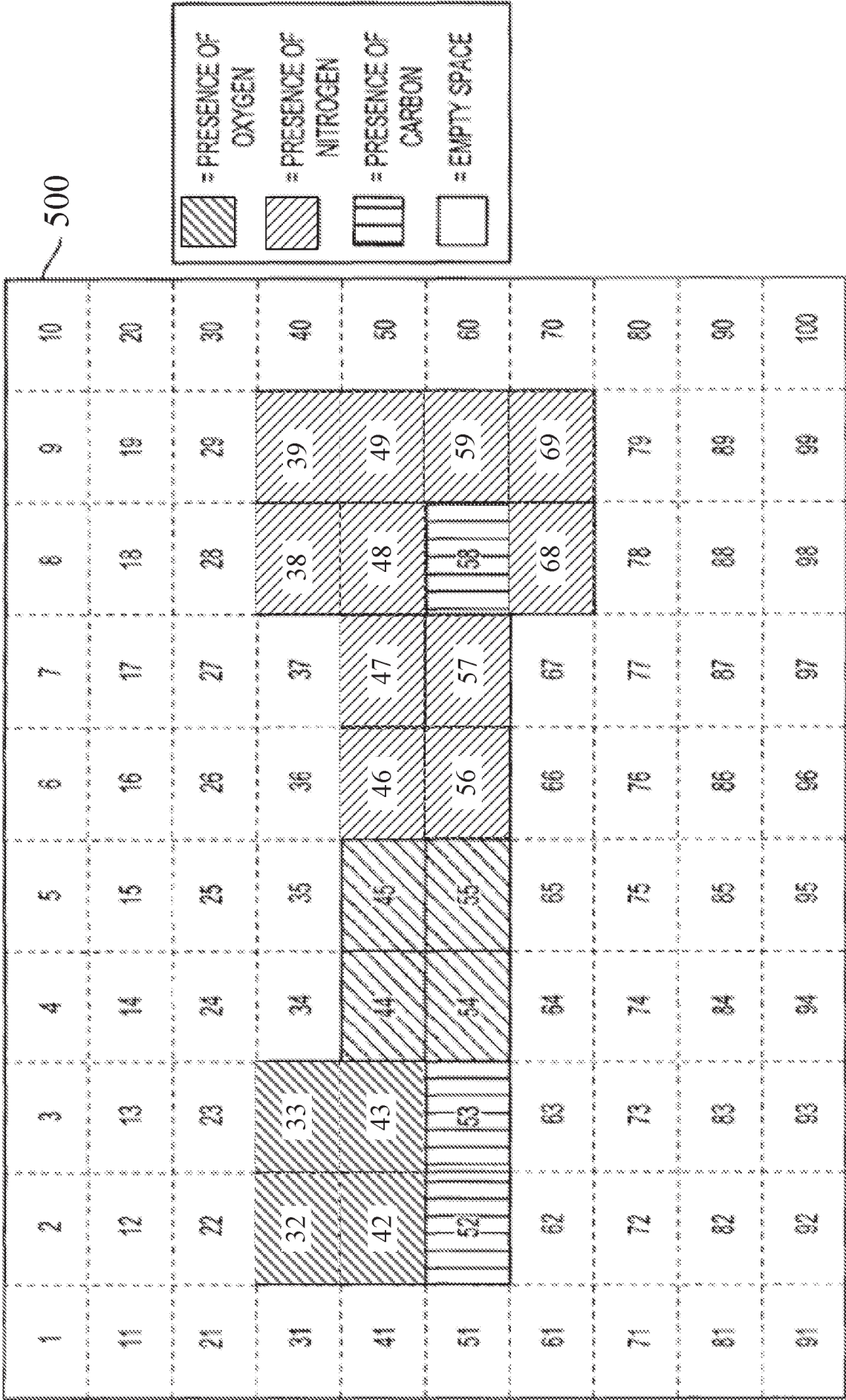


Fig. 7

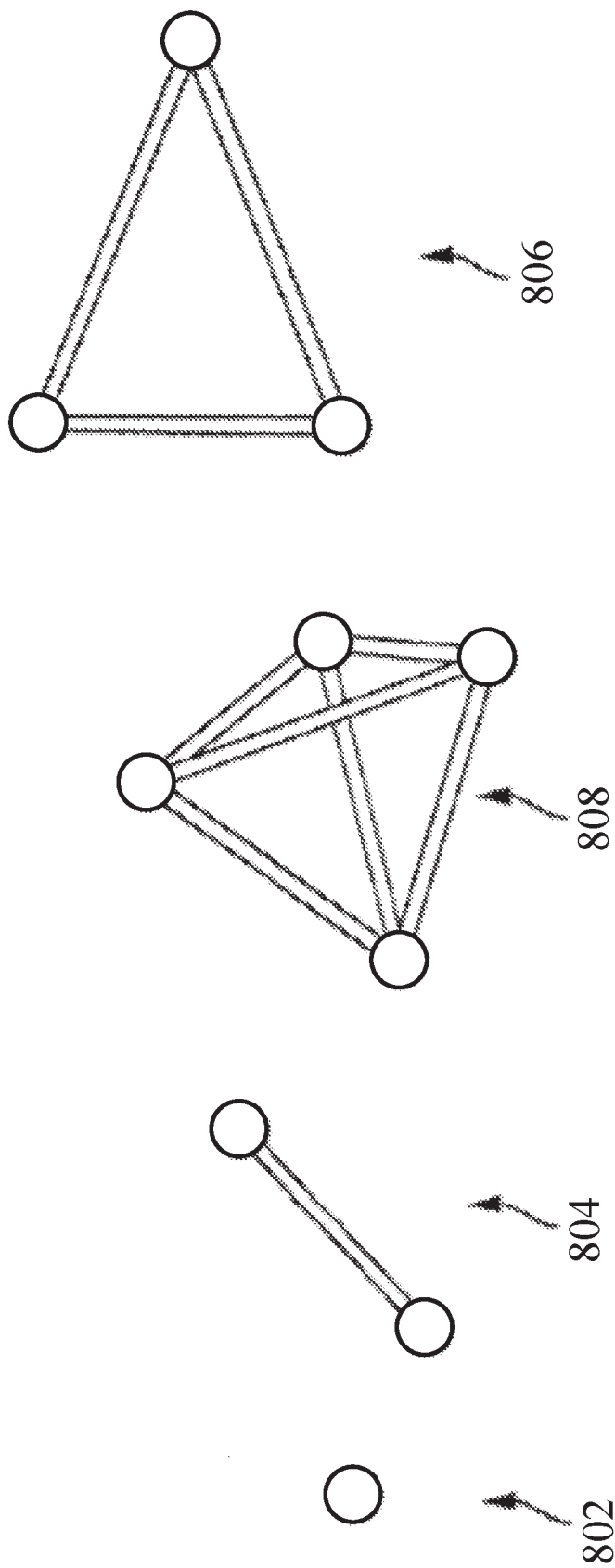


Fig. 8

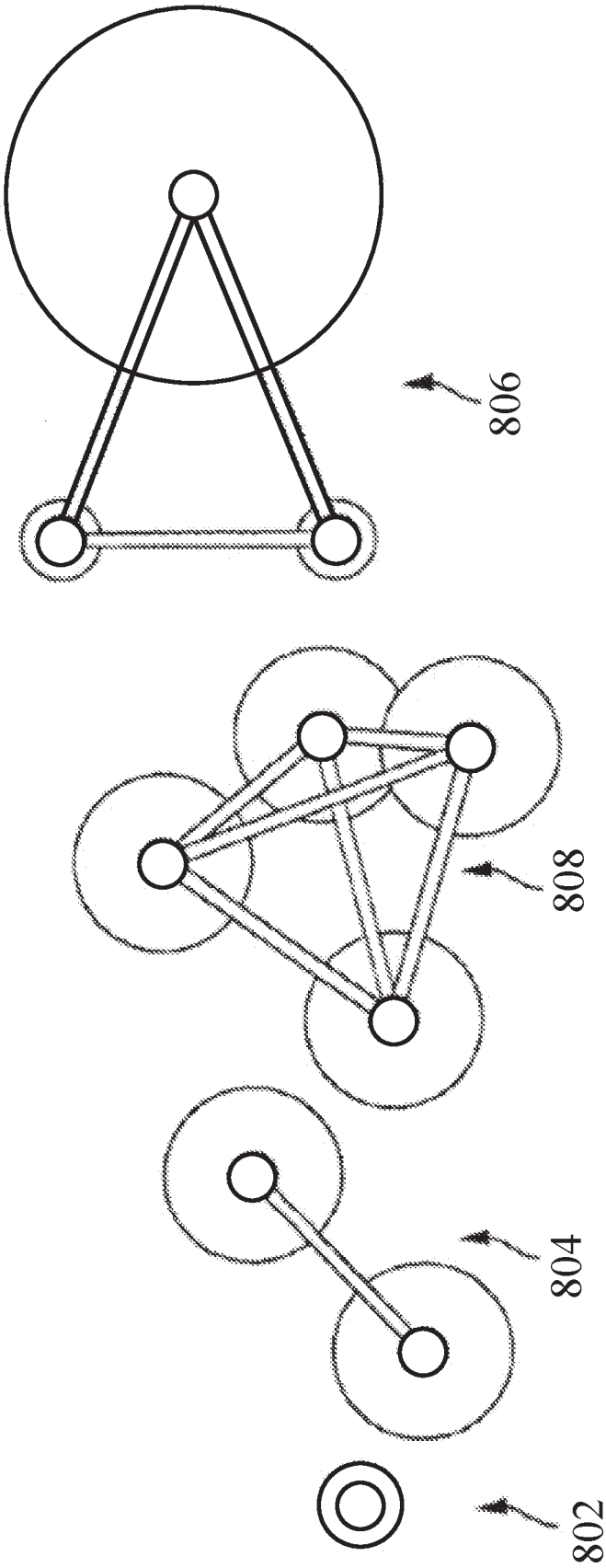


