

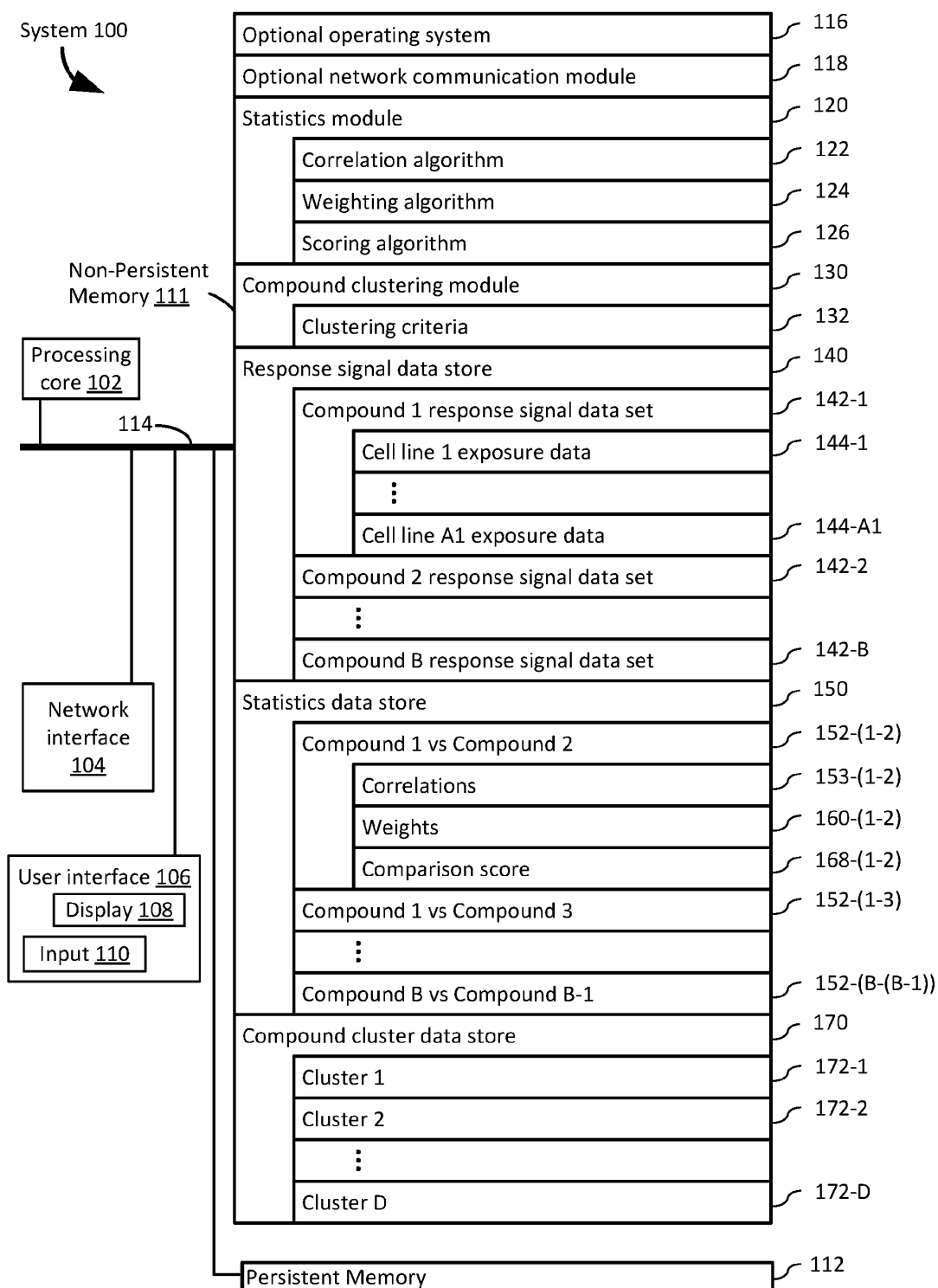


FIG. 1A

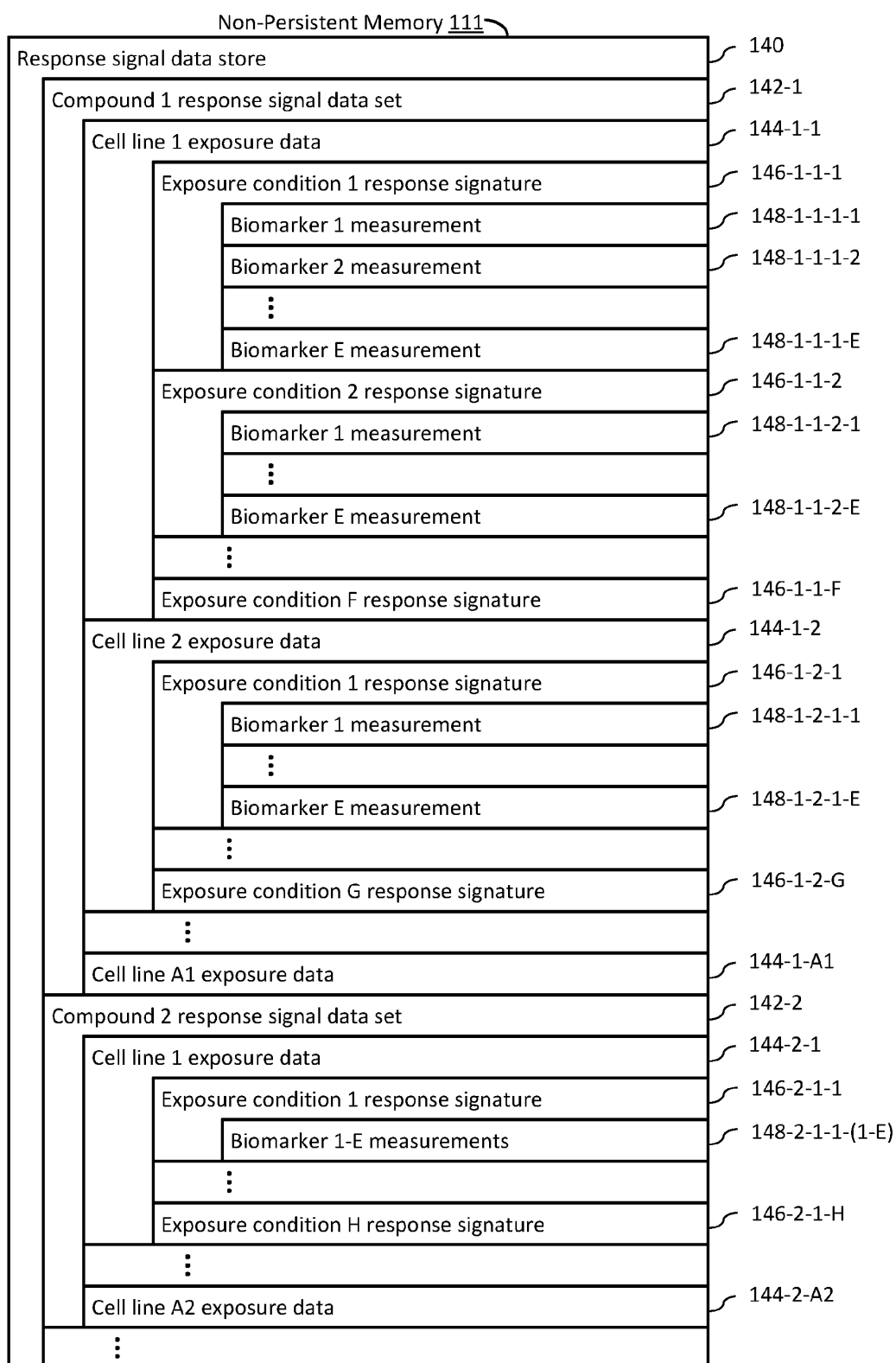


FIG. 1B

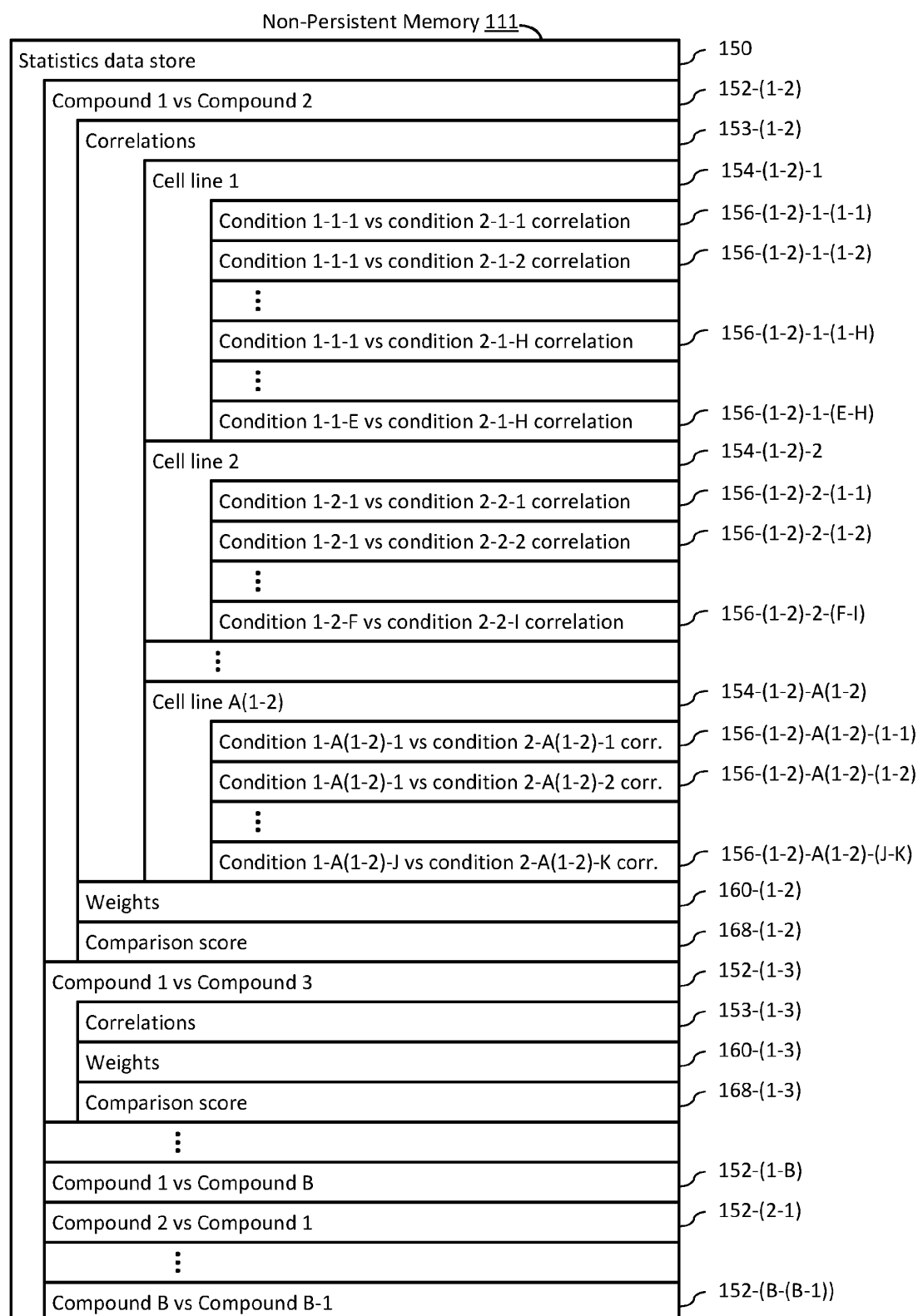


FIG. 1C

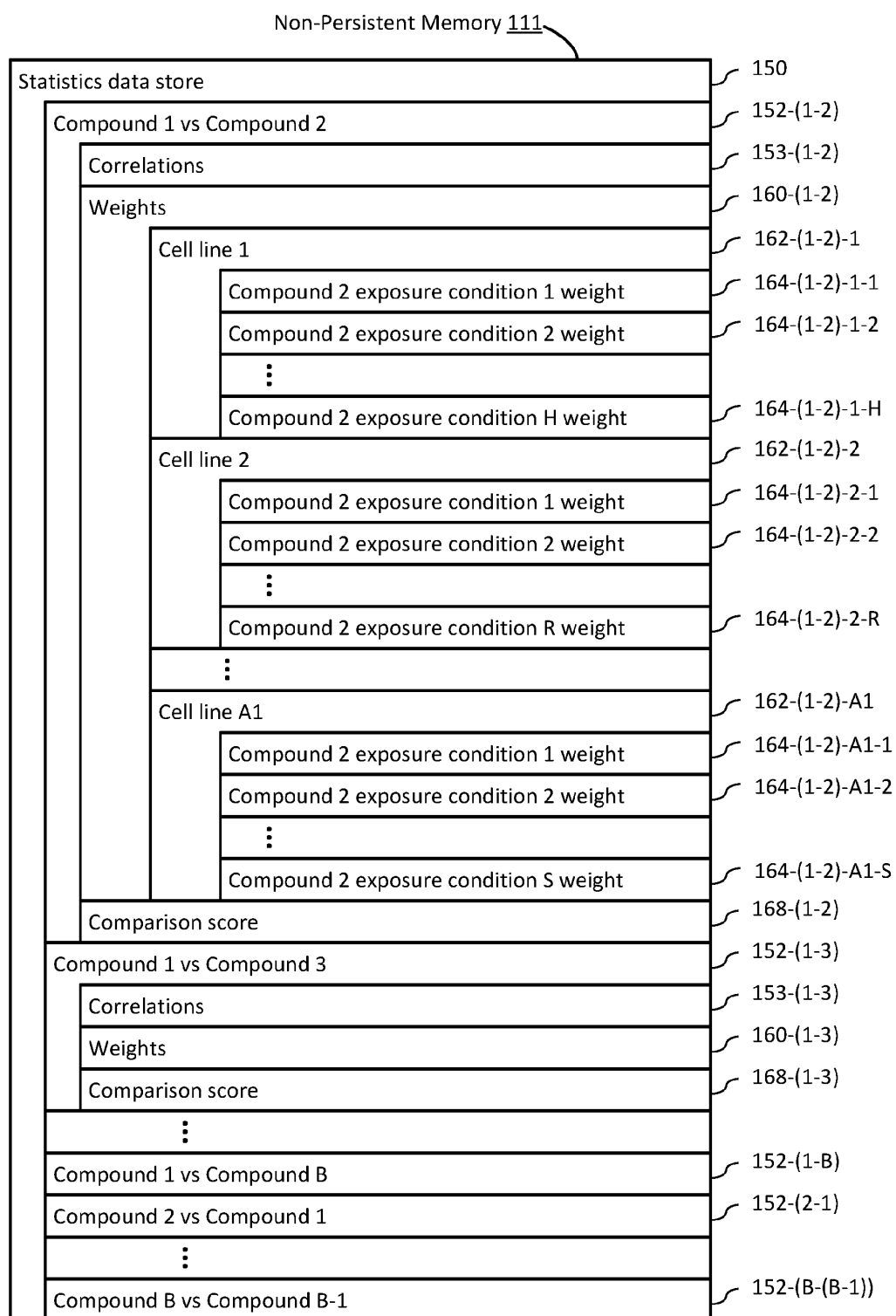


FIG. 1D

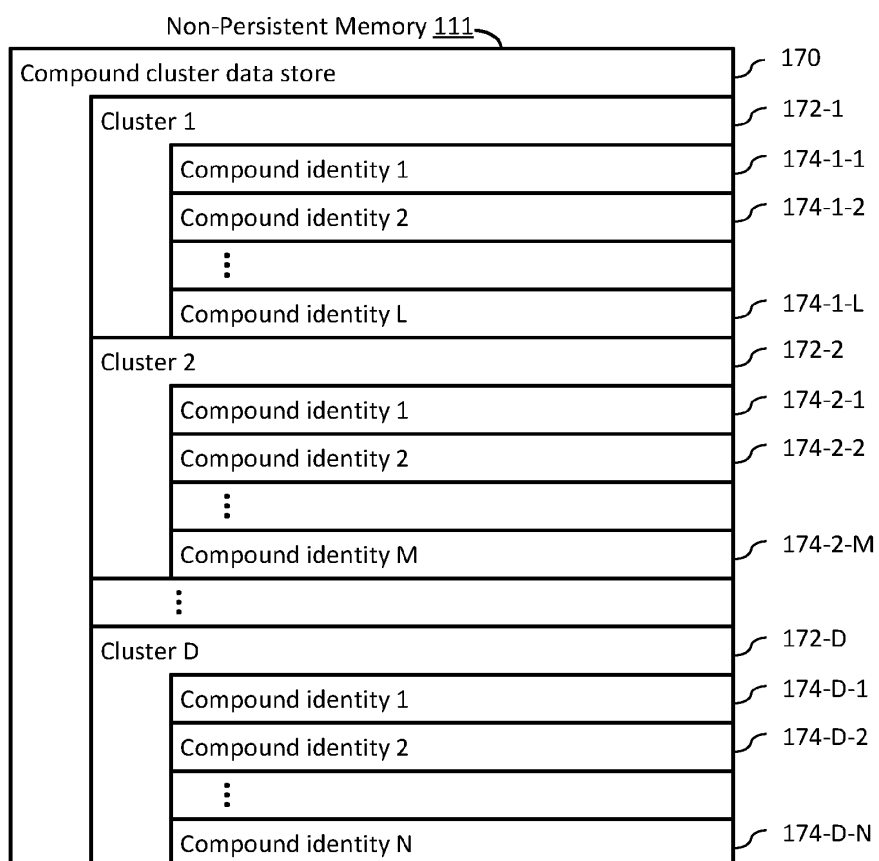


FIG. 1E

Comparison between compound 1 and compound 2

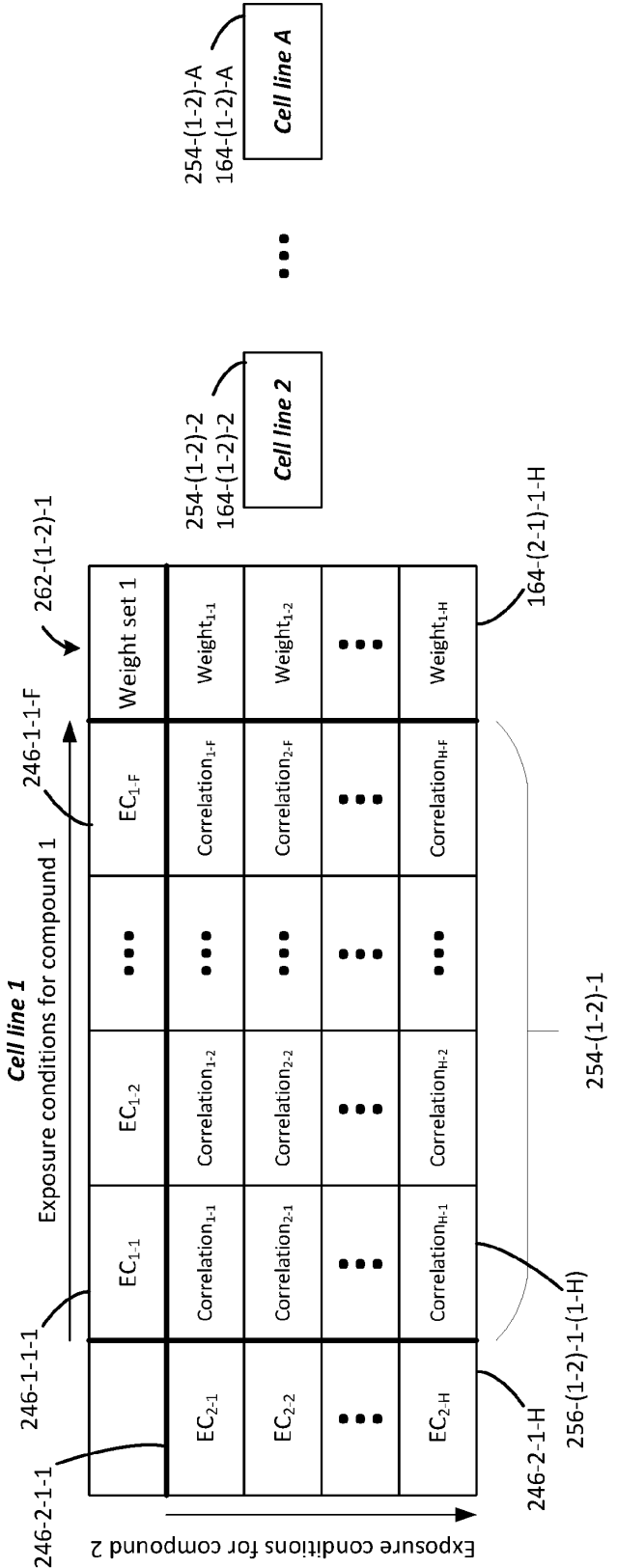


