WHAT IS CLAIMED IS:

1. A method of screening a plurality of compounds comprising at least 50 compounds, wherein each compound in the plurality of compounds is associated with a corresponding plurality of exposure conditions, the method using a plurality of cells lines that comprises 5 or more cell lines and a plurality of biomarkers that comprises 25 or more different biomarkers, the method comprising:

(A) for each combination of (i) a compound in the plurality of compounds and (ii) an exposure condition in the corresponding plurality of exposure conditions associated with the compound:

(a) exposing an aliquot of each cell line in the plurality of cell lines to the compound in the plurality of compounds under the exposure condition in the corresponding plurality of exposure conditions associated with the compound, and

(b) obtaining a response signature for each aliquot of each cell line in the plurality of cell lines, that comprises a plurality of quantitative biomarker measurements of the aliquot of the cell line, the plurality of quantitative biomarker measurements including a separate quantitative biomarker measurement for each biomarker in the plurality of biomarkers, upon exposure of the aliquot of the cell line to the compound in the plurality of compounds under the exposure condition in the corresponding plurality of exposure conditions associated with the compound,

thereby obtaining a plurality of response signatures, wherein

the plurality of response signatures includes a response signature for each aliquot of each cell line in the plurality of cell lines for each combination of (i) a compound in the plurality of compounds and (ii) an exposure condition in the corresponding plurality of exposure conditions associated with the compound,

each corresponding plurality of exposure conditions for each compound in the plurality of compounds comprises at least five exposure conditions for the compound, and

each exposure condition in the corresponding plurality of exposure conditions for a compound comprises a combination of a duration of exposure and a concentration of the compound for exposure;

at a computer system comprising a memory and one or more processors:

(B) determining, for each combination of (i) a first compound in the plurality of compounds and an exposure condition in the corresponding plurality of exposure conditions associated with the first compound and (ii) a second compound in the plurality of compounds

and an exposure condition in the corresponding plurality of exposure conditions associated with the second compound:

a correlation value for each cell line in the plurality of cell lines that is a correlation of (1) the plurality of quantitative biomarker measurements of the cell line in the response signature in the plurality of response signatures that represents the cell line upon exposing an aliquot of the cell line to the first compound at the exposure condition in the corresponding plurality of exposure conditions associated with the first compound and (2) the plurality of quantitative biomarker measurements of the cell line in the response signature in the plurality of response signatures that represents the cell line upon exposing an aliquot of the cell line to the second compound at the exposure condition in the corresponding plurality of exposure conditions associated with the second compound,

thereby determining a corresponding plurality of correlation values for each pair of first and second compounds in the plurality of compounds for each cell in the plurality of cells;

(C) for each corresponding plurality of correlation values, for each pair of first and second compounds in the plurality of compounds, for each cell line in the plurality of cell lines, determining a first weight that represents a maximum value or a measure of central tendency of the corresponding plurality of correlation values;

(D) obtaining an upper correlation bound that is a maximum correlation value determined for any combination of (i) a first compound in the plurality of compounds and an exposure condition in the corresponding plurality of exposure conditions associated with the first compound and (ii) a second compound in the plurality of compounds and an exposure condition in the corresponding plurality of exposure conditions associated with the second compound evaluated by the determining (B);

(E) forming a plurality of compound clusters using the first weight for each cell type in the plurality of cell types, wherein a first compound cluster in the plurality of compound clusters is for a first compound in the plurality of compounds and includes each compound in each pair of compounds in the plurality of compounds that:

(1) includes the first compound, and

(2) is associated with a first weight, for each cell type in the plurality of cell types, that is within a threshold percent of the upper correlation bound;

(F) determining that a test compound is in one or more compound clusters in the plurality of compound clusters, including the first cluster, that contains the first compound, wherein the first compound is associated with a disease; and

(G) responsive to determining that the test compound is in one or more compound clusters in the plurality of compound clusters, including the first cluster, that contains the first compound, associating the test compound with the disease,

wherein the plurality of biomarkers is any combination of nucleic acids, ribonucleic acids, carbohydrates, lipids, epigenetic features, metabolites, and proteins.

2. The method of claim 1, wherein the threshold percent is between five percent and fifty percent.

3. The method of claim 1, wherein the threshold percent is five, ten, fifteen, twenty, twenty-five, thirty, thirty-five, forty, forty-five, or fifty percent.

4. The method of any one of claims 1-3, wherein each plurality of quantitative biomarker measurements in each response signature is normalized against a response signature of one or more control genes in the respective cell line.

5. The method of any one of claims 1-4, wherein the plurality of cell lines comprises 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 30, 40, 50, 60, or 100 different cell lines.

6. The method of any one of claims 1-5, wherein the plurality of compounds is between 100 and 1×10^7 compounds, between 1000 and 1×10^6 compounds or between 10,000 and 100,000 compounds.