Fig. 9

## ChEMBL-20 PMD Benchmark Results

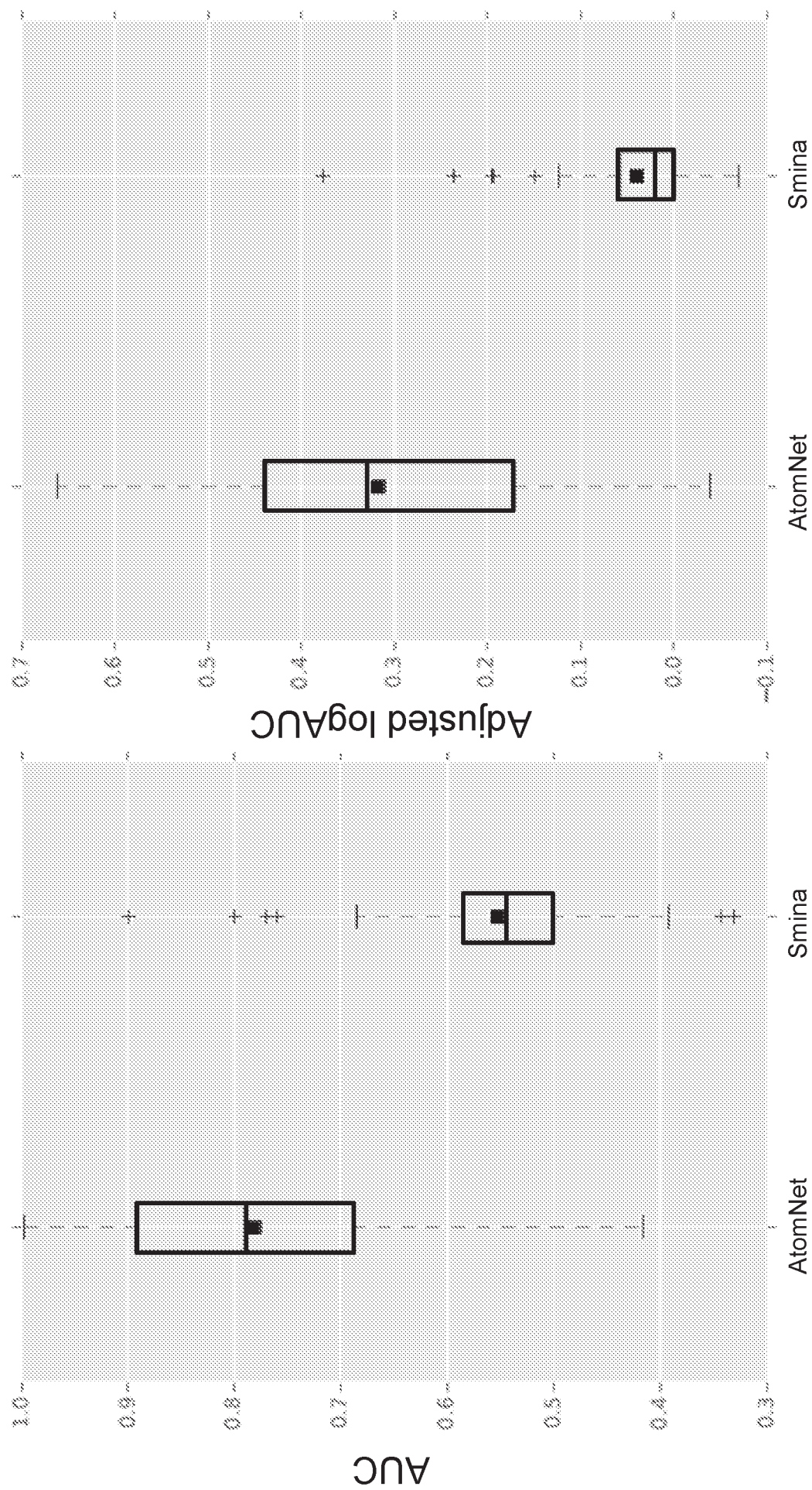


Fig. 10

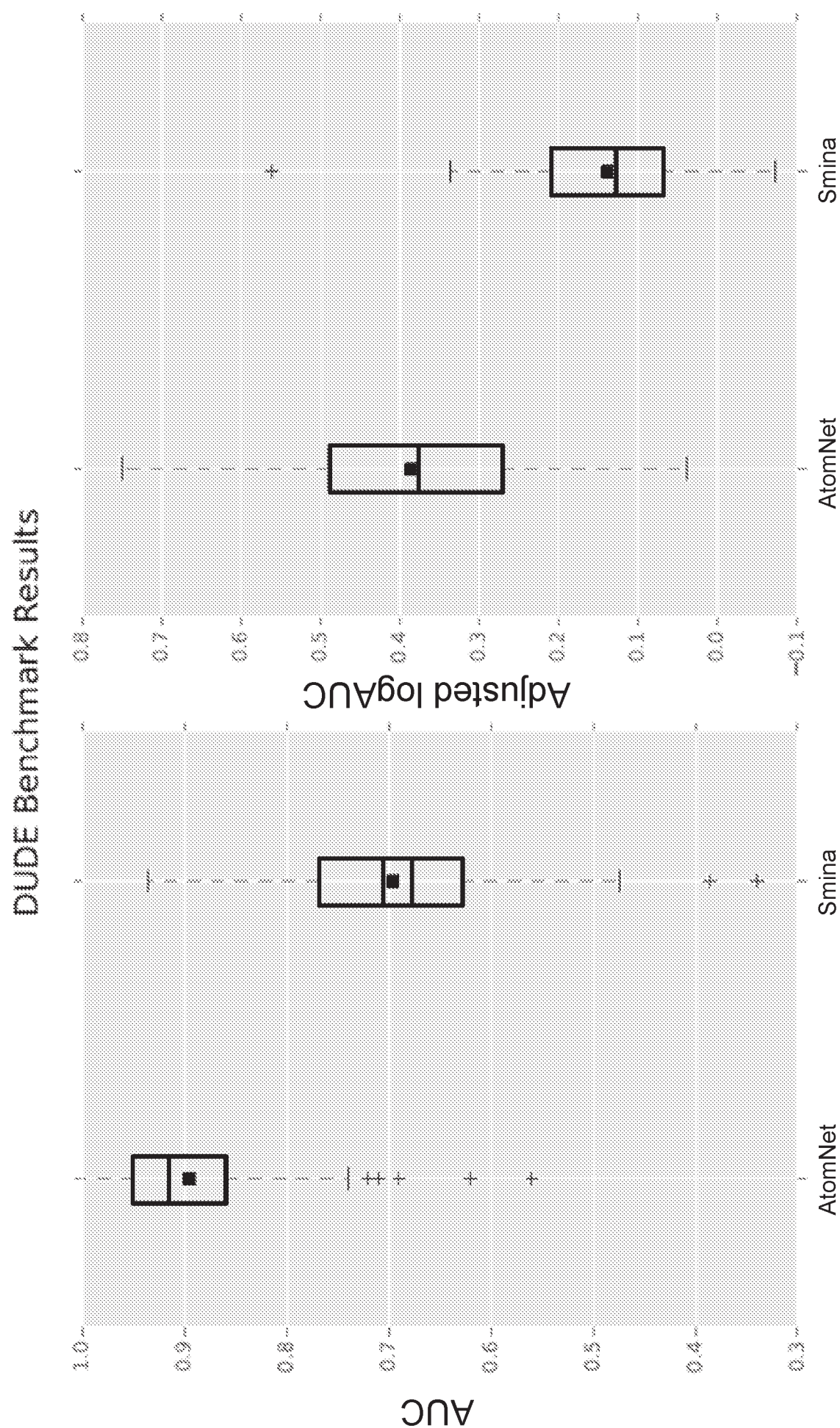