FIG. 2A

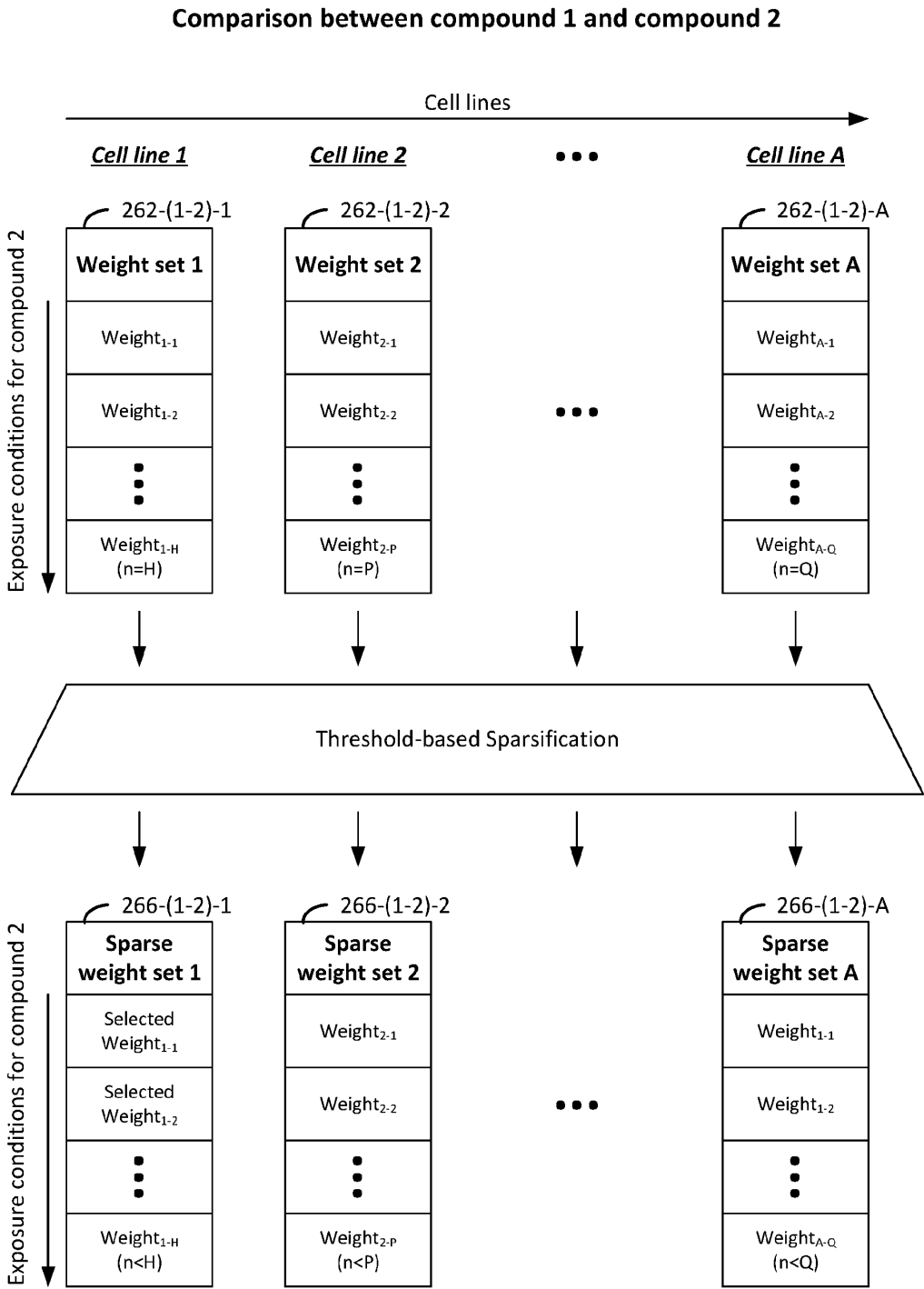


FIG. 2B

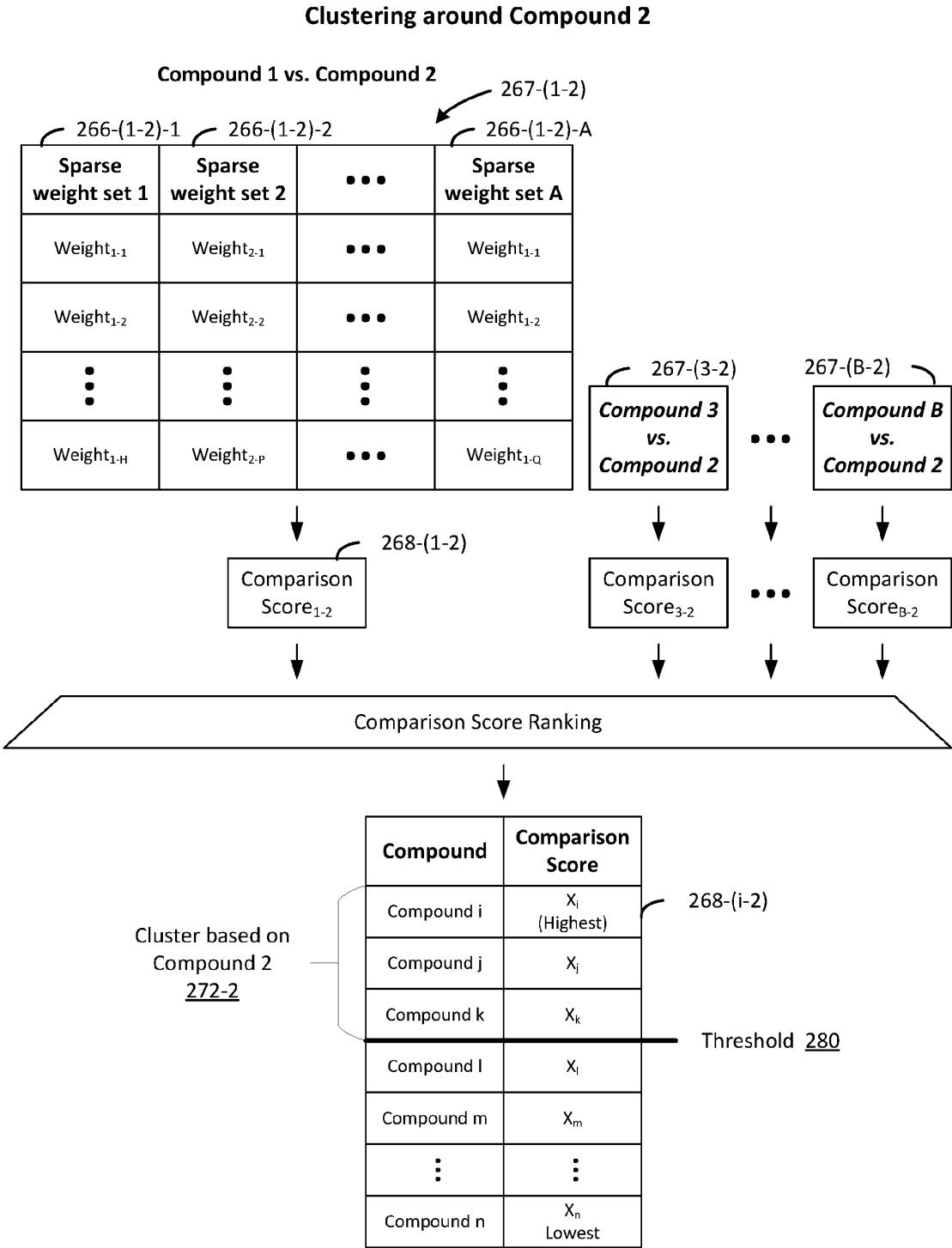


FIG. 2C

300

302 Obtain one or more datasets in electronic form, the one or more datasets including or collectively including: for each respective cell line in a plurality of cell lines, where the plurality of cell lines includes five or more cell lines: for each respective compound in a plurality of compounds: for each respective exposure condition in one or more exposure conditions for the respective compound: a corresponding response signature for the respective compound in the respective cell line under the respective exposure condition, the corresponding response signature including a corresponding plurality of quantitative biomarker measurements of the respective cell line across a plurality of biomarkers upon exposure of the respective cell line to the respective compound at the respective exposure condition, where the plurality of biomarkers includes one hundred or more biomarkers.