7. The method of any one of claims 1-6, wherein an exposure condition in the corresponding plurality of exposure conditions for a compound in the plurality of compounds is a duration of exposure of the compound to a cell line, a concentration of the compound upon exposure to a cell line, an environmental condition of the exposure of a cell line upon exposure to the compound, or a combination thereof.

8. The method of any one of claims 1-7, wherein, for a pair of first and second compounds in the plurality of compounds, the first weight for the pair of first and second compounds is a measure of central tendency of the corresponding plurality of correlation values determined for the pair of compounds.

9. The method of any one of claims 1-8, wherein the correlation value for a cell line in the plurality of cell lines that is correlation of (1) the plurality of quantitative biomarker measurements of the cell line in the response signature in the plurality of response signatures that represents the cell line upon exposing an aliquot of the cell line to the first compound at the exposure condition in the corresponding plurality of exposure conditions associated with the first compound and (2) the plurality of quantitative biomarker measurements of the cell line in the response signature in the plurality of response signatures that represents the cell line upon exposing an aliquot of the cell line to the second compound at the exposure condition in the corresponding plurality of exposure conditions associated with the second compound is a Pearson correlation value.

10. The method of any one of claims 1-9, wherein

the one or more compound clusters in the plurality of compound clusters contains the test compound, and the method further comprises:

associating the test compound as being a drug for a second disease indication on the basis that one or more properties of one or more compounds, in the one or more compound clusters in the plurality of compound clusters, including the first cluster, that contains the test compound, is associated with the second disease condition, thereby repurposing the drug for the second disease indication.

11. The method of any one of claims 1-10, the method further comprising performing pharmacophore analysis of one or more compounds, in the one or more compound clusters in the plurality of compound clusters, including the first cluster, that contain the test compound.

12. The method of any one of claims 1-10, wherein the method further comprises determining that the test compound and the first compound share a common mechanism-of-action annotation responsive to the determining that the test compound is in one or more compound clusters in the plurality of compound clusters, including the first cluster, that contains the first compound.

13. The method of any one of claims 1-12, the method further comprising using the test compound and the one or more compounds in the one or more compound clusters in the plurality of compound clusters that contains the test compound to identify a molecular target for a disease indication.

14. The method of any one of claims 1-13, wherein each quantitative biomarker measurement in the plurality of quantitative biomarker measurements is a colorimetric measurement, a fluorescence measurement, a luminescence measurement, or a resonance energy transfer (FRET) measurement.

15. The method of any one of claims 1-14, wherein a Tanimoto coefficient between a fingerprint of the test compound and a fingerprint of the first compound is less than 0.80, less than 0.70, less than 0.60, less than 0.50, or less than 0.40 or wherein a Tanimoto coefficient between the fingerprint of the test compound and the fingerprint of the first compound is less than a threshold value, wherein the threshold value is a predetermined value between 0.30 and 0.99.

16. The method of claim 15, wherein the fingerprint is a Daylight fingerprint, a BCI fingerprint, an ECFP4 fingerprint, an EcFC fingerprint, an MDL fingerprint, an atom pair fingerprint (APFP fingerprint), a topological torsion fingerprint (TTFP), a UNITY 2D fingerprint, an RNNS2S fingerprint, or a GraphConv fingerprint.

17. The method of any one of claims 1-16, wherein a cell line in the plurality of cell lines is drawn from cells of an organ, is drawn from cells of a tissue, is drawn from cells of a plurality of stem cells, is drawn from a plurality of primary human cells, is drawn from cells in umbilical cord blood, in peripheral blood, or in bone marrow, is drawn from a solid tissue, or is drawn from a plurality of differentiated cells.

18. The method of any one of claims 1-17, wherein the plurality of quantitative biomarker measurements of the (A)(b) obtaining for a cell line in the plurality of cell lines is a plurality of cell-based assay abundance values for the plurality of biomarkers from single-cell ribonucleic acid (RNA) sequencing (scRNA-seq) data of the aliquot of the cell line.

19. Use of the test compound of claim 10 in the manufacture of a medicament for treating the second disease indication in a subject in need of treatment.

20. The method of any one of claims 1-18, wherein the plurality of compounds comprises at least 2500 compounds and the plurality of biomarkers comprises 150 or more biomarkers.

21. The method of any one of claims 1-18 and 20, wherein the plurality of biomarkers is nucleic acids.

22. The method of any one of claims 1-18 and 20-21, wherein the plurality of biomarkers is ribonucleic acids.

23. The method of any one of claims 1-18 and 20-22, wherein the plurality of biomarkers is proteins.

24. The method of any one of claims 1-18 and 20-23, wherein the disease is hyperparathyroidism, metabolic bone disease, chronic kidney failure, asthma, or chronic obstructive pulmonary disease.