Fig. 11

## ChEMBL-20 with Inactives Benchmark Results

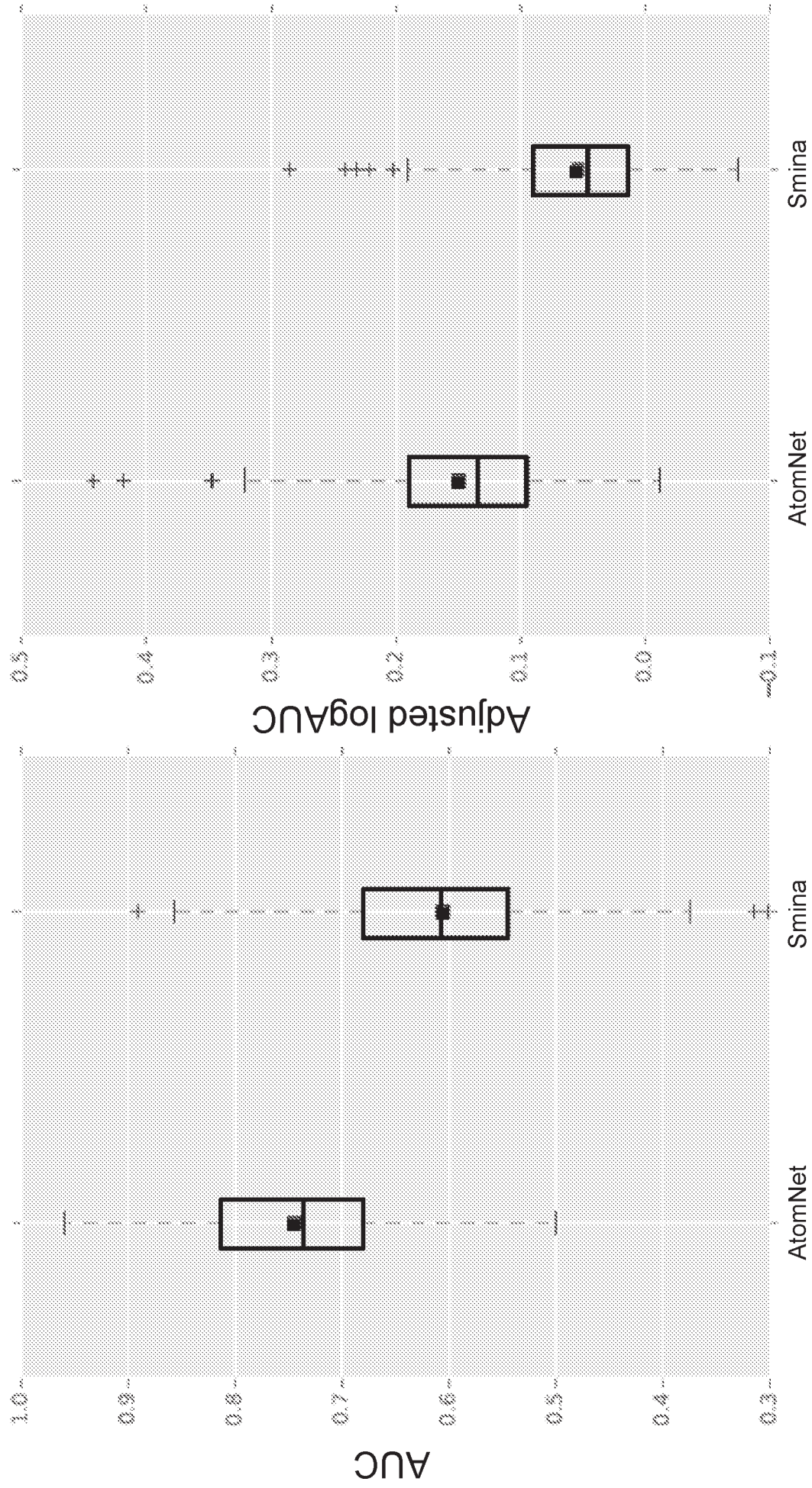


Fig. 12

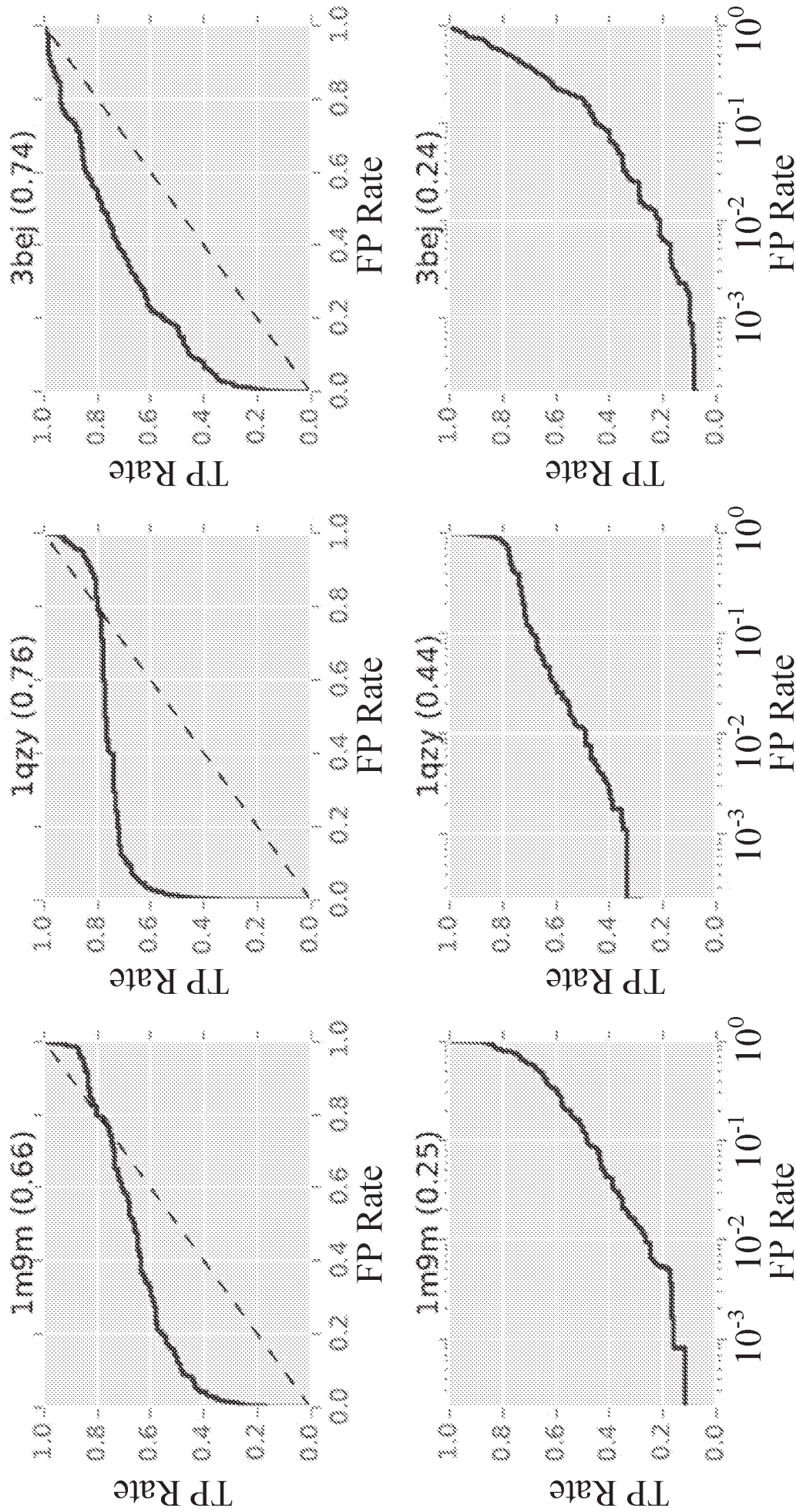