304 Each corresponding response signature is normalized against a response signature of one or more control genes in the respective cell line.

306 The plurality of cell lines includes 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, or more than 25 cell lines.

308 The plurality of compounds is between 10 and 1×10^8 compounds, between 100 and 1×10^7 compounds, between 1000 and 1×10^5 compounds, or between 10,000 and 100,000 compounds.

310 The respective exposure condition is a duration of exposure, a concentration of the respective compound, an environmental condition of the exposure, or a combination thereof.

312 The plurality of biomarkers are nucleic acids, ribonucleic acids, carbohydrates, lipids, epigenetic features, metabolites, proteins, cell morphological features, or a combination thereof.

314 Each quantitative biomarker measurement in the corresponding plurality of quantitative biomarker measurement is a colorimetric measurement, a fluorescence measurement, a luminescence measurement, or a resonance energy transfer (FRET) measurement.



FIG. 3A

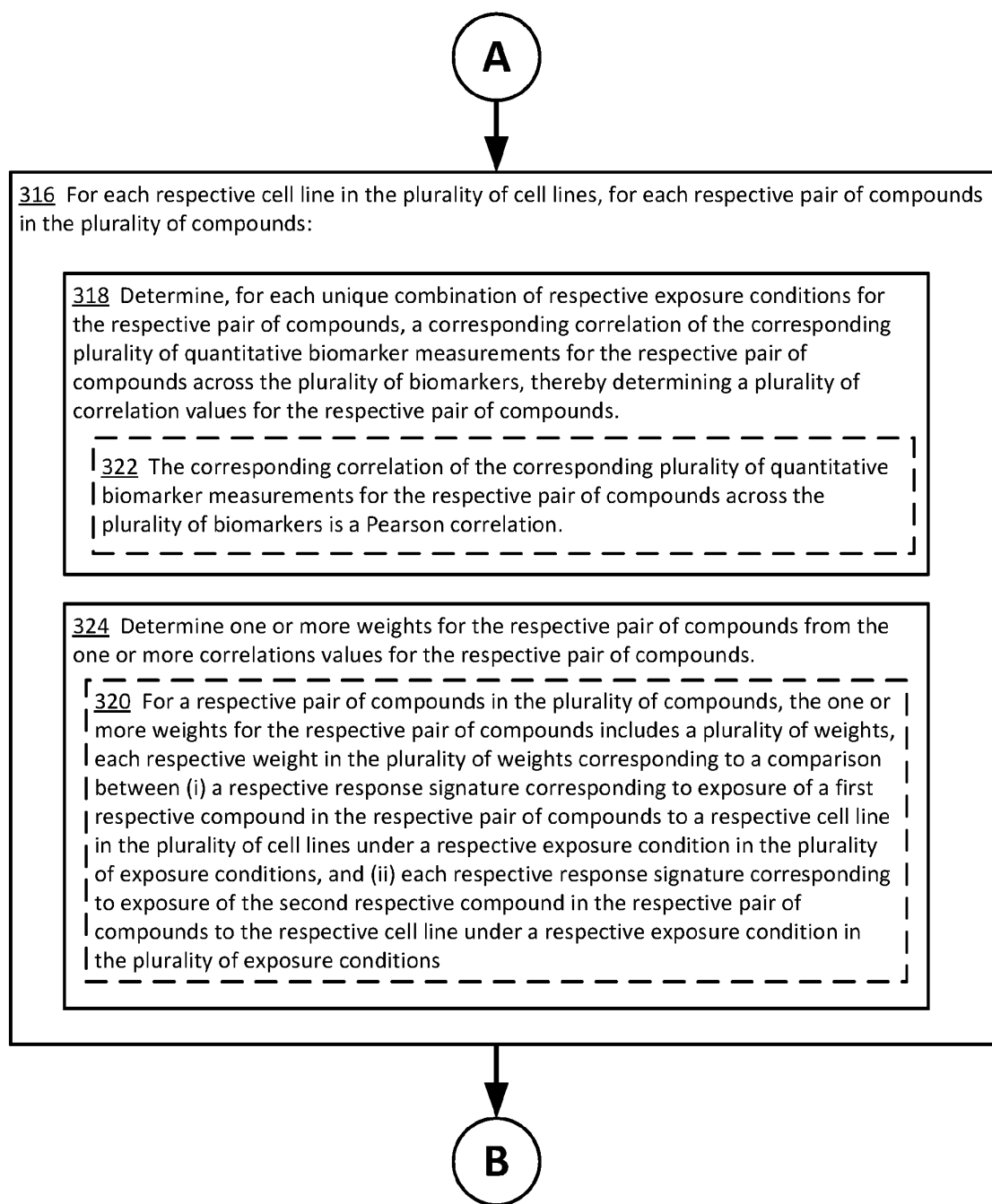
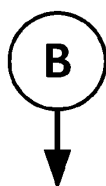


FIG. 3B



326 Form a plurality of compound clusters, each respective compound cluster representing a first respective compound in the plurality of compounds and including a corresponding subset of compounds in the plurality of compounds, where each respective compound in the corresponding subset of compounds satisfies one or more weight criteria with respect to the first respective compound.

328 The one or more weight criteria includes a requirement that the respective pair of compounds in the corresponding unique subset of compounds have a correlation value across all or a subset of the plurality of cell lines that is within a threshold percent of an upper correlation bound identified for the plurality of compounds across the plurality of cell lines.

330 The threshold percent is between five percent and fifty percent (e.g., five, ten, fifteen, twenty, twenty-five, thirty, thirty-five, forty, forty-five, or fifty percent).

332 The one or more weight criteria is a plurality of weight criterion and the plurality of weight criteria further includes a requirement that the subset of the plurality of cells lines be at least five different cell lines.

334 The one or more weight criteria is a plurality of weight criterion and the plurality of weight criteria further includes a requirement that the subset of the plurality of cells lines be at least 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, or 20 different cell lines.

336 One or more compound clusters in the plurality of compound clusters that contain the test compound for test compound is a drug for a first disease indication, and the method further includes using the identifying the compound property of test compound from one or more properties of one or more compounds in one or more compound clusters in the plurality of compound clusters to repurpose the drug for a second disease indication.

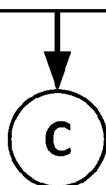


FIG. 3C

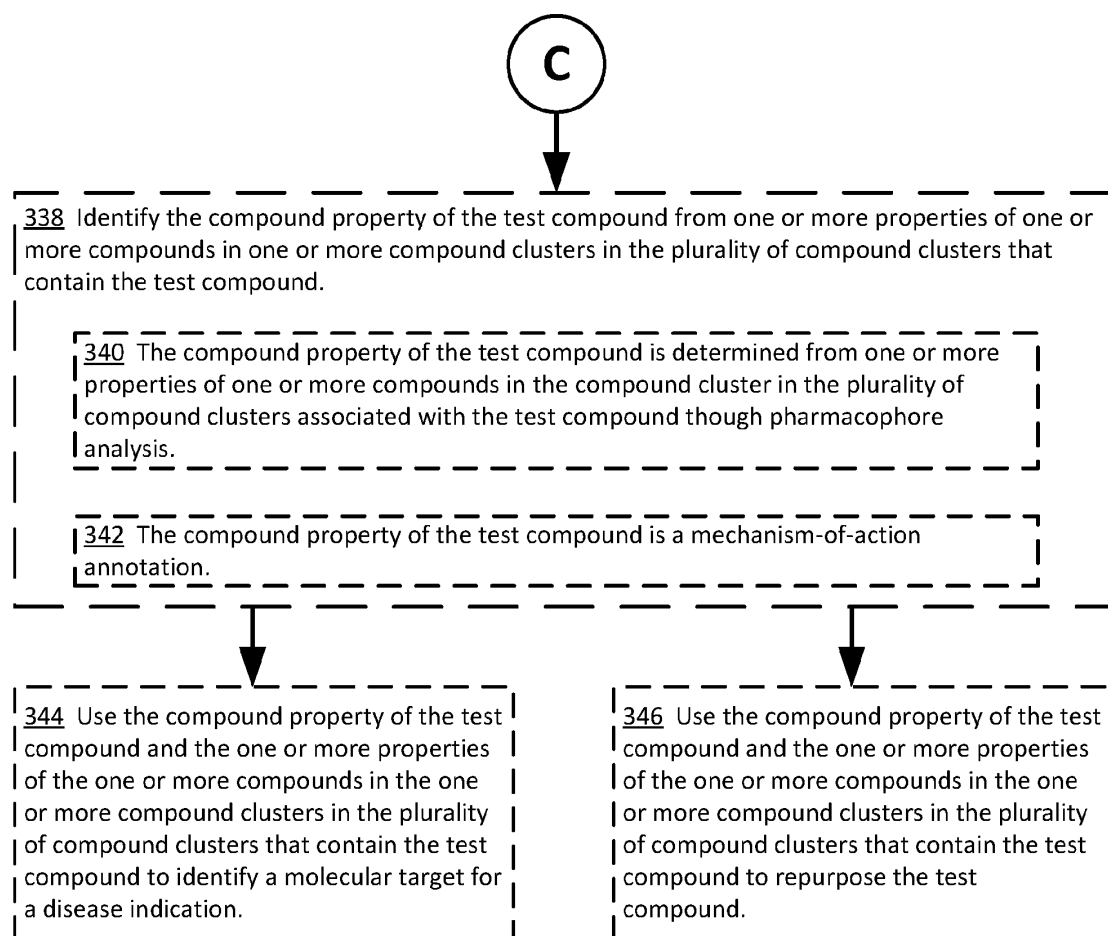


FIG. 3D