Fig. 13A

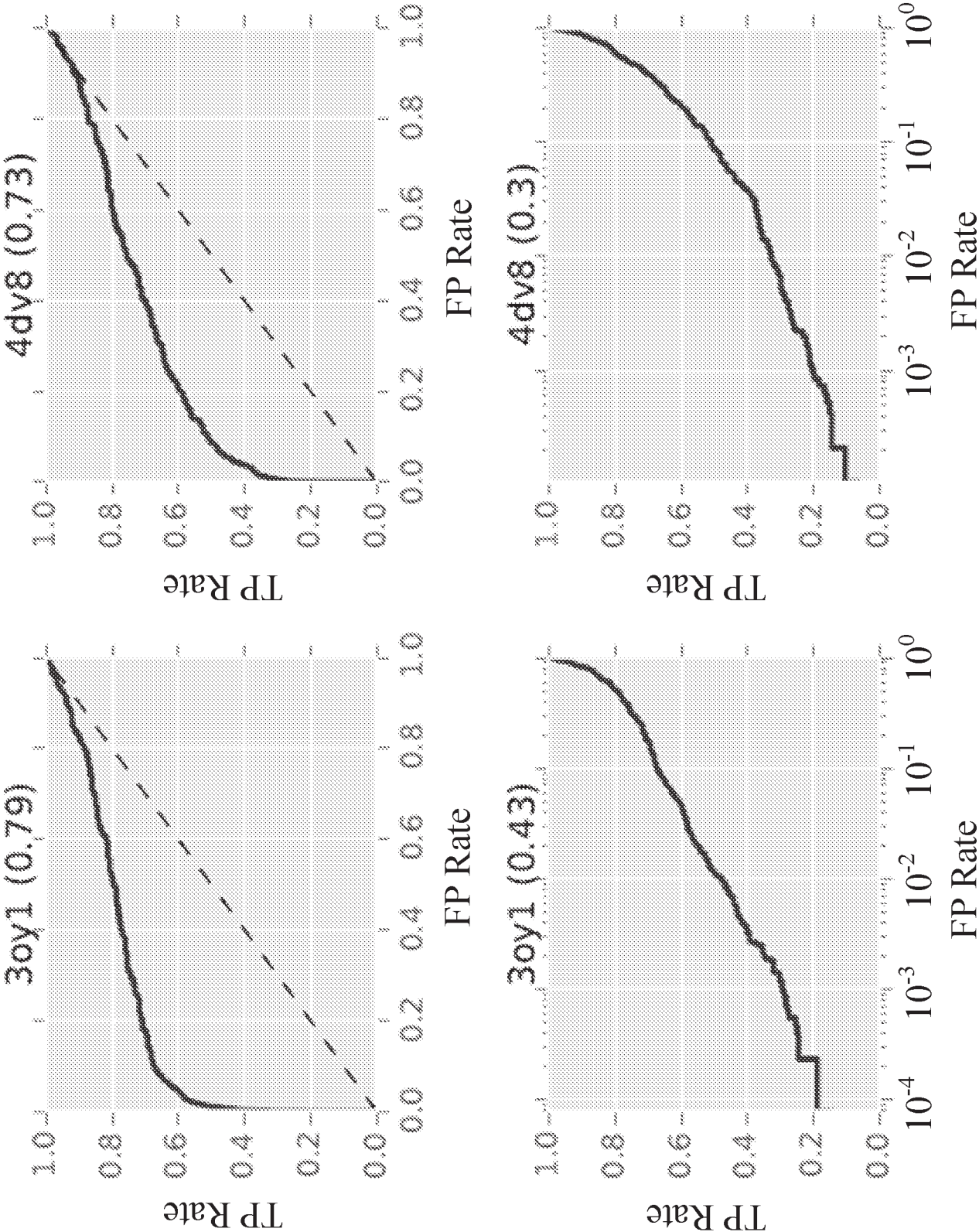


Fig. 13B

$$f(\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_{100}}) = g\big(g_0(\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_{100}}), g_1(\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_{100}}), \dots, g_n(\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_{100}})\big)$$
$$\overrightarrow{x_1} = (x_1^1, \ x_1^2, \ x_1^3, \dots, \ x_1^{40})$$
$$\overrightarrow{x_2} = (x_2^1, \ x_2^2, \ x_2^3, \dots, \ x_2^{40})$$

Fig. 14



Fig. 15A



Fig. 15B