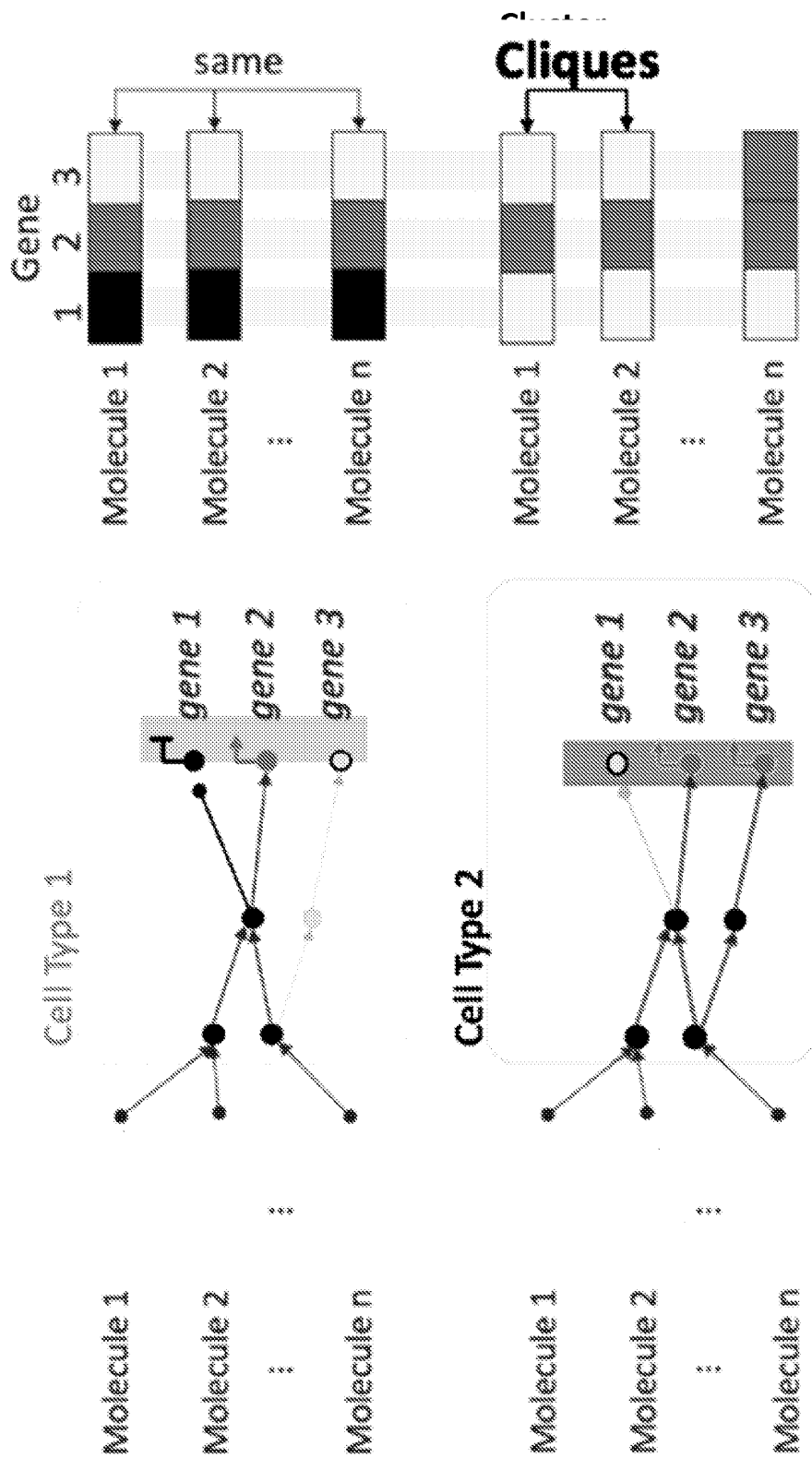


FIG. 4

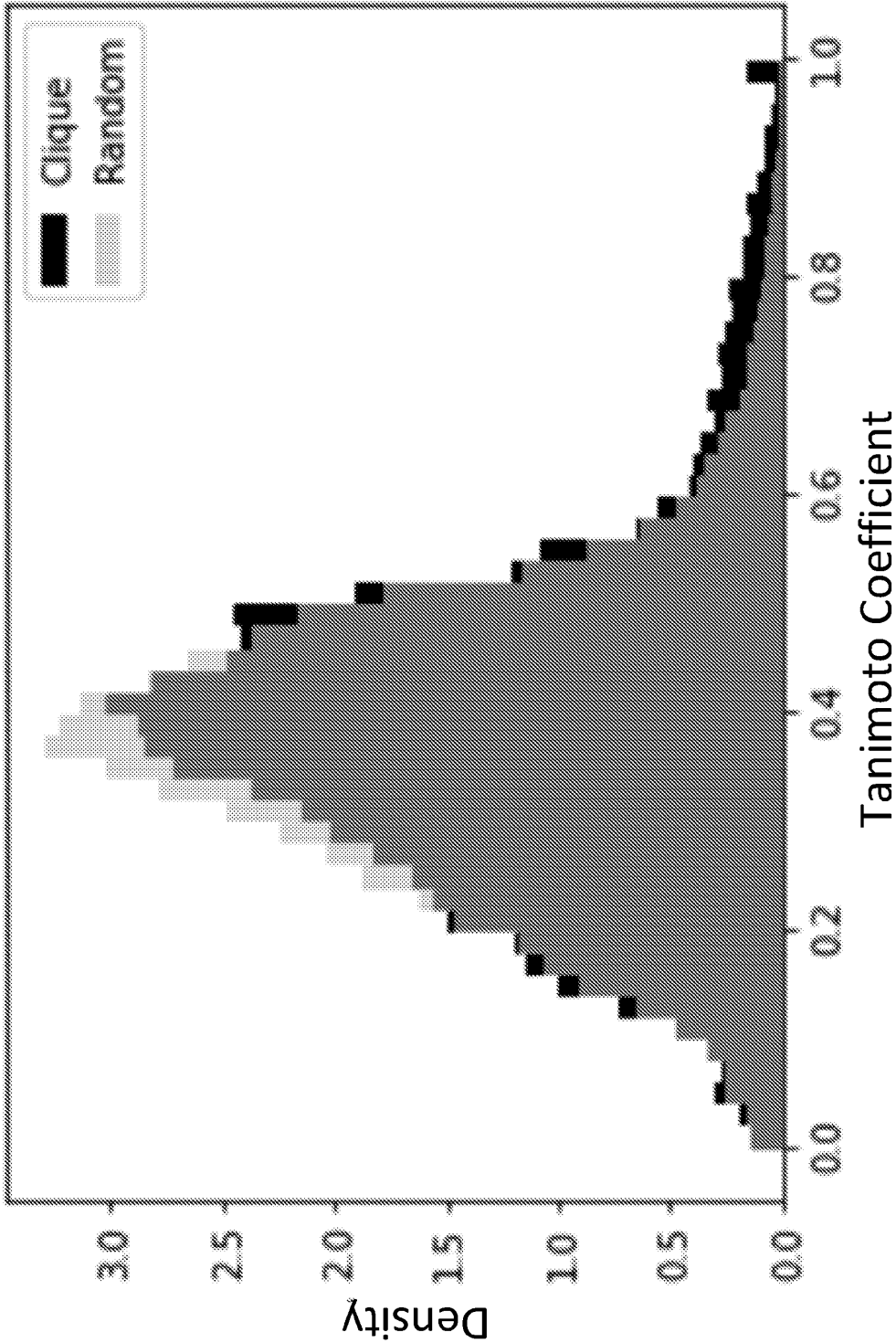


FIG. 5

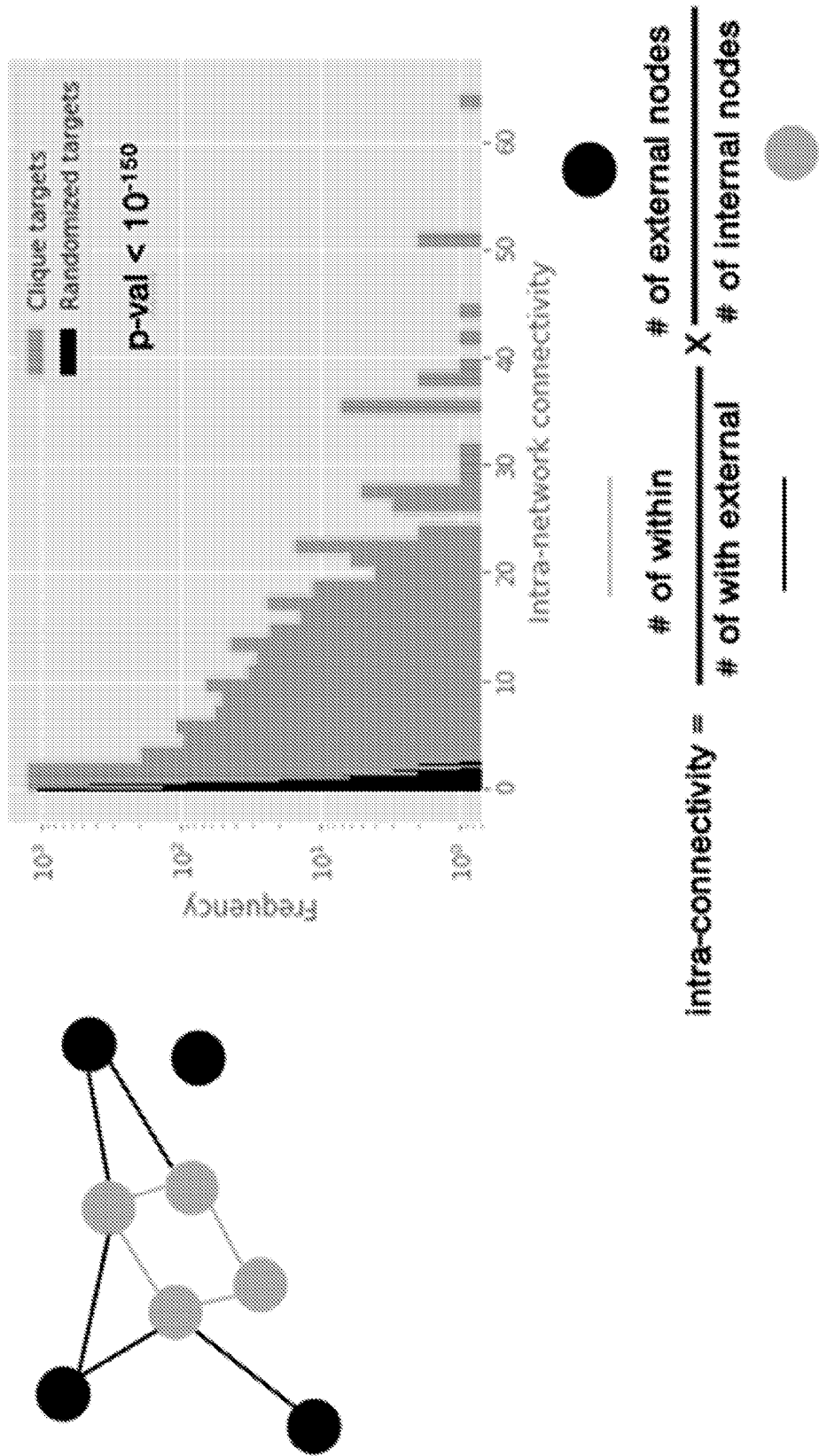


FIG. 6

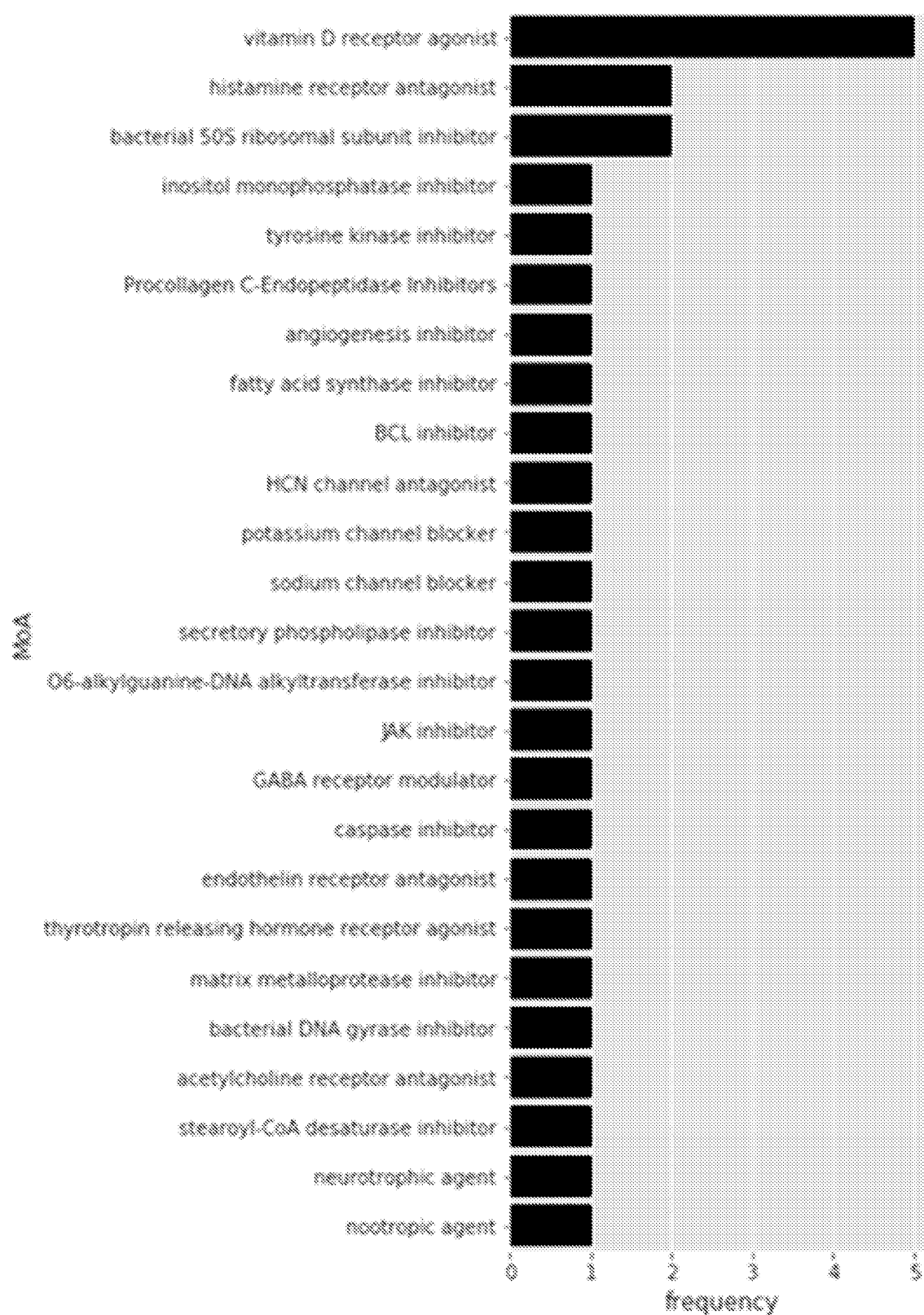


FIG. 7

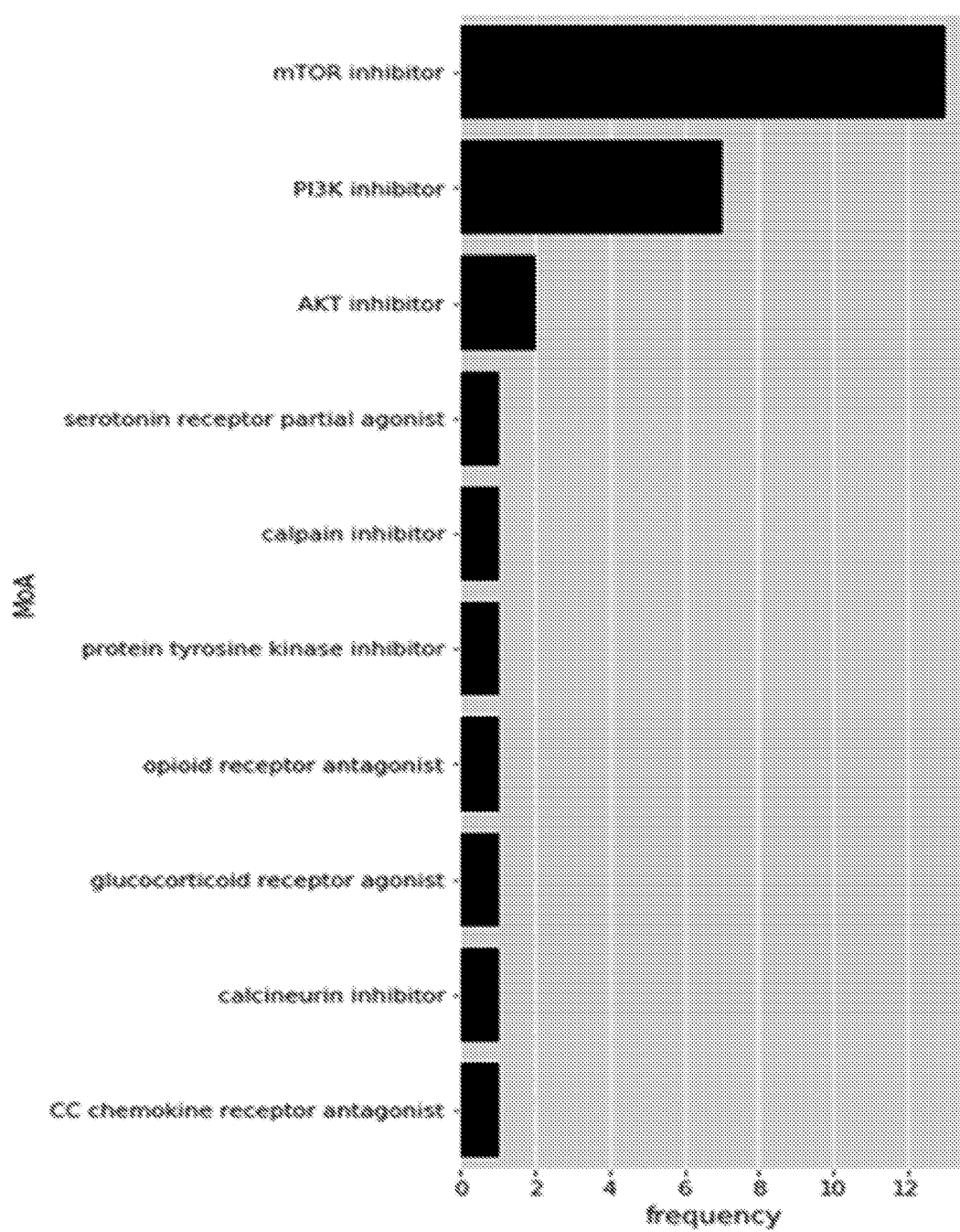


FIG. 8